



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:25 PM UTC

PDB ID : 6JH6 / pdb_00006jh6
EMDB ID : EMD-9825
Title : Structure of RyR2 (F/A/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 : 2019-02-17
Resolution : 4.80 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

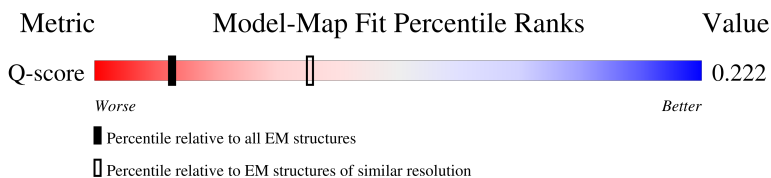
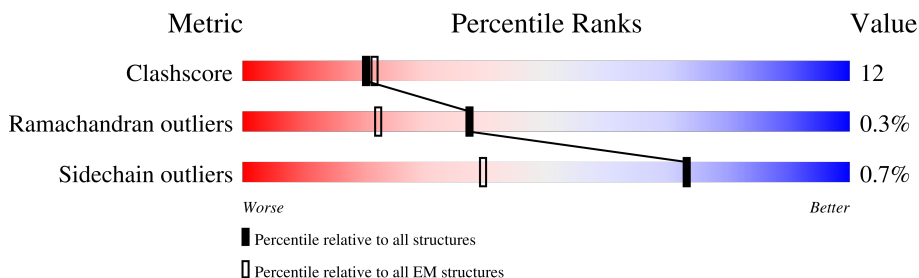
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1575 (4.30 - 5.30)

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	

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Mol	Chain	Length	Quality of chain
2	B	4968	6% 51% 18% 30%
2	D	4968	6% 52% 17% 30%
2	F	4968	6% 52% 17% 30%
2	H	4968	6% 52% 17% 30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 108924 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.

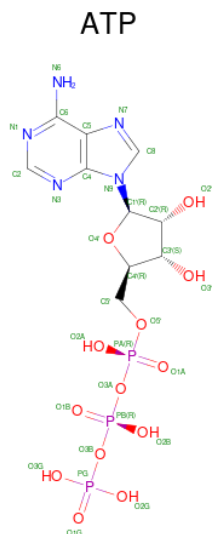
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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	3454	Total	C	N	O	S	0	0
			26380	16798	4512	4915	155		
2	D	3454	Total	C	N	O	S	0	0
			26380	16798	4512	4915	155		
2	F	3454	Total	C	N	O	S	0	0
			26380	16798	4512	4915	155		
2	H	3454	Total	C	N	O	S	0	0
			26380	16798	4512	4915	155		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0
3	F	1	Total 31	C 10	N 5	O 13	P 3	0
3	H	1	Total 31	C 10	N 5	O 13	P 3	0

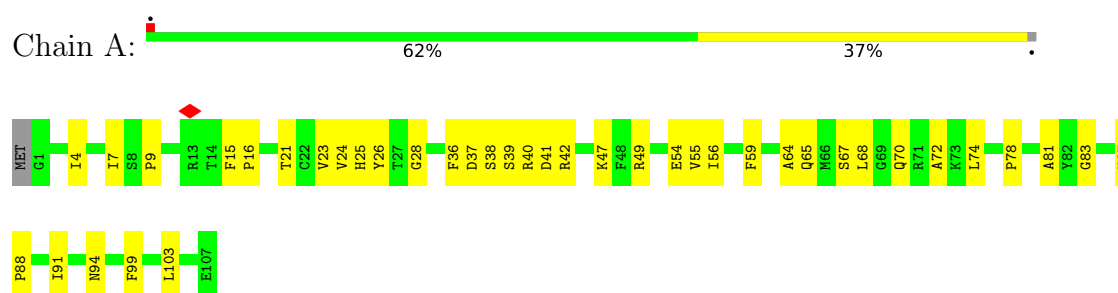
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

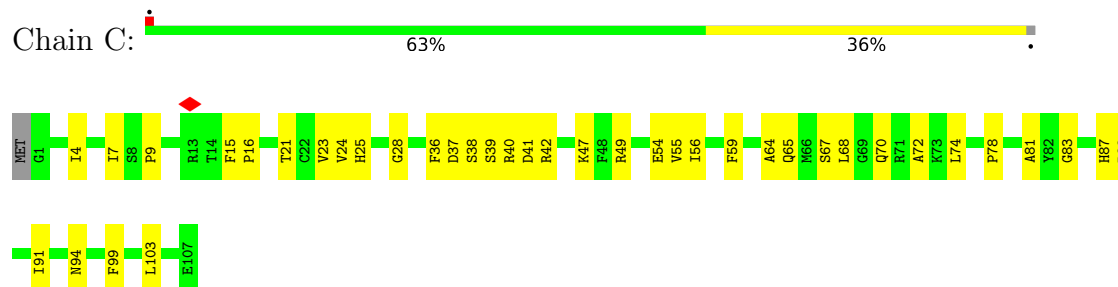
3 Residue-property plots

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

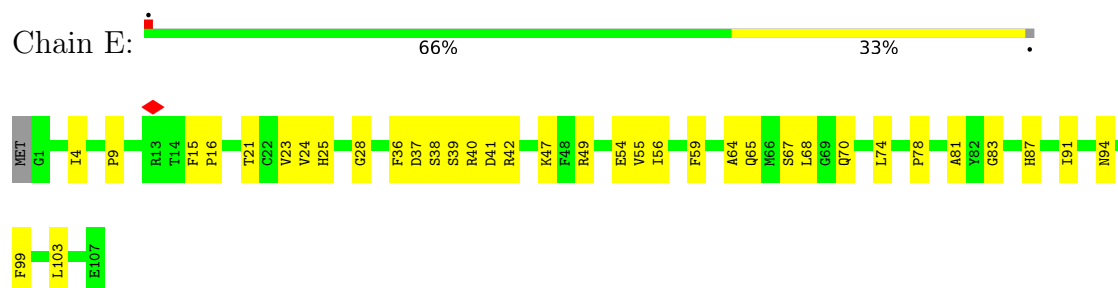
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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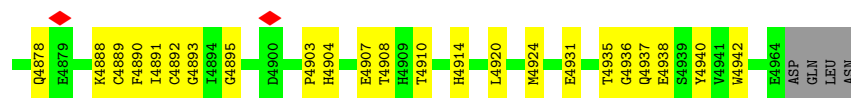




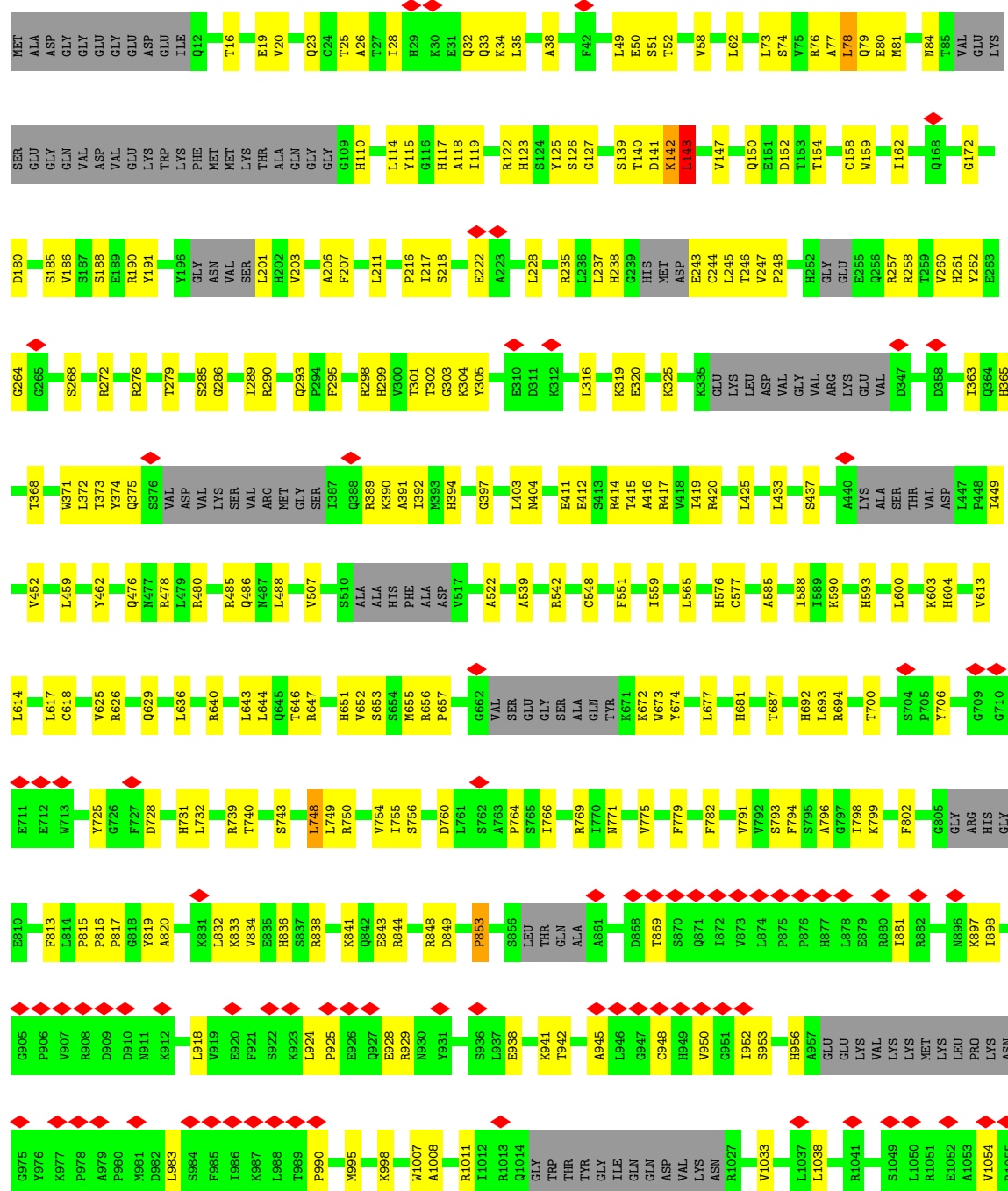








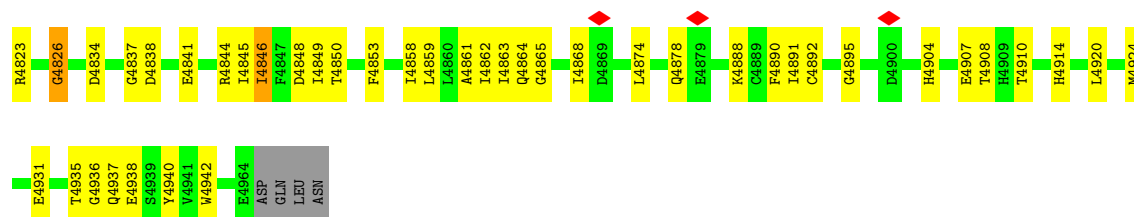
Molecule 2: RyR2



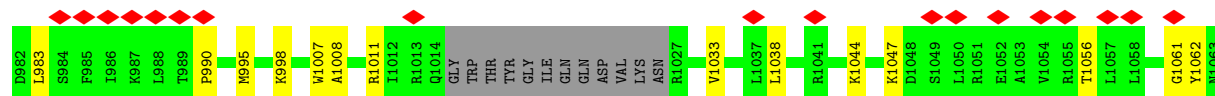
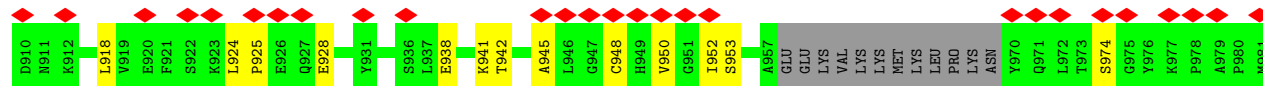
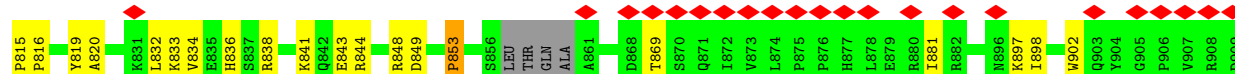
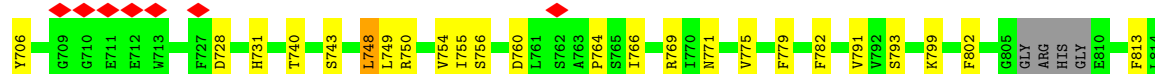
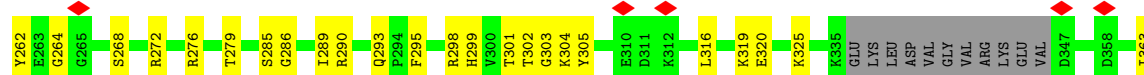
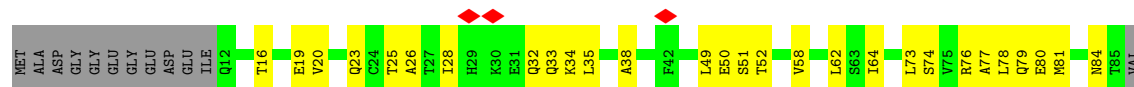
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N2211	V2082	E2011	V1934	I1830	L1719	V1619	Y1543	I1446	ARG	PRO	Y1236	R1144	G1061
Q2212	R2083	D2012	V1934	E1847	M1722	C1620	F1543	H1451	LYS	ALA	F1239	W1145	Y1062
Y2221	A2084	D2013	Q1938	P1848	M1723	L1622	A1545	T1455	GLN	GLY	N1242	Q1147	N1063
L2222	R2085	GLU	P1839	S1849	I1726	L1625	Q1546	L1459	ARG	PHE	W1250	E1150	E1065
N2225	L2089	ASP	N1940	V1848	V1727	Q1626	S1549	ASP	LEU	GLY	L1251	H1151	A1066
S2226	R2090	GLY	Q1941	PHE	L1738	S1629	P1550	ARG	LEU	PRO	S1252	Y1152	PRO
S2227	R2091	SER	F1942	GLU	L1738	L1630	N1551	VAL	ARG	ASN	G1153	R1154	ASP
V2228	Q2092	ASP	F1943	GLU	H1631	L1632	Q1554	ARG	THR	LEU	S1155	W1156	ASP
	L2096	GLY	R1944	ALA	D1741	I1632	F1555	THR	LYS	LEU	L1255	Q1157	HIS
	ASN	ASN	V1948	GLY	GLU	E1635	E1556	V1485	PRO	GLU	P1256	Q1158	ALA
S2232	V2100	D2022	GLN	PRO	ASN	E1635	LEU	L1489	TYR	ASP	Q1257	A1160	ALA
P2233	R2101	D2023	ALA	GLU	LYS	S1638	GLY	L1489	THR	ALA	F1258	D1160	ALA
A2102	A2102	L2024	LEU	GLU	HIS	G1470	ARG	D1471	THR	ASP	H1267	M1165	GLU
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V2248	T2106	I2026	MET	SER	L1748	I1642	LYS	K1475	HIS	ASP	R1272	T1172	CYS
N2249	Y2107	R2027	THR	THR	P1749	L1643	ASN	V1476	ALA	PHE	I1273	M1173	GLY
L2254	T2108	G2028	GLU	LEU	G1750	E1643	VAL	H1477	ARG	GLU	D1274	M1174	THR
A2255	I2109	L2030	ALA	GLU	S1756	Y1655	MET	E1478	LEU	VAL	GLY	L1177	GLY
L2256	L2109	L2030	LEU	LYS	L1757	R1659	PRO	S1479	THR	LEU	THR	N1178	GLU
	D2116	L2031	THR	GLU	R1758	R1659	LEU		GLU	MET	ILE	N1178	R1084
R2259	T2117	ALA	ALA	PRO	M1761	L1667	SER	R1482	ASP	LYS	ASP	G1179	F1085
V2267	I2118	ARG	ARG	CYS	Q1762	G1668	A1568	S1483	VAL	THR	SER	E1180	R1086
	L2121	LYS	LYS	ALA	S1767	M1669	L1570	N1484	LEU	ALA	PRO	I1181	
L2270	L2121	THR	GLU	GLU	S1767	H1670	CYS	Y1486	ALA	HIS	SER	L1182	R1089
	V2133	LYS	ASP	ASP	S1770	R1671	S1573	GLY	ASP	GLY	CYS	L1183	
G2274	R2134	LYS	PHE	SER	S1770	V1672	V1579	M1487	ASP	HIS	LEU	D1184	Y1102
LEU	R2135	LYS	ARG	ARG	I1771	A1673	P1580	V1488	ASP	LEU	V1285	G1187	E1106
GLN	G2136	GLN	SER	GLU	N1773	L1676	Q1581	C1489	ASP	PRO	TL286	S1188	T1109
CYS	L2142	ALA	PRO	GLY	E1774	H1679	C1582	A1490	TYR	ARG	GLI291	E1189	A1110
GLN	R2145	LYS	GLU	ALA	S1779	V1680	L1586	GLY	ASP	ARG	GLI291	A1190	G1111
MET		LYS	GLU	GLU	P1783	D1681	H1587	SER	TYR	VAL	N1294	F1192	M1112
LEU	N2153	VAL	ILE	GLU	Q1786	Q1684	F1590	GLY	LEU	LYS	M1300	D1196	M1113
SER	N2161	GLU	ASN	GLU	I1786	Q1684	L1591	GLY	GLN	ASP	F1301	S1206	V1115
GLY	N2173	ASP	LEU	LYS	L1795	Y1687	S1592	GLY	THR	LYS	Y1302	L1207	G1116
TYR		SER	LEU	GLY	L1795	A1688	H1593	GLY	SER	ALA	R1303	L1207	W1117
PRO		LYS	ASN	GLY	V1799	I1689	H1596	ARG	THR	ALA	L1304	Q1211	S1118
ASP		SER	PHE	LYS	W1799	E1690	W1596	ASN	PRO	LYS	S1305	P1212	R1119
ILE	V2177	ASP	LYS	ARG	S1803	N1691	P1600	N1502	GLU	GLY	G1213	G1213	P1120
GLY	G2181	SER	ASP	PRO	S1803	G1696	N1601	N1502	PHE	PHE	R1214		G121
TRP	GLY	L2058	LYS	GLU	R1807	G1696	Q1602	I1507	ASN	ASN	C1310		F1124
ASN	GLU	L2059	LYS	GLU	D1808	R1699	Q1602	C1508	GLY	GLU	ALA		
P2293	SER	Q2060	SER	G1893	P1809	R1699	D1607	C1509	GLY	ASN	VAL	S1222	E1127
G2296	GLU	M2067	GLU	L1894	V1810	Y1703	I1611	V1510	GLU	HIS	T1223	L1224	L1128
E2297	LYS	PRO	CYS	P1902	G1811	I1707	I1612	V1511	PRO	LYS	PHE		
R2298	THR	CYS	CYS	L1905	G1812	I1707	S1613	ASP	ALA	TYR	SER	F1227	E1132
Y2299	ILE	PRO	PRO	L1905	F1816	L1711	R1614	ALA	ALA	ALA	LYS	T1228	R1133
L2300	F2190	GLU	GLU	R1920	L1817	T1716	Q1615	SER	V1441	THR	THR		
	F2191	ILE	ILE	H1921	P1820	A1717	W1617	ALA	W1442	GLN	SER	L1232	A1136
R2304	F2191			R1922				G1516	W1443	GLY	ALA	G1231	F1137
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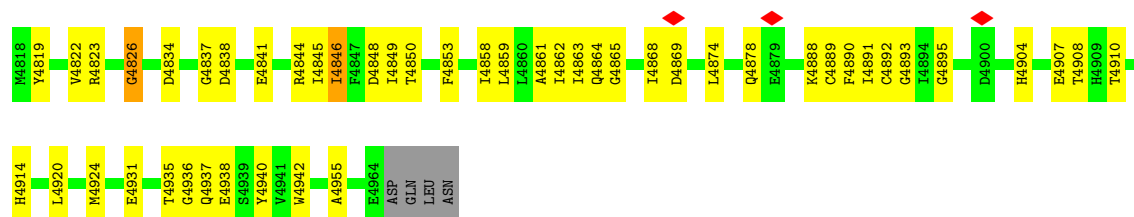
• Molecule 2: RyR2



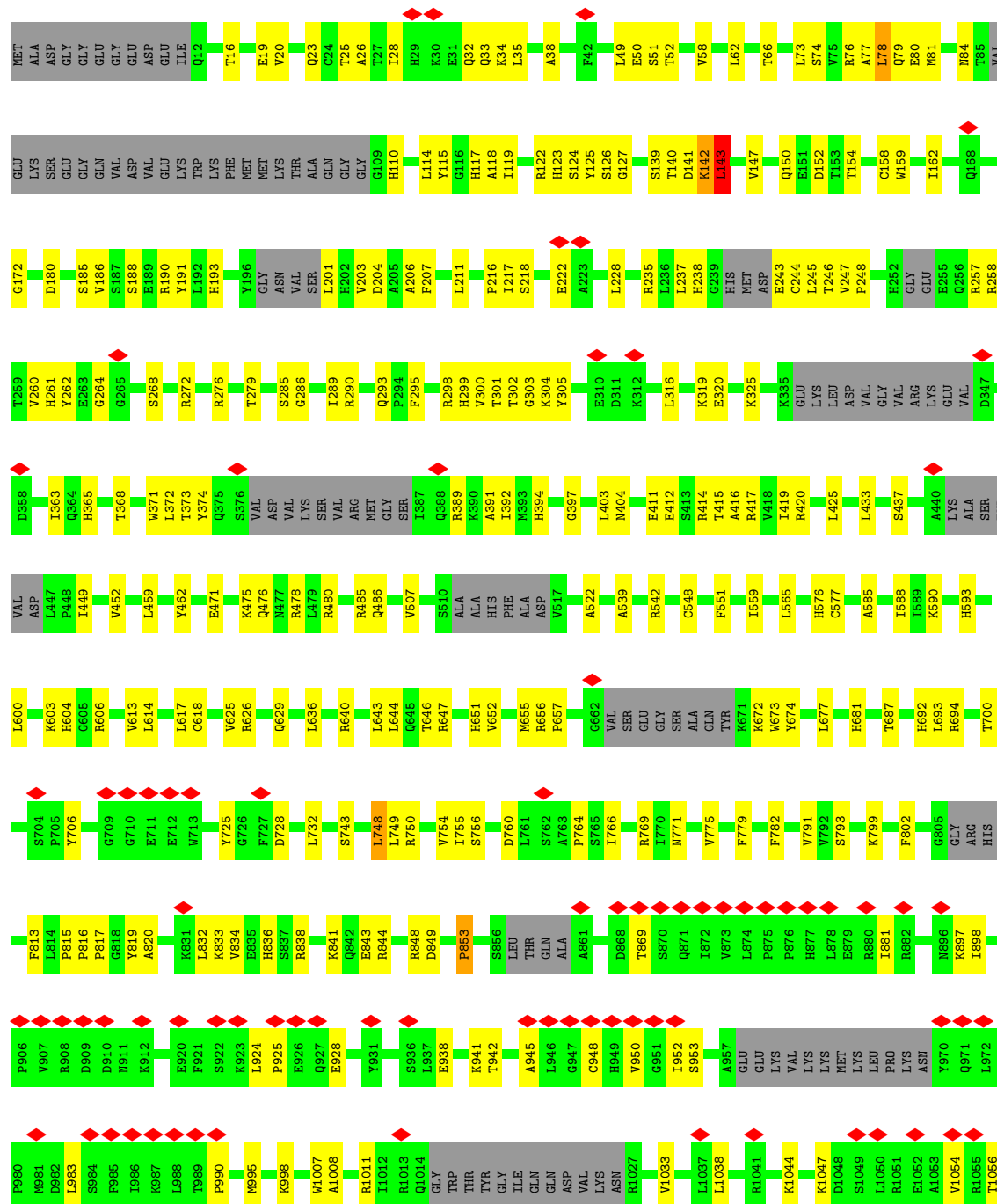








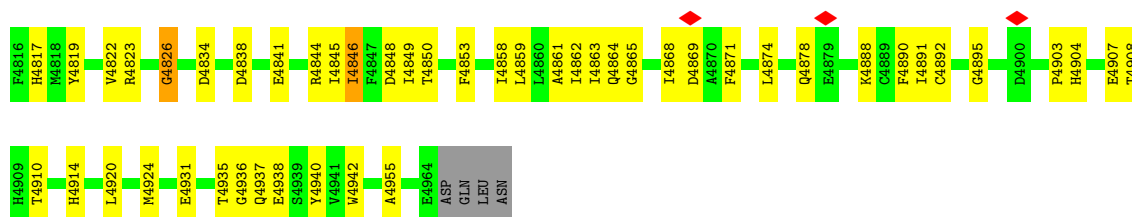
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GLU	SER	W2070	W2071	S2074	V2075	I2076	L2081	L2082	L2083	L2084	L2085	L2089	H2090	H2091	Q2092	I2096	S2226	S2227	V2228	S2232	P2233	S2247	V2248	M2249	L2254	L2255	L2256	R2259	V2267	L2270	G2274	LEU	GLN	SER	CYS	GLN	MET	LEU	VAL	SER	LYS	GLY	THR	PRO	ILE	GLY	TRP	ASN					
F2190	P2191	M2193	N2196	N2211	Q2212	Y2221	L2222	N2225	S2226	V2228	S2232	P2233	S2247	V2248	M2249	L2254	L2255	L2256	R2259	V2267	L2270	G2274	LEU	GLN	SER	CYS	GLN	MET	LEU	VAL	SER	LYS	GLY	THR	PRO	ILE	GLY	TRP	ASN														
PRO	GLU	ILE	L1997	L1998	D1999	E2011	L2012	D2013	ASP	GLY	SER	LEU	ASP	ASN	GLY	ASN	S2022	D2023	L2024	T2025	L2026	R2027	G2028	L2029	H2030	L2031	E2035	K2036	T2037	T2038	Y2039	L2040	LYS	LYS	GLN	ALA	GLU	GLY	LEU	VAL	SER	ASP	SER	LYS	ASP	LYS	SER	T2058	L2059	Q2060	M2067		
L1905	R1920	H1921	R1922	V1927	V1934	Q1938	D1939	N1940	Q1941	R1942	F1943	R1944	V1948	MET	GLN	ALA	S2022	D2023	L2024	T2025	L2026	R2027	G2028	L2029	H2030	L2031	E2035	K2036	T2037	T2038	Y2039	L2040	LYS	LYS	GLN	ALA	GLU	GLY	LEU	VAL	SER	ASP	SER	LYS	ASP	LYS	SER	T2058	L2059	Q2060	M2067		
F1816	L1817	P1820	L1821	I1830	E1847	P1848	S1849	VAL	PHE	LYS	GLU	ALA	ALA	GLY	PRO	GLU	S2022	D2023	L2024	T2025	L2026	R2027	G2028	L2029	H2030	L2031	E2035	K2036	T2037	T2038	Y2039	L2040	LYS	LYS	GLN	ALA	GLU	GLY	LEU	VAL	SER	ASP	SER	LYS	ASP	LYS	SER	T2058	L2059	Q2060	M2067		
R1718	L1719	M1722	M1723	L1726	V1727	T1730	T1733	L1738	D1741	GLU	ASN	LYS	LYS	LYS	HIS	G1747	L1748	P1749	G1750	S1756	L1757	R1758	M1761	Q1762	P1766	S1767	S1770	I1771	N1772	E1774	S1779	P1783	I1786	L1795	V1799	S1803	R1807	G1808	P1809	V1810	G1812	G1813	L1894	P1902	CYS								
V1619	Q1620	C1621	L1622	L1625	Q1626	S1629	H1631	I1632	P1633	E1634	E1635	S1638	T1641	L1642	E1643	Y1655	Y1655	G1659	L1667	G1668	N1669	R1670	H1671	V1672	A1673	L1676	H1679	V1680	D1681	Q1684	Y1687	A1688	I1689	N1691	G1696	R1699	Y1703	S1803	R1807	G1808	P1809	V1810	G1812	G1813	L1894	P1902	CYS						
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Y1531	V1543	F1544	A1545	Q1546	S1549	P1550	N1551	Q1554	F1555	E1556	LEU	GLY	ILE	ASN	LYS	VAL	PRO	SER	A1568	G1569	L1570	S1573	V1579	P1580	Q1581	C1582	L1586	H1587	F1590	L1591	S1592	H1593	W1596	P1600	N1601	Q1602	D1607	I1611	S1612	E1613	R1614	Q1615	G1616	W1617	L1618								
V1619	Q1620	C1621	L1622	L1625	Q1626	S1629	H1631	I1632	P1633	E1634	E1635	S1638	T1641	L1642	E1643	Y1655	Y1655	G1659	L1667	G1668	N1669	R1670	H1671	V1672	A1673	L1676	H1679	V1680	D1681	Q1684	Y1687	A1688	I1689	N1691	G1696	R1699	Y1703	S1803	R1807	G1808	P1809	V1810	G1812	G1813	L1894	P1902	CYS						
F1816	L1817	P1820	L1821	I1830	E1847	P1848	S1849	VAL	PHE	LYS	GLU	ALA	ALA	GLY	PRO	GLU	S2022	D2023	L2024	T2025	L2026	R2027	G2028	L2029	H2030	L2031	E2035	K2036	T2037	T2038	Y2039	L2040	LYS	LYS	GLN	ALA	GLU	GLY	LEU	VAL	SER	ASP	SER	LYS	ASP	LYS	SER	T2058	L2059	Q2060	M2067		
W2070	A2071	S2074	S2075	L2076	L2081	L2082	L2083	L2084	L2085	L2089	L2090	L2091	Q2092	I2096	S2226	S2227	S2228	S2232	P2233	S2247	V2248	M2249	L2254	L2255	L2256	R2259	V2267	L2270	G2274	LEU	GLN	SER	CYS	GLN	MET	LEU	VAL	SER	LYS	GLY	THR	PRO	ILE	GLY	TRP	ASN							
Y1062	H1063	L1064	E1065	A1066	PRO	ASP	GLN	ASP	HIS	ALA	ALA	ARG	ALA	GLU	VAL	CYS	SER	GLY	THR	GLY	GLU	F1084	F1085	R1086	R1089	A1098	V1101	Y1102	E1106	T1109	A1110	G1111	D1112	M1113	R1114	V1115	G1116	V1117	G1121	P1124	E1127	L1128	R1133	A1136	F1137	D1138	Q1143	R1144					
W1145	H1146	E1150	H1151	Y1152	G1153	R1154	S1155	W1156	Q1157	A1158	G1159	D1160	V1161	V1162	M1165	T1172	M1173	M1174	F1175	T1176	L1177	N1178	G1179	H1180	I1181	L1182	L1183	D1184	G1187	E1189	A1190	A1191	F1192	S1206	M1207	Q1211	V1212	G1213	R1214	S1222	T1223	L1224	F1227	T1228	G1231	F1232	D1233	G1235	Y1236				
F1239	M1242	W1250	L1251	K1252	R1253	L1254	L1255	P1256	Q1257	F1258	H1267	I1268	R1272	I1273	D1274	GLY	THR	ILE	ASP	SER	GLY	PRO	T1285	T1286	G1291	M1294	F1301	Y1302	R1303	L1304	S1305	M1306	C1310	ALA	GLU	VAL	PHE	LYS	THR	SER	ALA	GLY	PRO	ILE	PRO								
GLY	ALA	SER	PHE	GLY	PRO	LYS	ASN	ASP	THR	TYR	ASP	ALA	SER	ASP	PHE	GLU	VAL	MET	LEU	THR	ALA	HIS	GLY	VAL	ASP	TYR	ASP	TYR	VAL	ASP	LYS	ASP	GLN	MET	GLN	THR	T1425	S1429	V1430	R1431	P1434	GLY	GLN	GLU	PRO	ALA	N1440	V1441	V1442	V1443	G1444	W1445	I1446







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	44288	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	0.071	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.017	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: ATP, 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	0.23	0/835	0.49	0/1123
1	C	0.24	0/835	0.49	0/1123
1	E	0.24	0/835	0.49	0/1123
1	G	0.24	0/835	0.49	0/1123
2	B	0.27	0/26871	0.62	26/36338 (0.1%)
2	D	0.27	0/26871	0.62	26/36338 (0.1%)
2	F	0.27	0/26871	0.62	26/36338 (0.1%)
2	H	0.27	0/26871	0.62	26/36338 (0.1%)
All	All	0.27	0/110824	0.62	104/149844 (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	21
2	D	0	21
2	F	0	21
2	H	0	21
All	All	0	84

There are no bond length outliers.

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2327	ARG	N-CA-C	-8.65	101.17	112.68
2	B	2039	TYR	N-CA-C	8.12	126.03	113.28
2	F	2039	TYR	N-CA-C	8.12	126.03	113.28
2	D	2039	TYR	N-CA-C	8.12	126.03	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2039	TYR	N-CA-C	8.12	126.02	113.28
2	F	2327	ARG	N-CA-C	-7.95	102.10	112.68
2	B	2327	ARG	N-CA-C	-7.93	102.13	112.68
2	H	139	SER	CA-C-N	7.33	134.89	121.70
2	H	139	SER	C-N-CA	7.33	134.89	121.70
2	D	139	SER	CA-C-N	7.33	134.88	121.70
2	D	139	SER	C-N-CA	7.33	134.88	121.70
2	B	139	SER	CA-C-N	7.32	134.87	121.70
2	B	139	SER	C-N-CA	7.32	134.87	121.70
2	F	2022	SER	CA-C-N	7.32	134.87	121.70
2	F	2022	SER	C-N-CA	7.32	134.87	121.70
2	F	139	SER	CA-C-N	7.31	134.86	121.70
2	F	139	SER	C-N-CA	7.31	134.86	121.70
2	B	2022	SER	CA-C-N	7.28	134.81	121.70
2	B	2022	SER	C-N-CA	7.28	134.81	121.70
2	D	2022	SER	CA-C-N	7.28	134.81	121.70
2	D	2022	SER	C-N-CA	7.28	134.81	121.70
2	H	2022	SER	CA-C-N	7.28	134.81	121.70
2	H	2022	SER	C-N-CA	7.28	134.81	121.70
2	H	2327	ARG	N-CA-C	-7.18	103.12	112.68
2	D	2133	VAL	CA-C-N	6.53	133.45	121.70
2	D	2133	VAL	C-N-CA	6.53	133.45	121.70
2	B	2133	VAL	CA-C-N	6.52	133.43	121.70
2	B	2133	VAL	C-N-CA	6.52	133.43	121.70
2	H	2133	VAL	CA-C-N	6.51	133.43	121.70
2	H	2133	VAL	C-N-CA	6.51	133.43	121.70
2	D	2038	THR	CA-C-N	6.49	137.94	126.45
2	D	2038	THR	C-N-CA	6.49	137.94	126.45
2	F	2133	VAL	CA-C-N	6.48	133.36	121.70
2	F	2133	VAL	C-N-CA	6.48	133.36	121.70
2	B	2038	THR	CA-C-N	6.48	137.91	126.45
2	B	2038	THR	C-N-CA	6.48	137.91	126.45
2	H	2038	THR	CA-C-N	6.46	137.88	126.45
2	H	2038	THR	C-N-CA	6.46	137.88	126.45
2	F	2038	THR	CA-C-N	6.45	137.86	126.45
2	F	2038	THR	C-N-CA	6.45	137.86	126.45
2	D	507	VAL	N-CA-C	-5.88	107.18	112.12
2	F	507	VAL	N-CA-C	-5.88	107.18	112.12
2	B	507	VAL	N-CA-C	-5.84	107.22	112.12
2	H	507	VAL	N-CA-C	-5.84	107.22	112.12
2	D	4826	GLY	N-CA-C	-5.72	105.86	112.50
2	F	4826	GLY	N-CA-C	-5.72	105.86	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	4826	GLY	N-CA-C	-5.72	105.86	112.50
2	B	4826	GLY	N-CA-C	-5.71	105.88	112.50
2	F	140	THR	CA-C-N	5.69	131.94	121.70
2	F	140	THR	C-N-CA	5.69	131.94	121.70
2	D	140	THR	CA-C-N	5.67	131.90	121.70
2	D	140	THR	C-N-CA	5.67	131.90	121.70
2	B	140	THR	CA-C-N	5.67	131.90	121.70
2	B	140	THR	C-N-CA	5.67	131.90	121.70
2	H	140	THR	CA-C-N	5.66	131.88	121.70
2	H	140	THR	C-N-CA	5.66	131.88	121.70
2	F	1474	GLY	CA-C-N	5.28	131.62	121.54
2	F	1474	GLY	C-N-CA	5.28	131.62	121.54
2	B	1474	GLY	CA-C-N	5.26	131.59	121.54
2	B	1474	GLY	C-N-CA	5.26	131.59	121.54
2	H	1474	GLY	CA-C-N	5.26	131.59	121.54
2	H	1474	GLY	C-N-CA	5.26	131.59	121.54
2	D	1474	GLY	CA-C-N	5.26	131.58	121.54
2	D	1474	GLY	C-N-CA	5.26	131.58	121.54
2	D	1773	ASN	CA-C-N	5.23	131.52	121.54
2	D	1773	ASN	C-N-CA	5.23	131.52	121.54
2	H	1773	ASN	CA-C-N	5.22	131.50	121.54
2	H	1773	ASN	C-N-CA	5.22	131.50	121.54
2	B	1773	ASN	CA-C-N	5.21	131.48	121.54
2	B	1773	ASN	C-N-CA	5.21	131.48	121.54
2	F	222	GLU	CA-C-N	5.20	131.07	121.70
2	F	222	GLU	C-N-CA	5.20	131.07	121.70
2	D	222	GLU	CA-C-N	5.19	131.05	121.70
2	D	222	GLU	C-N-CA	5.19	131.05	121.70
2	F	1773	ASN	CA-C-N	5.18	131.44	121.54
2	F	1773	ASN	C-N-CA	5.18	131.44	121.54
2	B	222	GLU	CA-C-N	5.18	131.03	121.70
2	B	222	GLU	C-N-CA	5.18	131.03	121.70
2	F	1471	ASP	CA-C-N	5.16	131.39	121.54
2	F	1471	ASP	C-N-CA	5.16	131.39	121.54
2	H	222	GLU	CA-C-N	5.15	130.97	121.70
2	H	222	GLU	C-N-CA	5.15	130.97	121.70
2	D	1471	ASP	CA-C-N	5.15	131.38	121.54
2	D	1471	ASP	C-N-CA	5.15	131.38	121.54
2	H	1471	ASP	CA-C-N	5.15	131.38	121.54
2	H	1471	ASP	C-N-CA	5.15	131.38	121.54
2	B	1471	ASP	CA-C-N	5.14	131.37	121.54
2	B	1471	ASP	C-N-CA	5.14	131.37	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1772	ASN	N-CA-C	5.11	118.37	111.17
2	B	2039	TYR	CA-C-N	5.11	130.89	121.70
2	B	2039	TYR	C-N-CA	5.11	130.89	121.70
2	F	2039	TYR	CA-C-N	5.10	130.89	121.70
2	F	2039	TYR	C-N-CA	5.10	130.89	121.70
2	H	2039	TYR	CA-C-N	5.10	130.89	121.70
2	H	2039	TYR	C-N-CA	5.10	130.89	121.70
2	F	2228	VAL	N-CA-C	-5.10	108.87	113.71
2	H	2228	VAL	N-CA-C	-5.10	108.87	113.71
2	D	1772	ASN	N-CA-C	5.09	118.35	111.17
2	F	1772	ASN	N-CA-C	5.09	118.35	111.17
2	H	1772	ASN	N-CA-C	5.09	118.35	111.17
2	D	2039	TYR	CA-C-N	5.09	130.86	121.70
2	D	2039	TYR	C-N-CA	5.09	130.86	121.70
2	B	2228	VAL	N-CA-C	-5.09	108.88	113.71
2	D	2228	VAL	N-CA-C	-5.07	108.89	113.71

There are no chirality outliers.

All (84) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1102	TYR	Peptide
2	B	1127	GLU	Peptide
2	B	141	ASP	Peptide
2	B	142	LYS	Peptide
2	B	143	LEU	Peptide
2	B	1551	ASN	Peptide
2	B	1579	VAL	Peptide
2	B	1596	TRP	Peptide
2	B	1622	LEU	Peptide
2	B	1635	GLU	Peptide
2	B	1756	SER	Peptide
2	B	1847	GLU	Peptide
2	B	2075	VAL	Peptide
2	B	2232	SER	Peptide
2	B	3633	GLU	Peptide
2	B	4594	LEU	Peptide
2	B	4751	PHE	Peptide
2	B	748	LEU	Peptide
2	B	816	PRO	Peptide
2	B	819	TYR	Peptide
2	B	838	ARG	Peptide

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Mol	Chain	Res	Type	Group
2	D	1102	TYR	Peptide
2	D	1127	GLU	Peptide
2	D	141	ASP	Peptide
2	D	142	LYS	Peptide
2	D	143	LEU	Peptide
2	D	1551	ASN	Peptide
2	D	1579	VAL	Peptide
2	D	1596	TRP	Peptide
2	D	1622	LEU	Peptide
2	D	1635	GLU	Peptide
2	D	1756	SER	Peptide
2	D	1847	GLU	Peptide
2	D	2075	VAL	Peptide
2	D	2232	SER	Peptide
2	D	3633	GLU	Peptide
2	D	4594	LEU	Peptide
2	D	4751	PHE	Peptide
2	D	748	LEU	Peptide
2	D	816	PRO	Peptide
2	D	819	TYR	Peptide
2	D	838	ARG	Peptide
2	F	1102	TYR	Peptide
2	F	1127	GLU	Peptide
2	F	141	ASP	Peptide
2	F	142	LYS	Peptide
2	F	143	LEU	Peptide
2	F	1551	ASN	Peptide
2	F	1579	VAL	Peptide
2	F	1596	TRP	Peptide
2	F	1622	LEU	Peptide
2	F	1635	GLU	Peptide
2	F	1756	SER	Peptide
2	F	1847	GLU	Peptide
2	F	2075	VAL	Peptide
2	F	2232	SER	Peptide
2	F	3633	GLU	Peptide
2	F	4594	LEU	Peptide
2	F	4751	PHE	Peptide
2	F	748	LEU	Peptide
2	F	816	PRO	Peptide
2	F	819	TYR	Peptide
2	F	838	ARG	Peptide

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Mol	Chain	Res	Type	Group
2	H	1102	TYR	Peptide
2	H	1127	GLU	Peptide
2	H	141	ASP	Peptide
2	H	142	LYS	Peptide
2	H	143	LEU	Peptide
2	H	1551	ASN	Peptide
2	H	1579	VAL	Peptide
2	H	1596	TRP	Peptide
2	H	1622	LEU	Peptide
2	H	1635	GLU	Peptide
2	H	1756	SER	Peptide
2	H	1847	GLU	Peptide
2	H	2075	VAL	Peptide
2	H	2232	SER	Peptide
2	H	3633	GLU	Peptide
2	H	4594	LEU	Peptide
2	H	4751	PHE	Peptide
2	H	748	LEU	Peptide
2	H	816	PRO	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	30	0
1	C	819	0	824	29	0
1	E	819	0	824	26	0
1	G	819	0	824	28	0
2	B	26380	0	24897	714	0
2	D	26380	0	24897	704	0
2	F	26380	0	24897	701	0
2	H	26380	0	24897	706	0
3	B	31	0	12	2	0
3	D	31	0	12	2	0
3	F	31	0	12	2	0
3	H	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
All	All	108924	0	102932	2582	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 (2582) 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:B:4861:ALA:CB	2:D:4864:GLN:HG2	1.60	1.32
2:D:4861:ALA:CB	2:F:4864:GLN:HG2	1.61	1.30
2:F:4861:ALA:CB	2:H:4864:GLN:HG2	1.65	1.27
2:F:4814:TYR:CE2	2:H:4518:LEU:HD13	1.71	1.24
2:D:4780:TYR:CE1	2:F:4518:LEU:HD22	1.73	1.23
2:B:4864:GLN:HG2	2:H:4861:ALA:CB	1.70	1.22
2:F:4780:TYR:CE1	2:H:4518:LEU:HD22	1.74	1.22
2:F:4780:TYR:CD1	2:H:4518:LEU:HD22	1.74	1.21
2:B:4861:ALA:HB2	2:D:4864:GLN:CG	1.70	1.21
2:D:4814:TYR:CE2	2:F:4518:LEU:HD13	1.76	1.20
2:D:4861:ALA:HB2	2:F:4864:GLN:CG	1.72	1.20
2:B:4518:LEU:HD13	2:H:4814:TYR:CE2	1.75	1.20
2:B:4814:TYR:CE2	2:D:4518:LEU:HD13	1.76	1.20
2:B:4518:LEU:HD22	2:H:4780:TYR:CE1	1.75	1.19
2:B:4518:LEU:HD22	2:H:4780:TYR:CD1	1.78	1.19
2:B:4780:TYR:CE1	2:D:4518:LEU:HD22	1.75	1.18
2:B:4780:TYR:CD1	2:D:4518:LEU:HD22	1.79	1.18
2:D:4780:TYR:CD1	2:F:4518:LEU:HD22	1.76	1.18
2:F:4774:LEU:HD22	2:H:4754:LEU:HD21	1.26	1.17
2:D:4780:TYR:CE1	2:F:4518:LEU:CD2	2.28	1.17
2:F:4780:TYR:CE1	2:H:4518:LEU:CD2	2.28	1.16
2:F:4780:TYR:HE1	2:H:4518:LEU:CB	1.56	1.16
2:D:4780:TYR:HE1	2:F:4518:LEU:CB	1.57	1.15
2:B:4518:LEU:CB	2:H:4780:TYR:HE1	1.59	1.15
2:D:73:LEU:HD13	2:D:77:ALA:HB1	1.15	1.15
2:F:4861:ALA:HB2	2:H:4864:GLN:CG	1.76	1.15
2:B:4518:LEU:CD2	2:H:4780:TYR:CE1	2.31	1.13
2:B:4780:TYR:CE1	2:D:4518:LEU:CD2	2.31	1.13
2:B:4780:TYR:HE1	2:D:4518:LEU:CB	1.59	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:73:LEU:HD13	2:H:77:ALA:HB1	1.14	1.13
2:B:4523:VAL:HA	2:B:4559:HIS:ND1	1.64	1.13
2:F:4523:VAL:HA	2:F:4559:HIS:ND1	1.64	1.12
2:F:73:LEU:HD13	2:F:77:ALA:HB1	1.14	1.12
2:B:4754:LEU:HD21	2:H:4774:LEU:HD22	1.26	1.11
2:D:4523:VAL:HA	2:D:4559:HIS:ND1	1.64	1.11
2:D:4774:LEU:HD22	2:F:4754:LEU:HD21	1.25	1.11
2:F:4811:LEU:HB2	2:H:4519:LEU:HD22	1.30	1.10
2:B:73:LEU:HD13	2:B:77:ALA:HB1	1.14	1.09
2:H:4523:VAL:HA	2:H:4559:HIS:ND1	1.64	1.09
2:B:4864:GLN:CG	2:H:4861:ALA:HB2	1.80	1.09
2:B:4774:LEU:HD22	2:D:4754:LEU:HD21	1.25	1.08
2:B:4811:LEU:HB2	2:D:4519:LEU:HD22	1.32	1.08
2:F:4814:TYR:HE2	2:H:4518:LEU:CD1	1.66	1.07
2:B:4519:LEU:HD22	2:H:4811:LEU:HB2	1.31	1.06
2:D:143:LEU:H	2:F:2427:LEU:HD21	1.21	1.05
2:D:4814:TYR:HE2	2:F:4518:LEU:HD13	0.88	1.04
2:F:4849:ILE:HA	2:H:4822:VAL:HG21	1.39	1.04
2:D:4811:LEU:HB2	2:F:4519:LEU:HD22	1.34	1.04
2:D:4849:ILE:HA	2:F:4822:VAL:HG21	1.36	1.04
2:B:4822:VAL:HG21	2:H:4849:ILE:HA	1.38	1.03
2:D:4523:VAL:HA	2:D:4559:HIS:HD1	1.16	1.03
2:B:143:LEU:H	2:D:2427:LEU:HD21	1.24	1.03
2:D:4814:TYR:HE2	2:F:4518:LEU:CD1	1.70	1.03
2:B:4518:LEU:CD1	2:H:4814:TYR:HE2	1.70	1.03
2:B:4814:TYR:HE2	2:D:4518:LEU:CD1	1.71	1.02
2:B:4849:ILE:HA	2:D:4822:VAL:HG21	1.35	1.02
2:B:4814:TYR:HE2	2:D:4518:LEU:HD13	0.87	1.01
2:B:4518:LEU:HD13	2:H:4814:TYR:HE2	0.86	1.00
2:B:2427:LEU:HD21	2:H:143:LEU:H	1.23	1.00
2:F:143:LEU:H	2:H:2427:LEU:HD21	1.22	1.00
2:D:4780:TYR:CE1	2:F:4518:LEU:CB	2.46	0.99
2:B:4523:VAL:HA	2:B:4559:HIS:HD1	1.16	0.99
2:F:4780:TYR:CE1	2:H:4518:LEU:CB	2.45	0.99
2:F:4814:TYR:HE2	2:H:4518:LEU:HD13	0.83	0.98
2:H:4523:VAL:HA	2:H:4559:HIS:HD1	1.16	0.97
2:F:4774:LEU:CD2	2:H:4754:LEU:HD21	1.95	0.97
2:B:4780:TYR:CE1	2:D:4518:LEU:CB	2.48	0.96
2:B:4518:LEU:CB	2:H:4780:TYR:CE1	2.48	0.96
2:B:4523:VAL:HA	2:B:4559:HIS:CE1	2.01	0.95
2:H:4523:VAL:HA	2:H:4559:HIS:CE1	2.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4523:VAL:HA	2:D:4559:HIS:CE1	2.01	0.95
2:F:4523:VAL:HA	2:F:4559:HIS:CE1	2.01	0.95
2:B:4754:LEU:HD21	2:H:4774:LEU:CD2	1.97	0.95
2:B:4774:LEU:CD2	2:D:4754:LEU:HD21	1.97	0.95
2:D:4774:LEU:CD2	2:F:4754:LEU:HD21	1.96	0.95
2:B:73:LEU:HB3	2:B:77:ALA:HB3	1.49	0.94
2:B:4904:HIS:NE2	2:H:4184:LYS:CD	2.30	0.94
2:H:73:LEU:HB3	2:H:77:ALA:HB3	1.50	0.94
2:D:73:LEU:HB3	2:D:77:ALA:HB3	1.50	0.94
2:F:73:LEU:HB3	2:F:77:ALA:HB3	1.49	0.94
2:F:4523:VAL:HA	2:F:4559:HIS:HD1	1.16	0.93
2:B:4184:LYS:CD	2:D:4904:HIS:NE2	2.32	0.93
2:F:4780:TYR:CE1	2:H:4518:LEU:HB3	2.03	0.93
2:D:143:LEU:N	2:F:2427:LEU:HD21	1.84	0.93
2:B:73:LEU:CD1	2:B:77:ALA:HB1	2.00	0.91
2:B:2427:LEU:HD21	2:H:143:LEU:N	1.85	0.91
2:B:4849:ILE:O	2:D:4822:VAL:HG23	1.70	0.91
2:F:143:LEU:N	2:H:2427:LEU:HD21	1.84	0.91
2:F:4184:LYS:CD	2:H:4904:HIS:NE2	2.34	0.91
2:D:4780:TYR:CE1	2:F:4518:LEU:HB3	2.06	0.91
2:H:73:LEU:CD1	2:H:77:ALA:HB1	2.00	0.91
2:D:4849:ILE:O	2:F:4822:VAL:HG23	1.70	0.90
2:D:143:LEU:H	2:F:2427:LEU:CD2	1.85	0.90
2:D:73:LEU:CD1	2:D:77:ALA:HB1	2.01	0.90
2:F:73:LEU:CD1	2:F:77:ALA:HB1	2.00	0.90
2:D:4184:LYS:CD	2:F:4904:HIS:NE2	2.34	0.89
2:F:143:LEU:H	2:H:2427:LEU:CD2	1.84	0.89
2:B:4518:LEU:HB3	2:H:4780:TYR:CE1	2.07	0.89
2:B:4819:TYR:O	2:B:4822:VAL:HG12	1.73	0.89
2:B:143:LEU:N	2:D:2427:LEU:HD21	1.87	0.88
2:B:4780:TYR:CE1	2:D:4518:LEU:HB3	2.08	0.88
2:B:4846:ILE:HD11	2:D:4815:MET:SD	2.14	0.88
2:F:4819:TYR:O	2:F:4822:VAL:HG12	1.73	0.88
2:F:73:LEU:HB3	2:F:77:ALA:CB	2.04	0.88
2:B:73:LEU:HB3	2:B:77:ALA:CB	2.04	0.88
2:B:2427:LEU:CD2	2:H:143:LEU:H	1.86	0.88
2:F:4780:TYR:HE1	2:H:4518:LEU:HB3	1.35	0.87
2:B:4780:TYR:HE1	2:D:4518:LEU:HB3	1.39	0.87
2:B:143:LEU:H	2:D:2427:LEU:CD2	1.87	0.87
2:D:4819:TYR:O	2:D:4822:VAL:HG12	1.73	0.87
2:B:4815:MET:SD	2:H:4846:ILE:HD11	2.15	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4819:TYR:O	2:H:4822:VAL:HG12	1.74	0.87
2:H:73:LEU:HB3	2:H:77:ALA:CB	2.04	0.86
2:B:4849:ILE:CA	2:D:4822:VAL:HG21	2.04	0.86
2:D:4849:ILE:CA	2:F:4822:VAL:HG21	2.04	0.86
2:B:4822:VAL:HG23	2:H:4849:ILE:O	1.74	0.86
2:F:4849:ILE:O	2:H:4822:VAL:HG23	1.74	0.86
2:D:4780:TYR:HE1	2:F:4518:LEU:HB3	1.39	0.85
2:D:4846:ILE:HD11	2:F:4815:MET:SD	2.16	0.85
2:D:73:LEU:HB3	2:D:77:ALA:CB	2.06	0.85
2:F:74:SER:O	2:F:78:LEU:CD1	2.25	0.84
2:B:74:SER:O	2:B:78:LEU:CD1	2.26	0.84
2:F:4849:ILE:CA	2:H:4822:VAL:HG21	2.07	0.84
2:B:4822:VAL:HG21	2:H:4849:ILE:CA	2.07	0.83
2:B:4849:ILE:O	2:D:4822:VAL:CG2	2.27	0.83
2:F:4846:ILE:HD11	2:H:4815:MET:SD	2.19	0.83
2:D:4849:ILE:O	2:F:4822:VAL:CG2	2.27	0.83
2:B:4774:LEU:HD22	2:D:4754:LEU:CD2	2.10	0.82
2:D:2326:ILE:O	2:D:2326:ILE:HG22	1.78	0.82
2:B:4754:LEU:CD2	2:H:4774:LEU:HD22	2.10	0.82
2:B:76:ARG:CB	2:D:3891:TRP:CB	2.58	0.81
2:F:74:SER:O	2:F:78:LEU:HD12	1.80	0.81
2:D:76:ARG:CB	2:F:3891:TRP:CB	2.59	0.81
2:F:4774:LEU:HD22	2:H:4754:LEU:CD2	2.09	0.80
2:B:3891:TRP:CB	2:H:76:ARG:CB	2.60	0.80
2:F:76:ARG:CB	2:H:3891:TRP:CB	2.60	0.79
2:B:4822:VAL:CG2	2:H:4849:ILE:O	2.31	0.79
2:B:4864:GLN:HG2	2:H:4861:ALA:HB2	0.86	0.79
2:B:4823:ARG:HA	2:H:4826:GLY:CA	2.14	0.78
2:D:4780:TYR:HE1	2:F:4518:LEU:HB2	1.48	0.78
2:F:4849:ILE:O	2:H:4822:VAL:CG2	2.31	0.78
2:F:4175:PHE:O	2:F:4179:ASN:HB2	1.83	0.78
2:F:4780:TYR:HE1	2:H:4518:LEU:CG	1.96	0.78
2:F:4780:TYR:HE1	2:H:4518:LEU:HB2	1.49	0.78
2:B:74:SER:O	2:B:78:LEU:HD12	1.81	0.78
2:B:4780:TYR:HE1	2:D:4518:LEU:HB2	1.49	0.78
2:D:4175:PHE:O	2:D:4179:ASN:HB2	1.83	0.77
2:D:4774:LEU:HD22	2:F:4754:LEU:CD2	2.10	0.77
2:B:4175:PHE:O	2:B:4179:ASN:HB2	1.83	0.77
2:B:4046:LYS:H	2:B:4077:GLU:HB3	1.50	0.77
2:H:4046:LYS:H	2:H:4077:GLU:HB3	1.50	0.77
2:D:4780:TYR:HE1	2:F:4518:LEU:CG	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4175:PHE:O	2:H:4179:ASN:HB2	1.83	0.77
2:B:4518:LEU:HB3	2:H:4780:TYR:HE1	1.39	0.77
2:B:4849:ILE:HB	2:D:4822:VAL:CB	2.15	0.76
2:B:4849:ILE:CG2	2:D:4822:VAL:HG11	2.15	0.76
1:A:87:HIS:H	1:A:91:ILE:HB	1.51	0.76
2:B:4849:ILE:HB	2:D:4822:VAL:HB	1.66	0.76
2:D:4849:ILE:HB	2:F:4822:VAL:CB	2.15	0.76
2:F:2326:ILE:O	2:F:2326:ILE:HG22	1.86	0.76
2:F:4861:ALA:HB2	2:H:4864:GLN:HG2	0.82	0.76
1:G:87:HIS:H	1:G:91:ILE:HB	1.51	0.76
2:B:4518:LEU:CG	2:H:4780:TYR:HE1	1.99	0.75
1:C:87:HIS:H	1:C:91:ILE:HB	1.51	0.75
2:D:4046:LYS:H	2:D:4077:GLU:HB3	1.50	0.75
2:F:4046:LYS:H	2:F:4077:GLU:HB3	1.50	0.75
2:B:4904:HIS:NE2	2:H:4184:LYS:HD2	2.00	0.75
2:H:4845:ILE:O	2:H:4849:ILE:HG12	1.87	0.75
2:F:4845:ILE:O	2:F:4849:ILE:HG12	1.87	0.75
2:D:4849:ILE:CG2	2:F:4822:VAL:HG11	2.16	0.75
2:B:4518:LEU:HB2	2:H:4780:TYR:HE1	1.50	0.75
2:B:4780:TYR:HE1	2:D:4518:LEU:CG	2.00	0.75
2:B:4845:ILE:O	2:B:4849:ILE:HG12	1.87	0.75
2:D:4849:ILE:HB	2:F:4822:VAL:HB	1.67	0.74
2:D:4845:ILE:O	2:D:4849:ILE:HG12	1.87	0.74
2:F:4849:ILE:HB	2:H:4822:VAL:HB	1.68	0.74
2:B:2326:ILE:HG22	2:B:2326:ILE:O	1.86	0.74
2:B:4826:GLY:CA	2:D:4823:ARG:HA	2.18	0.74
2:F:4849:ILE:HB	2:H:4822:VAL:CB	2.17	0.74
2:D:4569:MET:O	2:D:4573:LEU:HB2	1.88	0.74
2:F:4569:MET:O	2:F:4573:LEU:HB2	1.88	0.74
2:F:4811:LEU:HB2	2:H:4519:LEU:CD2	2.16	0.74
2:H:74:SER:O	2:H:78:LEU:CD1	2.36	0.73
2:B:4822:VAL:HB	2:H:4849:ILE:HB	1.68	0.73
2:B:4569:MET:O	2:B:4573:LEU:HB2	1.88	0.73
1:E:87:HIS:H	1:E:91:ILE:HB	1.51	0.73
2:F:4826:GLY:CA	2:H:4823:ARG:HA	2.18	0.73
2:D:4849:ILE:HB	2:F:4822:VAL:CG1	2.18	0.73
2:B:4822:VAL:CB	2:H:4849:ILE:HB	2.18	0.73
2:B:4849:ILE:HB	2:D:4822:VAL:CG1	2.18	0.73
2:D:4826:GLY:CA	2:F:4823:ARG:HA	2.19	0.73
2:H:74:SER:O	2:H:78:LEU:HD12	1.89	0.73
2:H:4569:MET:O	2:H:4573:LEU:HB2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4849:ILE:CG2	2:H:4822:VAL:HG11	2.19	0.72
2:B:4822:VAL:HG11	2:H:4849:ILE:CG2	2.18	0.72
2:B:4811:LEU:HB2	2:D:4519:LEU:CD2	2.16	0.72
2:B:4184:LYS:HD2	2:D:4904:HIS:NE2	2.02	0.72
2:D:74:SER:O	2:D:78:LEU:CD1	2.37	0.72
2:D:4861:ALA:HB2	2:F:4864:GLN:HG2	0.79	0.72
2:B:4823:ARG:CB	2:H:4826:GLY:HA3	2.20	0.72
2:B:4907:GLU:OE1	2:H:4184:LYS:HB2	1.90	0.72
2:B:4861:ALA:HB2	2:D:4864:GLN:HG2	0.77	0.72
2:B:4823:ARG:CA	2:H:4826:GLY:CA	2.68	0.71
2:D:4184:LYS:HD2	2:F:4904:HIS:NE2	2.04	0.71
2:B:4819:TYR:O	2:B:4822:VAL:CG1	2.39	0.71
2:B:4823:ARG:CB	2:H:4826:GLY:C	2.64	0.71
2:D:74:SER:O	2:D:78:LEU:HD12	1.91	0.71
2:F:4811:LEU:CB	2:H:4519:LEU:HD22	2.16	0.71
2:F:4780:TYR:CE1	2:H:4518:LEU:HD23	2.25	0.71
2:D:4819:TYR:O	2:D:4822:VAL:CG1	2.39	0.70
2:B:4822:VAL:HG11	2:H:4849:ILE:HG22	1.73	0.70
2:H:4819:TYR:O	2:H:4822:VAL:CG1	2.39	0.70
2:B:4849:ILE:HG22	2:D:4822:VAL:HG11	1.72	0.70
2:F:4780:TYR:HE1	2:H:4518:LEU:CD2	1.87	0.70
2:B:4904:HIS:NE2	2:H:4184:LYS:HD3	2.05	0.70
2:F:4819:TYR:O	2:F:4822:VAL:CG1	2.39	0.70
2:F:4826:GLY:HA3	2:H:4823:ARG:CB	2.21	0.70
2:F:4849:ILE:HB	2:H:4822:VAL:CG1	2.22	0.70
2:D:4811:LEU:HB2	2:F:4519:LEU:CD2	2.19	0.70
2:B:4519:LEU:CD2	2:H:4811:LEU:HB2	2.16	0.70
2:B:4826:GLY:C	2:D:4823:ARG:CB	2.65	0.70
2:B:4822:VAL:CG1	2:H:4849:ILE:HB	2.22	0.69
2:F:4184:LYS:HD3	2:H:4904:HIS:NE2	2.08	0.69
2:B:4184:LYS:HB2	2:D:4907:GLU:OE1	1.93	0.69
2:H:2067:MET:HE2	2:H:2089:LEU:HB2	1.75	0.69
2:D:4826:GLY:C	2:F:4823:ARG:CB	2.65	0.69
2:F:2067:MET:HE2	2:F:2089:LEU:HB2	1.75	0.69
2:D:4826:GLY:HA3	2:F:4823:ARG:CB	2.23	0.69
2:D:4849:ILE:HG22	2:F:4822:VAL:HG11	1.73	0.69
2:F:4184:LYS:HD2	2:H:4904:HIS:NE2	2.06	0.69
2:F:4184:LYS:HB2	2:H:4907:GLU:OE1	1.93	0.69
2:F:4780:TYR:CE1	2:H:4518:LEU:HB2	2.24	0.69
2:B:4184:LYS:HD3	2:D:4904:HIS:NE2	2.07	0.68
2:B:4519:LEU:HD22	2:H:4811:LEU:CB	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4184:LYS:HD3	2:F:4904:HIS:NE2	2.08	0.68
2:B:4849:ILE:HB	2:D:4822:VAL:HG11	1.75	0.68
2:B:74:SER:O	2:B:78:LEU:HD13	1.93	0.68
2:B:4826:GLY:HA3	2:D:4823:ARG:CB	2.23	0.68
2:F:694:ARG:HB2	2:F:793:SER:HB2	1.76	0.68
2:F:4849:ILE:HG22	2:H:4822:VAL:HG11	1.75	0.68
2:B:4515:ASN:O	2:B:4518:LEU:HG	1.94	0.68
2:D:4515:ASN:O	2:D:4518:LEU:HG	1.94	0.68
2:D:2067:MET:HE2	2:D:2089:LEU:HB2	1.75	0.68
2:D:4780:TYR:CE1	2:F:4518:LEU:HD23	2.27	0.68
2:F:4515:ASN:O	2:F:4518:LEU:HG	1.94	0.68
2:H:843:GLU:HA	2:H:848:ARG:HG2	1.76	0.68
2:B:143:LEU:CB	2:D:2427:LEU:HD21	2.24	0.68
2:B:4826:GLY:CA	2:D:4823:ARG:CA	2.72	0.68
2:D:843:GLU:HA	2:D:848:ARG:HG2	1.76	0.68
2:D:4184:LYS:HB2	2:F:4907:GLU:OE1	1.94	0.68
2:D:694:ARG:HB2	2:D:793:SER:HB2	1.76	0.67
2:H:4515:ASN:O	2:H:4518:LEU:HG	1.94	0.67
2:B:4621:GLN:HE22	2:B:4633:ARG:HH12	1.42	0.67
2:D:4826:GLY:CA	2:F:4823:ARG:CA	2.72	0.67
2:F:748:LEU:HD13	2:F:750:ARG:HE	1.60	0.67
2:F:4826:GLY:CA	2:H:4823:ARG:CA	2.72	0.67
2:B:2067:MET:HE2	2:B:2089:LEU:HB2	1.75	0.67
2:B:4904:HIS:CD2	2:H:4184:LYS:HG3	2.29	0.67
2:B:4823:ARG:HA	2:H:4826:GLY:C	2.20	0.67
2:D:1114:ARG:HB2	2:D:1206:SER:HB3	1.77	0.67
2:H:748:LEU:HD13	2:H:750:ARG:HE	1.60	0.67
2:D:4849:ILE:HB	2:F:4822:VAL:HG11	1.75	0.67
2:F:74:SER:O	2:F:78:LEU:HD13	1.93	0.67
2:F:1114:ARG:HB2	2:F:1206:SER:HB3	1.77	0.67
2:H:4621:GLN:HE22	2:H:4633:ARG:HH12	1.42	0.67
2:B:1114:ARG:HB2	2:B:1206:SER:HB3	1.77	0.67
2:D:748:LEU:HD13	2:D:750:ARG:HE	1.60	0.67
2:F:4826:GLY:C	2:H:4823:ARG:CB	2.67	0.67
2:B:4518:LEU:HD23	2:H:4780:TYR:CE1	2.29	0.67
2:F:843:GLU:HA	2:F:848:ARG:HG2	1.76	0.67
2:B:843:GLU:HA	2:B:848:ARG:HG2	1.76	0.66
2:H:694:ARG:HB2	2:H:793:SER:HB2	1.76	0.66
2:D:4523:VAL:CA	2:D:4559:HIS:CE1	2.78	0.66
2:D:4621:GLN:HE22	2:D:4633:ARG:HH12	1.42	0.66
2:D:4780:TYR:HE1	2:F:4518:LEU:CD2	1.87	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:694:ARG:HB2	2:B:793:SER:HB2	1.76	0.66
2:B:4780:TYR:CE1	2:D:4518:LEU:HD23	2.29	0.66
2:D:4811:LEU:CB	2:F:4519:LEU:HD22	2.20	0.66
2:H:1114:ARG:HB2	2:H:1206:SER:HB3	1.77	0.66
2:B:748:LEU:HD13	2:B:750:ARG:HE	1.60	0.66
2:H:2326:ILE:O	2:H:2326:ILE:HG22	1.95	0.66
2:B:4849:ILE:CB	2:D:4822:VAL:HG11	2.26	0.65
2:D:4780:TYR:CE1	2:F:4518:LEU:HB2	2.24	0.65
2:F:4621:GLN:HE22	2:F:4633:ARG:HH12	1.43	0.65
2:H:4523:VAL:CA	2:H:4559:HIS:CE1	2.78	0.65
2:D:1487:MET:HE1	2:D:1531:TYR:HB2	1.79	0.65
2:F:1165:MET:HB2	2:F:1174:MET:HB2	1.79	0.65
2:F:1487:MET:HE1	2:F:1531:TYR:HB2	1.79	0.65
2:F:4849:ILE:HB	2:H:4822:VAL:HG11	1.78	0.65
2:D:4849:ILE:CB	2:F:4822:VAL:HG11	2.26	0.65
2:B:4826:GLY:C	2:D:4823:ARG:HA	2.22	0.65
2:B:2427:LEU:HD21	2:H:143:LEU:CB	2.27	0.65
2:B:4184:LYS:HG3	2:D:4904:HIS:CD2	2.31	0.65
2:B:4518:LEU:HB2	2:H:4780:TYR:CE1	2.26	0.65
2:B:4780:TYR:HE1	2:D:4518:LEU:CD2	1.89	0.65
2:B:4642:PRO:HG2	2:B:4648:LYS:HD3	1.79	0.64
2:D:1165:MET:HB2	2:D:1174:MET:HB2	1.79	0.64
2:D:1602:GLN:HE22	2:D:1642:LEU:HB3	1.63	0.64
2:D:3860:ARG:HH21	2:D:3932:ASN:HB2	1.62	0.64
2:D:3996:ILE:HG12	2:D:4000:MET:HE3	1.79	0.64
2:B:1602:GLN:HE22	2:B:1642:LEU:HB3	1.63	0.64
2:H:4642:PRO:HG2	2:H:4648:LYS:HD3	1.79	0.64
2:B:3860:ARG:HH21	2:B:3932:ASN:HB2	1.62	0.64
2:B:1487:MET:HE1	2:B:1531:TYR:HB2	1.79	0.64
2:B:4523:VAL:CA	2:B:4559:HIS:CE1	2.78	0.64
2:F:4523:VAL:CA	2:F:4559:HIS:CE1	2.78	0.64
2:F:3996:ILE:HG12	2:F:4000:MET:HE3	1.79	0.64
2:F:4184:LYS:HG3	2:H:4904:HIS:CD2	2.33	0.64
2:H:1487:MET:HE1	2:H:1531:TYR:HB2	1.79	0.64
2:F:143:LEU:CB	2:H:2427:LEU:HD21	2.28	0.64
2:H:1602:GLN:HE22	2:H:1642:LEU:HB3	1.63	0.64
2:F:1602:GLN:HE22	2:F:1642:LEU:HB3	1.63	0.63
2:B:1165:MET:HB2	2:B:1174:MET:HB2	1.79	0.63
2:D:833:LYS:HA	2:D:1614:ARG:HH12	1.64	0.63
2:B:3996:ILE:HG12	2:B:4000:MET:HE3	1.79	0.63
2:F:833:LYS:HA	2:F:1614:ARG:HH12	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3860:ARG:HH21	2:F:3932:ASN:HB2	1.62	0.63
2:H:3860:ARG:HH21	2:H:3932:ASN:HB2	1.62	0.63
2:F:207:PHE:CB	2:H:2326:ILE:O	2.46	0.63
2:D:4642:PRO:HG2	2:D:4648:LYS:HD3	1.79	0.63
2:F:1442:TRP:HB2	2:F:1544:PHE:HB2	1.81	0.63
2:D:4184:LYS:HG3	2:F:4904:HIS:CD2	2.34	0.63
2:H:1165:MET:HB2	2:H:1174:MET:HB2	1.79	0.63
2:H:2067:MET:HE1	2:H:2085:MET:HB3	1.80	0.63
2:B:4811:LEU:CB	2:D:4519:LEU:HD22	2.19	0.63
2:D:143:LEU:CB	2:F:2427:LEU:HD21	2.29	0.63
2:D:3748:SER:HB2	2:D:3751:GLU:HB2	1.81	0.63
2:B:1442:TRP:HB2	2:B:1544:PHE:HB2	1.81	0.63
2:F:3645:LEU:HB3	2:F:3665:LEU:HB2	1.81	0.63
2:B:1258:PHE:HB2	2:B:1593:HIS:HB3	1.80	0.62
2:F:4642:PRO:HG2	2:F:4648:LYS:HD3	1.80	0.62
2:B:4518:LEU:CD2	2:H:4780:TYR:HE1	1.88	0.62
2:H:3996:ILE:HG12	2:H:4000:MET:HE3	1.79	0.62
2:B:833:LYS:HA	2:B:1614:ARG:HH12	1.64	0.62
2:B:3748:SER:HB2	2:B:3751:GLU:HB2	1.81	0.62
2:B:4822:VAL:HG11	2:H:4849:ILE:HB	1.79	0.62
2:F:3748:SER:HB2	2:F:3751:GLU:HB2	1.81	0.62
2:H:1938:GLN:NE2	2:H:3611:ASN:O	2.33	0.62
2:H:3748:SER:HB2	2:H:3751:GLU:HB2	1.81	0.62
2:D:3645:LEU:HB3	2:D:3665:LEU:HB2	1.81	0.62
2:F:4849:ILE:CB	2:H:4822:VAL:HG11	2.30	0.62
2:H:1258:PHE:HB2	2:H:1593:HIS:HB3	1.80	0.62
2:D:2067:MET:HE1	2:D:2085:MET:HB3	1.80	0.62
2:D:4826:GLY:C	2:F:4823:ARG:HA	2.23	0.62
2:B:4823:ARG:CB	2:H:4826:GLY:CA	2.78	0.62
2:B:924:LEU:HB3	2:B:928:GLU:HB3	1.81	0.62
2:B:2067:MET:HE1	2:B:2085:MET:HB3	1.80	0.62
2:H:1442:TRP:HB2	2:H:1544:PHE:HB2	1.81	0.62
2:D:924:LEU:HB3	2:D:928:GLU:HB3	1.81	0.62
2:H:122:ARG:HE	2:H:127:GLY:HA2	1.65	0.62
2:B:1938:GLN:NE2	2:B:3611:ASN:O	2.33	0.62
2:D:1938:GLN:NE2	2:D:3611:ASN:O	2.33	0.62
2:B:1703:TYR:HD2	2:B:1820:PRO:HB2	1.65	0.61
2:B:4822:VAL:HG11	2:H:4849:ILE:CB	2.30	0.61
2:F:1258:PHE:HB2	2:F:1593:HIS:HB3	1.80	0.61
2:F:1703:TYR:HD2	2:F:1820:PRO:HB2	1.65	0.61
2:B:3880:LEU:HD23	2:B:3944:ALA:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4659:GLY:HA3	2:F:4664:ARG:HH21	1.65	0.61
2:H:3645:LEU:HB3	2:H:3665:LEU:HB2	1.81	0.61
2:D:1258:PHE:HB2	2:D:1593:HIS:HB3	1.80	0.61
2:H:833:LYS:HA	2:H:1614:ARG:HH12	1.64	0.61
2:B:4659:GLY:HA3	2:B:4664:ARG:HH21	1.65	0.61
2:F:1938:GLN:NE2	2:F:3611:ASN:O	2.33	0.61
2:B:1111:GLY:HA3	2:B:1211:GLN:HE21	1.66	0.61
2:D:1442:TRP:HB2	2:D:1544:PHE:HB2	1.81	0.61
2:H:1429:SER:HA	2:H:1507:ILE:HG12	1.82	0.61
2:F:1111:GLY:HA3	2:F:1211:GLN:HE21	1.66	0.61
2:F:2067:MET:HE1	2:F:2085:MET:HB3	1.80	0.61
2:H:1703:TYR:HD2	2:H:1820:PRO:HB2	1.65	0.61
2:B:1425:THR:N	2:B:1510:VAL:O	2.34	0.61
2:D:1703:TYR:HD2	2:D:1820:PRO:HB2	1.65	0.61
2:F:4826:GLY:C	2:H:4823:ARG:HA	2.25	0.61
2:H:1696:GLY:HA2	2:H:1699:ARG:HB3	1.82	0.61
2:B:1304:LEU:HD23	2:B:1306:MET:H	1.66	0.61
2:B:3645:LEU:HB3	2:B:3665:LEU:HB2	1.81	0.61
2:D:1429:SER:HA	2:D:1507:ILE:HG12	1.82	0.61
2:F:924:LEU:HB3	2:F:928:GLU:HB3	1.81	0.61
2:F:2060:GLN:NE2	2:F:2092:GLN:O	2.34	0.61
2:H:841:LYS:HD3	2:H:848:ARG:HD3	1.83	0.61
2:H:4047:ARG:NH1	2:H:4077:GLU:OE2	2.34	0.61
2:F:123:HIS:HD2	2:F:126:SER:H	1.49	0.61
2:F:3880:LEU:HD23	2:F:3944:ALA:HB2	1.82	0.61
2:H:1111:GLY:HA3	2:H:1211:GLN:HE21	1.66	0.61
2:H:4659:GLY:HA3	2:H:4664:ARG:HH21	1.65	0.61
2:D:123:HIS:HD2	2:D:126:SER:H	1.49	0.60
2:H:924:LEU:HB3	2:H:928:GLU:HB3	1.81	0.60
2:D:2060:GLN:NE2	2:D:2092:GLN:O	2.34	0.60
2:D:2326:ILE:O	2:D:2326:ILE:CG2	2.45	0.60
2:F:122:ARG:HE	2:F:127:GLY:HA2	1.65	0.60
2:F:1304:LEU:HD23	2:F:1306:MET:H	1.66	0.60
2:F:1696:GLY:HA2	2:F:1699:ARG:HB3	1.82	0.60
2:F:4826:GLY:CA	2:H:4823:ARG:CB	2.80	0.60
2:H:123:HIS:HD2	2:H:126:SER:H	1.49	0.60
2:H:1425:THR:N	2:H:1510:VAL:O	2.34	0.60
2:F:243:GLU:HA	2:F:264:GLY:HA2	1.84	0.60
2:H:672:LYS:HA	2:H:760:ASP:HA	1.84	0.60
2:B:2718:LEU:HB3	2:B:2780:LEU:HD13	1.84	0.60
1:C:74:LEU:HB2	1:C:99:PHE:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1425:THR:N	2:D:1510:VAL:O	2.34	0.60
2:F:672:LYS:HA	2:F:760:ASP:HA	1.84	0.60
2:F:4047:ARG:NH1	2:F:4077:GLU:OE2	2.34	0.60
2:B:122:ARG:HE	2:B:127:GLY:HA2	1.65	0.60
2:B:1696:GLY:HA2	2:B:1699:ARG:HB3	1.82	0.60
2:B:4047:ARG:NH1	2:B:4077:GLU:OE2	2.34	0.60
2:B:4823:ARG:CA	2:H:4826:GLY:HA3	2.32	0.60
2:F:244:CYS:SG	2:F:245:LEU:N	2.75	0.60
2:H:2060:GLN:NE2	2:H:2092:GLN:O	2.34	0.60
2:H:3880:LEU:HD23	2:H:3944:ALA:HB2	1.82	0.60
2:B:4780:TYR:CE1	2:D:4518:LEU:HB2	2.26	0.60
2:D:1111:GLY:HA3	2:D:1211:GLN:HE21	1.66	0.60
2:D:4659:GLY:HA3	2:D:4664:ARG:HH21	1.65	0.60
2:B:1429:SER:HA	2:B:1507:ILE:HG12	1.82	0.60
2:D:1696:GLY:HA2	2:D:1699:ARG:HB3	1.82	0.60
1:E:74:LEU:HB2	1:E:99:PHE:HB2	1.84	0.60
2:F:841:LYS:HD3	2:F:848:ARG:HD3	1.83	0.60
2:H:1146:HIS:HB2	2:H:1192:PHE:HE1	1.67	0.60
2:H:1445:TRP:HE1	2:H:1508:GLY:HA3	1.67	0.60
2:B:123:HIS:HD2	2:B:126:SER:H	1.49	0.60
2:B:1146:HIS:HB2	2:B:1192:PHE:HE1	1.67	0.60
2:B:1810:VAL:H	2:B:1817:LEU:HD13	1.67	0.60
2:H:2718:LEU:HB3	2:H:2780:LEU:HD13	1.84	0.60
2:D:3880:LEU:HD23	2:D:3944:ALA:HB2	1.82	0.60
2:B:748:LEU:HB2	2:B:750:ARG:HG3	1.83	0.60
2:D:243:GLU:HA	2:D:264:GLY:HA2	1.84	0.60
2:D:1445:TRP:HE1	2:D:1508:GLY:HA3	1.67	0.60
2:F:1272:ARG:NH2	2:F:1590:PHE:O	2.35	0.60
2:D:4826:GLY:CA	2:F:4823:ARG:CB	2.80	0.59
2:F:2536:PHE:O	2:F:2539:THR:N	2.35	0.59
2:H:1304:LEU:HD23	2:H:1306:MET:H	1.66	0.59
2:B:841:LYS:HD3	2:B:848:ARG:HD3	1.83	0.59
2:B:2060:GLN:NE2	2:B:2092:GLN:O	2.34	0.59
2:D:748:LEU:HB2	2:D:750:ARG:HG3	1.83	0.59
2:D:1146:HIS:HB2	2:D:1192:PHE:HE1	1.67	0.59
2:D:4838:ASP:HB3	2:D:4841:GLU:HB2	1.84	0.59
2:F:1425:THR:N	2:F:1510:VAL:O	2.34	0.59
2:H:1810:VAL:H	2:H:1817:LEU:HD13	1.67	0.59
2:B:243:GLU:HA	2:B:264:GLY:HA2	1.84	0.59
2:D:122:ARG:HE	2:D:127:GLY:HA2	1.65	0.59
2:D:1304:LEU:HD23	2:D:1306:MET:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:CYS:SG	2:B:245:LEU:N	2.75	0.59
2:B:672:LYS:HA	2:B:760:ASP:HA	1.84	0.59
2:B:4838:ASP:HB3	2:B:4841:GLU:HB2	1.84	0.59
2:D:1272:ARG:NH2	2:D:1590:PHE:O	2.35	0.59
2:D:1809:PRO:HB2	2:D:1812:GLY:H	1.68	0.59
2:D:4047:ARG:NH1	2:D:4077:GLU:OE2	2.34	0.59
2:F:1146:HIS:HB2	2:F:1192:PHE:HE1	1.67	0.59
2:H:1655:TYR:OH	2:H:1659:ARG:NH2	2.36	0.59
2:D:2718:LEU:HB3	2:D:2780:LEU:HD13	1.84	0.59
2:F:844:ARG:HD3	2:F:1214:ARG:HH21	1.68	0.59
2:H:365:HIS:HD2	2:H:368:THR:H	1.50	0.59
2:B:1809:PRO:HB2	2:B:1812:GLY:H	1.68	0.59
2:D:672:LYS:HA	2:D:760:ASP:HA	1.84	0.59
2:D:4861:ALA:CB	2:F:4864:GLN:CG	2.52	0.59
2:F:1810:VAL:H	2:F:1817:LEU:HD13	1.67	0.59
2:B:1445:TRP:HE1	2:B:1508:GLY:HA3	1.67	0.59
2:D:244:CYS:SG	2:D:245:LEU:N	2.75	0.59
2:D:365:HIS:HD2	2:D:368:THR:H	1.50	0.59
2:F:1429:SER:HA	2:F:1507:ILE:HG12	1.82	0.59
1:G:54:GLU:O	2:H:1772:ASN:ND2	2.36	0.59
2:B:4826:GLY:CA	2:D:4823:ARG:CB	2.80	0.59
2:H:244:CYS:SG	2:H:245:LEU:N	2.75	0.59
2:H:748:LEU:HB2	2:H:750:ARG:HG3	1.83	0.59
2:B:1272:ARG:NH2	2:B:1590:PHE:O	2.35	0.59
2:H:235:ARG:NH2	2:H:268:SER:O	2.36	0.59
2:B:844:ARG:HD3	2:B:1214:ARG:HH21	1.68	0.59
2:D:4931:GLU:OE2	2:D:4942:TRP:NE1	2.36	0.59
2:F:748:LEU:HB2	2:F:750:ARG:HG3	1.83	0.59
2:F:2326:ILE:O	2:F:2326:ILE:CG2	2.51	0.59
2:B:1242:ASN:HB3	2:B:1807:ARG:HB2	1.85	0.58
2:B:3810:GLU:O	2:B:3814:LYS:HB2	2.03	0.58
2:B:4874:LEU:O	2:B:4878:GLN:NE2	2.36	0.58
1:C:54:GLU:O	2:D:1772:ASN:ND2	2.36	0.58
2:F:1655:TYR:OH	2:F:1659:ARG:NH2	2.36	0.58
2:F:2718:LEU:HB3	2:F:2780:LEU:HD13	1.84	0.58
1:G:74:LEU:HB2	1:G:99:PHE:HB2	1.84	0.58
2:B:1655:TYR:OH	2:B:1659:ARG:NH2	2.36	0.58
2:D:841:LYS:HD3	2:D:848:ARG:HD3	1.83	0.58
2:D:844:ARG:HD3	2:D:1214:ARG:HH21	1.68	0.58
2:F:4819:TYR:C	2:F:4822:VAL:HG12	2.28	0.58
2:F:4931:GLU:OE2	2:F:4942:TRP:NE1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.84	0.58
2:B:235:ARG:NH2	2:B:268:SER:O	2.36	0.58
2:B:4758:LEU:HD21	2:H:4774:LEU:HD21	1.85	0.58
2:D:1242:ASN:HB3	2:D:1807:ARG:HB2	1.85	0.58
2:D:4054:GLU:HG2	2:D:4061:GLN:HE21	1.69	0.58
2:F:235:ARG:NH2	2:F:268:SER:O	2.36	0.58
2:H:246:THR:OG1	2:H:272:ARG:NH1	2.37	0.58
2:H:1272:ARG:NH2	2:H:1590:PHE:O	2.35	0.58
2:D:4807:CYS:SG	2:D:4812:THR:OG1	2.61	0.58
2:F:1445:TRP:HE1	2:F:1508:GLY:HA3	1.67	0.58
2:F:4838:ASP:HB3	2:F:4841:GLU:HB2	1.84	0.58
2:H:4807:CYS:SG	2:H:4812:THR:OG1	2.61	0.58
2:H:4838:ASP:HB3	2:H:4841:GLU:HB2	1.84	0.58
2:B:4054:GLU:HG2	2:B:4061:GLN:HE21	1.69	0.58
2:F:3810:GLU:O	2:F:3814:LYS:HB2	2.03	0.58
2:B:4616:LEU:HA	2:B:4620:GLU:HB2	1.85	0.58
2:B:4807:CYS:SG	2:B:4812:THR:OG1	2.61	0.58
2:D:3899:ILE:O	2:D:3904:GLN:NE2	2.36	0.58
2:D:4819:TYR:C	2:D:4822:VAL:HG12	2.28	0.58
2:F:246:THR:OG1	2:F:272:ARG:NH1	2.37	0.58
2:H:1809:PRO:HB2	2:H:1812:GLY:H	1.68	0.58
2:H:3810:GLU:O	2:H:3814:LYS:HB2	2.03	0.58
2:B:4931:GLU:OE2	2:B:4942:TRP:NE1	2.36	0.58
2:F:1272:ARG:NH1	2:F:1587:HIS:O	2.37	0.58
2:F:4807:CYS:SG	2:F:4812:THR:OG1	2.61	0.58
1:G:37:ASP:OD1	1:G:42:ARG:NH2	2.37	0.58
2:H:4054:GLU:HG2	2:H:4061:GLN:HE21	1.69	0.58
2:H:4874:LEU:O	2:H:4878:GLN:NE2	2.36	0.58
1:C:37:ASP:OD1	1:C:42:ARG:NH2	2.37	0.58
2:D:1810:VAL:H	2:D:1817:LEU:HD13	1.67	0.58
2:H:243:GLU:HA	2:H:264:GLY:HA2	1.84	0.58
2:H:3899:ILE:O	2:H:3904:GLN:NE2	2.36	0.58
1:A:37:ASP:OD1	1:A:42:ARG:NH2	2.37	0.58
1:A:54:GLU:O	2:B:1772:ASN:ND2	2.36	0.58
2:D:1442:TRP:HD1	2:D:1488:VAL:HG13	1.68	0.58
2:D:4013:MET:N	2:D:4013:MET:SD	2.77	0.58
2:F:365:HIS:HD2	2:F:368:THR:H	1.50	0.58
2:F:3899:ILE:O	2:F:3904:GLN:NE2	2.36	0.58
2:B:363:ILE:HD12	2:B:372:LEU:HD22	1.86	0.58
2:B:2326:ILE:O	2:B:2326:ILE:CG2	2.51	0.58
1:E:54:GLU:O	2:F:1772:ASN:ND2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4655:MET:HA	2:F:4667:ILE:HD12	1.86	0.58
2:H:844:ARG:HD3	2:H:1214:ARG:HH21	1.68	0.58
2:B:4861:ALA:CB	2:D:4864:GLN:CG	2.51	0.57
2:D:235:ARG:NH2	2:D:268:SER:O	2.36	0.57
2:F:4616:LEU:HA	2:F:4620:GLU:HB2	1.85	0.57
2:B:365:HIS:HD2	2:B:368:THR:H	1.50	0.57
2:D:246:THR:OG1	2:D:272:ARG:NH1	2.37	0.57
2:D:1655:TYR:OH	2:D:1659:ARG:NH2	2.36	0.57
2:D:4655:MET:HA	2:D:4667:ILE:HD12	1.86	0.57
2:F:1809:PRO:HB2	2:F:1812:GLY:H	1.68	0.57
2:H:1242:ASN:HB3	2:H:1807:ARG:HB2	1.85	0.57
2:H:4931:GLU:OE2	2:H:4942:TRP:NE1	2.36	0.57
2:B:246:THR:OG1	2:B:272:ARG:NH1	2.37	0.57
2:D:4616:LEU:HA	2:D:4620:GLU:HB2	1.85	0.57
2:H:4655:MET:HA	2:H:4667:ILE:HD12	1.86	0.57
2:B:1630:LEU:HD22	2:B:1641:ILE:HD13	1.86	0.57
2:B:1696:GLY:HA3	2:B:1816:PHE:HB3	1.86	0.57
2:D:3810:GLU:O	2:D:3814:LYS:HB2	2.03	0.57
2:F:1242:ASN:HB3	2:F:1807:ARG:HB2	1.85	0.57
2:F:4874:LEU:O	2:F:4878:GLN:NE2	2.36	0.57
2:H:1696:GLY:HA3	2:H:1816:PHE:HB3	1.86	0.57
2:H:4013:MET:SD	2:H:4013:MET:N	2.77	0.57
2:B:756:SER:HB3	2:B:769:ARG:HB2	1.86	0.57
2:D:258:ARG:NH1	2:D:316:LEU:O	2.38	0.57
2:D:1305:SER:HB2	2:D:1591:LEU:HB2	1.87	0.57
2:D:1630:LEU:HD22	2:D:1641:ILE:HD13	1.86	0.57
2:F:118:ALA:HB1	2:F:159:TRP:HB3	1.86	0.57
2:F:1696:GLY:HA3	2:F:1816:PHE:HB3	1.86	0.57
2:H:1231:GLY:O	2:H:1235:GLY:N	2.37	0.57
2:H:4616:LEU:HA	2:H:4620:GLU:HB2	1.85	0.57
2:B:1231:GLY:O	2:B:1235:GLY:N	2.37	0.57
2:B:1442:TRP:HD1	2:B:1488:VAL:HG13	1.68	0.57
2:B:4013:MET:N	2:B:4013:MET:SD	2.77	0.57
2:B:4819:TYR:C	2:B:4822:VAL:HG12	2.28	0.57
2:D:4874:LEU:O	2:D:4878:GLN:NE2	2.36	0.57
2:F:325:LYS:O	2:F:365:HIS:NE2	2.38	0.57
2:F:1231:GLY:O	2:F:1235:GLY:N	2.37	0.57
2:F:1305:SER:HB2	2:F:1591:LEU:HB2	1.86	0.57
2:H:1305:SER:HB2	2:H:1591:LEU:HB2	1.87	0.57
2:H:1442:TRP:HD1	2:H:1488:VAL:HG13	1.68	0.57
2:H:1630:LEU:HD22	2:H:1641:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4819:TYR:C	2:H:4822:VAL:HG12	2.28	0.57
2:B:832:LEU:O	2:B:1614:ARG:NH1	2.38	0.57
2:B:1143:GLN:HA	2:B:1151:HIS:HA	1.87	0.57
2:B:1305:SER:HB2	2:B:1591:LEU:HB2	1.87	0.57
2:D:118:ALA:HB1	2:D:159:TRP:HB3	1.86	0.57
2:F:4774:LEU:HD22	2:H:4754:LEU:HD11	1.85	0.57
2:F:4861:ALA:CB	2:H:4864:GLN:CG	2.56	0.57
2:H:363:ILE:HD12	2:H:372:LEU:HD22	1.86	0.57
2:B:4655:MET:HA	2:B:4667:ILE:HD12	1.86	0.57
2:D:58:VAL:HG22	2:D:320:GLU:HA	1.87	0.57
2:D:2027:ARG:HH12	2:D:2031:LEU:HB2	1.70	0.57
2:F:4013:MET:N	2:F:4013:MET:SD	2.77	0.57
2:H:651:HIS:N	2:H:1625:LEU:O	2.37	0.57
2:H:1272:ARG:NH1	2:H:1587:HIS:O	2.37	0.57
2:B:3160:LEU:O	2:B:3164:ALA:HB2	2.05	0.57
2:B:4774:LEU:HD21	2:D:4758:LEU:HD21	1.87	0.57
2:D:363:ILE:HD12	2:D:372:LEU:HD22	1.86	0.57
2:D:1272:ARG:NH1	2:D:1587:HIS:O	2.37	0.57
2:F:58:VAL:HG22	2:F:320:GLU:HA	1.87	0.57
2:F:651:HIS:N	2:F:1625:LEU:O	2.37	0.57
2:F:3914:ALA:HA	2:F:3917:VAL:HG12	1.86	0.57
2:H:756:SER:HB3	2:H:769:ARG:HB2	1.86	0.57
2:H:1143:GLN:HA	2:H:1151:HIS:HA	1.87	0.57
1:E:37:ASP:OD1	1:E:42:ARG:NH2	2.37	0.57
2:F:1922:ARG:NH1	2:F:2037:VAL:O	2.38	0.57
2:B:2027:ARG:HH12	2:B:2031:LEU:HB2	1.70	0.56
2:B:3899:ILE:O	2:B:3904:GLN:NE2	2.36	0.56
2:B:4864:GLN:CG	2:H:4861:ALA:CB	2.61	0.56
2:D:74:SER:O	2:D:78:LEU:HD13	2.05	0.56
2:D:1922:ARG:NH1	2:D:2037:VAL:O	2.38	0.56
2:H:2011:GLU:O	2:H:2027:ARG:NH2	2.37	0.56
2:B:1922:ARG:NH1	2:B:2037:VAL:O	2.38	0.56
2:D:832:LEU:O	2:D:1614:ARG:NH1	2.38	0.56
2:F:363:ILE:HD12	2:F:372:LEU:HD22	1.86	0.56
2:H:832:LEU:O	2:H:1614:ARG:NH1	2.38	0.56
2:B:3904:GLN:HG2	2:B:3965:GLN:HE22	1.70	0.56
1:C:36:PHE:HB3	2:D:640:ARG:HH12	1.71	0.56
2:D:290:ARG:H	2:D:293:GLN:HE21	1.53	0.56
2:D:647:ARG:NH1	2:D:1681:ASP:OD2	2.39	0.56
2:D:1143:GLN:HA	2:D:1151:HIS:HA	1.87	0.56
2:D:1696:GLY:HA3	2:D:1816:PHE:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:258:ARG:NH1	2:F:316:LEU:O	2.38	0.56
2:F:290:ARG:H	2:F:293:GLN:HE21	1.53	0.56
2:F:647:ARG:NH1	2:F:1681:ASP:OD2	2.39	0.56
2:F:1302:TYR:HB2	2:F:1543:VAL:HB	1.87	0.56
2:F:4826:GLY:HA3	2:H:4823:ARG:CA	2.35	0.56
2:H:58:VAL:HG22	2:H:320:GLU:HA	1.87	0.56
2:H:4002:ASP:OD1	2:H:4115:ARG:NH1	2.38	0.56
2:B:651:HIS:N	2:B:1625:LEU:O	2.37	0.56
2:B:1128:LEU:HD13	2:B:1206:SER:HB2	1.88	0.56
2:B:1302:TYR:HB2	2:B:1543:VAL:HB	1.87	0.56
2:D:756:SER:HB3	2:D:769:ARG:HB2	1.86	0.56
2:D:848:ARG:HH22	2:D:1607:ASP:H	1.54	0.56
2:D:1302:TYR:HB2	2:D:1543:VAL:HB	1.87	0.56
2:F:476:GLN:NE2	2:F:3679:GLU:OE1	2.39	0.56
2:F:4054:GLU:HG2	2:F:4061:GLN:HE21	1.69	0.56
2:F:4752:LYS:HA	2:F:4755:ARG:HD3	1.88	0.56
2:H:258:ARG:NH1	2:H:316:LEU:O	2.38	0.56
2:H:1302:TYR:HB2	2:H:1543:VAL:HB	1.87	0.56
2:B:118:ALA:HB1	2:B:159:TRP:HB3	1.86	0.56
2:B:258:ARG:NH1	2:B:316:LEU:O	2.38	0.56
2:B:411:GLU:HB3	2:B:414:ARG:HH21	1.71	0.56
2:B:647:ARG:NH1	2:B:1681:ASP:OD2	2.39	0.56
2:B:844:ARG:NH1	2:B:849:ASP:OD2	2.39	0.56
2:B:848:ARG:HH22	2:B:1607:ASP:H	1.54	0.56
2:B:4623:SER:O	2:B:4630:GLN:NE2	2.39	0.56
2:B:4826:GLY:HA3	2:D:4823:ARG:CA	2.36	0.56
2:B:4858:ILE:HG23	2:B:4862:ILE:HD12	1.88	0.56
2:D:3160:LEU:O	2:D:3164:ALA:HB2	2.05	0.56
2:F:832:LEU:O	2:F:1614:ARG:NH1	2.38	0.56
2:F:1442:TRP:HD1	2:F:1488:VAL:HG13	1.68	0.56
2:F:4780:TYR:CZ	2:H:4518:LEU:HB3	2.40	0.56
2:H:1922:ARG:NH1	2:H:2037:VAL:O	2.38	0.56
2:H:3160:LEU:O	2:H:3164:ALA:HB2	2.05	0.56
2:H:4623:SER:O	2:H:4630:GLN:NE2	2.39	0.56
2:B:58:VAL:HG22	2:B:320:GLU:HA	1.87	0.56
2:B:1267:HIS:O	2:B:1294:ASN:ND2	2.38	0.56
2:D:207:PHE:CB	2:F:2326:ILE:O	2.54	0.56
2:D:476:GLN:NE2	2:D:3679:GLU:OE1	2.39	0.56
2:D:3914:ALA:HA	2:D:3917:VAL:HG12	1.86	0.56
2:F:2011:GLU:O	2:F:2027:ARG:NH2	2.37	0.56
2:D:1128:LEU:HD13	2:D:1206:SER:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:PHE:HB3	2:F:640:ARG:HH12	1.71	0.56
2:F:1143:GLN:HA	2:F:1151:HIS:HA	1.87	0.56
2:F:1630:LEU:HD22	2:F:1641:ILE:HD13	1.86	0.56
2:H:476:GLN:NE2	2:H:3679:GLU:OE1	2.39	0.56
2:H:848:ARG:HH22	2:H:1607:ASP:H	1.54	0.56
2:B:476:GLN:NE2	2:B:3679:GLU:OE1	2.39	0.56
2:D:411:GLU:HB3	2:D:414:ARG:HH21	1.71	0.56
2:D:1267:HIS:O	2:D:1294:ASN:ND2	2.38	0.56
2:D:3904:GLN:HG2	2:D:3965:GLN:HE22	1.71	0.56
2:F:848:ARG:HH22	2:F:1607:ASP:H	1.54	0.56
2:F:1128:LEU:HD13	2:F:1206:SER:HB2	1.88	0.56
2:F:2027:ARG:HH12	2:F:2031:LEU:HB2	1.70	0.56
2:F:3160:LEU:O	2:F:3164:ALA:HB2	2.05	0.56
2:F:4800:GLY:HA2	2:F:4804:ASP:HB3	1.88	0.56
2:H:118:ALA:HB1	2:H:159:TRP:HB3	1.86	0.56
2:B:1272:ARG:NH1	2:B:1587:HIS:O	2.37	0.56
2:D:3663:ASP:OD2	2:D:3735:ARG:NH2	2.39	0.56
2:D:4623:SER:O	2:D:4630:GLN:NE2	2.39	0.56
2:D:4888:LYS:HG2	2:D:4895:GLY:HA2	1.88	0.56
2:F:4002:ASP:OD1	2:F:4115:ARG:NH1	2.38	0.56
2:D:1469:LEU:HB2	2:D:1477:HIS:HA	1.88	0.56
2:F:756:SER:HB3	2:F:769:ARG:HB2	1.86	0.56
2:H:74:SER:O	2:H:78:LEU:HD13	2.05	0.56
2:H:2027:ARG:HH12	2:H:2031:LEU:HB2	1.70	0.56
2:H:3970:LYS:HA	2:H:3973:MET:HE2	1.88	0.56
2:H:4752:LYS:HA	2:H:4755:ARG:HD3	1.88	0.56
2:H:4800:GLY:HA2	2:H:4804:ASP:HB3	1.88	0.56
1:A:36:PHE:HB3	2:B:640:ARG:HH12	1.71	0.55
2:B:3970:LYS:HA	2:B:3973:MET:HE2	1.88	0.55
2:D:4002:ASP:OD1	2:D:4115:ARG:NH1	2.38	0.55
2:D:4858:ILE:HG23	2:D:4862:ILE:HD12	1.88	0.55
2:F:3970:LYS:HA	2:F:3973:MET:HE2	1.88	0.55
2:H:647:ARG:NH1	2:H:1681:ASP:OD2	2.39	0.55
2:H:3914:ALA:HA	2:H:3917:VAL:HG12	1.87	0.55
2:B:150:GLN:NE2	2:B:158:CYS:SG	2.78	0.55
2:B:3914:ALA:HA	2:B:3917:VAL:HG12	1.87	0.55
2:B:4752:LYS:HA	2:B:4755:ARG:HD3	1.88	0.55
2:B:4888:LYS:HG2	2:B:4895:GLY:HA2	1.88	0.55
2:D:1231:GLY:O	2:D:1235:GLY:N	2.37	0.55
2:D:4780:TYR:CZ	2:F:4518:LEU:HB3	2.41	0.55
2:F:78:LEU:HD21	2:F:118:ALA:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1128:LEU:HD13	2:H:1206:SER:HB2	1.88	0.55
2:B:78:LEU:HD21	2:B:118:ALA:HB3	1.88	0.55
2:D:3970:LYS:HA	2:D:3973:MET:HE2	1.88	0.55
2:D:4662:TYR:HB3	2:D:4666:ARG:HG3	1.88	0.55
2:F:844:ARG:NH1	2:F:849:ASP:OD2	2.39	0.55
2:F:4888:LYS:HG2	2:F:4895:GLY:HA2	1.88	0.55
2:H:150:GLN:NE2	2:H:158:CYS:SG	2.78	0.55
2:H:1469:LEU:HB2	2:H:1477:HIS:HA	1.88	0.55
2:B:1761:MET:SD	2:B:1761:MET:N	2.76	0.55
2:B:4002:ASP:OD1	2:B:4115:ARG:NH1	2.38	0.55
2:H:4936:GLY:O	2:H:4940:TYR:HB2	2.07	0.55
2:B:4907:GLU:CD	2:H:4184:LYS:HD3	2.32	0.55
2:H:844:ARG:NH1	2:H:849:ASP:OD2	2.39	0.55
2:B:4936:GLY:O	2:B:4940:TYR:HB2	2.07	0.55
2:D:657:PRO:HA	2:D:834:VAL:HA	1.88	0.55
2:D:2296:GLY:HA2	2:D:2299:TYR:HD2	1.71	0.55
2:D:4826:GLY:HA3	2:F:4823:ARG:CA	2.37	0.55
2:D:4936:GLY:O	2:D:4940:TYR:HB2	2.07	0.55
2:F:4662:TYR:HB3	2:F:4666:ARG:HG3	1.88	0.55
2:H:411:GLU:HB3	2:H:414:ARG:HH21	1.71	0.55
2:H:2296:GLY:HA2	2:H:2299:TYR:HD2	1.71	0.55
2:H:4858:ILE:HG23	2:H:4862:ILE:HD12	1.88	0.55
2:H:4888:LYS:HG2	2:H:4895:GLY:HA2	1.88	0.55
2:B:2296:GLY:HA2	2:B:2299:TYR:HD2	1.71	0.55
2:F:3960:SER:HG	2:F:4070:CYS:HG	1.53	0.55
2:F:4936:GLY:O	2:F:4940:TYR:HB2	2.07	0.55
2:B:23:GLN:NE2	2:B:52:THR:OG1	2.40	0.55
2:B:4904:HIS:NE2	2:H:4184:LYS:CG	2.69	0.55
2:H:3904:GLN:HG2	2:H:3965:GLN:HE22	1.71	0.55
2:B:2011:GLU:O	2:B:2027:ARG:NH2	2.37	0.55
2:B:3663:ASP:OD2	2:B:3735:ARG:NH2	2.39	0.55
2:F:4774:LEU:HD21	2:H:4758:LEU:HD21	1.88	0.55
2:H:218:SER:HB3	2:H:286:GLY:HA3	1.89	0.55
2:H:4024:LEU:HD11	2:H:4084:PHE:HE2	1.72	0.55
2:B:262:TYR:HB2	2:B:389:ARG:HB3	1.89	0.55
2:B:4754:LEU:HD11	2:H:4774:LEU:HD22	1.88	0.55
2:F:898:ILE:HD13	2:F:974:SER:H	1.72	0.55
2:F:3845:GLN:HB2	2:F:3920:THR:HG22	1.89	0.55
2:B:1469:LEU:HB2	2:B:1477:HIS:HA	1.88	0.54
2:B:4662:TYR:HB3	2:B:4666:ARG:HG3	1.88	0.54
2:D:1089:ARG:HH21	2:D:1600:PRO:HG3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3845:GLN:HB2	2:D:3920:THR:HG22	1.89	0.54
2:F:23:GLN:NE2	2:F:52:THR:OG1	2.40	0.54
2:F:150:GLN:NE2	2:F:158:CYS:SG	2.78	0.54
2:F:2296:GLY:HA2	2:F:2299:TYR:HD2	1.71	0.54
2:F:3763:GLY:HA2	2:F:3766:ILE:HD12	1.90	0.54
2:F:4623:SER:O	2:F:4630:GLN:NE2	2.39	0.54
2:H:23:GLN:NE2	2:H:52:THR:OG1	2.40	0.54
2:H:290:ARG:H	2:H:293:GLN:HE21	1.53	0.54
2:H:1267:HIS:O	2:H:1294:ASN:ND2	2.38	0.54
2:H:3663:ASP:OD2	2:H:3735:ARG:NH2	2.39	0.54
2:B:394:HIS:HD2	2:B:397:GLY:H	1.56	0.54
2:D:651:HIS:N	2:D:1625:LEU:O	2.37	0.54
2:F:218:SER:HB3	2:F:286:GLY:HA3	1.89	0.54
2:F:411:GLU:HB3	2:F:414:ARG:HH21	1.71	0.54
2:F:657:PRO:HA	2:F:834:VAL:HA	1.88	0.54
2:F:4089:HIS:O	2:F:4093:LYS:N	2.40	0.54
1:G:67:SER:H	1:G:70:GLN:HB3	1.72	0.54
2:D:3786:LYS:NZ	2:D:3864:GLY:O	2.40	0.54
2:H:3845:GLN:HB2	2:H:3920:THR:HG22	1.89	0.54
2:B:325:LYS:O	2:B:365:HIS:NE2	2.38	0.54
2:B:1611:ILE:O	2:B:1620:GLN:N	2.40	0.54
2:B:4024:LEU:HD11	2:B:4084:PHE:HE2	1.72	0.54
2:F:1267:HIS:O	2:F:1294:ASN:ND2	2.38	0.54
2:F:4858:ILE:HG23	2:F:4862:ILE:HD12	1.88	0.54
2:H:898:ILE:HD13	2:H:974:SER:H	1.72	0.54
2:H:3763:GLY:HA2	2:H:3766:ILE:HD12	1.90	0.54
2:B:1722:ASN:OD1	2:B:1758:ARG:NH2	2.41	0.54
2:B:4823:ARG:CA	2:H:4826:GLY:C	2.81	0.54
2:D:844:ARG:NH1	2:D:849:ASP:OD2	2.39	0.54
2:D:4800:GLY:HA2	2:D:4804:ASP:HB3	1.88	0.54
1:E:67:SER:H	1:E:70:GLN:HB3	1.72	0.54
2:F:243:GLU:OE2	2:F:389:ARG:NH1	2.41	0.54
2:F:1469:LEU:HB2	2:F:1477:HIS:HA	1.88	0.54
2:F:1722:ASN:OD1	2:F:1758:ARG:NH2	2.41	0.54
2:H:1612:SER:HA	2:H:1619:VAL:HA	1.90	0.54
2:B:290:ARG:H	2:B:293:GLN:HE21	1.53	0.54
2:B:1089:ARG:HH21	2:B:1600:PRO:HG3	1.73	0.54
1:G:36:PHE:HB3	2:H:640:ARG:HH12	1.71	0.54
2:H:262:TYR:HB2	2:H:389:ARG:HB3	1.89	0.54
2:H:3876:VAL:HG13	2:H:3941:LEU:HB3	1.90	0.54
2:B:3763:GLY:HA2	2:B:3766:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:SER:H	1:C:70:GLN:HB3	1.72	0.54
2:D:1253:LYS:HD2	2:D:1255:LEU:HB2	1.89	0.54
2:D:1722:ASN:OD1	2:D:1758:ARG:NH2	2.41	0.54
2:D:2779:SER:OG	2:D:2849:TYR:OH	2.22	0.54
2:D:4752:LYS:HA	2:D:4755:ARG:HD3	1.88	0.54
2:F:1938:GLN:HE22	2:F:3611:ASN:HB2	1.73	0.54
2:H:1089:ARG:HH21	2:H:1600:PRO:HG3	1.72	0.54
2:H:1722:ASN:OD1	2:H:1758:ARG:NH2	2.41	0.54
2:B:218:SER:HB3	2:B:286:GLY:HA3	1.89	0.54
2:B:898:ILE:HD13	2:B:974:SER:H	1.73	0.54
2:B:3845:GLN:HB2	2:B:3920:THR:HG22	1.89	0.54
2:B:4518:LEU:HB3	2:H:4780:TYR:CZ	2.43	0.54
2:D:23:GLN:NE2	2:D:52:THR:OG1	2.40	0.54
2:D:4774:LEU:HD22	2:F:4754:LEU:HD11	1.90	0.54
2:H:1938:GLN:HE22	2:H:3611:ASN:HB2	1.73	0.54
2:H:4662:TYR:HB3	2:H:4666:ARG:HG3	1.88	0.54
2:H:4751:PHE:O	2:H:4755:ARG:NH1	2.41	0.54
2:B:2326:ILE:O	2:H:207:PHE:CB	2.55	0.54
2:B:4568:TYR:O	2:B:4572:THR:OG1	2.23	0.54
2:B:4800:GLY:HA2	2:B:4804:ASP:HB3	1.88	0.54
2:B:4841:GLU:OE2	2:B:4844:ARG:NH2	2.41	0.54
2:B:4853:PHE:CZ	2:D:4859:LEU:HD12	2.43	0.54
2:D:898:ILE:HD13	2:D:974:SER:H	1.73	0.54
2:D:948:CYS:HB3	2:D:1064:LEU:HD22	1.90	0.54
2:F:644:LEU:HD22	2:F:1632:ILE:HG22	1.90	0.54
2:F:2779:SER:OG	2:F:2849:TYR:OH	2.22	0.54
2:F:3663:ASP:OD2	2:F:3735:ARG:NH2	2.39	0.54
2:H:243:GLU:OE2	2:H:389:ARG:NH1	2.41	0.54
2:H:657:PRO:HA	2:H:834:VAL:HA	1.88	0.54
2:B:66:THR:HG1	2:B:124:SER:HG	1.53	0.54
2:B:4184:LYS:HD3	2:D:4907:GLU:CD	2.33	0.54
2:B:4751:PHE:O	2:B:4755:ARG:NH1	2.41	0.54
2:D:3763:GLY:HA2	2:D:3766:ILE:HD12	1.90	0.54
2:F:1089:ARG:HH21	2:F:1600:PRO:HG3	1.72	0.54
2:F:1116:GLY:HA3	2:F:1136:ALA:HA	1.90	0.54
2:F:3904:GLN:HG2	2:F:3965:GLN:HE22	1.71	0.54
2:F:4024:LEU:HD11	2:F:4084:PHE:HE2	1.72	0.54
2:H:3786:LYS:NZ	2:H:3864:GLY:O	2.40	0.54
1:A:21:THR:OG1	1:A:49:ARG:NH2	2.40	0.53
2:B:657:PRO:HA	2:B:834:VAL:HA	1.88	0.53
2:B:1172:THR:HG21	2:B:1190:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2221:TYR:O	2:B:2225:ASN:ND2	2.42	0.53
2:B:4774:LEU:HD22	2:D:4754:LEU:HD11	1.90	0.53
2:D:1938:GLN:HE22	2:D:3611:ASN:HB2	1.73	0.53
2:F:1253:LYS:HD2	2:F:1255:LEU:HB2	1.89	0.53
2:H:2221:TYR:O	2:H:2225:ASN:ND2	2.41	0.53
2:B:644:LEU:HD22	2:B:1632:ILE:HG22	1.90	0.53
2:B:948:CYS:HB3	2:B:1064:LEU:HD22	1.90	0.53
2:B:4868:ILE:HG12	2:H:4865:GLY:HA3	1.91	0.53
2:D:2011:GLU:O	2:D:2027:ARG:NH2	2.37	0.53
2:D:4774:LEU:HD21	2:F:4758:LEU:HD21	1.89	0.53
2:F:802:PHE:HB2	2:F:1617:TRP:HB2	1.90	0.53
2:H:644:LEU:HD22	2:H:1632:ILE:HG22	1.90	0.53
2:B:1106:GLU:OE1	2:B:1214:ARG:NH1	2.42	0.53
2:D:802:PHE:HB2	2:D:1617:TRP:HB2	1.91	0.53
2:D:2221:TYR:O	2:D:2225:ASN:ND2	2.41	0.53
2:F:4751:PHE:O	2:F:4755:ARG:NH1	2.41	0.53
2:F:4841:GLU:OE2	2:F:4844:ARG:NH2	2.41	0.53
2:B:279:THR:HA	2:B:295:PHE:HD1	1.74	0.53
2:D:1172:THR:HG21	2:D:1190:LEU:HD13	1.90	0.53
2:F:1612:SER:HA	2:F:1619:VAL:HA	1.90	0.53
2:F:2116:ASP:OD1	2:F:2153:ASN:ND2	2.41	0.53
2:F:3876:VAL:HG13	2:F:3941:LEU:HB3	1.90	0.53
1:G:39:SER:HA	1:G:42:ARG:HG2	1.90	0.53
2:H:1253:LYS:HD2	2:H:1255:LEU:HB2	1.89	0.53
2:H:4841:GLU:OE2	2:H:4844:ARG:NH2	2.41	0.53
1:A:67:SER:H	1:A:70:GLN:HB3	1.72	0.53
2:B:62:LEU:HB3	2:B:276:ARG:HH21	1.74	0.53
2:B:243:GLU:OE2	2:B:389:ARG:NH1	2.41	0.53
2:B:1160:ASP:OD1	2:B:1178:ASN:ND2	2.41	0.53
2:B:2102:ALA:HA	2:B:2105:LYS:HZ2	1.73	0.53
2:D:1761:MET:SD	2:D:1761:MET:N	2.76	0.53
2:D:3876:VAL:HG13	2:D:3941:LEU:HB3	1.90	0.53
2:B:656:ARG:HH12	2:B:700:THR:HG22	1.74	0.53
2:B:1253:LYS:HD2	2:B:1255:LEU:HB2	1.89	0.53
2:B:4089:HIS:O	2:B:4093:LYS:N	2.40	0.53
2:D:150:GLN:NE2	2:D:158:CYS:SG	2.78	0.53
2:D:218:SER:HB3	2:D:286:GLY:HA3	1.89	0.53
2:D:262:TYR:HB2	2:D:389:ARG:HB3	1.89	0.53
2:D:644:LEU:HD22	2:D:1632:ILE:HG22	1.90	0.53
2:D:1116:GLY:HA3	2:D:1136:ALA:HA	1.90	0.53
2:D:4751:PHE:O	2:D:4755:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:262:TYR:HB2	2:F:389:ARG:HB3	1.89	0.53
2:F:1033:VAL:HG23	2:F:1038:LEU:HB3	1.91	0.53
1:G:21:THR:OG1	1:G:49:ARG:NH2	2.40	0.53
2:H:394:HIS:HD2	2:H:397:GLY:H	1.56	0.53
2:H:802:PHE:HB2	2:H:1617:TRP:HB2	1.91	0.53
2:B:1612:SER:HA	2:B:1619:VAL:HA	1.90	0.53
2:B:1938:GLN:HE22	2:B:3611:ASN:HB2	1.73	0.53
2:B:3876:VAL:HG13	2:B:3941:LEU:HB3	1.90	0.53
2:D:279:THR:HA	2:D:295:PHE:HD1	1.74	0.53
2:F:1172:THR:HG21	2:F:1190:LEU:HD13	1.90	0.53
2:H:62:LEU:HB3	2:H:276:ARG:HH21	1.74	0.53
2:H:325:LYS:O	2:H:365:HIS:NE2	2.38	0.53
2:H:1116:GLY:HA3	2:H:1136:ALA:HA	1.90	0.53
2:B:4868:ILE:CD1	2:H:4865:GLY:HA2	2.39	0.53
2:D:1106:GLU:OE1	2:D:1214:ARG:NH1	2.42	0.53
2:D:4750:GLY:H	2:D:4755:ARG:HE	1.56	0.53
1:E:39:SER:HA	1:E:42:ARG:HG2	1.90	0.53
2:F:4750:GLY:H	2:F:4755:ARG:HE	1.56	0.53
2:H:1224:LEU:HB3	2:H:1227:PHE:HB3	1.91	0.53
2:H:3858:TYR:OH	2:H:3865:ASN:ND2	2.42	0.53
1:A:39:SER:HA	1:A:42:ARG:HG2	1.90	0.53
1:C:39:SER:HA	1:C:42:ARG:HG2	1.90	0.53
2:D:243:GLU:OE2	2:D:389:ARG:NH1	2.41	0.53
2:D:4841:GLU:OE2	2:D:4844:ARG:NH2	2.41	0.53
2:F:394:HIS:HD2	2:F:397:GLY:H	1.56	0.53
2:F:590:LYS:H	2:F:593:HIS:HD2	1.57	0.53
2:F:656:ARG:HH12	2:F:700:THR:HG22	1.74	0.53
2:B:4859:LEU:HD12	2:H:4853:PHE:CZ	2.43	0.53
2:D:73:LEU:CB	2:D:77:ALA:HB3	2.33	0.53
2:D:2418:ILE:HA	2:D:2421:ARG:HD3	1.91	0.53
2:F:948:CYS:HB3	2:F:1064:LEU:HD22	1.90	0.53
2:F:2418:ILE:HA	2:F:2421:ARG:HD3	1.91	0.53
2:F:4184:LYS:CG	2:H:4904:HIS:NE2	2.72	0.53
2:H:656:ARG:HH12	2:H:700:THR:HG22	1.74	0.53
2:H:3904:GLN:NE2	2:H:3965:GLN:OE1	2.42	0.53
2:B:1033:VAL:HG23	2:B:1038:LEU:HB3	1.91	0.52
2:B:2418:ILE:HA	2:B:2421:ARG:HD3	1.91	0.52
2:D:3904:GLN:NE2	2:D:3965:GLN:OE1	2.42	0.52
2:F:2221:TYR:O	2:F:2225:ASN:ND2	2.42	0.52
2:F:2860:GLU:O	2:F:2864:LYS:NZ	2.39	0.52
2:H:948:CYS:HB3	2:H:1064:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1033:VAL:HG23	2:H:1038:LEU:HB3	1.91	0.52
2:H:4089:HIS:O	2:H:4093:LYS:N	2.41	0.52
2:B:1224:LEU:HB3	2:B:1227:PHE:HB3	1.91	0.52
2:F:1224:LEU:HB3	2:F:1227:PHE:HB3	1.91	0.52
2:F:3805:ASP:OD2	2:F:3808:ALA:N	2.43	0.52
2:B:299:HIS:HD2	2:B:302:THR:H	1.57	0.52
2:B:1116:GLY:HA3	2:B:1136:ALA:HA	1.90	0.52
2:D:115:TYR:HB2	2:D:172:GLY:H	1.75	0.52
2:D:299:HIS:HD2	2:D:302:THR:H	1.57	0.52
2:D:1224:LEU:HB3	2:D:1227:PHE:HB3	1.91	0.52
2:D:2070:TRP:O	2:D:2074:SER:OG	2.28	0.52
2:H:73:LEU:CB	2:H:77:ALA:HB3	2.32	0.52
2:H:480:ARG:NH2	2:H:3679:GLU:OE2	2.43	0.52
2:H:897:LYS:HB3	2:H:902:TRP:HB2	1.92	0.52
2:H:1160:ASP:OD1	2:H:1178:ASN:ND2	2.41	0.52
2:H:1172:THR:HG21	2:H:1190:LEU:HD13	1.90	0.52
2:B:3904:GLN:NE2	2:B:3965:GLN:OE1	2.42	0.52
2:B:4759:SER:HA	2:B:4762:THR:HG22	1.92	0.52
2:D:656:ARG:HH12	2:D:700:THR:HG22	1.74	0.52
2:F:78:LEU:HD21	2:F:118:ALA:CB	2.40	0.52
2:F:1106:GLU:OE1	2:F:1214:ARG:NH1	2.42	0.52
2:H:228:LEU:HB3	2:H:289:ILE:HD12	1.91	0.52
2:H:646:THR:OG1	2:H:1684:GLN:NE2	2.42	0.52
2:H:2418:ILE:HA	2:H:2421:ARG:HD3	1.91	0.52
2:H:3917:VAL:O	2:H:3920:THR:OG1	2.23	0.52
2:B:1762:GLN:O	2:B:1779:SER:OG	2.25	0.52
2:B:4184:LYS:CG	2:D:4904:HIS:NE2	2.72	0.52
2:B:4826:GLY:C	2:D:4823:ARG:CA	2.83	0.52
2:D:62:LEU:HB3	2:D:276:ARG:HH21	1.74	0.52
2:D:228:LEU:HB3	2:D:289:ILE:HD12	1.91	0.52
2:D:1612:SER:HA	2:D:1619:VAL:HA	1.90	0.52
2:D:4759:SER:HA	2:D:4762:THR:HG22	1.92	0.52
2:D:4853:PHE:CZ	2:F:4859:LEU:HD12	2.45	0.52
1:E:21:THR:OG1	1:E:49:ARG:NH2	2.40	0.52
2:F:115:TYR:HB2	2:F:172:GLY:H	1.75	0.52
2:F:1756:SER:O	2:F:1920:ARG:NH2	2.43	0.52
2:H:25:THR:O	2:H:32:GLN:NE2	2.43	0.52
2:H:4750:GLY:H	2:H:4755:ARG:HE	1.56	0.52
2:B:646:THR:OG1	2:B:1684:GLN:NE2	2.42	0.52
2:B:897:LYS:HB3	2:B:902:TRP:HB2	1.92	0.52
2:B:2070:TRP:O	2:B:2074:SER:OG	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1783:PRO:HB3	2:D:1786:ILE:HD12	1.92	0.52
2:D:3805:ASP:OD2	2:D:3808:ALA:N	2.43	0.52
2:F:4780:TYR:HD1	2:H:4518:LEU:HD22	1.59	0.52
2:H:2070:TRP:O	2:H:2074:SER:OG	2.28	0.52
2:B:1756:SER:O	2:B:1920:ARG:NH2	2.43	0.52
2:D:4024:LEU:HD11	2:D:4084:PHE:HE2	1.72	0.52
2:D:4780:TYR:HD1	2:F:4518:LEU:HD22	1.63	0.52
2:D:4849:ILE:HG13	2:D:4850:THR:N	2.25	0.52
2:B:115:TYR:HB2	2:B:172:GLY:H	1.75	0.52
2:B:411:GLU:HA	2:B:414:ARG:HE	1.75	0.52
2:B:417:ARG:HD2	2:B:420:ARG:HD3	1.92	0.52
2:B:802:PHE:HB2	2:B:1617:TRP:HB2	1.90	0.52
2:B:1783:PRO:HB3	2:B:1786:ILE:HD12	1.92	0.52
2:D:1756:SER:O	2:D:1920:ARG:NH2	2.43	0.52
2:F:62:LEU:HB3	2:F:276:ARG:HH21	1.74	0.52
2:F:298:ARG:HE	2:F:303:GLY:HA2	1.75	0.52
2:H:279:THR:HA	2:H:295:PHE:HD1	1.74	0.52
2:H:590:LYS:H	2:H:593:HIS:HD2	1.57	0.52
2:H:1106:GLU:OE1	2:H:1214:ARG:NH1	2.42	0.52
2:H:2326:ILE:O	2:H:2326:ILE:CG2	2.57	0.52
2:B:73:LEU:CB	2:B:77:ALA:HB3	2.32	0.52
2:B:646:THR:OG1	2:B:1629:SER:O	2.26	0.52
2:D:411:GLU:HA	2:D:414:ARG:HE	1.75	0.52
2:F:3904:GLN:NE2	2:F:3965:GLN:OE1	2.42	0.52
2:H:1601:ASN:ND2	2:H:1643:GLU:OE2	2.43	0.52
2:B:25:THR:O	2:B:32:GLN:NE2	2.43	0.52
2:B:2308:PHE:HA	2:B:2313:SER:HA	1.92	0.52
2:D:636:LEU:HD21	2:D:643:LEU:HD21	1.92	0.52
2:D:1033:VAL:HG23	2:D:1038:LEU:HB3	1.91	0.52
2:D:2116:ASP:OD1	2:D:2153:ASN:ND2	2.42	0.52
2:F:897:LYS:HB3	2:F:902:TRP:HB2	1.92	0.52
2:F:1228:THR:HA	2:F:1232:LEU:HD12	1.92	0.52
2:B:1228:THR:HA	2:B:1232:LEU:HD12	1.92	0.51
2:B:4750:GLY:H	2:B:4755:ARG:HE	1.56	0.51
2:D:325:LYS:O	2:D:365:HIS:NE2	2.38	0.51
2:D:590:LYS:H	2:D:593:HIS:HD2	1.57	0.51
2:D:1228:THR:HA	2:D:1232:LEU:HD12	1.92	0.51
2:F:228:LEU:HB3	2:F:289:ILE:HD12	1.91	0.51
2:F:279:THR:HA	2:F:295:PHE:HD1	1.74	0.51
2:F:480:ARG:NH2	2:F:3679:GLU:OE2	2.43	0.51
1:A:9:PRO:HA	1:A:70:GLN:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1601:ASN:ND2	2:B:1643:GLU:OE2	2.43	0.51
2:B:3786:LYS:NZ	2:B:3864:GLY:O	2.40	0.51
2:F:646:THR:OG1	2:F:1684:GLN:NE2	2.43	0.51
2:H:115:TYR:HB2	2:H:172:GLY:H	1.75	0.51
2:H:4052:ALA:O	2:H:4056:HIS:ND1	2.39	0.51
2:B:677:LEU:HB2	2:B:755:ILE:HB	1.92	0.51
2:D:2308:PHE:HA	2:D:2313:SER:HA	1.92	0.51
2:F:2070:TRP:O	2:F:2074:SER:OG	2.28	0.51
2:H:411:GLU:HA	2:H:414:ARG:HE	1.75	0.51
2:H:636:LEU:HD21	2:H:643:LEU:HD21	1.92	0.51
2:H:1256:PRO:O	2:H:1451:HIS:ND1	2.44	0.51
2:H:1756:SER:O	2:H:1920:ARG:NH2	2.43	0.51
2:B:480:ARG:NH2	2:B:3679:GLU:OE2	2.43	0.51
2:B:4823:ARG:HA	2:H:4826:GLY:HA2	1.92	0.51
1:C:9:PRO:HA	1:C:70:GLN:HG3	1.93	0.51
2:D:25:THR:O	2:D:32:GLN:NE2	2.43	0.51
2:D:394:HIS:HD2	2:D:397:GLY:H	1.56	0.51
2:D:4568:TYR:O	2:D:4572:THR:OG1	2.23	0.51
1:E:9:PRO:HA	1:E:70:GLN:HG3	1.93	0.51
2:H:298:ARG:HE	2:H:303:GLY:HA2	1.75	0.51
2:H:1228:THR:HA	2:H:1232:LEU:HD12	1.92	0.51
2:H:4655:MET:O	2:H:4664:ARG:NH2	2.42	0.51
2:B:952:ILE:HA	2:B:1062:TYR:HE1	1.75	0.51
2:D:952:ILE:HA	2:D:1062:TYR:HE1	1.75	0.51
2:D:4522:LYS:O	2:D:4559:HIS:ND1	2.42	0.51
2:F:1783:PRO:HB3	2:F:1786:ILE:HD12	1.92	0.51
2:F:4849:ILE:HG13	2:F:4850:THR:N	2.25	0.51
2:H:417:ARG:HD2	2:H:420:ARG:HD3	1.92	0.51
2:H:4759:SER:HA	2:H:4762:THR:HG22	1.91	0.51
2:B:228:LEU:HB3	2:B:289:ILE:HD12	1.91	0.51
2:B:298:ARG:HE	2:B:303:GLY:HA2	1.75	0.51
2:B:299:HIS:NE2	2:B:301:THR:OG1	2.37	0.51
2:B:486:GLN:NE2	2:B:539:ALA:O	2.44	0.51
2:B:1183:LEU:HB3	2:B:1187:GLY:HA2	1.93	0.51
2:B:2096:ILE:O	2:B:2100:VAL:N	2.44	0.51
2:D:486:GLN:NE2	2:D:539:ALA:O	2.44	0.51
2:D:1601:ASN:ND2	2:D:1643:GLU:OE2	2.43	0.51
2:D:3853:SER:HB2	2:D:3929:CYS:HB3	1.92	0.51
2:D:4089:HIS:O	2:D:4093:LYS:N	2.41	0.51
2:F:25:THR:O	2:F:32:GLN:NE2	2.43	0.51
2:F:299:HIS:CD2	2:F:302:THR:H	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:299:HIS:HD2	2:F:302:THR:H	1.57	0.51
2:F:486:GLN:NE2	2:F:539:ALA:O	2.44	0.51
2:F:677:LEU:HB2	2:F:755:ILE:HB	1.92	0.51
2:F:1160:ASP:OD1	2:F:1178:ASN:ND2	2.41	0.51
2:F:1601:ASN:ND2	2:F:1643:GLU:OE2	2.43	0.51
2:F:2308:PHE:HA	2:F:2313:SER:HA	1.92	0.51
2:F:4655:MET:O	2:F:4664:ARG:NH2	2.42	0.51
2:H:299:HIS:CD2	2:H:302:THR:H	2.29	0.51
2:H:299:HIS:HD2	2:H:302:THR:H	1.57	0.51
2:H:2116:ASP:OD1	2:H:2153:ASN:ND2	2.42	0.51
2:H:4649:PHE:HB3	2:H:4653:LYS:HE3	1.93	0.51
2:B:78:LEU:HD21	2:B:118:ALA:CB	2.40	0.51
2:B:4649:PHE:HB3	2:B:4653:LYS:HE3	1.93	0.51
2:B:4780:TYR:CZ	2:D:4518:LEU:HB3	2.44	0.51
2:D:480:ARG:NH2	2:D:3679:GLU:OE2	2.43	0.51
2:D:646:THR:OG1	2:D:1684:GLN:NE2	2.42	0.51
2:D:897:LYS:HB3	2:D:902:TRP:HB2	1.92	0.51
2:F:2035:GLU:O	2:F:2038:THR:OG1	2.29	0.51
2:H:2860:GLU:O	2:H:2864:LYS:NZ	2.39	0.51
2:B:590:LYS:H	2:B:593:HIS:HD2	1.57	0.51
1:C:21:THR:HG1	1:C:49:ARG:HH21	1.57	0.51
2:D:299:HIS:CD2	2:D:302:THR:H	2.29	0.51
2:D:646:THR:OG1	2:D:1629:SER:O	2.26	0.51
2:D:4184:LYS:CG	2:F:4904:HIS:NE2	2.74	0.51
2:F:3786:LYS:NZ	2:F:3864:GLY:O	2.40	0.51
1:G:9:PRO:HA	1:G:70:GLN:HG3	1.93	0.51
2:H:2308:PHE:HA	2:H:2313:SER:HA	1.92	0.51
2:D:123:HIS:CD2	2:D:126:SER:H	2.28	0.51
2:D:417:ARG:HD2	2:D:420:ARG:HD3	1.92	0.51
2:D:1611:ILE:O	2:D:1620:GLN:N	2.40	0.51
2:F:1256:PRO:O	2:F:1451:HIS:ND1	2.44	0.51
2:H:180:ASP:HB3	2:H:211:LEU:HB3	1.93	0.51
2:H:1183:LEU:HB3	2:H:1187:GLY:HA2	1.93	0.51
2:H:2715:PRO:HD2	2:H:2718:LEU:HD12	1.93	0.51
2:B:4834:ASP:O	2:B:4844:ARG:NH2	2.45	0.51
2:D:119:ILE:HD13	2:D:162:ILE:HD11	1.93	0.51
2:D:1183:LEU:HB3	2:D:1187:GLY:HA2	1.93	0.51
2:D:1256:PRO:O	2:D:1451:HIS:ND1	2.44	0.51
2:H:4834:ASP:O	2:H:4844:ARG:NH2	2.44	0.51
2:H:4849:ILE:HG13	2:H:4850:THR:N	2.25	0.51
2:B:299:HIS:CD2	2:B:302:THR:H	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:636:LEU:HD21	2:B:643:LEU:HD21	1.92	0.50
2:B:2116:ASP:OD1	2:B:2153:ASN:ND2	2.41	0.50
2:B:3805:ASP:OD2	2:B:3808:ALA:N	2.43	0.50
2:B:4722:TYR:HD2	2:B:4723:LEU:HD12	1.76	0.50
1:C:23:VAL:HG22	1:C:47:LYS:HG2	1.93	0.50
2:D:4649:PHE:HB3	2:D:4653:LYS:HE3	1.93	0.50
2:D:4834:ASP:O	2:D:4844:ARG:NH2	2.44	0.50
1:E:23:VAL:HG22	1:E:47:LYS:HG2	1.93	0.50
2:F:143:LEU:CA	2:H:2427:LEU:HD21	2.41	0.50
2:F:1183:LEU:HB3	2:F:1187:GLY:HA2	1.93	0.50
2:F:1227:PHE:HE1	2:F:1236:TYR:HB2	1.76	0.50
2:F:3853:SER:HB2	2:F:3929:CYS:HB3	1.92	0.50
2:H:952:ILE:HA	2:H:1062:TYR:HE1	1.75	0.50
2:B:4796:LYS:HB2	2:B:4805:MET:HB3	1.93	0.50
2:B:4849:ILE:HG13	2:B:4850:THR:N	2.25	0.50
2:D:180:ASP:HB3	2:D:211:LEU:HB3	1.93	0.50
2:D:677:LEU:HB2	2:D:755:ILE:HB	1.92	0.50
2:D:4160:GLN:NE2	2:D:4201:MET:O	2.44	0.50
2:D:4184:LYS:HD3	2:F:4907:GLU:CD	2.35	0.50
2:D:4523:VAL:CA	2:D:4559:HIS:HD1	2.06	0.50
2:F:119:ILE:HD13	2:F:162:ILE:HD11	1.93	0.50
2:F:411:GLU:HA	2:F:414:ARG:HE	1.75	0.50
2:F:952:ILE:HA	2:F:1062:TYR:HE1	1.75	0.50
2:F:4160:GLN:NE2	2:F:4201:MET:O	2.44	0.50
1:G:23:VAL:HG22	1:G:47:LYS:HG2	1.93	0.50
2:H:486:GLN:NE2	2:H:539:ALA:O	2.44	0.50
2:B:123:HIS:CD2	2:B:126:SER:H	2.29	0.50
2:B:3853:SER:HB2	2:B:3929:CYS:HB3	1.92	0.50
2:B:3915:LYS:O	2:B:3919:ASN:ND2	2.45	0.50
2:F:3915:LYS:O	2:F:3919:ASN:ND2	2.45	0.50
2:F:4759:SER:HA	2:F:4762:THR:HG22	1.92	0.50
2:H:119:ILE:HD13	2:H:162:ILE:HD11	1.93	0.50
2:H:646:THR:HA	2:H:1630:LEU:HA	1.92	0.50
2:H:2779:SER:OG	2:H:2849:TYR:OH	2.22	0.50
2:B:119:ILE:HD13	2:B:162:ILE:HD11	1.93	0.50
2:B:2715:PRO:HD2	2:B:2718:LEU:HD12	1.93	0.50
1:C:4:ILE:O	1:C:65:GLN:NE2	2.45	0.50
2:D:298:ARG:HE	2:D:303:GLY:HA2	1.75	0.50
2:D:1184:ASP:OD2	2:D:1188:SER:OG	2.29	0.50
2:D:4651:LYS:NZ	2:D:4670:LEU:O	2.45	0.50
2:D:4780:TYR:OH	2:F:4518:LEU:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:417:ARG:HD2	2:F:420:ARG:HD3	1.92	0.50
2:F:4597:PRO:HA	2:F:4600:ILE:HG22	1.94	0.50
2:F:4649:PHE:HB3	2:F:4653:LYS:HE3	1.93	0.50
2:H:73:LEU:CB	2:H:77:ALA:CB	2.86	0.50
2:H:1783:PRO:HB3	2:H:1786:ILE:HD12	1.92	0.50
2:H:3915:LYS:O	2:H:3919:ASN:ND2	2.45	0.50
2:B:4849:ILE:CA	2:D:4822:VAL:CG2	2.86	0.50
2:B:4865:GLY:HA2	2:D:4868:ILE:CD1	2.42	0.50
2:D:1250:TRP:HB3	2:D:1600:PRO:HB2	1.93	0.50
2:D:2035:GLU:O	2:D:2038:THR:OG1	2.29	0.50
2:D:4722:TYR:HD2	2:D:4723:LEU:HD12	1.76	0.50
2:D:4796:LYS:HB2	2:D:4805:MET:HB3	1.93	0.50
2:D:4826:GLY:C	2:F:4823:ARG:CA	2.84	0.50
2:F:1184:ASP:OD2	2:F:1188:SER:OG	2.29	0.50
2:H:4597:PRO:HA	2:H:4600:ILE:HG22	1.94	0.50
2:H:4722:TYR:HD2	2:H:4723:LEU:HD12	1.76	0.50
2:B:2860:GLU:O	2:B:2864:LYS:NZ	2.39	0.50
2:B:4865:GLY:HA3	2:D:4868:ILE:HG12	1.94	0.50
2:D:147:VAL:HG21	2:D:203:VAL:HG12	1.94	0.50
2:D:373:THR:HG23	2:D:392:ILE:HG13	1.93	0.50
2:D:4826:GLY:O	2:F:4823:ARG:HA	2.12	0.50
2:F:646:THR:HA	2:F:1630:LEU:HA	1.93	0.50
1:G:4:ILE:O	1:G:65:GLN:NE2	2.45	0.50
2:H:1250:TRP:HB3	2:H:1600:PRO:HB2	1.93	0.50
2:H:2528:LEU:HD11	2:H:2568:ASP:HA	1.93	0.50
2:H:3853:SER:HB2	2:H:3929:CYS:HB3	1.92	0.50
2:B:180:ASP:HB3	2:B:211:LEU:HB3	1.93	0.50
2:B:1184:ASP:OD2	2:B:1188:SER:OG	2.29	0.50
2:D:2715:PRO:HD2	2:D:2718:LEU:HD12	1.93	0.50
2:D:3915:LYS:O	2:D:3919:ASN:ND2	2.45	0.50
2:F:585:ALA:HA	2:F:588:ILE:HD12	1.94	0.50
2:F:1115:VAL:O	2:F:1137:PHE:N	2.45	0.50
2:F:2462:CYS:O	2:F:2520:TYR:OH	2.30	0.50
2:H:373:THR:HG23	2:H:392:ILE:HG13	1.93	0.50
2:H:1227:PHE:HE1	2:H:1236:TYR:HB2	1.76	0.50
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.93	0.50
2:B:585:ALA:HA	2:B:588:ILE:HD12	1.94	0.50
2:B:1227:PHE:HE1	2:B:1236:TYR:HB2	1.76	0.50
2:B:4160:GLN:NE2	2:B:4201:MET:O	2.44	0.50
1:C:21:THR:OG1	1:C:49:ARG:NH2	2.40	0.50
2:D:4652:ARG:HA	2:D:4655:MET:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:180:ASP:HB3	2:F:211:LEU:HB3	1.93	0.50
2:F:299:HIS:NE2	2:F:301:THR:OG1	2.37	0.50
2:F:4834:ASP:O	2:F:4844:ARG:NH2	2.45	0.50
1:G:4:ILE:HD13	1:G:74:LEU:HG	1.94	0.50
2:H:123:HIS:CD2	2:H:126:SER:H	2.29	0.50
2:H:677:LEU:HB2	2:H:755:ILE:HB	1.92	0.50
2:H:1154:ARG:HH21	2:H:1177:LEU:HD23	1.77	0.50
2:H:1184:ASP:OD2	2:H:1188:SER:OG	2.29	0.50
2:H:4160:GLN:NE2	2:H:4201:MET:O	2.44	0.50
2:B:147:VAL:HG21	2:B:203:VAL:HG12	1.94	0.50
2:B:1154:ARG:HH21	2:B:1177:LEU:HD23	1.77	0.50
2:B:4822:VAL:O	2:H:4826:GLY:O	2.29	0.50
2:D:1154:ARG:HH21	2:D:1177:LEU:HD23	1.77	0.50
2:D:1227:PHE:HE1	2:D:1236:TYR:HB2	1.76	0.50
2:D:2860:GLU:O	2:D:2864:LYS:NZ	2.39	0.50
2:D:4594:LEU:O	2:D:4596:VAL:N	2.45	0.50
2:F:2835:SER:O	2:F:2839:HIS:N	2.40	0.50
2:F:4722:TYR:HD2	2:F:4723:LEU:HD12	1.76	0.50
2:H:416:ALA:HA	2:H:419:ILE:HD12	1.94	0.50
2:H:1748:LEU:HD22	2:H:1749:PRO:HD2	1.94	0.50
1:A:4:ILE:HD13	1:A:74:LEU:HG	1.94	0.49
2:B:1256:PRO:O	2:B:1451:HIS:ND1	2.44	0.49
2:B:2835:SER:O	2:B:2839:HIS:N	2.40	0.49
2:D:585:ALA:HA	2:D:588:ILE:HD12	1.94	0.49
2:D:655:MET:HE2	2:D:834:VAL:HG12	1.94	0.49
2:D:3858:TYR:OH	2:D:3865:ASN:ND2	2.42	0.49
2:D:3919:ASN:O	2:D:3922:THR:OG1	2.26	0.49
2:D:3921:LEU:HB3	2:D:3982:MET:HE3	1.94	0.49
2:D:4849:ILE:C	2:F:4822:VAL:HG21	2.37	0.49
2:F:1250:TRP:HB3	2:F:1600:PRO:HB2	1.93	0.49
2:F:4651:LYS:NZ	2:F:4670:LEU:O	2.45	0.49
2:H:1611:ILE:O	2:H:1620:GLN:N	2.40	0.49
2:B:416:ALA:HA	2:B:419:ILE:HD12	1.94	0.49
2:B:2528:LEU:HD11	2:B:2568:ASP:HA	1.93	0.49
2:B:2878:LEU:HB2	2:B:2883:LYS:HE3	1.95	0.49
2:B:3919:ASN:O	2:B:3922:THR:OG1	2.26	0.49
2:B:4652:ARG:HA	2:B:4655:MET:HB2	1.94	0.49
2:D:260:VAL:HG12	2:D:391:ALA:HB3	1.95	0.49
2:D:416:ALA:HA	2:D:419:ILE:HD12	1.94	0.49
2:D:869:THR:OG1	2:D:938:GLU:OE1	2.31	0.49
1:E:4:ILE:O	1:E:65:GLN:NE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:ILE:HD13	1:E:74:LEU:HG	1.94	0.49
2:F:123:HIS:CD2	2:F:126:SER:H	2.29	0.49
2:F:1154:ARG:HH21	2:F:1177:LEU:HD23	1.77	0.49
2:F:1431:ARG:HB3	2:F:1554:GLN:HB2	1.94	0.49
2:F:1748:LEU:HD22	2:F:1749:PRO:HD2	1.94	0.49
2:F:4184:LYS:HD3	2:H:4907:GLU:CD	2.37	0.49
2:F:4826:GLY:HA2	2:H:4823:ARG:HA	1.95	0.49
2:H:49:LEU:HD12	2:H:201:LEU:HB3	1.94	0.49
2:H:299:HIS:N	2:H:304:LYS:O	2.44	0.49
2:H:585:ALA:HA	2:H:588:ILE:HD12	1.94	0.49
2:H:2096:ILE:O	2:H:2100:VAL:N	2.44	0.49
2:H:4651:LYS:NZ	2:H:4670:LEU:O	2.45	0.49
1:A:4:ILE:O	1:A:65:GLN:NE2	2.45	0.49
2:D:1115:VAL:O	2:D:1137:PHE:N	2.45	0.49
2:D:1688:ALA:HA	2:D:1691:ASN:HD22	1.77	0.49
2:F:147:VAL:HG21	2:F:203:VAL:HG12	1.94	0.49
2:F:646:THR:OG1	2:F:1629:SER:O	2.26	0.49
1:G:16:PRO:HD2	1:G:64:ALA:HA	1.95	0.49
2:H:3805:ASP:OD2	2:H:3808:ALA:N	2.43	0.49
2:H:4522:LYS:O	2:H:4559:HIS:ND1	2.42	0.49
2:H:4652:ARG:HA	2:H:4655:MET:HB2	1.94	0.49
2:B:4849:ILE:C	2:D:4822:VAL:CG2	2.85	0.49
1:C:4:ILE:HD13	1:C:74:LEU:HG	1.94	0.49
2:D:25:THR:HA	2:D:34:LYS:HA	1.94	0.49
2:D:4597:PRO:HA	2:D:4600:ILE:HG22	1.94	0.49
2:D:4849:ILE:C	2:F:4822:VAL:CG2	2.85	0.49
2:F:25:THR:HA	2:F:34:LYS:HA	1.94	0.49
2:F:636:LEU:HD21	2:F:643:LEU:HD21	1.92	0.49
2:H:1455:THR:HB	2:H:1546:GLN:HE21	1.78	0.49
2:H:2462:CYS:O	2:H:2520:TYR:OH	2.30	0.49
2:B:260:VAL:HG12	2:B:391:ALA:HB3	1.95	0.49
2:B:646:THR:HA	2:B:1630:LEU:HA	1.92	0.49
2:B:4826:GLY:O	2:D:4823:ARG:HA	2.11	0.49
2:D:248:PRO:HG2	2:D:257:ARG:HA	1.95	0.49
2:D:646:THR:HA	2:D:1630:LEU:HA	1.92	0.49
2:F:373:THR:HG23	2:F:392:ILE:HG13	1.93	0.49
2:F:4796:LYS:HB2	2:F:4805:MET:HB3	1.93	0.49
2:H:2558:LYS:O	2:H:2562:LEU:N	2.44	0.49
2:B:26:ALA:O	2:B:33:GLN:N	2.43	0.49
2:B:1748:LEU:HD22	2:B:1749:PRO:HD2	1.94	0.49
2:B:3858:TYR:OH	2:B:3865:ASN:ND2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4823:ARG:HA	2:H:4826:GLY:O	2.11	0.49
2:D:1160:ASP:OD1	2:D:1178:ASN:ND2	2.41	0.49
2:D:1767:SER:OG	2:D:1770:SER:OG	2.31	0.49
2:D:2462:CYS:O	2:D:2520:TYR:OH	2.30	0.49
2:D:2878:LEU:HB2	2:D:2883:LYS:HE3	1.95	0.49
2:D:3680:LYS:NZ	2:D:3684:GLU:OE2	2.46	0.49
2:D:4025:LYS:HE2	2:D:4086:LYS:HA	1.95	0.49
2:F:2558:LYS:O	2:F:2562:LEU:N	2.44	0.49
2:F:4594:LEU:O	2:F:4596:VAL:N	2.45	0.49
2:F:4652:ARG:HA	2:F:4655:MET:HB2	1.94	0.49
1:G:55:VAL:HG12	2:H:1770:SER:HB3	1.95	0.49
2:H:25:THR:HA	2:H:34:LYS:HA	1.94	0.49
2:B:655:MET:HE2	2:B:834:VAL:HG12	1.94	0.49
2:B:4594:LEU:O	2:B:4596:VAL:N	2.45	0.49
2:B:4651:LYS:NZ	2:B:4670:LEU:O	2.45	0.49
2:D:143:LEU:CA	2:F:2427:LEU:HD21	2.43	0.49
2:D:3988:GLU:OE1	2:D:4937:GLN:NE2	2.46	0.49
1:E:55:VAL:HG12	2:F:1770:SER:HB3	1.95	0.49
2:F:49:LEU:HD12	2:F:201:LEU:HB3	1.94	0.49
2:F:869:THR:OG1	2:F:938:GLU:OE1	2.31	0.49
2:F:2715:PRO:HD2	2:F:2718:LEU:HD12	1.93	0.49
2:F:3009:PHE:O	2:F:3013:GLY:N	2.46	0.49
2:F:3779:LEU:HD13	2:F:3855:PHE:HD1	1.78	0.49
2:F:3919:ASN:O	2:F:3922:THR:OG1	2.26	0.49
2:F:4522:LYS:O	2:F:4559:HIS:ND1	2.42	0.49
2:H:248:PRO:HG2	2:H:257:ARG:HA	1.95	0.49
2:H:853:PRO:HB3	2:H:1086:ARG:HH21	1.77	0.49
2:H:1086:ARG:HB2	2:H:1207:LEU:HB2	1.95	0.49
2:H:3779:LEU:HD13	2:H:3855:PHE:HD1	1.78	0.49
2:B:248:PRO:HG2	2:B:257:ARG:HA	1.95	0.49
2:B:299:HIS:N	2:B:304:LYS:O	2.44	0.49
2:B:1250:TRP:HB3	2:B:1600:PRO:HB2	1.93	0.49
2:B:3680:LYS:NZ	2:B:3684:GLU:OE2	2.46	0.49
2:B:3862:GLN:HB3	2:B:3865:ASN:HB2	1.95	0.49
2:F:260:VAL:HG12	2:F:391:ALA:HB3	1.95	0.49
2:F:1455:THR:HB	2:F:1546:GLN:HE21	1.78	0.49
2:F:1630:LEU:O	2:F:1638:SER:OG	2.30	0.49
2:F:4713:VAL:O	2:F:4716:THR:OG1	2.30	0.49
2:H:1431:ARG:HB3	2:H:1554:GLN:HB2	1.94	0.49
2:H:2878:LEU:HB2	2:H:2883:LYS:HE3	1.95	0.49
2:H:3009:PHE:O	2:H:3013:GLY:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3988:GLU:OE1	2:H:4937:GLN:NE2	2.46	0.49
2:B:869:THR:OG1	2:B:938:GLU:OE1	2.31	0.49
2:B:3779:LEU:HD13	2:B:3855:PHE:HD1	1.78	0.49
2:D:3779:LEU:HD13	2:D:3855:PHE:HD1	1.78	0.49
2:D:4865:GLY:HA2	2:F:4868:ILE:CD1	2.43	0.49
2:F:19:GLU:OE1	2:F:218:SER:OG	2.29	0.49
2:F:1144:ARG:N	2:F:1150:GLU:O	2.41	0.49
2:F:1511:VAL:HG22	2:F:1516:GLY:HA2	1.95	0.49
2:F:2528:LEU:HD11	2:F:2568:ASP:HA	1.93	0.49
2:F:3862:GLN:HB3	2:F:3865:ASN:HB2	1.95	0.49
2:F:4114:THR:HA	2:F:4117:GLN:HB2	1.95	0.49
2:H:260:VAL:HG12	2:H:391:ALA:HB3	1.95	0.49
2:H:576:HIS:HB2	2:H:613:VAL:HG22	1.95	0.49
2:H:693:LEU:HB3	2:H:749:LEU:HD22	1.95	0.49
2:H:4594:LEU:O	2:H:4596:VAL:N	2.45	0.49
2:B:73:LEU:CB	2:B:77:ALA:CB	2.85	0.49
2:B:576:HIS:HB2	2:B:613:VAL:HG22	1.95	0.49
2:B:853:PRO:HB3	2:B:1086:ARG:HH21	1.77	0.49
2:B:2779:SER:OG	2:B:2849:TYR:OH	2.22	0.49
2:B:3921:LEU:HB3	2:B:3982:MET:HE3	1.94	0.49
2:D:1124:PRO:HG3	2:D:1600:PRO:HD3	1.95	0.49
2:D:2096:ILE:O	2:D:2100:VAL:N	2.44	0.49
2:D:3862:GLN:HB3	2:D:3865:ASN:HB2	1.95	0.49
1:E:16:PRO:HD2	1:E:64:ALA:HA	1.95	0.49
2:F:416:ALA:HA	2:F:419:ILE:HD12	1.94	0.49
2:F:576:HIS:HB2	2:F:613:VAL:HG22	1.95	0.49
2:F:1251:LEU:O	2:F:1601:ASN:N	2.46	0.49
2:F:3988:GLU:OE1	2:F:4937:GLN:NE2	2.46	0.49
2:F:4025:LYS:HE2	2:F:4086:LYS:HA	1.95	0.49
2:H:4796:LYS:HB2	2:H:4805:MET:HB3	1.93	0.49
1:A:16:PRO:HD2	1:A:64:ALA:HA	1.95	0.48
2:B:49:LEU:HD12	2:B:201:LEU:HB3	1.94	0.48
2:B:1748:LEU:HD13	2:B:1750:GLY:H	1.78	0.48
2:B:4597:PRO:HA	2:B:4600:ILE:HG22	1.94	0.48
2:B:4717:ASP:HB3	2:B:4720:PHE:HB3	1.95	0.48
2:D:1511:VAL:HG22	2:D:1516:GLY:HA2	1.95	0.48
2:D:1748:LEU:HD13	2:D:1750:GLY:H	1.78	0.48
2:D:2528:LEU:HD11	2:D:2568:ASP:HA	1.93	0.48
2:D:4717:ASP:HB3	2:D:4720:PHE:HB3	1.95	0.48
2:F:655:MET:HE2	2:F:834:VAL:HG12	1.94	0.48
2:F:3921:LEU:HB3	2:F:3982:MET:HE3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:147:VAL:HG21	2:H:203:VAL:HG12	1.94	0.48
2:H:371:TRP:N	2:H:394:HIS:O	2.46	0.48
2:H:626:ARG:NH1	2:H:1667:LEU:O	2.46	0.48
2:H:3680:LYS:NZ	2:H:3684:GLU:OE2	2.46	0.48
2:H:4515:ASN:O	2:H:4518:LEU:CG	2.60	0.48
2:H:4717:ASP:HB3	2:H:4720:PHE:HB3	1.95	0.48
1:A:55:VAL:HG12	2:B:1770:SER:HB3	1.95	0.48
2:B:4025:LYS:HE2	2:B:4086:LYS:HA	1.95	0.48
2:B:4655:MET:O	2:B:4664:ARG:NH2	2.42	0.48
2:D:1431:ARG:HB3	2:D:1554:GLN:HB2	1.94	0.48
2:D:1748:LEU:HD22	2:D:1749:PRO:HD2	1.94	0.48
2:F:626:ARG:NH1	2:F:1667:LEU:O	2.46	0.48
2:F:853:PRO:HB3	2:F:1086:ARG:HH21	1.77	0.48
2:F:1611:ILE:O	2:F:1620:GLN:N	2.40	0.48
2:F:1767:SER:OG	2:F:1770:SER:OG	2.31	0.48
2:F:2878:LEU:HB2	2:F:2883:LYS:HE3	1.95	0.48
2:F:4515:ASN:O	2:F:4518:LEU:CD2	2.61	0.48
2:H:3862:GLN:HB3	2:H:3865:ASN:HB2	1.95	0.48
2:B:143:LEU:CA	2:D:2427:LEU:HD21	2.42	0.48
2:B:2462:CYS:O	2:B:2520:TYR:OH	2.30	0.48
2:D:185:SER:OG	2:D:186:VAL:N	2.46	0.48
2:D:1718:ARG:NH1	2:D:1830:ILE:O	2.46	0.48
2:F:217:ILE:HG23	2:F:285:SER:HB3	1.96	0.48
2:F:248:PRO:HG2	2:F:257:ARG:HA	1.95	0.48
2:F:1086:ARG:HB2	2:F:1207:LEU:HB2	1.95	0.48
2:F:1688:ALA:HA	2:F:1691:ASN:HD22	1.77	0.48
2:F:4515:ASN:O	2:F:4518:LEU:CG	2.60	0.48
2:H:217:ILE:HG23	2:H:285:SER:HB3	1.96	0.48
2:H:1761:MET:SD	2:H:1761:MET:N	2.76	0.48
2:B:373:THR:HG23	2:B:392:ILE:HG13	1.93	0.48
2:B:1431:ARG:HB3	2:B:1554:GLN:HB2	1.94	0.48
2:B:1719:LEU:HA	2:B:1722:ASN:HD22	1.79	0.48
2:B:3988:GLU:OE1	2:B:4937:GLN:NE2	2.46	0.48
2:B:4861:ALA:N	2:D:4864:GLN:NE2	2.61	0.48
2:D:16:THR:N	2:D:110:HIS:O	2.44	0.48
2:D:693:LEU:HB3	2:D:749:LEU:HD22	1.95	0.48
2:D:853:PRO:HB3	2:D:1086:ARG:HH21	1.77	0.48
2:D:1944:ARG:HH22	2:D:2024:LEU:HD12	1.79	0.48
2:D:4861:ALA:N	2:F:4864:GLN:NE2	2.62	0.48
2:F:185:SER:OG	2:F:186:VAL:N	2.46	0.48
2:F:2107:TYR:HE1	2:F:2161:ASN:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4717:ASP:HB3	2:F:4720:PHE:HB3	1.95	0.48
1:G:24:VAL:HG12	1:G:103:LEU:HA	1.95	0.48
2:H:25:THR:HG22	2:H:34:LYS:HG2	1.95	0.48
2:H:1115:VAL:O	2:H:1137:PHE:N	2.45	0.48
2:H:1944:ARG:HH22	2:H:2024:LEU:HD12	1.79	0.48
2:H:2035:GLU:O	2:H:2038:THR:OG1	2.29	0.48
2:H:2107:TYR:HE1	2:H:2161:ASN:HB2	1.79	0.48
2:H:2835:SER:O	2:H:2839:HIS:N	2.40	0.48
2:B:1688:ALA:HA	2:B:1691:ASN:HD22	1.77	0.48
2:B:2035:GLU:O	2:B:2038:THR:OG1	2.29	0.48
2:B:2419:ARG:O	2:B:2422:SER:OG	2.31	0.48
2:B:4523:VAL:CB	2:B:4559:HIS:HE1	2.26	0.48
2:B:4891:ILE:HD13	2:B:4914:HIS:HB3	1.95	0.48
2:D:26:ALA:O	2:D:33:GLN:N	2.43	0.48
2:D:1455:THR:HB	2:D:1546:GLN:HE21	1.78	0.48
2:F:476:GLN:NE2	2:F:3677:LEU:O	2.43	0.48
2:F:1124:PRO:HG3	2:F:1600:PRO:HD3	1.95	0.48
2:F:1434:PRO:HD3	2:F:1549:SER:HB2	1.96	0.48
2:F:2096:ILE:O	2:F:2100:VAL:N	2.44	0.48
2:F:3680:LYS:NZ	2:F:3684:GLU:OE2	2.46	0.48
2:F:3917:VAL:O	2:F:3920:THR:OG1	2.23	0.48
2:F:4853:PHE:CZ	2:H:4859:LEU:HD12	2.48	0.48
2:H:1124:PRO:HG3	2:H:1600:PRO:HD3	1.95	0.48
2:H:1630:LEU:O	2:H:1638:SER:OG	2.30	0.48
2:H:4515:ASN:O	2:H:4518:LEU:CD2	2.61	0.48
2:B:25:THR:HG22	2:B:34:LYS:HG2	1.96	0.48
2:B:1124:PRO:HG3	2:B:1600:PRO:HD3	1.95	0.48
2:B:1944:ARG:HH22	2:B:2024:LEU:HD12	1.79	0.48
2:B:3009:PHE:O	2:B:3013:GLY:N	2.46	0.48
2:B:3911:ILE:HG21	2:B:3971:GLU:HB3	1.96	0.48
2:B:4085:VAL:O	2:B:4089:HIS:N	2.41	0.48
2:B:4515:ASN:O	2:B:4518:LEU:CG	2.60	0.48
2:B:4522:LYS:O	2:B:4559:HIS:ND1	2.42	0.48
2:B:4849:ILE:C	2:D:4822:VAL:HG21	2.38	0.48
1:C:55:VAL:HG12	2:D:1770:SER:HB3	1.95	0.48
2:D:237:LEU:HB2	2:D:404:ASN:HB3	1.96	0.48
2:D:576:HIS:HB2	2:D:613:VAL:HG22	1.95	0.48
2:D:3009:PHE:O	2:D:3013:GLY:N	2.46	0.48
2:D:4515:ASN:O	2:D:4518:LEU:CG	2.60	0.48
2:D:4515:ASN:O	2:D:4518:LEU:CD2	2.61	0.48
2:F:25:THR:HG22	2:F:34:LYS:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2102:ALA:HA	2:F:2105:LYS:HZ2	1.79	0.48
2:H:185:SER:OG	2:H:186:VAL:N	2.46	0.48
2:H:869:THR:OG1	2:H:938:GLU:OE1	2.31	0.48
2:H:1251:LEU:O	2:H:1601:ASN:N	2.46	0.48
2:H:1719:LEU:HA	2:H:1722:ASN:HD22	1.79	0.48
2:H:3921:LEU:HB3	2:H:3982:MET:HE3	1.94	0.48
2:H:4523:VAL:CB	2:H:4559:HIS:HE1	2.26	0.48
2:B:2427:LEU:HD21	2:H:143:LEU:CA	2.42	0.48
2:D:2419:ARG:O	2:D:2422:SER:OG	2.31	0.48
2:D:4114:THR:HA	2:D:4117:GLN:HB2	1.95	0.48
2:D:4865:GLY:HA3	2:F:4868:ILE:HG12	1.95	0.48
2:F:2142:LEU:HD23	2:F:2145:ARG:HD2	1.96	0.48
2:F:4826:GLY:C	2:H:4823:ARG:CA	2.86	0.48
2:F:4853:PHE:HB2	2:H:4822:VAL:HG23	1.96	0.48
2:H:4891:ILE:HD13	2:H:4914:HIS:HB3	1.95	0.48
2:B:25:THR:HA	2:B:34:LYS:HA	1.94	0.48
2:B:1251:LEU:O	2:B:1601:ASN:N	2.46	0.48
2:B:3983:LEU:O	2:B:3987:LEU:HB2	2.14	0.48
2:B:4713:VAL:O	2:B:4716:THR:OG1	2.30	0.48
2:D:559:ILE:HD13	2:D:593:HIS:HB3	1.96	0.48
2:D:2835:SER:O	2:D:2839:HIS:N	2.40	0.48
2:F:3983:LEU:O	2:F:3987:LEU:HB2	2.14	0.48
2:H:655:MET:HE2	2:H:834:VAL:HG12	1.94	0.48
2:H:3911:ILE:HG21	2:H:3971:GLU:HB3	1.96	0.48
2:B:237:LEU:HB2	2:B:404:ASN:HB3	1.96	0.48
2:B:1086:ARG:HB2	2:B:1207:LEU:HB2	1.95	0.48
2:B:1115:VAL:O	2:B:1137:PHE:N	2.45	0.48
2:B:1455:THR:HB	2:B:1546:GLN:HE21	1.78	0.48
2:B:1511:VAL:HG22	2:B:1516:GLY:HA2	1.95	0.48
2:B:2107:TYR:HE1	2:B:2161:ASN:HB2	1.79	0.48
2:D:299:HIS:N	2:D:304:LYS:O	2.44	0.48
2:D:3911:ILE:HG21	2:D:3971:GLU:HB3	1.96	0.48
2:F:73:LEU:CB	2:F:77:ALA:CB	2.85	0.48
2:F:1177:LEU:N	2:F:1180:GLU:O	2.43	0.48
2:F:2894:LEU:HD23	2:F:2897:LEU:HD12	1.96	0.48
2:F:4780:TYR:OH	2:H:4518:LEU:HB3	2.14	0.48
2:F:4891:ILE:HD13	2:F:4914:HIS:HB3	1.95	0.48
2:H:16:THR:N	2:H:110:HIS:O	2.44	0.48
2:H:706:TYR:HE2	2:H:1253:LYS:HG2	1.79	0.48
2:H:1511:VAL:HG22	2:H:1516:GLY:HA2	1.95	0.48
2:H:3956:GLN:HE21	2:H:3976:GLN:HE22	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:HIS:NE2	2:B:1774:GLU:OE2	2.47	0.48
2:B:626:ARG:NH1	2:B:1667:LEU:O	2.46	0.48
1:C:16:PRO:HD2	1:C:64:ALA:HA	1.95	0.48
2:D:217:ILE:HG23	2:D:285:SER:HB3	1.96	0.48
2:D:4891:ILE:HD13	2:D:4914:HIS:HB3	1.95	0.48
1:E:24:VAL:HG12	1:E:103:LEU:HA	1.95	0.48
1:E:87:HIS:NE2	2:F:1774:GLU:OE2	2.47	0.48
2:F:35:LEU:HA	2:F:51:SER:HA	1.96	0.48
2:F:559:ILE:HD13	2:F:593:HIS:HB3	1.96	0.48
2:F:693:LEU:HB3	2:F:749:LEU:HD22	1.95	0.48
2:F:3956:GLN:HE21	2:F:3976:GLN:HE22	1.62	0.48
2:H:673:TRP:HA	2:H:820:ALA:HB3	1.95	0.48
2:H:2894:LEU:HD23	2:H:2897:LEU:HD12	1.96	0.48
2:H:4114:THR:HA	2:H:4117:GLN:HB2	1.95	0.48
2:B:706:TYR:HE2	2:B:1253:LYS:HG2	1.79	0.47
2:B:4515:ASN:O	2:B:4518:LEU:CD2	2.61	0.47
2:D:2107:TYR:HE1	2:D:2161:ASN:HB2	1.79	0.47
2:D:3983:LEU:O	2:D:3987:LEU:HB2	2.14	0.47
2:D:4523:VAL:CB	2:D:4559:HIS:HE1	2.26	0.47
2:F:1444:GLY:HA2	2:F:1487:MET:HB2	1.96	0.47
2:F:4523:VAL:CB	2:F:4559:HIS:HE1	2.26	0.47
2:H:412:GLU:O	2:H:415:THR:OG1	2.31	0.47
2:H:3919:ASN:O	2:H:3922:THR:OG1	2.26	0.47
2:B:1510:VAL:HG12	2:B:1511:VAL:HG23	1.96	0.47
2:D:49:LEU:HD12	2:D:201:LEU:HB3	1.94	0.47
2:D:673:TRP:HA	2:D:820:ALA:HB3	1.95	0.47
2:D:706:TYR:HE2	2:D:1253:LYS:HG2	1.79	0.47
2:F:299:HIS:N	2:F:304:LYS:O	2.44	0.47
2:F:471:GLU:O	2:F:475:LYS:N	2.44	0.47
2:F:1762:GLN:O	2:F:1779:SER:OG	2.25	0.47
2:F:2193:MET:HA	2:F:2196:ASN:HD22	1.79	0.47
2:F:3911:ILE:HG21	2:F:3971:GLU:HB3	1.96	0.47
2:F:4052:ALA:O	2:F:4056:HIS:ND1	2.39	0.47
2:F:4865:GLY:HA3	2:H:4868:ILE:HG12	1.96	0.47
2:H:646:THR:OG1	2:H:1629:SER:O	2.26	0.47
2:H:1688:ALA:HA	2:H:1691:ASN:HD22	1.77	0.47
2:H:2026:ILE:HG13	2:H:2029:ARG:HH12	1.80	0.47
2:H:2256:LEU:HD11	2:H:3815:ALA:HB3	1.96	0.47
2:H:2419:ARG:O	2:H:2422:SER:OG	2.31	0.47
1:A:24:VAL:HG12	1:A:103:LEU:HA	1.95	0.47
2:B:217:ILE:HG23	2:B:285:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:TRP:N	2:B:394:HIS:O	2.46	0.47
2:B:559:ILE:HD13	2:B:593:HIS:HB3	1.96	0.47
2:B:4780:TYR:HD1	2:D:4518:LEU:HD22	1.65	0.47
2:D:542:ARG:NE	2:D:577:CYS:SG	2.78	0.47
2:D:626:ARG:NH1	2:D:1667:LEU:O	2.46	0.47
2:D:1922:ARG:NH2	2:D:2039:TYR:OH	2.47	0.47
2:D:4655:MET:O	2:D:4664:ARG:NH2	2.42	0.47
2:F:706:TYR:HE2	2:F:1253:LYS:HG2	1.79	0.47
2:H:1434:PRO:HD3	2:H:1549:SER:HB2	1.95	0.47
2:H:1748:LEU:HD13	2:H:1750:GLY:H	1.79	0.47
2:H:4025:LYS:HE2	2:H:4086:LYS:HA	1.95	0.47
2:B:35:LEU:HA	2:B:51:SER:HA	1.96	0.47
2:B:673:TRP:HA	2:B:820:ALA:HB3	1.95	0.47
2:B:2558:LYS:O	2:B:2562:LEU:N	2.44	0.47
2:D:25:THR:HG22	2:D:34:LYS:HG2	1.95	0.47
2:D:1251:LEU:O	2:D:1601:ASN:N	2.46	0.47
2:D:3831:LEU:HA	2:D:3832:GLN:HA	1.64	0.47
2:D:4750:GLY:H	2:D:4755:ARG:NE	2.12	0.47
2:F:191:TYR:N	2:F:206:ALA:O	2.47	0.47
2:F:673:TRP:HA	2:F:820:ALA:HB3	1.95	0.47
2:F:2419:ARG:O	2:F:2422:SER:OG	2.31	0.47
2:H:1998:LEU:HA	2:H:1999:ASP:HA	1.57	0.47
2:H:2142:LEU:HD23	2:H:2145:ARG:HD2	1.96	0.47
2:H:3983:LEU:O	2:H:3987:LEU:HB2	2.14	0.47
2:H:4518:LEU:HD12	2:H:4519:LEU:N	2.30	0.47
2:H:4750:GLY:H	2:H:4755:ARG:NE	2.12	0.47
2:B:1303:ARG:O	2:B:1593:HIS:N	2.48	0.47
2:B:4853:PHE:HB2	2:D:4822:VAL:HG23	1.96	0.47
2:D:1086:ARG:HB2	2:D:1207:LEU:HB2	1.95	0.47
2:D:1444:GLY:HA2	2:D:1487:MET:HB2	1.96	0.47
2:D:1669:ASN:O	2:D:1673:ALA:N	2.47	0.47
2:D:1719:LEU:HA	2:D:1722:ASN:HD22	1.79	0.47
2:D:2142:LEU:HD23	2:D:2145:ARG:HD2	1.96	0.47
2:D:2193:MET:HA	2:D:2196:ASN:HD22	1.79	0.47
2:D:2894:LEU:HD23	2:D:2897:LEU:HD12	1.96	0.47
2:F:237:LEU:HB2	2:F:404:ASN:HB3	1.96	0.47
2:F:1507:ILE:O	2:F:1521:THR:OG1	2.33	0.47
2:F:1748:LEU:HD13	2:F:1750:GLY:H	1.78	0.47
2:F:4518:LEU:HD12	2:F:4519:LEU:N	2.30	0.47
1:G:87:HIS:NE2	2:H:1774:GLU:OE2	2.47	0.47
2:H:1303:ARG:O	2:H:1593:HIS:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1630:LEU:O	2:B:1638:SER:OG	2.30	0.47
2:D:299:HIS:NE2	2:D:301:THR:OG1	2.37	0.47
2:D:1809:PRO:HA	2:D:1817:LEU:HD22	1.97	0.47
2:F:1303:ARG:O	2:F:1593:HIS:N	2.48	0.47
2:H:1738:LEU:HG	2:H:2037:VAL:HG22	1.96	0.47
2:H:1922:ARG:NH2	2:H:2039:TYR:OH	2.47	0.47
2:B:1434:PRO:HD3	2:B:1549:SER:HB2	1.95	0.47
2:B:1809:PRO:HA	2:B:1817:LEU:HD22	1.97	0.47
2:B:2026:ILE:HG13	2:B:2029:ARG:HH12	1.80	0.47
2:B:2142:LEU:HD23	2:B:2145:ARG:HD2	1.96	0.47
2:B:2256:LEU:HD11	2:B:3815:ALA:HB3	1.96	0.47
2:B:3956:GLN:HE21	2:B:3976:GLN:HE22	1.62	0.47
2:B:4780:TYR:OH	2:D:4518:LEU:HB3	2.15	0.47
2:B:4853:PHE:CZ	2:D:4859:LEU:CD1	2.98	0.47
1:C:24:VAL:HG12	1:C:103:LEU:HA	1.95	0.47
1:C:87:HIS:NE2	2:D:1774:GLU:OE2	2.47	0.47
2:D:1177:LEU:N	2:D:1180:GLU:O	2.43	0.47
2:D:1303:ARG:O	2:D:1593:HIS:N	2.48	0.47
2:D:2026:ILE:HG13	2:D:2029:ARG:HH12	1.79	0.47
2:D:4138:GLU:OE2	2:D:4148:ARG:NH1	2.48	0.47
2:D:4518:LEU:HD12	2:D:4519:LEU:N	2.30	0.47
2:D:4853:PHE:HB2	2:F:4822:VAL:HG23	1.95	0.47
2:F:1719:LEU:HA	2:F:1722:ASN:HD22	1.79	0.47
2:F:2256:LEU:HD11	2:F:3815:ALA:HB3	1.96	0.47
2:F:3858:TYR:OH	2:F:3865:ASN:ND2	2.42	0.47
2:F:4920:LEU:HG	2:F:4924:MET:HE3	1.96	0.47
2:H:559:ILE:HD13	2:H:593:HIS:HB3	1.96	0.47
2:B:298:ARG:HA	2:B:305:TYR:HA	1.96	0.47
2:B:766:ILE:HB	2:B:779:PHE:HB2	1.97	0.47
2:B:1799:VAL:HG22	2:B:1894:LEU:HD13	1.97	0.47
2:B:4114:THR:HA	2:B:4117:GLN:HB2	1.95	0.47
2:B:4518:LEU:HB3	2:H:4780:TYR:OH	2.15	0.47
2:B:4518:LEU:HD12	2:B:4519:LEU:N	2.30	0.47
2:D:298:ARG:HA	2:D:305:TYR:HA	1.96	0.47
2:D:4523:VAL:CB	2:D:4559:HIS:CE1	2.98	0.47
2:D:4920:LEU:HG	2:D:4924:MET:HE3	1.96	0.47
2:F:1510:VAL:HG12	2:F:1511:VAL:HG23	1.96	0.47
2:F:1944:ARG:HH22	2:F:2024:LEU:HD12	1.79	0.47
2:F:2177:VAL:HG22	2:F:2221:TYR:CZ	2.50	0.47
2:H:35:LEU:HA	2:H:51:SER:HA	1.96	0.47
2:H:299:HIS:NE2	2:H:301:THR:OG1	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:GLU:OE1	2:B:218:SER:OG	2.29	0.47
2:B:1718:ARG:NH1	2:B:1830:ILE:O	2.46	0.47
2:B:1922:ARG:NH2	2:B:2039:TYR:OH	2.47	0.47
2:B:4138:GLU:OE2	2:B:4148:ARG:NH1	2.48	0.47
2:B:4920:LEU:HG	2:B:4924:MET:HE3	1.96	0.47
2:D:1144:ARG:N	2:D:1150:GLU:O	2.41	0.47
2:D:1253:LYS:HZ1	2:D:1257:GLN:HG3	1.80	0.47
2:H:1723:ASN:O	2:H:2105:LYS:NZ	2.41	0.47
2:B:693:LEU:HB3	2:B:749:LEU:HD22	1.95	0.47
2:B:1173:MET:O	2:B:1191:ALA:N	2.49	0.47
2:B:1444:GLY:HA2	2:B:1487:MET:HB2	1.96	0.47
2:B:1738:LEU:HG	2:B:2037:VAL:HG22	1.96	0.47
2:B:4052:ALA:O	2:B:4056:HIS:ND1	2.39	0.47
2:B:4750:GLY:H	2:B:4755:ARG:NE	2.12	0.47
2:F:73:LEU:CB	2:F:77:ALA:HB3	2.32	0.47
2:F:2026:ILE:HG13	2:F:2029:ARG:HH12	1.80	0.47
2:F:4826:GLY:O	2:H:4822:VAL:O	2.33	0.47
2:H:237:LEU:HB2	2:H:404:ASN:HB3	1.96	0.47
2:H:548:CYS:HA	2:H:551:PHE:HB2	1.97	0.47
2:H:1510:VAL:HG12	2:H:1511:VAL:HG23	1.96	0.47
2:H:3831:LEU:HA	2:H:3832:GLN:HA	1.65	0.47
2:H:4822:VAL:HG13	2:H:4823:ARG:N	2.31	0.47
2:B:4617:TYR:OH	2:B:4629:GLY:O	2.26	0.46
1:C:16:PRO:HG3	1:C:103:LEU:HD22	1.98	0.46
2:D:1434:PRO:HD3	2:D:1549:SER:HB2	1.95	0.46
2:D:2177:VAL:HG22	2:D:2221:TYR:CZ	2.50	0.46
2:D:2558:LYS:O	2:D:2562:LEU:N	2.44	0.46
2:D:3748:SER:O	2:D:3793:SER:OG	2.29	0.46
2:D:3956:GLN:HE21	2:D:3976:GLN:HE22	1.62	0.46
2:F:412:GLU:O	2:F:415:THR:OG1	2.31	0.46
2:F:1253:LYS:HZ1	2:F:1257:GLN:HG3	1.81	0.46
2:F:1738:LEU:HG	2:F:2037:VAL:HG22	1.96	0.46
2:F:1809:PRO:HA	2:F:1817:LEU:HD22	1.97	0.46
2:F:4750:GLY:H	2:F:4755:ARG:NE	2.12	0.46
2:H:766:ILE:HB	2:H:779:PHE:HB2	1.97	0.46
2:H:1799:VAL:HG22	2:H:1894:LEU:HD13	1.97	0.46
2:H:3803:VAL:HG21	2:H:3881:ARG:HD2	1.98	0.46
2:H:4920:LEU:HG	2:H:4924:MET:HE3	1.96	0.46
2:B:2177:VAL:HG22	2:B:2221:TYR:CZ	2.50	0.46
2:B:2894:LEU:HD23	2:B:2897:LEU:HD12	1.96	0.46
2:B:4523:VAL:CB	2:B:4559:HIS:CE1	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:LEU:HA	2:D:51:SER:HA	1.96	0.46
2:D:1109:THR:OG1	2:D:1212:VAL:N	2.48	0.46
2:D:1510:VAL:HG12	2:D:1511:VAL:HG23	1.96	0.46
2:D:2256:LEU:HD11	2:D:3815:ALA:HB3	1.96	0.46
2:D:4822:VAL:HG13	2:D:4823:ARG:N	2.31	0.46
2:F:754:VAL:HG11	2:F:813:PHE:HD2	1.80	0.46
2:F:766:ILE:HB	2:F:779:PHE:HB2	1.97	0.46
2:F:1998:LEU:HA	2:F:1999:ASP:HA	1.57	0.46
2:F:3748:SER:O	2:F:3793:SER:OG	2.29	0.46
2:F:4617:TYR:OH	2:F:4629:GLY:O	2.26	0.46
2:F:4865:GLY:HA2	2:H:4868:ILE:CD1	2.45	0.46
2:H:1718:ARG:NH1	2:H:1830:ILE:O	2.46	0.46
2:H:2177:VAL:HG22	2:H:2221:TYR:CZ	2.50	0.46
2:B:28:ILE:HD12	2:B:33:GLN:HE21	1.81	0.46
2:D:4826:GLY:O	2:F:4822:VAL:O	2.33	0.46
2:D:4890:PHE:H	3:D:5101:ATP:N6	2.14	0.46
2:F:1109:THR:OG1	2:F:1212:VAL:N	2.48	0.46
2:H:1444:GLY:HA2	2:H:1487:MET:HB2	1.96	0.46
2:H:1809:PRO:HA	2:H:1817:LEU:HD22	1.97	0.46
2:H:2193:MET:HA	2:H:2196:ASN:HD22	1.79	0.46
2:H:4523:VAL:CA	2:H:4559:HIS:HD1	2.06	0.46
2:B:16:THR:N	2:B:110:HIS:O	2.44	0.46
2:B:1253:LYS:HZ1	2:B:1257:GLN:HG3	1.80	0.46
2:B:3803:VAL:HG21	2:B:3881:ARG:HD2	1.97	0.46
2:D:4052:ALA:O	2:D:4056:HIS:ND1	2.39	0.46
2:F:1922:ARG:NH2	2:F:2039:TYR:OH	2.47	0.46
2:F:4794:TYR:HE2	2:F:4817:HIS:HE1	1.64	0.46
2:H:298:ARG:HA	2:H:305:TYR:HA	1.96	0.46
2:H:1687:TYR:O	2:H:1691:ASN:ND2	2.49	0.46
2:H:4138:GLU:OE2	2:H:4148:ARG:NH1	2.48	0.46
2:B:185:SER:OG	2:B:186:VAL:N	2.47	0.46
2:B:478:ARG:HE	2:B:485:ARG:HH22	1.64	0.46
2:B:548:CYS:HA	2:B:551:PHE:HB2	1.97	0.46
2:B:2108:THR:OG1	2:B:3615:HIS:O	2.34	0.46
2:B:4826:GLY:O	2:D:4822:VAL:O	2.33	0.46
2:D:28:ILE:HD12	2:D:33:GLN:HE21	1.81	0.46
2:D:433:LEU:O	2:D:437:SER:HB3	2.16	0.46
2:F:298:ARG:HA	2:F:305:TYR:HA	1.96	0.46
2:F:1669:ASN:O	2:F:1673:ALA:N	2.47	0.46
2:F:1799:VAL:HG22	2:F:1894:LEU:HD13	1.97	0.46
2:F:4811:LEU:CB	2:H:4519:LEU:CD2	2.87	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:26:ALA:O	2:H:33:GLN:N	2.43	0.46
2:H:1258:PHE:HB3	2:H:1303:ARG:NH2	2.31	0.46
2:H:1446:ILE:HG12	2:H:1487:MET:H	1.81	0.46
2:H:4085:VAL:O	2:H:4089:HIS:N	2.41	0.46
2:B:25:THR:HB	2:B:32:GLN:HB3	1.98	0.46
2:B:114:LEU:HB2	2:B:117:HIS:CE1	2.51	0.46
2:B:1109:THR:OG1	2:B:1212:VAL:N	2.48	0.46
2:B:1144:ARG:N	2:B:1150:GLU:O	2.41	0.46
2:B:1258:PHE:HB3	2:B:1303:ARG:NH2	2.31	0.46
2:B:2345:LEU:HD21	2:B:2434:VAL:HB	1.98	0.46
2:D:25:THR:HB	2:D:32:GLN:HB3	1.98	0.46
2:D:478:ARG:HE	2:D:485:ARG:HH22	1.64	0.46
2:D:1738:LEU:HG	2:D:2037:VAL:HG22	1.96	0.46
2:F:25:THR:HB	2:F:32:GLN:HB3	1.98	0.46
2:F:1687:TYR:O	2:F:1691:ASN:ND2	2.49	0.46
2:F:4138:GLU:OE2	2:F:4148:ARG:NH1	2.48	0.46
2:F:4523:VAL:CB	2:F:4559:HIS:CE1	2.99	0.46
2:H:114:LEU:HB2	2:H:117:HIS:CE1	2.51	0.46
2:H:478:ARG:HE	2:H:485:ARG:HH22	1.64	0.46
2:H:754:VAL:HG11	2:H:813:PHE:HD2	1.80	0.46
2:H:1109:THR:OG1	2:H:1212:VAL:N	2.48	0.46
2:H:4794:TYR:HE2	2:H:4817:HIS:HE1	1.64	0.46
2:B:2193:MET:HA	2:B:2196:ASN:HD22	1.79	0.46
1:C:28:GLY:N	1:C:37:ASP:O	2.49	0.46
2:D:114:LEU:HB2	2:D:117:HIS:CE1	2.51	0.46
2:D:449:ILE:HG13	2:D:522:ALA:HB1	1.97	0.46
2:D:1173:MET:O	2:D:1191:ALA:N	2.49	0.46
2:D:1258:PHE:HB3	2:D:1303:ARG:NH2	2.31	0.46
2:D:1446:ILE:HG12	2:D:1487:MET:H	1.81	0.46
2:F:478:ARG:HE	2:F:485:ARG:HH22	1.64	0.46
2:F:1258:PHE:HB3	2:F:1303:ARG:NH2	2.31	0.46
2:F:4164:PRO:HA	2:F:4167:LYS:HB2	1.98	0.46
2:F:4890:PHE:H	3:F:5101:ATP:N6	2.14	0.46
1:G:28:GLY:N	1:G:37:ASP:O	2.49	0.46
2:H:983:LEU:HD23	2:H:1056:THR:HA	1.98	0.46
2:H:4890:PHE:H	3:H:5101:ATP:N6	2.14	0.46
1:A:16:PRO:HG3	1:A:103:LEU:HD22	1.98	0.46
2:B:764:PRO:HG3	2:B:782:PHE:H	1.81	0.46
2:B:4794:TYR:HE2	2:B:4817:HIS:HE1	1.64	0.46
2:B:4822:VAL:CG2	2:H:4849:ILE:CA	2.90	0.46
2:D:754:VAL:HG11	2:D:813:PHE:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1762:GLN:O	2:D:1779:SER:OG	2.25	0.46
2:D:2108:THR:OG1	2:D:3615:HIS:O	2.34	0.46
2:D:2222:LEU:O	2:D:2226:SER:N	2.49	0.46
2:D:4853:PHE:CZ	2:F:4859:LEU:CD1	2.99	0.46
2:F:247:VAL:O	2:F:272:ARG:NH1	2.48	0.46
2:F:2108:THR:OG1	2:F:3615:HIS:O	2.34	0.46
2:F:2770:GLU:HA	2:F:2773:ARG:HB2	1.98	0.46
2:F:4849:ILE:C	2:H:4822:VAL:HG21	2.41	0.46
2:H:28:ILE:HD12	2:H:33:GLN:HE21	1.81	0.46
2:H:449:ILE:HG13	2:H:522:ALA:HB1	1.98	0.46
2:H:2108:THR:OG1	2:H:3615:HIS:O	2.34	0.46
2:H:2135:MET:HA	2:H:2136:GLY:HA3	1.67	0.46
2:B:983:LEU:HD23	2:B:1056:THR:HA	1.98	0.46
2:B:1669:ASN:O	2:B:1673:ALA:N	2.47	0.46
2:B:4518:LEU:HD22	2:H:4780:TYR:HD1	1.64	0.46
2:B:4822:VAL:CG2	2:H:4849:ILE:C	2.89	0.46
2:D:764:PRO:HG3	2:D:782:PHE:H	1.81	0.46
2:D:4849:ILE:CA	2:F:4822:VAL:CG2	2.87	0.46
2:F:433:LEU:O	2:F:437:SER:HB3	2.16	0.46
2:F:1117:TRP:HH2	2:F:1239:PHE:HZ	1.64	0.46
2:F:1446:ILE:HG12	2:F:1487:MET:H	1.81	0.46
2:F:4610:LYS:O	2:F:4615:GLY:N	2.38	0.46
1:G:16:PRO:HG3	1:G:103:LEU:HD22	1.98	0.46
2:H:1162:VAL:O	2:H:1176:THR:OG1	2.30	0.46
1:A:28:GLY:N	1:A:37:ASP:O	2.49	0.46
2:B:754:VAL:HG11	2:B:813:PHE:HD2	1.80	0.46
2:B:4822:VAL:HG23	2:H:4853:PHE:HB2	1.96	0.46
2:D:1676:LEU:HA	2:D:1679:HIS:HB2	1.98	0.46
2:F:548:CYS:HA	2:F:551:PHE:HB2	1.97	0.46
2:F:983:LEU:HD23	2:F:1056:THR:HA	1.98	0.46
2:H:247:VAL:O	2:H:272:ARG:NH1	2.48	0.46
2:H:4523:VAL:CB	2:H:4559:HIS:CE1	2.99	0.46
2:B:1446:ILE:HG12	2:B:1487:MET:H	1.81	0.45
2:B:1482:ARG:HD3	2:B:1531:TYR:HD1	1.81	0.45
2:B:1570:LEU:HD23	2:B:1570:LEU:HA	1.81	0.45
2:B:1676:LEU:HA	2:B:1679:HIS:HB2	1.98	0.45
2:B:3729:GLN:HE22	2:B:3769:GLY:H	1.64	0.45
2:D:38:ALA:HB2	2:D:50:GLU:HB2	1.98	0.45
2:D:766:ILE:HB	2:D:779:PHE:HB2	1.97	0.45
2:D:1687:TYR:O	2:D:1691:ASN:ND2	2.49	0.45
2:D:2345:LEU:HD21	2:D:2434:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4640:SER:O	2:D:4648:LYS:NZ	2.50	0.45
2:D:4814:TYR:CE2	2:F:4518:LEU:CD1	2.63	0.45
2:F:1114:ARG:HG2	2:F:1138:ASP:HB2	1.98	0.45
2:H:25:THR:HB	2:H:32:GLN:HB3	1.98	0.45
2:H:1253:LYS:HZ1	2:H:1257:GLN:HG3	1.80	0.45
2:B:247:VAL:O	2:B:272:ARG:NH1	2.48	0.45
2:B:542:ARG:NE	2:B:577:CYS:SG	2.78	0.45
2:B:1687:TYR:O	2:B:1691:ASN:ND2	2.49	0.45
2:B:4523:VAL:CA	2:B:4559:HIS:HD1	2.06	0.45
2:B:4640:SER:O	2:B:4648:LYS:NZ	2.49	0.45
2:B:4890:PHE:H	3:B:5101:ATP:N6	2.14	0.45
2:D:371:TRP:N	2:D:394:HIS:O	2.46	0.45
2:D:1799:VAL:HG22	2:D:1894:LEU:HD13	1.97	0.45
2:D:4164:PRO:HA	2:D:4167:LYS:HB2	1.98	0.45
2:F:449:ILE:HG13	2:F:522:ALA:HB1	1.98	0.45
2:F:764:PRO:HG3	2:F:782:PHE:H	1.81	0.45
2:H:1114:ARG:HG2	2:H:1138:ASP:HB2	1.98	0.45
2:B:188:SER:HB2	2:B:190:ARG:HH21	1.82	0.45
2:B:2770:GLU:HA	2:B:2773:ARG:HB2	1.98	0.45
2:B:4822:VAL:HG13	2:B:4823:ARG:N	2.31	0.45
2:B:4826:GLY:HA2	2:D:4823:ARG:HA	1.96	0.45
2:D:983:LEU:HD23	2:D:1056:THR:HA	1.98	0.45
2:D:2425:ARG:O	2:D:2477:TYR:OH	2.32	0.45
2:D:3729:GLN:HE22	2:D:3769:GLY:H	1.64	0.45
2:F:26:ALA:O	2:F:33:GLN:N	2.43	0.45
2:F:1173:MET:O	2:F:1191:ALA:N	2.49	0.45
2:F:3803:VAL:HG21	2:F:3881:ARG:HD2	1.97	0.45
2:F:4811:LEU:CA	2:H:4519:LEU:CD2	2.94	0.45
2:H:191:TYR:N	2:H:206:ALA:O	2.47	0.45
2:D:1117:TRP:HH2	2:D:1239:PHE:HZ	1.64	0.45
2:D:1507:ILE:O	2:D:1521:THR:OG1	2.33	0.45
2:F:655:MET:HG2	2:F:836:HIS:HA	1.98	0.45
2:F:1137:PHE:HA	2:F:1144:ARG:HA	1.99	0.45
2:F:4822:VAL:HG13	2:F:4823:ARG:N	2.31	0.45
2:H:802:PHE:N	2:H:1616:GLY:O	2.48	0.45
2:B:1507:ILE:O	2:B:1521:THR:OG1	2.33	0.45
2:B:4822:VAL:HG21	2:H:4849:ILE:C	2.42	0.45
1:E:28:GLY:N	1:E:37:ASP:O	2.49	0.45
2:F:1761:MET:SD	2:F:1761:MET:N	2.76	0.45
2:F:4640:SER:O	2:F:4648:LYS:NZ	2.49	0.45
2:H:565:LEU:HD11	2:H:603:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1121:GLY:O	2:H:1133:ARG:NH1	2.50	0.45
2:H:2345:LEU:HD21	2:H:2434:VAL:HB	1.98	0.45
2:B:433:LEU:O	2:B:437:SER:HB3	2.16	0.45
2:B:655:MET:HG2	2:B:836:HIS:HA	1.98	0.45
2:B:1121:GLY:O	2:B:1133:ARG:NH1	2.50	0.45
2:D:548:CYS:HA	2:D:551:PHE:HB2	1.97	0.45
2:D:1137:PHE:HA	2:D:1144:ARG:HA	1.99	0.45
2:D:1940:ASN:HA	2:D:1943:PHE:HD2	1.82	0.45
2:D:3803:VAL:HG21	2:D:3881:ARG:HD2	1.97	0.45
2:F:28:ILE:HD12	2:F:33:GLN:HE21	1.81	0.45
2:F:114:LEU:HB2	2:F:117:HIS:CE1	2.51	0.45
2:F:425:LEU:HD21	2:F:452:VAL:HA	1.99	0.45
2:F:1484:ASN:H	2:F:1486:TYR:HA	1.81	0.45
2:F:4523:VAL:CA	2:F:4559:HIS:HD1	2.06	0.45
2:F:4814:TYR:CE2	2:H:4518:LEU:CD1	2.59	0.45
2:F:4826:GLY:O	2:H:4823:ARG:HA	2.16	0.45
2:H:66:THR:OG1	2:H:124:SER:OG	2.26	0.45
2:H:152:ASP:HB3	2:H:154:THR:H	1.82	0.45
2:H:1117:TRP:HH2	2:H:1239:PHE:HZ	1.64	0.45
2:H:3926:GLN:HE21	2:H:4935:THR:HA	1.82	0.45
2:B:38:ALA:HB2	2:B:50:GLU:HB2	1.98	0.45
2:B:449:ILE:HG13	2:B:522:ALA:HB1	1.98	0.45
2:B:3831:LEU:HA	2:B:3832:GLN:HA	1.65	0.45
2:B:3858:TYR:CZ	2:B:3862:GLN:HG2	2.52	0.45
2:D:191:TYR:N	2:D:206:ALA:O	2.47	0.45
2:D:1482:ARG:HD3	2:D:1531:TYR:HD1	1.81	0.45
2:F:1718:ARG:NH1	2:F:1830:ILE:O	2.46	0.45
2:H:425:LEU:HD21	2:H:452:VAL:HA	1.99	0.45
2:H:614:LEU:HD23	2:H:617:LEU:HD12	1.99	0.45
2:H:3986:MET:HE3	2:H:3986:MET:HB2	1.86	0.45
2:B:152:ASP:HB3	2:B:154:THR:H	1.82	0.45
2:B:207:PHE:CB	2:D:2326:ILE:O	2.65	0.45
2:B:3993:ASN:HD22	2:B:4110:MET:HG3	1.82	0.45
2:D:73:LEU:CB	2:D:77:ALA:CB	2.87	0.45
2:D:2135:MET:HA	2:D:2136:GLY:HA3	1.67	0.45
2:D:2770:GLU:HA	2:D:2773:ARG:HB2	1.98	0.45
2:D:4794:TYR:HE2	2:D:4817:HIS:HE1	1.64	0.45
2:F:799:LYS:HE2	2:F:1618:LEU:HB3	1.99	0.45
2:F:2521:LEU:HD22	2:F:2565:ALA:HB2	1.99	0.45
2:H:1676:LEU:HA	2:H:1679:HIS:HB2	1.98	0.45
1:A:26:TYR:O	1:A:38:SER:OG	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:565:LEU:HD11	2:B:603:LYS:HG2	1.99	0.45
2:B:3926:GLN:HE21	2:B:4935:THR:HA	1.82	0.45
2:B:4907:GLU:OE1	2:H:4184:LYS:HD3	2.16	0.45
2:D:425:LEU:HD21	2:D:452:VAL:HA	1.99	0.45
2:D:652:VAL:HG13	2:D:692:HIS:CE1	2.52	0.45
2:D:3858:TYR:CZ	2:D:3862:GLN:HG2	2.52	0.45
2:F:188:SER:HB2	2:F:190:ARG:HH21	1.82	0.45
2:F:1482:ARG:HD3	2:F:1531:TYR:HD1	1.81	0.45
2:F:2345:LEU:HD21	2:F:2434:VAL:HB	1.98	0.45
2:F:4028:THR:HA	2:F:4033:PHE:CD2	2.52	0.45
2:F:4889:CYS:O	2:F:4893:GLY:N	2.46	0.45
2:H:433:LEU:O	2:H:437:SER:HB3	2.16	0.45
2:H:1137:PHE:HA	2:H:1144:ARG:HA	1.99	0.45
2:H:1573:SER:HB3	2:H:1582:CYS:HA	1.99	0.45
2:B:1137:PHE:HA	2:B:1144:ARG:HA	1.99	0.45
2:B:1722:ASN:HA	2:B:1758:ARG:HH21	1.82	0.45
2:B:2027:ARG:NH1	2:B:2031:LEU:HB2	2.32	0.45
2:B:3871:ILE:O	2:B:3874:SER:OG	2.31	0.45
2:B:4028:THR:HA	2:B:4033:PHE:CD2	2.52	0.45
2:B:4849:ILE:O	2:D:4822:VAL:HG21	2.13	0.45
2:D:476:GLN:NE2	2:D:3677:LEU:O	2.43	0.45
2:D:754:VAL:HB	2:D:771:ASN:HA	1.99	0.45
2:F:1102:TYR:HB2	2:F:1236:TYR:HB3	1.99	0.45
2:F:1940:ASN:HA	2:F:1943:PHE:HD2	1.82	0.45
2:F:3742:LEU:HD23	2:F:3781:TYR:HD2	1.82	0.45
2:F:4849:ILE:C	2:H:4822:VAL:CG2	2.88	0.45
2:H:1482:ARG:HD3	2:H:1531:TYR:HD1	1.81	0.45
2:H:2837:ASP:OD1	2:H:2906:ARG:NE	2.50	0.45
2:H:4164:PRO:HA	2:H:4167:LYS:HB2	1.98	0.45
2:H:4568:TYR:O	2:H:4572:THR:OG1	2.23	0.45
2:B:425:LEU:HD21	2:B:452:VAL:HA	1.99	0.44
2:B:1102:TYR:HB2	2:B:1236:TYR:HB3	1.99	0.44
2:B:1940:ASN:HA	2:B:1943:PHE:HD2	1.82	0.44
2:B:2222:LEU:O	2:B:2226:SER:N	2.49	0.44
2:B:3628:SER:HG	2:B:3629:TRP:CD1	2.35	0.44
2:B:3917:VAL:O	2:B:3920:THR:OG1	2.23	0.44
2:B:4859:LEU:HD12	2:H:4853:PHE:HZ	1.82	0.44
1:C:25:HIS:CG	1:C:40:ARG:HE	2.35	0.44
2:D:1114:ARG:HG2	2:D:1138:ASP:HB2	1.98	0.44
2:D:4028:THR:HA	2:D:4033:PHE:CD2	2.52	0.44
2:F:565:LEU:HD11	2:F:603:LYS:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4568:TYR:O	2:F:4572:THR:OG1	2.23	0.44
2:H:652:VAL:HG13	2:H:692:HIS:CE1	2.52	0.44
2:H:1144:ARG:N	2:H:1150:GLU:O	2.41	0.44
2:H:1762:GLN:O	2:H:1779:SER:OG	2.25	0.44
2:H:3998:LYS:HA	2:H:4110:MET:HE1	1.99	0.44
2:B:191:TYR:N	2:B:206:ALA:O	2.47	0.44
2:B:4859:LEU:CD1	2:H:4853:PHE:CZ	2.99	0.44
2:D:655:MET:HG2	2:D:836:HIS:HA	1.98	0.44
2:D:1008:ALA:HA	2:D:1011:ARG:HB2	1.99	0.44
2:D:4910:THR:HB	3:D:5101:ATP:H1'	1.99	0.44
2:F:614:LEU:HD23	2:F:617:LEU:HD12	1.99	0.44
2:F:618:CYS:SG	2:F:629:GLN:NE2	2.87	0.44
2:F:652:VAL:HG13	2:F:692:HIS:CE1	2.52	0.44
2:F:1121:GLY:O	2:F:1133:ARG:NH1	2.50	0.44
2:F:1676:LEU:HA	2:F:1679:HIS:HB2	1.98	0.44
2:F:3805:ASP:N	2:F:3832:GLN:OE1	2.50	0.44
2:H:655:MET:HG2	2:H:836:HIS:HA	1.98	0.44
2:H:764:PRO:HG3	2:H:782:PHE:H	1.81	0.44
2:H:799:LYS:HE2	2:H:1618:LEU:HB3	1.99	0.44
2:H:1173:MET:O	2:H:1191:ALA:N	2.49	0.44
2:B:476:GLN:NE2	2:B:3677:LEU:O	2.43	0.44
2:B:674:TYR:OH	2:B:815:PRO:O	2.36	0.44
2:B:4002:ASP:HA	2:B:4115:ARG:HH12	1.82	0.44
2:B:4184:LYS:HD3	2:D:4907:GLU:OE1	2.17	0.44
2:D:188:SER:HB2	2:D:190:ARG:HH21	1.82	0.44
2:D:1102:TYR:HB2	2:D:1236:TYR:HB3	1.99	0.44
2:D:1573:SER:HB3	2:D:1582:CYS:HA	1.99	0.44
2:D:1723:ASN:O	2:D:2105:LYS:NZ	2.41	0.44
2:D:2027:ARG:NH1	2:D:2031:LEU:HB2	2.32	0.44
2:D:2304:ARG:HG3	2:D:2402:ARG:HG3	2.00	0.44
2:D:2521:LEU:HD22	2:D:2565:ALA:HB2	1.99	0.44
2:F:38:ALA:HB2	2:F:50:GLU:HB2	1.98	0.44
2:F:1570:LEU:HD23	2:F:1570:LEU:HA	1.81	0.44
2:F:3926:GLN:HE21	2:F:4935:THR:HA	1.82	0.44
2:H:3993:ASN:HD22	2:H:4110:MET:HG3	1.82	0.44
2:H:4005:VAL:HG21	2:H:4115:ARG:HB3	1.98	0.44
2:B:246:THR:N	2:B:261:HIS:O	2.40	0.44
2:B:652:VAL:HG13	2:B:692:HIS:CE1	2.52	0.44
2:B:1114:ARG:HG2	2:B:1138:ASP:HB2	1.98	0.44
2:B:1941:GLN:HE22	2:B:3611:ASN:H	1.66	0.44
2:B:2514:ALA:HA	2:B:2517:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4164:PRO:HA	2:B:4167:LYS:HB2	1.98	0.44
2:D:19:GLU:OE1	2:D:218:SER:OG	2.29	0.44
2:D:78:LEU:HD21	2:D:118:ALA:HB3	2.00	0.44
2:D:1722:ASN:HA	2:D:1758:ARG:HH21	1.82	0.44
2:D:3687:PHE:HA	2:D:3690:MET:HB2	2.00	0.44
2:D:3856:GLN:NE2	2:D:3923:GLU:O	2.51	0.44
2:D:4713:VAL:O	2:D:4716:THR:OG1	2.30	0.44
2:D:4826:GLY:HA2	2:F:4823:ARG:HA	1.96	0.44
1:E:15:PHE:HA	1:E:67:SER:HA	1.99	0.44
2:F:16:THR:N	2:F:110:HIS:O	2.44	0.44
2:F:674:TYR:OH	2:F:815:PRO:O	2.36	0.44
2:F:1008:ALA:HA	2:F:1011:ARG:HB2	2.00	0.44
2:F:1722:ASN:HA	2:F:1758:ARG:HH21	1.82	0.44
2:F:2259:ARG:HH22	2:F:3831:LEU:HD11	1.82	0.44
2:F:2425:ARG:O	2:F:2477:TYR:OH	2.32	0.44
2:H:600:LEU:HA	2:H:603:LYS:HB2	2.00	0.44
2:H:3742:LEU:HD23	2:H:3781:TYR:HD2	1.82	0.44
2:H:4515:ASN:O	2:H:4518:LEU:HD23	2.18	0.44
2:H:4640:SER:O	2:H:4648:LYS:NZ	2.50	0.44
2:B:1117:TRP:HH2	2:B:1239:PHE:HZ	1.64	0.44
2:B:1727:VAL:HG11	2:B:1927:VAL:HG21	2.00	0.44
2:B:2837:ASP:OD1	2:B:2906:ARG:NE	2.50	0.44
2:B:3805:ASP:N	2:B:3832:GLN:OE1	2.50	0.44
2:B:4005:VAL:HG21	2:B:4115:ARG:HB3	1.99	0.44
2:D:1726:ILE:HD11	2:D:2121:LEU:HD11	2.00	0.44
2:D:4002:ASP:HA	2:D:4115:ARG:HH12	1.82	0.44
1:E:16:PRO:HG3	1:E:103:LEU:HD22	1.98	0.44
2:F:459:LEU:HA	2:F:462:TYR:HB3	2.00	0.44
2:F:2884:ALA:HA	2:F:2887:ARG:HB3	1.99	0.44
2:F:3729:GLN:HE22	2:F:3769:GLY:H	1.64	0.44
2:F:3907:PHE:HD2	2:F:3968:LEU:HD11	1.83	0.44
2:H:1102:TYR:HB2	2:H:1236:TYR:HB3	1.99	0.44
2:H:1177:LEU:N	2:H:1180:GLU:O	2.43	0.44
2:H:1941:GLN:HE22	2:H:3611:ASN:H	1.66	0.44
2:H:2770:GLU:HA	2:H:2773:ARG:HB2	1.98	0.44
2:H:3729:GLN:HE22	2:H:3769:GLY:H	1.64	0.44
2:B:373:THR:OG1	2:B:374:TYR:N	2.51	0.44
2:B:1484:ASN:H	2:B:1486:TYR:HA	1.81	0.44
2:B:2259:ARG:HH22	2:B:3831:LEU:HD11	1.82	0.44
2:B:2304:ARG:HG3	2:B:2402:ARG:HG3	2.00	0.44
2:B:3748:SER:O	2:B:3793:SER:OG	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1630:LEU:O	2:D:1638:SER:OG	2.30	0.44
2:D:3742:LEU:HD23	2:D:3781:TYR:HD2	1.82	0.44
2:D:3993:ASN:HD22	2:D:4110:MET:HG3	1.82	0.44
2:D:4085:VAL:O	2:D:4089:HIS:N	2.41	0.44
2:F:371:TRP:N	2:F:394:HIS:O	2.46	0.44
2:F:373:THR:OG1	2:F:374:TYR:N	2.51	0.44
2:F:754:VAL:HB	2:F:771:ASN:HA	1.99	0.44
2:F:1727:VAL:HG11	2:F:1927:VAL:HG21	2.00	0.44
2:F:2222:LEU:O	2:F:2226:SER:N	2.49	0.44
2:F:3858:TYR:CZ	2:F:3862:GLN:HG2	2.52	0.44
2:F:3993:ASN:HD22	2:F:4110:MET:HG3	1.82	0.44
1:G:68:LEU:HA	1:G:103:LEU:HD23	2.00	0.44
1:G:78:PRO:HA	1:G:81:ALA:HB3	2.00	0.44
2:H:188:SER:HB2	2:H:190:ARG:HH21	1.82	0.44
2:H:459:LEU:HA	2:H:462:TYR:HB3	2.00	0.44
2:H:3856:GLN:NE2	2:H:3923:GLU:O	2.51	0.44
1:A:25:HIS:CG	1:A:40:ARG:HE	2.35	0.44
2:B:1726:ILE:HD11	2:B:2121:LEU:HD11	2.00	0.44
2:B:2884:ALA:HA	2:B:2887:ARG:HB3	1.99	0.44
2:B:3687:PHE:HA	2:B:3690:MET:HB2	2.00	0.44
2:B:4871:PHE:HB3	2:H:4869:ASP:OD2	2.17	0.44
2:B:4910:THR:HB	3:B:5101:ATP:H1'	1.99	0.44
2:D:2102:ALA:HA	2:D:2105:LYS:HZ2	1.83	0.44
2:D:2259:ARG:HH22	2:D:3831:LEU:HD11	1.82	0.44
2:D:3926:GLN:HE21	2:D:4935:THR:HA	1.82	0.44
2:D:4515:ASN:O	2:D:4518:LEU:HD23	2.18	0.44
2:D:4811:LEU:CB	2:F:4519:LEU:CD2	2.91	0.44
2:H:942:THR:HA	2:H:945:ALA:HB3	2.00	0.44
2:H:1570:LEU:HD23	2:H:1570:LEU:HA	1.81	0.44
2:H:1727:VAL:HG11	2:H:1927:VAL:HG21	2.00	0.44
2:H:3805:ASP:N	2:H:3832:GLN:OE1	2.50	0.44
2:H:3858:TYR:CZ	2:H:3862:GLN:HG2	2.52	0.44
2:H:4028:THR:HA	2:H:4033:PHE:CD2	2.52	0.44
2:H:4713:VAL:O	2:H:4716:THR:OG1	2.30	0.44
2:H:4910:THR:HB	3:H:5101:ATP:H1'	1.99	0.44
2:B:1114:ARG:NH1	2:B:1128:LEU:O	2.51	0.44
2:B:1119:ARG:NH2	2:B:1196:ASP:O	2.45	0.44
2:B:1573:SER:HB3	2:B:1582:CYS:HA	1.99	0.44
2:B:3638:GLU:HB3	2:B:3695:ILE:HG23	2.00	0.44
2:D:152:ASP:HB3	2:D:154:THR:H	1.82	0.44
2:D:3907:PHE:HD2	2:D:3968:LEU:HD11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:228:LEU:HD23	2:F:228:LEU:HA	1.82	0.44
2:F:542:ARG:NE	2:F:577:CYS:SG	2.78	0.44
2:F:600:LEU:HA	2:F:603:LYS:HB2	2.00	0.44
2:F:802:PHE:N	2:F:1616:GLY:O	2.48	0.44
2:F:1726:ILE:HB	2:F:2109:ILE:HD11	2.00	0.44
2:F:3638:GLU:HB3	2:F:3695:ILE:HG23	2.00	0.44
2:F:3687:PHE:HA	2:F:3690:MET:HB2	2.00	0.44
2:F:4005:VAL:HG21	2:F:4115:ARG:HB3	1.99	0.44
2:F:4955:ALA:CB	2:H:4903:PRO:HB3	2.48	0.44
2:H:373:THR:OG1	2:H:374:TYR:N	2.51	0.44
2:H:471:GLU:O	2:H:475:LYS:N	2.44	0.44
2:H:1114:ARG:NH1	2:H:1128:LEU:O	2.51	0.44
2:H:2521:LEU:HD22	2:H:2565:ALA:HB2	1.99	0.44
2:H:2743:ILE:HB	2:H:2754:VAL:HG22	2.00	0.44
2:H:3748:SER:O	2:H:3793:SER:OG	2.29	0.44
1:A:78:PRO:HA	1:A:81:ALA:HB3	2.00	0.44
2:B:412:GLU:O	2:B:415:THR:OG1	2.31	0.44
2:B:606:ARG:NE	2:B:1634:GLU:OE2	2.41	0.44
2:B:3627:LYS:HE2	2:B:3627:LYS:HB3	1.84	0.44
2:D:799:LYS:HE2	2:D:1618:LEU:HB3	1.99	0.44
2:D:1121:GLY:O	2:D:1133:ARG:NH1	2.50	0.44
2:D:1484:ASN:H	2:D:1486:TYR:HA	1.81	0.44
2:D:3998:LYS:HA	2:D:4110:MET:HE1	1.99	0.44
2:D:4617:TYR:OH	2:D:4629:GLY:O	2.26	0.44
1:E:25:HIS:CG	1:E:40:ARG:HE	2.35	0.44
2:F:606:ARG:NE	2:F:1634:GLU:OE2	2.41	0.44
2:F:2743:ILE:HB	2:F:2754:VAL:HG22	2.00	0.44
2:F:3998:LYS:HA	2:F:4110:MET:HE1	1.99	0.44
2:F:4002:ASP:HA	2:F:4115:ARG:HH12	1.81	0.44
1:G:15:PHE:HA	1:G:67:SER:HA	1.99	0.44
2:H:1484:ASN:H	2:H:1486:TYR:HA	1.82	0.44
2:H:1726:ILE:HB	2:H:2109:ILE:HD11	2.00	0.44
2:H:1726:ILE:HD11	2:H:2121:LEU:HD11	2.00	0.44
2:H:1905:LEU:HB2	2:H:2081:LEU:HD12	2.00	0.44
2:H:1940:ASN:HA	2:H:1943:PHE:HD2	1.82	0.44
2:B:614:LEU:HD23	2:B:617:LEU:HD12	1.99	0.43
2:B:4515:ASN:O	2:B:4518:LEU:HD23	2.18	0.43
2:B:4853:PHE:HZ	2:D:4859:LEU:HD12	1.83	0.43
1:C:78:PRO:HA	1:C:81:ALA:HB3	2.00	0.43
2:D:565:LEU:HD11	2:D:603:LYS:HG2	1.99	0.43
2:D:600:LEU:HA	2:D:603:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1726:ILE:HB	2:D:2109:ILE:HD11	2.00	0.43
2:D:2884:ALA:HA	2:D:2887:ARG:HB3	1.99	0.43
2:D:3638:GLU:HB3	2:D:3695:ILE:HG23	2.00	0.43
1:E:38:SER:HB3	1:E:41:ASP:HB2	2.00	0.43
1:E:68:LEU:HA	1:E:103:LEU:HD23	2.00	0.43
2:F:2038:THR:HB	2:F:2040:LEU:HD23	2.00	0.43
2:F:2514:ALA:HA	2:F:2517:LEU:HD23	1.99	0.43
2:F:3854:ASP:N	2:F:3854:ASP:OD1	2.50	0.43
1:G:25:HIS:CG	1:G:40:ARG:HE	2.35	0.43
2:H:3907:PHE:HD2	2:H:3968:LEU:HD11	1.83	0.43
1:A:15:PHE:HA	1:A:67:SER:HA	1.99	0.43
2:B:2038:THR:HB	2:B:2040:LEU:HD23	2.00	0.43
2:B:2521:LEU:HD22	2:B:2565:ALA:HB2	1.99	0.43
2:B:3856:GLN:NE2	2:B:3923:GLU:O	2.51	0.43
2:B:4811:LEU:CB	2:D:4519:LEU:CD2	2.89	0.43
1:C:15:PHE:HA	1:C:67:SER:HA	1.99	0.43
2:D:3805:ASP:N	2:D:3832:GLN:OE1	2.50	0.43
2:F:1941:GLN:HE22	2:F:3611:ASN:H	1.66	0.43
2:F:2304:ARG:HG3	2:F:2402:ARG:HG3	2.00	0.43
2:F:4910:THR:HB	3:F:5101:ATP:H1'	1.99	0.43
2:H:38:ALA:HB2	2:H:50:GLU:HB2	1.98	0.43
2:H:78:LEU:HD11	2:H:118:ALA:HB3	2.01	0.43
2:H:2027:ARG:NH1	2:H:2031:LEU:HB2	2.32	0.43
2:H:2259:ARG:HH22	2:H:3831:LEU:HD11	1.82	0.43
2:B:1707:ILE:HG23	2:B:1711:LEU:HB2	2.01	0.43
2:B:2425:ARG:O	2:B:2477:TYR:OH	2.32	0.43
2:B:4889:CYS:O	2:B:4893:GLY:N	2.46	0.43
2:D:614:LEU:HD23	2:D:617:LEU:HD12	1.99	0.43
2:D:1727:VAL:HG11	2:D:1927:VAL:HG21	2.00	0.43
2:D:2520:TYR:HA	2:D:2523:THR:HB	2.01	0.43
2:F:152:ASP:HB3	2:F:154:THR:H	1.82	0.43
2:F:942:THR:HA	2:F:945:ALA:HB3	2.00	0.43
2:F:2520:TYR:HA	2:F:2523:THR:HB	2.01	0.43
2:F:3856:GLN:NE2	2:F:3923:GLU:O	2.51	0.43
2:F:4811:LEU:HA	2:H:4519:LEU:CD2	2.49	0.43
2:H:565:LEU:HG	2:H:604:HIS:CE1	2.54	0.43
2:H:754:VAL:HB	2:H:771:ASN:HA	1.99	0.43
2:H:1707:ILE:HG23	2:H:1711:LEU:HB2	2.01	0.43
2:H:4002:ASP:HA	2:H:4115:ARG:HH12	1.81	0.43
2:B:471:GLU:O	2:B:475:LYS:N	2.44	0.43
2:B:1905:LEU:HB2	2:B:2081:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1941:GLN:HE22	2:D:3611:ASN:H	1.66	0.43
2:D:3854:ASP:OD1	2:D:3854:ASP:N	2.50	0.43
2:D:4640:SER:HB3	2:D:4643:ASN:HD21	1.84	0.43
1:E:78:PRO:HA	1:E:81:ALA:HB3	2.00	0.43
2:F:4640:SER:HB3	2:F:4643:ASN:HD21	1.84	0.43
2:H:246:THR:N	2:H:261:HIS:O	2.40	0.43
2:H:2304:ARG:HG3	2:H:2402:ARG:HG3	2.00	0.43
2:B:374:TYR:HA	2:B:391:ALA:HA	2.00	0.43
2:B:1113:MET:HG3	2:B:1156:TRP:HZ2	1.84	0.43
2:B:1726:ILE:HB	2:B:2109:ILE:HD11	2.00	0.43
2:B:3998:LYS:HA	2:B:4110:MET:HE1	1.99	0.43
2:B:4504:ARG:NH2	2:B:4587:CYS:SG	2.92	0.43
2:D:373:THR:OG1	2:D:374:TYR:N	2.51	0.43
2:D:374:TYR:HA	2:D:391:ALA:HA	2.00	0.43
2:D:2212:GLN:HG2	2:D:2254:LEU:HD22	2.00	0.43
2:F:1573:SER:HB3	2:F:1582:CYS:HA	1.99	0.43
2:F:4124:GLU:HG3	2:F:4128:ASN:HD21	1.83	0.43
1:G:56:ILE:HG13	1:G:59:PHE:H	1.84	0.43
2:H:476:GLN:NE2	2:H:3677:LEU:O	2.43	0.43
2:H:4640:SER:HB3	2:H:4643:ASN:HD21	1.84	0.43
2:B:754:VAL:HB	2:B:771:ASN:HA	1.99	0.43
2:B:942:THR:HA	2:B:945:ALA:HB3	2.00	0.43
2:B:1007:TRP:O	2:B:1011:ARG:N	2.51	0.43
2:B:1008:ALA:HA	2:B:1011:ARG:HB2	2.00	0.43
2:B:1177:LEU:N	2:B:1180:GLU:O	2.43	0.43
2:B:2520:TYR:HA	2:B:2523:THR:HB	2.01	0.43
2:D:674:TYR:OH	2:D:815:PRO:O	2.36	0.43
2:D:1007:TRP:O	2:D:1011:ARG:N	2.51	0.43
2:D:2038:THR:HB	2:D:2040:LEU:HD23	2.00	0.43
1:E:56:ILE:HG13	1:E:59:PHE:H	1.84	0.43
2:F:1113:MET:HG3	2:F:1156:TRP:HZ2	1.84	0.43
2:F:1905:LEU:HB2	2:F:2081:LEU:HD12	2.00	0.43
2:F:3733:HIS:CD2	2:F:3774:VAL:HG22	2.54	0.43
2:H:1722:ASN:HA	2:H:1758:ARG:HH21	1.82	0.43
2:H:3733:HIS:CD2	2:H:3774:VAL:HG22	2.54	0.43
1:A:38:SER:HB3	1:A:41:ASP:HB2	2.00	0.43
2:B:565:LEU:HG	2:B:604:HIS:CE1	2.54	0.43
2:B:799:LYS:HE2	2:B:1618:LEU:HB3	1.99	0.43
2:B:4904:HIS:NE2	2:H:4184:LYS:HG3	2.33	0.43
1:C:56:ILE:HG13	1:C:59:PHE:H	1.84	0.43
2:F:2869:HIS:HE1	2:F:2871:LEU:HD12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3977:LYS:HE2	2:F:3977:LYS:HB3	1.90	0.43
2:F:4805:MET:HE3	2:F:4807:CYS:HA	2.01	0.43
2:H:228:LEU:HA	2:H:228:LEU:HD23	1.82	0.43
2:H:1008:ALA:HA	2:H:1011:ARG:HB2	1.99	0.43
2:H:1669:ASN:O	2:H:1673:ALA:N	2.47	0.43
2:H:3638:GLU:HB3	2:H:3695:ILE:HG23	2.00	0.43
1:A:56:ILE:HG13	1:A:59:PHE:H	1.84	0.43
2:B:459:LEU:HA	2:B:462:TYR:HB3	2.00	0.43
2:B:1689:ILE:HG12	2:B:1703:TYR:HE1	1.83	0.43
2:B:2029:ARG:O	2:B:2032:SER:OG	2.37	0.43
2:B:2843:GLU:OE2	2:B:2875:TYR:OH	2.34	0.43
2:B:4124:GLU:HG3	2:B:4128:ASN:HD21	1.83	0.43
1:C:68:LEU:HA	1:C:103:LEU:HD23	2.00	0.43
2:D:246:THR:N	2:D:261:HIS:O	2.40	0.43
2:D:459:LEU:HA	2:D:462:TYR:HB3	2.00	0.43
2:D:1114:ARG:NH1	2:D:1128:LEU:O	2.51	0.43
2:D:1689:ILE:HG12	2:D:1703:TYR:HE1	1.83	0.43
2:D:4005:VAL:HG21	2:D:4115:ARG:HB3	1.99	0.43
2:F:4753:THR:O	2:F:4756:THR:OG1	2.32	0.43
2:F:4869:ASP:OD2	2:H:4871:PHE:HB3	2.19	0.43
2:H:1098:ALA:O	2:H:1101:TRP:NE1	2.52	0.43
2:H:2102:ALA:HA	2:H:2105:LYS:HZ2	1.83	0.43
2:H:2520:TYR:HA	2:H:2523:THR:HB	2.01	0.43
2:H:2869:HIS:HE1	2:H:2871:LEU:HD12	1.84	0.43
2:H:4504:ARG:NH2	2:H:4587:CYS:SG	2.92	0.43
2:H:4610:LYS:O	2:H:4615:GLY:N	2.38	0.43
1:A:68:LEU:HA	1:A:103:LEU:HD23	2.00	0.43
2:B:1716:THR:HA	2:B:1719:LEU:HD12	2.01	0.43
2:B:1799:VAL:O	2:B:1803:SER:CB	2.67	0.43
2:B:2743:ILE:HB	2:B:2754:VAL:HG22	2.00	0.43
2:B:3742:LEU:HD23	2:B:3781:TYR:HD2	1.83	0.43
2:B:4519:LEU:CD2	2:H:4811:LEU:CB	2.88	0.43
2:D:1707:ILE:HG23	2:D:1711:LEU:HB2	2.00	0.43
2:D:1716:THR:HA	2:D:1719:LEU:HD12	2.01	0.43
2:D:1905:LEU:HB2	2:D:2081:LEU:HD12	2.00	0.43
2:D:3665:LEU:HD23	2:D:3735:ARG:HH11	1.84	0.43
2:D:4184:LYS:HD3	2:F:4907:GLU:OE1	2.19	0.43
2:D:4504:ARG:NH2	2:D:4587:CYS:SG	2.92	0.43
2:F:20:VAL:HG12	2:F:216:PRO:HA	2.01	0.43
2:F:565:LEU:HG	2:F:604:HIS:CE1	2.54	0.43
2:F:694:ARG:O	2:F:793:SER:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1696:GLY:H	2:F:1811:GLY:HA2	1.84	0.43
2:F:1726:ILE:HD11	2:F:2121:LEU:HD11	2.00	0.43
2:F:3665:LEU:HD23	2:F:3735:ARG:HH11	1.84	0.43
2:F:4504:ARG:NH2	2:F:4587:CYS:SG	2.92	0.43
2:H:238:HIS:HA	2:H:403:LEU:HD22	2.01	0.43
2:H:2514:ALA:HA	2:H:2517:LEU:HD23	1.99	0.43
2:H:2884:ALA:HA	2:H:2887:ARG:HB3	1.99	0.43
2:H:3857:ASN:OD1	2:H:3860:ARG:NH1	2.46	0.43
2:B:600:LEU:HA	2:B:603:LYS:HB2	2.00	0.43
2:B:618:CYS:SG	2:B:629:GLN:NE2	2.87	0.43
1:C:38:SER:HB3	1:C:41:ASP:HB2	2.00	0.43
2:D:1570:LEU:HD23	2:D:1570:LEU:HA	1.81	0.43
2:D:1696:GLY:H	2:D:1811:GLY:HA2	1.84	0.43
2:D:2743:ILE:HB	2:D:2754:VAL:HG22	2.00	0.43
2:D:4834:ASP:N	2:D:4834:ASP:OD1	2.52	0.43
2:F:238:HIS:HA	2:F:403:LEU:HD22	2.01	0.43
2:F:1689:ILE:HG12	2:F:1703:TYR:HE1	1.83	0.43
2:F:2135:MET:HA	2:F:2136:GLY:HA3	1.67	0.43
2:H:1113:MET:HG3	2:H:1156:TRP:HZ2	1.84	0.43
2:H:2038:THR:HB	2:H:2040:LEU:HD23	2.00	0.43
2:H:2212:GLN:HG2	2:H:2254:LEU:HD22	2.00	0.43
2:H:3665:LEU:HD23	2:H:3735:ARG:HH11	1.84	0.43
2:B:2658:TYR:O	2:B:2662:LEU:N	2.50	0.42
2:B:4002:ASP:HA	2:B:4115:ARG:HH22	1.84	0.42
2:D:78:LEU:HD11	2:D:118:ALA:HB3	2.01	0.42
2:D:2067:MET:HE3	2:D:2067:MET:HB3	1.87	0.42
2:D:2090:HIS:HD2	2:D:3695:ILE:HD11	1.84	0.42
2:D:2514:ALA:HA	2:D:2517:LEU:HD23	1.99	0.42
2:D:4002:ASP:HA	2:D:4115:ARG:HH22	1.84	0.42
2:D:4805:MET:HE3	2:D:4807:CYS:HA	2.01	0.42
2:F:1007:TRP:O	2:F:1011:ARG:N	2.51	0.42
2:F:1707:ILE:HG23	2:F:1711:LEU:HB2	2.01	0.42
2:F:2090:HIS:HD2	2:F:3695:ILE:HD11	1.84	0.42
2:F:3986:MET:HE3	2:F:3986:MET:HB2	1.86	0.42
2:H:20:VAL:HG12	2:H:216:PRO:HA	2.01	0.42
2:H:1716:THR:HA	2:H:1719:LEU:HD12	2.01	0.42
2:H:1799:VAL:O	2:H:1803:SER:CB	2.67	0.42
2:H:2222:LEU:O	2:H:2226:SER:N	2.49	0.42
2:H:2249:MET:HG2	2:H:2305:PHE:HB3	2.01	0.42
2:H:3854:ASP:OD1	2:H:3854:ASP:N	2.50	0.42
2:H:4124:GLU:HG3	2:H:4128:ASN:HD21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4805:MET:HE3	2:H:4807:CYS:HA	2.01	0.42
2:B:238:HIS:HA	2:B:403:LEU:HD22	2.01	0.42
2:B:3665:LEU:HD23	2:B:3735:ARG:HH11	1.84	0.42
2:B:3854:ASP:OD1	2:B:3854:ASP:N	2.50	0.42
2:B:4804:ASP:N	2:B:4804:ASP:OD1	2.51	0.42
2:D:247:VAL:O	2:D:272:ARG:NH1	2.48	0.42
2:D:681:HIS:HB2	2:D:799:LYS:HG2	2.02	0.42
2:D:953:SER:OG	2:D:1061:GLY:O	2.37	0.42
2:F:677:LEU:N	2:F:755:ILE:O	2.48	0.42
2:F:1114:ARG:NH1	2:F:1128:LEU:O	2.51	0.42
2:F:1716:THR:HA	2:F:1719:LEU:HD12	2.01	0.42
2:F:4861:ALA:N	2:H:4864:GLN:NE2	2.66	0.42
2:H:674:TYR:OH	2:H:815:PRO:O	2.36	0.42
2:H:681:HIS:HB2	2:H:799:LYS:HG2	2.01	0.42
2:H:1696:GLY:H	2:H:1811:GLY:HA2	1.84	0.42
2:H:3687:PHE:HA	2:H:3690:MET:HB2	2.00	0.42
2:B:20:VAL:HG12	2:B:216:PRO:HA	2.01	0.42
2:B:620:CYS:N	2:B:623:VAL:O	2.45	0.42
2:B:3733:HIS:CD2	2:B:3774:VAL:HG22	2.54	0.42
2:D:565:LEU:HG	2:D:604:HIS:CE1	2.54	0.42
2:D:4892:CYS:HB2	2:D:4914:HIS:CD2	2.54	0.42
2:F:305:TYR:HE2	2:F:319:LYS:HG2	1.85	0.42
2:F:1626:GLN:O	2:F:1687:TYR:OH	2.37	0.42
2:F:2832:VAL:O	2:F:2895:LYS:NZ	2.38	0.42
2:H:1507:ILE:O	2:H:1521:THR:OG1	2.33	0.42
2:H:4892:CYS:HB2	2:H:4914:HIS:CD2	2.54	0.42
2:B:1696:GLY:H	2:B:1811:GLY:HA2	1.84	0.42
2:B:2869:HIS:HE1	2:B:2871:LEU:HD12	1.84	0.42
2:B:4892:CYS:HB2	2:B:4914:HIS:CD2	2.54	0.42
2:D:938:GLU:HA	2:D:941:LYS:HB2	2.02	0.42
2:D:995:MET:HA	2:D:998:LYS:HB2	2.01	0.42
2:D:4804:ASP:OD1	2:D:4804:ASP:N	2.51	0.42
2:F:246:THR:N	2:F:261:HIS:O	2.40	0.42
2:F:1482:ARG:HH11	2:F:1531:TYR:HA	1.85	0.42
2:F:1902:PRO:HA	2:F:1905:LEU:HB3	2.02	0.42
2:F:2212:GLN:HG2	2:F:2254:LEU:HD22	2.00	0.42
2:F:4611:LEU:HA	2:F:4615:GLY:HA2	2.02	0.42
2:H:728:ASP:HA	2:H:748:LEU:HA	2.01	0.42
2:H:1902:PRO:HA	2:H:1905:LEU:HB3	2.02	0.42
2:B:2212:GLN:HG2	2:B:2254:LEU:HD22	2.00	0.42
2:B:2249:MET:HG2	2:B:2305:PHE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3907:PHE:HD2	2:B:3968:LEU:HD11	1.83	0.42
2:B:4519:LEU:CD2	2:H:4811:LEU:CA	2.98	0.42
2:D:942:THR:HA	2:D:945:ALA:HB3	2.00	0.42
2:D:1113:MET:HG3	2:D:1156:TRP:HZ2	1.84	0.42
2:D:1153:GLY:HA3	2:D:1182:LEU:HB3	2.01	0.42
2:D:1482:ARG:HH11	2:D:1531:TYR:HA	1.85	0.42
2:D:1799:VAL:O	2:D:1803:SER:CB	2.67	0.42
2:D:2658:TYR:O	2:D:2662:LEU:N	2.50	0.42
2:F:374:TYR:HA	2:F:391:ALA:HA	2.00	0.42
2:F:657:PRO:HB3	2:F:834:VAL:HG22	2.02	0.42
2:F:2027:ARG:NH1	2:F:2031:LEU:HB2	2.32	0.42
2:H:995:MET:HA	2:H:998:LYS:HB2	2.02	0.42
2:H:1689:ILE:HG12	2:H:1703:TYR:HE1	1.83	0.42
2:B:681:HIS:HB2	2:B:799:LYS:HG2	2.02	0.42
2:B:4752:LYS:H	2:B:4752:LYS:HD2	1.85	0.42
2:B:4753:THR:O	2:B:4756:THR:OG1	2.32	0.42
2:B:4808:ASP:CB	2:D:4523:VAL:CB	2.98	0.42
2:D:3733:HIS:CD2	2:D:3774:VAL:HG22	2.54	0.42
2:F:953:SER:OG	2:F:1061:GLY:O	2.38	0.42
2:F:1799:VAL:O	2:F:1803:SER:CB	2.67	0.42
1:G:38:SER:HB3	1:G:41:ASP:HB2	2.00	0.42
2:H:374:TYR:HA	2:H:391:ALA:HA	2.00	0.42
2:H:2071:ALA:HA	2:H:2076:ILE:HD11	2.02	0.42
2:H:2090:HIS:HD2	2:H:3695:ILE:HD11	1.84	0.42
2:H:2843:GLU:OE2	2:H:2875:TYR:OH	2.34	0.42
2:H:4611:LEU:HA	2:H:4615:GLY:HA2	2.02	0.42
2:H:4753:THR:O	2:H:4756:THR:OG1	2.32	0.42
2:B:3997:GLY:HA2	2:B:4000:MET:SD	2.60	0.42
2:D:20:VAL:HG12	2:D:216:PRO:HA	2.01	0.42
2:D:618:CYS:SG	2:D:629:GLN:NE2	2.87	0.42
2:D:2267:VAL:HA	2:D:2270:LEU:HB2	2.01	0.42
2:D:2837:ASP:OD1	2:D:2906:ARG:NE	2.50	0.42
2:D:4124:GLU:HG3	2:D:4128:ASN:HD21	1.83	0.42
2:D:4853:PHE:HZ	2:F:4859:LEU:HD12	1.84	0.42
2:F:1098:ALA:O	2:F:1101:TRP:NE1	2.52	0.42
2:F:4515:ASN:O	2:F:4518:LEU:HD23	2.18	0.42
2:H:305:TYR:HE2	2:H:319:LYS:HG2	1.85	0.42
2:H:3997:GLY:HA2	2:H:4000:MET:SD	2.60	0.42
2:H:4068:LEU:HA	2:H:4071:ALA:HB2	2.02	0.42
2:B:2267:VAL:HA	2:B:2270:LEU:HB2	2.01	0.42
2:B:2424:LEU:HD23	2:B:2476:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4138:GLU:HA	2:B:4148:ARG:HA	2.02	0.42
2:B:4523:VAL:CB	2:H:4808:ASP:CB	2.98	0.42
2:B:4611:LEU:HD23	2:B:4615:GLY:HA2	2.02	0.42
2:B:4640:SER:HB3	2:B:4643:ASN:HD21	1.84	0.42
2:D:728:ASP:HA	2:D:748:LEU:HA	2.01	0.42
2:D:2519:ARG:O	2:D:2523:THR:OG1	2.35	0.42
2:D:2869:HIS:HE1	2:D:2871:LEU:HD12	1.84	0.42
2:D:3917:VAL:O	2:D:3920:THR:OG1	2.23	0.42
2:D:4611:LEU:HD23	2:D:4615:GLY:HA2	2.02	0.42
2:F:681:HIS:HB2	2:F:799:LYS:HG2	2.01	0.42
2:F:1799:VAL:O	2:F:1803:SER:HB3	2.20	0.42
2:F:2267:VAL:HA	2:F:2270:LEU:HB2	2.01	0.42
2:F:3844:LEU:HA	2:F:3847:LEU:HD13	2.01	0.42
2:F:4892:CYS:HB2	2:F:4914:HIS:CD2	2.54	0.42
1:G:88:PRO:O	2:H:1671:ARG:NH2	2.46	0.42
2:H:78:LEU:HD21	2:H:118:ALA:HB3	2.01	0.42
2:H:657:PRO:HB3	2:H:834:VAL:HG22	2.02	0.42
2:H:1007:TRP:O	2:H:1011:ARG:N	2.51	0.42
2:H:4138:GLU:HA	2:H:4148:ARG:HA	2.02	0.42
2:B:728:ASP:HA	2:B:748:LEU:HA	2.01	0.42
2:B:3841:PHE:HB3	2:B:3920:THR:HG21	2.02	0.42
2:B:4903:PRO:HB3	2:H:4955:ALA:CB	2.50	0.42
2:D:1799:VAL:O	2:D:1803:SER:HB3	2.20	0.42
2:D:2212:GLN:HG3	2:D:2247:SER:HA	2.02	0.42
2:F:938:GLU:HA	2:F:941:LYS:HB2	2.02	0.42
2:F:1723:ASN:O	2:F:2105:LYS:NZ	2.41	0.42
2:F:4780:TYR:CE1	2:H:4518:LEU:CG	2.81	0.42
2:H:677:LEU:N	2:H:755:ILE:O	2.48	0.42
2:H:1482:ARG:HH11	2:H:1531:TYR:HA	1.85	0.42
2:H:2143:MET:HE2	2:H:2143:MET:HB3	1.94	0.42
2:H:2424:LEU:HD23	2:H:2476:VAL:HG22	2.02	0.42
2:H:4002:ASP:HA	2:H:4115:ARG:HH22	1.84	0.42
2:H:4611:LEU:HD23	2:H:4615:GLY:HA2	2.02	0.42
2:B:305:TYR:HE2	2:B:319:LYS:HG2	1.85	0.42
2:B:687:THR:HG23	2:B:1626:GLN:HE21	1.85	0.42
2:B:743:SER:HB3	2:B:775:VAL:HG13	2.02	0.42
2:B:4068:LEU:HA	2:B:4071:ALA:HB2	2.02	0.42
2:B:4184:LYS:HG3	2:D:4904:HIS:NE2	2.35	0.42
2:D:799:LYS:HB3	2:D:1620:GLN:HB2	2.02	0.42
2:D:2038:THR:OG1	2:D:2039:TYR:N	2.52	0.42
2:D:4138:GLU:HA	2:D:4148:ARG:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4611:LEU:HA	2:D:4615:GLY:HA2	2.02	0.42
2:F:1934:VAL:HB	2:F:3618:VAL:HG22	2.02	0.42
2:F:2212:GLN:HG3	2:F:2247:SER:HA	2.02	0.42
2:F:2249:MET:HG2	2:F:2305:PHE:HB3	2.01	0.42
2:F:3831:LEU:HD23	2:F:3831:LEU:HA	1.89	0.42
2:F:3857:ASN:OD1	2:F:3860:ARG:NH1	2.46	0.42
2:F:4002:ASP:HA	2:F:4115:ARG:HH22	1.85	0.42
2:F:4804:ASP:OD1	2:F:4804:ASP:N	2.51	0.42
2:H:78:LEU:HD21	2:H:118:ALA:CB	2.50	0.42
2:H:618:CYS:SG	2:H:629:GLN:NE2	2.87	0.42
2:H:2425:ARG:O	2:H:2477:TYR:OH	2.32	0.42
2:H:3841:PHE:HB3	2:H:3920:THR:HG21	2.02	0.42
1:A:83:GLY:C	1:A:94:ASN:H	2.28	0.41
2:B:1156:TRP:HZ3	2:B:1158:ALA:HA	1.85	0.41
2:B:2071:ALA:HA	2:B:2076:ILE:HD11	2.02	0.41
2:B:3847:LEU:HB3	2:B:3855:PHE:HE2	1.85	0.41
2:B:4805:MET:HE3	2:B:4807:CYS:HA	2.01	0.41
2:B:4834:ASP:OD1	2:B:4834:ASP:N	2.52	0.41
2:B:4907:GLU:OE2	2:H:4184:LYS:HD3	2.19	0.41
2:D:815:PRO:HB2	2:D:817:PRO:HD3	2.02	0.41
2:D:1902:PRO:HA	2:D:1905:LEU:HB3	2.02	0.41
1:E:83:GLY:C	1:E:94:ASN:H	2.28	0.41
2:F:2071:ALA:HA	2:F:2076:ILE:HD11	2.02	0.41
2:F:3841:PHE:HB3	2:F:3920:THR:HG21	2.02	0.41
2:F:4068:LEU:HA	2:F:4071:ALA:HB2	2.02	0.41
2:F:4844:ARG:O	2:F:4848:ASP:HB2	2.20	0.41
2:H:3983:LEU:HD12	2:H:3983:LEU:HA	1.91	0.41
2:H:4093:LYS:HE2	2:H:4093:LYS:HB3	1.92	0.41
2:H:4804:ASP:OD1	2:H:4804:ASP:N	2.51	0.41
2:H:4834:ASP:OD1	2:H:4834:ASP:N	2.52	0.41
2:B:1795:LEU:HD21	2:B:1821:LEU:HB3	2.03	0.41
2:B:2090:HIS:HD2	2:B:3695:ILE:HD11	1.84	0.41
2:B:2124:LEU:HA	2:B:2127:ILE:HG22	2.03	0.41
2:B:4015:LEU:HD23	2:B:4015:LEU:HA	1.91	0.41
1:C:83:GLY:C	1:C:94:ASN:H	2.28	0.41
2:D:238:HIS:HA	2:D:403:LEU:HD22	2.01	0.41
2:D:1156:TRP:HZ3	2:D:1158:ALA:HA	1.85	0.41
2:D:3997:GLY:HA2	2:D:4000:MET:SD	2.60	0.41
2:D:4068:LEU:HA	2:D:4071:ALA:HB2	2.02	0.41
2:H:125:TYR:CZ	2:H:417:ARG:HB3	2.55	0.41
2:H:1626:GLN:O	2:H:1687:TYR:OH	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4635:VAL:O	2:H:4638:THR:OG1	2.36	0.41
2:B:1291:GLY:HA2	2:B:1551:ASN:H	1.85	0.41
2:B:1799:VAL:O	2:B:1803:SER:HB3	2.20	0.41
2:B:3808:ALA:HA	2:B:3811:ARG:HD3	2.02	0.41
2:B:4184:LYS:HD3	2:D:4907:GLU:OE2	2.20	0.41
2:D:305:TYR:HE2	2:D:319:LYS:HG2	1.85	0.41
2:D:375:GLN:N	2:D:390:LYS:O	2.45	0.41
2:D:3841:PHE:HB3	2:D:3920:THR:HG21	2.02	0.41
2:D:4935:THR:H	2:D:4938:GLU:HB2	1.85	0.41
2:F:1153:GLY:HA3	2:F:1182:LEU:HB3	2.01	0.41
2:F:4085:VAL:O	2:F:4089:HIS:N	2.41	0.41
2:F:4808:ASP:CB	2:H:4523:VAL:CB	2.98	0.41
2:H:815:PRO:HB2	2:H:817:PRO:HD3	2.02	0.41
2:H:1253:LYS:HB3	2:H:1255:LEU:H	1.86	0.41
2:H:3844:LEU:HA	2:H:3847:LEU:HD13	2.01	0.41
2:H:4752:LYS:H	2:H:4752:LYS:HD2	1.85	0.41
2:B:1098:ALA:O	2:B:1101:TRP:NE1	2.52	0.41
2:B:1482:ARG:HH11	2:B:1531:TYR:HA	1.85	0.41
2:B:2038:THR:OG1	2:B:2039:TYR:N	2.52	0.41
2:B:2828:ASP:OD2	2:B:2831:ASN:ND2	2.53	0.41
2:B:4811:LEU:CA	2:D:4519:LEU:CD2	2.98	0.41
2:B:4935:THR:H	2:B:4938:GLU:HB2	1.85	0.41
2:D:412:GLU:O	2:D:415:THR:OG1	2.31	0.41
2:D:1934:VAL:HB	2:D:3618:VAL:HG22	2.02	0.41
2:D:4844:ARG:O	2:D:4848:ASP:HB2	2.20	0.41
2:F:125:TYR:CZ	2:F:417:ARG:HB3	2.55	0.41
2:F:1291:GLY:HA2	2:F:1551:ASN:H	1.85	0.41
2:F:4653:LYS:O	2:F:4657:LYS:HB2	2.21	0.41
2:H:953:SER:OG	2:H:1061:GLY:O	2.38	0.41
2:H:1291:GLY:HA2	2:H:1551:ASN:H	1.85	0.41
2:H:2828:ASP:OD2	2:H:2831:ASN:ND2	2.53	0.41
2:H:3808:ALA:HA	2:H:3811:ARG:HD3	2.02	0.41
2:B:938:GLU:HA	2:B:941:LYS:HB2	2.02	0.41
2:D:78:LEU:HD21	2:D:118:ALA:CB	2.50	0.41
2:D:125:TYR:CZ	2:D:417:ARG:HB3	2.55	0.41
2:D:1253:LYS:HB3	2:D:1255:LEU:H	1.86	0.41
2:D:2424:LEU:HD23	2:D:2476:VAL:HG22	2.02	0.41
2:D:3808:ALA:HA	2:D:3811:ARG:HD3	2.02	0.41
2:D:4653:LYS:O	2:D:4657:LYS:HB2	2.21	0.41
2:F:551:PHE:HD1	2:F:551:PHE:HA	1.73	0.41
2:F:687:THR:HG23	2:F:1626:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1705:LEU:HA	2:F:1705:LEU:HD23	1.85	0.41
2:F:3997:GLY:HA2	2:F:4000:MET:SD	2.60	0.41
2:F:4611:LEU:HD23	2:F:4615:GLY:HA2	2.02	0.41
2:B:375:GLN:N	2:B:390:LYS:O	2.45	0.41
2:B:653:SER:OG	2:B:794:PHE:O	2.27	0.41
2:B:773:GLN:HA	2:B:774:PRO:HD3	1.94	0.41
2:B:953:SER:OG	2:B:1061:GLY:O	2.37	0.41
2:B:1153:GLY:HA3	2:B:1182:LEU:HB3	2.01	0.41
2:B:3922:THR:O	2:B:3926:GLN:N	2.54	0.41
2:B:4653:LYS:O	2:B:4657:LYS:HB2	2.21	0.41
2:B:4904:HIS:CD2	2:H:4184:LYS:CG	3.03	0.41
2:D:802:PHE:N	2:D:1616:GLY:O	2.48	0.41
2:D:2071:ALA:HA	2:D:2076:ILE:HD11	2.02	0.41
2:D:3844:LEU:HA	2:D:3847:LEU:HD13	2.01	0.41
2:D:4754:LEU:HA	2:D:4757:ILE:HD12	2.03	0.41
2:F:2424:LEU:HD23	2:F:2476:VAL:HG22	2.02	0.41
2:F:2828:ASP:OD2	2:F:2831:ASN:ND2	2.53	0.41
2:F:3847:LEU:HB3	2:F:3855:PHE:HE2	1.85	0.41
2:F:4138:GLU:HA	2:F:4148:ARG:HA	2.02	0.41
2:F:4752:LYS:H	2:F:4752:LYS:HD2	1.85	0.41
2:H:542:ARG:NE	2:H:577:CYS:SG	2.78	0.41
2:H:743:SER:HB3	2:H:775:VAL:HG13	2.02	0.41
2:H:799:LYS:HB3	2:H:1620:GLN:HB2	2.02	0.41
2:H:1156:TRP:HZ3	2:H:1158:ALA:HA	1.85	0.41
2:H:1795:LEU:HD21	2:H:1821:LEU:HB3	2.03	0.41
2:H:4935:THR:H	2:H:4938:GLU:HB2	1.86	0.41
2:B:802:PHE:N	2:B:1616:GLY:O	2.48	0.41
2:B:995:MET:HA	2:B:998:LYS:HB2	2.02	0.41
2:B:1268:ILE:HG21	2:B:1300:MET:HE2	2.03	0.41
2:B:2297:GLU:HA	2:B:2300:LEU:HD12	2.03	0.41
2:B:3686:ASP:HB2	2:B:3755:MET:HE1	2.03	0.41
2:B:4631:TRP:CZ2	2:B:4712:GLY:HA3	2.56	0.41
2:B:4904:HIS:HD1	2:B:4908:THR:HG23	1.86	0.41
2:D:687:THR:HG23	2:D:1626:GLN:HE21	1.85	0.41
2:D:2083:ARG:HG3	2:D:3688:LEU:HD22	2.03	0.41
2:D:2843:GLU:OE2	2:D:2875:TYR:OH	2.34	0.41
2:D:4518:LEU:HD12	2:D:4518:LEU:C	2.46	0.41
2:D:4631:TRP:CZ2	2:D:4712:GLY:HA3	2.56	0.41
2:F:728:ASP:HA	2:F:748:LEU:HA	2.01	0.41
2:F:3983:LEU:HD12	2:F:3983:LEU:HA	1.91	0.41
2:F:4853:PHE:CZ	2:H:4859:LEU:CD1	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:603:LYS:HG3	2:H:1587:HIS:CE1	2.56	0.41
2:H:938:GLU:HA	2:H:941:LYS:HB2	2.02	0.41
2:H:1153:GLY:HA3	2:H:1182:LEU:HB3	2.01	0.41
2:H:2124:LEU:HA	2:H:2127:ILE:HG22	2.02	0.41
2:H:2267:VAL:HA	2:H:2270:LEU:HB2	2.01	0.41
2:H:4653:LYS:O	2:H:4657:LYS:HB2	2.21	0.41
2:B:125:TYR:CZ	2:B:417:ARG:HB3	2.55	0.41
2:B:1934:VAL:HB	2:B:3618:VAL:HG22	2.02	0.41
2:B:2083:ARG:HG3	2:B:3688:LEU:HD22	2.03	0.41
2:B:3798:MET:SD	2:B:3874:SER:OG	2.79	0.41
2:B:4611:LEU:HA	2:B:4615:GLY:HA2	2.02	0.41
2:B:4670:LEU:HD13	2:B:4670:LEU:HA	1.97	0.41
2:D:2192:LYS:O	2:D:2196:ASN:ND2	2.54	0.41
2:D:2249:MET:HG2	2:D:2305:PHE:HB3	2.01	0.41
2:F:603:LYS:HG3	2:F:1587:HIS:CE1	2.56	0.41
2:F:1255:LEU:HA	2:F:1256:PRO:HD3	1.90	0.41
2:H:606:ARG:NE	2:H:1634:GLU:OE2	2.41	0.41
2:H:687:THR:HG23	2:H:1626:GLN:HE21	1.85	0.41
2:B:657:PRO:HB3	2:B:834:VAL:HG22	2.02	0.41
2:B:1902:PRO:HA	2:B:1905:LEU:HB3	2.02	0.41
2:B:4093:LYS:HE2	2:B:4093:LYS:HB3	1.92	0.41
2:B:4610:LYS:O	2:B:4615:GLY:N	2.38	0.41
2:B:4754:LEU:HA	2:B:4757:ILE:HD12	2.03	0.41
2:B:4844:ARG:O	2:B:4848:ASP:HB2	2.20	0.41
2:D:228:LEU:HD23	2:D:228:LEU:HA	1.82	0.41
2:D:1124:PRO:HB2	2:D:1252:SER:HB3	2.03	0.41
2:D:1268:ILE:HG21	2:D:1300:MET:HE2	2.03	0.41
2:D:1291:GLY:HA2	2:D:1551:ASN:H	1.85	0.41
2:D:2297:GLU:HA	2:D:2300:LEU:HD12	2.03	0.41
2:D:2828:ASP:OD2	2:D:2831:ASN:ND2	2.53	0.41
2:D:3847:LEU:HB3	2:D:3855:PHE:HE2	1.85	0.41
2:D:4184:LYS:HD3	2:F:4907:GLU:OE2	2.21	0.41
2:D:4837:GLY:N	2:D:4841:GLU:OE1	2.54	0.41
2:F:64:ILE:H	2:F:64:ILE:HG13	1.80	0.41
2:F:728:ASP:HB2	2:F:748:LEU:HG	2.03	0.41
2:F:743:SER:HB3	2:F:775:VAL:HG13	2.02	0.41
2:F:799:LYS:HB3	2:F:1620:GLN:HB2	2.02	0.41
2:F:902:TRP:HB3	2:F:918:LEU:HD11	2.02	0.41
2:F:1044:LYS:HA	2:F:1047:LYS:HB2	2.02	0.41
2:F:1124:PRO:HB2	2:F:1252:SER:HB3	2.03	0.41
2:F:1156:TRP:HZ3	2:F:1158:ALA:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1268:ILE:HG21	2:F:1300:MET:HE2	2.03	0.41
2:F:1286:THR:HA	2:F:1586:LEU:HD11	2.03	0.41
2:F:2192:LYS:O	2:F:2196:ASN:ND2	2.54	0.41
2:F:3686:ASP:HB2	2:F:3755:MET:HE1	2.03	0.41
2:F:3922:THR:O	2:F:3926:GLN:N	2.54	0.41
2:F:4754:LEU:HA	2:F:4757:ILE:HD12	2.03	0.41
2:F:4935:THR:H	2:F:4938:GLU:HB2	1.86	0.41
2:H:193:HIS:N	2:H:204:ASP:O	2.43	0.41
2:H:725:TYR:HA	2:H:732:LEU:HA	2.03	0.41
2:H:1176:THR:HG22	2:H:1181:ILE:HG23	2.03	0.41
2:H:1286:THR:HA	2:H:1586:LEU:HD11	2.03	0.41
2:H:1767:SER:HG	2:H:1770:SER:HG	1.55	0.41
2:H:2127:ILE:HD11	2:H:2143:MET:HG3	2.03	0.41
2:H:3647:LYS:HA	2:H:3648:PRO:HD3	1.95	0.41
2:H:3798:MET:SD	2:H:3874:SER:OG	2.79	0.41
2:H:3871:ILE:O	2:H:3874:SER:OG	2.31	0.41
2:H:4068:LEU:HA	2:H:4068:LEU:HD23	1.95	0.41
2:H:4631:TRP:CZ2	2:H:4712:GLY:HA3	2.56	0.41
2:H:4754:LEU:HA	2:H:4757:ILE:HD12	2.03	0.41
2:H:4844:ARG:O	2:H:4848:ASP:HB2	2.20	0.41
2:H:4904:HIS:HD1	2:H:4908:THR:HG23	1.86	0.41
2:B:193:HIS:N	2:B:204:ASP:O	2.43	0.41
2:B:548:CYS:HB2	2:B:582:SER:HB3	2.03	0.41
2:B:815:PRO:HB2	2:B:817:PRO:HD3	2.02	0.41
2:B:1165:MET:O	2:B:1174:MET:N	2.52	0.41
2:B:1176:THR:HG22	2:B:1181:ILE:HG23	2.03	0.41
2:B:2127:ILE:HD11	2:B:2143:MET:HG3	2.03	0.41
2:B:2192:LYS:O	2:B:2196:ASN:ND2	2.54	0.41
2:B:2201:LEU:HD23	2:B:2201:LEU:HA	1.95	0.41
2:B:2212:GLN:HG3	2:B:2247:SER:HA	2.02	0.41
2:B:3844:LEU:HA	2:B:3847:LEU:HD13	2.01	0.41
1:C:4:ILE:HG12	1:C:74:LEU:HA	2.03	0.41
2:D:657:PRO:HB3	2:D:834:VAL:HG22	2.02	0.41
2:D:1119:ARG:NH2	2:D:1196:ASP:O	2.45	0.41
2:D:3686:ASP:HB2	2:D:3755:MET:HE1	2.03	0.41
2:F:1669:ASN:HB3	2:F:1672:VAL:HB	2.03	0.41
2:F:2658:TYR:O	2:F:2662:LEU:N	2.50	0.41
2:F:2837:ASP:OD1	2:F:2906:ARG:NE	2.50	0.41
2:H:19:GLU:OE1	2:H:218:SER:OG	2.29	0.41
2:H:3686:ASP:HB2	2:H:3755:MET:HE1	2.03	0.41
2:H:3922:THR:O	2:H:3926:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:HG21	1:A:59:PHE:HD2	1.86	0.40
2:B:732:LEU:HD11	2:B:739:ARG:HB2	2.03	0.40
2:B:902:TRP:HB3	2:B:918:LEU:HD11	2.02	0.40
1:C:7:ILE:H	1:C:72:ALA:HA	1.86	0.40
2:D:290:ARG:H	2:D:293:GLN:NE2	2.19	0.40
2:D:725:TYR:HA	2:D:732:LEU:HA	2.03	0.40
2:D:728:ASP:HB2	2:D:748:LEU:HG	2.03	0.40
2:D:3959:LEU:HD13	2:D:3969:LEU:HA	2.03	0.40
2:F:3798:MET:SD	2:F:3874:SER:OG	2.79	0.40
2:F:3871:ILE:O	2:F:3874:SER:OG	2.31	0.40
2:F:4631:TRP:CZ2	2:F:4712:GLY:HA3	2.56	0.40
2:F:4904:HIS:HD1	2:F:4908:THR:HG23	1.86	0.40
2:H:300:VAL:O	2:H:420:ARG:NH2	2.55	0.40
2:H:1268:ILE:HG21	2:H:1300:MET:HE2	2.03	0.40
2:B:603:LYS:HG3	2:B:1587:HIS:CE1	2.56	0.40
2:B:679:VAL:HG13	2:B:800:VAL:HG12	2.04	0.40
2:B:1286:THR:HA	2:B:1586:LEU:HD11	2.03	0.40
2:B:1654:HIS:O	2:B:1657:THR:OG1	2.27	0.40
2:B:1669:ASN:HB3	2:B:1672:VAL:HB	2.03	0.40
1:C:88:PRO:O	2:D:1671:ARG:NH2	2.46	0.40
2:D:743:SER:HB3	2:D:775:VAL:HG13	2.02	0.40
2:D:956:HIS:HA	2:D:1060:TYR:HB3	2.03	0.40
2:D:1795:LEU:HD21	2:D:1821:LEU:HB3	2.03	0.40
2:D:3665:LEU:HD11	2:D:3696:MET:HE2	2.04	0.40
2:D:3871:ILE:O	2:D:3874:SER:OG	2.31	0.40
2:D:4904:HIS:HD1	2:D:4908:THR:HG23	1.86	0.40
2:F:995:MET:HA	2:F:998:LYS:HB2	2.02	0.40
2:F:4036:TYR:HE2	2:F:4048:ASP:HB3	1.86	0.40
1:G:55:VAL:HG21	1:G:59:PHE:HD2	1.86	0.40
2:H:1173:MET:HE2	2:H:1192:PHE:HB2	2.03	0.40
2:H:1452:GLN:NE2	2:H:1459:LEU:O	2.54	0.40
2:H:1799:VAL:O	2:H:1803:SER:HB3	2.20	0.40
2:H:3847:LEU:HB3	2:H:3855:PHE:HE2	1.85	0.40
2:H:4005:VAL:HG11	2:H:4115:ARG:HB3	2.04	0.40
1:A:4:ILE:HG12	1:A:74:LEU:HA	2.04	0.40
1:A:7:ILE:H	1:A:72:ALA:HA	1.86	0.40
2:B:956:HIS:HA	2:B:1060:TYR:HB3	2.03	0.40
2:B:1124:PRO:HB2	2:B:1252:SER:HB3	2.03	0.40
2:B:1132:GLU:HB3	2:B:1147:GLN:HE21	1.86	0.40
2:B:1173:MET:HE2	2:B:1192:PHE:HB2	2.03	0.40
2:B:1452:GLN:NE2	2:B:1459:LEU:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3665:LEU:HD11	2:B:3696:MET:HE2	2.04	0.40
2:D:488:LEU:HD23	2:D:488:LEU:HA	1.94	0.40
2:D:732:LEU:HD11	2:D:739:ARG:HB2	2.03	0.40
2:D:902:TRP:HB3	2:D:918:LEU:HD11	2.02	0.40
2:D:924:LEU:HB2	2:D:929:ARG:HB2	2.04	0.40
2:D:1669:ASN:HB3	2:D:1672:VAL:HB	2.03	0.40
2:D:4612:GLU:O	2:D:4658:TYR:OH	2.35	0.40
2:F:290:ARG:H	2:F:293:GLN:NE2	2.19	0.40
2:F:1253:LYS:HB3	2:F:1255:LEU:H	1.86	0.40
2:F:3925:ILE:HD11	2:F:3936:LEU:HD13	2.04	0.40
1:G:83:GLY:C	1:G:94:ASN:H	2.28	0.40
2:H:1669:ASN:HB3	2:H:1672:VAL:HB	2.03	0.40
2:H:2212:GLN:HG3	2:H:2247:SER:HA	2.02	0.40
2:H:4004:LEU:HD13	2:H:4004:LEU:HA	1.97	0.40
1:A:88:PRO:O	2:B:1671:ARG:NH2	2.46	0.40
2:B:551:PHE:HD1	2:B:551:PHE:HA	1.73	0.40
2:B:731:HIS:CG	2:B:740:THR:HA	2.57	0.40
2:B:2832:VAL:O	2:B:2895:LYS:NZ	2.38	0.40
2:B:3857:ASN:OD1	2:B:3860:ARG:NH1	2.46	0.40
2:B:4005:VAL:HG11	2:B:4115:ARG:HB3	2.04	0.40
2:B:4837:GLY:N	2:B:4841:GLU:OE1	2.54	0.40
2:D:551:PHE:HD1	2:D:551:PHE:HA	1.73	0.40
2:D:731:HIS:CG	2:D:740:THR:HA	2.57	0.40
2:D:1132:GLU:HB3	2:D:1147:GLN:HE21	1.86	0.40
2:D:1173:MET:HE2	2:D:1192:PHE:HB2	2.03	0.40
2:D:1286:THR:HA	2:D:1586:LEU:HD11	2.03	0.40
2:D:3798:MET:SD	2:D:3874:SER:OG	2.79	0.40
2:D:3925:ILE:HD11	2:D:3936:LEU:HD13	2.04	0.40
2:D:4005:VAL:HG11	2:D:4115:ARG:HB3	2.04	0.40
2:D:4752:LYS:HD2	2:D:4752:LYS:H	1.85	0.40
2:F:731:HIS:CG	2:F:740:THR:HA	2.57	0.40
2:F:1795:LEU:HD21	2:F:1821:LEU:HB3	2.03	0.40
2:F:2127:ILE:HD11	2:F:2143:MET:HG3	2.03	0.40
2:F:4808:ASP:O	2:H:4521:TYR:O	2.38	0.40
2:F:4837:GLY:N	2:F:4841:GLU:OE1	2.54	0.40
1:G:42:ARG:HH21	2:H:1766:PRO:HG2	1.87	0.40
2:H:1044:LYS:HA	2:H:1047:LYS:HB2	2.03	0.40
2:H:1934:VAL:HB	2:H:3618:VAL:HG22	2.02	0.40
2:B:464:HIS:HA	2:B:465:PRO:HD3	1.98	0.40
2:D:603:LYS:HG3	2:D:1587:HIS:CE1	2.56	0.40
2:D:653:SER:OG	2:D:794:PHE:O	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:694:ARG:O	2:D:793:SER:N	2.46	0.40
2:D:796:ALA:HB3	2:D:798:ILE:HG13	2.04	0.40
2:D:2173:MET:HE3	2:D:2173:MET:HB2	1.97	0.40
2:D:2832:VAL:O	2:D:2895:LYS:NZ	2.38	0.40
2:D:4811:LEU:CA	2:F:4519:LEU:CD2	2.99	0.40
1:E:42:ARG:HH21	2:F:1766:PRO:HG2	1.87	0.40
2:F:1452:GLN:NE2	2:F:1459:LEU:O	2.54	0.40
2:F:2124:LEU:HA	2:F:2127:ILE:HG22	2.03	0.40
2:H:1730:THR:O	2:H:1733:THR:OG1	2.28	0.40
2:H:2083:ARG:HG3	2:H:3688:LEU:HD22	2.03	0.40
2:H:2192:LYS:O	2:H:2196:ASN:ND2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	C	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	E	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
1	G	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	B	3332/4968 (67%)	2955 (89%)	368 (11%)	9 (0%)	36	71
2	D	3332/4968 (67%)	2955 (89%)	368 (11%)	9 (0%)	36	71
2	F	3332/4968 (67%)	2955 (89%)	368 (11%)	9 (0%)	36	71
2	H	3332/4968 (67%)	2958 (89%)	365 (11%)	9 (0%)	36	71
All	All	13748/20304 (68%)	12227 (89%)	1485 (11%)	36 (0%)	37	71

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4595	LYS
2	D	4595	LYS
2	F	4595	LYS
2	H	4595	LYS
2	B	143	LEU
2	D	143	LEU
2	F	143	LEU
2	H	143	LEU
2	B	1580	PRO
2	B	1581	GLN
2	D	1580	PRO
2	D	1581	GLN
2	F	1580	PRO
2	F	1581	GLN
2	H	1580	PRO
2	H	1581	GLN
2	B	4071	ALA
2	D	4071	ALA
2	F	4071	ALA
2	H	4071	ALA
2	B	142	LYS
2	B	853	PRO
2	B	2233	PRO
2	D	142	LYS
2	D	853	PRO
2	D	2233	PRO
2	F	142	LYS
2	F	853	PRO
2	F	2233	PRO
2	H	142	LYS
2	H	853	PRO
2	H	2233	PRO
2	B	1848	PRO
2	D	1848	PRO
2	F	1848	PRO
2	H	1848	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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	2657/4355 (61%)	2641 (99%)	16 (1%)	78	81
2	D	2658/4355 (61%)	2639 (99%)	19 (1%)	76	79
2	F	2657/4355 (61%)	2640 (99%)	17 (1%)	78	81
2	H	2658/4355 (61%)	2638 (99%)	20 (1%)	73	78
All	All	10982/17776 (62%)	10910 (99%)	72 (1%)	73	79

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	79	GLN
2	B	80	GLU
2	B	81	MET
2	B	625	VAL
2	B	791	VAL
2	B	881	ILE
2	B	925	PRO
2	B	950	VAL
2	B	990	PRO
2	B	1089	ARG
2	B	1997	LEU
2	B	2118	ILE
2	B	2211	ASN
2	B	4139	ILE
2	B	4846	ILE
2	B	4863	ILE
2	D	78	LEU
2	D	79	GLN
2	D	80	GLU
2	D	81	MET
2	D	84	ASN
2	D	625	VAL
2	D	791	VAL
2	D	881	ILE
2	D	925	PRO

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Mol	Chain	Res	Type
2	D	950	VAL
2	D	990	PRO
2	D	1054	VAL
2	D	1089	ARG
2	D	1997	LEU
2	D	2118	ILE
2	D	2211	ASN
2	D	4139	ILE
2	D	4846	ILE
2	D	4863	ILE
2	F	79	GLN
2	F	80	GLU
2	F	81	MET
2	F	84	ASN
2	F	625	VAL
2	F	791	VAL
2	F	881	ILE
2	F	925	PRO
2	F	950	VAL
2	F	990	PRO
2	F	1089	ARG
2	F	1997	LEU
2	F	2118	ILE
2	F	2211	ASN
2	F	4139	ILE
2	F	4846	ILE
2	F	4863	ILE
2	H	78	LEU
2	H	79	GLN
2	H	80	GLU
2	H	81	MET
2	H	84	ASN
2	H	625	VAL
2	H	791	VAL
2	H	881	ILE
2	H	925	PRO
2	H	950	VAL
2	H	990	PRO
2	H	1054	VAL
2	H	1089	ARG
2	H	1738	LEU
2	H	1997	LEU

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Mol	Chain	Res	Type
2	H	2118	ILE
2	H	2211	ASN
2	H	4139	ILE
2	H	4846	ILE
2	H	4863	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (243) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
2	B	23	GLN
2	B	33	GLN
2	B	44	ASN
2	B	84	ASN
2	B	117	HIS
2	B	202	HIS
2	B	394	HIS
2	B	490	GLN
2	B	531	ASN
2	B	604	HIS
2	B	607	ASN
2	B	628	ASN
2	B	776	GLN
2	B	914	GLN
2	B	1123	GLN
2	B	1147	GLN
2	B	1257	GLN
2	B	1452	GLN
2	B	1503	ASN
2	B	1546	GLN
2	B	1602	GLN
2	B	1626	GLN
2	B	1670	HIS
2	B	1684	GLN
2	B	1691	ASN
2	B	1918	GLN
2	B	1938	GLN
2	B	1940	ASN
2	B	2090	HIS
2	B	2119	ASN
2	B	2196	ASN
2	B	2211	ASN

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Mol	Chain	Res	Type
2	B	2218	HIS
2	B	2317	ASN
2	B	2755	GLN
2	B	2831	ASN
2	B	2868	ASN
2	B	3635	HIS
2	B	3813	ASN
2	B	3870	ASN
2	B	3904	GLN
2	B	3906	ASN
2	B	3916	GLN
2	B	3919	ASN
2	B	3932	ASN
2	B	3956	GLN
2	B	3965	GLN
2	B	3993	ASN
2	B	3999	GLN
2	B	4061	GLN
2	B	4098	ASN
2	B	4128	ASN
2	B	4160	GLN
2	B	4172	GLN
2	B	4179	ASN
2	B	4499	ASN
2	B	4621	GLN
2	B	4643	ASN
2	B	4864	GLN
2	B	4918	ASN
1	C	31	GLN
2	D	23	GLN
2	D	33	GLN
2	D	44	ASN
2	D	84	ASN
2	D	117	HIS
2	D	202	HIS
2	D	252	HIS
2	D	394	HIS
2	D	398	HIS
2	D	531	ASN
2	D	604	HIS
2	D	607	ASN
2	D	628	ASN

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Mol	Chain	Res	Type
2	D	776	GLN
2	D	914	GLN
2	D	1002	ASN
2	D	1123	GLN
2	D	1147	GLN
2	D	1257	GLN
2	D	1452	GLN
2	D	1503	ASN
2	D	1546	GLN
2	D	1602	GLN
2	D	1626	GLN
2	D	1670	HIS
2	D	1684	GLN
2	D	1691	ASN
2	D	1918	GLN
2	D	1938	GLN
2	D	1940	ASN
2	D	2090	HIS
2	D	2196	ASN
2	D	2211	ASN
2	D	2317	ASN
2	D	2755	GLN
2	D	2831	ASN
2	D	2868	ASN
2	D	3611	ASN
2	D	3635	HIS
2	D	3813	ASN
2	D	3845	GLN
2	D	3865	ASN
2	D	3870	ASN
2	D	3904	GLN
2	D	3906	ASN
2	D	3919	ASN
2	D	3932	ASN
2	D	3965	GLN
2	D	3976	GLN
2	D	3993	ASN
2	D	3999	GLN
2	D	4061	GLN
2	D	4098	ASN
2	D	4128	ASN
2	D	4160	GLN

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Mol	Chain	Res	Type
2	D	4179	ASN
2	D	4499	ASN
2	D	4621	GLN
2	D	4643	ASN
2	D	4864	GLN
2	D	4918	ASN
1	E	31	GLN
2	F	23	GLN
2	F	33	GLN
2	F	44	ASN
2	F	84	ASN
2	F	117	HIS
2	F	202	HIS
2	F	252	HIS
2	F	394	HIS
2	F	490	GLN
2	F	531	ASN
2	F	604	HIS
2	F	607	ASN
2	F	628	ASN
2	F	776	GLN
2	F	914	GLN
2	F	1002	ASN
2	F	1123	GLN
2	F	1147	GLN
2	F	1257	GLN
2	F	1452	GLN
2	F	1503	ASN
2	F	1546	GLN
2	F	1602	GLN
2	F	1626	GLN
2	F	1670	HIS
2	F	1684	GLN
2	F	1691	ASN
2	F	1918	GLN
2	F	1938	GLN
2	F	1940	ASN
2	F	2090	HIS
2	F	2196	ASN
2	F	2211	ASN
2	F	2755	GLN
2	F	2831	ASN

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Mol	Chain	Res	Type
2	F	2868	ASN
2	F	3635	HIS
2	F	3813	ASN
2	F	3845	GLN
2	F	3870	ASN
2	F	3904	GLN
2	F	3906	ASN
2	F	3919	ASN
2	F	3932	ASN
2	F	3965	GLN
2	F	3976	GLN
2	F	3993	ASN
2	F	3999	GLN
2	F	4050	HIS
2	F	4061	GLN
2	F	4098	ASN
2	F	4128	ASN
2	F	4160	GLN
2	F	4172	GLN
2	F	4179	ASN
2	F	4499	ASN
2	F	4621	GLN
2	F	4643	ASN
2	F	4864	GLN
2	F	4918	ASN
1	G	31	GLN
2	H	23	GLN
2	H	33	GLN
2	H	44	ASN
2	H	84	ASN
2	H	117	HIS
2	H	202	HIS
2	H	252	HIS
2	H	394	HIS
2	H	490	GLN
2	H	531	ASN
2	H	604	HIS
2	H	607	ASN
2	H	628	ASN
2	H	776	GLN
2	H	914	GLN
2	H	1002	ASN

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Mol	Chain	Res	Type
2	H	1123	GLN
2	H	1147	GLN
2	H	1257	GLN
2	H	1452	GLN
2	H	1503	ASN
2	H	1546	GLN
2	H	1602	GLN
2	H	1626	GLN
2	H	1670	HIS
2	H	1691	ASN
2	H	1918	GLN
2	H	1938	GLN
2	H	2090	HIS
2	H	2119	ASN
2	H	2196	ASN
2	H	2211	ASN
2	H	2317	ASN
2	H	2755	GLN
2	H	2831	ASN
2	H	2868	ASN
2	H	3635	HIS
2	H	3813	ASN
2	H	3845	GLN
2	H	3870	ASN
2	H	3904	GLN
2	H	3906	ASN
2	H	3919	ASN
2	H	3932	ASN
2	H	3956	GLN
2	H	3965	GLN
2	H	3993	ASN
2	H	3999	GLN
2	H	4061	GLN
2	H	4098	ASN
2	H	4128	ASN
2	H	4160	GLN
2	H	4172	GLN
2	H	4179	ASN
2	H	4499	ASN
2	H	4621	GLN
2	H	4864	GLN
2	H	4918	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	F	5101	-	32,33,33	1.33	4 (12%)	48,52,52	1.92	12 (25%)
3	ATP	B	5101	-	32,33,33	1.34	4 (12%)	48,52,52	1.92	12 (25%)
3	ATP	D	5101	-	32,33,33	1.34	4 (12%)	48,52,52	1.92	12 (25%)
3	ATP	H	5101	-	32,33,33	1.34	4 (12%)	48,52,52	1.92	12 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	F	5101	-	-	7/22/38/38	0/3/3/3
3	ATP	B	5101	-	-	7/22/38/38	0/3/3/3
3	ATP	D	5101	-	-	7/22/38/38	0/3/3/3
3	ATP	H	5101	-	-	7/22/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5101	ATP	C5-C4	4.27	1.46	1.39
3	H	5101	ATP	C5-C4	4.27	1.46	1.39
3	B	5101	ATP	C5-C4	4.25	1.46	1.39
3	F	5101	ATP	C5-C4	4.24	1.46	1.39
3	B	5101	ATP	C5-C6	2.58	1.48	1.41
3	F	5101	ATP	C5-C6	2.57	1.48	1.41
3	D	5101	ATP	C5-C6	2.55	1.48	1.41
3	H	5101	ATP	C5-C6	2.55	1.48	1.41
3	B	5101	ATP	C5-N7	-2.44	1.34	1.39
3	D	5101	ATP	C5-N7	-2.44	1.34	1.39
3	F	5101	ATP	C5-N7	-2.44	1.34	1.39
3	H	5101	ATP	C5-N7	-2.44	1.34	1.39
3	D	5101	ATP	C8-N7	2.19	1.35	1.31
3	H	5101	ATP	C8-N7	2.19	1.35	1.31
3	B	5101	ATP	C8-N7	2.19	1.35	1.31
3	F	5101	ATP	C8-N7	2.17	1.35	1.31

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5101	ATP	C5-C4-N3	-6.31	118.03	126.72
3	B	5101	ATP	C5-C4-N3	-6.30	118.04	126.72
3	D	5101	ATP	C5-C4-N3	-6.30	118.04	126.72
3	H	5101	ATP	C5-C4-N3	-6.30	118.04	126.72
3	D	5101	ATP	N3-C4-N9	5.08	135.80	127.17
3	B	5101	ATP	N3-C4-N9	5.07	135.79	127.17
3	H	5101	ATP	N3-C4-N9	5.07	135.79	127.17
3	F	5101	ATP	N3-C4-N9	5.05	135.76	127.17
3	D	5101	ATP	C2-N3-C4	4.07	121.78	111.83
3	H	5101	ATP	C2-N3-C4	4.07	121.78	111.83
3	B	5101	ATP	C2-N3-C4	4.07	121.77	111.83
3	F	5101	ATP	C2-N3-C4	4.05	121.72	111.83
3	D	5101	ATP	N3-C2-N1	-3.44	123.37	128.58
3	H	5101	ATP	N3-C2-N1	-3.44	123.37	128.58
3	B	5101	ATP	N3-C2-N1	-3.41	123.41	128.58
3	F	5101	ATP	N3-C2-N1	-3.38	123.47	128.58
3	F	5101	ATP	C4-C5-N7	-3.35	106.75	110.58
3	D	5101	ATP	C4-C5-N7	-3.35	106.75	110.58
3	H	5101	ATP	C4-C5-N7	-3.35	106.75	110.58
3	B	5101	ATP	C4-C5-N7	-3.33	106.78	110.58
3	B	5101	ATP	C2'-C1'-N9	-3.21	105.32	113.30
3	F	5101	ATP	C2'-C1'-N9	-3.21	105.32	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	5101	ATP	C2'-C1'-N9	-3.21	105.32	113.30
3	D	5101	ATP	C2'-C1'-N9	-3.21	105.33	113.30
3	B	5101	ATP	C3'-C2'-C1'	3.08	107.29	101.46
3	H	5101	ATP	C3'-C2'-C1'	3.08	107.29	101.46
3	F	5101	ATP	C3'-C2'-C1'	3.08	107.28	101.46
3	D	5101	ATP	C3'-C2'-C1'	3.07	107.27	101.46
3	H	5101	ATP	C4-N9-C8	2.72	108.59	105.74
3	D	5101	ATP	C4-N9-C8	2.70	108.58	105.74
3	B	5101	ATP	C4-N9-C8	2.70	108.58	105.74
3	F	5101	ATP	C4-N9-C8	2.67	108.54	105.74
3	D	5101	ATP	C5-N7-C8	2.59	107.52	103.45
3	H	5101	ATP	C5-N7-C8	2.59	107.52	103.45
3	F	5101	ATP	C5-N7-C8	2.57	107.50	103.45
3	B	5101	ATP	C5-N7-C8	2.56	107.48	103.45
3	F	5101	ATP	C6-C5-N7	2.19	136.32	132.09
3	D	5101	ATP	C6-C5-N7	2.19	136.30	132.09
3	H	5101	ATP	C6-C5-N7	2.19	136.30	132.09
3	B	5101	ATP	C6-C5-N7	2.17	136.28	132.09
3	F	5101	ATP	O4'-C1'-N9	2.11	112.14	108.09
3	H	5101	ATP	O4'-C1'-N9	2.11	112.14	108.09
3	H	5101	ATP	N9-C8-N7	-2.10	110.96	113.94
3	B	5101	ATP	O4'-C1'-N9	2.09	112.10	108.09
3	D	5101	ATP	N9-C8-N7	-2.08	110.98	113.94
3	B	5101	ATP	N9-C8-N7	-2.07	111.00	113.94
3	D	5101	ATP	O4'-C1'-N9	2.06	112.05	108.09
3	F	5101	ATP	N9-C8-N7	-2.06	111.01	113.94

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	D	5101	ATP	C5'-O5'-PA-O2A
3	D	5101	ATP	C5'-O5'-PA-O3A
3	F	5101	ATP	C5'-O5'-PA-O2A
3	F	5101	ATP	C5'-O5'-PA-O3A
3	H	5101	ATP	C5'-O5'-PA-O2A
3	H	5101	ATP	C5'-O5'-PA-O3A
3	B	5101	ATP	O4'-C4'-C5'-O5'
3	B	5101	ATP	C3'-C4'-C5'-O5'
3	D	5101	ATP	O4'-C4'-C5'-O5'

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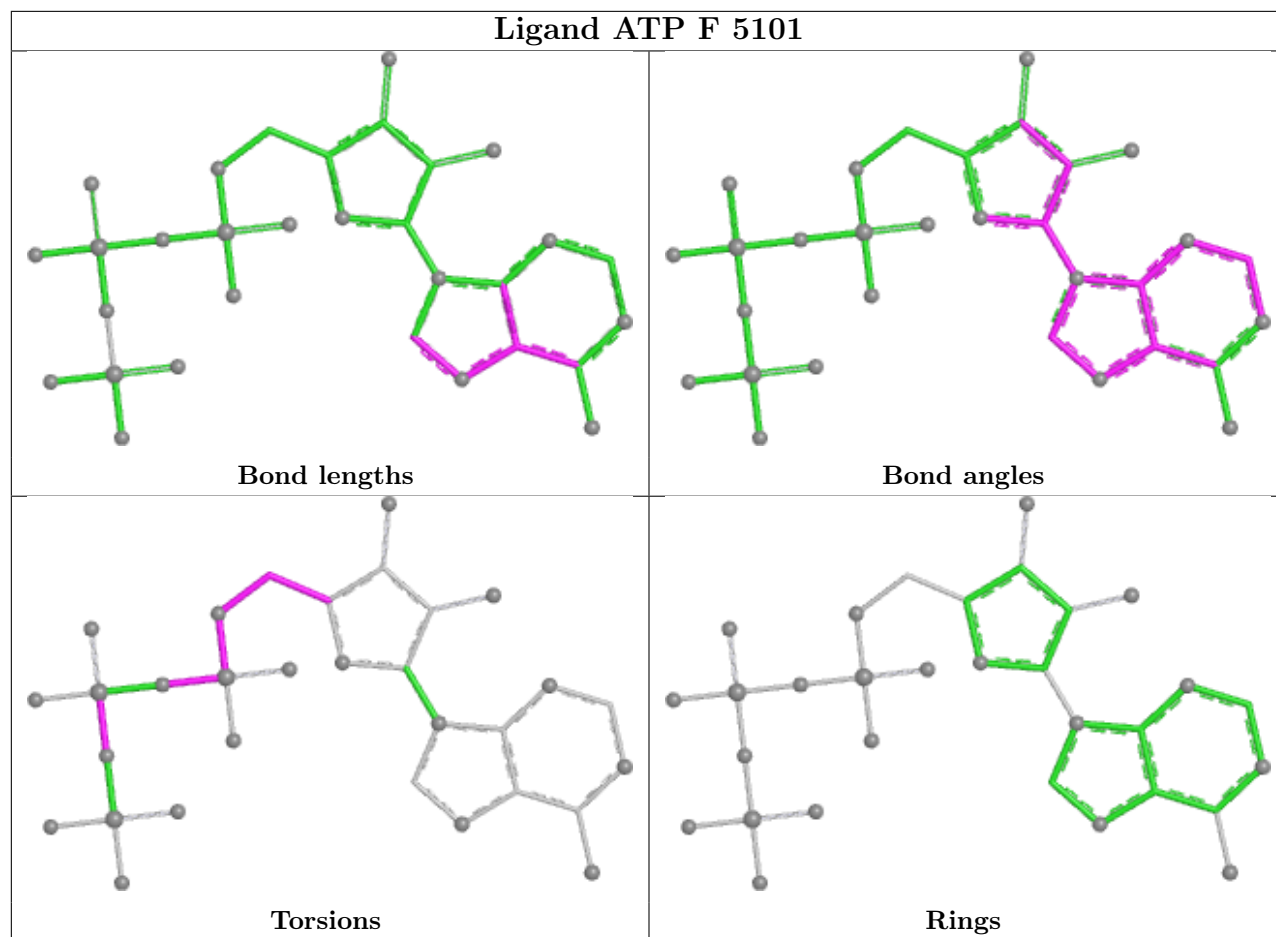
Mol	Chain	Res	Type	Atoms
3	D	5101	ATP	C3'-C4'-C5'-O5'
3	F	5101	ATP	O4'-C4'-C5'-O5'
3	F	5101	ATP	C3'-C4'-C5'-O5'
3	H	5101	ATP	O4'-C4'-C5'-O5'
3	H	5101	ATP	C3'-C4'-C5'-O5'
3	B	5101	ATP	PB-O3A-PA-O5'
3	D	5101	ATP	PB-O3A-PA-O5'
3	F	5101	ATP	PB-O3A-PA-O5'
3	H	5101	ATP	PB-O3A-PA-O5'
3	B	5101	ATP	C4'-C5'-O5'-PA
3	D	5101	ATP	C4'-C5'-O5'-PA
3	F	5101	ATP	C4'-C5'-O5'-PA
3	H	5101	ATP	C4'-C5'-O5'-PA
3	B	5101	ATP	PG-O3B-PB-O1B
3	D	5101	ATP	PG-O3B-PB-O1B
3	F	5101	ATP	PG-O3B-PB-O1B
3	H	5101	ATP	PG-O3B-PB-O1B

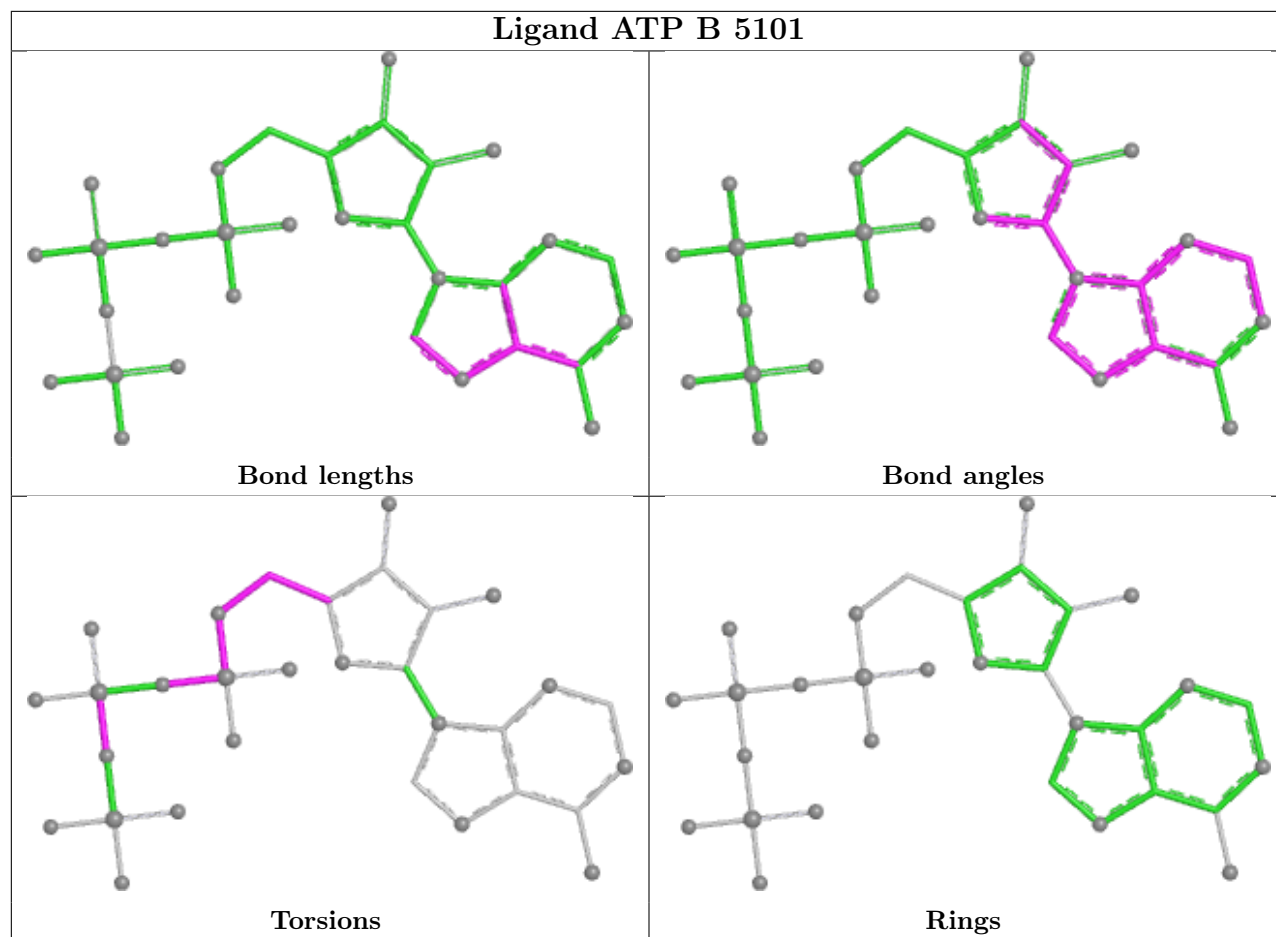
There are no ring outliers.

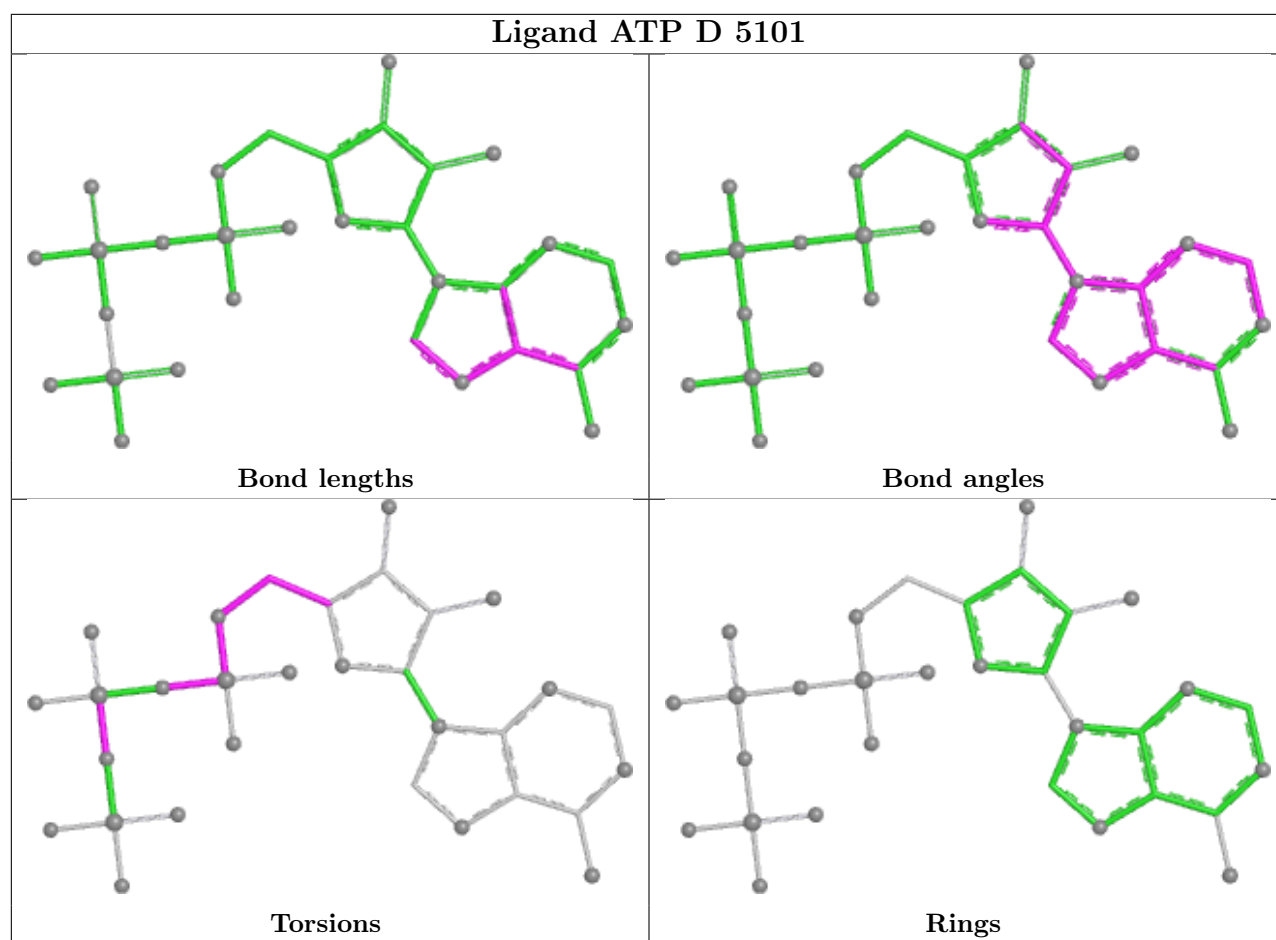
4 monomers are involved in 8 short contacts:

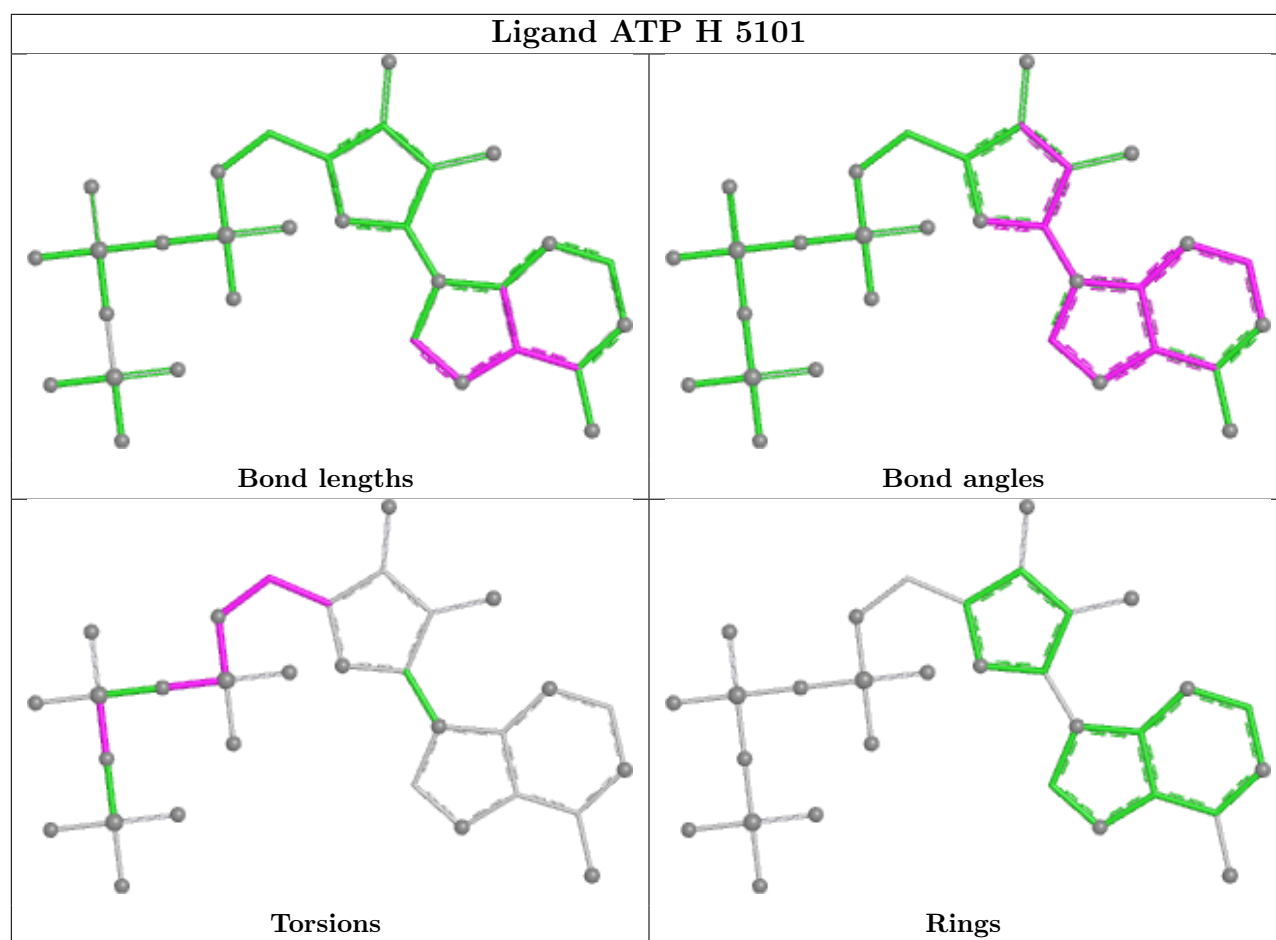
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	5101	ATP	2	0
3	B	5101	ATP	2	0
3	D	5101	ATP	2	0
3	H	5101	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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.

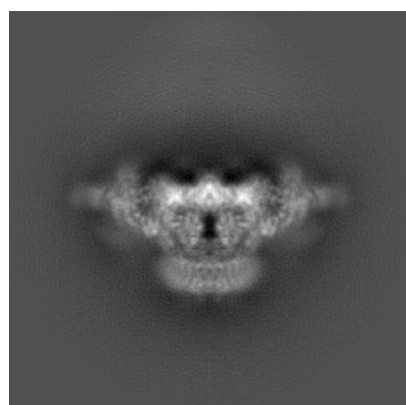
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9825. These allow visual inspection of the internal detail of the map and identification of artifacts.

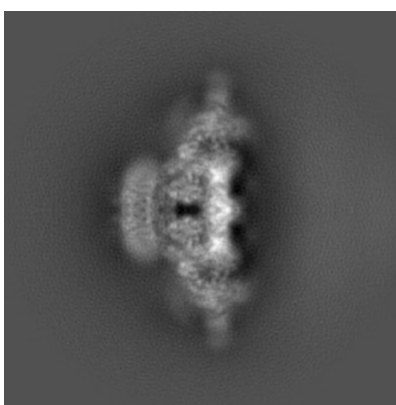
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

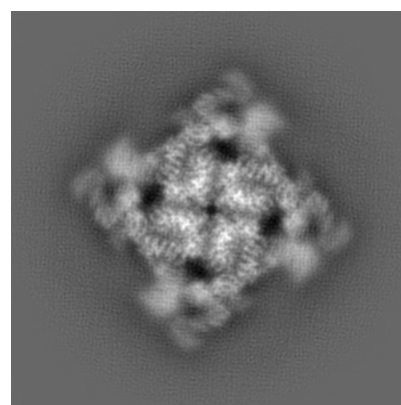
6.1.1 Primary map



X



Y

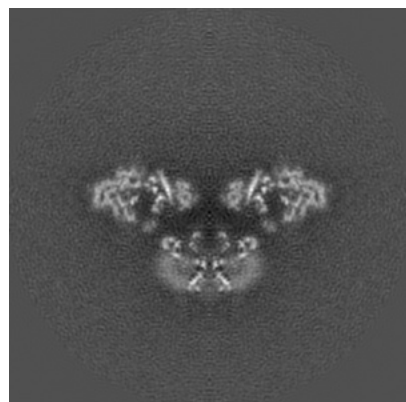


Z

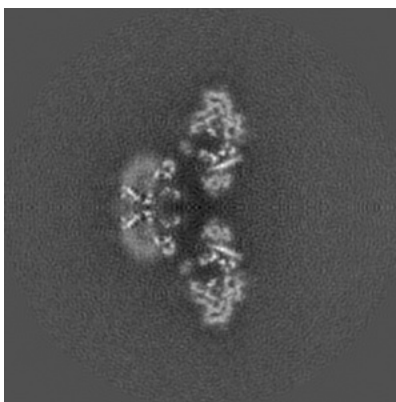
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

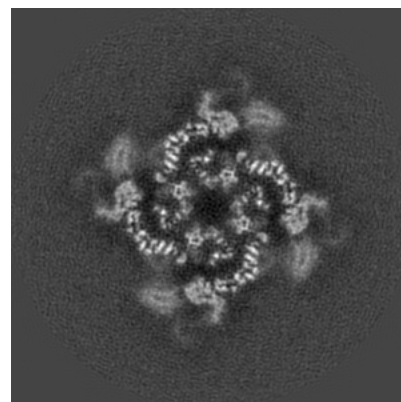
6.2.1 Primary map



X Index: 200



Y Index: 200

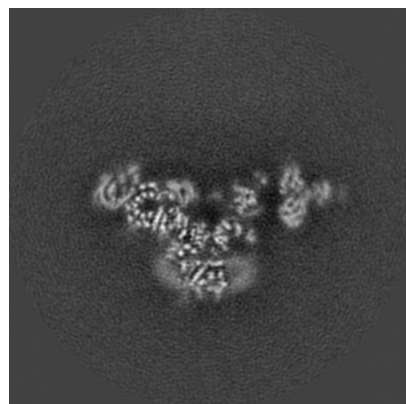


Z Index: 200

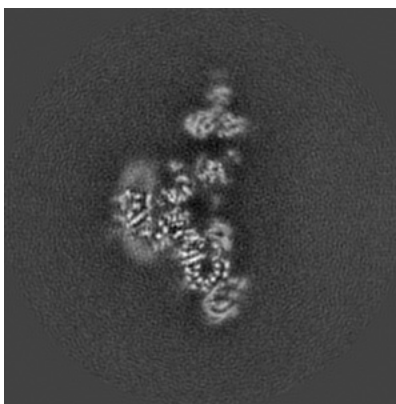
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

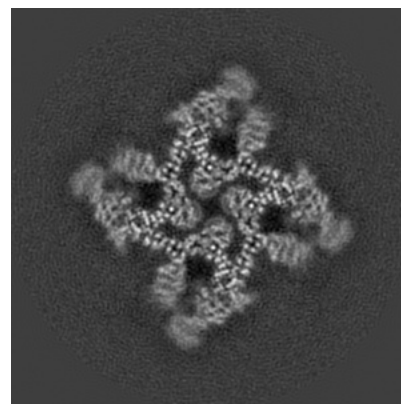
6.3.1 Primary map



X Index: 211



Y Index: 189

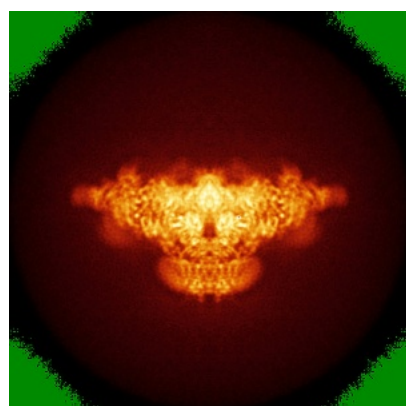


Z Index: 212

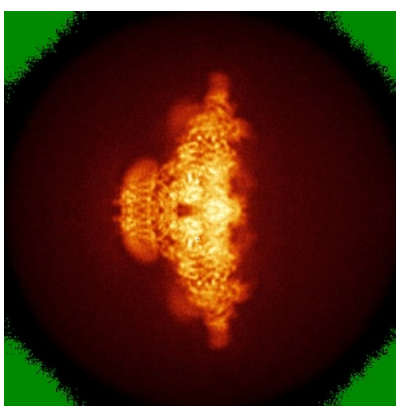
The images above show the largest variance slices of the map in three orthogonal directions.

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

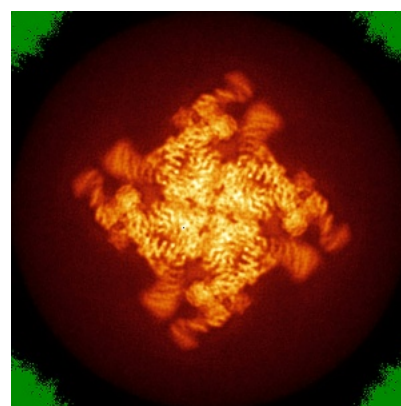
6.4.1 Primary map



X



Y

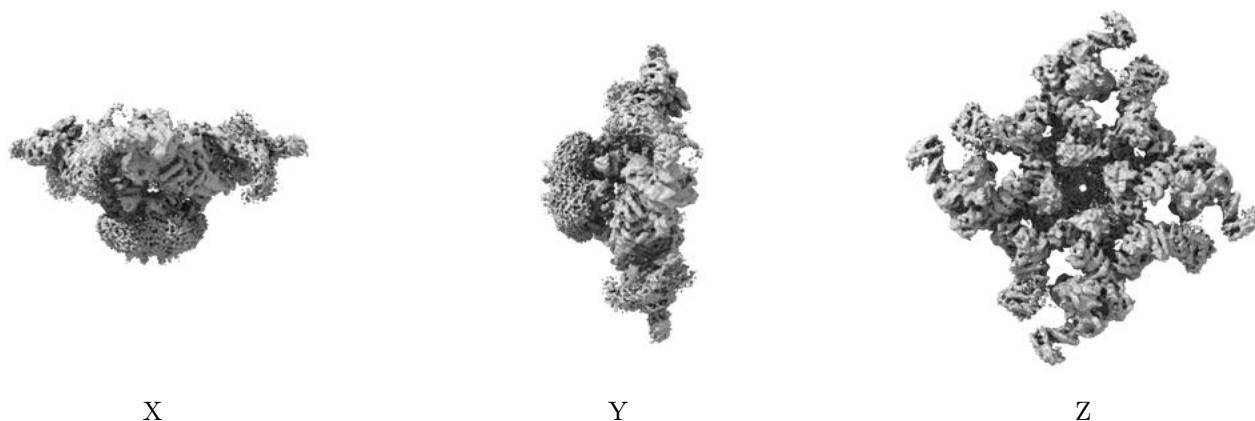


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

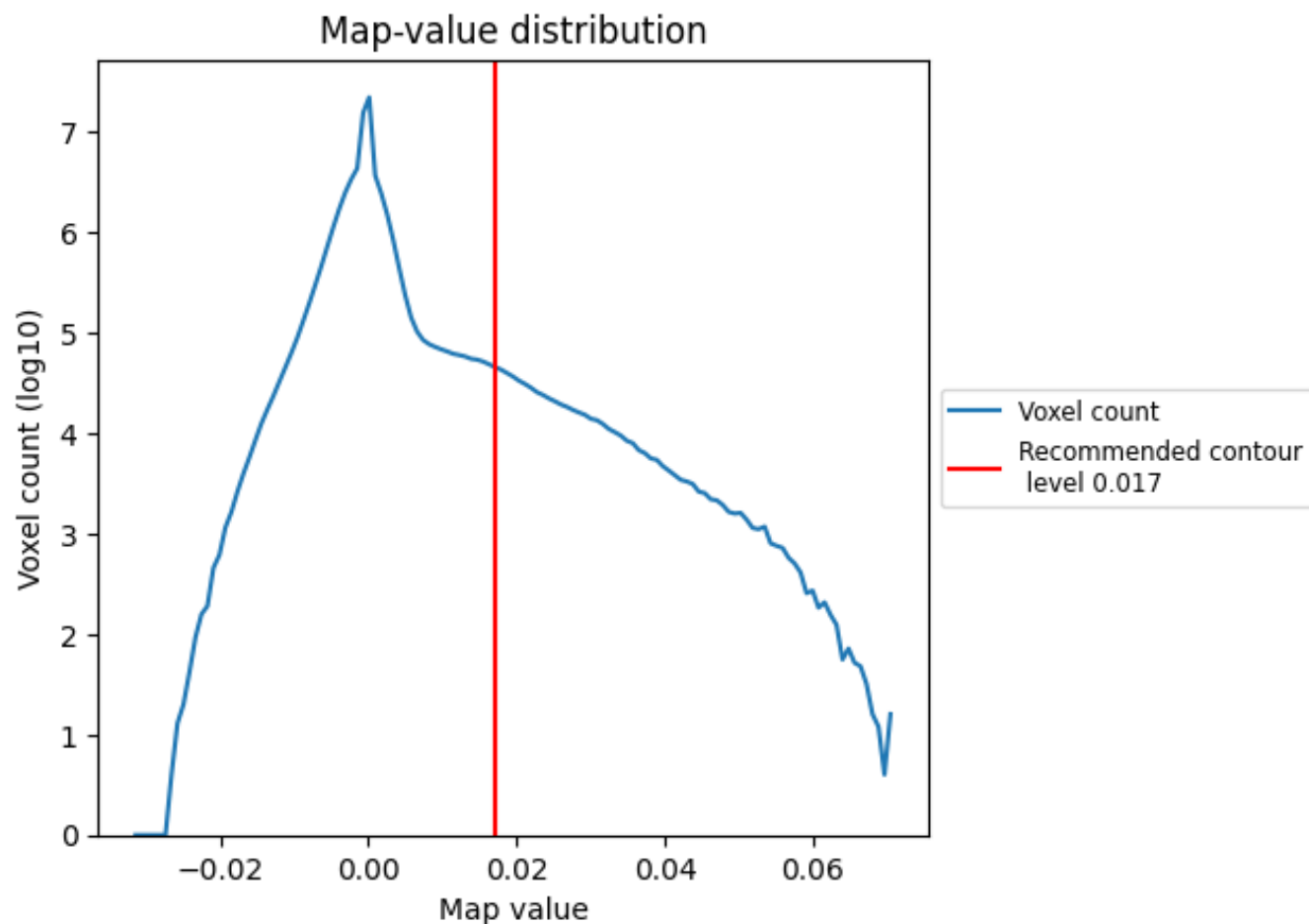
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

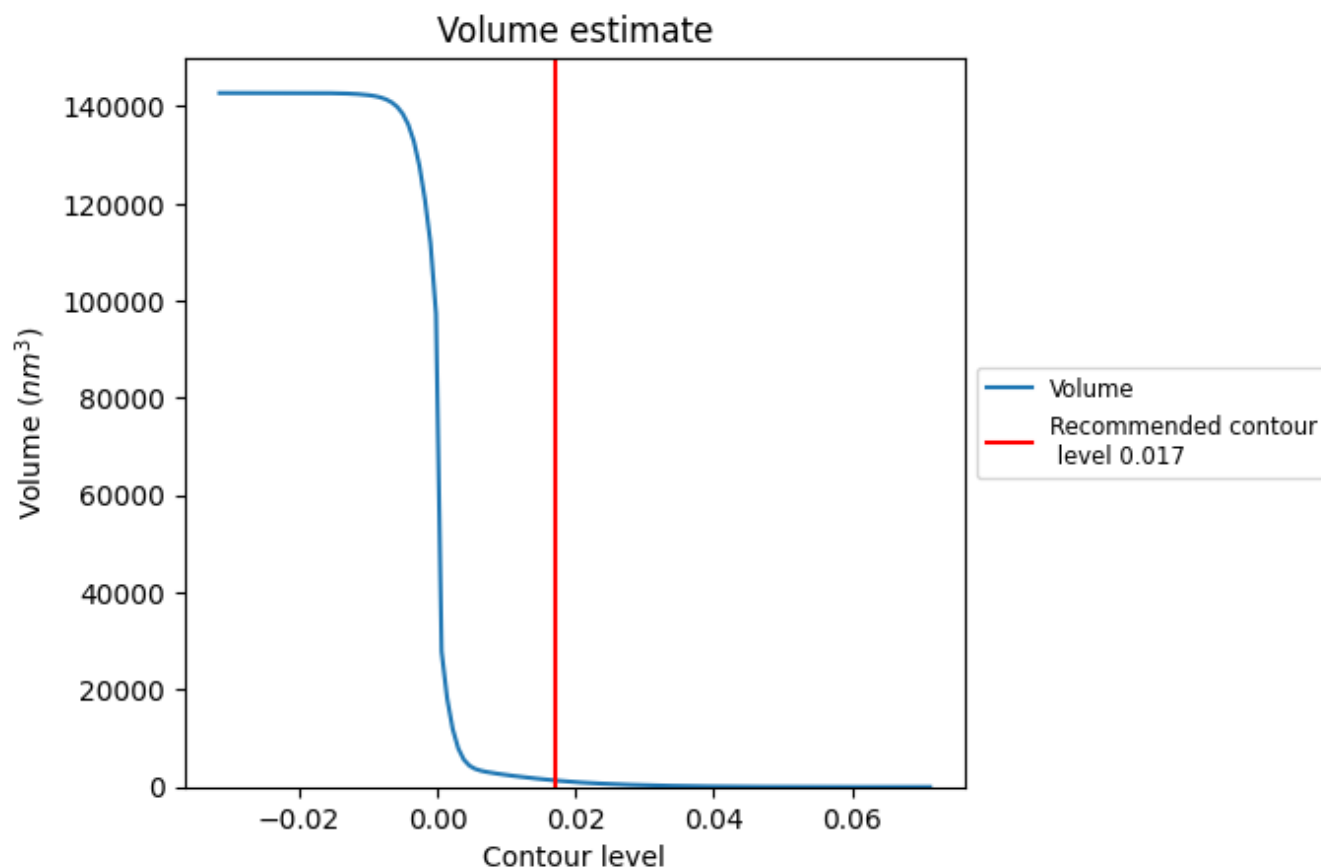
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

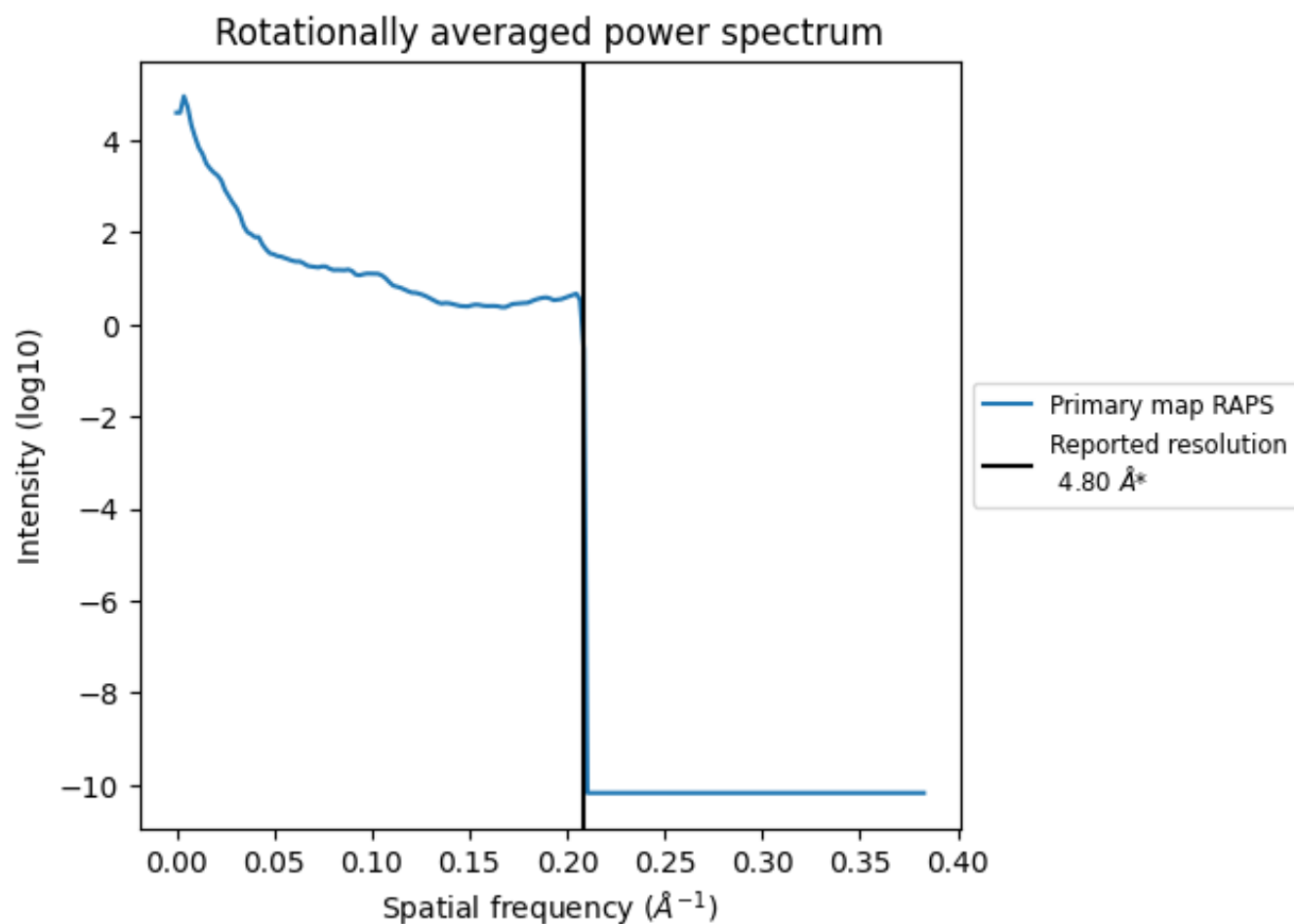
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1350 nm^3 ; this corresponds to an approximate mass of 1219 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 ⓘ

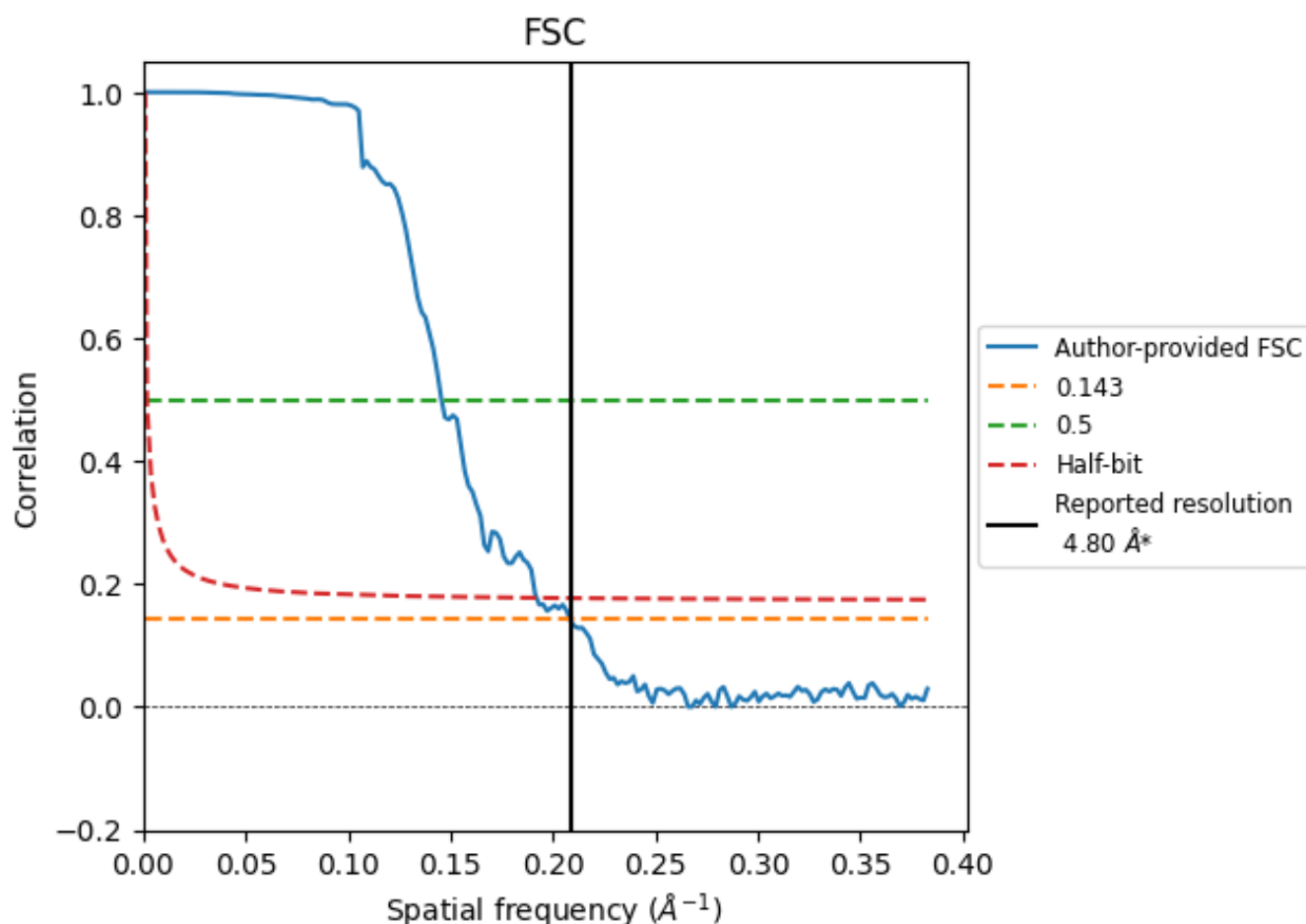


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

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 0.208 Å⁻¹

8.2 Resolution estimates [i](#)

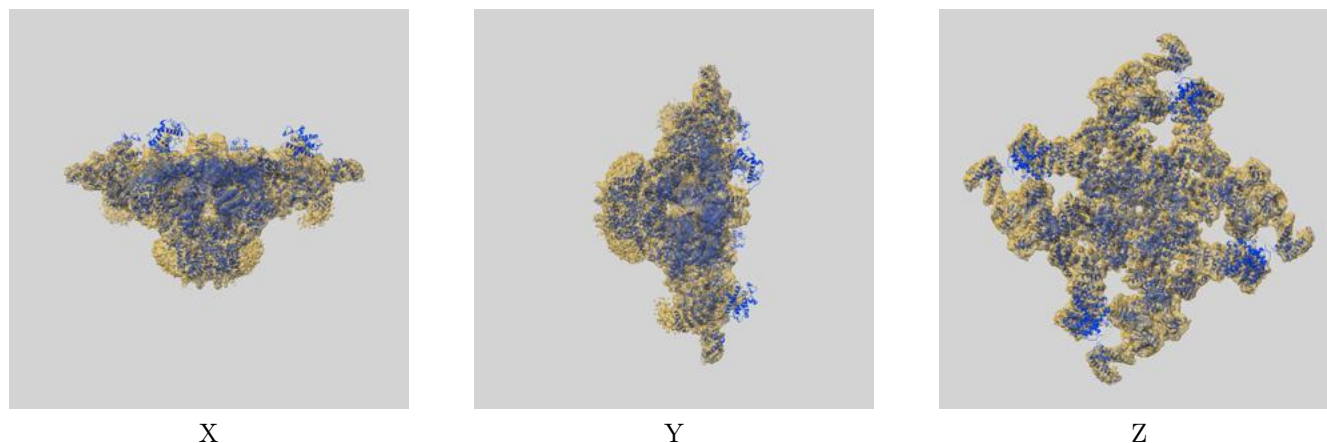
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.81	6.87	5.21
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

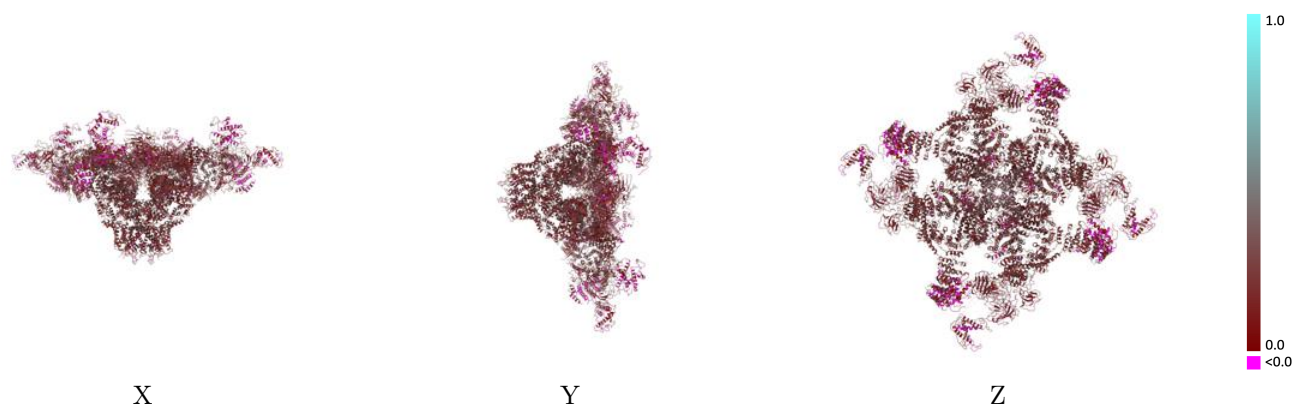
This section contains information regarding the fit between EMDB map EMD-9825 and PDB model 6JH6. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



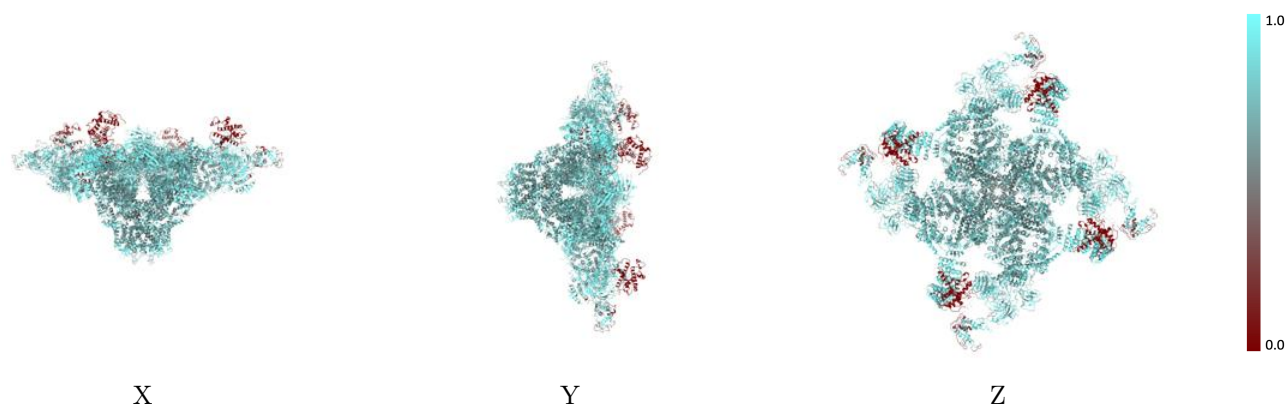
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



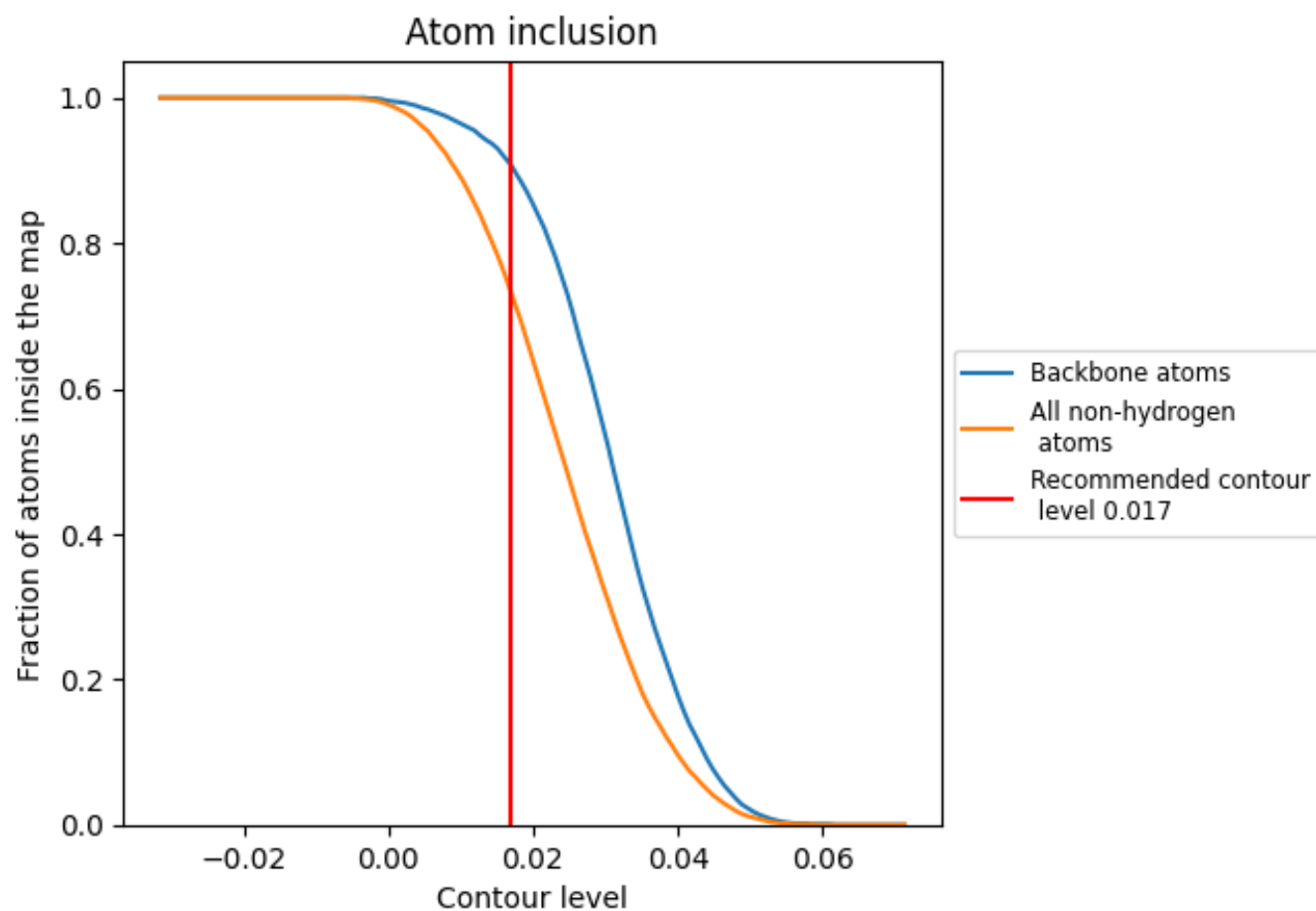
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 73% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7310	0.2220
A	0.7920	0.2290
B	0.7300	0.2220
C	0.7920	0.2300
D	0.7290	0.2220
E	0.7880	0.2300
F	0.7290	0.2220
G	0.7890	0.2260
H	0.7290	0.2210

