



Full wwPDB EM Validation Report ⓘ

Feb 24, 2025 – 05:03 PM JST

PDB ID : 8X4E
EMDB ID : EMD-38048
Title : Cryo-EM structure of Ryanodine receptor 1 (TM helix S0, 5 mM Ca2+)
Authors : Chen, Q.; Hu, H.
Deposited on : 2023-11-15
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

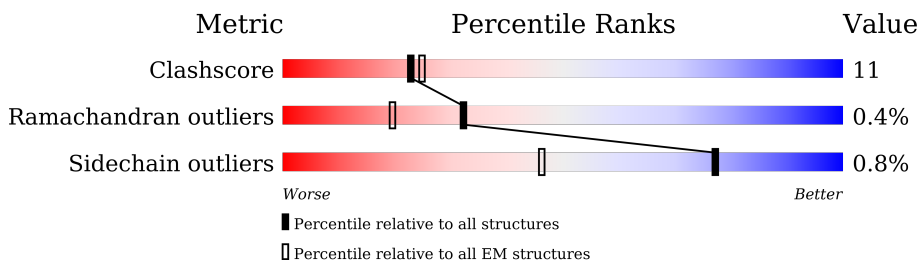
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	5037	
1	B	5037	
1	C	5037	
1	D	5037	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 118280 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3982	Total	C	N	O	S	0	0
			29568	18816	5133	5431	188		
1	B	3982	Total	C	N	O	S	0	0
			29568	18816	5133	5431	188		
1	C	3982	Total	C	N	O	S	0	0
			29568	18816	5133	5431	188		
1	D	3982	Total	C	N	O	S	0	0
			29568	18816	5133	5431	188		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

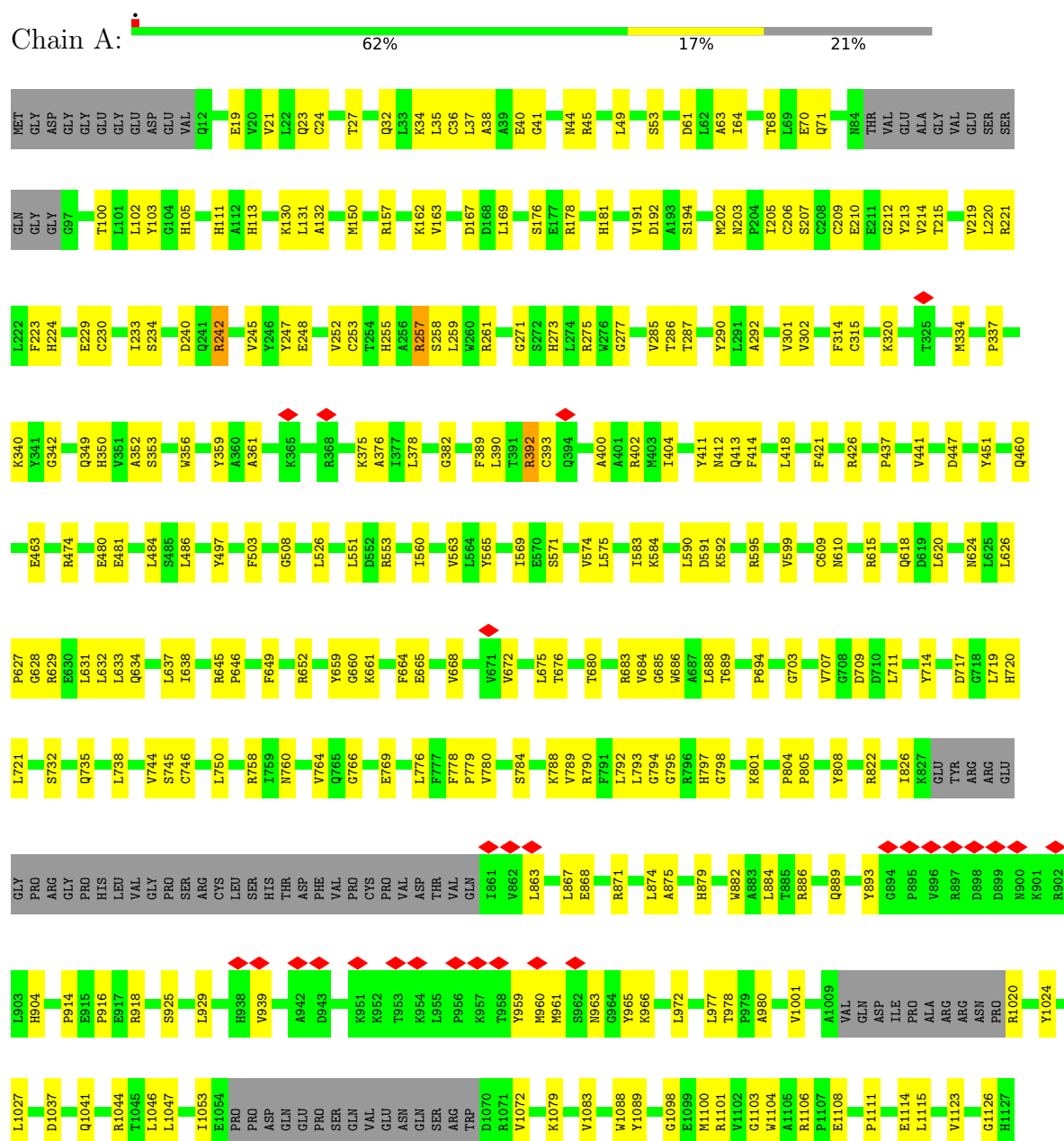
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	
3	B	1	Total	Ca	0
			1	1	
3	C	1	Total	Ca	0
			1	1	
3	D	1	Total	Ca	0
			1	1	

3 Residue-property plots

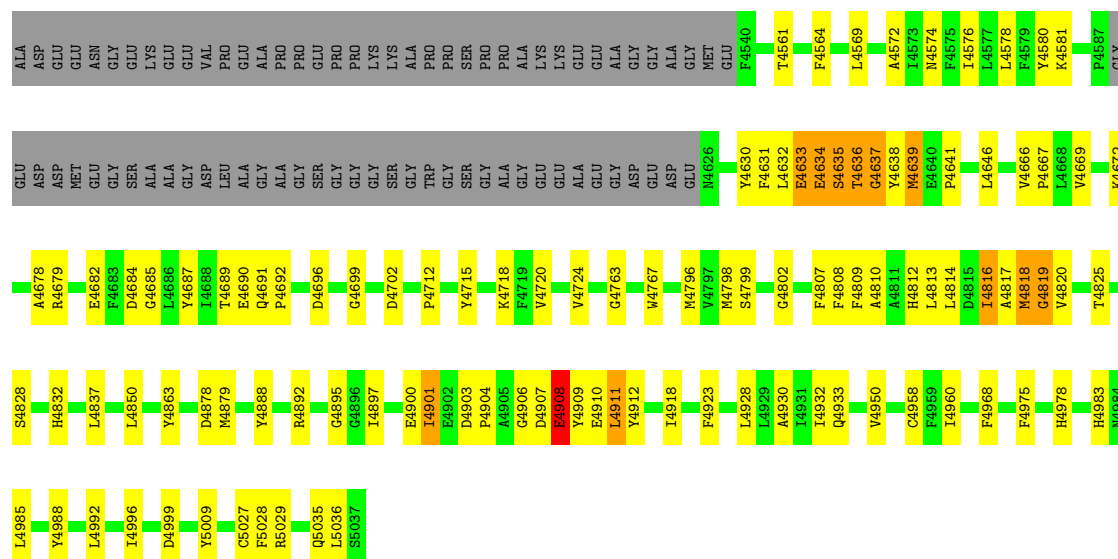
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ryanodine receptor 1



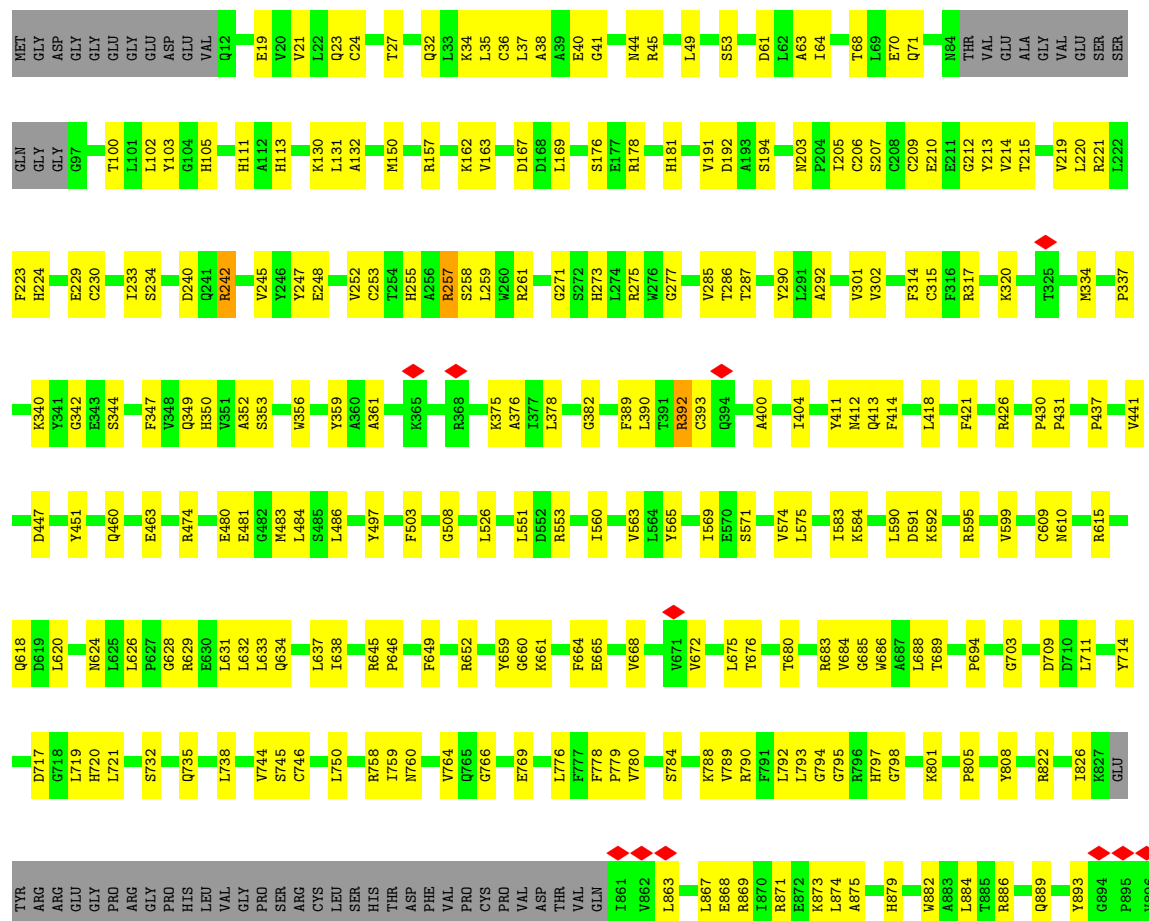






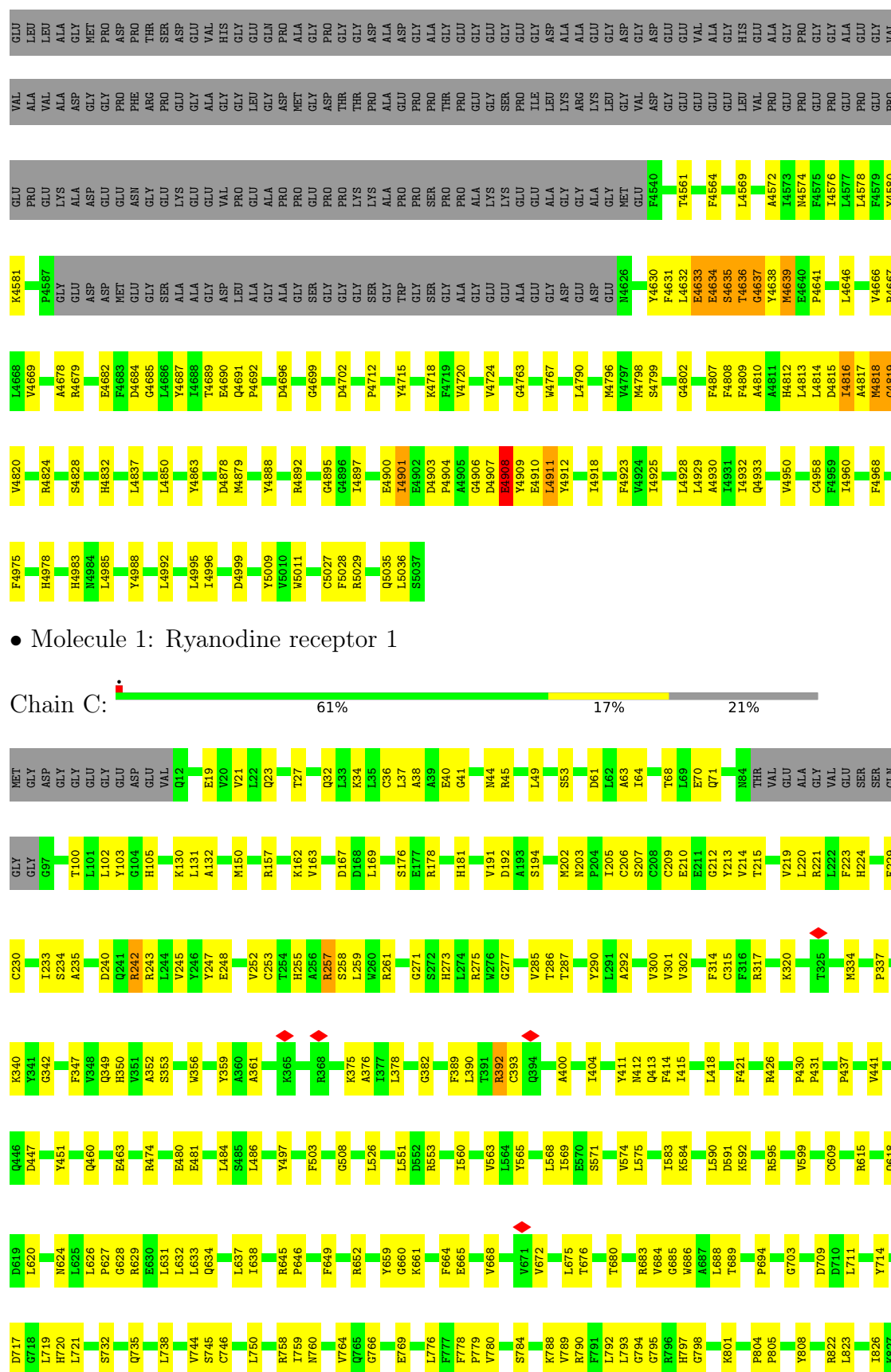
• Molecule 1: Ryanodine receptor 1

Chain B: 61% 17% 21%



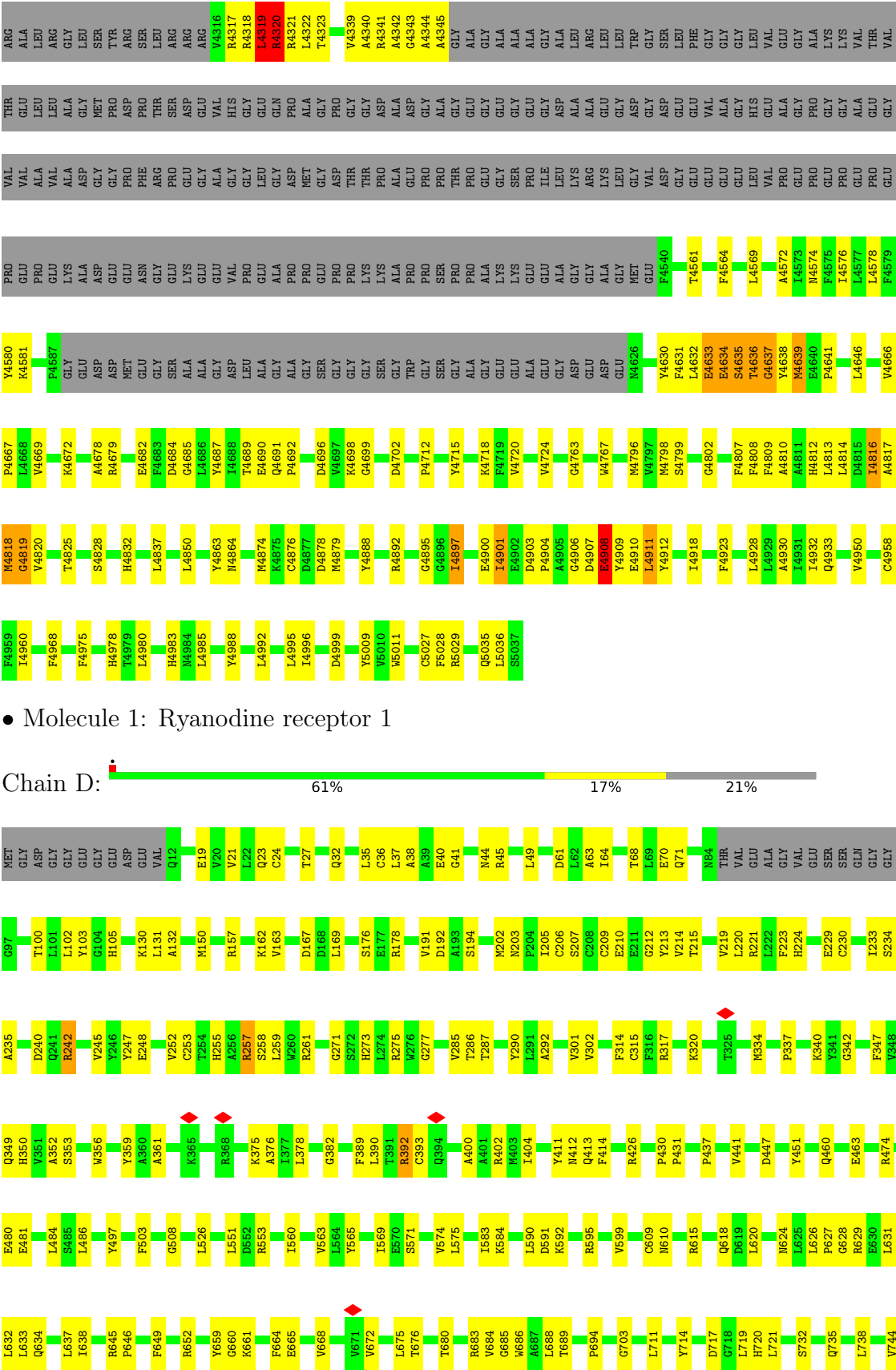








F4219	E4227	A4228	E4229	D4240	I4247	E4253	PRO	GLU	GLY	GLU	PRO	GLU	ALA	ASP	GLU	ASP	GLY	GLY	GLU	PRO	GLU	ALA	ALA	GLY	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY	GLU	GLY
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L2166	G1832	G1677	R1584	V1483	GLN	GLY	P1263	D1147	L1047	S925	PRO	S745
I2167	S1833	R1680	C1591	H1484	PRO	TRP	H1254	V1148	G1048	L929	SER	C746
V2168	E1835	R1680	C1591	K1488	ALA	GLY	Y1255	C1151	I1053	L750	ARG	L750
E2174	F1836	H1683	R1594	K1488	THR	ALA	R1259	C1151	E1054	H938	LEU	R758
E2175	F1838	L1694	L1600	C1492	ALA	GLY	C1269	M1152	PRO	V939	HIS	I759
S2181	V1839	E1699	M1601	V1495	LEU	GLY	C1269	D1154	ASP	A942	THR	N760
I2182	P1840	E1699	P1602	V1496	PRO	LYS	H1274	L1155	GLN	D943	ASP	V764
I2185	V1841	G1705	M1605	G1497	ARG	GLY	L1287	M1158	PRO	R951	VAL	Q765
H2184	V1859	L1706	S1606	V1501	LEU	THR	L1293	I1161	SER	R951	PRO	G766
L2197	K1860	L1707	R1607	S1502	HIS	ALA	P1294	R952	GLN	R952	CYS	E769
L2197	K1862	R1708	M1608	P1503	ASP	LYS	P1295	M1165	VAL	T953	PRO	L776
V2207	I1863	Y1712	P1609	G1507	VAL	GLY	Q1296	R954	ASN	R954	VAL	F777
V2210	K1864	L1715	M1615	R1508	PRO	THR	Q1297	D1172	GLN	L955	THR	F778
L2215	M1865	L1716	GLY	V1515	ALA	GLY	HIS	E1176	ARG	P956	VAL	P779
L2215	E1867	S1717	THR	V1515	GLY	GLY	GLN	T1177	TRP	R957	GLN	V780
T2220	E1868	M1730	ARG	C1518	THR	THR	PHE	R1180	D1070	T958	I861	
V2229	E1869	G1765	ALA	L1526	ASP	PRO	ARG	R1180	R1071	Y959	V862	
I2223	V1870	G1766	GLY	L1526	ASP	GLN	CYS	E1183	V1072	M960	L863	
P2226	F1871	P1750	E1822	N1532	PRO	THR	THR	K1079	K1079	R961	L867	
K2227	E1874	G1755	GLY	G1533	ILE	VAL	GLY	F1188	N963	S962	E868	
N2228	GLU	G1755	THR	L1534	ILE	GLY	ALA	L1189	N963	N963	V789	
V2229	GLU	G1765	ARG	E1535	LEU	GLY	ALA	P1190	G964	N963	R790	
C2240	GLU	G1766	ALA	S1536	LEU	GLN	THR	Y965	Y965	N963	F791	
S2243	GLU	S1770	E1633	T1538	VAL	VAL	ALA	G1195	W1088	K966	L792	
N2246	GLU	R1772	M1637	F1540	ARG	ARG	PRO	Q1198	G1098	L972	L874	
Q2247	GLU	ALA	A1638	Q1541	GLY	ALA	PRO	G1205	E1099	L977	A875	
C2240	GLU	ALA	L1639	V1542	GLY	GLY	GLY	G1205	M1100	L977	H879	
D2252	GLU	ALA	L1639	E1543	GLY	ASN	GLY	V1208	R1101	T978	G798	
S2279	GLU	ALA	E1643	P1544	ASP	GLY	GLN	V1208	V1102	P979	K801	
E2296	ASP	E1793	E1643	P1544	ASP	LYS	PRO	R1212	G1103	A980	L884	
V2289	GLU	A1796	C1647	V1554	ALA	ASP	PRO	A1215	A1105	V1001	T885	
S2300	GLU	R1797	M1648	L1555	THR	ALA	ALA	A1215	R1106	A1009	R886	
L2302	GLU	P1800	D1649	P1556	THR	THR	ASP	G1218	P1107	VAL	Q889	
L2302	LYS	P1800	L1651	F1564	GLY	GLY	ALA	L1219	E1108	GLN	Y893	
K2316	GLU	E1806	E1652	GLY	LEU	LYS	ALA	Q1220	P1111	ASP	G894	
G2317	GLU	R1808	L1653	LEU	LEU	LYS	ALA	E1221	P1111	ILE	P895	
Y2318	ASP	K1810	S1654	GLY	LYS	LYS	ALA	G1222	E1114	PRO	V896	
V2323	GLU	M1814	E1655	LYS	LYS	ARG	GLY	F1223	L1115	ALA	R897	
N2324	PRO	A1826	D1658	GLN	GLY	GLY	PRO	E1224	V1123	ARG	D898	
P2325	GLU	A1826	L1659	LYS	PHE	ASP	ASP	T1228	V1123	ASN	D899	
Y2331	GLU	P1829	Q1660	ASN	LEU	LEU	PRO	N1229	G1126	PRO	N900	
L2332	ASP	A1675	M1573	ILE	PHE	PHE	TYR	H1127	R1020	R1020	GLY	
L2332	ALA	L1676	P1574	LYS	LYS	LYS	TYR	R1128	Y1024	Y1024	PRO	
			L1575	LYS	LYS	LYS	ASN	F1139	L1027	L1027	ARG	
			A1578	LYS	LYS	LYS	LEU	G1140	P1037	P1037	GLY	
			M1579	ALA	ALA	ALA	ARG	R1141	D1041	D1041	HIS	
			F1580	MET	ALA	ALA	SER	P1142	Q1041	Q1041	LEU	
						THR	GLY	H1262	R1044	R1044	VAL	
									T1045	T1045	GLY	
									L1046	L1046		



C4958	H4812	L4646	L4577	GLU	VAL	ALA	R4192
F4969	L4813		L4578	PRO	THR	ALA	F4193
I4960	L4814	V4666	F4579	GLU	VAL	ALA	Y4194
	D4815	P4667	Y4580	PRO	THR	ARG	
F4968	I4816	L4668	K4581	VAL	GLU	ALA	F4219
A4817		V4669		PRO	ALA	LEU	
M4818			F4587	VAL	LEU	ARG	E4227
G4819	V4520	K4672	GLY	LYS	ALA	GLY	A4228
			GLU	ALA	ALA	LEU	E4229
H4978			GLU	ASP	GLY	SER	
		A4678	ASP	GLY	MET	TYR	D4240
H4983	T4325	R4679	GLU	PRO	ASP	ARG	
N4984		K4680	GLU	PRO	ASP	ARG	T4247
L4985	S4328	L4681	GLY	PHE	THR	LEU	
		E4682	GLY	ARG	THR	ARG	E4253
Y4988	H4832	F4683	SER	PRO	SER	ARG	PRO
		D4684	GLU	GLY	ASP	ARG	
L4992	L4837	G4685	ALA	GLY	GLU	ARG	GLY
M4993		L4686	ALA	GLY	VAL	GLY	GLU
Y4994	L4850	Y4687	ASP	VAL	HIS	R4317	PRO
L4995		T4688	LEU	PRO	GLY	R4318	ALA
I4996	Y4863	T4689	ALA	GLU	LEU	R4319	ALA
	D4878	E4690	GLY	ALA	GLN	R4320	ASP
D4999	M4879	Q4691	ALA	PRO	ASP	R4321	GLY
		P4692	GLY	PRO	MET	L4322	ASP
Y5009			SER	GLY	GLY	T4323	GLY
V5010	Y4888	D4696	GLY	PRO	ASP		GLU
W5011		V4697	GLY	THR	THR	V4339	GLY
	R4892	K4698	GLY	PRO	THR	A4340	MET
C5027		G4699	SER	LYS	GLY	R4341	GLY
F5028	G4895		GLY	ALA	ALA	A4342	GLY
R5029	G4896	D4702	TRP	PRO	GLU	G4343	ALA
	I4897		GLY	PRO	GLY	A4344	ALA
		P4712	SER	SER	ALA	A4345	ALA
	E4900		GLY	PRO	GLY		GLY
	I4901	Y4715	ALA	PRO	GLU	ALA	GLY
E4902			GLY	PRO	GLY	ALA	ALA
D4903		K4718	GLU	LYS	GLY	ALA	GLU
P4904		F4719	GLU	LYS	GLY	ALA	GLU
A4905		V4720	ALA	GLU	PRO	GLY	GLY
G4906			GLU	GLU	GLY	ALA	ALA
D4907	V4724		GLY	ALA	ASP	ALA	ALA
		V4724	ASP	GLY	LYS	LEU	GLY
E4908		G4763	GLY	GLY	ARG	ALA	ALA
Y4909			ASP	ALA	LYS	LEU	GLU
E4910			GLU	GLY	LEU	LEU	GLY
L4911		W4767	GLU	GLY	GLY	TRP	ALA
Y4912			F4526	MET	VAL	GLY	ALA
	L4790			GLU	GLY	THR	VAL
I4918		M4796	Y4630	F4540	GLY	LEU	ALA
		V4797	F4631		GLY	SER	ALA
F4923			L4632	T4561	GLY	PHE	ALA
		M4798	E4633		GLY	GLY	ALA
L4928			E4634	F4564	VAL	GLY	ALA
L4929		S4799	S4635		GLY	GLY	GLY
A4930			T4636	L4569	GLY	LEU	ALA
I4931		G4802	Q4637		HIS	LEU	ALA
			Y4638		VAL	GLU	THR
I4932		F4807	M4639	A4572	ALA	GLU	ALA
Q4933		F4808	E4640	I4573	GLY	GLY	ARG
		F4809		M4574	PRO	ALA	LEU
		A4810	P4641	F4575	GLY	LYS	ALA
	V4950			I4576	PRO	GLY	ALA
		A4811				LYS	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	279704	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	3.162	Depositor
Minimum map value	-1.419	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.182	Depositor
Map size (\AA)	643.2, 643.2, 643.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.072, 1.072, 1.072	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.32	0/30188	0.46	0/41084
1	B	0.32	0/30188	0.46	0/41084
1	C	0.32	0/30188	0.46	0/41084
1	D	0.32	0/30188	0.46	0/41084
All	All	0.32	0/120752	0.46	0/164336

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29568	0	27784	634	0
1	B	29568	0	27784	641	0
1	C	29568	0	27784	643	0
1	D	29568	0	27784	647	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	118280	0	111136	2512	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 11.

All (2512) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4634:GLU:HG3	1:B:4636:THR:HG22	1.46	0.97
1:C:4634:GLU:HG3	1:C:4636:THR:HG22	1.46	0.97
1:A:4634:GLU:HG3	1:A:4636:THR:HG22	1.46	0.94
1:D:4634:GLU:HG3	1:D:4636:THR:HG22	1.46	0.94
1:D:4069:LYS:HB2	1:D:4133:GLN:HE22	1.41	0.85
1:B:4069:LYS:HB2	1:B:4133:GLN:HE22	1.41	0.84
1:A:4069:LYS:HB2	1:A:4133:GLN:HE22	1.41	0.84
1:C:4069:LYS:HB2	1:C:4133:GLN:HE22	1.41	0.83
1:D:3051:ARG:HH22	1:D:3182:TYR:HB2	1.44	0.83
1:A:3051:ARG:HH22	1:A:3182:TYR:HB2	1.44	0.82
1:C:3051:ARG:HH22	1:C:3182:TYR:HB2	1.44	0.82
1:A:1492:CYS:H	1:A:1540:PHE:HE1	1.27	0.82
1:A:3285:TRP:HE1	1:A:3293:PRO:HG3	1.44	0.82
1:B:3285:TRP:HE1	1:B:3293:PRO:HG3	1.44	0.81
1:A:1501:VAL:HG12	1:A:1503:PRO:HD3	1.62	0.81
1:D:1492:CYS:H	1:D:1540:PHE:HE1	1.27	0.81
1:B:1501:VAL:HG12	1:B:1503:PRO:HD3	1.62	0.81
1:B:3051:ARG:HH22	1:B:3182:TYR:HB2	1.44	0.81
1:C:1501:VAL:HG12	1:C:1503:PRO:HD3	1.62	0.81
1:D:3285:TRP:HE1	1:D:3293:PRO:HG3	1.44	0.80
1:C:3285:TRP:HE1	1:C:3293:PRO:HG3	1.44	0.80
1:C:1492:CYS:H	1:C:1540:PHE:HE1	1.27	0.80
1:D:1501:VAL:HG12	1:D:1503:PRO:HD3	1.62	0.80
1:B:4679:ARG:NH1	1:B:4715:TYR:OH	2.15	0.80
1:C:4679:ARG:NH1	1:C:4715:TYR:OH	2.15	0.80
1:B:1492:CYS:H	1:B:1540:PHE:HE1	1.27	0.79
1:D:4679:ARG:NH1	1:D:4715:TYR:OH	2.15	0.79
1:A:4679:ARG:NH1	1:A:4715:TYR:OH	2.15	0.78
1:A:745:SER:HB2	1:A:758:ARG:HB2	1.66	0.78
1:B:745:SER:HB2	1:B:758:ARG:HB2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3990:VAL:HG23	1:D:4051:SER:HB3	1.67	0.77
1:A:3990:VAL:HG23	1:A:4051:SER:HB3	1.67	0.77
1:C:745:SER:HB2	1:C:758:ARG:HB2	1.66	0.77
1:C:4344:ALA:HB3	1:C:4564:PHE:CD2	2.20	0.77
1:C:3990:VAL:HG23	1:C:4051:SER:HB3	1.67	0.77
1:D:745:SER:HB2	1:D:758:ARG:HB2	1.66	0.77
1:C:626:LEU:HG	1:C:628:GLY:H	1.50	0.76
1:D:4344:ALA:HB3	1:D:4564:PHE:CD2	2.20	0.76
1:A:4581:LYS:HD2	1:A:4632:LEU:HD22	1.67	0.76
1:B:3990:VAL:HG23	1:B:4051:SER:HB3	1.67	0.76
1:B:4344:ALA:HB3	1:B:4564:PHE:CD2	2.20	0.76
1:A:626:LEU:HG	1:A:628:GLY:H	1.50	0.76
1:A:4344:ALA:HB3	1:A:4564:PHE:CD2	2.20	0.76
1:C:4340:ALA:C	1:C:4342:ALA:H	1.89	0.76
1:B:626:LEU:HG	1:B:628:GLY:H	1.50	0.76
1:D:626:LEU:HG	1:D:628:GLY:H	1.50	0.76
1:C:4581:LYS:HD2	1:C:4632:LEU:HD22	1.67	0.75
1:C:4345:ALA:CB	1:C:4561:THR:HG22	2.17	0.75
1:A:760:ASN:O	1:A:801:LYS:NZ	2.20	0.75
1:B:4581:LYS:HD2	1:B:4632:LEU:HD22	1.67	0.75
1:D:4340:ALA:C	1:D:4342:ALA:H	1.89	0.75
1:B:4345:ALA:CB	1:B:4561:THR:HG22	2.17	0.74
1:A:4345:ALA:CB	1:A:4561:THR:HG22	2.17	0.74
1:C:760:ASN:O	1:C:801:LYS:NZ	2.20	0.74
1:D:4581:LYS:HD2	1:D:4632:LEU:HD22	1.67	0.74
1:D:4345:ALA:CB	1:D:4561:THR:HG22	2.17	0.74
1:C:1208:VAL:O	1:D:3577:ARG:NH2	2.21	0.74
1:A:1208:VAL:O	1:B:3577:ARG:NH2	2.21	0.74
1:B:760:ASN:O	1:B:801:LYS:NZ	2.20	0.74
1:D:760:ASN:O	1:D:801:LYS:NZ	2.20	0.74
1:A:3577:ARG:NH2	1:D:1208:VAL:O	2.21	0.74
1:A:4340:ALA:C	1:A:4342:ALA:H	1.89	0.73
1:B:100:THR:HG21	1:B:162:LYS:HE3	1.69	0.73
1:B:1208:VAL:O	1:C:3577:ARG:NH2	2.21	0.73
1:A:1835:GLU:O	1:A:1837:GLN:N	2.21	0.73
1:C:1147:ASP:OD1	1:C:1165:ASN:ND2	2.22	0.73
1:B:1835:GLU:O	1:B:1837:GLN:N	2.21	0.73
1:B:4340:ALA:C	1:B:4342:ALA:H	1.89	0.73
1:D:1839:VAL:HB	1:D:1840:PRO:HD3	1.70	0.73
1:B:1839:VAL:HB	1:B:1840:PRO:HD3	1.70	0.73
1:C:1835:GLU:O	1:C:1837:GLN:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:THR:HG21	1:C:162:LYS:HE3	1.69	0.72
1:A:1147:ASP:OD1	1:A:1165:ASN:ND2	2.22	0.72
1:A:3733:CYS:HG	1:A:3803:SER:HG	1.36	0.72
1:A:100:THR:HG21	1:A:162:LYS:HE3	1.69	0.72
1:B:1834:VAL:O	1:B:1837:GLN:HB3	1.90	0.72
1:C:1834:VAL:O	1:C:1837:GLN:HB3	1.90	0.72
1:D:315:CYS:SG	1:D:349:GLN:NE2	2.62	0.72
1:D:100:THR:HG21	1:D:162:LYS:HE3	1.69	0.72
1:D:1147:ASP:OD1	1:D:1165:ASN:ND2	2.22	0.72
1:D:1835:GLU:O	1:D:1837:GLN:N	2.21	0.72
1:A:1834:VAL:O	1:A:1837:GLN:HB3	1.90	0.72
1:D:4635:SER:C	1:D:4637:GLY:N	2.41	0.72
1:A:315:CYS:SG	1:A:349:GLN:NE2	2.62	0.72
1:B:315:CYS:SG	1:B:349:GLN:NE2	2.62	0.72
1:B:1147:ASP:OD1	1:B:1165:ASN:ND2	2.22	0.72
1:B:3733:CYS:HG	1:B:3803:SER:HG	1.36	0.72
1:C:315:CYS:SG	1:C:349:GLN:NE2	2.62	0.72
1:C:1839:VAL:HB	1:C:1840:PRO:HD3	1.70	0.72
1:A:1839:VAL:HB	1:A:1840:PRO:HD3	1.70	0.71
1:D:4958:CYS:SG	1:D:4978:HIS:CD2	2.82	0.71
1:A:3891:LEU:HB3	1:A:3899:PHE:HE2	1.56	0.71
1:B:3891:LEU:HB3	1:B:3899:PHE:HE2	1.56	0.71
1:C:3891:LEU:HB3	1:C:3899:PHE:HE2	1.56	0.71
1:A:1578:ALA:O	1:A:1584:ARG:NH2	2.24	0.71
1:D:2644:LEU:HG	1:D:2645:THR:HG23	1.73	0.71
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.72	0.71
1:B:1578:ALA:O	1:B:1584:ARG:NH2	2.24	0.71
1:C:683:ARG:HB3	1:C:717:ASP:HB3	1.73	0.70
1:D:3891:LEU:HB3	1:D:3899:PHE:HE2	1.56	0.70
1:A:2644:LEU:HG	1:A:2645:THR:HG23	1.73	0.70
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.72	0.70
1:D:1834:VAL:O	1:D:1837:GLN:HB3	1.90	0.70
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.72	0.70
1:C:1578:ALA:O	1:C:1584:ARG:NH2	2.24	0.70
1:C:2644:LEU:HG	1:C:2645:THR:HG23	1.73	0.70
1:C:4958:CYS:SG	1:C:4978:HIS:CD2	2.82	0.70
1:D:1578:ALA:O	1:D:1584:ARG:NH2	2.24	0.70
1:D:3817:LEU:HD13	1:D:3899:PHE:HD1	1.57	0.70
1:A:3817:LEU:HD13	1:A:3899:PHE:HD1	1.57	0.70
1:C:3817:LEU:HD13	1:C:3899:PHE:HD1	1.57	0.70
1:D:683:ARG:HB3	1:D:717:ASP:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:ASP:O	1:A:1041:GLN:NE2	2.25	0.70
1:D:1037:ASP:O	1:D:1041:GLN:NE2	2.25	0.70
1:B:1453:VAL:HG23	1:B:1454:THR:H	1.58	0.69
1:B:3817:LEU:HD13	1:B:3899:PHE:HD1	1.57	0.69
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.72	0.69
1:C:4635:SER:C	1:C:4637:GLY:N	2.41	0.69
1:A:4635:SER:C	1:A:4637:GLY:N	2.41	0.69
1:B:1037:ASP:O	1:B:1041:GLN:NE2	2.25	0.69
1:A:683:ARG:HB3	1:A:717:ASP:HB3	1.73	0.69
1:B:36:CYS:SG	1:B:37:LEU:N	2.65	0.69
1:C:1037:ASP:O	1:C:1041:GLN:NE2	2.25	0.69
1:D:36:CYS:SG	1:D:37:LEU:N	2.65	0.69
1:D:794:GLY:H	1:D:798:GLY:HA3	1.57	0.69
1:B:683:ARG:HB3	1:B:717:ASP:HB3	1.73	0.69
1:C:1453:VAL:HG23	1:C:1454:THR:H	1.58	0.69
1:A:36:CYS:SG	1:A:37:LEU:N	2.65	0.69
1:D:4344:ALA:HB3	1:D:4564:PHE:HD2	1.57	0.69
1:B:2644:LEU:HG	1:B:2645:THR:HG23	1.73	0.68
1:A:638:ILE:HG21	1:A:703:GLY:HA3	1.75	0.68
1:A:794:GLY:H	1:A:798:GLY:HA3	1.57	0.68
1:C:36:CYS:SG	1:C:37:LEU:N	2.65	0.68
1:C:3733:CYS:SG	1:C:3803:SER:OG	2.52	0.68
1:D:1453:VAL:HG23	1:D:1454:THR:H	1.58	0.68
1:A:209:CYS:SG	1:A:210:GLU:N	2.67	0.68
1:A:4630:TYR:HE2	1:A:4632:LEU:HD13	1.57	0.68
1:B:638:ILE:HG21	1:B:703:GLY:HA3	1.75	0.68
1:C:794:GLY:H	1:C:798:GLY:HA3	1.57	0.68
1:A:1453:VAL:HG23	1:A:1454:THR:H	1.58	0.68
1:A:4958:CYS:SG	1:A:4978:HIS:CD2	2.82	0.68
1:C:3446:SER:HA	1:C:3449:HIS:HB3	1.76	0.68
1:C:4344:ALA:HB3	1:C:4564:PHE:HD2	1.57	0.68
1:D:209:CYS:SG	1:D:210:GLU:N	2.67	0.68
1:A:4344:ALA:HB3	1:A:4564:PHE:HD2	1.57	0.68
1:B:794:GLY:H	1:B:798:GLY:HA3	1.57	0.68
1:B:4863:TYR:HA	1:B:4901:ILE:HD11	1.75	0.68
1:B:4344:ALA:HB3	1:B:4564:PHE:HD2	1.57	0.68
1:D:3733:CYS:SG	1:D:3803:SER:OG	2.52	0.68
1:C:4630:TYR:HE2	1:C:4632:LEU:HD13	1.57	0.68
1:D:4345:ALA:HB2	1:D:4561:THR:HG22	1.76	0.68
1:D:4630:TYR:HE2	1:D:4632:LEU:HD13	1.57	0.68
1:A:4863:TYR:HA	1:A:4901:ILE:HD11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2102:VAL:HG13	1:D:2120:MET:HG2	1.76	0.67
1:B:4635:SER:C	1:B:4637:GLY:N	2.41	0.67
1:B:4152:GLU:OE1	1:B:4194:TYR:OH	2.12	0.67
1:D:3446:SER:HA	1:D:3449:HIS:HB3	1.76	0.67
1:A:2495:VAL:HG22	1:A:2497:ASP:H	1.59	0.67
1:B:2495:VAL:HG22	1:B:2497:ASP:H	1.59	0.67
1:C:2021:CYS:SG	1:C:2028:ARG:NH1	2.68	0.67
1:A:2131:LEU:HB2	1:A:3662:ILE:HG12	1.77	0.67
1:A:4345:ALA:HB2	1:A:4561:THR:HG22	1.76	0.67
1:D:638:ILE:HG21	1:D:703:GLY:HA3	1.75	0.67
1:D:2021:CYS:SG	1:D:2028:ARG:NH1	2.68	0.67
1:B:3446:SER:HA	1:B:3449:HIS:HB3	1.76	0.67
1:D:2131:LEU:HB2	1:D:3662:ILE:HG12	1.77	0.67
1:D:2495:VAL:HG22	1:D:2497:ASP:H	1.59	0.67
1:D:4863:TYR:HA	1:D:4901:ILE:HD11	1.75	0.67
1:B:209:CYS:SG	1:B:210:GLU:N	2.67	0.67
1:C:209:CYS:SG	1:C:210:GLU:N	2.67	0.67
1:C:4863:TYR:HA	1:C:4901:ILE:HD11	1.75	0.67
1:A:2102:VAL:HG13	1:A:2120:MET:HG2	1.76	0.67
1:A:4152:GLU:OE1	1:A:4194:TYR:OH	2.12	0.67
1:C:2131:LEU:HB2	1:C:3662:ILE:HG12	1.77	0.67
1:D:3552:PHE:O	1:D:3555:ASN:ND2	2.28	0.67
1:A:27:THR:HG22	1:A:32:GLN:HA	1.77	0.67
1:B:2131:LEU:HB2	1:B:3662:ILE:HG12	1.77	0.67
1:B:3733:CYS:SG	1:B:3803:SER:OG	2.52	0.67
1:B:4630:TYR:HE2	1:B:4632:LEU:HD13	1.57	0.67
1:A:3733:CYS:SG	1:A:3803:SER:OG	2.52	0.66
1:B:2021:CYS:SG	1:B:2028:ARG:NH1	2.68	0.66
1:C:273:HIS:O	1:C:275:ARG:NH2	2.28	0.66
1:C:632:LEU:O	1:C:634:GLN:NE2	2.28	0.66
1:C:2102:VAL:HG13	1:C:2120:MET:HG2	1.76	0.66
1:A:273:HIS:O	1:A:275:ARG:NH2	2.28	0.66
1:A:2456:ILE:HD11	1:D:176:SER:HA	1.78	0.66
1:B:3552:PHE:O	1:B:3555:ASN:ND2	2.28	0.66
1:B:4345:ALA:HB2	1:B:4561:THR:HG22	1.76	0.66
1:C:3552:PHE:O	1:C:3555:ASN:ND2	2.28	0.66
1:C:4152:GLU:OE1	1:C:4194:TYR:OH	2.12	0.66
1:C:638:ILE:HG21	1:C:703:GLY:HA3	1.75	0.66
1:C:4345:ALA:HB2	1:C:4561:THR:HG22	1.76	0.66
1:D:4807:PHE:O	1:D:4809:PHE:N	2.29	0.66
1:A:4933:GLN:HG2	1:D:4930:ALA:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4958:CYS:SG	1:B:4978:HIS:CD2	2.82	0.66
1:A:2021:CYS:SG	1:A:2028:ARG:NH1	2.68	0.66
1:B:27:THR:HG22	1:B:32:GLN:HA	1.77	0.66
1:C:2495:VAL:HG22	1:C:2497:ASP:H	1.59	0.66
1:A:2570:ALA:O	1:A:2574:HIS:ND1	2.29	0.66
1:B:273:HIS:O	1:B:275:ARG:NH2	2.28	0.66
1:B:2102:VAL:HG13	1:B:2120:MET:HG2	1.76	0.66
1:B:2570:ALA:O	1:B:2574:HIS:ND1	2.29	0.66
1:C:176:SER:HA	1:D:2456:ILE:HD11	1.78	0.66
1:C:27:THR:HG22	1:C:32:GLN:HA	1.77	0.66
1:B:4807:PHE:O	1:B:4809:PHE:N	2.29	0.66
1:D:632:LEU:O	1:D:634:GLN:NE2	2.28	0.66
1:B:4930:ALA:HB2	1:C:4933:GLN:HG2	1.77	0.66
1:C:652:ARG:NH1	1:C:750:LEU:O	2.29	0.66
1:C:4807:PHE:O	1:C:4809:PHE:N	2.29	0.66
1:D:4152:GLU:OE1	1:D:4194:TYR:OH	2.12	0.66
1:A:3552:PHE:O	1:A:3555:ASN:ND2	2.28	0.65
1:A:176:SER:HA	1:B:2456:ILE:HD11	1.78	0.65
1:A:392:ARG:NH1	1:A:393:CYS:O	2.29	0.65
1:A:660:GLY:HA3	1:A:750:LEU:HD13	1.77	0.65
1:A:3446:SER:HA	1:A:3449:HIS:HB3	1.76	0.65
1:B:652:ARG:NH1	1:B:750:LEU:O	2.29	0.65
1:B:1215:ALA:HA	1:B:1219:LEU:HB3	1.78	0.65
1:C:1772:ARG:NH2	1:C:1952:GLN:OE1	2.29	0.65
1:D:27:THR:HG22	1:D:32:GLN:HA	1.77	0.65
1:D:660:GLY:HA3	1:D:750:LEU:HD13	1.77	0.65
1:B:660:GLY:HA3	1:B:750:LEU:HD13	1.77	0.65
1:D:652:ARG:NH1	1:D:750:LEU:O	2.29	0.65
1:A:652:ARG:NH1	1:A:750:LEU:O	2.29	0.65
1:A:4807:PHE:O	1:A:4809:PHE:N	2.29	0.65
1:C:392:ARG:NH1	1:C:393:CYS:O	2.29	0.65
1:A:4930:ALA:HB2	1:B:4933:GLN:HG2	1.77	0.65
1:A:2651:CYS:HA	1:A:2695:LEU:HB2	1.78	0.65
1:B:615:ARG:NH2	1:B:1677:GLY:O	2.30	0.65
1:A:632:LEU:O	1:A:634:GLN:NE2	2.28	0.65
1:B:176:SER:HA	1:C:2456:ILE:HD11	1.78	0.65
1:C:4930:ALA:HB2	1:D:4933:GLN:HG2	1.77	0.65
1:C:2182:ILE:HD13	1:C:2185:ILE:HD11	1.79	0.65
1:D:392:ARG:NH1	1:D:393:CYS:O	2.29	0.65
1:A:615:ARG:NH2	1:A:1677:GLY:O	2.30	0.65
1:B:2651:CYS:HA	1:B:2695:LEU:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1215:ALA:HA	1:C:1219:LEU:HB3	1.78	0.65
1:D:273:HIS:O	1:D:275:ARG:NH2	2.28	0.65
1:D:615:ARG:NH2	1:D:1677:GLY:O	2.30	0.65
1:A:1772:ARG:NH2	1:A:1952:GLN:OE1	2.29	0.65
1:B:1772:ARG:NH2	1:B:1952:GLN:OE1	2.29	0.65
1:D:2182:ILE:HD13	1:D:2185:ILE:HD11	1.79	0.65
1:B:961:MET:SD	1:B:963:ASN:ND2	2.70	0.64
1:B:2182:ILE:HD13	1:B:2185:ILE:HD11	1.79	0.64
1:C:615:ARG:NH2	1:C:1677:GLY:O	2.30	0.64
1:C:1712:TYR:OH	1:C:1814:MET:SD	2.55	0.64
1:D:1712:TYR:OH	1:D:1814:MET:SD	2.55	0.64
1:D:1772:ARG:NH2	1:D:1952:GLN:OE1	2.29	0.64
1:B:40:GLU:HB3	1:B:44:ASN:HD21	1.62	0.64
1:C:4807:PHE:C	1:C:4809:PHE:H	2.00	0.64
1:A:40:GLU:HB3	1:A:44:ASN:HD21	1.62	0.64
1:D:2570:ALA:O	1:D:2574:HIS:ND1	2.29	0.64
1:D:2651:CYS:HA	1:D:2695:LEU:HB2	1.78	0.64
1:B:4863:TYR:HA	1:B:4901:ILE:CD1	2.28	0.64
1:C:4863:TYR:HA	1:C:4901:ILE:CD1	2.28	0.64
1:D:1215:ALA:HA	1:D:1219:LEU:HB3	1.78	0.64
1:A:1215:ALA:HA	1:A:1219:LEU:HB3	1.78	0.64
1:A:4863:TYR:HA	1:A:4901:ILE:CD1	2.28	0.64
1:B:1699:GLU:OE1	1:B:1810:LYS:NZ	2.30	0.64
1:C:660:GLY:HA3	1:C:750:LEU:HD13	1.77	0.64
1:C:1699:GLU:OE1	1:C:1810:LYS:NZ	2.30	0.64
1:D:40:GLU:HB3	1:D:44:ASN:HD21	1.62	0.64
1:D:961:MET:SD	1:D:963:ASN:ND2	2.70	0.64
1:C:961:MET:SD	1:C:963:ASN:ND2	2.70	0.64
1:D:4863:TYR:HA	1:D:4901:ILE:CD1	2.28	0.64
1:A:961:MET:SD	1:A:963:ASN:ND2	2.70	0.64
1:A:4807:PHE:C	1:A:4809:PHE:H	2.00	0.64
1:B:392:ARG:NH1	1:B:393:CYS:O	2.29	0.64
1:B:4807:PHE:C	1:B:4809:PHE:H	2.00	0.64
1:A:2182:ILE:HD13	1:A:2185:ILE:HD11	1.79	0.64
1:B:1243:PRO:HB2	1:B:1600:LEU:HD21	1.80	0.64
1:D:4345:ALA:CB	1:D:4561:THR:HA	2.28	0.64
1:C:40:GLU:HB3	1:C:44:ASN:HD21	1.62	0.63
1:C:2651:CYS:HA	1:C:2695:LEU:HB2	1.78	0.63
1:C:4085:ARG:HH11	1:C:4087:LEU:HD12	1.64	0.63
1:A:1243:PRO:HB2	1:A:1600:LEU:HD21	1.80	0.63
1:B:1508:ARG:O	1:B:1537:ASN:ND2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3971:GLY:O	1:B:3973:CYS:N	2.31	0.63
1:C:1243:PRO:HB2	1:C:1600:LEU:HD21	1.80	0.63
1:D:4085:ARG:HH11	1:D:4087:LEU:HD12	1.64	0.63
1:A:4345:ALA:CB	1:A:4561:THR:HA	2.28	0.63
1:D:1508:ARG:O	1:D:1537:ASN:ND2	2.32	0.63
1:A:1712:TYR:OH	1:A:1814:MET:SD	2.55	0.63
1:B:632:LEU:O	1:B:634:GLN:NE2	2.28	0.63
1:D:1243:PRO:HB2	1:D:1600:LEU:HD21	1.80	0.63
1:D:1699:GLU:OE1	1:D:1810:LYS:NZ	2.30	0.63
1:B:4085:ARG:HH11	1:B:4087:LEU:HD12	1.64	0.63
1:D:4807:PHE:C	1:D:4809:PHE:H	2.00	0.63
1:A:3971:GLY:O	1:A:3973:CYS:N	2.31	0.63
1:A:4340:ALA:O	1:A:4343:GLY:N	2.31	0.63
1:B:686:TRP:NE1	1:B:746:CYS:SG	2.72	0.63
1:C:3971:GLY:O	1:C:3973:CYS:N	2.31	0.63
1:D:686:TRP:NE1	1:D:746:CYS:SG	2.72	0.63
1:D:719:LEU:O	1:D:720:HIS:ND1	2.31	0.63
1:D:4340:ALA:C	1:D:4342:ALA:N	2.51	0.63
1:A:719:LEU:O	1:A:720:HIS:ND1	2.31	0.63
1:B:1712:TYR:OH	1:B:1814:MET:SD	2.55	0.63
1:C:686:TRP:NE1	1:C:746:CYS:SG	2.72	0.63
1:C:4345:ALA:CB	1:C:4561:THR:HA	2.28	0.63
1:A:4085:ARG:HH11	1:A:4087:LEU:HD12	1.64	0.63
1:A:4340:ALA:C	1:A:4342:ALA:N	2.51	0.63
1:B:4340:ALA:C	1:B:4342:ALA:N	2.51	0.63
1:B:4345:ALA:CB	1:B:4561:THR:HA	2.28	0.63
1:C:4344:ALA:O	1:C:4345:ALA:C	2.37	0.63
1:D:3971:GLY:O	1:D:3973:CYS:N	2.31	0.63
1:B:719:LEU:O	1:B:720:HIS:ND1	2.31	0.63
1:D:1439:VAL:HG21	1:D:1543:GLU:HG3	1.81	0.63
1:D:4817:ALA:C	1:D:4819:GLY:H	2.02	0.63
1:A:1508:ARG:O	1:A:1537:ASN:ND2	2.32	0.62
1:B:3426:GLU:O	1:B:3430:ASN:N	2.27	0.62
1:C:4817:ALA:C	1:C:4819:GLY:H	2.02	0.62
1:D:871:ARG:HH22	1:D:918:ARG:HH12	1.47	0.62
1:A:686:TRP:NE1	1:A:746:CYS:SG	2.72	0.62
1:A:871:ARG:HH22	1:A:918:ARG:HH12	1.47	0.62
1:A:1439:VAL:HG21	1:A:1543:GLU:HG3	1.81	0.62
1:C:719:LEU:O	1:C:720:HIS:ND1	2.31	0.62
1:C:1508:ARG:O	1:C:1537:ASN:ND2	2.32	0.62
1:C:1439:VAL:HG21	1:C:1543:GLU:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:THR:HG23	1:A:784:SER:HB2	1.81	0.62
1:A:1699:GLU:OE1	1:A:1810:LYS:NZ	2.30	0.62
1:A:3891:LEU:HB3	1:A:3899:PHE:CE2	2.35	0.62
1:A:4817:ALA:C	1:A:4819:GLY:H	2.02	0.62
1:B:1219:LEU:HG	1:B:1220:GLN:HG3	1.82	0.62
1:D:3657:TYR:HB3	1:D:3661:TRP:HE1	1.65	0.62
1:B:4817:ALA:C	1:B:4819:GLY:H	2.02	0.62
1:C:680:THR:HG23	1:C:784:SER:HB2	1.81	0.62
1:D:1730:MET:O	1:D:1772:ARG:NH1	2.33	0.62
1:A:1024:TYR:HA	1:A:1027:LEU:HB2	1.81	0.62
1:B:1024:TYR:HA	1:B:1027:LEU:HB2	1.81	0.62
1:A:1730:MET:O	1:A:1772:ARG:NH1	2.33	0.62
1:C:3657:TYR:HB3	1:C:3661:TRP:HE1	1.65	0.62
1:D:1024:TYR:HA	1:D:1027:LEU:HB2	1.81	0.62
1:D:1219:LEU:HG	1:D:1220:GLN:HG3	1.82	0.62
1:A:3657:TYR:HB3	1:A:3661:TRP:HE1	1.65	0.61
1:B:1439:VAL:HG21	1:B:1543:GLU:HG3	1.81	0.61
1:B:1973:GLN:OE1	1:B:1976:ARG:NH2	2.33	0.61
1:D:4340:ALA:O	1:D:4343:GLY:N	2.31	0.61
1:B:1730:MET:O	1:B:1772:ARG:NH1	2.33	0.61
1:B:3657:TYR:HB3	1:B:3661:TRP:HE1	1.65	0.61
1:C:4340:ALA:C	1:C:4342:ALA:N	2.51	0.61
1:C:4340:ALA:O	1:C:4343:GLY:N	2.31	0.61
1:C:1219:LEU:HG	1:C:1220:GLN:HG3	1.82	0.61
1:C:1973:GLN:OE1	1:C:1976:ARG:NH2	2.33	0.61
1:C:2012:PHE:HD2	1:C:2022:PRO:HD3	1.65	0.61
1:C:2570:ALA:O	1:C:2574:HIS:ND1	2.29	0.61
1:C:3891:LEU:HB3	1:C:3899:PHE:CE2	2.35	0.61
1:B:4636:THR:C	1:B:4638:TYR:H	2.04	0.61
1:D:939:VAL:HA	1:D:1053:ILE:HD12	1.83	0.61
1:A:939:VAL:HA	1:A:1053:ILE:HD12	1.83	0.61
1:A:4069:LYS:HB2	1:A:4133:GLN:NE2	2.15	0.61
1:C:871:ARG:HH22	1:C:918:ARG:HH12	1.47	0.61
1:D:680:THR:HG23	1:D:784:SER:HB2	1.81	0.61
1:A:1219:LEU:HG	1:A:1220:GLN:HG3	1.82	0.61
1:D:3768:SER:O	1:D:3773:ARG:NH1	2.29	0.61
1:D:4344:ALA:O	1:D:4345:ALA:C	2.37	0.61
1:A:1148:VAL:HG21	1:A:1212:ARG:HG3	1.83	0.61
1:A:1973:GLN:OE1	1:A:1976:ARG:NH2	2.33	0.61
1:A:3799:LYS:NZ	1:A:3883:ASP:OD2	2.33	0.61
1:C:219:VAL:HG13	1:C:285:VAL:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1730:MET:O	1:C:1772:ARG:NH1	2.33	0.61
1:C:3426:GLU:O	1:C:3430:ASN:N	2.27	0.61
1:D:1973:GLN:OE1	1:D:1976:ARG:NH2	2.33	0.61
1:D:2012:PHE:HD2	1:D:2022:PRO:HD3	1.65	0.61
1:D:3891:LEU:HB3	1:D:3899:PHE:CE2	2.35	0.61
1:B:680:THR:HG23	1:B:784:SER:HB2	1.81	0.60
1:B:871:ARG:HH22	1:B:918:ARG:HH12	1.47	0.60
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.34	0.60
1:C:4636:THR:C	1:C:4638:TYR:H	2.04	0.60
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.34	0.60
1:A:4344:ALA:O	1:A:4345:ALA:C	2.37	0.60
1:B:1148:VAL:HG21	1:B:1212:ARG:HG3	1.83	0.60
1:C:1024:TYR:HA	1:C:1027:LEU:HB2	1.81	0.60
1:D:219:VAL:HG13	1:D:285:VAL:HG21	1.83	0.60
1:A:4636:THR:C	1:A:4638:TYR:H	2.04	0.60
1:B:4345:ALA:HB1	1:B:4561:THR:HG22	1.83	0.60
1:B:3768:SER:O	1:B:3773:ARG:NH1	2.29	0.60
1:C:4069:LYS:HB2	1:C:4133:GLN:NE2	2.15	0.60
1:A:1676:LEU:HD12	1:A:2167:ILE:HD12	1.84	0.60
1:A:2012:PHE:HD2	1:A:2022:PRO:HD3	1.65	0.60
1:B:1458:HIS:NE2	1:B:1483:VAL:HG21	2.17	0.60
1:C:1458:HIS:NE2	1:C:1483:VAL:HG21	2.17	0.60
1:D:764:VAL:HG12	1:D:766:GLY:H	1.67	0.60
1:D:977:LEU:HD23	1:D:1047:LEU:HD22	1.84	0.60
1:C:977:LEU:HD23	1:C:1047:LEU:HD22	1.84	0.60
1:C:3799:LYS:NZ	1:C:3883:ASP:OD2	2.33	0.60
1:D:3799:LYS:NZ	1:D:3883:ASP:OD2	2.33	0.60
1:B:3891:LEU:HB3	1:B:3899:PHE:CE2	2.35	0.60
1:C:1969:LEU:HD12	1:C:2009:LEU:HD21	1.84	0.60
1:D:4069:LYS:HB2	1:D:4133:GLN:NE2	2.15	0.60
1:B:63:ALA:HB2	1:B:261:ARG:HH12	1.67	0.60
1:B:1708:ARG:NH1	1:B:1837:GLN:HA	2.17	0.60
1:B:2012:PHE:HD2	1:B:2022:PRO:HD3	1.65	0.60
1:C:1708:ARG:NH1	1:C:1837:GLN:HA	2.17	0.60
1:C:1805:GLU:OE1	1:C:1808:ARG:NH2	2.30	0.60
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.34	0.60
1:D:1708:ARG:NH1	1:D:1837:GLN:HA	2.17	0.60
1:B:1676:LEU:HD12	1:B:2167:ILE:HD12	1.84	0.60
1:B:1805:GLU:OE1	1:B:1808:ARG:NH2	2.30	0.60
1:B:4344:ALA:O	1:B:4345:ALA:C	2.37	0.60
1:D:1838:PHE:O	1:D:1839:VAL:C	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1708:ARG:NH1	1:A:1837:GLN:HA	2.17	0.60
1:A:3768:SER:O	1:A:3773:ARG:NH1	2.29	0.60
1:B:591:ASP:O	1:B:1594:ARG:NH2	2.35	0.60
1:B:1838:PHE:O	1:B:1839:VAL:C	2.39	0.60
1:B:3657:TYR:HB3	1:B:3661:TRP:NE1	2.17	0.60
1:C:4345:ALA:HB1	1:C:4561:THR:HG22	1.83	0.60
1:D:4636:THR:C	1:D:4638:TYR:H	2.04	0.60
1:A:219:VAL:HG13	1:A:285:VAL:HG21	1.83	0.59
1:A:221:ARG:NH1	1:A:253:CYS:O	2.35	0.59
1:A:63:ALA:HB2	1:A:261:ARG:HH12	1.67	0.59
1:A:3657:TYR:HB3	1:A:3661:TRP:NE1	2.17	0.59
1:B:3799:LYS:NZ	1:B:3883:ASP:OD2	2.33	0.59
1:C:63:ALA:HB2	1:C:261:ARG:HH12	1.67	0.59
1:D:591:ASP:O	1:D:1594:ARG:NH2	2.35	0.59
1:D:1148:VAL:HG21	1:D:1212:ARG:HG3	1.83	0.59
1:D:1676:LEU:HD12	1:D:2167:ILE:HD12	1.84	0.59
1:A:1969:LEU:HD12	1:A:2009:LEU:HD21	1.84	0.59
1:B:939:VAL:HA	1:B:1053:ILE:HD12	1.83	0.59
1:B:3292:PRO:O	1:B:3294:PRO:HD3	2.03	0.59
1:A:1458:HIS:NE2	1:A:1483:VAL:HG21	2.17	0.59
1:A:3292:PRO:O	1:A:3294:PRO:HD3	2.03	0.59
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.34	0.59
1:C:1148:VAL:HG21	1:C:1212:ARG:HG3	1.83	0.59
1:D:221:ARG:NH1	1:D:253:CYS:O	2.35	0.59
1:D:1458:HIS:NE2	1:D:1483:VAL:HG21	2.17	0.59
1:A:764:VAL:HG12	1:A:766:GLY:H	1.67	0.59
1:A:4345:ALA:HB1	1:A:4561:THR:HG22	1.83	0.59
1:B:221:ARG:NH1	1:B:253:CYS:O	2.35	0.59
1:B:1969:LEU:HD12	1:B:2009:LEU:HD21	1.84	0.59
1:B:4340:ALA:O	1:B:4343:GLY:N	2.31	0.59
1:C:3768:SER:O	1:C:3773:ARG:NH1	2.29	0.59
1:A:234:SER:HB2	1:A:242:ARG:HA	1.85	0.59
1:B:219:VAL:HG13	1:B:285:VAL:HG21	1.83	0.59
1:B:977:LEU:HD23	1:B:1047:LEU:HD22	1.84	0.59
1:C:591:ASP:O	1:C:1594:ARG:NH2	2.35	0.59
1:C:764:VAL:HG12	1:C:766:GLY:H	1.67	0.59
1:C:2044:ILE:HD11	1:C:2131:LEU:HD13	1.85	0.59
1:C:4633:GLU:HB2	1:C:4639:MET:HG3	1.84	0.59
1:D:2044:ILE:HD11	1:D:2131:LEU:HD13	1.85	0.59
1:D:3292:PRO:O	1:D:3294:PRO:HD3	2.03	0.59
1:C:1676:LEU:HD12	1:C:2167:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3657:TYR:HB3	1:C:3661:TRP:NE1	2.17	0.59
1:D:1805:GLU:OE1	1:D:1808:ARG:NH2	2.30	0.59
1:A:2044:ILE:HD11	1:A:2131:LEU:HD13	1.85	0.59
1:B:1161:ILE:HD11	1:B:1223:PHE:HE2	1.68	0.59
1:C:939:VAL:HA	1:C:1053:ILE:HD12	1.83	0.59
1:C:978:THR:HG23	1:C:980:ALA:H	1.67	0.59
1:D:978:THR:HG23	1:D:980:ALA:H	1.67	0.59
1:D:3657:TYR:HB3	1:D:3661:TRP:NE1	2.17	0.59
1:B:4633:GLU:HB2	1:B:4639:MET:HG3	1.84	0.59
1:B:4817:ALA:O	1:B:4819:GLY:N	2.36	0.59
1:C:3292:PRO:O	1:C:3294:PRO:HD3	2.03	0.59
1:A:977:LEU:HD23	1:A:1047:LEU:HD22	1.84	0.58
1:A:1161:ILE:HD11	1:A:1223:PHE:HE2	1.68	0.58
1:A:1607:ARG:NH1	1:A:1610:ASN:OD1	2.36	0.58
1:B:1607:ARG:NH1	1:B:1610:ASN:OD1	2.36	0.58
1:B:4807:PHE:C	1:B:4809:PHE:N	2.55	0.58
1:C:2474:LEU:HD22	1:C:2494:PHE:HD2	1.68	0.58
1:D:63:ALA:HB2	1:D:261:ARG:HH12	1.67	0.58
1:D:1867:GLU:O	1:D:1871:PHE:N	2.36	0.58
1:A:1838:PHE:O	1:A:1839:VAL:C	2.39	0.58
1:B:2474:LEU:HD22	1:B:2494:PHE:HD2	1.68	0.58
1:D:234:SER:HB2	1:D:242:ARG:HA	1.85	0.58
1:D:4345:ALA:HB1	1:D:4561:THR:HG22	1.83	0.58
1:D:4633:GLU:HB2	1:D:4639:MET:HG3	1.84	0.58
1:A:3426:GLU:O	1:A:3430:ASN:N	2.27	0.58
1:B:215:THR:OG1	1:B:271:GLY:O	2.20	0.58
1:B:234:SER:HB2	1:B:242:ARG:HA	1.85	0.58
1:A:591:ASP:O	1:A:1594:ARG:NH2	2.35	0.58
1:B:1867:GLU:O	1:B:1871:PHE:N	2.36	0.58
1:C:3145:GLN:O	1:C:3149:GLN:NE2	2.37	0.58
1:D:1607:ARG:NH1	1:D:1610:ASN:OD1	2.36	0.58
1:D:1969:LEU:HD12	1:D:2009:LEU:HD21	1.84	0.58
1:A:1867:GLU:O	1:A:1871:PHE:N	2.36	0.58
1:A:4633:GLU:HB2	1:A:4639:MET:HG3	1.84	0.58
1:B:252:VAL:HG12	1:B:258:SER:HB3	1.85	0.58
1:B:978:THR:HG23	1:B:980:ALA:H	1.67	0.58
1:B:2458:ARG:HH21	1:B:2510:TYR:HA	1.69	0.58
1:A:252:VAL:HG12	1:A:258:SER:HB3	1.85	0.58
1:B:764:VAL:HG12	1:B:766:GLY:H	1.67	0.58
1:C:1607:ARG:NH1	1:C:1610:ASN:OD1	2.36	0.58
1:D:1647:CYS:SG	1:D:1648:MET:N	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2587:TYR:O	1:A:2590:SER:N	2.36	0.58
1:D:2587:TYR:O	1:D:2590:SER:N	2.36	0.58
1:B:1101:ARG:NH2	1:B:1114:GLU:OE2	2.37	0.58
1:B:2044:ILE:HD11	1:B:2131:LEU:HD13	1.85	0.58
1:B:3145:GLN:O	1:B:3149:GLN:NE2	2.37	0.58
1:B:4069:LYS:HB2	1:B:4133:GLN:NE2	2.15	0.58
1:C:1647:CYS:SG	1:C:1648:MET:N	2.77	0.58
1:D:2474:LEU:HD22	1:D:2494:PHE:HD2	1.68	0.58
1:D:3946:GLN:OE1	1:D:3949:ARG:NH1	2.37	0.58
1:B:3946:GLN:OE1	1:B:3949:ARG:NH1	2.37	0.58
1:C:221:ARG:NH1	1:C:253:CYS:O	2.35	0.58
1:C:1101:ARG:NH2	1:C:1114:GLU:OE2	2.37	0.58
1:D:4633:GLU:HG2	1:D:4635:SER:N	2.19	0.58
1:D:4807:PHE:C	1:D:4809:PHE:N	2.55	0.58
1:A:2458:ARG:HH21	1:A:2510:TYR:HA	1.69	0.58
1:C:1867:GLU:O	1:C:1871:PHE:N	2.36	0.58
1:C:3786:CYS:SG	1:C:3794:VAL:HG22	2.44	0.58
1:D:252:VAL:HG12	1:D:258:SER:HB3	1.85	0.58
1:B:3786:CYS:SG	1:B:3794:VAL:HG22	2.44	0.57
1:C:788:LYS:HG2	1:C:1629:GLN:HA	1.85	0.57
1:C:1161:ILE:HD11	1:C:1223:PHE:HE2	1.68	0.57
1:D:3786:CYS:SG	1:D:3794:VAL:HG22	2.44	0.57
1:D:5027:CYS:O	1:D:5029:ARG:N	2.37	0.57
1:A:978:THR:HG23	1:A:980:ALA:H	1.67	0.57
1:A:2474:LEU:HD22	1:A:2494:PHE:HD2	1.68	0.57
1:A:3228:ALA:HA	1:A:3302:PRO:HG3	1.86	0.57
1:A:4574:ASN:ND2	1:A:4813:LEU:HG	2.20	0.57
1:B:1647:CYS:SG	1:B:1648:MET:N	2.77	0.57
1:C:1838:PHE:O	1:C:1839:VAL:C	2.39	0.57
1:C:3946:GLN:OE1	1:C:3949:ARG:NH1	2.37	0.57
1:D:1161:ILE:HD11	1:D:1223:PHE:HE2	1.68	0.57
1:D:2458:ARG:HH21	1:D:2510:TYR:HA	1.69	0.57
1:A:1101:ARG:NH2	1:A:1114:GLU:OE2	2.37	0.57
1:B:206:CYS:SG	1:B:207:SER:N	2.77	0.57
1:C:234:SER:HB2	1:C:242:ARG:HA	1.85	0.57
1:C:252:VAL:HG12	1:C:258:SER:HB3	1.85	0.57
1:C:3228:ALA:HA	1:C:3302:PRO:HG3	1.86	0.57
1:A:1269:CYS:HB3	1:A:1473:THR:HG23	1.87	0.57
1:A:3767:GLN:OE1	1:A:3809:ASN:ND2	2.38	0.57
1:A:4895:GLY:O	1:B:4892:ARG:NH2	2.38	0.57
1:C:3767:GLN:OE1	1:C:3809:ASN:ND2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4321:ARG:NH2	1:C:4323:THR:HG22	2.19	0.57
1:C:5027:CYS:O	1:C:5029:ARG:N	2.37	0.57
1:D:584:LYS:NZ	1:D:624:ASN:OD1	2.35	0.57
1:A:206:CYS:SG	1:A:207:SER:N	2.77	0.57
1:A:1647:CYS:SG	1:A:1648:MET:N	2.77	0.57
1:A:4321:ARG:NH2	1:A:4323:THR:HG22	2.19	0.57
1:A:4678:ALA:HB1	1:A:4720:VAL:HG21	1.86	0.57
1:B:4574:ASN:ND2	1:B:4813:LEU:HG	2.20	0.57
1:C:2587:TYR:O	1:C:2590:SER:N	2.36	0.57
1:D:3145:GLN:O	1:D:3149:GLN:NE2	2.37	0.57
1:A:3786:CYS:SG	1:A:3794:VAL:HG22	2.44	0.57
1:D:3228:ALA:HA	1:D:3302:PRO:HG3	1.86	0.57
1:D:4574:ASN:ND2	1:D:4813:LEU:HG	2.20	0.57
1:A:5027:CYS:O	1:A:5029:ARG:N	2.37	0.57
1:B:788:LYS:HG2	1:B:1629:GLN:HA	1.85	0.57
1:B:3228:ALA:HA	1:B:3302:PRO:HG3	1.86	0.57
1:A:3143:LEU:HD13	1:A:3146:HIS:CE1	2.40	0.57
1:A:3946:GLN:OE1	1:A:3949:ARG:NH1	2.37	0.57
1:B:1269:CYS:HB3	1:B:1473:THR:HG23	1.87	0.57
1:B:2587:TYR:O	1:B:2590:SER:N	2.36	0.57
1:B:3143:LEU:HD13	1:B:3146:HIS:CE1	2.40	0.57
1:C:1139:PHE:CZ	1:C:1177:THR:HG22	2.40	0.57
1:C:4633:GLU:HG2	1:C:4635:SER:N	2.19	0.57
1:C:4807:PHE:C	1:C:4809:PHE:N	2.55	0.57
1:D:675:LEU:HG	1:D:676:THR:H	1.69	0.57
1:D:788:LYS:HG2	1:D:1629:GLN:HA	1.85	0.57
1:D:206:CYS:SG	1:D:207:SER:N	2.77	0.57
1:D:234:SER:HB2	1:D:242:ARG:HG3	1.87	0.57
1:D:1101:ARG:NH2	1:D:1114:GLU:OE2	2.37	0.57
1:D:1139:PHE:CZ	1:D:1177:THR:HG22	2.40	0.57
1:D:1269:CYS:HB3	1:D:1473:THR:HG23	1.87	0.57
1:D:4678:ALA:HB1	1:D:4720:VAL:HG21	1.86	0.57
1:A:1437:VAL:HG11	1:A:1538:THR:HG21	1.87	0.57
1:B:350:HIS:HD2	1:B:352:ALA:H	1.53	0.57
1:B:3767:GLN:OE1	1:B:3809:ASN:ND2	2.38	0.57
1:C:234:SER:HB2	1:C:242:ARG:HG3	1.87	0.57
1:A:788:LYS:HG2	1:A:1629:GLN:HA	1.85	0.56
1:A:1501:VAL:HG13	1:A:1534:LYS:HD3	1.87	0.56
1:A:4817:ALA:O	1:A:4819:GLY:N	2.36	0.56
1:B:694:PRO:HG3	1:B:826:ILE:HG13	1.87	0.56
1:B:1139:PHE:CZ	1:B:1177:THR:HG22	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4633:GLU:HG2	1:B:4635:SER:N	2.19	0.56
1:B:5027:CYS:O	1:B:5029:ARG:N	2.37	0.56
1:C:215:THR:OG1	1:C:271:GLY:O	2.20	0.56
1:C:2458:ARG:HH21	1:C:2510:TYR:HA	1.69	0.56
1:D:3767:GLN:OE1	1:D:3809:ASN:ND2	2.38	0.56
1:A:1805:GLU:OE1	1:A:1808:ARG:NH2	2.30	0.56
1:A:3145:GLN:O	1:A:3149:GLN:NE2	2.37	0.56
1:A:4633:GLU:HG2	1:A:4635:SER:N	2.19	0.56
1:B:1437:VAL:HG11	1:B:1538:THR:HG21	1.87	0.56
1:B:4574:ASN:HD22	1:B:4813:LEU:HG	1.70	0.56
1:B:4906:GLY:O	1:B:4907:ASP:C	2.43	0.56
1:C:4906:GLY:O	1:C:4907:ASP:C	2.43	0.56
1:A:584:LYS:NZ	1:A:624:ASN:OD1	2.35	0.56
1:A:4807:PHE:C	1:A:4809:PHE:N	2.55	0.56
1:A:4892:ARG:NH2	1:D:4895:GLY:O	2.38	0.56
1:B:4895:GLY:O	1:C:4892:ARG:NH2	2.38	0.56
1:C:206:CYS:SG	1:C:207:SER:N	2.77	0.56
1:C:350:HIS:HD2	1:C:352:ALA:H	1.53	0.56
1:C:675:LEU:HG	1:C:676:THR:H	1.69	0.56
1:C:1437:VAL:HG11	1:C:1538:THR:HG21	1.87	0.56
1:C:4895:GLY:O	1:D:4892:ARG:NH2	2.38	0.56
1:D:1501:VAL:HG13	1:D:1534:LYS:HD3	1.87	0.56
1:D:3426:GLU:O	1:D:3430:ASN:N	2.27	0.56
1:D:3578:GLY:O	1:D:3582:ARG:N	2.37	0.56
1:D:4321:ARG:NH2	1:D:4323:THR:HG22	2.19	0.56
1:A:3059:THR:O	1:A:3187:ARG:NH2	2.39	0.56
1:A:4712:PRO:O	1:A:4718:LYS:NZ	2.38	0.56
1:A:4906:GLY:O	1:A:4907:ASP:C	2.43	0.56
1:C:3315:LEU:O	1:C:3318:ASN:ND2	2.39	0.56
1:C:4678:ALA:HB1	1:C:4720:VAL:HG21	1.86	0.56
1:A:178:ARG:NE	1:A:194:SER:O	2.38	0.56
1:A:1189:LEU:HD12	1:A:1190:PRO:HD2	1.87	0.56
1:A:1650:ILE:HG23	1:A:1651:LEU:HD22	1.87	0.56
1:B:1189:LEU:HD12	1:B:1190:PRO:HD2	1.87	0.56
1:B:1765:VAL:HG22	1:B:1766:GLY:H	1.71	0.56
1:C:1269:CYS:HB3	1:C:1473:THR:HG23	1.87	0.56
1:C:3059:THR:O	1:C:3187:ARG:NH2	2.39	0.56
1:C:4574:ASN:ND2	1:C:4813:LEU:HG	2.20	0.56
1:D:1835:GLU:C	1:D:1837:GLN:N	2.59	0.56
1:A:1139:PHE:CZ	1:A:1177:THR:HG22	2.40	0.56
1:B:4321:ARG:NH2	1:B:4323:THR:HG22	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4574:ASN:HD22	1:C:4813:LEU:HG	1.70	0.56
1:D:3143:LEU:HD13	1:D:3146:HIS:CE1	2.40	0.56
1:D:4817:ALA:O	1:D:4819:GLY:N	2.36	0.56
1:A:1765:VAL:HG22	1:A:1766:GLY:H	1.71	0.56
1:A:2548:LEU:O	1:A:2552:ARG:NH1	2.39	0.56
1:A:3315:LEU:O	1:A:3318:ASN:ND2	2.39	0.56
1:B:3059:THR:O	1:B:3187:ARG:NH2	2.39	0.56
1:B:4678:ALA:HB1	1:B:4720:VAL:HG21	1.86	0.56
1:D:1072:VAL:HG12	1:D:1195:GLY:HA2	1.88	0.56
1:D:4906:GLY:O	1:D:4907:ASP:C	2.43	0.56
1:A:694:PRO:HG3	1:A:826:ILE:HG13	1.87	0.56
1:A:1835:GLU:HG2	1:A:1932:PRO:HG2	1.87	0.56
1:A:4574:ASN:HD22	1:A:4813:LEU:HG	1.70	0.56
1:B:1650:ILE:HG23	1:B:1651:LEU:HD22	1.87	0.56
1:B:2548:LEU:O	1:B:2552:ARG:NH1	2.39	0.56
1:C:3143:LEU:HD13	1:C:3146:HIS:CE1	2.40	0.56
1:D:350:HIS:HD2	1:D:352:ALA:H	1.53	0.56
1:B:863:LEU:HD22	1:B:868:GLU:HG2	1.88	0.56
1:B:4712:PRO:O	1:B:4718:LYS:NZ	2.38	0.56
1:D:1765:VAL:HG22	1:D:1766:GLY:H	1.71	0.56
1:D:4574:ASN:HD22	1:D:4813:LEU:HG	1.70	0.56
1:A:1072:VAL:HG12	1:A:1195:GLY:HA2	1.88	0.56
1:A:3652:MET:O	1:A:3656:SER:OG	2.24	0.56
1:C:1554:VAL:HG12	1:C:1556:PRO:HD3	1.88	0.56
1:A:675:LEU:HG	1:A:676:THR:H	1.69	0.55
1:C:694:PRO:HG3	1:C:826:ILE:HG13	1.87	0.55
1:C:2548:LEU:O	1:C:2552:ARG:NH1	2.39	0.55
1:D:1189:LEU:HD12	1:D:1190:PRO:HD2	1.87	0.55
1:A:793:LEU:HD21	1:A:797:HIS:H	1.71	0.55
1:B:977:LEU:HB3	1:B:1047:LEU:HD22	1.88	0.55
1:B:1501:VAL:HG13	1:B:1534:LYS:HD3	1.87	0.55
1:B:1554:VAL:HG12	1:B:1556:PRO:HD3	1.88	0.55
1:D:694:PRO:HG3	1:D:826:ILE:HG13	1.87	0.55
1:D:3315:LEU:O	1:D:3318:ASN:ND2	2.39	0.55
1:A:350:HIS:HD2	1:A:352:ALA:H	1.53	0.55
1:B:234:SER:HB2	1:B:242:ARG:HG3	1.87	0.55
1:B:3315:LEU:O	1:B:3318:ASN:ND2	2.39	0.55
1:C:70:GLU:O	1:C:71:GLN:NE2	2.39	0.55
1:D:1554:VAL:HG12	1:D:1556:PRO:HD3	1.88	0.55
1:C:1650:ILE:HG23	1:C:1651:LEU:HD22	1.87	0.55
1:D:1287:LEU:HB2	1:D:1460:HIS:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1437:VAL:HG11	1:D:1538:THR:HG21	1.87	0.55
1:D:1650:ILE:HG23	1:D:1651:LEU:HD22	1.87	0.55
1:D:3654:LEU:O	1:D:3661:TRP:NE1	2.38	0.55
1:A:1287:LEU:HB2	1:A:1460:HIS:HB2	1.88	0.55
1:A:4345:ALA:HB3	1:A:4561:THR:HA	1.89	0.55
1:C:1189:LEU:HD12	1:C:1190:PRO:HD2	1.87	0.55
1:D:793:LEU:HD21	1:D:797:HIS:H	1.71	0.55
1:D:1835:GLU:HG2	1:D:1932:PRO:HG2	1.87	0.55
1:D:4813:LEU:O	1:D:4816:ILE:HB	2.07	0.55
1:B:675:LEU:HG	1:B:676:THR:H	1.69	0.55
1:C:1765:VAL:HG22	1:C:1766:GLY:H	1.71	0.55
1:C:1835:GLU:HG2	1:C:1932:PRO:HG2	1.87	0.55
1:A:234:SER:HB2	1:A:242:ARG:HG3	1.87	0.55
1:A:1554:VAL:HG12	1:A:1556:PRO:HD3	1.88	0.55
1:A:4813:LEU:O	1:A:4816:ILE:HB	2.07	0.55
1:C:1501:VAL:HG13	1:C:1534:LYS:HD3	1.87	0.55
1:C:4813:LEU:O	1:C:4816:ILE:HB	2.07	0.55
1:D:70:GLU:O	1:D:71:GLN:NE2	2.39	0.55
1:D:215:THR:OG1	1:D:271:GLY:O	2.20	0.55
1:D:2556:LEU:HD13	1:D:2597:LYS:HA	1.89	0.55
1:D:3059:THR:O	1:D:3187:ARG:NH2	2.39	0.55
1:D:4345:ALA:HB3	1:D:4561:THR:HA	1.89	0.55
1:B:584:LYS:NZ	1:B:624:ASN:OD1	2.35	0.55
1:C:1126:GLY:HA3	1:C:1143:TRP:CE2	2.42	0.55
1:C:4635:SER:C	1:C:4637:GLY:H	2.11	0.55
1:A:3187:ARG:HH12	1:A:3190:LEU:HD12	1.72	0.55
1:B:2556:LEU:HD13	1:B:2597:LYS:HA	1.89	0.55
1:B:3187:ARG:HH12	1:B:3190:LEU:HD12	1.72	0.55
1:C:977:LEU:HB3	1:C:1047:LEU:HD22	1.88	0.55
1:D:863:LEU:HD22	1:D:868:GLU:HG2	1.88	0.55
1:D:3524:MET:O	1:D:3528:THR:OG1	2.24	0.55
1:D:4696:ASP:OD1	1:D:4696:ASP:N	2.40	0.55
1:A:70:GLU:O	1:A:71:GLN:NE2	2.39	0.55
1:A:977:LEU:HB3	1:A:1047:LEU:HD22	1.88	0.55
1:A:2556:LEU:HD13	1:A:2597:LYS:HA	1.89	0.55
1:A:3578:GLY:O	1:A:3582:ARG:N	2.37	0.55
1:B:178:ARG:NE	1:B:194:SER:O	2.38	0.55
1:B:277:GLY:HA2	1:B:315:CYS:HB2	1.89	0.55
1:B:4345:ALA:HB3	1:B:4561:THR:HA	1.89	0.55
1:D:1126:GLY:HA3	1:D:1143:TRP:CE2	2.42	0.55
1:A:1141:ARG:HH22	1:A:1144:GLN:HE22	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLU:O	1:B:71:GLN:NE2	2.39	0.54
1:D:2548:LEU:O	1:D:2552:ARG:NH1	2.39	0.54
1:B:1126:GLY:HA3	1:B:1143:TRP:CE2	2.42	0.54
1:B:1835:GLU:HG2	1:B:1932:PRO:HG2	1.87	0.54
1:B:3578:GLY:O	1:B:3582:ARG:N	2.37	0.54
1:C:1072:VAL:HG12	1:C:1195:GLY:HA2	1.88	0.54
1:C:2556:LEU:HD13	1:C:2597:LYS:HA	1.89	0.54
1:D:102:LEU:HB2	1:D:105:HIS:HD2	1.73	0.54
1:A:215:THR:OG1	1:A:271:GLY:O	2.20	0.54
1:A:4635:SER:C	1:A:4637:GLY:H	2.11	0.54
1:A:4900:GLU:O	1:A:4901:ILE:HD13	2.07	0.54
1:B:320:LYS:HE2	1:B:382:GLY:HA3	1.90	0.54
1:C:320:LYS:HE2	1:C:382:GLY:HA3	1.90	0.54
1:C:1287:LEU:HB2	1:C:1460:HIS:HB2	1.88	0.54
1:C:4090:LYS:HG3	1:C:4112:LEU:HD22	1.90	0.54
1:D:977:LEU:HB3	1:D:1047:LEU:HD22	1.88	0.54
1:D:3652:MET:O	1:D:3656:SER:OG	2.24	0.54
1:D:4090:LYS:HG3	1:D:4112:LEU:HD22	1.90	0.54
1:D:4900:GLU:O	1:D:4901:ILE:HD13	2.07	0.54
1:A:2512:ILE:HD11	1:A:2558:VAL:HG11	1.89	0.54
1:B:1072:VAL:HG12	1:B:1195:GLY:HA2	1.88	0.54
1:B:4090:LYS:HG3	1:B:4112:LEU:HD22	1.90	0.54
1:B:4813:LEU:O	1:B:4816:ILE:HB	2.07	0.54
1:C:4345:ALA:HB3	1:C:4561:THR:HA	1.89	0.54
1:D:4635:SER:C	1:D:4637:GLY:H	2.11	0.54
1:D:4712:PRO:O	1:D:4718:LYS:NZ	2.38	0.54
1:A:863:LEU:HD22	1:A:868:GLU:HG2	1.88	0.54
1:A:977:LEU:HD12	1:A:978:THR:N	2.23	0.54
1:B:793:LEU:HD21	1:B:797:HIS:H	1.71	0.54
1:B:4635:SER:C	1:B:4637:GLY:H	2.11	0.54
1:B:4684:ASP:OD1	1:B:4685:GLY:N	2.41	0.54
1:A:3524:MET:O	1:A:3528:THR:OG1	2.24	0.54
1:B:3654:LEU:O	1:B:3661:TRP:NE1	2.38	0.54
1:C:102:LEU:HB2	1:C:105:HIS:HD2	1.73	0.54
1:B:977:LEU:HD12	1:B:978:THR:N	2.23	0.54
1:C:863:LEU:HD22	1:C:868:GLU:HG2	1.88	0.54
1:C:2512:ILE:HD11	1:C:2558:VAL:HG11	1.89	0.54
1:C:4817:ALA:O	1:C:4819:GLY:N	2.36	0.54
1:C:4900:GLU:O	1:C:4901:ILE:HD13	2.07	0.54
1:D:2512:ILE:HD11	1:D:2558:VAL:HG11	1.89	0.54
1:D:3200:ALA:O	1:D:3204:ALA:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3654:LEU:O	1:A:3661:TRP:NE1	2.38	0.54
1:B:2512:ILE:HD11	1:B:2558:VAL:HG11	1.89	0.54
1:B:4900:GLU:O	1:B:4901:ILE:HD13	2.07	0.54
1:C:793:LEU:HD21	1:C:797:HIS:H	1.71	0.54
1:C:3919:THR:HG21	1:C:3968:TYR:HE2	1.73	0.54
1:A:102:LEU:HB2	1:A:105:HIS:HD2	1.73	0.54
1:B:4912:TYR:OH	1:D:4320:ARG:HG2	2.08	0.54
1:C:1141:ARG:HH22	1:C:1144:GLN:HE22	1.55	0.54
1:C:1970:GLN:NE2	1:C:3641:LEU:O	2.36	0.54
1:D:1141:ARG:HH22	1:D:1144:GLN:HE22	1.55	0.54
1:A:3200:ALA:O	1:A:3204:ALA:N	2.40	0.53
1:A:4912:TYR:OH	1:C:4320:ARG:HG2	2.08	0.53
1:C:575:LEU:HD22	1:C:609:CYS:HB3	1.90	0.53
1:D:3187:ARG:HH12	1:D:3190:LEU:HD12	1.72	0.53
1:A:320:LYS:HE2	1:A:382:GLY:HA3	1.90	0.53
1:A:4090:LYS:HG3	1:A:4112:LEU:HD22	1.90	0.53
1:B:575:LEU:HD22	1:B:609:CYS:HB3	1.90	0.53
1:B:1088:TRP:HA	1:B:1224:GLU:O	2.09	0.53
1:B:1141:ARG:HH22	1:B:1144:GLN:HE22	1.55	0.53
1:C:3187:ARG:HH12	1:C:3190:LEU:HD12	1.72	0.53
1:D:4576:ILE:HG22	1:D:4631:PHE:CE2	2.44	0.53
1:A:2358:ILE:HD13	1:A:2460:LEU:HD12	1.91	0.53
1:B:664:PHE:HB3	1:B:746:CYS:HB3	1.91	0.53
1:C:277:GLY:HA2	1:C:315:CYS:HB2	1.89	0.53
1:D:320:LYS:HE2	1:D:382:GLY:HA3	1.90	0.53
1:D:3232:LEU:HB3	1:D:3235:SER:HB3	1.91	0.53
1:D:3657:TYR:HB3	1:D:3661:TRP:CD1	2.44	0.53
1:A:664:PHE:HB3	1:A:746:CYS:HB3	1.91	0.53
1:B:1287:LEU:HB2	1:B:1460:HIS:HB2	1.88	0.53
1:B:1835:GLU:C	1:B:1837:GLN:N	2.59	0.53
1:B:3657:TYR:HB3	1:B:3661:TRP:CD1	2.44	0.53
1:C:3232:LEU:HB3	1:C:3235:SER:HB3	1.91	0.53
1:A:575:LEU:HD22	1:A:609:CYS:HB3	1.90	0.53
1:A:4684:ASP:OD1	1:A:4685:GLY:N	2.41	0.53
1:C:4576:ILE:HG22	1:C:4631:PHE:CE2	2.44	0.53
1:D:1835:GLU:C	1:D:1837:GLN:H	2.12	0.53
1:D:2358:ILE:HD13	1:D:2460:LEU:HD12	1.91	0.53
1:A:1126:GLY:HA3	1:A:1143:TRP:CE2	2.42	0.53
1:A:3919:THR:HG21	1:A:3968:TYR:HE2	1.73	0.53
1:A:4320:ARG:HG2	1:C:4912:TYR:OH	2.08	0.53
1:B:1835:GLU:C	1:B:1837:GLN:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4320:ARG:HG2	1:D:4912:TYR:OH	2.08	0.53
1:C:1835:GLU:C	1:C:1837:GLN:H	2.12	0.53
1:D:277:GLY:HA2	1:D:315:CYS:HB2	1.89	0.53
1:A:4687:TYR:OH	1:A:4699:GLY:O	2.20	0.53
1:B:2358:ILE:HD13	1:B:2460:LEU:HD12	1.91	0.53
1:C:150:MET:HB2	1:C:169:LEU:HD23	1.91	0.53
1:C:977:LEU:HD12	1:C:978:THR:N	2.23	0.53
1:C:1859:VAL:HA	1:C:1862:ILE:HG22	1.91	0.53
1:C:4684:ASP:OD1	1:C:4685:GLY:N	2.41	0.53
1:C:4712:PRO:O	1:C:4718:LYS:NZ	2.38	0.53
1:A:150:MET:HB2	1:A:169:LEU:HD23	1.91	0.53
1:A:595:ARG:NH1	1:A:631:LEU:O	2.42	0.53
1:A:1088:TRP:HA	1:A:1224:GLU:O	2.09	0.53
1:A:1835:GLU:C	1:A:1837:GLN:N	2.59	0.53
1:A:3657:TYR:HB3	1:A:3661:TRP:CD1	2.44	0.53
1:B:102:LEU:HB2	1:B:105:HIS:HD2	1.73	0.53
1:C:675:LEU:HD21	1:C:1633:PRO:HB3	1.90	0.53
1:C:1088:TRP:HA	1:C:1224:GLU:O	2.09	0.53
1:C:3200:ALA:O	1:C:3204:ALA:N	2.40	0.53
1:D:977:LEU:HD12	1:D:978:THR:N	2.23	0.53
1:D:1088:TRP:HA	1:D:1224:GLU:O	2.09	0.53
1:A:675:LEU:HD21	1:A:1633:PRO:HB3	1.90	0.53
1:A:1835:GLU:C	1:A:1837:GLN:H	2.12	0.53
1:B:150:MET:HB2	1:B:169:LEU:HD23	1.91	0.53
1:B:1859:VAL:HA	1:B:1862:ILE:HG22	1.91	0.53
1:B:3919:THR:HG21	1:B:3968:TYR:HE2	1.73	0.53
1:C:584:LYS:NZ	1:C:624:ASN:OD1	2.35	0.53
1:C:4691:GLN:OE1	1:C:4692:PRO:HD2	2.09	0.53
1:D:675:LEU:HD21	1:D:1633:PRO:HB3	1.90	0.53
1:D:1859:VAL:HA	1:D:1862:ILE:HG22	1.91	0.53
1:D:2961:GLN:O	1:D:2965:ARG:NH1	2.42	0.53
1:D:4180:ARG:HD3	1:D:4192:ARG:HH21	1.74	0.53
1:D:4691:GLN:OE1	1:D:4692:PRO:HD2	2.09	0.53
1:A:1970:GLN:NE2	1:A:3641:LEU:O	2.36	0.53
1:A:3232:LEU:HB3	1:A:3235:SER:HB3	1.91	0.53
1:A:4576:ILE:HG22	1:A:4631:PHE:CE2	2.44	0.53
1:B:234:SER:OG	1:B:240:ASP:OD2	2.27	0.53
1:B:2961:GLN:O	1:B:2965:ARG:NH1	2.42	0.53
1:C:664:PHE:HB3	1:C:746:CYS:HB3	1.91	0.53
1:D:1259:ARG:NH2	1:D:1591:CYS:SG	2.82	0.53
1:A:1259:ARG:NH2	1:A:1591:CYS:SG	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4909:TYR:CZ	1:D:4319:LEU:HD12	2.45	0.52
1:C:3654:LEU:O	1:C:3661:TRP:NE1	2.38	0.52
1:A:102:LEU:HB2	1:A:105:HIS:CD2	2.44	0.52
1:A:4909:TYR:CZ	1:C:4319:LEU:HD12	2.45	0.52
1:B:102:LEU:HB2	1:B:105:HIS:CD2	2.44	0.52
1:B:595:ARG:NH1	1:B:631:LEU:O	2.42	0.52
1:B:4576:ILE:HG22	1:B:4631:PHE:CE2	2.44	0.52
1:C:684:VAL:HG21	1:C:744:VAL:HG11	1.91	0.52
1:C:4321:ARG:HH11	1:C:4321:ARG:HG2	1.74	0.52
1:D:595:ARG:NH1	1:D:631:LEU:O	2.42	0.52
1:D:664:PHE:HB3	1:D:746:CYS:HB3	1.91	0.52
1:D:4684:ASP:OD1	1:D:4685:GLY:N	2.41	0.52
1:A:2961:GLN:O	1:A:2965:ARG:NH1	2.42	0.52
1:B:3232:LEU:HB3	1:B:3235:SER:HB3	1.91	0.52
1:B:4321:ARG:HG2	1:B:4321:ARG:HH11	1.74	0.52
1:C:595:ARG:NH1	1:C:631:LEU:O	2.42	0.52
1:C:2358:ILE:HD13	1:C:2460:LEU:HD12	1.91	0.52
1:C:3657:TYR:HB3	1:C:3661:TRP:CD1	2.44	0.52
1:C:4052:SER:O	1:C:4056:GLU:HG2	2.09	0.52
1:A:2042:CYS:SG	1:A:2043:GLY:N	2.83	0.52
1:B:4691:GLN:OE1	1:B:4692:PRO:HD2	2.09	0.52
1:C:1712:TYR:CD2	1:C:1840:PRO:O	2.63	0.52
1:D:102:LEU:HB2	1:D:105:HIS:CD2	2.44	0.52
1:D:178:ARG:NE	1:D:194:SER:O	2.38	0.52
1:A:277:GLY:HA2	1:A:315:CYS:HB2	1.89	0.52
1:B:1712:TYR:CD2	1:B:1840:PRO:O	2.63	0.52
1:D:575:LEU:HD22	1:D:609:CYS:HB3	1.90	0.52
1:D:3919:THR:HG21	1:D:3968:TYR:HE2	1.73	0.52
1:A:1712:TYR:CD2	1:A:1840:PRO:O	2.63	0.52
1:A:4321:ARG:HG2	1:A:4321:ARG:HH11	1.74	0.52
1:B:684:VAL:HG21	1:B:744:VAL:HG11	1.91	0.52
1:B:1259:ARG:NH2	1:B:1591:CYS:SG	2.82	0.52
1:B:2042:CYS:SG	1:B:2043:GLY:N	2.83	0.52
1:B:4052:SER:O	1:B:4056:GLU:HG2	2.09	0.52
1:C:1835:GLU:C	1:C:1837:GLN:N	2.59	0.52
1:C:3524:MET:O	1:C:3528:THR:OG1	2.24	0.52
1:D:1712:TYR:CD2	1:D:1840:PRO:O	2.63	0.52
1:D:4798:MET:O	1:D:4802:GLY:N	2.43	0.52
1:A:214:VAL:HG21	1:A:390:LEU:HD11	1.91	0.52
1:A:1859:VAL:HA	1:A:1862:ILE:HG22	1.91	0.52
1:A:4052:SER:O	1:A:4056:GLU:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LYS:HD2	1:B:131:LEU:N	2.25	0.52
1:B:3652:MET:O	1:B:3656:SER:OG	2.24	0.52
1:C:102:LEU:HB2	1:C:105:HIS:CD2	2.44	0.52
1:C:1259:ARG:NH2	1:C:1591:CYS:SG	2.82	0.52
1:C:2042:CYS:SG	1:C:2043:GLY:N	2.83	0.52
1:C:2961:GLN:O	1:C:2965:ARG:NH1	2.42	0.52
1:A:4888:TYR:HA	1:D:4918:ILE:HD11	1.92	0.52
1:B:3524:MET:O	1:B:3528:THR:OG1	2.24	0.52
1:D:214:VAL:HG21	1:D:390:LEU:HD11	1.91	0.52
1:A:3771:HIS:HB3	1:A:3774:GLY:H	1.75	0.52
1:A:4319:LEU:HD12	1:C:4909:TYR:CZ	2.45	0.52
1:A:4636:THR:O	1:A:4638:TYR:N	2.43	0.52
1:B:4636:THR:O	1:B:4638:TYR:N	2.43	0.52
1:C:4918:ILE:HD11	1:D:4888:TYR:HA	1.92	0.52
1:D:350:HIS:HB3	1:D:353:SER:HB2	1.92	0.52
1:D:2042:CYS:SG	1:D:2043:GLY:N	2.83	0.52
1:D:4321:ARG:HG2	1:D:4321:ARG:HH11	1.74	0.52
1:A:130:LYS:HD2	1:A:131:LEU:N	2.25	0.52
1:A:4798:MET:O	1:A:4802:GLY:N	2.43	0.52
1:B:1089:TYR:HB2	1:B:1152:MET:SD	2.50	0.52
1:C:130:LYS:HD2	1:C:131:LEU:N	2.25	0.52
1:C:234:SER:OG	1:C:240:ASP:OD2	2.27	0.52
1:C:1469:VAL:HG23	1:C:1488:LYS:HD3	1.92	0.52
1:C:3960:GLN:NE2	1:C:3960:GLN:O	2.43	0.52
1:D:150:MET:HB2	1:D:169:LEU:HD23	1.91	0.52
1:D:3960:GLN:O	1:D:3960:GLN:NE2	2.43	0.52
1:A:668:VAL:HA	1:A:789:VAL:HG12	1.92	0.51
1:A:689:THR:HA	1:A:778:PHE:CE2	2.45	0.51
1:B:411:TYR:HB2	1:B:486:LEU:HD21	1.93	0.51
1:B:1469:VAL:HG23	1:B:1488:LYS:HD3	1.92	0.51
1:B:4180:ARG:HD3	1:B:4192:ARG:HH21	1.74	0.51
1:B:4319:LEU:HD12	1:D:4909:TYR:CZ	2.45	0.51
1:B:4918:ILE:HD11	1:C:4888:TYR:HA	1.92	0.51
1:C:350:HIS:HB3	1:C:353:SER:HB2	1.92	0.51
1:C:4180:ARG:HD3	1:C:4192:ARG:HH21	1.74	0.51
1:A:4180:ARG:HD3	1:A:4192:ARG:HH21	1.74	0.51
1:D:130:LYS:HD2	1:D:131:LEU:N	2.25	0.51
1:D:411:TYR:HB2	1:D:486:LEU:HD21	1.93	0.51
1:D:4052:SER:O	1:D:4056:GLU:HG2	2.09	0.51
1:A:350:HIS:HB3	1:A:353:SER:HB2	1.92	0.51
1:A:4691:GLN:OE1	1:A:4692:PRO:HD2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:VAL:HG21	1:B:390:LEU:HD11	1.91	0.51
1:C:252:VAL:HG22	1:C:257:ARG:NH2	2.26	0.51
1:C:1100:MET:HB2	1:C:1143:TRP:HZ3	1.75	0.51
1:C:3051:ARG:NH2	1:C:3179:LYS:O	2.44	0.51
1:D:689:THR:HA	1:D:778:PHE:CE2	2.45	0.51
1:D:1100:MET:HB2	1:D:1143:TRP:HZ3	1.75	0.51
1:D:1240:LYS:HE2	1:D:1606:SER:HB2	1.92	0.51
1:A:3680:ALA:HB3	1:A:3697:PRO:HG2	1.93	0.51
1:A:3729:MET:HB3	1:A:3770:LEU:HD21	1.92	0.51
1:B:689:THR:HA	1:B:778:PHE:CE2	2.45	0.51
1:B:4635:SER:O	1:B:4636:THR:C	2.49	0.51
1:C:646:PRO:HG2	1:C:779:PRO:HG2	1.93	0.51
1:C:668:VAL:HA	1:C:789:VAL:HG12	1.92	0.51
1:D:668:VAL:HA	1:D:789:VAL:HG12	1.92	0.51
1:A:221:ARG:NH2	1:A:259:LEU:HD21	2.26	0.51
1:A:1089:TYR:HB2	1:A:1152:MET:SD	2.50	0.51
1:A:4918:ILE:HD11	1:B:4888:TYR:HA	1.92	0.51
1:B:675:LEU:HD21	1:B:1633:PRO:HB3	1.90	0.51
1:B:3960:GLN:O	1:B:3960:GLN:NE2	2.43	0.51
1:B:4798:MET:O	1:B:4802:GLY:N	2.43	0.51
1:C:221:ARG:NH2	1:C:259:LEU:HD21	2.26	0.51
1:C:3578:GLY:O	1:C:3582:ARG:N	2.37	0.51
1:C:4634:GLU:HG3	1:C:4636:THR:CG2	2.32	0.51
1:C:4636:THR:O	1:C:4638:TYR:N	2.43	0.51
1:D:3680:ALA:HB3	1:D:3697:PRO:HG2	1.93	0.51
1:D:3729:MET:HB3	1:D:3770:LEU:HD21	1.92	0.51
1:A:411:TYR:HB2	1:A:486:LEU:HD21	1.93	0.51
1:A:3960:GLN:NE2	1:A:3960:GLN:O	2.43	0.51
1:A:4638:TYR:O	1:A:4641:PRO:HD2	2.11	0.51
1:B:668:VAL:HA	1:B:789:VAL:HG12	1.92	0.51
1:D:23:GLN:HE21	1:D:203:ASN:HD22	1.58	0.51
1:D:4636:THR:O	1:D:4638:TYR:N	2.43	0.51
1:B:221:ARG:NH2	1:B:259:LEU:HD21	2.26	0.51
1:C:411:TYR:HB2	1:C:486:LEU:HD21	1.93	0.51
1:C:497:TYR:HD1	1:C:503:PHE:HB3	1.76	0.51
1:C:3729:MET:HB3	1:C:3770:LEU:HD21	1.92	0.51
1:C:4635:SER:O	1:C:4637:GLY:N	2.44	0.51
1:C:4798:MET:O	1:C:4802:GLY:N	2.43	0.51
1:D:665:GLU:HG3	1:D:792:LEU:HD12	1.93	0.51
1:D:4638:TYR:O	1:D:4641:PRO:HD2	2.11	0.51
1:A:23:GLN:HE21	1:A:203:ASN:HD22	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:TYR:HD1	1:A:503:PHE:HB3	1.76	0.51
1:A:684:VAL:HG21	1:A:744:VAL:HG11	1.91	0.51
1:A:4635:SER:O	1:A:4636:THR:C	2.49	0.51
1:B:350:HIS:HB3	1:B:353:SER:HB2	1.92	0.51
1:B:1970:GLN:NE2	1:B:3641:LEU:O	2.36	0.51
1:C:689:THR:HA	1:C:778:PHE:CE2	2.45	0.51
1:C:1089:TYR:HB2	1:C:1152:MET:SD	2.50	0.51
1:D:1079:LYS:NZ	1:D:1655:GLU:OE2	2.35	0.51
1:A:252:VAL:HG22	1:A:257:ARG:NH2	2.26	0.51
1:B:3200:ALA:O	1:B:3204:ALA:N	2.40	0.51
1:B:3771:HIS:HB3	1:B:3774:GLY:H	1.75	0.51
1:C:2149:VAL:HA	1:C:2152:THR:HG22	1.93	0.51
1:D:684:VAL:HG21	1:D:744:VAL:HG11	1.91	0.51
1:D:1161:ILE:HG13	1:D:1161:ILE:O	2.11	0.51
1:D:4635:SER:O	1:D:4637:GLY:N	2.44	0.51
1:A:1161:ILE:HG13	1:A:1161:ILE:O	2.11	0.51
1:A:1469:VAL:HG23	1:A:1488:LYS:HD3	1.92	0.51
1:A:4098:ASP:OD1	1:A:4098:ASP:N	2.41	0.51
1:B:3729:MET:HB3	1:B:3770:LEU:HD21	1.92	0.51
1:C:178:ARG:NE	1:C:194:SER:O	2.38	0.51
1:C:2961:GLN:NE2	1:C:3037:GLU:OE2	2.44	0.51
1:D:497:TYR:HD1	1:D:503:PHE:HB3	1.76	0.51
1:D:583:ILE:CD1	1:D:620:LEU:HB3	2.42	0.51
1:D:646:PRO:HG2	1:D:779:PRO:HG2	1.93	0.51
1:A:583:ILE:CD1	1:A:620:LEU:HB3	2.42	0.50
1:A:665:GLU:OE1	1:A:745:SER:OG	2.23	0.50
1:A:665:GLU:HG3	1:A:792:LEU:HD12	1.93	0.50
1:A:2961:GLN:NE2	1:A:3037:GLU:OE2	2.44	0.50
1:B:3680:ALA:HB3	1:B:3697:PRO:HG2	1.93	0.50
1:B:4635:SER:O	1:B:4637:GLY:N	2.44	0.50
1:C:214:VAL:HG21	1:C:390:LEU:HD11	1.91	0.50
1:C:583:ILE:CD1	1:C:620:LEU:HB3	2.42	0.50
1:D:252:VAL:HG22	1:D:257:ARG:NH2	2.26	0.50
1:A:4227:GLU:HG2	1:A:4229:GLU:H	1.76	0.50
1:B:583:ILE:CD1	1:B:620:LEU:HB3	2.42	0.50
1:B:1161:ILE:O	1:B:1161:ILE:HG13	2.11	0.50
1:B:1240:LYS:HE2	1:B:1606:SER:HB2	1.92	0.50
1:C:1161:ILE:HG13	1:C:1161:ILE:O	2.11	0.50
1:C:4036:VAL:O	1:C:4037:ASN:ND2	2.44	0.50
1:C:4638:TYR:O	1:C:4641:PRO:HD2	2.11	0.50
1:C:4696:ASP:OD1	1:C:4696:ASP:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ARG:NH2	1:D:259:LEU:HD21	2.26	0.50
1:A:646:PRO:HG2	1:A:779:PRO:HG2	1.93	0.50
1:B:252:VAL:HG22	1:B:257:ARG:NH2	2.26	0.50
1:B:2149:VAL:HA	1:B:2152:THR:HG22	1.93	0.50
1:C:2175:GLU:HB2	1:C:2228:MET:HE3	1.93	0.50
1:C:3652:MET:O	1:C:3656:SER:OG	2.24	0.50
1:A:1224:GLU:OE2	1:A:1228:ILE:HB	2.11	0.50
1:B:497:TYR:HD1	1:B:503:PHE:HB3	1.76	0.50
1:B:4687:TYR:OH	1:B:4699:GLY:O	2.20	0.50
1:C:711:LEU:HB3	1:C:1532:ASN:ND2	2.27	0.50
1:C:1293:LEU:CD2	1:C:1579:MET:HB3	2.42	0.50
1:D:1089:TYR:HB2	1:D:1152:MET:SD	2.50	0.50
1:D:1224:GLU:OE2	1:D:1228:ILE:HB	2.11	0.50
1:D:2441:HIS:HA	1:D:2444:GLN:HG2	1.94	0.50
1:D:4036:VAL:O	1:D:4037:ASN:ND2	2.44	0.50
1:D:4999:ASP:OD1	1:D:4999:ASP:N	2.45	0.50
1:C:23:GLN:HE21	1:C:203:ASN:HD22	1.58	0.50
1:D:378:LEU:HD12	1:D:378:LEU:O	2.12	0.50
1:D:1469:VAL:HG23	1:D:1488:LYS:HD3	1.92	0.50
1:A:378:LEU:O	1:A:378:LEU:HD12	2.12	0.50
1:A:2149:VAL:HA	1:A:2152:THR:HG22	1.93	0.50
1:B:378:LEU:HD12	1:B:378:LEU:O	2.12	0.50
1:B:4036:VAL:O	1:B:4037:ASN:ND2	2.44	0.50
1:B:4638:TYR:O	1:B:4641:PRO:HD2	2.11	0.50
1:C:350:HIS:CD2	1:C:352:ALA:H	2.30	0.50
1:C:3771:HIS:HB3	1:C:3774:GLY:H	1.75	0.50
1:D:350:HIS:CD2	1:D:352:ALA:H	2.30	0.50
1:D:2149:VAL:HA	1:D:2152:THR:HG22	1.93	0.50
1:A:1100:MET:HB2	1:A:1143:TRP:HZ3	1.75	0.50
1:A:1240:LYS:HE2	1:A:1606:SER:HB2	1.92	0.50
1:A:2441:HIS:HA	1:A:2444:GLN:HG2	1.94	0.50
1:A:4320:ARG:HB3	1:A:4320:ARG:CZ	2.42	0.50
1:A:4635:SER:O	1:A:4637:GLY:N	2.44	0.50
1:B:224:HIS:HB3	1:B:229:GLU:HB3	1.94	0.50
1:B:1104:TRP:NE1	1:B:1151:CYS:SG	2.85	0.50
1:B:1293:LEU:CD2	1:B:1579:MET:HB3	2.42	0.50
1:C:378:LEU:HD12	1:C:378:LEU:O	2.12	0.50
1:C:3680:ALA:HB3	1:C:3697:PRO:HG2	1.93	0.50
1:D:3051:ARG:NH2	1:D:3179:LYS:O	2.44	0.50
1:A:4036:VAL:O	1:A:4037:ASN:ND2	2.44	0.50
1:B:646:PRO:HG2	1:B:779:PRO:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4633:GLU:CB	1:B:4639:MET:HG3	2.42	0.50
1:D:224:HIS:HB3	1:D:229:GLU:HB3	1.94	0.50
1:D:711:LEU:HB3	1:D:1532:ASN:ND2	2.27	0.50
1:D:4687:TYR:OH	1:D:4699:GLY:O	2.20	0.50
1:A:223:PHE:N	1:A:389:PHE:O	2.45	0.50
1:B:23:GLN:HE21	1:B:203:ASN:HD22	1.58	0.50
1:B:1735:ILE:HG13	1:B:1771:LEU:HD23	1.94	0.50
1:B:2175:GLU:HB2	1:B:2228:MET:HE3	1.94	0.50
1:B:2961:GLN:NE2	1:B:3037:GLU:OE2	2.44	0.50
1:C:665:GLU:HG3	1:C:792:LEU:HD12	1.93	0.50
1:D:665:GLU:OE1	1:D:745:SER:OG	2.23	0.50
1:D:3771:HIS:HB3	1:D:3774:GLY:H	1.75	0.50
1:D:3878:ASP:OD1	1:D:3879:GLU:N	2.45	0.50
1:A:711:LEU:HB3	1:A:1532:ASN:ND2	2.27	0.49
1:B:412:ASN:OD1	1:B:413:GLN:N	2.46	0.49
1:B:1100:MET:HB2	1:B:1143:TRP:HZ3	1.75	0.49
1:B:1224:GLU:OE2	1:B:1228:ILE:HB	2.11	0.49
1:B:4227:GLU:HG2	1:B:4229:GLU:H	1.76	0.49
1:C:1240:LYS:HE2	1:C:1606:SER:HB2	1.92	0.49
1:C:1653:LEU:HD13	1:C:1660:GLN:HA	1.94	0.49
1:D:4666:VAL:HA	1:D:4669:VAL:HG22	1.94	0.49
1:A:350:HIS:CD2	1:A:352:ALA:H	2.30	0.49
1:A:1104:TRP:NE1	1:A:1151:CYS:SG	2.85	0.49
1:B:4817:ALA:C	1:B:4819:GLY:N	2.66	0.49
1:C:1507:GLY:O	1:C:1508:ARG:NE	2.42	0.49
1:C:4999:ASP:N	1:C:4999:ASP:OD1	2.45	0.49
1:D:412:ASN:OD1	1:D:413:GLN:N	2.46	0.49
1:D:2961:GLN:NE2	1:D:3037:GLU:OE2	2.44	0.49
1:A:2174:GLU:OE1	1:A:2174:GLU:N	2.39	0.49
1:A:4240:ASP:OD2	1:A:4672:LYS:NZ	2.39	0.49
1:B:959:TYR:HE2	1:B:966:LYS:HD2	1.78	0.49
1:B:3878:ASP:OD1	1:B:3879:GLU:N	2.45	0.49
1:C:224:HIS:HB3	1:C:229:GLU:HB3	1.94	0.49
1:C:1735:ILE:HG13	1:C:1771:LEU:HD23	1.94	0.49
1:C:1839:VAL:O	1:C:1841:VAL:N	2.46	0.49
1:C:4227:GLU:HG2	1:C:4229:GLU:H	1.76	0.49
1:C:4633:GLU:CB	1:C:4639:MET:HG3	2.42	0.49
1:D:4320:ARG:HB3	1:D:4320:ARG:CZ	2.42	0.49
1:A:224:HIS:HB3	1:A:229:GLU:HB3	1.94	0.49
1:B:665:GLU:HG3	1:B:792:LEU:HD12	1.93	0.49
1:B:1653:LEU:HD13	1:B:1660:GLN:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2441:HIS:HA	1:B:2444:GLN:HG2	1.94	0.49
1:B:4320:ARG:CZ	1:B:4320:ARG:HB3	2.42	0.49
1:C:359:TYR:HD2	1:C:361:ALA:HB2	1.77	0.49
1:C:1224:GLU:OE2	1:C:1228:ILE:HB	2.11	0.49
1:D:223:PHE:N	1:D:389:PHE:O	2.45	0.49
1:D:2243:SER:O	1:D:2247:GLN:NE2	2.46	0.49
1:A:412:ASN:OD1	1:A:413:GLN:N	2.46	0.49
1:B:40:GLU:H	1:B:44:ASN:HD21	1.60	0.49
1:C:412:ASN:OD1	1:C:413:GLN:N	2.46	0.49
1:D:1104:TRP:NE1	1:D:1151:CYS:SG	2.85	0.49
1:D:2175:GLU:HB2	1:D:2228:MET:HE3	1.94	0.49
1:A:1839:VAL:O	1:A:1841:VAL:N	2.46	0.49
1:B:649:PHE:HB3	1:B:776:LEU:HD22	1.95	0.49
1:C:2243:SER:O	1:C:2247:GLN:NE2	2.46	0.49
1:C:3838:THR:OG1	1:C:3838:THR:O	2.29	0.49
1:C:4636:THR:C	1:C:4638:TYR:N	2.66	0.49
1:C:4666:VAL:HA	1:C:4669:VAL:HG22	1.94	0.49
1:A:649:PHE:HB3	1:A:776:LEU:HD22	1.95	0.49
1:A:1293:LEU:CD2	1:A:1579:MET:HB3	2.42	0.49
1:A:1576:SER:HA	1:A:1579:MET:HG2	1.94	0.49
1:B:223:PHE:N	1:B:389:PHE:O	2.45	0.49
1:B:350:HIS:CD2	1:B:352:ALA:H	2.30	0.49
1:B:1507:GLY:O	1:B:1508:ARG:NE	2.42	0.49
1:B:1839:VAL:O	1:B:1841:VAL:N	2.46	0.49
1:D:1293:LEU:CD2	1:D:1579:MET:HB3	2.42	0.49
1:D:4227:GLU:HG2	1:D:4229:GLU:H	1.76	0.49
1:A:255:HIS:HB3	1:A:480:GLU:HG3	1.94	0.49
1:A:359:TYR:HD2	1:A:361:ALA:HB2	1.77	0.49
1:A:2175:GLU:HB2	1:A:2228:MET:HE3	1.95	0.49
1:A:3385:ALA:HB1	1:A:3400:VAL:HG13	1.95	0.49
1:A:4340:ALA:O	1:A:4342:ALA:N	2.46	0.49
1:A:4666:VAL:HA	1:A:4669:VAL:HG22	1.94	0.49
1:A:4696:ASP:OD1	1:A:4696:ASP:N	2.40	0.49
1:B:2243:SER:O	1:B:2247:GLN:NE2	2.46	0.49
1:D:359:TYR:HD2	1:D:361:ALA:HB2	1.77	0.49
1:D:2010:LEU:HD13	1:D:3657:TYR:HD1	1.77	0.49
1:D:4635:SER:O	1:D:4636:THR:C	2.49	0.49
1:A:959:TYR:HE2	1:A:966:LYS:HD2	1.78	0.49
1:A:3657:TYR:CE1	1:A:3660:ALA:HB3	2.48	0.49
1:B:717:ASP:OD1	1:B:720:HIS:HB2	2.13	0.49
1:B:2252:ASP:OD1	1:B:2252:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1104:TRP:NE1	1:C:1151:CYS:SG	2.85	0.49
1:C:3657:TYR:CE1	1:C:3660:ALA:HB3	2.48	0.49
1:C:3878:ASP:OD1	1:C:3879:GLU:N	2.45	0.49
1:D:1839:VAL:O	1:D:1841:VAL:N	2.46	0.49
1:D:2243:SER:HB3	1:D:2246:ASN:HD22	1.78	0.49
1:D:3657:TYR:CE1	1:D:3660:ALA:HB3	2.48	0.49
1:D:4340:ALA:O	1:D:4342:ALA:N	2.46	0.49
1:D:4633:GLU:CB	1:D:4639:MET:HG3	2.42	0.49
1:A:717:ASP:OD1	1:A:720:HIS:HB2	2.13	0.49
1:A:1735:ILE:HG13	1:A:1771:LEU:HD23	1.94	0.49
1:B:711:LEU:HB3	1:B:1532:ASN:ND2	2.27	0.49
1:B:4340:ALA:O	1:B:4342:ALA:N	2.46	0.49
1:C:40:GLU:H	1:C:44:ASN:HD21	1.60	0.49
1:C:290:TYR:O	1:C:302:VAL:N	2.46	0.49
1:C:959:TYR:HE2	1:C:966:LYS:HD2	1.78	0.49
1:D:290:TYR:O	1:D:302:VAL:N	2.46	0.49
1:D:959:TYR:HE2	1:D:966:LYS:HD2	1.78	0.49
1:D:1507:GLY:O	1:D:1508:ARG:NE	2.42	0.49
1:D:4049:VAL:HG11	1:D:4159:ARG:HB3	1.95	0.49
1:D:4634:GLU:HG3	1:D:4636:THR:CG2	2.32	0.49
1:A:1543:GLU:HB2	1:A:1544:PRO:HD3	1.95	0.48
1:B:4666:VAL:HA	1:B:4669:VAL:HG22	1.94	0.48
1:C:3285:TRP:NE1	1:C:3293:PRO:HG3	2.23	0.48
1:D:592:LYS:HG2	1:D:1580:PHE:CD2	2.49	0.48
1:D:1576:SER:HA	1:D:1579:MET:HG2	1.94	0.48
1:D:3385:ALA:HB1	1:D:3400:VAL:HG13	1.95	0.48
1:A:1653:LEU:HD13	1:A:1660:GLN:HA	1.94	0.48
1:A:4049:VAL:HG11	1:A:4159:ARG:HB3	1.95	0.48
1:B:893:TYR:OH	1:B:904:HIS:O	2.32	0.48
1:B:2223:ILE:O	1:B:2223:ILE:HG22	2.13	0.48
1:B:4049:VAL:HG11	1:B:4159:ARG:HB3	1.95	0.48
1:C:893:TYR:OH	1:C:904:HIS:O	2.32	0.48
1:C:2441:HIS:HA	1:C:2444:GLN:HG2	1.94	0.48
1:C:4635:SER:O	1:C:4636:THR:C	2.49	0.48
1:D:40:GLU:H	1:D:44:ASN:HD21	1.60	0.48
1:D:221:ARG:HH21	1:D:259:LEU:HD21	1.78	0.48
1:D:1458:HIS:CE1	1:D:1483:VAL:HG21	2.48	0.48
1:D:1653:LEU:HD13	1:D:1660:GLN:HA	1.94	0.48
1:D:4636:THR:C	1:D:4638:TYR:N	2.66	0.48
1:A:867:LEU:HD11	1:A:929:LEU:HD22	1.95	0.48
1:A:2463:LEU:HG	1:A:2464:ASP:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3569:LEU:HG	1:A:3574:ALA:HB3	1.95	0.48
1:A:3761:GLN:C	1:A:3763:LEU:H	2.17	0.48
1:A:4636:THR:C	1:A:4638:TYR:N	2.66	0.48
1:B:592:LYS:HG2	1:B:1580:PHE:CD2	2.49	0.48
1:B:1458:HIS:CE1	1:B:1483:VAL:HG21	2.48	0.48
1:B:2243:SER:HB3	1:B:2246:ASN:HD22	1.78	0.48
1:B:3657:TYR:CE1	1:B:3660:ALA:HB3	2.48	0.48
1:B:4126:GLU:O	1:B:4130:ASN:ND2	2.35	0.48
1:C:223:PHE:N	1:C:389:PHE:O	2.45	0.48
1:C:649:PHE:HB3	1:C:776:LEU:HD22	1.95	0.48
1:C:1576:SER:HA	1:C:1579:MET:HG2	1.94	0.48
1:C:4186:ALA:H	1:C:4188:ARG:HH22	1.60	0.48
1:D:565:TYR:CZ	1:D:569:ILE:HD11	2.49	0.48
1:D:867:LEU:HD11	1:D:929:LEU:HD22	1.95	0.48
1:D:2223:ILE:HG22	1:D:2223:ILE:O	2.13	0.48
1:D:2463:LEU:HG	1:D:2464:ASP:H	1.79	0.48
1:D:3761:GLN:C	1:D:3763:LEU:H	2.17	0.48
1:A:290:TYR:O	1:A:302:VAL:N	2.46	0.48
1:A:2223:ILE:HG22	1:A:2223:ILE:O	2.13	0.48
1:A:4999:ASP:N	1:A:4999:ASP:OD1	2.45	0.48
1:B:359:TYR:HD2	1:B:361:ALA:HB2	1.77	0.48
1:B:3163:VAL:HG12	1:B:3173:TYR:HD1	1.79	0.48
1:C:255:HIS:HB3	1:C:480:GLU:HG3	1.94	0.48
1:C:1139:PHE:HZ	1:C:1177:THR:HG22	1.79	0.48
1:C:3385:ALA:HB1	1:C:3400:VAL:HG13	1.95	0.48
1:C:4049:VAL:HG11	1:C:4159:ARG:HB3	1.95	0.48
1:D:649:PHE:HB3	1:D:776:LEU:HD22	1.95	0.48
1:D:717:ASP:OD1	1:D:720:HIS:HB2	2.13	0.48
1:D:1139:PHE:HZ	1:D:1177:THR:HG22	1.79	0.48
1:D:1252:HIS:CE1	1:D:1255:TYR:HD2	2.32	0.48
1:D:1543:GLU:HB2	1:D:1544:PRO:HD3	1.95	0.48
1:D:1735:ILE:HG13	1:D:1771:LEU:HD23	1.94	0.48
1:A:248:GLU:HG2	1:A:252:VAL:HG23	1.96	0.48
1:A:1139:PHE:HZ	1:A:1177:THR:HG22	1.79	0.48
1:A:3878:ASP:OD1	1:A:3879:GLU:N	2.45	0.48
1:A:4633:GLU:CB	1:A:4639:MET:HG3	2.42	0.48
1:B:248:GLU:HG2	1:B:252:VAL:HG23	1.96	0.48
1:B:255:HIS:HB3	1:B:480:GLU:HG3	1.94	0.48
1:B:1252:HIS:CE1	1:B:1255:TYR:HD2	2.32	0.48
1:B:3385:ALA:HB1	1:B:3400:VAL:HG13	1.95	0.48
1:B:3761:GLN:C	1:B:3763:LEU:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4999:ASP:OD1	1:B:4999:ASP:N	2.45	0.48
1:C:565:TYR:CZ	1:C:569:ILE:HD11	2.49	0.48
1:D:255:HIS:HB3	1:D:480:GLU:HG3	1.94	0.48
1:A:40:GLU:H	1:A:44:ASN:HD21	1.60	0.48
1:A:221:ARG:HH21	1:A:259:LEU:HD21	1.78	0.48
1:A:592:LYS:HG2	1:A:1580:PHE:CD2	2.49	0.48
1:A:874:LEU:HB2	1:A:1046:LEU:HD21	1.96	0.48
1:A:2243:SER:O	1:A:2247:GLN:NE2	2.46	0.48
1:A:2243:SER:HB3	1:A:2246:ASN:HD22	1.78	0.48
1:A:4186:ALA:H	1:A:4188:ARG:HH22	1.60	0.48
1:C:37:LEU:HD13	1:C:191:VAL:HG21	1.95	0.48
1:C:592:LYS:HG2	1:C:1580:PHE:CD2	2.49	0.48
1:C:717:ASP:OD1	1:C:720:HIS:HB2	2.13	0.48
1:C:3343:GLN:O	1:C:3347:SER:OG	2.25	0.48
1:D:886:ARG:NH1	1:D:889:GLN:OE1	2.47	0.48
1:A:2010:LEU:HD13	1:A:3657:TYR:HD1	1.77	0.48
1:B:41:GLY:O	1:B:45:ARG:NH1	2.47	0.48
1:B:290:TYR:O	1:B:302:VAL:N	2.46	0.48
1:B:1543:GLU:HB2	1:B:1544:PRO:HD3	1.95	0.48
1:B:1576:SER:HA	1:B:1579:MET:HG2	1.94	0.48
1:B:3569:LEU:HG	1:B:3574:ALA:HB3	1.95	0.48
1:D:1861:GLN:HA	1:D:1864:LYS:HE3	1.95	0.48
1:A:234:SER:OG	1:A:240:ASP:OD2	2.27	0.48
1:A:1507:GLY:O	1:A:1508:ARG:NE	2.42	0.48
1:A:1861:GLN:HA	1:A:1864:LYS:HE3	1.95	0.48
1:A:2220:THR:HA	1:A:2223:ILE:HD11	1.96	0.48
1:A:4837:LEU:HD11	1:A:4932:ILE:HG23	1.96	0.48
1:B:2131:LEU:HB2	1:B:3662:ILE:CG1	2.44	0.48
1:B:3343:GLN:O	1:B:3347:SER:OG	2.25	0.48
1:B:4636:THR:C	1:B:4638:TYR:N	2.66	0.48
1:C:1295:VAL:O	1:C:1453:VAL:HA	2.14	0.48
1:C:1458:HIS:CE1	1:C:1483:VAL:HG21	2.48	0.48
1:C:2463:LEU:HG	1:C:2464:ASP:H	1.79	0.48
1:C:4320:ARG:CZ	1:C:4320:ARG:HB3	2.42	0.48
1:D:2207:VAL:HA	1:D:2210:VAL:HG12	1.96	0.48
1:A:2252:ASP:N	1:A:2252:ASP:OD1	2.45	0.48
1:A:3051:ARG:NH2	1:A:3179:LYS:O	2.44	0.48
1:B:37:LEU:HD13	1:B:191:VAL:HG21	1.95	0.48
1:B:1219:LEU:HD11	1:C:3528:THR:HG23	1.96	0.48
1:B:2463:LEU:HG	1:B:2464:ASP:H	1.79	0.48
1:B:2586:VAL:HG22	1:B:2591:ARG:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:822:ARG:HH21	1:C:1626:TRP:HB3	1.79	0.48
1:C:1219:LEU:HD11	1:D:3528:THR:HG23	1.96	0.48
1:C:1861:GLN:HA	1:C:1864:LYS:HE3	1.95	0.48
1:C:2207:VAL:HA	1:C:2210:VAL:HG12	1.96	0.48
1:C:2457:LEU:HD21	1:C:2505:PHE:CE1	2.49	0.48
1:C:4340:ALA:O	1:C:4342:ALA:N	2.46	0.48
1:D:37:LEU:HD13	1:D:191:VAL:HG21	1.95	0.48
1:D:822:ARG:HH21	1:D:1626:TRP:HB3	1.79	0.48
1:D:1453:VAL:HG23	1:D:1454:THR:N	2.28	0.48
1:A:1458:HIS:CE1	1:A:1483:VAL:HG21	2.48	0.48
1:A:2457:LEU:HD21	1:A:2505:PHE:CE1	2.49	0.48
1:C:41:GLY:O	1:C:45:ARG:NH1	2.47	0.48
1:C:221:ARG:HH21	1:C:259:LEU:HD21	1.78	0.48
1:C:886:ARG:NH1	1:C:889:GLN:OE1	2.47	0.48
1:C:1218:GLY:HA2	1:C:1223:PHE:HB2	1.96	0.48
1:C:2010:LEU:HD13	1:C:3657:TYR:HD1	1.77	0.48
1:C:2181:SER:O	1:C:2185:ILE:HG12	2.14	0.48
1:C:2243:SER:HB3	1:C:2246:ASN:HD22	1.78	0.48
1:C:4104:THR:HG22	1:C:4106:PRO:HD2	1.96	0.48
1:C:4219:PHE:CD1	1:C:4950:VAL:HG21	2.49	0.48
1:D:41:GLY:O	1:D:45:ARG:NH1	2.47	0.48
1:D:2174:GLU:OE1	1:D:2174:GLU:N	2.39	0.48
1:D:2457:LEU:HD21	1:D:2505:PHE:CE1	2.49	0.48
1:D:4837:LEU:HD11	1:D:4932:ILE:HG23	1.96	0.48
1:A:1833:SER:O	1:A:1834:VAL:C	2.51	0.47
1:A:2586:VAL:HG22	1:A:2591:ARG:HB2	1.96	0.47
1:B:867:LEU:HD11	1:B:929:LEU:HD22	1.95	0.47
1:B:886:ARG:NH1	1:B:889:GLN:OE1	2.47	0.47
1:B:1861:GLN:HA	1:B:1864:LYS:HE3	1.95	0.47
1:B:2010:LEU:HD13	1:B:3657:TYR:HD1	1.77	0.47
1:B:2457:LEU:HD21	1:B:2505:PHE:CE1	2.49	0.47
1:B:4104:THR:HG22	1:B:4106:PRO:HD2	1.96	0.47
1:C:2223:ILE:O	1:C:2223:ILE:HG22	2.13	0.47
1:C:4114:CYS:O	1:C:4131:ARG:NH2	2.47	0.47
1:D:4114:CYS:O	1:D:4131:ARG:NH2	2.47	0.47
1:A:571:SER:O	1:A:574:VAL:HG12	2.15	0.47
1:A:668:VAL:HG11	1:A:738:LEU:HD12	1.96	0.47
1:A:1218:GLY:HA2	1:A:1223:PHE:HB2	1.96	0.47
1:A:3558:HIS:CE1	1:A:3593:VAL:HG22	2.49	0.47
1:B:4186:ALA:H	1:B:4188:ARG:HH22	1.60	0.47
1:C:1683:HIS:CD2	1:C:1800:PRO:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4837:LEU:HD11	1:C:4932:ILE:HG23	1.96	0.47
1:D:874:LEU:HB2	1:D:1046:LEU:HD21	1.96	0.47
1:D:2252:ASP:OD1	1:D:2252:ASP:N	2.45	0.47
1:D:3163:VAL:HG12	1:D:3173:TYR:HD1	1.79	0.47
1:A:37:LEU:HD13	1:A:191:VAL:HG21	1.95	0.47
1:A:1252:HIS:CE1	1:A:1255:TYR:HD2	2.32	0.47
1:A:3163:VAL:HG12	1:A:3173:TYR:HD1	1.79	0.47
1:B:19:GLU:HB2	1:B:206:CYS:HB3	1.96	0.47
1:B:1658:ASP:OD1	1:B:1658:ASP:N	2.46	0.47
1:B:4696:ASP:OD1	1:B:4696:ASP:N	2.40	0.47
1:C:2174:GLU:OE1	1:C:2174:GLU:N	2.39	0.47
1:D:893:TYR:OH	1:D:904:HIS:O	2.32	0.47
1:D:1218:GLY:HA2	1:D:1223:PHE:HB2	1.96	0.47
1:D:2220:THR:HA	1:D:2223:ILE:HD11	1.96	0.47
1:D:3285:TRP:NE1	1:D:3293:PRO:HG3	2.23	0.47
1:D:4219:PHE:CD1	1:D:4950:VAL:HG21	2.49	0.47
1:A:1295:VAL:O	1:A:1453:VAL:HA	2.14	0.47
1:A:4114:CYS:O	1:A:4131:ARG:NH2	2.47	0.47
1:B:565:TYR:CZ	1:B:569:ILE:HD11	2.49	0.47
1:B:1683:HIS:CD2	1:B:1800:PRO:HG3	2.49	0.47
1:B:4837:LEU:HD11	1:B:4932:ILE:HG23	1.96	0.47
1:C:665:GLU:OE1	1:C:745:SER:OG	2.23	0.47
1:C:1252:HIS:CE1	1:C:1255:TYR:HD2	2.32	0.47
1:C:1543:GLU:HB2	1:C:1544:PRO:HD3	1.95	0.47
1:C:3569:LEU:HG	1:C:3574:ALA:HB3	1.95	0.47
1:D:793:LEU:HG	1:D:795:GLY:H	1.79	0.47
1:D:3838:THR:O	1:D:3838:THR:OG1	2.29	0.47
1:A:565:TYR:CZ	1:A:569:ILE:HD11	2.49	0.47
1:A:893:TYR:OH	1:A:904:HIS:O	2.32	0.47
1:A:2181:SER:O	1:A:2185:ILE:HG12	2.14	0.47
1:A:4219:PHE:CD1	1:A:4950:VAL:HG21	2.49	0.47
1:B:1833:SER:O	1:B:1834:VAL:C	2.51	0.47
1:B:2220:THR:HA	1:B:2223:ILE:HD11	1.96	0.47
1:B:4119:GLU:HG2	1:B:4121:GLU:HG2	1.97	0.47
1:B:4219:PHE:CD1	1:B:4950:VAL:HG21	2.49	0.47
1:B:4907:ASP:O	1:B:4909:TYR:N	2.48	0.47
1:B:4908:GLU:H	1:B:4908:GLU:HG3	1.34	0.47
1:C:1653:LEU:HB3	1:C:1660:GLN:HB2	1.97	0.47
1:C:1658:ASP:OD1	1:C:1658:ASP:N	2.46	0.47
1:C:2316:LYS:HE2	1:C:2318:TYR:HE2	1.79	0.47
1:D:207:SER:HB3	1:D:334:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4186:ALA:H	1:D:4188:ARG:HH22	1.60	0.47
1:A:19:GLU:HB2	1:A:206:CYS:HB3	1.96	0.47
1:A:41:GLY:O	1:A:45:ARG:NH1	2.47	0.47
1:A:1219:LEU:HD11	1:B:3528:THR:HG23	1.96	0.47
1:A:2131:LEU:HB2	1:A:3662:ILE:CG1	2.44	0.47
1:A:3528:THR:HG23	1:D:1219:LEU:HD11	1.96	0.47
1:A:4126:GLU:O	1:A:4130:ASN:ND2	2.35	0.47
1:A:4904:PRO:O	1:A:4910:GLU:HG3	2.15	0.47
1:B:822:ARG:HH21	1:B:1626:TRP:HB3	1.79	0.47
1:B:874:LEU:HB2	1:B:1046:LEU:HD21	1.96	0.47
1:B:1218:GLY:HA2	1:B:1223:PHE:HB2	1.96	0.47
1:B:1295:VAL:O	1:B:1453:VAL:HA	2.14	0.47
1:B:1708:ARG:HH12	1:B:1837:GLN:HA	1.80	0.47
1:B:3174:SER:OG	1:B:3175:LEU:N	2.48	0.47
1:B:4904:PRO:O	1:B:4910:GLU:HG3	2.15	0.47
1:C:248:GLU:HG2	1:C:252:VAL:HG23	1.96	0.47
1:C:1208:VAL:HA	1:D:3573:MET:CE	2.45	0.47
1:C:3163:VAL:HG12	1:C:3173:TYR:HD1	1.79	0.47
1:D:3569:LEU:HG	1:D:3574:ALA:HB3	1.95	0.47
1:D:3927:GLN:HB3	1:D:3992:PHE:CE2	2.50	0.47
1:D:4633:GLU:HG3	1:D:4637:GLY:H	1.80	0.47
1:D:4907:ASP:O	1:D:4909:TYR:N	2.48	0.47
1:A:822:ARG:HH21	1:A:1626:TRP:HB3	1.79	0.47
1:A:1683:HIS:CD2	1:A:1800:PRO:HG3	2.49	0.47
1:A:2512:ILE:O	1:A:2512:ILE:HG13	2.15	0.47
1:A:3573:MET:CE	1:D:1208:VAL:HA	2.45	0.47
1:A:4807:PHE:O	1:A:4810:ALA:N	2.48	0.47
1:A:4825:THR:O	1:A:4828:SER:OG	2.23	0.47
1:B:1653:LEU:HB3	1:B:1660:GLN:HB2	1.97	0.47
1:B:2316:LYS:HE2	1:B:2318:TYR:HE2	1.79	0.47
1:B:4968:PHE:O	1:B:4975:PHE:N	2.48	0.47
1:C:793:LEU:HG	1:C:795:GLY:H	1.79	0.47
1:C:2220:THR:HA	1:C:2223:ILE:HD11	1.96	0.47
1:C:4908:GLU:H	1:C:4908:GLU:HG3	1.34	0.47
1:D:234:SER:OG	1:D:240:ASP:OD2	2.27	0.47
1:D:248:GLU:HG2	1:D:252:VAL:HG23	1.96	0.47
1:D:1108:GLU:OE1	1:D:1108:GLU:N	2.48	0.47
1:D:1683:HIS:CD2	1:D:1800:PRO:HG3	2.49	0.47
1:D:4104:THR:HG22	1:D:4106:PRO:HD2	1.96	0.47
1:D:4580:TYR:HD2	1:D:4807:PHE:CZ	2.33	0.47
1:A:886:ARG:NH1	1:A:889:GLN:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1708:ARG:HH12	1:A:1837:GLN:HA	1.80	0.47
1:A:3927:GLN:HB3	1:A:3992:PHE:CE2	2.50	0.47
1:A:5035:GLN:O	1:A:5036:LEU:HD22	2.15	0.47
1:B:571:SER:O	1:B:574:VAL:HG12	2.15	0.47
1:B:2181:SER:O	1:B:2185:ILE:HG12	2.14	0.47
1:B:3558:HIS:CE1	1:B:3593:VAL:HG22	2.49	0.47
1:B:3927:GLN:HB3	1:B:3992:PHE:CE2	2.50	0.47
1:C:867:LEU:HD11	1:C:929:LEU:HD22	1.95	0.47
1:C:1694:LEU:HB3	1:C:1715:LEU:HD12	1.96	0.47
1:C:2252:ASP:N	1:C:2252:ASP:OD1	2.45	0.47
1:C:4907:ASP:O	1:C:4909:TYR:N	2.48	0.47
1:D:590:LEU:HB2	1:D:599:VAL:HG11	1.97	0.47
1:D:1295:VAL:O	1:D:1453:VAL:HA	2.14	0.47
1:D:1694:LEU:HB3	1:D:1715:LEU:HD12	1.96	0.47
1:D:2512:ILE:O	1:D:2512:ILE:HG13	2.15	0.47
1:D:3558:HIS:CE1	1:D:3593:VAL:HG22	2.49	0.47
1:A:793:LEU:HG	1:A:795:GLY:H	1.79	0.47
1:A:1079:LYS:NZ	1:A:1655:GLU:OE2	2.35	0.47
1:A:1653:LEU:HB3	1:A:1660:GLN:HB2	1.97	0.47
1:B:668:VAL:HG11	1:B:738:LEU:HD12	1.96	0.47
1:B:2174:GLU:OE1	1:B:2174:GLU:N	2.39	0.47
1:B:2512:ILE:HG13	1:B:2512:ILE:O	2.15	0.47
1:B:4569:LEU:HD22	1:B:4646:LEU:HD22	1.97	0.47
1:C:192:ASP:N	1:C:192:ASP:OD1	2.48	0.47
1:C:207:SER:HB3	1:C:334:MET:SD	2.55	0.47
1:C:571:SER:O	1:C:574:VAL:HG12	2.15	0.47
1:C:1833:SER:O	1:C:1834:VAL:C	2.51	0.47
1:C:2131:LEU:HB2	1:C:3662:ILE:CG1	2.44	0.47
1:C:2512:ILE:HG13	1:C:2512:ILE:O	2.15	0.47
1:C:4098:ASP:OD1	1:C:4098:ASP:N	2.41	0.47
1:C:4569:LEU:HD22	1:C:4646:LEU:HD22	1.97	0.47
1:C:4633:GLU:HG3	1:C:4637:GLY:H	1.80	0.47
1:D:1658:ASP:OD1	1:D:1658:ASP:N	2.46	0.47
1:D:2340:PHE:HD1	1:D:2435:ARG:HG3	1.79	0.47
1:A:2207:VAL:HA	1:A:2210:VAL:HG12	1.96	0.47
1:A:2316:LYS:HE2	1:A:2318:TYR:HE2	1.79	0.47
1:A:2340:PHE:HD1	1:A:2435:ARG:HG3	1.79	0.47
1:A:3174:SER:OG	1:A:3175:LEU:N	2.48	0.47
1:A:4580:TYR:HD2	1:A:4807:PHE:CZ	2.33	0.47
1:A:4634:GLU:HG3	1:A:4636:THR:CG2	2.32	0.47
1:A:4814:LEU:HD21	1:D:4850:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:977:LEU:HD12	1:B:978:THR:H	1.80	0.47
1:B:4339:VAL:HG21	1:B:4816:ILE:HD11	1.97	0.47
1:C:2131:LEU:HD12	1:C:3662:ILE:HG13	1.97	0.47
1:C:3927:GLN:HB3	1:C:3992:PHE:CE2	2.50	0.47
1:C:4580:TYR:HD2	1:C:4807:PHE:CZ	2.33	0.47
1:D:2131:LEU:HD12	1:D:3662:ILE:HG13	1.97	0.47
1:D:4085:ARG:NH1	1:D:4087:LEU:HD12	2.29	0.47
1:A:4339:VAL:HG21	1:A:4816:ILE:HD11	1.97	0.46
1:A:4907:ASP:O	1:A:4909:TYR:N	2.48	0.46
1:B:61:ASP:OD1	1:B:61:ASP:N	2.48	0.46
1:B:192:ASP:N	1:B:192:ASP:OD1	2.48	0.46
1:B:221:ARG:HH21	1:B:259:LEU:HD21	1.78	0.46
1:B:1208:VAL:HA	1:C:3573:MET:CE	2.45	0.46
1:B:2207:VAL:HA	1:B:2210:VAL:HG12	1.96	0.46
1:B:4796:MET:O	1:B:4799:SER:OG	2.27	0.46
1:C:61:ASP:OD1	1:C:61:ASP:N	2.48	0.46
1:C:874:LEU:HB2	1:C:1046:LEU:HD21	1.96	0.46
1:C:2368:LEU:HD13	1:C:2376:LEU:HB2	1.97	0.46
1:C:3761:GLN:C	1:C:3763:LEU:H	2.17	0.46
1:C:4119:GLU:HG2	1:C:4121:GLU:HG2	1.97	0.46
1:C:4960:ILE:HD11	1:C:4985:LEU:HB3	1.97	0.46
1:D:4321:ARG:HG2	1:D:4321:ARG:NH1	2.31	0.46
1:D:4968:PHE:O	1:D:4975:PHE:N	2.48	0.46
1:A:192:ASP:OD1	1:A:192:ASP:N	2.48	0.46
1:B:207:SER:HB3	1:B:334:MET:SD	2.55	0.46
1:B:871:ARG:HH22	1:B:918:ARG:NH1	2.13	0.46
1:B:871:ARG:NH2	1:B:918:ARG:HH22	2.14	0.46
1:B:2368:LEU:HD13	1:B:2376:LEU:HB2	1.97	0.46
1:B:3051:ARG:NH2	1:B:3179:LYS:O	2.44	0.46
1:B:4321:ARG:HG2	1:B:4321:ARG:NH1	2.31	0.46
1:C:1079:LYS:NZ	1:C:1655:GLU:OE2	2.35	0.46
1:C:2586:VAL:HG22	1:C:2591:ARG:HB2	1.96	0.46
1:C:4850:LEU:HD22	1:D:4814:LEU:HD21	1.97	0.46
1:C:5035:GLN:O	1:C:5036:LEU:HD22	2.15	0.46
1:D:1866:ILE:C	1:D:1868:PRO:HD2	2.36	0.46
1:D:2181:SER:O	1:D:2185:ILE:HG12	2.14	0.46
1:D:4904:PRO:O	1:D:4910:GLU:HG3	2.15	0.46
1:A:61:ASP:OD1	1:A:61:ASP:N	2.48	0.46
1:A:207:SER:HB3	1:A:334:MET:SD	2.55	0.46
1:A:590:LEU:HB2	1:A:599:VAL:HG11	1.97	0.46
1:A:1126:GLY:HA3	1:A:1143:TRP:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2301:TYR:HB3	1:A:2331:TYR:CE2	2.51	0.46
1:A:4321:ARG:HG2	1:A:4321:ARG:NH1	2.31	0.46
1:B:2301:TYR:HB3	1:B:2331:TYR:CE2	2.51	0.46
1:B:4807:PHE:O	1:B:4810:ALA:N	2.48	0.46
1:C:19:GLU:HB2	1:C:206:CYS:HB3	1.96	0.46
1:C:793:LEU:HD23	1:C:793:LEU:H	1.80	0.46
1:C:1083:VAL:HG21	1:C:1088:TRP:CE2	2.51	0.46
1:C:1126:GLY:HA3	1:C:1143:TRP:CD2	2.50	0.46
1:C:4321:ARG:HG2	1:C:4321:ARG:NH1	2.31	0.46
1:C:4339:VAL:HG21	1:C:4816:ILE:HD11	1.97	0.46
1:D:4339:VAL:HG21	1:D:4816:ILE:HD11	1.97	0.46
1:D:4807:PHE:O	1:D:4810:ALA:N	2.48	0.46
1:D:5035:GLN:O	1:D:5036:LEU:HD22	2.15	0.46
1:A:960:MET:HA	1:A:960:MET:HE3	1.98	0.46
1:A:1208:VAL:HA	1:B:3573:MET:CE	2.45	0.46
1:B:618:GLN:NE2	1:B:1675:ALA:H	2.14	0.46
1:B:793:LEU:H	1:B:793:LEU:HD23	1.80	0.46
1:B:1079:LYS:NZ	1:B:1655:GLU:OE2	2.35	0.46
1:B:2302:LEU:HD11	1:B:2332:LEU:HB2	1.97	0.46
1:B:3285:TRP:NE1	1:B:3293:PRO:HG3	2.23	0.46
1:B:4633:GLU:HG3	1:B:4637:GLY:H	1.80	0.46
1:C:668:VAL:HG11	1:C:738:LEU:HD12	1.96	0.46
1:C:871:ARG:NH2	1:C:918:ARG:HH22	2.14	0.46
1:C:3721:LEU:HD11	1:C:3725:TYR:HE2	1.80	0.46
1:C:4085:ARG:NH1	1:C:4087:LEU:HD12	2.29	0.46
1:D:1832:GLY:O	1:D:1833:SER:CB	2.64	0.46
1:D:2368:LEU:HD13	1:D:2376:LEU:HB2	1.97	0.46
1:D:2586:VAL:HG22	1:D:2591:ARG:HB2	1.96	0.46
1:D:4960:ILE:HD11	1:D:4985:LEU:HB3	1.97	0.46
1:A:209:CYS:HG	1:A:210:GLU:N	2.12	0.46
1:A:460:GLN:HB2	1:A:463:GLU:OE2	2.16	0.46
1:A:4104:THR:HG22	1:A:4106:PRO:HD2	1.96	0.46
1:A:4633:GLU:HG3	1:A:4637:GLY:H	1.80	0.46
1:A:4968:PHE:O	1:A:4975:PHE:N	2.48	0.46
1:B:1126:GLY:HA3	1:B:1143:TRP:CD2	2.50	0.46
1:B:1139:PHE:HZ	1:B:1177:THR:HG22	1.79	0.46
1:B:3721:LEU:HD11	1:B:3725:TYR:HE2	1.80	0.46
1:B:4580:TYR:HD2	1:B:4807:PHE:CZ	2.33	0.46
1:C:590:LEU:HB2	1:C:599:VAL:HG11	1.97	0.46
1:C:4968:PHE:O	1:C:4975:PHE:N	2.48	0.46
1:D:668:VAL:HG11	1:D:738:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:793:LEU:HD23	1:D:793:LEU:H	1.80	0.46
1:D:977:LEU:HD12	1:D:978:THR:H	1.80	0.46
1:D:1653:LEU:HB3	1:D:1660:GLN:HB2	1.97	0.46
1:D:2302:LEU:HD11	1:D:2332:LEU:HB2	1.97	0.46
1:A:4085:ARG:NH1	1:A:4087:LEU:HD12	2.29	0.46
1:A:4817:ALA:C	1:A:4819:GLY:N	2.66	0.46
1:B:793:LEU:HG	1:B:795:GLY:H	1.79	0.46
1:B:2142:TYR:CG	1:B:2197:LEU:HD13	2.50	0.46
1:B:4114:CYS:O	1:B:4131:ARG:NH2	2.47	0.46
1:C:3558:HIS:CE1	1:C:3593:VAL:HG22	2.49	0.46
1:D:167:ASP:N	1:D:167:ASP:OD1	2.48	0.46
1:D:169:LEU:HD13	1:D:202:MET:HE1	1.98	0.46
1:D:460:GLN:HB2	1:D:463:GLU:OE2	2.16	0.46
1:D:1083:VAL:HG21	1:D:1088:TRP:CE2	2.51	0.46
1:D:2142:TYR:CG	1:D:2197:LEU:HD13	2.50	0.46
1:D:4060:LYS:NZ	1:D:4107:GLU:OE2	2.39	0.46
1:D:4569:LEU:HD22	1:D:4646:LEU:HD22	1.97	0.46
1:A:1463:ASN:N	1:A:1492:CYS:SG	2.82	0.46
1:A:1658:ASP:OD1	1:A:1658:ASP:N	2.46	0.46
1:A:2368:LEU:HD13	1:A:2376:LEU:HB2	1.97	0.46
1:A:4960:ILE:HD11	1:A:4985:LEU:HB3	1.97	0.46
1:B:1083:VAL:HG21	1:B:1088:TRP:CE2	2.51	0.46
1:B:2131:LEU:HD12	1:B:3662:ILE:HG13	1.97	0.46
1:C:871:ARG:HH22	1:C:918:ARG:NH1	2.13	0.46
1:C:2301:TYR:HB3	1:C:2331:TYR:CE2	2.51	0.46
1:D:481:GLU:OE1	1:D:481:GLU:N	2.49	0.46
1:D:1970:GLN:NE2	1:D:3641:LEU:O	2.36	0.46
1:D:2301:TYR:HB3	1:D:2331:TYR:CE2	2.51	0.46
1:D:2316:LYS:HE2	1:D:2318:TYR:HE2	1.79	0.46
1:A:414:PHE:HD1	1:A:437:PRO:HD2	1.81	0.46
1:A:793:LEU:HD23	1:A:793:LEU:H	1.80	0.46
1:A:871:ARG:NH2	1:A:918:ARG:HH22	2.14	0.46
1:A:977:LEU:HD12	1:A:978:THR:H	1.80	0.46
1:A:1079:LYS:HG3	1:A:1655:GLU:OE2	2.16	0.46
1:A:1108:GLU:OE1	1:A:1108:GLU:N	2.48	0.46
1:A:1694:LEU:HB3	1:A:1715:LEU:HD12	1.96	0.46
1:A:3645:PRO:HB2	1:A:3647:HIS:HD1	1.81	0.46
1:A:4569:LEU:HD22	1:A:4646:LEU:HD22	1.97	0.46
1:B:5035:GLN:O	1:B:5036:LEU:HD22	2.15	0.46
1:C:414:PHE:HD1	1:C:437:PRO:HD2	1.81	0.46
1:C:460:GLN:HB2	1:C:463:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2340:PHE:HD1	1:C:2435:ARG:HG3	1.79	0.46
1:C:4825:THR:O	1:C:4828:SER:OG	2.23	0.46
1:D:571:SER:O	1:D:574:VAL:HG12	2.15	0.46
1:D:1111:PRO:HD3	1:D:1605:TRP:HE1	1.81	0.46
1:D:1126:GLY:HA3	1:D:1143:TRP:CD2	2.50	0.46
1:D:2131:LEU:HB2	1:D:3662:ILE:CG1	2.44	0.46
1:D:4814:LEU:C	1:D:4816:ILE:N	2.69	0.46
1:A:1238:PHE:CD1	1:A:1608:MET:HG2	2.51	0.46
1:B:460:GLN:HB2	1:B:463:GLU:OE2	2.16	0.46
1:B:1434:TYR:HA	1:B:1449:TRP:HB3	1.98	0.46
1:B:2340:PHE:HD1	1:B:2435:ARG:HG3	1.79	0.46
1:B:3014:CYS:SG	1:B:3015:LEU:N	2.89	0.46
1:C:132:ALA:O	1:C:194:SER:OG	2.34	0.46
1:C:871:ARG:NE	1:C:925:SER:OG	2.49	0.46
1:C:977:LEU:HD12	1:C:978:THR:H	1.80	0.46
1:C:1708:ARG:HH12	1:C:1837:GLN:HA	1.80	0.46
1:C:1866:ILE:C	1:C:1868:PRO:HD2	2.36	0.46
1:C:3174:SER:OG	1:C:3175:LEU:N	2.48	0.46
1:C:4807:PHE:O	1:C:4810:ALA:N	2.48	0.46
1:C:4923:PHE:O	1:C:4928:LEU:HD23	2.16	0.46
1:D:871:ARG:NE	1:D:925:SER:OG	2.49	0.46
1:D:1708:ARG:HH12	1:D:1837:GLN:HA	1.80	0.46
1:D:4119:GLU:HG2	1:D:4121:GLU:HG2	1.97	0.46
1:D:4634:GLU:C	1:D:4636:THR:H	2.19	0.46
1:A:688:LEU:H	1:A:688:LEU:HD23	1.81	0.46
1:A:2142:TYR:CG	1:A:2197:LEU:HD13	2.50	0.46
1:A:3014:CYS:SG	1:A:3015:LEU:N	2.89	0.46
1:B:132:ALA:O	1:B:194:SER:OG	2.34	0.46
1:B:1694:LEU:HB3	1:B:1715:LEU:HD12	1.96	0.46
1:B:4850:LEU:HD22	1:C:4814:LEU:HD21	1.97	0.46
1:C:1106:ARG:NH2	1:C:1183:GLU:OE2	2.49	0.46
1:C:1111:PRO:HD3	1:C:1605:TRP:HE1	1.81	0.46
1:C:1238:PHE:CD1	1:C:1608:MET:HG2	2.51	0.46
1:D:400:ALA:O	1:D:404:ILE:HG13	2.16	0.46
1:D:4067:LYS:HD3	1:D:4102:GLN:HG3	1.98	0.46
1:A:1083:VAL:HG21	1:A:1088:TRP:CE2	2.51	0.45
1:A:1111:PRO:HD3	1:A:1605:TRP:HE1	1.81	0.45
1:A:1453:VAL:HG23	1:A:1454:THR:N	2.28	0.45
1:A:1832:GLY:O	1:A:1833:SER:CB	2.64	0.45
1:B:167:ASP:N	1:B:167:ASP:OD1	2.48	0.45
1:B:590:LEU:HB2	1:B:599:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1001:VAL:HA	1:B:1020:ARG:NH2	2.31	0.45
1:B:3645:PRO:HB2	1:B:3647:HIS:HD1	1.81	0.45
1:B:4085:ARG:NH1	1:B:4087:LEU:HD12	2.29	0.45
1:C:4067:LYS:HD3	1:C:4102:GLN:HG3	1.98	0.45
1:D:3014:CYS:SG	1:D:3015:LEU:N	2.89	0.45
1:D:3555:ASN:HA	1:D:3558:HIS:HD1	1.82	0.45
1:A:871:ARG:NE	1:A:925:SER:OG	2.49	0.45
1:A:1001:VAL:HA	1:A:1020:ARG:NH2	2.31	0.45
1:A:1866:ILE:C	1:A:1868:PRO:HD2	2.36	0.45
1:A:2131:LEU:HD12	1:A:3662:ILE:HG13	1.97	0.45
1:A:3721:LEU:HD11	1:A:3725:TYR:HE2	1.80	0.45
1:A:4879:MET:HG2	1:B:4578:LEU:HA	1.99	0.45
1:B:414:PHE:HD1	1:B:437:PRO:HD2	1.81	0.45
1:B:481:GLU:OE1	1:B:481:GLU:N	2.49	0.45
1:B:1866:ILE:C	1:B:1868:PRO:HD2	2.36	0.45
1:B:4923:PHE:O	1:B:4928:LEU:HD23	2.16	0.45
1:C:430:PRO:HA	1:C:431:PRO:HD3	1.86	0.45
1:C:1453:VAL:HG23	1:C:1454:THR:N	2.28	0.45
1:C:1495:VAL:HG11	1:C:1536:SER:O	2.16	0.45
1:C:4634:GLU:C	1:C:4636:THR:H	2.19	0.45
1:C:4796:MET:O	1:C:4799:SER:OG	2.27	0.45
1:C:4904:PRO:O	1:C:4910:GLU:HG3	2.15	0.45
1:D:192:ASP:OD1	1:D:192:ASP:N	2.48	0.45
1:D:1457:TYR:O	1:D:1497:GLY:N	2.47	0.45
1:D:1463:ASN:N	1:D:1492:CYS:SG	2.82	0.45
1:D:3174:SER:OG	1:D:3175:LEU:N	2.48	0.45
1:A:2302:LEU:HD11	1:A:2332:LEU:HB2	1.97	0.45
1:A:4067:LYS:HD3	1:A:4102:GLN:HG3	1.98	0.45
1:A:4578:LEU:HA	1:D:4879:MET:HG2	1.99	0.45
1:B:213:TYR:CZ	1:B:337:PRO:HB2	2.52	0.45
1:B:400:ALA:O	1:B:404:ILE:HG13	2.16	0.45
1:B:871:ARG:NE	1:B:925:SER:OG	2.49	0.45
1:B:960:MET:HA	1:B:960:MET:HE3	1.99	0.45
1:B:4634:GLU:HG3	1:B:4636:THR:CG2	2.32	0.45
1:C:481:GLU:OE1	1:C:481:GLU:N	2.49	0.45
1:C:1079:LYS:HG3	1:C:1655:GLU:OE2	2.16	0.45
1:C:1161:ILE:HA	1:C:1177:THR:OG1	2.16	0.45
1:D:213:TYR:CZ	1:D:337:PRO:HB2	2.52	0.45
1:D:484:LEU:HD11	1:D:526:LEU:HD12	1.99	0.45
1:D:688:LEU:HD23	1:D:688:LEU:H	1.81	0.45
1:D:4763:GLY:HA3	1:D:4767:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ALA:O	1:A:194:SER:OG	2.34	0.45
1:A:213:TYR:CZ	1:A:337:PRO:HB2	2.52	0.45
1:A:484:LEU:HD11	1:A:526:LEU:HD12	1.99	0.45
1:A:1176:GLU:O	1:A:1180:ARG:NH2	2.44	0.45
1:B:4067:LYS:HD3	1:B:4102:GLN:HG3	1.98	0.45
1:C:688:LEU:HD23	1:C:688:LEU:H	1.81	0.45
1:C:1108:GLU:OE1	1:C:1108:GLU:N	2.48	0.45
1:C:3645:PRO:HB2	1:C:3647:HIS:HD1	1.81	0.45
1:C:4687:TYR:OH	1:C:4699:GLY:O	2.20	0.45
1:C:4698:LYS:HD3	1:C:4698:LYS:HA	1.72	0.45
1:C:4763:GLY:HA3	1:C:4767:TRP:CE2	2.52	0.45
1:D:19:GLU:HB2	1:D:206:CYS:HB3	1.96	0.45
1:D:871:ARG:NH2	1:D:918:ARG:HH22	2.14	0.45
1:D:1079:LYS:HG3	1:D:1655:GLU:OE2	2.16	0.45
1:D:4923:PHE:O	1:D:4928:LEU:HD23	2.16	0.45
1:A:914:PRO:HB2	1:A:916:PRO:HD2	1.99	0.45
1:A:3143:LEU:HD13	1:A:3146:HIS:HE1	1.81	0.45
1:A:4763:GLY:HA3	1:A:4767:TRP:CE2	2.52	0.45
1:A:4850:LEU:HD22	1:B:4814:LEU:HD21	1.97	0.45
1:B:914:PRO:HB2	1:B:916:PRO:HD2	1.99	0.45
1:B:1079:LYS:HG3	1:B:1655:GLU:OE2	2.16	0.45
1:B:1115:LEU:HG	1:B:1123:VAL:HG11	1.99	0.45
1:B:1457:TYR:O	1:B:1497:GLY:N	2.47	0.45
1:C:484:LEU:HD11	1:C:526:LEU:HD12	1.99	0.45
1:C:618:GLN:NE2	1:C:1675:ALA:H	2.14	0.45
1:A:167:ASP:N	1:A:167:ASP:OD1	2.48	0.45
1:A:1842:LEU:HD12	1:A:1842:LEU:HA	1.77	0.45
1:A:3285:TRP:NE1	1:A:3293:PRO:HG3	2.23	0.45
1:A:4322:LEU:HD23	1:A:4322:LEU:HA	1.84	0.45
1:B:1106:ARG:NH2	1:B:1183:GLU:OE2	2.49	0.45
1:B:1238:PHE:CD1	1:B:1608:MET:HG2	2.51	0.45
1:B:1495:VAL:HG11	1:B:1536:SER:O	2.16	0.45
1:C:2142:TYR:CG	1:C:2197:LEU:HD13	2.50	0.45
1:C:3555:ASN:HA	1:C:3558:HIS:HD1	1.82	0.45
1:C:4814:LEU:C	1:C:4816:ILE:N	2.69	0.45
1:C:4879:MET:HG2	1:D:4578:LEU:HA	1.99	0.45
1:D:103:TYR:HE2	1:D:157:ARG:HD3	1.82	0.45
1:D:132:ALA:O	1:D:194:SER:OG	2.34	0.45
1:D:3645:PRO:HB2	1:D:3647:HIS:HD1	1.81	0.45
1:A:1106:ARG:NH2	1:A:1183:GLU:OE2	2.49	0.45
1:B:688:LEU:HD23	1:B:688:LEU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1111:PRO:HD3	1:B:1605:TRP:HE1	1.81	0.45
1:B:2093:SER:OG	1:B:2094:LEU:N	2.50	0.45
1:B:4634:GLU:C	1:B:4636:THR:H	2.19	0.45
1:B:4960:ILE:HD11	1:B:4985:LEU:HB3	1.97	0.45
1:C:213:TYR:CZ	1:C:337:PRO:HB2	2.52	0.45
1:C:1832:GLY:O	1:C:1833:SER:CB	2.64	0.45
1:C:3668:SER:O	1:C:3672:ARG:NH2	2.47	0.45
1:D:1001:VAL:HA	1:D:1020:ARG:NH2	2.31	0.45
1:D:1495:VAL:HG11	1:D:1536:SER:O	2.16	0.45
1:D:1663:HIS:O	1:D:1666:THR:HG22	2.17	0.45
1:A:103:TYR:HE2	1:A:157:ARG:HD3	1.82	0.45
1:A:618:GLN:NE2	1:A:1675:ALA:H	2.14	0.45
1:A:871:ARG:HH22	1:A:918:ARG:NH1	2.13	0.45
1:A:1634:LEU:HD12	1:A:1634:LEU:HA	1.86	0.45
1:A:4119:GLU:HG2	1:A:4121:GLU:HG2	1.97	0.45
1:A:4923:PHE:O	1:A:4928:LEU:HD23	2.16	0.45
1:C:1001:VAL:HA	1:C:1020:ARG:NH2	2.31	0.45
1:C:2243:SER:OG	1:C:2246:ASN:HB2	2.17	0.45
1:D:1294:PRO:HB3	1:D:1455:PRO:HG3	1.99	0.45
1:D:2093:SER:OG	1:D:2094:LEU:N	2.50	0.45
1:D:2155:LEU:HD12	1:D:2185:ILE:HG22	1.99	0.45
1:D:3721:LEU:HD11	1:D:3725:TYR:HE2	1.80	0.45
1:D:4240:ASP:OD2	1:D:4672:LYS:NZ	2.39	0.45
1:D:4908:GLU:H	1:D:4908:GLU:HG3	1.34	0.45
1:A:481:GLU:N	1:A:481:GLU:OE1	2.49	0.45
1:B:411:TYR:HE1	1:B:441:VAL:HG23	1.82	0.45
1:B:1161:ILE:HA	1:B:1177:THR:OG1	2.16	0.45
1:B:1832:GLY:O	1:B:1833:SER:CB	2.64	0.45
1:B:4901:ILE:HD12	1:B:4901:ILE:HA	1.65	0.45
1:C:45:ARG:NH2	1:C:447:ASP:OD2	2.50	0.45
1:C:224:HIS:H	1:C:230:CYS:HA	1.82	0.45
1:C:3143:LEU:HD13	1:C:3146:HIS:HE1	1.81	0.45
1:D:414:PHE:HD1	1:D:437:PRO:HD2	1.81	0.45
1:D:618:GLN:NE2	1:D:1675:ALA:H	2.14	0.45
1:D:1106:ARG:NH2	1:D:1183:GLU:OE2	2.49	0.45
1:D:1238:PHE:CD1	1:D:1608:MET:HG2	2.51	0.45
1:D:3667:HIS:ND1	1:D:3667:HIS:O	2.50	0.45
1:A:400:ALA:O	1:A:404:ILE:HG13	2.16	0.45
1:A:2093:SER:OG	1:A:2094:LEU:N	2.50	0.45
1:A:4634:GLU:C	1:A:4636:THR:H	2.19	0.45
1:A:4814:LEU:C	1:A:4816:ILE:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:709:ASP:OD1	1:B:709:ASP:N	2.43	0.45
1:B:1437:VAL:HA	1:B:1556:PRO:HA	1.99	0.45
1:B:4879:MET:HG2	1:C:4578:LEU:HA	1.99	0.45
1:D:1176:GLU:O	1:D:1180:ARG:NH2	2.44	0.45
1:D:1839:VAL:HG12	1:D:1840:PRO:N	2.32	0.45
1:D:2243:SER:OG	1:D:2246:ASN:HB2	2.17	0.45
1:D:3641:LEU:HD23	1:D:3641:LEU:H	1.82	0.45
1:A:3555:ASN:HA	1:A:3558:HIS:HD1	1.82	0.44
1:B:1839:VAL:HG12	1:B:1840:PRO:N	2.32	0.44
1:B:3274:LEU:N	1:B:3275:PRO:HD2	2.32	0.44
1:B:4012:LEU:HD23	1:B:4012:LEU:HA	1.84	0.44
1:C:400:ALA:O	1:C:404:ILE:HG13	2.16	0.44
1:C:914:PRO:HB2	1:C:916:PRO:HD2	1.99	0.44
1:C:1294:PRO:HB3	1:C:1455:PRO:HG3	1.99	0.44
1:C:3641:LEU:H	1:C:3641:LEU:HD23	1.82	0.44
1:C:3973:CYS:SG	1:C:3976:ASN:ND2	2.90	0.44
1:C:4185:GLY:HA3	1:C:5009:TYR:CE2	2.53	0.44
1:A:1839:VAL:HG12	1:A:1840:PRO:N	2.32	0.44
1:C:1434:TYR:HA	1:C:1449:TRP:HB3	1.98	0.44
1:C:1663:HIS:O	1:C:1666:THR:HG22	2.17	0.44
1:C:3014:CYS:SG	1:C:3015:LEU:N	2.89	0.44
1:D:233:ILE:HD11	1:D:301:VAL:HG21	1.99	0.44
1:D:1473:THR:N	1:D:1484:HIS:O	2.47	0.44
1:D:4817:ALA:C	1:D:4819:GLY:N	2.66	0.44
1:A:1931:LEU:HD22	1:A:1935:VAL:HG11	1.99	0.44
1:A:3973:CYS:SG	1:A:3976:ASN:ND2	2.90	0.44
1:B:1931:LEU:HD22	1:B:1935:VAL:HG11	1.99	0.44
1:B:2243:SER:OG	1:B:2246:ASN:HB2	2.17	0.44
1:B:2323:TRP:HZ3	1:B:2325:PRO:HB3	1.83	0.44
1:B:3667:HIS:ND1	1:B:3667:HIS:O	2.50	0.44
1:B:4185:GLY:HA3	1:B:5009:TYR:CE2	2.53	0.44
1:C:233:ILE:HD11	1:C:301:VAL:HG21	1.99	0.44
1:C:411:TYR:HE1	1:C:441:VAL:HG23	1.82	0.44
1:C:560:ILE:HA	1:C:563:VAL:HG12	2.00	0.44
1:C:2383:ALA:O	1:C:2386:ILE:HG22	2.18	0.44
1:C:4799:SER:HB3	1:C:4812:HIS:HE1	1.83	0.44
1:D:1161:ILE:HA	1:D:1177:THR:OG1	2.16	0.44
1:D:1434:TYR:HA	1:D:1449:TRP:HB3	1.98	0.44
1:D:2360:LYS:HD2	1:D:2360:LYS:HA	1.77	0.44
1:A:1161:ILE:HA	1:A:1177:THR:OG1	2.16	0.44
1:A:3274:LEU:N	1:A:3275:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:HIS:H	1:B:230:CYS:HA	1.82	0.44
1:B:1108:GLU:OE1	1:B:1108:GLU:N	2.48	0.44
1:B:2458:ARG:NH2	1:B:2510:TYR:HA	2.33	0.44
1:B:3973:CYS:SG	1:B:3976:ASN:ND2	2.90	0.44
1:C:1437:VAL:HA	1:C:1556:PRO:HA	1.99	0.44
1:C:2093:SER:OG	1:C:2094:LEU:N	2.50	0.44
1:C:2302:LEU:HD11	1:C:2332:LEU:HB2	1.97	0.44
1:D:626:LEU:HG	1:D:628:GLY:N	2.27	0.44
1:D:1115:LEU:HG	1:D:1123:VAL:HG11	1.99	0.44
1:A:1434:TYR:HA	1:A:1449:TRP:HB3	1.98	0.44
1:A:3667:HIS:ND1	1:A:3667:HIS:O	2.50	0.44
1:B:224:HIS:N	1:B:229:GLU:O	2.51	0.44
1:B:3641:LEU:HD23	1:B:3641:LEU:H	1.82	0.44
1:B:3798:LEU:O	1:B:3802:ILE:HG12	2.18	0.44
1:C:167:ASP:OD1	1:C:167:ASP:N	2.48	0.44
1:C:2323:TRP:HZ3	1:C:2325:PRO:HB3	1.83	0.44
1:C:3274:LEU:N	1:C:3275:PRO:HD2	2.32	0.44
1:D:1833:SER:O	1:D:1834:VAL:C	2.51	0.44
1:D:3143:LEU:HD13	1:D:3146:HIS:HE1	1.81	0.44
1:D:3292:PRO:HB2	1:D:3293:PRO:HD3	2.00	0.44
1:D:4799:SER:HB3	1:D:4812:HIS:HE1	1.83	0.44
1:A:233:ILE:HD11	1:A:301:VAL:HG21	1.99	0.44
1:A:292:ALA:HA	1:A:314:PHE:HZ	1.83	0.44
1:A:2155:LEU:HD12	1:A:2185:ILE:HG22	1.99	0.44
1:A:3569:LEU:C	1:A:3571:TRP:H	2.21	0.44
1:A:4185:GLY:HA3	1:A:5009:TYR:CE2	2.53	0.44
1:B:484:LEU:HD11	1:B:526:LEU:HD12	1.99	0.44
1:B:1663:HIS:O	1:B:1666:THR:HG22	2.17	0.44
1:B:4322:LEU:HD23	1:B:4322:LEU:HA	1.84	0.44
1:B:4799:SER:HB3	1:B:4812:HIS:HE1	1.83	0.44
1:C:626:LEU:HG	1:C:628:GLY:N	2.27	0.44
1:C:3569:LEU:C	1:C:3571:TRP:H	2.21	0.44
1:D:3435:PHE:HA	1:D:3438:VAL:HG13	2.00	0.44
1:A:719:LEU:O	1:A:719:LEU:HG	2.18	0.44
1:A:3570:ARG:HA	1:A:3574:ALA:O	2.18	0.44
1:A:3798:LEU:O	1:A:3802:ILE:HG12	2.18	0.44
1:B:45:ARG:NH2	1:B:447:ASP:OD2	2.50	0.44
1:B:1176:GLU:O	1:B:1180:ARG:NH2	2.44	0.44
1:C:103:TYR:HE2	1:C:157:ARG:HD3	1.82	0.44
1:C:342:GLY:H	1:C:389:PHE:HE1	1.66	0.44
1:C:1115:LEU:HG	1:C:1123:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1221:GLU:OE2	1:C:1221:GLU:N	2.51	0.44
1:C:1931:LEU:HD22	1:C:1935:VAL:HG11	1.99	0.44
1:D:292:ALA:HA	1:D:314:PHE:HZ	1.83	0.44
1:D:411:TYR:HE1	1:D:441:VAL:HG23	1.82	0.44
1:D:3798:LEU:O	1:D:3802:ILE:HG12	2.18	0.44
1:D:3973:CYS:SG	1:D:3976:ASN:ND2	2.90	0.44
1:A:224:HIS:H	1:A:230:CYS:HA	1.82	0.44
1:A:769:GLU:O	1:A:1515:VAL:HG22	2.18	0.44
1:A:1663:HIS:O	1:A:1666:THR:HG22	2.17	0.44
1:A:3292:PRO:HB2	1:A:3293:PRO:HD3	2.00	0.44
1:B:3570:ARG:HA	1:B:3574:ALA:O	2.18	0.44
1:C:224:HIS:N	1:C:229:GLU:O	2.51	0.44
1:C:3435:PHE:HA	1:C:3438:VAL:HG13	2.00	0.44
1:C:3798:LEU:O	1:C:3802:ILE:HG12	2.18	0.44
1:D:212:GLY:O	1:D:340:LYS:HG3	2.18	0.44
1:D:560:ILE:HA	1:D:563:VAL:HG12	2.00	0.44
1:A:1437:VAL:HA	1:A:1556:PRO:HA	1.99	0.44
1:A:4799:SER:HB3	1:A:4812:HIS:HE1	1.83	0.44
1:B:3292:PRO:HB2	1:B:3293:PRO:HD3	2.00	0.44
1:B:3835:LEU:HD22	1:B:3880:PHE:HZ	1.83	0.44
1:B:4763:GLY:HA3	1:B:4767:TRP:CE2	2.52	0.44
1:C:3667:HIS:ND1	1:C:3667:HIS:O	2.50	0.44
1:D:224:HIS:H	1:D:230:CYS:HA	1.82	0.44
1:D:4698:LYS:HD3	1:D:4698:LYS:HA	1.72	0.44
1:A:1115:LEU:HG	1:A:1123:VAL:HG11	1.99	0.43
1:A:3641:LEU:HD23	1:A:3641:LEU:H	1.82	0.43
1:B:719:LEU:O	1:B:719:LEU:HG	2.18	0.43
1:B:3143:LEU:HD13	1:B:3146:HIS:HE1	1.81	0.43
1:B:3569:LEU:C	1:B:3571:TRP:H	2.21	0.43
1:D:615:ARG:CZ	1:D:2168:VAL:HG21	2.49	0.43
1:D:871:ARG:HH22	1:D:918:ARG:NH1	2.13	0.43
1:D:2383:ALA:O	1:D:2386:ILE:HG22	2.18	0.43
1:A:560:ILE:HA	1:A:563:VAL:HG12	2.00	0.43
1:A:1495:VAL:HG11	1:A:1536:SER:O	2.16	0.43
1:A:2243:SER:OG	1:A:2246:ASN:HB2	2.17	0.43
1:A:2383:ALA:O	1:A:2386:ILE:HG22	2.18	0.43
1:A:3835:LEU:HD22	1:A:3880:PHE:HZ	1.83	0.43
1:B:103:TYR:HE2	1:B:157:ARG:HD3	1.82	0.43
1:B:233:ILE:HD11	1:B:301:VAL:HG21	1.99	0.43
1:B:430:PRO:HA	1:B:431:PRO:HD3	1.86	0.43
1:B:1481:GLY:HA2	1:B:1573:MET:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4992:LEU:O	1:B:4996:ILE:HG13	2.19	0.43
1:C:247:TYR:CE2	1:C:376:ALA:HB2	2.54	0.43
1:C:292:ALA:HA	1:C:314:PHE:HZ	1.83	0.43
1:C:875:ALA:O	1:C:879:HIS:ND1	2.52	0.43
1:C:3292:PRO:HB2	1:C:3293:PRO:HD3	2.00	0.43
1:D:224:HIS:N	1:D:229:GLU:O	2.51	0.43
1:D:342:GLY:H	1:D:389:PHE:HE1	1.66	0.43
1:D:914:PRO:HB2	1:D:916:PRO:HD2	1.99	0.43
1:D:2138:LEU:HD12	1:D:2138:LEU:HA	1.84	0.43
1:D:4897:ILE:H	1:D:4897:ILE:HG13	1.59	0.43
1:A:224:HIS:N	1:A:229:GLU:O	2.51	0.43
1:B:317:ARG:N	1:B:347:PHE:O	2.48	0.43
1:B:628:GLY:C	1:B:629:ARG:HG2	2.39	0.43
1:B:2383:ALA:O	1:B:2386:ILE:HG22	2.18	0.43
1:B:4983:HIS:HB2	1:B:4988:TYR:HE1	1.83	0.43
1:C:615:ARG:CZ	1:C:2168:VAL:HG21	2.49	0.43
1:C:4983:HIS:HB2	1:C:4988:TYR:HE1	1.83	0.43
1:D:645:ARG:HB3	1:D:780:VAL:HG12	2.01	0.43
1:A:45:ARG:NH2	1:A:447:ASP:OD2	2.50	0.43
1:A:286:THR:HG23	1:A:287:THR:HG23	2.01	0.43
1:A:720:HIS:O	1:A:721:LEU:HD23	2.18	0.43
1:A:1221:GLU:OE2	1:A:1221:GLU:N	2.51	0.43
1:A:1294:PRO:HB3	1:A:1455:PRO:HG3	1.99	0.43
1:A:1481:GLY:HA2	1:A:1573:MET:O	2.18	0.43
1:A:3435:PHE:HA	1:A:3438:VAL:HG13	2.00	0.43
1:A:4992:LEU:O	1:A:4996:ILE:HG13	2.19	0.43
1:B:2155:LEU:HD12	1:B:2185:ILE:HG22	1.99	0.43
1:B:3817:LEU:HD13	1:B:3899:PHE:CD1	2.45	0.43
1:C:709:ASP:OD1	1:C:709:ASP:N	2.43	0.43
1:C:719:LEU:O	1:C:719:LEU:HG	2.18	0.43
1:D:3569:LEU:C	1:D:3571:TRP:H	2.21	0.43
1:D:3570:ARG:HA	1:D:3574:ALA:O	2.18	0.43
1:A:615:ARG:CZ	1:A:2168:VAL:HG21	2.49	0.43
1:A:875:ALA:O	1:A:879:HIS:ND1	2.52	0.43
1:B:615:ARG:CZ	1:B:2168:VAL:HG21	2.49	0.43
1:B:720:HIS:O	1:B:721:LEU:HD23	2.18	0.43
1:B:3716:LEU:HD12	1:B:3716:LEU:HA	1.86	0.43
1:C:628:GLY:C	1:C:629:ARG:HG2	2.39	0.43
1:C:720:HIS:O	1:C:721:LEU:HD23	2.18	0.43
1:C:2155:LEU:HD12	1:C:2185:ILE:HG22	1.99	0.43
1:D:19:GLU:HA	1:D:68:THR:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:720:HIS:O	1:D:721:LEU:HD23	2.18	0.43
1:D:1437:VAL:HA	1:D:1556:PRO:HA	1.99	0.43
1:D:1481:GLY:HA2	1:D:1573:MET:O	2.18	0.43
1:D:4185:GLY:HA3	1:D:5009:TYR:CE2	2.53	0.43
1:A:411:TYR:HE1	1:A:441:VAL:HG23	1.82	0.43
1:A:2458:ARG:NH2	1:A:2510:TYR:HA	2.33	0.43
1:A:3679:LYS:HB3	1:A:3679:LYS:HE3	1.84	0.43
1:A:3962:PHE:O	1:A:3966:THR:HG23	2.19	0.43
1:A:4983:HIS:HB2	1:A:4988:TYR:HE1	1.83	0.43
1:B:247:TYR:CE2	1:B:376:ALA:HB2	2.54	0.43
1:B:659:TYR:O	1:B:661:LYS:HG2	2.19	0.43
1:B:1294:PRO:HB3	1:B:1455:PRO:HG3	1.99	0.43
1:B:3435:PHE:HA	1:B:3438:VAL:HG13	2.00	0.43
1:B:3555:ASN:HA	1:B:3558:HIS:HD1	1.82	0.43
1:C:212:GLY:O	1:C:340:LYS:HG3	2.18	0.43
1:C:769:GLU:O	1:C:1515:VAL:HG22	2.18	0.43
1:C:1098:GLY:HA3	1:C:1198:GLN:NE2	2.34	0.43
1:C:3570:ARG:HA	1:C:3574:ALA:O	2.18	0.43
1:C:3657:TYR:O	1:C:3661:TRP:HD1	2.02	0.43
1:C:3835:LEU:HD22	1:C:3880:PHE:HZ	1.83	0.43
1:C:4126:GLU:O	1:C:4130:ASN:ND2	2.35	0.43
1:D:247:TYR:CE2	1:D:376:ALA:HB2	2.54	0.43
1:D:659:TYR:O	1:D:661:LYS:HG2	2.19	0.43
1:D:719:LEU:O	1:D:719:LEU:HG	2.18	0.43
1:D:1221:GLU:N	1:D:1221:GLU:OE2	2.51	0.43
1:D:2240:CYS:SG	1:D:2279:SER:HA	2.59	0.43
1:D:3274:LEU:N	1:D:3275:PRO:HD2	2.32	0.43
1:A:38:ALA:HB1	1:A:64:ILE:HG13	2.01	0.43
1:B:1103:GLY:HA3	1:B:1123:VAL:HA	2.01	0.43
1:C:645:ARG:HB3	1:C:780:VAL:HG12	2.01	0.43
1:C:711:LEU:HD23	1:C:711:LEU:H	1.84	0.43
1:D:61:ASP:N	1:D:61:ASP:OD1	2.48	0.43
1:D:875:ALA:O	1:D:879:HIS:ND1	2.52	0.43
1:D:1243:PRO:HB3	1:D:1602:PRO:HA	2.01	0.43
1:D:2165:LEU:HD23	1:D:2165:LEU:HA	1.85	0.43
1:D:2296:GLU:HA	1:D:2299:VAL:HG12	2.00	0.43
1:D:3533:ILE:H	1:D:3533:ILE:HD12	1.84	0.43
1:D:3534:MET:C	1:D:3535:LEU:HD12	2.39	0.43
1:D:3835:LEU:HD22	1:D:3880:PHE:HZ	1.83	0.43
1:A:672:VAL:HG11	1:A:675:LEU:HD13	2.01	0.43
1:A:711:LEU:HD23	1:A:711:LEU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2323:TRP:HZ3	1:A:2325:PRO:HB3	1.83	0.43
1:A:3534:MET:C	1:A:3535:LEU:HD12	2.39	0.43
1:A:3923:LEU:HD21	1:A:3962:PHE:HE1	1.84	0.43
1:A:4572:ALA:O	1:A:4576:ILE:HG12	2.19	0.43
1:B:103:TYR:CD2	1:B:163:VAL:HG22	2.54	0.43
1:B:245:VAL:O	1:B:375:LYS:HG3	2.19	0.43
1:B:292:ALA:HA	1:B:314:PHE:HZ	1.83	0.43
1:B:665:GLU:OE1	1:B:745:SER:OG	2.23	0.43
1:B:1671:ARG:HG2	1:B:1717:SER:HB3	2.01	0.43
1:B:3668:SER:O	1:B:3672:ARG:NH2	2.47	0.43
1:B:4343:GLY:O	1:B:4344:ALA:C	2.57	0.43
1:C:103:TYR:CD2	1:C:163:VAL:HG22	2.54	0.43
1:C:1839:VAL:CB	1:C:1840:PRO:HD3	2.45	0.43
1:C:4992:LEU:O	1:C:4996:ILE:HG13	2.19	0.43
1:D:672:VAL:HG11	1:D:675:LEU:HD13	2.01	0.43
1:D:3657:TYR:O	1:D:3661:TRP:HD1	2.02	0.43
1:D:3962:PHE:O	1:D:3966:THR:HG23	2.19	0.43
1:A:212:GLY:O	1:A:340:LYS:HG3	2.18	0.43
1:A:628:GLY:C	1:A:629:ARG:HG2	2.39	0.43
1:A:1103:GLY:HA3	1:A:1123:VAL:HA	2.01	0.43
1:A:1243:PRO:HB3	1:A:1602:PRO:HA	2.01	0.43
1:B:2240:CYS:SG	1:B:2279:SER:HA	2.59	0.43
1:C:19:GLU:HA	1:C:68:THR:HA	2.01	0.43
1:C:1671:ARG:HG2	1:C:1717:SER:HB3	2.01	0.43
1:C:1842:LEU:HD12	1:C:1842:LEU:HA	1.77	0.43
1:C:2438:PRO:HG3	1:C:2454:ARG:HG3	2.01	0.43
1:D:646:PRO:HD2	1:D:779:PRO:O	2.19	0.43
1:D:1238:PHE:HD1	1:D:1608:MET:HG2	1.84	0.43
1:D:1839:VAL:CB	1:D:1840:PRO:HD3	2.45	0.43
1:D:2458:ARG:NH2	1:D:2510:TYR:HA	2.33	0.43
1:D:4630:TYR:CE2	1:D:4632:LEU:HD13	2.46	0.43
1:D:4983:HIS:HB2	1:D:4988:TYR:HE1	1.83	0.43
1:A:19:GLU:HA	1:A:68:THR:HA	2.01	0.43
1:A:247:TYR:CE2	1:A:376:ALA:HB2	2.54	0.43
1:A:1952:GLN:O	1:A:1956:GLU:HG2	2.19	0.43
1:A:4021:LYS:HA	1:A:4139:ILE:HD13	2.01	0.43
1:B:560:ILE:HA	1:B:563:VAL:HG12	2.00	0.43
1:B:1243:PRO:HB3	1:B:1602:PRO:HA	2.01	0.43
1:C:1238:PHE:HD1	1:C:1608:MET:HG2	1.84	0.43
1:C:1243:PRO:HB3	1:C:1602:PRO:HA	2.01	0.43
1:C:1839:VAL:HG12	1:C:1840:PRO:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:711:LEU:H	1:D:711:LEU:HD23	1.84	0.43
1:A:169:LEU:HD13	1:A:202:MET:HE1	2.01	0.42
1:A:645:ARG:HB3	1:A:780:VAL:HG12	2.01	0.42
1:A:709:ASP:N	1:A:709:ASP:OD1	2.43	0.42
1:A:2637:ALA:O	1:A:2640:PRO:HD2	2.19	0.42
1:A:4828:SER:O	1:A:4832:HIS:N	2.52	0.42
1:B:711:LEU:HD23	1:B:711:LEU:H	1.84	0.42
1:B:875:ALA:O	1:B:879:HIS:ND1	2.52	0.42
1:B:4021:LYS:HA	1:B:4139:ILE:HD13	2.01	0.42
1:B:4572:ALA:O	1:B:4576:ILE:HG12	2.19	0.42
1:B:4814:LEU:C	1:B:4816:ILE:N	2.69	0.42
1:C:426:ARG:NH1	1:C:508:GLY:HA2	2.34	0.42
1:C:659:TYR:O	1:C:661:LYS:HG2	2.19	0.42
1:C:1103:GLY:HA3	1:C:1123:VAL:HA	2.01	0.42
1:C:1254:HIS:HB2	1:C:1274:HIS:ND1	2.34	0.42
1:C:1481:GLY:HA2	1:C:1573:MET:O	2.18	0.42
1:D:426:ARG:NH1	1:D:508:GLY:HA2	2.34	0.42
1:D:769:GLU:O	1:D:1515:VAL:HG22	2.18	0.42
1:D:1103:GLY:HA3	1:D:1123:VAL:HA	2.01	0.42
1:A:181:HIS:N	1:A:192:ASP:O	2.50	0.42
1:A:646:PRO:HD2	1:A:779:PRO:O	2.19	0.42
1:B:38:ALA:HB1	1:B:64:ILE:HG13	2.01	0.42
1:B:672:VAL:HG11	1:B:675:LEU:HD13	2.01	0.42
1:B:769:GLU:O	1:B:1515:VAL:HG22	2.18	0.42
1:B:2637:ALA:O	1:B:2640:PRO:HD2	2.19	0.42
1:B:3533:ILE:HD12	1:B:3533:ILE:H	1.84	0.42
1:B:3534:MET:C	1:B:3535:LEU:HD12	2.39	0.42
1:C:672:VAL:HG11	1:C:675:LEU:HD13	2.01	0.42
1:C:805:PRO:HB2	1:C:808:TYR:CE1	2.54	0.42
1:C:1172:ASP:OD1	1:C:1172:ASP:N	2.52	0.42
1:C:2240:CYS:SG	1:C:2279:SER:HA	2.59	0.42
1:C:3339:ALA:HB3	1:C:3343:GLN:HB2	2.01	0.42
1:C:3923:LEU:HD21	1:C:3962:PHE:HE1	1.84	0.42
1:C:3962:PHE:O	1:C:3966:THR:HG23	2.19	0.42
1:D:103:TYR:CD2	1:D:163:VAL:HG22	2.54	0.42
1:D:628:GLY:C	1:D:629:ARG:HG2	2.39	0.42
1:D:805:PRO:HB2	1:D:808:TYR:CE1	2.54	0.42
1:D:1098:GLY:HA3	1:D:1198:GLN:NE2	2.34	0.42
1:D:1671:ARG:HG2	1:D:1717:SER:HB3	2.01	0.42
1:D:2438:PRO:HG3	1:D:2454:ARG:HG3	2.01	0.42
1:D:4630:TYR:CD2	1:D:4631:PHE:O	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:PRO:HB2	1:A:808:TYR:CE1	2.54	0.42
1:A:2240:CYS:SG	1:A:2279:SER:HA	2.59	0.42
1:A:3668:SER:O	1:A:3672:ARG:NH2	2.47	0.42
1:A:4796:MET:O	1:A:4799:SER:OG	2.27	0.42
1:A:4908:GLU:H	1:A:4908:GLU:HG3	1.34	0.42
1:B:426:ARG:NH1	1:B:508:GLY:HA2	2.34	0.42
1:B:3309:SER:O	1:B:3312:LEU:HD23	2.20	0.42
1:C:2296:GLU:HA	1:C:2299:VAL:HG12	2.00	0.42
1:C:3533:ILE:H	1:C:3533:ILE:HD12	1.84	0.42
1:C:3842:LEU:HD23	1:C:3842:LEU:HA	1.83	0.42
1:D:1931:LEU:HD22	1:D:1935:VAL:HG11	1.99	0.42
1:D:2135:LEU:HD13	1:D:3662:ILE:HG22	2.01	0.42
1:D:3304:CYS:O	1:D:3308:THR:OG1	2.25	0.42
1:D:3309:SER:O	1:D:3312:LEU:HD23	2.20	0.42
1:D:4126:GLU:O	1:D:4130:ASN:ND2	2.35	0.42
1:A:245:VAL:O	1:A:375:LYS:HG3	2.19	0.42
1:A:342:GLY:H	1:A:389:PHE:HE1	1.66	0.42
1:A:426:ARG:NH1	1:A:508:GLY:HA2	2.34	0.42
1:A:1293:LEU:HD23	1:A:1579:MET:HB3	2.01	0.42
1:A:1671:ARG:HG2	1:A:1717:SER:HB3	2.01	0.42
1:A:2296:GLU:HA	1:A:2299:VAL:HG12	2.00	0.42
1:A:2368:LEU:HD22	1:A:2376:LEU:HD13	2.02	0.42
1:B:19:GLU:HA	1:B:68:THR:HA	2.01	0.42
1:B:212:GLY:O	1:B:340:LYS:HG3	2.18	0.42
1:B:286:THR:HG23	1:B:287:THR:HG23	2.01	0.42
1:B:342:GLY:H	1:B:389:PHE:HE1	1.66	0.42
1:B:805:PRO:HB2	1:B:808:TYR:CE1	2.54	0.42
1:B:882:TRP:HZ3	1:B:886:ARG:HD3	1.85	0.42
1:B:3962:PHE:O	1:B:3966:THR:HG23	2.19	0.42
1:C:317:ARG:N	1:C:347:PHE:O	2.48	0.42
1:C:882:TRP:HZ3	1:C:886:ARG:HD3	1.85	0.42
1:C:3534:MET:C	1:C:3535:LEU:HD12	2.39	0.42
1:C:3662:ILE:O	1:C:3664:THR:N	2.50	0.42
1:D:286:THR:HG23	1:D:287:THR:HG23	2.01	0.42
1:D:882:TRP:HZ3	1:D:886:ARG:HD3	1.85	0.42
1:D:2368:LEU:HD22	1:D:2376:LEU:HD13	2.02	0.42
1:D:2637:ALA:O	1:D:2640:PRO:HD2	2.19	0.42
1:D:4796:MET:O	1:D:4799:SER:OG	2.27	0.42
1:A:882:TRP:HZ3	1:A:886:ARG:HD3	1.85	0.42
1:A:3838:THR:O	1:A:3838:THR:OG1	2.29	0.42
1:B:645:ARG:HG2	1:B:826:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:884:LEU:HG	1:B:965:TYR:HD2	1.84	0.42
1:B:1254:HIS:HB2	1:B:1274:HIS:ND1	2.34	0.42
1:B:1683:HIS:HD2	1:B:1800:PRO:HG3	1.85	0.42
1:B:1952:GLN:O	1:B:1956:GLU:HG2	2.19	0.42
1:B:3802:ILE:HD12	1:B:3886:ARG:HG3	2.01	0.42
1:B:4247:ILE:HD11	1:B:4667:PRO:HB2	2.01	0.42
1:B:4630:TYR:CD2	1:B:4631:PHE:O	2.72	0.42
1:C:245:VAL:O	1:C:375:LYS:HG3	2.19	0.42
1:C:568:LEU:HD23	1:C:568:LEU:HA	1.89	0.42
1:C:3309:SER:O	1:C:3312:LEU:HD23	2.20	0.42
1:C:3771:HIS:HA	1:C:3773:ARG:NH1	2.35	0.42
1:C:4572:ALA:O	1:C:4576:ILE:HG12	2.19	0.42
1:D:1952:GLN:O	1:D:1956:GLU:HG2	2.19	0.42
1:D:2215:LEU:HD12	1:D:2229:VAL:HG11	2.02	0.42
1:D:2438:PRO:HG3	1:D:2454:ARG:HB2	2.02	0.42
1:D:3798:LEU:HD21	1:D:3884:LEU:HA	2.02	0.42
1:D:4646:LEU:HD23	1:D:4646:LEU:HA	1.91	0.42
1:D:4825:THR:O	1:D:4828:SER:OG	2.23	0.42
1:A:21:VAL:HG12	1:A:205:ILE:HB	2.02	0.42
1:A:2215:LEU:HD12	1:A:2229:VAL:HG11	2.02	0.42
1:A:2438:PRO:HG3	1:A:2454:ARG:HB2	2.02	0.42
1:A:3533:ILE:H	1:A:3533:ILE:HD12	1.84	0.42
1:A:4702:ASP:OD1	1:A:4702:ASP:N	2.53	0.42
1:B:1453:VAL:HG23	1:B:1454:THR:N	2.28	0.42
1:B:1829:PRO:HG2	1:B:1833:SER:H	1.85	0.42
1:B:3339:ALA:HB3	1:B:3343:GLN:HB2	2.01	0.42
1:C:451:TYR:OH	1:C:474:ARG:HD2	2.20	0.42
1:C:3679:LYS:HE3	1:C:3679:LYS:HB3	1.84	0.42
1:C:4630:TYR:CD2	1:C:4631:PHE:O	2.72	0.42
1:D:1108:GLU:CD	1:D:1108:GLU:H	2.23	0.42
1:A:1098:GLY:HA3	1:A:1198:GLN:NE2	2.34	0.42
1:A:1238:PHE:HD1	1:A:1608:MET:HG2	1.84	0.42
1:A:1444:GLU:HA	1:A:1445:PRO:HD3	1.92	0.42
1:A:1457:TYR:O	1:A:1497:GLY:N	2.47	0.42
1:A:1683:HIS:HD2	1:A:1800:PRO:HG3	1.85	0.42
1:A:4630:TYR:CD2	1:A:4631:PHE:O	2.72	0.42
1:B:1221:GLU:OE2	1:B:1221:GLU:N	2.51	0.42
1:B:1238:PHE:HD1	1:B:1608:MET:HG2	1.84	0.42
1:B:2296:GLU:HA	1:B:2299:VAL:HG12	2.00	0.42
1:B:4150:LEU:HD12	1:B:4150:LEU:HA	1.92	0.42
1:B:5027:CYS:C	1:B:5029:ARG:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:LEU:HD11	1:C:191:VAL:HG13	2.02	0.42
1:C:286:THR:HG23	1:C:287:THR:HG23	2.01	0.42
1:C:1539:PHE:O	1:C:1542:VAL:HG22	2.20	0.42
1:C:2458:ARG:NH2	1:C:2510:TYR:HA	2.33	0.42
1:D:451:TYR:OH	1:D:474:ARG:HD2	2.20	0.42
1:D:1483:VAL:HG12	1:D:1575:LEU:HD22	2.02	0.42
1:D:1927:LEU:HB3	1:D:1939:MET:SD	2.60	0.42
1:D:4247:ILE:HD11	1:D:4667:PRO:HB2	2.01	0.42
1:D:4992:LEU:O	1:D:4996:ILE:HG13	2.19	0.42
1:A:103:TYR:CD2	1:A:163:VAL:HG22	2.54	0.42
1:A:659:TYR:O	1:A:661:LYS:HG2	2.19	0.42
1:A:1108:GLU:H	1:A:1108:GLU:CD	2.23	0.42
1:A:1483:VAL:HG12	1:A:1575:LEU:HD22	2.02	0.42
1:A:2438:PRO:HG3	1:A:2454:ARG:HG3	2.01	0.42
1:A:3573:MET:HE3	1:D:1205:GLY:O	2.20	0.42
1:A:3657:TYR:O	1:A:3661:TRP:HD1	2.02	0.42
1:A:4247:ILE:HD11	1:A:4667:PRO:HB2	2.01	0.42
1:B:645:ARG:HB3	1:B:780:VAL:HG12	2.01	0.42
1:B:646:PRO:HD2	1:B:779:PRO:O	2.19	0.42
1:B:972:LEU:HD13	1:B:1044:ARG:HB3	2.01	0.42
1:B:2438:PRO:HG3	1:B:2454:ARG:HB2	2.02	0.42
1:C:415:ILE:HD12	1:C:415:ILE:HA	1.90	0.42
1:C:1483:VAL:HG12	1:C:1575:LEU:HD22	2.02	0.42
1:C:1952:GLN:O	1:C:1956:GLU:HG2	2.19	0.42
1:C:2438:PRO:HG3	1:C:2454:ARG:HB2	2.02	0.42
1:C:4021:LYS:HA	1:C:4139:ILE:HD13	2.01	0.42
1:C:4322:LEU:HD23	1:C:4322:LEU:HA	1.84	0.42
1:C:5027:CYS:C	1:C:5029:ARG:H	2.23	0.42
1:D:2323:TRP:HZ3	1:D:2325:PRO:HB3	1.83	0.42
1:D:3339:ALA:HB3	1:D:3343:GLN:HB2	2.01	0.42
1:D:4572:ALA:O	1:D:4576:ILE:HG12	2.19	0.42
1:D:4685:GLY:HA3	1:D:4689:THR:HB	2.02	0.42
1:A:1835:GLU:O	1:A:1838:PHE:N	2.53	0.42
1:A:4901:ILE:HD12	1:A:4901:ILE:HA	1.65	0.42
1:B:21:VAL:HG12	1:B:205:ILE:HB	2.02	0.42
1:B:1927:LEU:HB3	1:B:1939:MET:SD	2.60	0.42
1:B:3923:LEU:HD21	1:B:3962:PHE:HE1	1.84	0.42
1:B:5027:CYS:O	1:B:5027:CYS:SG	2.78	0.42
1:C:1207:ASP:OD1	1:C:1207:ASP:N	2.53	0.42
1:C:1829:PRO:HG2	1:C:1833:SER:H	1.85	0.42
1:C:1835:GLU:O	1:C:1838:PHE:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1927:LEU:HB3	1:C:1939:MET:SD	2.60	0.42
1:C:3980:LEU:HD23	1:C:3980:LEU:HA	1.85	0.42
1:C:4240:ASP:OD2	1:C:4672:LYS:NZ	2.39	0.42
1:D:192:ASP:OD2	1:D:194:SER:OG	2.29	0.42
1:D:627:PRO:O	1:D:629:ARG:NE	2.53	0.42
1:D:1254:HIS:HB2	1:D:1274:HIS:ND1	2.34	0.42
1:A:732:SER:O	1:A:735:GLN:HG2	2.20	0.42
1:A:790:ARG:NH1	1:A:797:HIS:HB3	2.35	0.42
1:A:1254:HIS:HB2	1:A:1274:HIS:ND1	2.34	0.42
1:A:3577:ARG:CZ	1:D:1208:VAL:O	2.68	0.42
1:A:3798:LEU:HD21	1:A:3884:LEU:HA	2.02	0.42
1:A:4630:TYR:CE2	1:A:4632:LEU:HD13	2.46	0.42
1:B:609:CYS:SG	1:B:610:ASN:N	2.93	0.42
1:B:1098:GLY:HA3	1:B:1198:GLN:NE2	2.34	0.42
1:B:1539:PHE:O	1:B:1542:VAL:HG22	2.20	0.42
1:B:2164:SER:O	1:B:2167:ILE:HG12	2.20	0.42
1:C:38:ALA:HB1	1:C:64:ILE:HG13	2.01	0.42
1:C:790:ARG:NH1	1:C:797:HIS:HB3	2.35	0.42
1:C:1518:CYS:O	1:C:1526:LEU:HA	2.20	0.42
1:C:1730:MET:SD	1:C:2163:ARG:NH1	2.93	0.42
1:C:2135:LEU:HD13	1:C:3662:ILE:HG22	2.01	0.42
1:C:4685:GLY:HA3	1:C:4689:THR:HB	2.02	0.42
1:C:4828:SER:O	1:C:4832:HIS:N	2.52	0.42
1:D:49:LEU:HD11	1:D:191:VAL:HG13	2.02	0.42
1:D:245:VAL:O	1:D:375:LYS:HG3	2.19	0.42
1:D:645:ARG:HG2	1:D:826:ILE:HG23	2.01	0.42
1:D:972:LEU:HD13	1:D:1044:ARG:HB3	2.01	0.42
1:D:1835:GLU:O	1:D:1838:PHE:N	2.53	0.42
1:D:3842:LEU:HA	1:D:3842:LEU:HD23	1.83	0.42
1:A:977:LEU:HD12	1:A:978:THR:HG22	2.02	0.41
1:A:1229:ASN:HB3	1:A:1826:ALA:HA	2.02	0.41
1:B:49:LEU:HD11	1:B:191:VAL:HG13	2.02	0.41
1:B:1172:ASP:N	1:B:1172:ASP:OD1	2.52	0.41
1:B:1295:VAL:N	1:B:1453:VAL:O	2.53	0.41
1:B:1483:VAL:HG12	1:B:1575:LEU:HD22	2.02	0.41
1:B:3657:TYR:O	1:B:3661:TRP:HD1	2.02	0.41
1:B:3771:HIS:HA	1:B:3773:ARG:NH1	2.35	0.41
1:C:1229:ASN:HB3	1:C:1826:ALA:HA	2.02	0.41
1:C:5027:CYS:O	1:C:5027:CYS:SG	2.78	0.41
1:D:732:SER:O	1:D:735:GLN:HG2	2.20	0.41
1:D:1730:MET:SD	1:D:2163:ARG:NH1	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1829:PRO:HG2	1:D:1833:SER:H	1.85	0.41
1:D:2695:LEU:HD12	1:D:2696:TYR:H	1.85	0.41
1:D:3716:LEU:HD12	1:D:3716:LEU:HA	1.86	0.41
1:D:4702:ASP:N	1:D:4702:ASP:OD1	2.53	0.41
1:A:40:GLU:HB3	1:A:44:ASN:ND2	2.33	0.41
1:A:609:CYS:SG	1:A:610:ASN:N	2.93	0.41
1:A:2194:HIS:HE1	1:A:3647:HIS:NE2	2.18	0.41
1:A:3716:LEU:HD12	1:A:3716:LEU:HA	1.86	0.41
1:A:3790:THR:HG22	1:A:3835:LEU:HD23	2.02	0.41
1:A:4343:GLY:O	1:A:4344:ALA:C	2.57	0.41
1:A:4816:ILE:O	1:A:4820:VAL:HG23	2.20	0.41
1:B:451:TYR:OH	1:B:474:ARG:HD2	2.20	0.41
1:B:790:ARG:NH1	1:B:797:HIS:HB3	2.35	0.41
1:B:1730:MET:SD	1:B:2163:ARG:NH1	2.93	0.41
1:B:3838:THR:O	1:B:3838:THR:OG1	2.29	0.41
1:B:4685:GLY:HA3	1:B:4689:THR:HB	2.02	0.41
1:C:646:PRO:HD2	1:C:779:PRO:O	2.19	0.41
1:C:884:LEU:HG	1:C:965:TYR:HD2	1.84	0.41
1:C:1208:VAL:O	1:D:3577:ARG:CZ	2.68	0.41
1:C:1463:ASN:N	1:C:1492:CYS:SG	2.82	0.41
1:C:1683:HIS:ND1	1:C:1797:ARG:HG2	2.35	0.41
1:C:2164:SER:O	1:C:2167:ILE:HG12	2.20	0.41
1:C:2637:ALA:O	1:C:2640:PRO:HD2	2.19	0.41
1:C:4816:ILE:O	1:C:4820:VAL:HG23	2.20	0.41
1:D:220:LEU:CB	1:D:392:ARG:HA	2.51	0.41
1:D:719:LEU:O	1:D:720:HIS:CG	2.73	0.41
1:D:884:LEU:HG	1:D:965:TYR:HD2	1.84	0.41
1:D:1172:ASP:OD1	1:D:1172:ASP:N	2.52	0.41
1:D:1539:PHE:O	1:D:1542:VAL:HG22	2.20	0.41
1:D:1683:HIS:ND1	1:D:1797:ARG:HG2	2.35	0.41
1:D:1683:HIS:HD2	1:D:1800:PRO:HG3	1.85	0.41
1:A:1730:MET:SD	1:A:2163:ARG:NH1	2.93	0.41
1:A:3339:ALA:HB3	1:A:3343:GLN:HB2	2.01	0.41
1:A:4690:GLU:O	1:A:4691:GLN:HG2	2.21	0.41
1:A:5027:CYS:O	1:A:5027:CYS:SG	2.78	0.41
1:B:220:LEU:CB	1:B:392:ARG:HA	2.51	0.41
1:B:1208:VAL:O	1:C:3577:ARG:CZ	2.68	0.41
1:B:1229:ASN:HB3	1:B:1826:ALA:HA	2.02	0.41
1:B:1293:LEU:HD23	1:B:1579:MET:HB3	2.01	0.41
1:B:1295:VAL:HB	1:B:1452:TRP:O	2.21	0.41
1:B:2094:LEU:O	1:B:2098:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2194:HIS:HE1	1:B:3647:HIS:NE2	2.18	0.41
1:B:3662:ILE:O	1:B:3664:THR:N	2.50	0.41
1:B:4630:TYR:CE2	1:B:4632:LEU:HD13	2.46	0.41
1:B:4828:SER:O	1:B:4832:HIS:N	2.52	0.41
1:C:732:SER:O	1:C:735:GLN:HG2	2.20	0.41
1:C:972:LEU:HD21	1:C:1048:GLY:HA3	2.03	0.41
1:C:1295:VAL:HB	1:C:1452:TRP:O	2.21	0.41
1:C:2695:LEU:HD12	1:C:2696:TYR:H	1.85	0.41
1:C:3802:ILE:HD12	1:C:3886:ARG:HG3	2.01	0.41
1:D:38:ALA:HB1	1:D:64:ILE:HG13	2.01	0.41
1:D:977:LEU:HD12	1:D:978:THR:HG22	2.02	0.41
1:D:1229:ASN:HB3	1:D:1826:ALA:HA	2.02	0.41
1:D:1293:LEU:HD23	1:D:1579:MET:HB3	2.01	0.41
1:D:3197:LEU:HD12	1:D:3197:LEU:HA	1.96	0.41
1:A:220:LEU:CB	1:A:392:ARG:HA	2.51	0.41
1:A:591:ASP:HB2	1:A:631:LEU:HD11	2.02	0.41
1:A:2226:PRO:C	1:A:2228:MET:H	2.24	0.41
1:A:3761:GLN:O	1:A:3762:ARG:HB2	2.20	0.41
1:A:3771:HIS:HA	1:A:3773:ARG:NH1	2.35	0.41
1:A:4633:GLU:C	1:A:4635:SER:H	2.24	0.41
1:A:5027:CYS:C	1:A:5029:ARG:H	2.23	0.41
1:B:40:GLU:HB3	1:B:44:ASN:ND2	2.33	0.41
1:B:591:ASP:HB2	1:B:631:LEU:HD11	2.02	0.41
1:B:1028:ASP:N	1:B:1028:ASP:OD1	2.54	0.41
1:B:1463:ASN:N	1:B:1492:CYS:SG	2.82	0.41
1:B:3532:LEU:HA	1:B:3535:LEU:HD13	2.03	0.41
1:C:252:VAL:HA	1:C:255:HIS:HB2	2.03	0.41
1:C:645:ARG:HG2	1:C:826:ILE:HG23	2.01	0.41
1:C:804:PRO:HA	1:C:805:PRO:HD3	1.91	0.41
1:C:977:LEU:HD12	1:C:978:THR:HG22	2.02	0.41
1:C:1108:GLU:H	1:C:1108:GLU:CD	2.23	0.41
1:C:1176:GLU:O	1:C:1180:ARG:NH2	2.44	0.41
1:C:1601:MET:HA	1:C:1602:PRO:HD3	1.92	0.41
1:C:2094:LEU:O	1:C:2098:VAL:HG12	2.20	0.41
1:C:2215:LEU:HD12	1:C:2229:VAL:HG11	2.02	0.41
1:C:3532:LEU:HA	1:C:3535:LEU:HD13	2.03	0.41
1:D:45:ARG:NH2	1:D:447:ASP:OD2	2.50	0.41
1:D:1518:CYS:O	1:D:1526:LEU:HA	2.20	0.41
1:D:1705:GLY:O	1:D:1708:ARG:N	2.54	0.41
1:D:1750:PRO:HD2	1:D:1755:GLY:HA3	2.02	0.41
1:D:2094:LEU:O	1:D:2098:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2164:SER:O	1:D:2167:ILE:HG12	2.20	0.41
1:D:3644:LEU:HD12	1:D:3645:PRO:HD2	2.03	0.41
1:D:3771:HIS:HA	1:D:3773:ARG:NH1	2.35	0.41
1:D:4021:LYS:HA	1:D:4139:ILE:HD13	2.01	0.41
1:A:451:TYR:OH	1:A:474:ARG:HD2	2.20	0.41
1:A:685:GLY:HA3	1:A:714:TYR:O	2.20	0.41
1:A:1539:PHE:O	1:A:1542:VAL:HG22	2.20	0.41
1:A:1653:LEU:HD12	1:A:1707:LEU:HD11	2.02	0.41
1:A:1829:PRO:HG2	1:A:1833:SER:H	1.85	0.41
1:A:1839:VAL:CB	1:A:1840:PRO:HD3	2.45	0.41
1:A:3802:ILE:HD12	1:A:3886:ARG:HG3	2.01	0.41
1:B:349:GLN:HG2	1:B:356:TRP:CH2	2.56	0.41
1:B:418:LEU:HA	1:B:421:PHE:HE1	1.86	0.41
1:B:2438:PRO:HG3	1:B:2454:ARG:HG3	2.01	0.41
1:B:3761:GLN:O	1:B:3762:ARG:HB2	2.20	0.41
1:B:4815:ASP:O	1:B:4816:ILE:C	2.57	0.41
1:B:4824:ARG:HE	1:B:4824:ARG:HB3	1.66	0.41
1:C:181:HIS:N	1:C:192:ASP:O	2.50	0.41
1:C:551:LEU:HD23	1:C:553:ARG:NH2	2.36	0.41
1:C:1028:ASP:N	1:C:1028:ASP:OD1	2.54	0.41
1:C:1293:LEU:HD23	1:C:1579:MET:HB3	2.01	0.41
1:C:3212:GLU:HA	1:C:3216:CYS:SG	2.61	0.41
1:C:3798:LEU:HD21	1:C:3884:LEU:HA	2.02	0.41
1:C:4247:ILE:HD11	1:C:4667:PRO:HB2	2.01	0.41
1:D:349:GLN:HG2	1:D:356:TRP:CH2	2.56	0.41
1:D:1444:GLU:HA	1:D:1445:PRO:HD3	1.92	0.41
1:D:1457:TYR:OH	1:D:1643:GLU:O	2.38	0.41
1:D:4995:LEU:HD23	1:D:5011:TRP:HB2	2.03	0.41
1:D:5027:CYS:O	1:D:5027:CYS:SG	2.78	0.41
1:A:252:VAL:HA	1:A:255:HIS:HB2	2.03	0.41
1:A:349:GLN:HG2	1:A:356:TRP:CH2	2.56	0.41
1:A:645:ARG:HG2	1:A:826:ILE:HG23	2.01	0.41
1:A:1683:HIS:ND1	1:A:1797:ARG:HG2	2.35	0.41
1:A:2094:LEU:O	1:A:2098:VAL:HG12	2.20	0.41
1:A:2418:LEU:HD12	1:A:2418:LEU:HA	1.94	0.41
1:A:2506:LEU:HD12	1:A:2510:TYR:HB2	2.03	0.41
1:A:3343:GLN:O	1:A:3347:SER:OG	2.25	0.41
1:A:4006:ASP:OD1	1:A:4008:SER:N	2.53	0.41
1:A:4685:GLY:HA3	1:A:4689:THR:HB	2.02	0.41
1:B:652:ARG:HD2	1:B:750:LEU:HB2	2.02	0.41
1:B:869:ARG:NH2	1:B:873:LYS:HZ3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:977:LEU:HD12	1:B:978:THR:HG22	2.02	0.41
1:B:1108:GLU:H	1:B:1108:GLU:CD	2.23	0.41
1:B:1750:PRO:HD2	1:B:1755:GLY:HA3	2.02	0.41
1:B:2215:LEU:HD12	1:B:2229:VAL:HG11	2.02	0.41
1:B:2695:LEU:HD12	1:B:2696:TYR:H	1.85	0.41
1:B:3842:LEU:HA	1:B:3842:LEU:HD23	1.83	0.41
1:B:4702:ASP:N	1:B:4702:ASP:OD1	2.53	0.41
1:B:4816:ILE:O	1:B:4820:VAL:HG23	2.20	0.41
1:C:220:LEU:HB2	1:C:392:ARG:HA	2.03	0.41
1:C:349:GLN:HG2	1:C:356:TRP:CH2	2.56	0.41
1:C:960:MET:HE3	1:C:960:MET:HA	2.02	0.41
1:C:1293:LEU:HD21	1:C:1579:MET:HB3	2.03	0.41
1:C:1634:LEU:HD12	1:C:1634:LEU:HA	1.86	0.41
1:C:1680:ARG:HA	1:C:1797:ARG:HD2	2.03	0.41
1:C:4112:LEU:O	1:C:4115:SER:OG	2.39	0.41
1:C:4802:GLY:HA3	1:C:4809:PHE:CE2	2.56	0.41
1:D:21:VAL:HG12	1:D:205:ILE:HB	2.02	0.41
1:D:3290:GLU:C	1:D:3293:PRO:HD2	2.41	0.41
1:D:4690:GLU:O	1:D:4691:GLN:HG2	2.21	0.41
1:A:884:LEU:HG	1:A:965:TYR:HD2	1.84	0.41
1:A:1205:GLY:O	1:B:3573:MET:HE3	2.20	0.41
1:A:1927:LEU:HB3	1:A:1939:MET:SD	2.60	0.41
1:A:2164:SER:O	1:A:2167:ILE:HG12	2.20	0.41
1:A:3309:SER:O	1:A:3312:LEU:HD23	2.20	0.41
1:B:63:ALA:HB2	1:B:261:ARG:NH1	2.36	0.41
1:B:719:LEU:O	1:B:720:HIS:CG	2.73	0.41
1:B:732:SER:O	1:B:735:GLN:HG2	2.20	0.41
1:B:1705:GLY:O	1:B:1708:ARG:N	2.54	0.41
1:B:2418:LEU:HD12	1:B:2418:LEU:HA	1.94	0.41
1:B:3212:GLU:HA	1:B:3216:CYS:SG	2.61	0.41
1:B:3790:THR:HG22	1:B:3835:LEU:HD23	2.02	0.41
1:B:4633:GLU:C	1:B:4635:SER:H	2.24	0.41
1:C:627:PRO:O	1:C:629:ARG:NE	2.53	0.41
1:C:759:ILE:HG22	1:C:760:ASN:H	1.86	0.41
1:C:972:LEU:HD13	1:C:1044:ARG:HB3	2.01	0.41
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.28	0.41
1:C:1240:LYS:HG3	1:C:1241:SER:H	1.86	0.41
1:C:4006:ASP:OD1	1:C:4008:SER:N	2.53	0.41
1:C:4817:ALA:C	1:C:4819:GLY:N	2.66	0.41
1:C:4878:ASP:OD1	1:C:4879:MET:N	2.54	0.41
1:C:4995:LEU:HD23	1:C:5011:TRP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:VAL:HA	1:D:255:HIS:HB2	2.03	0.41
1:D:317:ARG:N	1:D:347:PHE:O	2.48	0.41
1:D:646:PRO:HA	1:D:823:LEU:HA	2.03	0.41
1:D:972:LEU:HD21	1:D:1048:GLY:HA3	2.03	0.41
1:D:1240:LYS:HG3	1:D:1241:SER:H	1.86	0.41
1:D:2194:HIS:HE1	1:D:3647:HIS:NE2	2.18	0.41
1:D:2506:LEU:HD12	1:D:2510:TYR:HB2	2.03	0.41
1:D:3802:ILE:HD12	1:D:3886:ARG:HG3	2.01	0.41
1:D:3980:LEU:HD23	1:D:3980:LEU:HA	1.85	0.41
1:A:49:LEU:HD11	1:A:191:VAL:HG13	2.02	0.41
1:A:4802:GLY:HA3	1:A:4809:PHE:CE2	2.56	0.41
1:A:4878:ASP:OD1	1:A:4879:MET:N	2.54	0.41
1:B:181:HIS:N	1:B:192:ASP:O	2.50	0.41
1:B:759:ILE:HG22	1:B:760:ASN:H	1.86	0.41
1:B:1207:ASP:OD1	1:B:1207:ASP:N	2.53	0.41
1:B:1653:LEU:HD12	1:B:1707:LEU:HD11	2.02	0.41
1:B:1683:HIS:ND1	1:B:1797:ARG:HG2	2.35	0.41
1:B:1839:VAL:CB	1:B:1840:PRO:HD3	2.45	0.41
1:B:2226:PRO:C	1:B:2228:MET:H	2.24	0.41
1:B:4088:ILE:HD11	1:B:4093:PHE:HD2	1.86	0.41
1:B:4802:GLY:HA3	1:B:4809:PHE:CE2	2.56	0.41
1:C:1205:GLY:O	1:D:3573:MET:HE3	2.20	0.41
1:C:4980:LEU:HD23	1:C:4980:LEU:HA	1.96	0.41
1:D:2226:PRO:C	1:D:2228:MET:H	2.24	0.41
1:D:3761:GLN:O	1:D:3762:ARG:HB2	2.20	0.41
1:A:24:CYS:O	1:A:35:LEU:N	2.45	0.41
1:A:34:LYS:H	1:A:53:SER:HB2	1.86	0.41
1:A:418:LEU:HA	1:A:421:PHE:HE1	1.86	0.41
1:A:972:LEU:HD13	1:A:1044:ARG:HB3	2.01	0.41
1:A:1172:ASP:N	1:A:1172:ASP:OD1	2.52	0.41
1:A:1293:LEU:HD21	1:A:1579:MET:HB3	2.03	0.41
1:A:1705:GLY:O	1:A:1708:ARG:N	2.54	0.41
1:A:1849:LEU:HD12	1:A:1849:LEU:HA	1.84	0.41
1:A:2552:ARG:CZ	1:A:2552:ARG:HA	2.51	0.41
1:A:2695:LEU:HD12	1:A:2696:TYR:H	1.85	0.41
1:A:3532:LEU:HA	1:A:3535:LEU:HD13	2.03	0.41
1:A:4088:ILE:HD11	1:A:4093:PHE:HD2	1.86	0.41
1:A:4682:GLU:HA	1:A:4724:VAL:HG12	2.03	0.41
1:B:24:CYS:O	1:B:35:LEU:N	2.45	0.41
1:B:111:HIS:CE1	1:B:113:HIS:HB3	2.56	0.41
1:B:220:LEU:HB2	1:B:392:ARG:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:HA	1:B:255:HIS:HB2	2.03	0.41
1:B:633:LEU:HD23	1:B:1639:LEU:HD22	2.02	0.41
1:B:637:LEU:HD23	1:B:1637:MET:HB3	2.03	0.41
1:B:685:GLY:HA3	1:B:714:TYR:O	2.20	0.41
1:B:1154:ASP:O	1:B:1158:ASN:N	2.54	0.41
1:B:1176:GLU:O	1:B:1177:THR:OG1	2.38	0.41
1:B:1205:GLY:O	1:C:3573:MET:HE3	2.20	0.41
1:B:1601:MET:HA	1:B:1602:PRO:HD3	1.92	0.41
1:B:1842:LEU:HD12	1:B:1842:LEU:HA	1.77	0.41
1:B:2368:LEU:HD22	1:B:2376:LEU:HD13	2.02	0.41
1:B:4682:GLU:HA	1:B:4724:VAL:HG12	2.03	0.41
1:B:4690:GLU:O	1:B:4691:GLN:HG2	2.21	0.41
1:B:4878:ASP:OD1	1:B:4879:MET:N	2.54	0.41
1:B:4995:LEU:HD23	1:B:5011:TRP:HB2	2.03	0.41
1:C:21:VAL:HG12	1:C:205:ILE:HB	2.02	0.41
1:C:220:LEU:CB	1:C:392:ARG:HA	2.51	0.41
1:C:591:ASP:HB2	1:C:631:LEU:HD11	2.02	0.41
1:C:719:LEU:O	1:C:720:HIS:CG	2.73	0.41
1:C:1457:TYR:O	1:C:1497:GLY:N	2.47	0.41
1:C:1457:TYR:OH	1:C:1643:GLU:O	2.38	0.41
1:C:1683:HIS:HD2	1:C:1800:PRO:HG3	1.85	0.41
1:C:2138:LEU:N	1:C:2139:PRO:HD2	2.36	0.41
1:C:2368:LEU:HD22	1:C:2376:LEU:HD13	2.02	0.41
1:C:3716:LEU:HD12	1:C:3716:LEU:HA	1.86	0.41
1:C:4690:GLU:HG2	1:C:4691:GLN:H	1.86	0.41
1:D:591:ASP:HB2	1:D:631:LEU:HD11	2.02	0.41
1:D:685:GLY:HA3	1:D:714:TYR:O	2.20	0.41
1:D:759:ILE:HG22	1:D:760:ASN:H	1.86	0.41
1:D:1295:VAL:HB	1:D:1452:TRP:O	2.21	0.41
1:D:1540:PHE:O	1:D:1543:GLU:HG2	2.21	0.41
1:D:1867:GLU:O	1:D:1870:VAL:N	2.53	0.41
1:D:3662:ILE:O	1:D:3664:THR:N	2.50	0.41
1:D:3790:THR:HG22	1:D:3835:LEU:HD23	2.02	0.41
1:D:3923:LEU:HD21	1:D:3962:PHE:HE1	1.84	0.41
1:D:4088:ILE:HD11	1:D:4093:PHE:HD2	1.86	0.41
1:D:4682:GLU:HA	1:D:4724:VAL:HG12	2.03	0.41
1:D:4790:LEU:HA	1:D:4790:LEU:HD23	1.85	0.41
1:D:4802:GLY:HA3	1:D:4809:PHE:CE2	2.56	0.41
1:D:4816:ILE:O	1:D:4820:VAL:HG23	2.20	0.41
1:D:4878:ASP:OD1	1:D:4879:MET:N	2.54	0.41
1:D:4911:LEU:HD13	1:D:4911:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:HIS:CE1	1:A:113:HIS:HB3	2.56	0.41
1:A:551:LEU:HD23	1:A:553:ARG:NH2	2.36	0.41
1:A:719:LEU:O	1:A:720:HIS:CG	2.73	0.41
1:A:804:PRO:HA	1:A:805:PRO:HD3	1.91	0.41
1:A:1295:VAL:HB	1:A:1452:TRP:O	2.21	0.41
1:A:2135:LEU:HD13	1:A:3662:ILE:HG22	2.01	0.41
1:A:2138:LEU:N	1:A:2139:PRO:HD2	2.36	0.41
1:A:2420:HIS:HA	1:A:2423:MET:CE	2.51	0.41
1:B:404:ILE:HG23	1:B:483:MET:HE3	2.02	0.41
1:B:551:LEU:HD23	1:B:553:ARG:NH2	2.36	0.41
1:B:1663:HIS:HA	1:B:1666:THR:HG22	2.04	0.41
1:B:1680:ARG:HA	1:B:1797:ARG:HD2	2.03	0.41
1:B:1835:GLU:O	1:B:1838:PHE:N	2.53	0.41
1:B:4690:GLU:HG2	1:B:4691:GLN:H	1.86	0.41
1:C:637:LEU:HD23	1:C:1637:MET:HB3	2.03	0.41
1:C:1770:SER:HB2	1:C:1956:GLU:OE2	2.21	0.41
1:C:3290:GLU:C	1:C:3293:PRO:HD2	2.41	0.41
1:C:3761:GLN:O	1:C:3762:ARG:HB2	2.20	0.41
1:C:4088:ILE:HD11	1:C:4093:PHE:HD2	1.86	0.41
1:C:4682:GLU:HA	1:C:4724:VAL:HG12	2.03	0.41
1:D:24:CYS:O	1:D:35:LEU:N	2.45	0.41
1:D:178:ARG:HA	1:D:178:ARG:HD2	1.89	0.41
1:D:551:LEU:HD23	1:D:553:ARG:NH2	2.36	0.41
1:D:790:ARG:NH1	1:D:797:HIS:HB3	2.35	0.41
1:D:1155:LEU:HD11	1:D:1188:PHE:CD2	2.56	0.41
1:D:1651:LEU:HD13	1:D:1651:LEU:HA	1.95	0.41
1:D:3212:GLU:HA	1:D:3216:CYS:SG	2.61	0.41
1:D:4006:ASP:OD1	1:D:4008:SER:N	2.53	0.41
1:D:4828:SER:O	1:D:4832:HIS:N	2.52	0.41
1:A:633:LEU:HD23	1:A:1639:LEU:HD22	2.02	0.40
1:A:652:ARG:HD2	1:A:750:LEU:HB2	2.02	0.40
1:A:1208:VAL:O	1:B:3577:ARG:CZ	2.68	0.40
1:A:1540:PHE:O	1:A:1543:GLU:HG2	2.21	0.40
1:A:2456:ILE:HD12	1:D:131:LEU:HD11	2.03	0.40
1:A:3770:LEU:HD12	1:A:3770:LEU:HA	1.93	0.40
1:B:34:LYS:H	1:B:53:SER:HB2	1.86	0.40
1:B:1518:CYS:O	1:B:1526:LEU:HA	2.20	0.40
1:B:1770:SER:HB2	1:B:1956:GLU:OE2	2.21	0.40
1:B:2135:LEU:HD13	1:B:3662:ILE:HG22	2.01	0.40
1:B:3798:LEU:HD21	1:B:3884:LEU:HA	2.02	0.40
1:C:34:LYS:H	1:C:53:SER:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LEU:HD13	1:C:202:MET:HE1	2.03	0.40
1:C:646:PRO:HA	1:C:823:LEU:HA	2.03	0.40
1:C:652:ARG:HD2	1:C:750:LEU:HB2	2.02	0.40
1:C:1705:GLY:O	1:C:1708:ARG:N	2.54	0.40
1:C:1750:PRO:HD2	1:C:1755:GLY:HA3	2.02	0.40
1:C:4633:GLU:O	1:C:4635:SER:N	2.50	0.40
1:C:4897:ILE:H	1:C:4897:ILE:HG13	1.59	0.40
1:D:633:LEU:HD23	1:D:1639:LEU:HD22	2.02	0.40
1:D:1154:ASP:O	1:D:1158:ASN:N	2.54	0.40
1:D:2138:LEU:N	1:D:2139:PRO:HD2	2.36	0.40
1:D:2420:HIS:HA	1:D:2423:MET:CE	2.51	0.40
1:D:2552:ARG:CZ	1:D:2552:ARG:HA	2.51	0.40
1:A:402:ARG:HA	1:A:402:ARG:HD2	1.78	0.40
1:A:627:PRO:O	1:A:629:ARG:NE	2.53	0.40
1:A:1663:HIS:HA	1:A:1666:THR:HG22	2.04	0.40
1:A:3272:ILE:O	1:A:3272:ILE:HG13	2.21	0.40
1:A:3290:GLU:C	1:A:3293:PRO:HD2	2.41	0.40
1:A:3644:LEU:HD12	1:A:3645:PRO:HD2	2.03	0.40
1:A:4690:GLU:HG2	1:A:4691:GLN:H	1.86	0.40
1:B:3330:ASP:O	1:B:3333:THR:OG1	2.31	0.40
1:B:4925:ILE:O	1:B:4929:LEU:HB2	2.22	0.40
1:C:959:TYR:HD2	1:C:966:LYS:HB2	1.87	0.40
1:C:4690:GLU:O	1:C:4691:GLN:HG2	2.21	0.40
1:D:637:LEU:HD23	1:D:1637:MET:HB3	2.03	0.40
1:D:1653:LEU:HD12	1:D:1707:LEU:HD11	2.02	0.40
1:D:1835:GLU:O	1:D:1836:PHE:C	2.59	0.40
1:D:2654:TYR:O	1:D:2658:PRO:HD3	2.22	0.40
1:D:4112:LEU:O	1:D:4115:SER:OG	2.39	0.40
1:D:4993:MET:HE2	1:D:4993:MET:HB3	1.98	0.40
1:A:637:LEU:HD23	1:A:1637:MET:HB3	2.03	0.40
1:A:683:ARG:HD2	1:A:707:VAL:O	2.21	0.40
1:A:3212:GLU:HA	1:A:3216:CYS:SG	2.61	0.40
1:A:3996:PHE:O	1:A:4000:MET:HB2	2.22	0.40
1:B:626:LEU:HG	1:B:628:GLY:N	2.27	0.40
1:B:1155:LEU:HD11	1:B:1188:PHE:CD2	2.56	0.40
1:B:2420:HIS:HA	1:B:2423:MET:CE	2.51	0.40
1:B:2548:LEU:O	1:B:2552:ARG:HG2	2.22	0.40
1:B:3290:GLU:C	1:B:3293:PRO:HD2	2.41	0.40
1:C:418:LEU:HA	1:C:421:PHE:HE1	1.86	0.40
1:C:633:LEU:HD23	1:C:1639:LEU:HD22	2.02	0.40
1:C:660:GLY:O	1:C:750:LEU:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:GLY:HA3	1:C:714:TYR:O	2.20	0.40
1:C:1653:LEU:HD12	1:C:1707:LEU:HD11	2.02	0.40
1:C:2358:ILE:HD12	1:C:2358:ILE:HA	1.91	0.40
1:C:2654:TYR:O	1:C:2658:PRO:HD3	2.22	0.40
1:C:3644:LEU:HD12	1:C:3645:PRO:HD2	2.03	0.40
1:D:652:ARG:HD2	1:D:750:LEU:HB2	2.02	0.40
1:D:956:PRO:O	1:D:959:TYR:HD1	2.04	0.40
1:D:1176:GLU:O	1:D:1177:THR:OG1	2.38	0.40
1:D:2559:LEU:HD21	1:D:2603:ILE:HG22	2.04	0.40
1:D:3996:PHE:O	1:D:4000:MET:HB2	2.22	0.40
1:A:1240:LYS:HG3	1:A:1241:SER:H	1.86	0.40
1:A:1457:TYR:OH	1:A:1643:GLU:O	2.38	0.40
1:A:1518:CYS:O	1:A:1526:LEU:HA	2.20	0.40
1:B:583:ILE:HD11	1:B:620:LEU:HB3	2.04	0.40
1:B:956:PRO:O	1:B:959:TYR:HD1	2.04	0.40
1:B:972:LEU:HD21	1:B:1048:GLY:HA3	2.03	0.40
1:B:2138:LEU:N	1:B:2139:PRO:HD2	2.36	0.40
1:B:2538:THR:OG1	1:B:2539:ALA:N	2.55	0.40
1:B:2552:ARG:CZ	1:B:2552:ARG:HA	2.51	0.40
1:B:2559:LEU:HD21	1:B:2603:ILE:HG22	2.04	0.40
1:B:3005:LEU:HD11	1:B:3050:VAL:HB	2.04	0.40
1:C:235:ALA:HA	1:C:257:ARG:HH11	1.87	0.40
1:C:445:LEU:HD23	1:C:445:LEU:HA	1.91	0.40
1:C:805:PRO:HB2	1:C:808:TYR:CD1	2.57	0.40
1:C:1540:PHE:O	1:C:1543:GLU:HG2	2.21	0.40
1:C:1849:LEU:HA	1:C:1849:LEU:HD12	1.84	0.40
1:C:2194:HIS:HE1	1:C:3647:HIS:NE2	2.18	0.40
1:C:2226:PRO:C	1:C:2228:MET:H	2.24	0.40
1:C:2420:HIS:HA	1:C:2423:MET:CE	2.51	0.40
1:C:4864:ASN:HB3	1:C:4874:MET:SD	2.62	0.40
1:D:235:ALA:HA	1:D:257:ARG:HH11	1.87	0.40
1:D:402:ARG:HD2	1:D:402:ARG:HA	1.78	0.40
1:D:430:PRO:HA	1:D:431:PRO:HD3	1.86	0.40
1:D:1770:SER:HB2	1:D:1956:GLU:OE2	2.21	0.40
1:D:3668:SER:O	1:D:3672:ARG:NH2	2.47	0.40
1:D:3817:LEU:HD13	1:D:3899:PHE:CD1	2.45	0.40
1:D:4343:GLY:O	1:D:4344:ALA:C	2.57	0.40
1:D:4863:TYR:HA	1:D:4901:ILE:HD12	2.04	0.40
1:A:583:ILE:HD11	1:A:620:LEU:HB3	2.04	0.40
1:A:805:PRO:HB2	1:A:808:TYR:CD1	2.57	0.40
1:A:1155:LEU:HD11	1:A:1188:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1738:LEU:HD13	1:A:1738:LEU:HA	1.93	0.40
1:A:1750:PRO:HD2	1:A:1755:GLY:HA3	2.02	0.40
1:A:3224:PRO:HB2	1:A:3298:ALA:HB2	2.04	0.40
1:A:3832:ILE:HD13	1:A:3832:ILE:HA	1.98	0.40
1:B:340:LYS:O	1:B:344:SER:OG	2.31	0.40
1:B:4060:LYS:HD2	1:B:4060:LYS:HA	1.90	0.40
1:B:4790:LEU:HD23	1:B:4790:LEU:HA	1.85	0.40
1:C:243:ARG:HB3	1:C:300:VAL:HG23	2.04	0.40
1:C:956:PRO:O	1:C:959:TYR:HD1	2.04	0.40
1:C:1473:THR:N	1:C:1484:HIS:O	2.47	0.40
1:C:4184:MET:HB2	1:C:4190:ILE:HD13	2.04	0.40
1:C:4702:ASP:OD1	1:C:4702:ASP:N	2.53	0.40
1:C:4863:TYR:HB2	1:C:4876:CYS:SG	2.62	0.40
1:D:220:LEU:HB2	1:D:392:ARG:HA	2.03	0.40
1:D:609:CYS:SG	1:D:610:ASN:N	2.93	0.40
1:D:805:PRO:HB2	1:D:808:TYR:CD1	2.57	0.40
1:D:1663:HIS:HA	1:D:1666:THR:HG22	2.04	0.40
1:D:1680:ARG:HA	1:D:1797:ARG:HD2	2.03	0.40
1:D:1838:PHE:O	1:D:1841:VAL:N	2.53	0.40
1:D:3532:LEU:HA	1:D:3535:LEU:HD13	2.03	0.40
1:D:4184:MET:HB2	1:D:4190:ILE:HD13	2.04	0.40
1:D:4681:LEU:HD23	1:D:4681:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3934/5037 (78%)	3496 (89%)	423 (11%)	15 (0%)	30	61
1	B	3934/5037 (78%)	3496 (89%)	423 (11%)	15 (0%)	30	61
1	C	3934/5037 (78%)	3496 (89%)	423 (11%)	15 (0%)	30	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	3934/5037 (78%)	3496 (89%)	423 (11%)	15 (0%)	30	61
All	All	15736/20148 (78%)	13984 (89%)	1692 (11%)	60 (0%)	32	61

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4808	PHE
1	B	4808	PHE
1	C	4808	PHE
1	D	4808	PHE
1	A	1835	GLU
1	A	1836	PHE
1	A	4319	LEU
1	A	4341	ARG
1	A	4818	MET
1	A	4908	GLU
1	B	1835	GLU
1	B	1836	PHE
1	B	4319	LEU
1	B	4341	ARG
1	B	4818	MET
1	B	4908	GLU
1	C	1835	GLU
1	C	1836	PHE
1	C	4319	LEU
1	C	4341	ARG
1	C	4818	MET
1	C	4908	GLU
1	D	1835	GLU
1	D	1836	PHE
1	D	4319	LEU
1	D	4341	ARG
1	D	4818	MET
1	D	4908	GLU
1	A	4320	ARG
1	A	4911	LEU
1	B	4320	ARG
1	B	4911	LEU
1	C	4320	ARG
1	C	4911	LEU
1	D	4320	ARG
1	D	4911	LEU

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Mol	Chain	Res	Type
1	A	1833	SER
1	B	1833	SER
1	C	1833	SER
1	D	1833	SER
1	A	5028	PHE
1	B	5028	PHE
1	C	5028	PHE
1	D	5028	PHE
1	A	1839	VAL
1	A	1840	PRO
1	A	4637	GLY
1	B	1839	VAL
1	B	1840	PRO
1	B	4637	GLY
1	C	1839	VAL
1	C	1840	PRO
1	C	4637	GLY
1	D	1839	VAL
1	D	1840	PRO
1	D	4637	GLY
1	A	4819	GLY
1	B	4819	GLY
1	C	4819	GLY
1	D	4819	GLY

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	2905/4276 (68%)	2882 (99%)	23 (1%)	79	87
1	B	2905/4276 (68%)	2882 (99%)	23 (1%)	79	87
1	C	2905/4276 (68%)	2882 (99%)	23 (1%)	79	87
1	D	2905/4276 (68%)	2882 (99%)	23 (1%)	79	87
All	All	11620/17104 (68%)	11528 (99%)	92 (1%)	77	87

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	ARG
1	A	257	ARG
1	A	392	ARG
1	A	1128	ARG
1	A	1834	VAL
1	A	1842	LEU
1	A	4120	ASN
1	A	4317	ARG
1	A	4318	ARG
1	A	4319	LEU
1	A	4320	ARG
1	A	4633	GLU
1	A	4634	GLU
1	A	4635	SER
1	A	4636	THR
1	A	4639	MET
1	A	4816	ILE
1	A	4818	MET
1	A	4897	ILE
1	A	4901	ILE
1	A	4903	ASP
1	A	4908	GLU
1	A	4911	LEU
1	B	242	ARG
1	B	257	ARG
1	B	392	ARG
1	B	1128	ARG
1	B	1834	VAL
1	B	1842	LEU
1	B	4120	ASN
1	B	4317	ARG
1	B	4318	ARG
1	B	4319	LEU
1	B	4320	ARG
1	B	4633	GLU
1	B	4634	GLU
1	B	4635	SER
1	B	4636	THR
1	B	4639	MET
1	B	4816	ILE
1	B	4818	MET
1	B	4897	ILE

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Mol	Chain	Res	Type
1	B	4901	ILE
1	B	4903	ASP
1	B	4908	GLU
1	B	4911	LEU
1	C	242	ARG
1	C	257	ARG
1	C	392	ARG
1	C	1128	ARG
1	C	1834	VAL
1	C	1842	LEU
1	C	4120	ASN
1	C	4317	ARG
1	C	4318	ARG
1	C	4319	LEU
1	C	4320	ARG
1	C	4633	GLU
1	C	4634	GLU
1	C	4635	SER
1	C	4636	THR
1	C	4639	MET
1	C	4816	ILE
1	C	4818	MET
1	C	4897	ILE
1	C	4901	ILE
1	C	4903	ASP
1	C	4908	GLU
1	C	4911	LEU
1	D	242	ARG
1	D	257	ARG
1	D	392	ARG
1	D	1128	ARG
1	D	1834	VAL
1	D	1842	LEU
1	D	4120	ASN
1	D	4317	ARG
1	D	4318	ARG
1	D	4319	LEU
1	D	4320	ARG
1	D	4633	GLU
1	D	4634	GLU
1	D	4635	SER
1	D	4636	THR

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Mol	Chain	Res	Type
1	D	4639	MET
1	D	4816	ILE
1	D	4818	MET
1	D	4897	ILE
1	D	4901	ILE
1	D	4903	ASP
1	D	4908	GLU
1	D	4911	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	618	GLN
1	A	1041	GLN
1	A	1165	ASN
1	A	1220	GLN
1	A	1837	GLN
1	A	3146	HIS
1	A	3643	ASN
1	A	3809	ASN
1	A	3976	ASN
1	A	4133	GLN
1	A	4201	ASN
1	A	4574	ASN
1	B	23	GLN
1	B	618	GLN
1	B	1041	GLN
1	B	1165	ASN
1	B	1220	GLN
1	B	1837	GLN
1	B	3146	HIS
1	B	3809	ASN
1	B	3976	ASN
1	B	4133	GLN
1	B	4201	ASN
1	B	4574	ASN
1	C	23	GLN
1	C	44	ASN
1	C	618	GLN
1	C	1041	GLN
1	C	1165	ASN

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Mol	Chain	Res	Type
1	C	1220	GLN
1	C	1837	GLN
1	C	3146	HIS
1	C	3643	ASN
1	C	3809	ASN
1	C	3976	ASN
1	C	4133	GLN
1	C	4574	ASN
1	D	23	GLN
1	D	44	ASN
1	D	350	HIS
1	D	618	GLN
1	D	1041	GLN
1	D	1165	ASN
1	D	1220	GLN
1	D	1837	GLN
1	D	3146	HIS
1	D	3643	ASN
1	D	3809	ASN
1	D	3976	ASN
1	D	4133	GLN
1	D	4574	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, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

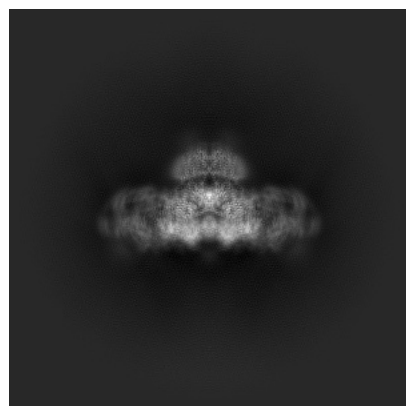
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38048. These allow visual inspection of the internal detail of the map and identification of artifacts.

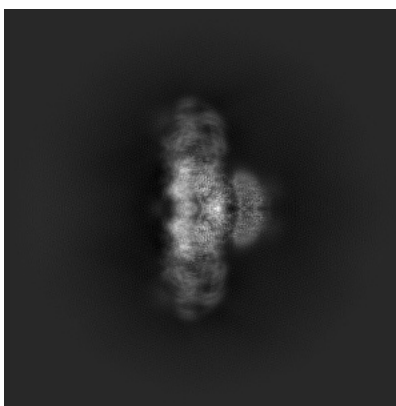
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

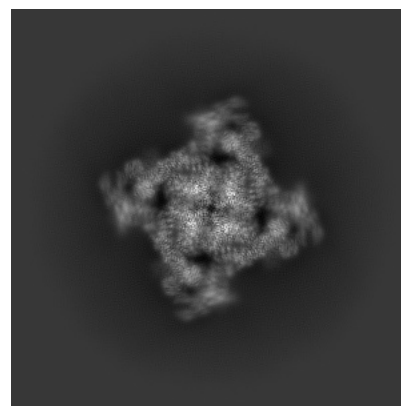
6.1.1 Primary map



X

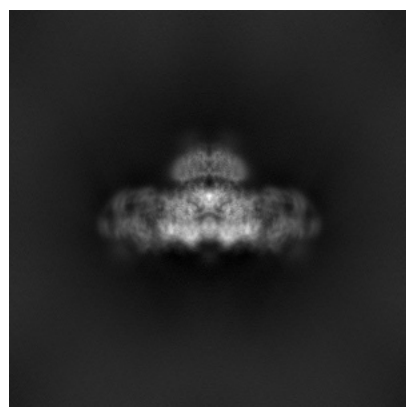


Y

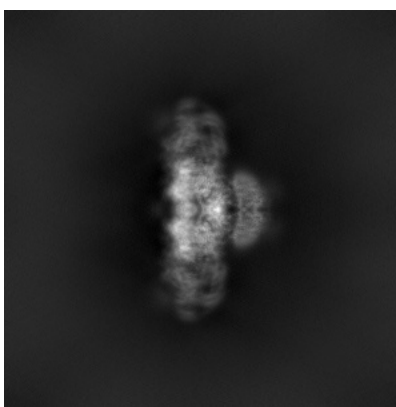


Z

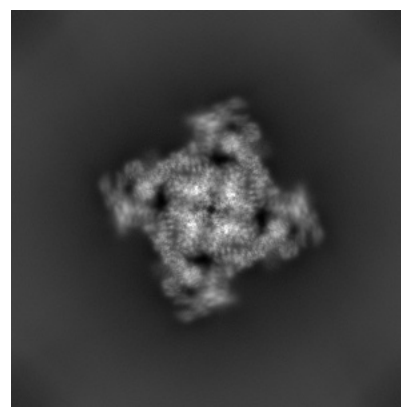
6.1.2 Raw map



X



Y

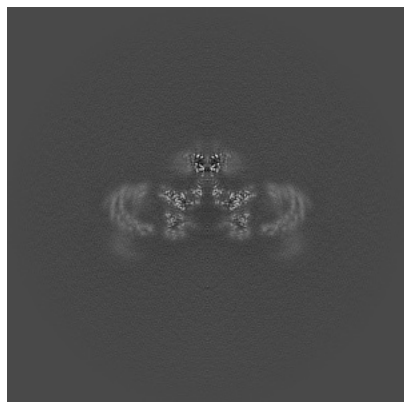


Z

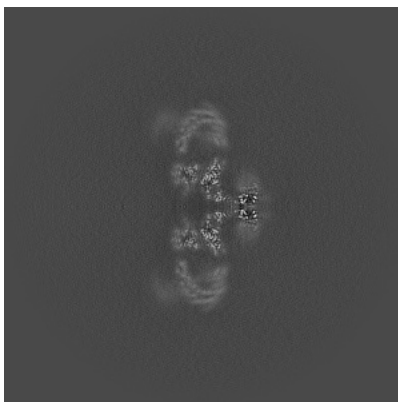
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

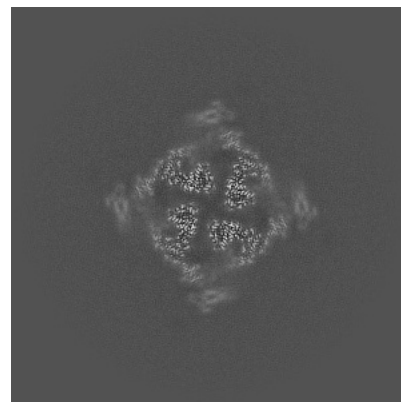
6.2.1 Primary map



X Index: 300

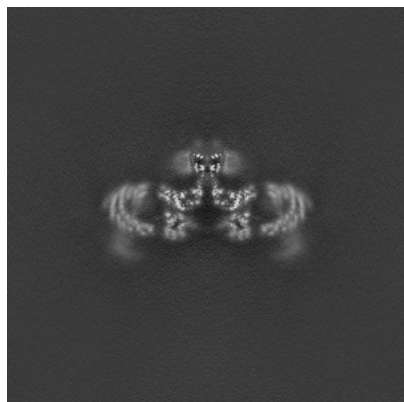


Y Index: 300

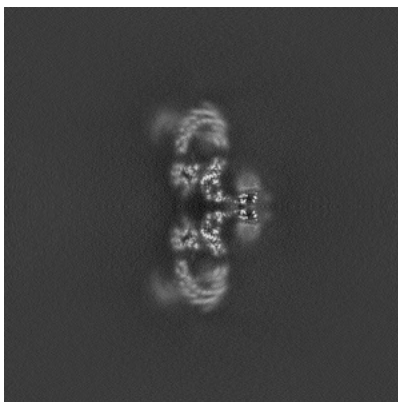


Z Index: 300

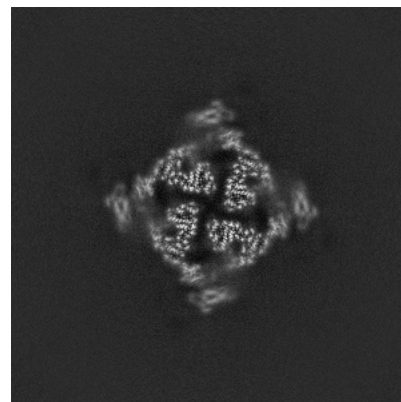
6.2.2 Raw map



X Index: 300



Y Index: 300

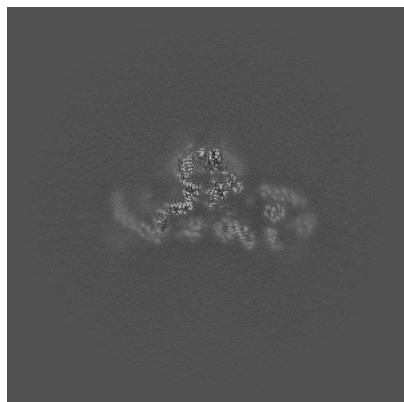


Z Index: 300

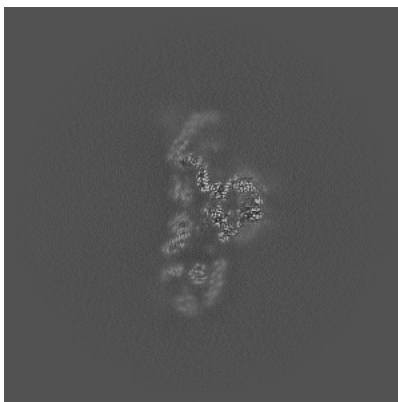
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

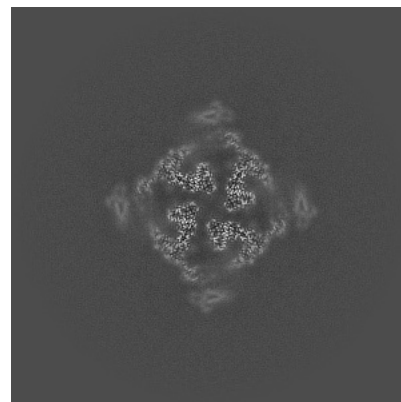
6.3.1 Primary map



X Index: 321

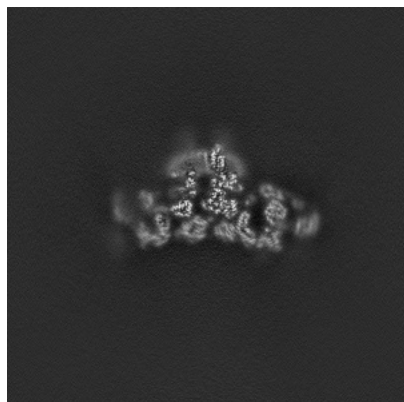


Y Index: 321

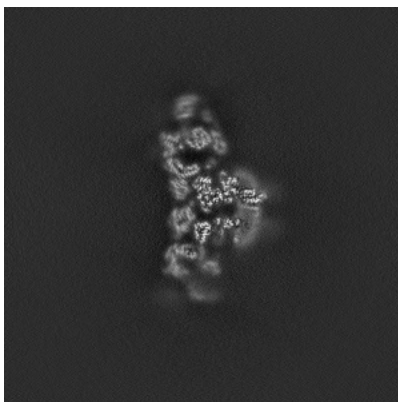


Z Index: 302

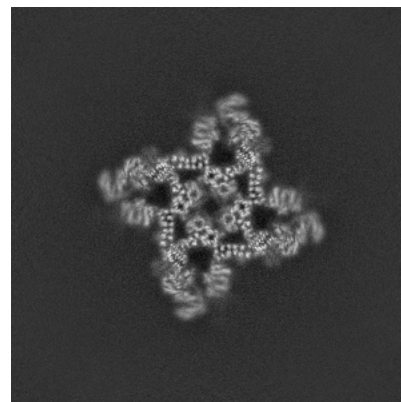
6.3.2 Raw map



X Index: 329



Y Index: 271

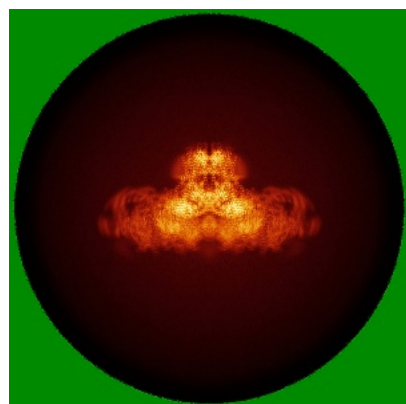


Z Index: 273

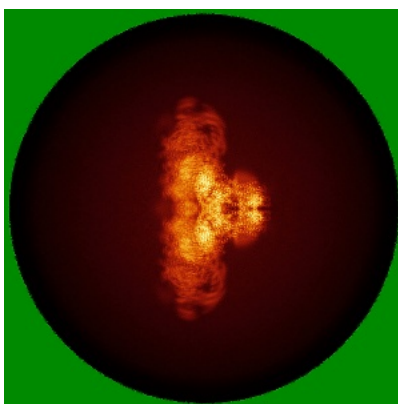
The images above show the largest variance slices of the map in three orthogonal directions.

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

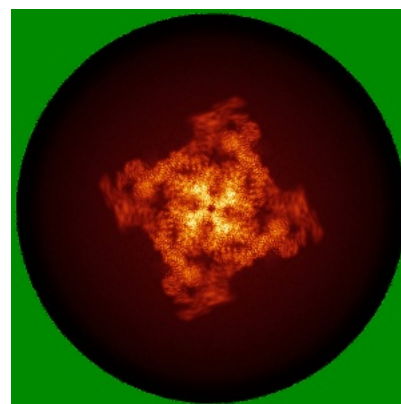
6.4.1 Primary map



X

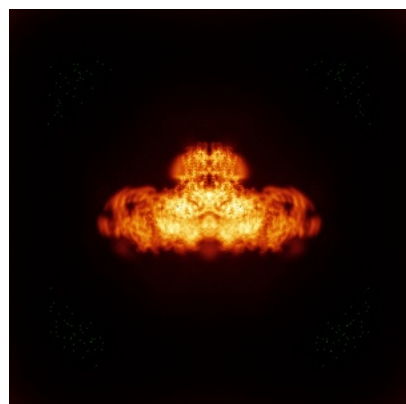


Y

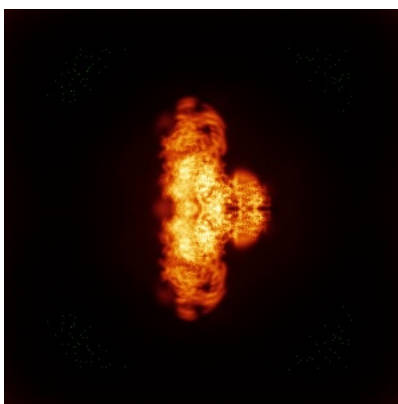


Z

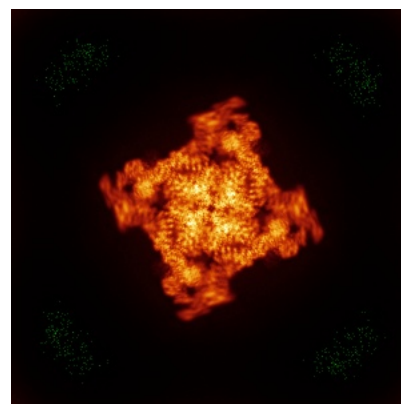
6.4.2 Raw map



X



Y

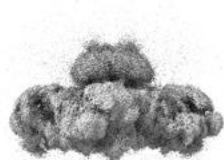


Z

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

6.5 Orthogonal surface views [i](#)

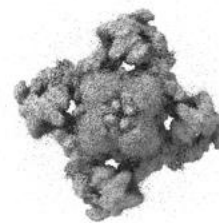
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.182. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

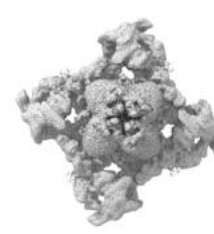
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

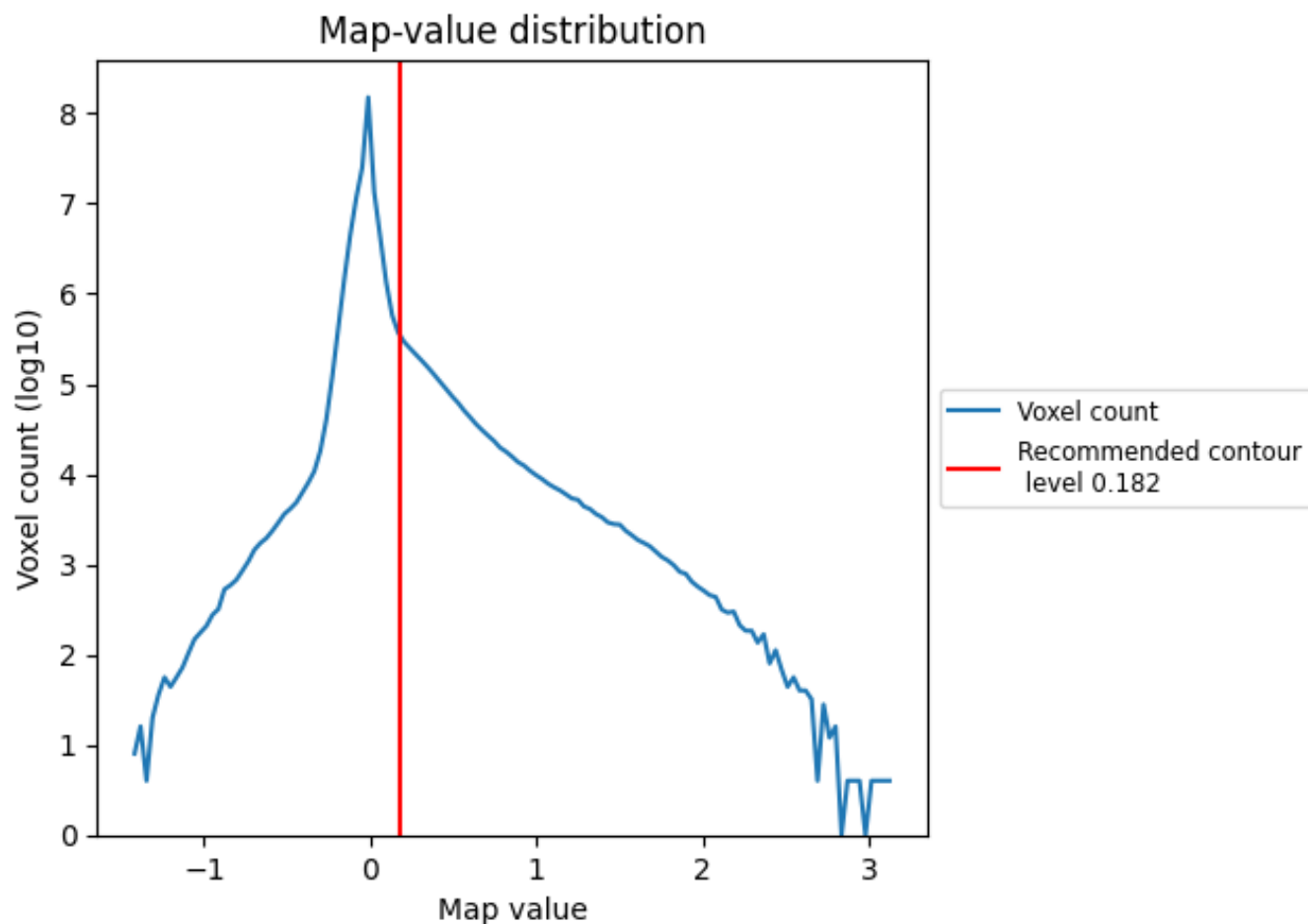
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

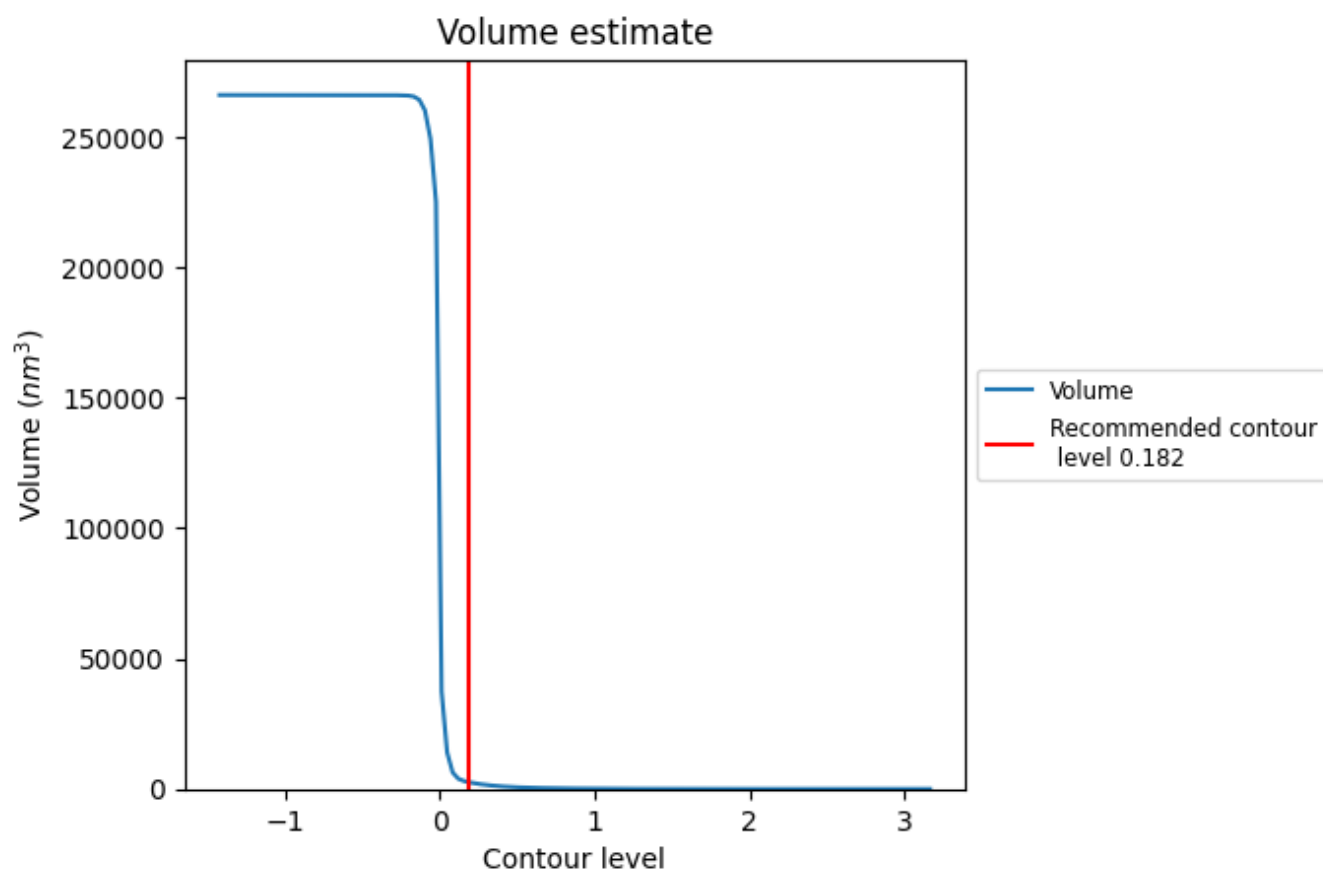
This section contains the results of statistical analysis of the map.

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.

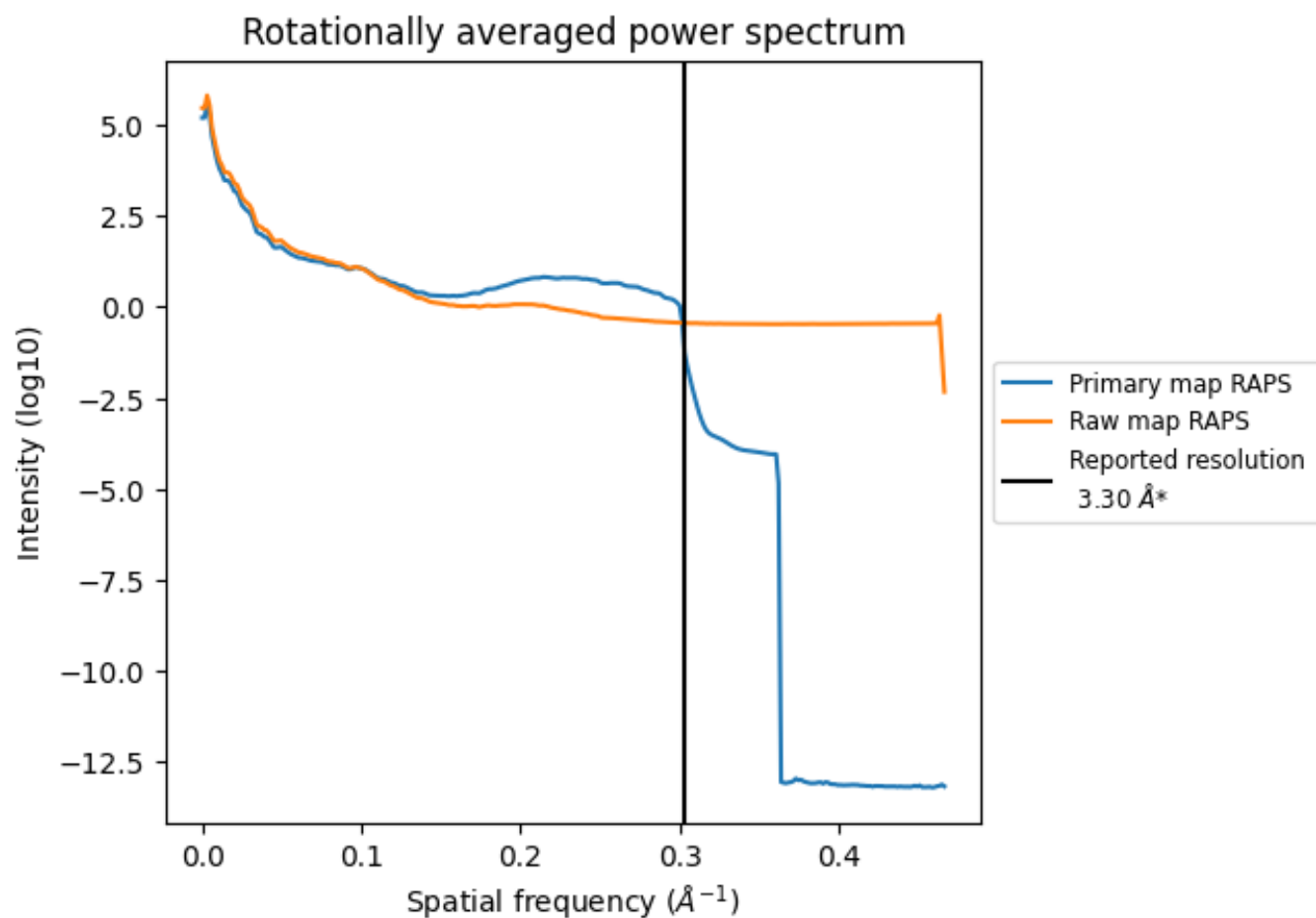
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2676 nm^3 ; this corresponds to an approximate mass of 2418 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

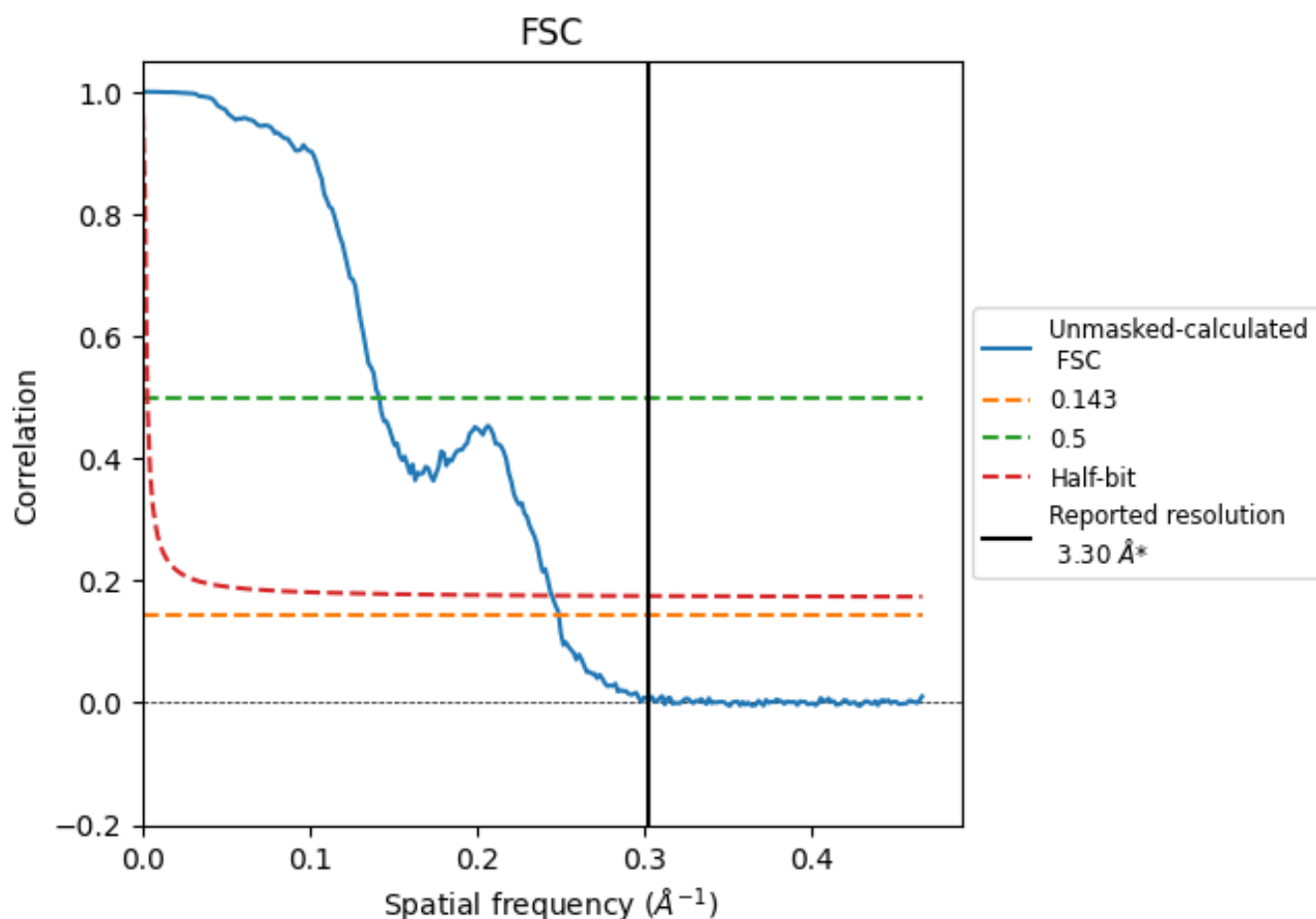


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

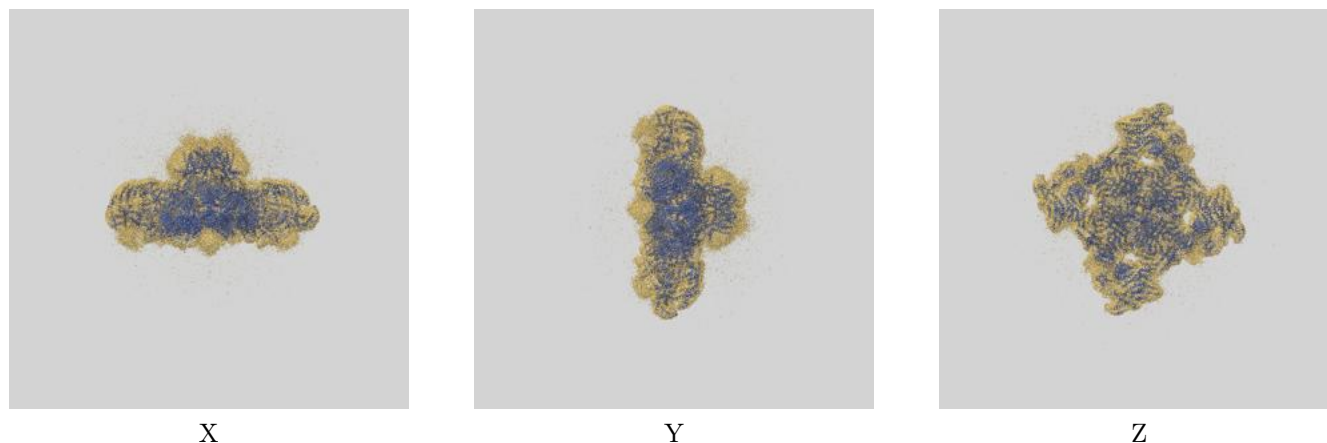
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.02	7.06	4.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

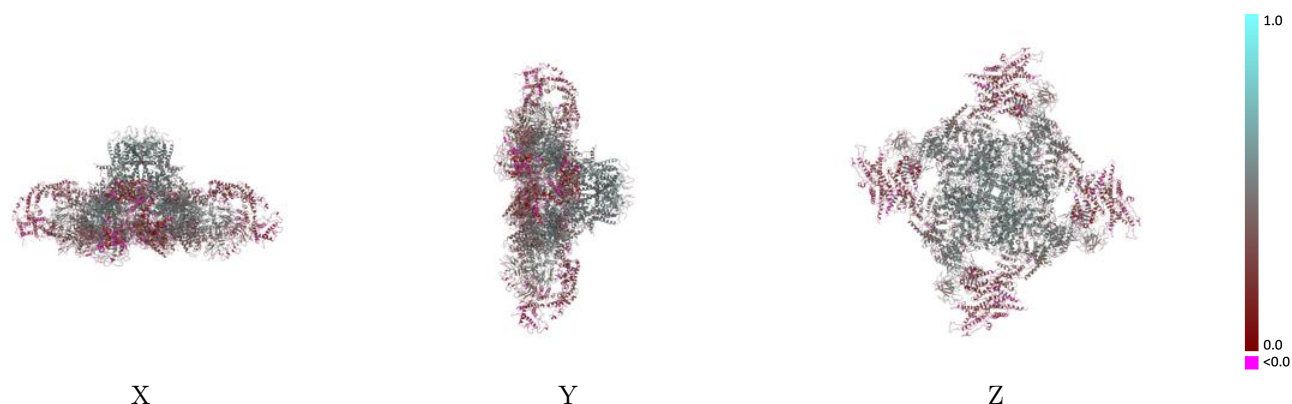
This section contains information regarding the fit between EMDB map EMD-38048 and PDB model 8X4E. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



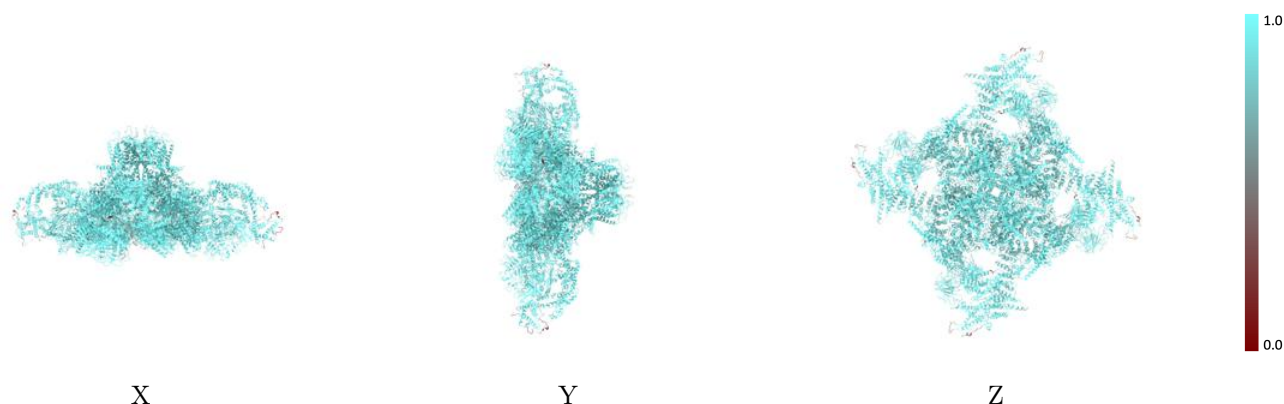
The images above show the 3D surface view of the map at the recommended contour level 0.182 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



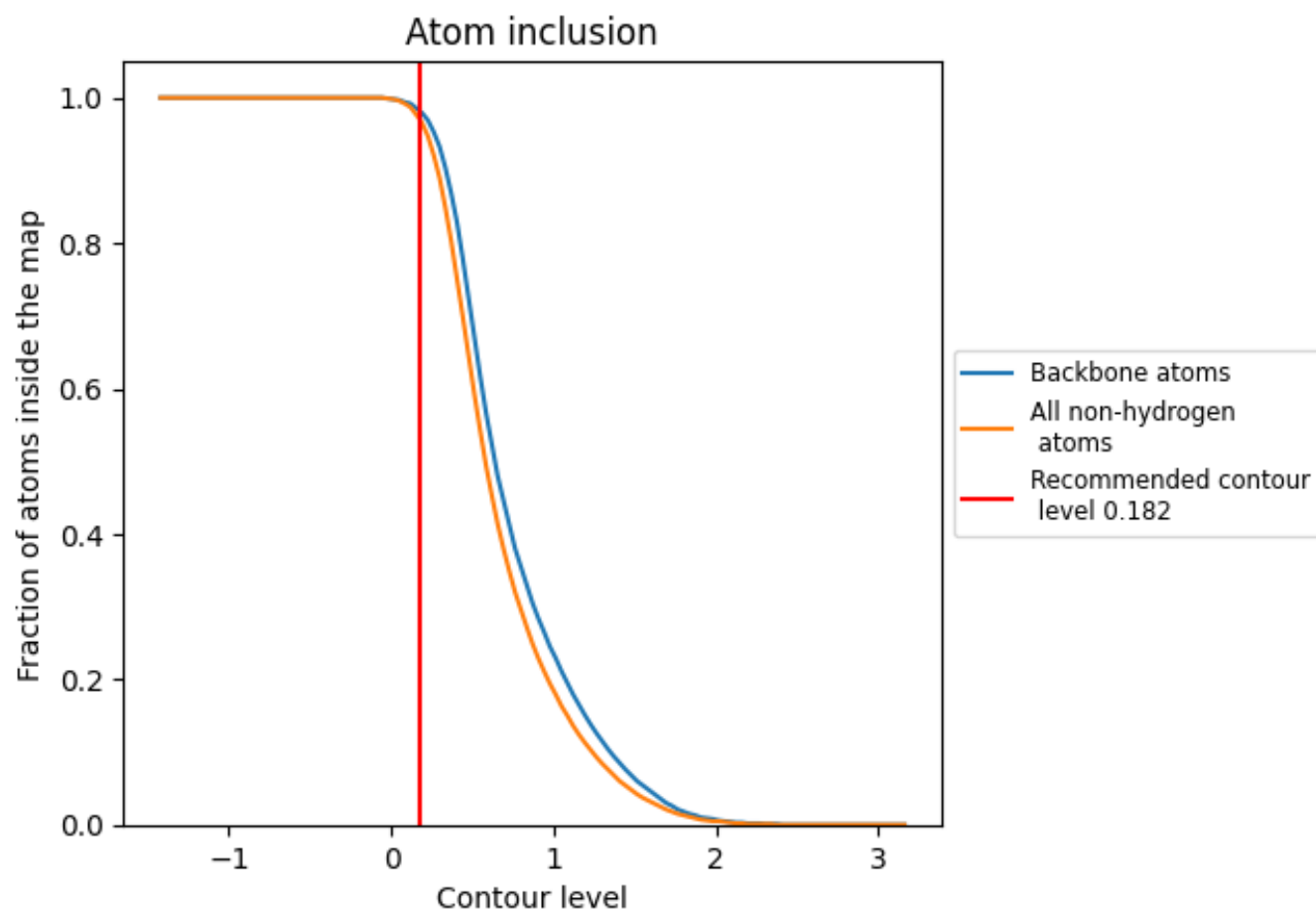
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.182).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.182) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9690	<div></div> 0.3850
A	<div></div> 0.9690	<div></div> 0.3840
B	<div></div> 0.9690	<div></div> 0.3850
C	<div></div> 0.9690	<div></div> 0.3850
D	<div></div> 0.9690	<div></div> 0.3850

