



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:54 AM UTC

PDB ID : 6FOO / pdb\_00006foo  
EMDB ID : EMD-4295  
Title : Structure of Ryanodine Receptor 1 in nanodiscs in the presence of calcium and ATP  
Authors : Willegems, K.; Efremov, R.G.  
Deposited on : 2018-02-08  
Resolution : 8.20 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](mailto: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>.

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

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

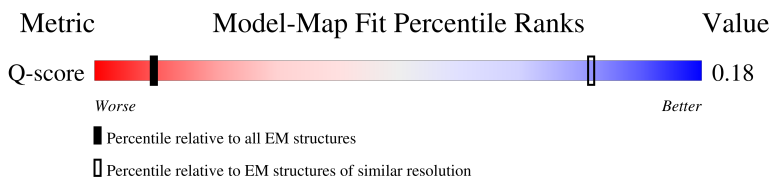
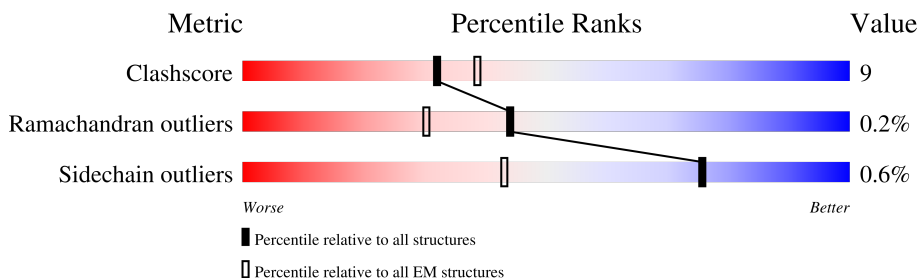
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	337 ( 7.70 - 8.70 )

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  $\geq 3$ , 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	<div> <div>11%</div> <div>67%</div> <div>16%</div> <div>17%</div> </div>
1	B	5037	<div> <div>11%</div> <div>67%</div> <div>16%</div> <div>17%</div> </div>
1	C	5037	<div> <div>11%</div> <div>67%</div> <div>16%</div> <div>17%</div> </div>
1	D	5037	<div> <div>11%</div> <div>67%</div> <div>16%</div> <div>17%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 117476 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	4168	Total 29368	C 18607	N 5202	O 5402	S 157	0	0
1	B	4168	Total 29368	C 18607	N 5202	O 5402	S 157	0	0
1	C	4168	Total 29368	C 18607	N 5202	O 5402	S 157	0	0
1	D	4168	Total 29368	C 18607	N 5202	O 5402	S 157	0	0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

### 3 Residue-property plots [i](#)

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

#### • Molecule 1: Ryanodine receptor 1









PRO	PRO	ASP	GLN	GLU	PRO	GLN	VAL	ASN	GLN	SER	ARG	TRP	D1070	R1071	V1072	R1073	R1076	A1077	E1078	K1079	S1080	Y1081	Q1084	Y1089	F1092	E1093	A1094	V1095	T1096	E1099	M1100	R1101	W1104	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	L1115	L1120	A1121	Y1122	F1123	E1124	F1225	F1226	F1238								
R1128	R1131	W1132	H1133	L1134	D1147	V1148	V1149	M1152	L1153	D1154	E1157	N1158	T1163	L1164	N1165	Y1168	L1169	M1170	S1171	D1172	E1176	G1187	F1188	L1189	V1189	G1200	H1201	L1202	M1203	S1210	L1211	R1212	C1217	G1218	F1223	E1224	F1225	F1226	F1238																			
L846	S847	H848	T849	D850	P853	C854	D857	THR	VAL	GLN	T861	V862	L863	P864	P865	H866	L867	E868	R869	I870	R886	I887	E888	Q889	G890	W891	V892	T893	G894	P895	V896	R897	D898	D899	N900	K901	R902	L903	L907	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	H938	V939	G940	M941					
A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	N960	M961	S962	N963	G964	A968	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ASN	PRO	R1020	R1044	T1045	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054					
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H725	V730	F733	G734	O735	F740	E741	V744	S745	G746	L750	I759	P763	F768	E769	A770	L773	D774	G775	L776	F777	R778	P779	V780	W781	A785	K788	L792	L793	H797	G798	E799	Y808	H812	L823	E824	R835	H838	P842																				
L846	S847	H848	T849	D850	P853	C854	D857	THR	VAL	GLN	T861	V862	L863	P864	P865	H866	L867	E868	R869	I870	R886	I887	E888	Q889	G890	W891	V892	T893	G894	P895	V896	R897	D898	D899	N900	K901	R902	L903	L907	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	H938	V939	G940	M941					
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VAL	GLU	ALA	GLY	VAL	SER	SER	GLN	GLY	GLY	G97	H98	R99	T100	H101	Y103	L102	G104	H105	A106	I107	L108	L109	R110	H111	A112	H113	S114	R115	M116	I117	L118	C206	S207	S119	C120	S124	R125	S126	K130	A132	F133	D134	V135	G136	L137	Q138	E139	E144	A145	C146	W147	W148	T149	M150	H151	N84	THR	
GLY	ASP	GLY	GLY	GLU	GLU	GLU	GLU	GLU	ASP	GLY	G97	H98	R99	T100	H101	Y103	L102	G104	H105	A106	I107	L108	L109	R110	H111	A112	H113	S114	R115	M116	I117	L118	C206	S207	S119	C120	S124	R125	S126	K130	A132	F133	D134	V135	G136	L137	Q138	E139	E144	A145	C146	W147	W148	T149	M150	H151	N84	THR
GLY	ASP	GLY	GLY	GLU	GLU	GLU	GLU	GLU	ASP	GLY	G97	H98	R99	T100	H101	Y103	L102	G104	H105	A106	I107	L108	L109	R110	H111	A112	H113	S114	R115	M116	I117	L118	C206	S207	S119	C120	S124	R125	S126	K130	A132	F133	D134	V135	G136	L137	Q138	E139	E144	A145	C146	W147	W148	T149	M150	H151	N84	THR
GLY	ASP	GLY	GLY	GLU	GLU	GLU	GLU	GLU	ASP	GLY	G97	H98	R99	T100	H101	Y103	L102	G104	H105	A106	I107	L108	L109	R110	H111	A112	H113	S114	R115	M116	I117	L118	C206	S207	S119	C120	S124	R125	S126	K130	A132	F133	D134	V135	G136	L137	Q138	E139	E144	A145	C146	W147	W148	T149	M150	H151	N84	THR
GLY	ASP	GLY	GLY	GLU	GLU	GLU	GLU	GLU	ASP	GLY	G97	H98	R99	T100	H101	Y103	L102	G104	H105	A106	I107	L108	L109	R110	H111	A112	H113	S114	R115	M116	I117	L118	C206	S207	S119	C120	S124	R125	S126	K130	A132	F133	D134	V135	G136	L137	Q138	E139	E144	A145	C146	W147	W148	T149	M150	H151	N84	THR
GLY	ASP	GLY	GLY	GLU	GLU	GLU	GLU	GLU	ASP	GLY	G97	H98	R99	T100	H101	Y103	L102	G104	H105	A106	I107	L108	L109	R110	H111	A112	H113	S114	R115	M116	I117	L118	C206	S207	S119	C120	S124	R125	S126	K130	A132	F133	D134	V135	G136	L137	Q138	E139	E144	A145	C146	W147	W148	T149	M150	H151	N84	THR
GLY	ASP	GLY	GLY	GLU	GLU	GLU	GLU	GLU	ASP	GLY	G97	H98	R99	T100	H101	Y103	L102	G104	H105	A106	I107	L108	L109	R110	H111	A112	H113	S114	R115	M116	I117	L118	C206	S207	S119	C120	S124	R125	S126	K130	A132	F133	D134	V135	G136	L137	Q138	E139	E144	A145	C146	W147	W148	T149	M150	H151	N84	THR
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GLY	ASP	GLY	GLY	GLU	GLU	GLU	GLU	GLU	ASP	GLY	G97	H98	R99	T100	H101	Y103	L102	G104	H105	A106	I107	L108	L109	R110	H111	A112	H113	S114	R115	M116	I117	L118	C206	S207	S119	C120	S124	R125	S126	K130	A132	F133	D134	V135	G136	L137	Q138	E139	E144	A145	C146	W147	W148	T149	M150	H151	N84	THR
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GLY	ASP	GLY	GLY	GLU	GLU	GLU	GLU	GLU	ASP	GLY	G97	H98	R99	T100	H101	Y103	L102	G104	H105	A106	I107	L108	L109	R110	H111	A112	H113	S114	R115	M116	I117	L118	C206	S207	S119	C120	S124	R125	S126	K130	A132	F133	D134	V135	G136	L137	Q138	E139	E144	A145	C146	W147	W148	T149	M150	H151	N84	THR
GLY	ASP	GLY	GLY	GLU	GLU	GLU	GLU	GLU	ASP	GLY	G97	H98	R99	T100	H101	Y103	L102	G104	H105	A106	I107	L108	L109	R110	H111	A112	H113	S114	R115	M116	I117	L118	C206	S207	S119	C120	S124	R125	S126	K130	A132	F133	D134	V135	G136	L137	Q138	E139	E144	A145	C146	W147	W148	T149	M150	H151	N84	THR
GLY	ASP	GLY	GLY	GLU	GLU	GLU	GLU	GLU	ASP	GLY	G97	H98	R99	T100	H101	Y103	L102	G104	H105	A106	I107	L108	L109	R110	H111	A112	H113	S114	R115	M116	I117	L118	C206	S207	S119	C120	S124	R125	S126	K130	A132	F133	D134	V135	G136	L137	Q138	E139	E144	A145	C146	W147	W148	T149	M150	H151	N84	THR
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GLY	ASP	GLY	GLY	GLU	GLU	GLU	GLU	GLU	ASP	GLY	G97	H98	R99	T100	H101	Y103	L102	G104	H105	A106	I107	L108	L109	R110	H111	A112	H113	S114	R115	M116	I117	L118	C206	S207	S119	C120	S124	R125	S126	K130	A132	F133	D134	V135	G136	L137	Q138	E139	E144	A145	C146	W147	W148	T149	M150	H151	N84	THR
GLY	ASP	GLY	GLY	GLU	GLU	GLU	GLU	GLU	ASP	GLY	G97	H98	R99	T100	H101	Y103	L102	G104	H105	A106	I107	L108	L109	R110	H111	A112	H113	S114	R115	M116	I117	L118	C206	S207	S119	C120	S124	R125	S126	K130	A132	F133	D134	V135	G136	L137	Q138	E139	E144	A145	C146	W147	W148	T149	M150	H151	N84	THR
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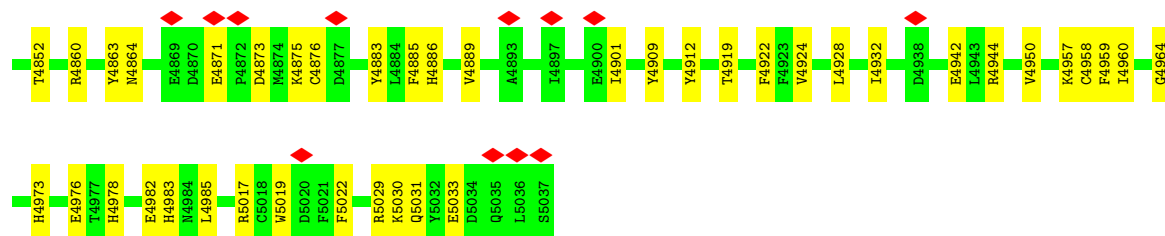




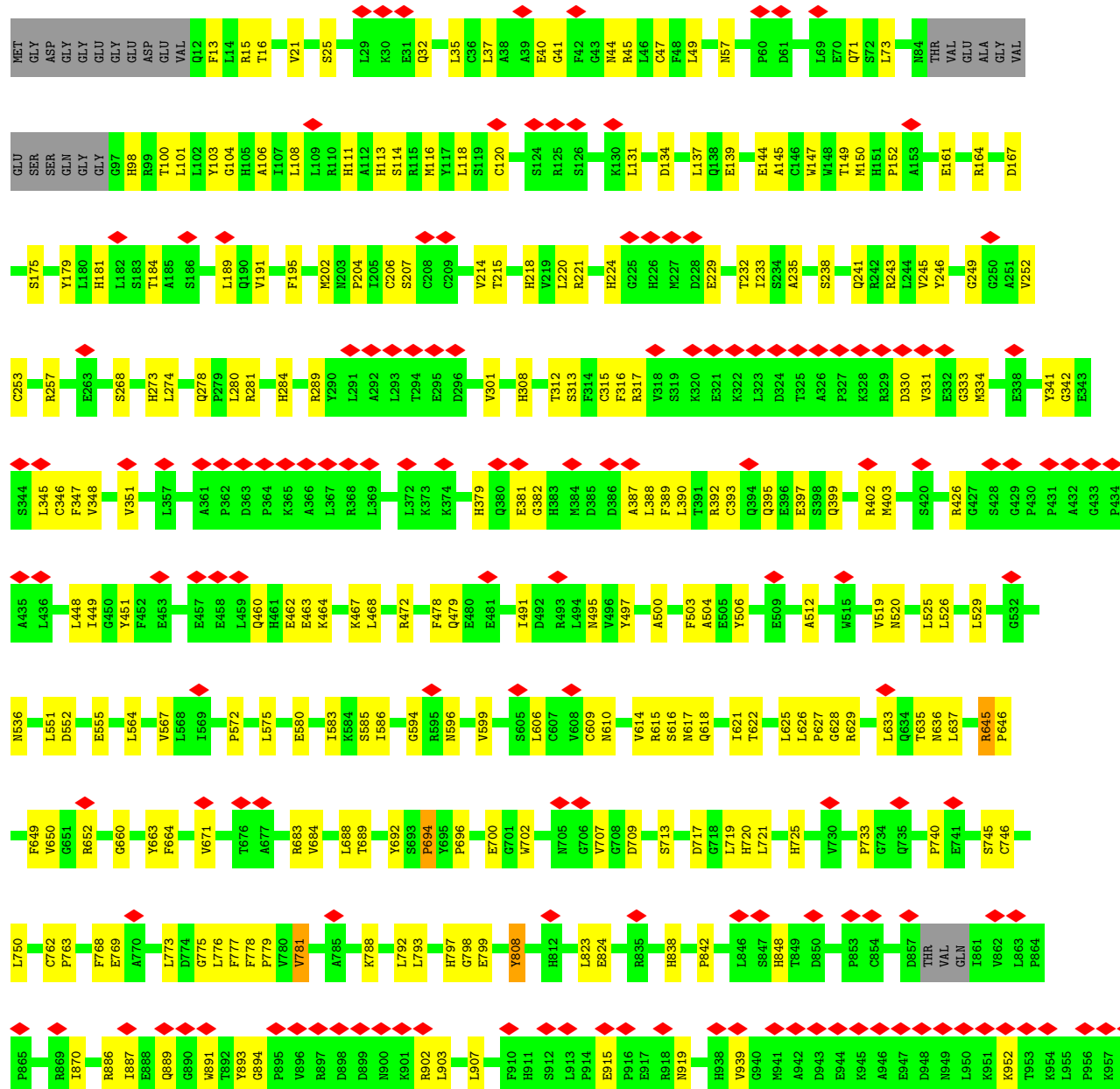
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D1154	E1157	N1158	T1163	L1164	N1165	V1168	L1169	M1170	S1171	D1172	S1175	E1176	G1187	F1188	L1189	P1190	V1191	C1192	S1193	L1194	G1195	Q1198	L1199	G1200	H1201	N1203	S1210	L1211	R1212	C1217	G1218	F1223	F1225	F1238	S1239	K1240	S1241	L1242	F1245	E1246	P1247	M1260	T1263	V1264									
D1265	T1266	C1269	L1270	R1271	M1281	S1282	L1283	V1284	E1285	M1286	L1289	L1293	P1294	F1297	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK		
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X1527	X1528	X1529	X1534	X1543	X1554	X1555	X1556	A1577	X1585	N1586	P1587	Q1590	R1594	V1597	Q1598	M1599	L1600	W1605	S1606	V1615	GLU	THR	ARG	ALA	GLY	E1622	C1630	L1634	M1637	A1638	L1639	H1640	R1646	C1647	M1648	D1649	L1650	L1651	E1652	L1653	D1658	L1659	Q1660										
R1661	F1662	H1663	L1667	R1671	A1672	V1673	C1674	A1675	L1676	M1679	L1685	H1688	E1699	L1707	R1708	A1709	G1710	Y1711	Y1712	D1713	L1714	L1715	I1716	I1718	H1719	L1720	E1721	R1725	R1728	I1735	L1738	T1739	T1742	R1743	T1746	G1751	R1752	K1753	G1754	P1763	G1764	V1767											
L1771	S1778	C1781	F1782	V1783	A1784	A1785	L1786	P1787	A1788	ALA	GLY	VAL	ALA	E1793	A1794	P1795	L1798	S1799	I1802	L1807	R1808	L1812	R1813	M1814	L1815	V1830	S1833	F1836	Q1837	F1838	V1839	P1840	V1841	L1842	V1845	L1849	I1853	F1854	V1859	K1860	Q1861	I1862	K1864	M1865									

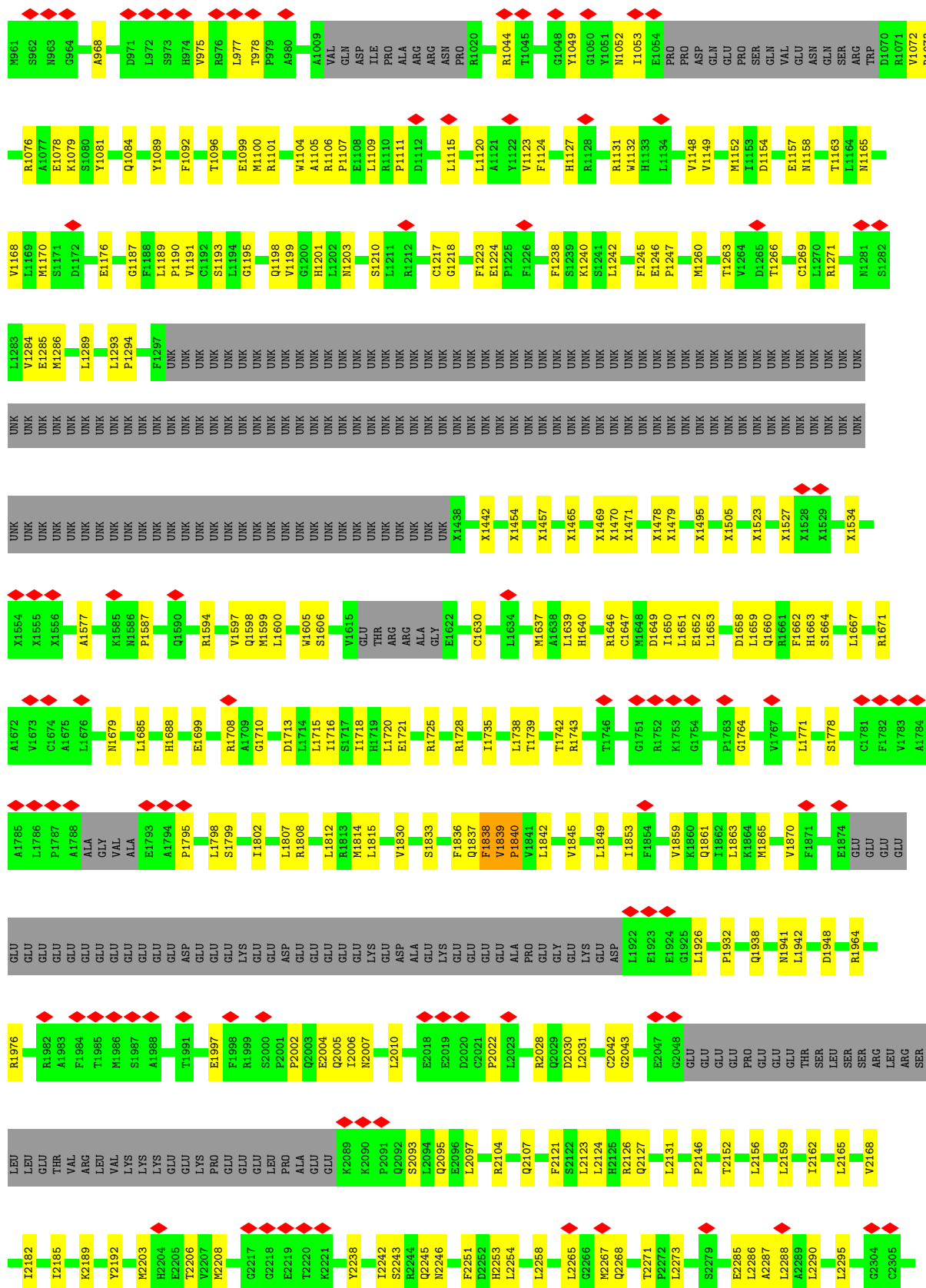






• Molecule 1: Ryanodine receptor 1











## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	42500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.7	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.281	Depositor
Minimum map value	-0.153	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	592.2, 592.2, 592.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.645, 1.645, 1.645	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.32	1/25537 (0.0%)	0.70	5/34686 (0.0%)
1	B	0.32	0/25537	0.70	5/34686 (0.0%)
1	C	0.32	0/25537	0.70	5/34686 (0.0%)
1	D	0.32	0/25537	0.70	5/34686 (0.0%)
All	All	0.32	1/102148 (0.0%)	0.70	20/138744 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16
1	B	0	16
1	C	0	16
1	D	0	16
All	All	0	64

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	802	PHE	C-N	-5.02	1.25	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1294	PRO	N-CA-CB	9.42	110.84	103.30
1	A	1294	PRO	N-CA-CB	9.35	110.78	103.30
1	B	1294	PRO	N-CA-CB	9.35	110.78	103.30
1	C	1294	PRO	N-CA-CB	9.31	110.75	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1838	PHE	CA-C-N	5.73	132.73	122.13
1	C	1838	PHE	C-N-CA	5.73	132.73	122.13
1	D	1838	PHE	CA-C-N	5.72	132.71	122.13
1	D	1838	PHE	C-N-CA	5.72	132.71	122.13
1	A	1838	PHE	CA-C-N	5.70	132.67	122.13
1	A	1838	PHE	C-N-CA	5.70	132.67	122.13
1	B	1838	PHE	CA-C-N	5.70	132.67	122.13
1	B	1838	PHE	C-N-CA	5.70	132.67	122.13
1	C	775	GLY	N-CA-C	5.38	117.55	111.85
1	A	775	GLY	N-CA-C	5.37	117.54	111.85
1	A	2473	PRO	N-CA-C	5.36	119.63	111.11
1	B	2473	PRO	N-CA-C	5.36	119.63	111.11
1	D	2473	PRO	N-CA-C	5.36	119.63	111.11
1	C	2473	PRO	N-CA-C	5.36	119.63	111.11
1	B	775	GLY	N-CA-C	5.35	117.53	111.85
1	D	775	GLY	N-CA-C	5.35	117.53	111.85

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	GLU	Peptide
1	A	1454	UNK	Peptide
1	A	1795	PRO	Peptide
1	A	1840	PRO	Peptide
1	A	2472	LEU	Peptide
1	A	3458	UNK	Peptide
1	A	3786	CYS	Peptide
1	A	4228	ALA	Peptide
1	A	4666	VAL	Peptide
1	A	478	PHE	Peptide
1	A	4807	PHE	Peptide
1	A	552	ASP	Peptide
1	A	645	ARG	Peptide
1	A	692	TYR	Peptide
1	A	694	PRO	Peptide
1	A	808	TYR	Peptide
1	B	139	GLU	Peptide
1	B	1454	UNK	Peptide
1	B	1795	PRO	Peptide
1	B	1840	PRO	Peptide
1	B	2472	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	B	3458	UNK	Peptide
1	B	3786	CYS	Peptide
1	B	4228	ALA	Peptide
1	B	4666	VAL	Peptide
1	B	478	PHE	Peptide
1	B	4807	PHE	Peptide
1	B	552	ASP	Peptide
1	B	645	ARG	Peptide
1	B	692	TYR	Peptide
1	B	694	PRO	Peptide
1	B	808	TYR	Peptide
1	C	139	GLU	Peptide
1	C	1454	UNK	Peptide
1	C	1795	PRO	Peptide
1	C	1840	PRO	Peptide
1	C	2472	LEU	Peptide
1	C	3458	UNK	Peptide
1	C	3786	CYS	Peptide
1	C	4228	ALA	Peptide
1	C	4666	VAL	Peptide
1	C	478	PHE	Peptide
1	C	4807	PHE	Peptide
1	C	552	ASP	Peptide
1	C	645	ARG	Peptide
1	C	692	TYR	Peptide
1	C	694	PRO	Peptide
1	C	808	TYR	Peptide
1	D	139	GLU	Peptide
1	D	1454	UNK	Peptide
1	D	1795	PRO	Peptide
1	D	1840	PRO	Peptide
1	D	2472	LEU	Peptide
1	D	3458	UNK	Peptide
1	D	3786	CYS	Peptide
1	D	4228	ALA	Peptide
1	D	4666	VAL	Peptide
1	D	478	PHE	Peptide
1	D	4807	PHE	Peptide
1	D	552	ASP	Peptide
1	D	645	ARG	Peptide
1	D	692	TYR	Peptide
1	D	694	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	D	808	TYR	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29368	0	24703	469	0
1	B	29368	0	24703	474	0
1	C	29368	0	24703	470	0
1	D	29368	0	24704	467	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
All	All	117476	0	98813	1863	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1863) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ILE:O	1:A:495:ASN:HB2	1.74	0.88
1:C:491:ILE:O	1:C:495:ASN:HB2	1.74	0.87
1:D:491:ILE:O	1:D:495:ASN:HB2	1.74	0.87
1:B:491:ILE:O	1:B:495:ASN:HB2	1.74	0.87
1:B:3802:ILE:O	1:B:3806:ASN:HB2	1.75	0.87
1:C:3802:ILE:O	1:C:3806:ASN:HB2	1.75	0.86
1:D:3802:ILE:O	1:D:3806:ASN:HB2	1.75	0.86
1:A:3802:ILE:O	1:A:3806:ASN:HB2	1.75	0.85
1:C:4172:GLU:HA	1:C:4175:ARG:HE	1.48	0.78
1:B:4172:GLU:HA	1:B:4175:ARG:HE	1.48	0.78
1:A:4172:GLU:HA	1:A:4175:ARG:HE	1.48	0.78
1:D:4172:GLU:HA	1:D:4175:ARG:HE	1.48	0.78
1:B:788:LYS:HG2	1:B:1630:CYS:H	1.51	0.76
1:A:788:LYS:HG2	1:A:1630:CYS:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:788:LYS:HG2	1:C:1630:CYS:H	1.51	0.75
1:C:664:PHE:O	1:C:745:SER:HA	1.88	0.74
1:A:664:PHE:O	1:A:745:SER:HA	1.88	0.74
1:D:664:PHE:O	1:D:745:SER:HA	1.88	0.74
1:D:788:LYS:HG2	1:D:1630:CYS:H	1.51	0.73
1:B:5029:ARG:O	1:B:5033:GLU:HB2	1.89	0.73
1:C:5029:ARG:O	1:C:5033:GLU:HB2	1.89	0.73
1:B:664:PHE:O	1:B:745:SER:HA	1.88	0.72
1:A:5029:ARG:O	1:A:5033:GLU:HB2	1.89	0.72
1:D:5029:ARG:O	1:D:5033:GLU:HB2	1.89	0.72
1:B:1101:ARG:HE	1:B:1115:LEU:HB3	1.55	0.71
1:A:1101:ARG:HE	1:A:1115:LEU:HB3	1.55	0.71
1:A:3805:LEU:HA	1:A:3809:ASN:HD22	1.56	0.71
1:D:3805:LEU:HA	1:D:3809:ASN:HD22	1.56	0.71
1:D:1101:ARG:HE	1:D:1115:LEU:HB3	1.55	0.71
1:C:1101:ARG:HE	1:C:1115:LEU:HB3	1.55	0.70
1:A:40:GLU:HB3	1:A:44:ASN:HB3	1.74	0.70
1:C:3805:LEU:HA	1:C:3809:ASN:HD22	1.56	0.70
1:B:3805:LEU:HA	1:B:3809:ASN:HD22	1.56	0.70
1:A:3882:GLN:HB2	1:A:3957:VAL:HG22	1.74	0.69
1:D:40:GLU:HB3	1:D:44:ASN:HB3	1.74	0.69
1:D:497:TYR:HB3	1:D:500:ALA:HB2	1.75	0.69
1:B:497:TYR:HB3	1:B:500:ALA:HB2	1.75	0.69
1:C:497:TYR:HB3	1:C:500:ALA:HB2	1.75	0.69
1:B:3882:GLN:HB2	1:B:3957:VAL:HG22	1.74	0.68
1:C:40:GLU:HB3	1:C:44:ASN:HB3	1.74	0.68
1:D:3882:GLN:HB2	1:D:3957:VAL:HG22	1.74	0.68
1:A:497:TYR:HB3	1:A:500:ALA:HB2	1.75	0.68
1:B:40:GLU:HB3	1:B:44:ASN:HB3	1.74	0.68
1:A:621:ILE:O	1:A:625:LEU:HB2	1.94	0.67
1:C:3882:GLN:HB2	1:C:3957:VAL:HG22	1.74	0.67
1:B:621:ILE:O	1:B:625:LEU:HB2	1.94	0.67
1:C:621:ILE:O	1:C:625:LEU:HB2	1.94	0.67
1:D:621:ILE:O	1:D:625:LEU:HB2	1.94	0.67
1:C:4239:GLU:OE2	1:C:5017:ARG:NH2	2.29	0.66
1:B:1653:LEU:HB3	1:B:1660:GLN:HB2	1.78	0.66
1:A:4239:GLU:OE2	1:A:5017:ARG:NH2	2.29	0.66
1:B:4239:GLU:OE2	1:B:5017:ARG:NH2	2.29	0.66
1:B:1640:HIS:HA	1:B:1647:CYS:HA	1.78	0.66
1:D:1640:HIS:HA	1:D:1647:CYS:HA	1.78	0.66
1:B:1260:MET:HB2	1:B:1269:CYS:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3904:ARG:NH2	1:D:3973:CYS:SG	2.69	0.66
1:C:1653:LEU:HB3	1:C:1660:GLN:HB2	1.78	0.65
1:A:1640:HIS:HA	1:A:1647:CYS:HA	1.78	0.65
1:D:4239:GLU:OE2	1:D:5017:ARG:NH2	2.29	0.65
1:C:792:LEU:HD22	1:C:799:GLU:H	1.61	0.65
1:C:1640:HIS:HA	1:C:1647:CYS:HA	1.78	0.65
1:A:1653:LEU:HB3	1:A:1660:GLN:HB2	1.78	0.65
1:A:3904:ARG:NH2	1:A:3973:CYS:SG	2.69	0.65
1:D:792:LEU:HD22	1:D:799:GLU:H	1.61	0.65
1:D:4048:LEU:O	1:D:4052:SER:HB2	1.97	0.65
1:A:1260:MET:HB2	1:A:1269:CYS:H	1.61	0.65
1:C:1260:MET:HB2	1:C:1269:CYS:H	1.61	0.64
1:C:2022:PRO:O	1:C:2028:ARG:NH2	2.30	0.64
1:D:1653:LEU:HB3	1:D:1660:GLN:HB2	1.78	0.64
1:B:4048:LEU:O	1:B:4052:SER:HB2	1.97	0.64
1:A:792:LEU:HD22	1:A:799:GLU:H	1.61	0.64
1:A:2022:PRO:O	1:A:2028:ARG:NH2	2.30	0.64
1:B:103:TYR:HB3	1:B:152:PRO:HD3	1.80	0.64
1:B:792:LEU:HD22	1:B:799:GLU:H	1.61	0.64
1:C:1104:TRP:HA	1:C:1190:PRO:HA	1.79	0.64
1:A:161:GLU:HG2	1:D:3984:ARG:HH12	1.63	0.64
1:A:4048:LEU:O	1:A:4052:SER:HB2	1.97	0.64
1:C:4048:LEU:O	1:C:4052:SER:HB2	1.97	0.64
1:D:1104:TRP:HA	1:D:1190:PRO:HA	1.79	0.64
1:A:2189:LYS:HA	1:A:2192:TYR:HD2	1.62	0.64
1:C:1671:ARG:NH2	1:C:1710:GLY:O	2.31	0.64
1:C:3904:ARG:NH2	1:C:3973:CYS:SG	2.69	0.63
1:D:103:TYR:HB3	1:D:152:PRO:HD3	1.80	0.63
1:D:2022:PRO:O	1:D:2028:ARG:NH2	2.30	0.63
1:D:2189:LYS:HA	1:D:2192:TYR:HD2	1.62	0.63
1:A:2265:LEU:HD22	1:A:2330:ARG:HB3	1.81	0.63
1:A:4149:ASN:OD1	1:A:4192:ARG:NH1	2.32	0.63
1:B:4149:ASN:OD1	1:B:4192:ARG:NH1	2.32	0.63
1:C:2189:LYS:HA	1:C:2192:TYR:HD2	1.62	0.63
1:D:4149:ASN:OD1	1:D:4192:ARG:NH1	2.32	0.63
1:A:1725:ARG:HA	1:A:1728:ARG:HG2	1.81	0.63
1:A:3984:ARG:HH12	1:B:161:GLU:HG2	1.63	0.63
1:B:2022:PRO:O	1:B:2028:ARG:NH2	2.30	0.63
1:C:4149:ASN:OD1	1:C:4192:ARG:NH1	2.32	0.63
1:A:103:TYR:HB3	1:A:152:PRO:HD3	1.80	0.63
1:B:1671:ARG:NH2	1:B:1710:GLY:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1764:GLY:HA3	1:C:1859:VAL:HG11	1.81	0.63
1:B:1104:TRP:HA	1:B:1190:PRO:HA	1.79	0.63
1:B:2189:LYS:HA	1:B:2192:TYR:HD2	1.62	0.63
1:A:1671:ARG:NH2	1:A:1710:GLY:O	2.32	0.63
1:D:1260:MET:HB2	1:D:1269:CYS:H	1.61	0.63
1:B:3904:ARG:NH2	1:B:3973:CYS:SG	2.69	0.63
1:D:4741:LEU:HB2	1:D:4743:MET:HE2	1.81	0.62
1:A:1104:TRP:HA	1:A:1190:PRO:HA	1.79	0.62
1:B:1725:ARG:HA	1:B:1728:ARG:HG2	1.81	0.62
1:C:317:ARG:HB2	1:C:347:PHE:HB2	1.82	0.62
1:A:317:ARG:HB2	1:A:347:PHE:HB2	1.82	0.62
1:B:1764:GLY:HA3	1:B:1859:VAL:HG11	1.81	0.62
1:B:4823:LEU:HD21	1:C:4839:MET:HE2	1.82	0.62
1:D:317:ARG:HB2	1:D:347:PHE:HB2	1.82	0.62
1:B:2265:LEU:HD22	1:B:2330:ARG:HB3	1.81	0.62
1:D:1671:ARG:NH2	1:D:1710:GLY:O	2.32	0.62
1:D:2093:SER:O	1:D:2097:LEU:HB2	1.99	0.62
1:A:1764:GLY:HA3	1:A:1859:VAL:HG11	1.81	0.62
1:D:1725:ARG:HA	1:D:1728:ARG:HG2	1.81	0.62
1:A:315:CYS:SG	1:A:316:PHE:N	2.73	0.62
1:C:4741:LEU:HB2	1:C:4743:MET:HE2	1.81	0.62
1:A:4839:MET:HE2	1:D:4823:LEU:HD21	1.82	0.62
1:C:2093:SER:O	1:C:2097:LEU:HB2	1.99	0.62
1:D:37:LEU:HD11	1:D:47:CYS:HB3	1.82	0.62
1:D:2265:LEU:HD22	1:D:2330:ARG:HB3	1.81	0.62
1:A:4741:LEU:HB2	1:A:4743:MET:HE2	1.81	0.61
1:B:2748:PRO:HD2	1:B:2751:LEU:HD12	1.81	0.61
1:C:37:LEU:HD11	1:C:47:CYS:HB3	1.82	0.61
1:A:3955:MET:HG3	1:A:4019:LEU:HD22	1.82	0.61
1:B:317:ARG:HB2	1:B:347:PHE:HB2	1.82	0.61
1:C:103:TYR:HB3	1:C:152:PRO:HD3	1.80	0.61
1:C:1725:ARG:HA	1:C:1728:ARG:HG2	1.81	0.61
1:C:3955:MET:HG3	1:C:4019:LEU:HD22	1.82	0.61
1:D:3955:MET:HG3	1:D:4019:LEU:HD22	1.82	0.61
1:C:315:CYS:SG	1:C:316:PHE:N	2.73	0.61
1:C:2265:LEU:HD22	1:C:2330:ARG:HB3	1.81	0.61
1:C:2285:GLU:HG3	1:C:2286:LEU:HG	1.82	0.61
1:C:3984:ARG:HH12	1:D:161:GLU:HG2	1.64	0.61
1:D:1764:GLY:HA3	1:D:1859:VAL:HG11	1.81	0.61
1:A:37:LEU:HD11	1:A:47:CYS:HB3	1.82	0.61
1:A:3990:VAL:HG13	1:A:4051:SER:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3984:ARG:HH12	1:C:161:GLU:HG2	1.66	0.61
1:B:4741:LEU:HB2	1:B:4743:MET:HE2	1.81	0.61
1:B:1289:LEU:HA	1:B:1597:VAL:HA	1.83	0.61
1:B:1833:SER:HG	1:B:1836:PHE:H	1.48	0.61
1:C:2748:PRO:HD2	1:C:2751:LEU:HD12	1.81	0.61
1:C:3676:ASP:N	1:C:3676:ASP:OD1	2.32	0.61
1:D:2748:PRO:HD2	1:D:2751:LEU:HD12	1.81	0.61
1:D:2285:GLU:HG3	1:D:2286:LEU:HG	1.82	0.61
1:A:1289:LEU:HA	1:A:1597:VAL:HA	1.83	0.61
1:A:2093:SER:O	1:A:2097:LEU:HB2	1.99	0.61
1:B:2093:SER:O	1:B:2097:LEU:HB2	1.99	0.61
1:B:37:LEU:HD11	1:B:47:CYS:HB3	1.82	0.61
1:C:3990:VAL:HG13	1:C:4051:SER:HB2	1.83	0.61
1:D:3676:ASP:OD1	1:D:3676:ASP:N	2.32	0.61
1:B:3955:MET:HG3	1:B:4019:LEU:HD22	1.82	0.61
1:D:2290:LEU:HB3	1:D:3849:ARG:HH12	1.66	0.60
1:A:4823:LEU:HD21	1:B:4839:MET:HE2	1.83	0.60
1:A:2748:PRO:HD2	1:A:2751:LEU:HD12	1.81	0.60
1:B:2290:LEU:HB3	1:B:3849:ARG:HH12	1.66	0.60
1:C:2290:LEU:HB3	1:C:3849:ARG:HH12	1.66	0.60
1:D:2737:PRO:O	1:D:2888:ARG:NH2	2.35	0.60
1:B:707:VAL:HG23	1:B:713:SER:HB2	1.84	0.60
1:B:3676:ASP:OD1	1:B:3676:ASP:N	2.32	0.60
1:D:3889:GLN:OE1	1:D:3960:GLN:NE2	2.35	0.60
1:B:2285:GLU:HG3	1:B:2286:LEU:HG	1.82	0.60
1:B:3990:VAL:HG13	1:B:4051:SER:HB2	1.82	0.60
1:C:3889:GLN:OE1	1:C:3960:GLN:NE2	2.35	0.60
1:D:3990:VAL:HG13	1:D:4051:SER:HB2	1.82	0.60
1:B:1286:MET:HA	1:B:1469:UNK:HA	1.83	0.60
1:C:2737:PRO:O	1:C:2888:ARG:NH2	2.35	0.60
1:A:2737:PRO:O	1:A:2888:ARG:NH2	2.35	0.60
1:A:2285:GLU:HG3	1:A:2286:LEU:HG	1.82	0.59
1:D:1289:LEU:HA	1:D:1597:VAL:HA	1.83	0.59
1:D:4673:ARG:HH22	1:D:4698:LYS:HB2	1.67	0.59
1:B:2737:PRO:O	1:B:2888:ARG:NH2	2.35	0.59
1:C:4823:LEU:HD21	1:D:4839:MET:HE2	1.84	0.59
1:A:460:GLN:O	1:A:464:LYS:HB2	2.02	0.59
1:A:3889:GLN:OE1	1:A:3960:GLN:NE2	2.35	0.59
1:C:626:LEU:HG	1:C:628:GLY:H	1.68	0.59
1:C:4673:ARG:HH22	1:C:4698:LYS:HB2	1.67	0.59
1:A:2290:LEU:HB3	1:A:3849:ARG:HH12	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1092:PHE:HB3	1:B:1149:VAL:HB	1.85	0.59
1:C:1286:MET:HA	1:C:1469:UNK:HA	1.83	0.59
1:D:1286:MET:HA	1:D:1469:UNK:HA	1.83	0.59
1:A:3695:PRO:HB2	1:A:3700:GLN:HG3	1.83	0.59
1:A:1092:PHE:HB3	1:A:1149:VAL:HB	1.84	0.59
1:B:3844:LEU:HD21	1:B:3933:PHE:HA	1.84	0.59
1:B:3889:GLN:OE1	1:B:3960:GLN:NE2	2.35	0.59
1:C:4860:ARG:HG3	1:C:4876:CYS:HB3	1.85	0.59
1:D:41:GLY:O	1:D:45:ARG:NH1	2.36	0.59
1:D:315:CYS:SG	1:D:316:PHE:N	2.73	0.59
1:D:3844:LEU:HD21	1:D:3933:PHE:HA	1.84	0.59
1:A:707:VAL:HG23	1:A:713:SER:HB2	1.84	0.59
1:A:1286:MET:HA	1:A:1469:UNK:HA	1.83	0.59
1:C:1289:LEU:HA	1:C:1597:VAL:HA	1.83	0.59
1:C:3695:PRO:HB2	1:C:3700:GLN:HG3	1.84	0.59
1:C:707:VAL:HG23	1:C:713:SER:HB2	1.84	0.59
1:D:4860:ARG:HG3	1:D:4876:CYS:HB3	1.85	0.59
1:A:41:GLY:O	1:A:45:ARG:NH1	2.36	0.59
1:B:626:LEU:HG	1:B:628:GLY:H	1.68	0.59
1:D:626:LEU:HG	1:D:628:GLY:H	1.68	0.59
1:D:3897:ASN:O	1:D:3901:ASN:ND2	2.36	0.59
1:A:596:ASN:HB3	1:A:599:VAL:HG22	1.85	0.59
1:C:1833:SER:HG	1:C:1836:PHE:H	1.48	0.59
1:C:2326:CYS:SG	1:C:2327:GLY:N	2.76	0.59
1:B:2254:LEU:O	1:B:2258:LEU:N	2.35	0.58
1:C:3695:PRO:HD2	1:C:3700:GLN:HE21	1.68	0.58
1:D:2326:CYS:SG	1:D:2327:GLY:N	2.76	0.58
1:A:626:LEU:HG	1:A:628:GLY:H	1.68	0.58
1:A:1948:ASP:OD1	1:A:2126:ARG:NH2	2.36	0.58
1:A:2420:HIS:ND1	1:A:2523:UNK:O	2.36	0.58
1:A:3847:PHE:HD1	1:A:3850:GLN:HE21	1.51	0.58
1:A:4673:ARG:HH22	1:A:4698:LYS:HB2	1.67	0.58
1:B:596:ASN:HB3	1:B:599:VAL:HG22	1.85	0.58
1:B:3695:PRO:HB2	1:B:3700:GLN:HG3	1.84	0.58
1:C:2420:HIS:ND1	1:C:2523:UNK:O	2.36	0.58
1:D:1092:PHE:HB3	1:D:1149:VAL:HB	1.84	0.58
1:D:2420:HIS:ND1	1:D:2523:UNK:O	2.36	0.58
1:B:3677:LEU:HB3	1:B:3698:LEU:HB2	1.85	0.58
1:A:3676:ASP:N	1:A:3676:ASP:OD1	2.32	0.58
1:A:3897:ASN:O	1:A:3901:ASN:ND2	2.36	0.58
1:B:460:GLN:O	1:B:464:LYS:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4860:ARG:HG3	1:B:4876:CYS:HB3	1.85	0.58
1:B:4944:ARG:HH12	1:C:4942:GLU:HB2	1.68	0.58
1:C:1092:PHE:HB3	1:C:1149:VAL:HB	1.84	0.58
1:C:1948:ASP:OD1	1:C:2126:ARG:NH2	2.36	0.58
1:A:1721:GLU:OE2	1:A:1725:ARG:NH2	2.37	0.58
1:A:3677:LEU:HB3	1:A:3698:LEU:HB2	1.85	0.58
1:A:4860:ARG:HG3	1:A:4876:CYS:HB3	1.85	0.58
1:B:2420:HIS:ND1	1:B:2523:UNK:O	2.36	0.58
1:B:4673:ARG:HH22	1:B:4698:LYS:HB2	1.67	0.58
1:C:1721:GLU:OE2	1:C:1725:ARG:NH2	2.37	0.58
1:C:3767:GLN:NE2	1:C:3804:ILE:O	2.37	0.58
1:D:460:GLN:O	1:D:464:LYS:HB2	2.03	0.58
1:D:1721:GLU:OE2	1:D:1725:ARG:NH2	2.37	0.58
1:D:3847:PHE:HD1	1:D:3850:GLN:HE21	1.51	0.58
1:D:4001:MET:HE1	1:D:4061:PHE:HB2	1.86	0.58
1:A:3767:GLN:NE2	1:A:3804:ILE:O	2.37	0.58
1:D:3695:PRO:HB2	1:D:3700:GLN:HG3	1.84	0.58
1:B:1948:ASP:OD1	1:B:2126:ARG:NH2	2.36	0.58
1:B:3695:PRO:HD2	1:B:3700:GLN:HE21	1.69	0.58
1:B:3897:ASN:O	1:B:3901:ASN:ND2	2.36	0.58
1:C:460:GLN:O	1:C:464:LYS:HB2	2.03	0.58
1:C:3844:LEU:HD21	1:C:3933:PHE:HA	1.84	0.58
1:C:3897:ASN:O	1:C:3901:ASN:ND2	2.36	0.58
1:D:3767:GLN:NE2	1:D:3804:ILE:O	2.37	0.58
1:A:3695:PRO:HD2	1:A:3700:GLN:HE21	1.69	0.58
1:D:707:VAL:HG23	1:D:713:SER:HB2	1.84	0.58
1:D:709:ASP:HA	1:D:725:HIS:H	1.69	0.58
1:A:379:HIS:HD2	1:A:382:GLY:H	1.52	0.58
1:A:664:PHE:HB2	1:A:746:CYS:HB2	1.86	0.58
1:B:3767:GLN:NE2	1:B:3804:ILE:O	2.37	0.58
1:A:3844:LEU:HD21	1:A:3933:PHE:HA	1.84	0.58
1:C:41:GLY:O	1:C:45:ARG:NH1	2.36	0.58
1:C:4001:MET:HE1	1:C:4061:PHE:HB2	1.86	0.58
1:D:664:PHE:HB2	1:D:746:CYS:HB2	1.86	0.58
1:A:2326:CYS:SG	1:A:2327:GLY:N	2.76	0.57
1:A:2770:LYS:HB3	1:A:2775:TRP:HB2	1.86	0.57
1:A:4942:GLU:HB2	1:D:4944:ARG:HH12	1.68	0.57
1:B:379:HIS:HD2	1:B:382:GLY:H	1.52	0.57
1:B:1721:GLU:OE2	1:B:1725:ARG:NH2	2.37	0.57
1:B:2326:CYS:SG	1:B:2327:GLY:N	2.76	0.57
1:B:4001:MET:HE1	1:B:4061:PHE:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2770:LYS:HB3	1:C:2775:TRP:HB2	1.86	0.57
1:A:4178:LEU:HD11	1:A:4194:TYR:HB3	1.87	0.57
1:A:4944:ARG:HH12	1:B:4942:GLU:HB2	1.68	0.57
1:C:709:ASP:HA	1:C:725:HIS:H	1.69	0.57
1:D:2770:LYS:HB3	1:D:2775:TRP:HB2	1.86	0.57
1:D:3695:PRO:HD2	1:D:3700:GLN:HE21	1.68	0.57
1:C:379:HIS:HD2	1:C:382:GLY:H	1.52	0.57
1:C:792:LEU:HB3	1:C:798:GLY:HA2	1.86	0.57
1:C:1685:LEU:HA	1:C:1688:HIS:HD2	1.70	0.57
1:C:3677:LEU:HB3	1:C:3698:LEU:HB2	1.85	0.57
1:D:379:HIS:HD2	1:D:382:GLY:H	1.52	0.57
1:D:1671:ARG:HH21	1:D:1713:ASP:HB3	1.70	0.57
1:D:1948:ASP:OD1	1:D:2126:ARG:NH2	2.36	0.57
1:A:2254:LEU:O	1:A:2258:LEU:N	2.35	0.57
1:B:41:GLY:O	1:B:45:ARG:NH1	2.36	0.57
1:B:2770:LYS:HB3	1:B:2775:TRP:HB2	1.86	0.57
1:C:16:THR:O	1:C:98:HIS:ND1	2.38	0.57
1:C:664:PHE:HB2	1:C:746:CYS:HB2	1.86	0.57
1:C:4687:TYR:OH	1:C:4699:GLY:O	2.22	0.57
1:A:1671:ARG:HH21	1:A:1713:ASP:HB3	1.70	0.57
1:C:4944:ARG:HH12	1:D:4942:GLU:HB2	1.69	0.57
1:B:664:PHE:HB2	1:B:746:CYS:HB2	1.86	0.57
1:B:2095:GLN:HA	1:B:2127:GLN:HE22	1.70	0.57
1:C:313:SER:HB3	1:C:351:VAL:HB	1.87	0.57
1:D:596:ASN:HB3	1:D:599:VAL:HG22	1.85	0.57
1:D:3677:LEU:HB3	1:D:3698:LEU:HB2	1.85	0.57
1:A:243:ARG:NH1	1:A:301:VAL:O	2.36	0.57
1:A:1833:SER:HG	1:A:1836:PHE:H	1.53	0.57
1:B:1743:ARG:O	1:B:1964:ARG:NH2	2.38	0.57
1:B:709:ASP:HA	1:B:725:HIS:H	1.69	0.57
1:C:1671:ARG:HH21	1:C:1713:ASP:HB3	1.70	0.57
1:D:2243:SER:HG	1:D:2245:GLN:H	1.50	0.57
1:A:4001:MET:HE1	1:A:4061:PHE:HB2	1.86	0.57
1:C:1240:LYS:HE3	1:C:1242:LEU:HB3	1.87	0.57
1:D:1716:ILE:O	1:D:1720:LEU:HB3	2.05	0.57
1:D:4674:GLU:HB3	1:D:4715:TYR:HB2	1.87	0.57
1:B:1685:LEU:HA	1:B:1688:HIS:HD2	1.70	0.57
1:B:1716:ILE:O	1:B:1720:LEU:HB3	2.05	0.57
1:C:2254:LEU:O	1:C:2258:LEU:N	2.35	0.57
1:C:3847:PHE:HD1	1:C:3850:GLN:HE21	1.51	0.57
1:B:792:LEU:HB3	1:B:798:GLY:HA2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4178:LEU:HD11	1:D:4194:TYR:HB3	1.87	0.56
1:A:709:ASP:HA	1:A:725:HIS:H	1.69	0.56
1:B:16:THR:O	1:B:98:HIS:ND1	2.38	0.56
1:B:313:SER:HB3	1:B:351:VAL:HB	1.87	0.56
1:C:596:ASN:HB3	1:C:599:VAL:HG22	1.85	0.56
1:D:2095:GLN:HA	1:D:2127:GLN:HE22	1.70	0.56
1:D:3780:LEU:HD11	1:D:3816:MET:HG3	1.87	0.56
1:A:792:LEU:HB3	1:A:798:GLY:HA2	1.86	0.56
1:A:2243:SER:HG	1:A:2245:GLN:H	1.52	0.56
1:B:1671:ARG:HH21	1:B:1713:ASP:HB3	1.70	0.56
1:B:1808:ARG:NH1	1:B:1853:ILE:O	2.39	0.56
1:C:21:VAL:O	1:C:202:MET:HA	2.06	0.56
1:C:2095:GLN:HA	1:C:2127:GLN:HE22	1.70	0.56
1:D:1685:LEU:HA	1:D:1688:HIS:HD2	1.70	0.56
1:D:1743:ARG:O	1:D:1964:ARG:NH2	2.38	0.56
1:D:4052:SER:O	1:D:4056:GLU:N	2.36	0.56
1:A:1716:ILE:O	1:A:1720:LEU:HB3	2.05	0.56
1:A:1743:ARG:O	1:A:1964:ARG:NH2	2.38	0.56
1:A:4674:GLU:HB3	1:A:4715:TYR:HB2	1.87	0.56
1:B:1240:LYS:HE3	1:B:1242:LEU:HB3	1.87	0.56
1:B:3847:PHE:HD1	1:B:3850:GLN:HE21	1.51	0.56
1:C:1808:ARG:NH1	1:C:1853:ILE:O	2.38	0.56
1:B:2265:LEU:HD21	1:B:2273:LEU:HD13	1.88	0.56
1:B:4178:LEU:HD11	1:B:4194:TYR:HB3	1.87	0.56
1:B:4674:GLU:HB3	1:B:4715:TYR:HB2	1.87	0.56
1:C:2318:TYR:HH	1:C:2414:ASN:N	2.03	0.56
1:D:21:VAL:O	1:D:202:MET:HA	2.06	0.56
1:A:120:CYS:HB3	1:A:145:ALA:HB1	1.87	0.56
1:A:1685:LEU:HA	1:A:1688:HIS:HD2	1.70	0.56
1:D:1079:LYS:NZ	1:D:1107:PRO:O	2.38	0.56
1:D:2318:TYR:HH	1:D:2414:ASN:N	2.03	0.56
1:A:1079:LYS:NZ	1:A:1107:PRO:O	2.39	0.56
1:B:278:GLN:N	1:B:315:CYS:SG	2.79	0.56
1:D:2042:CYS:SG	1:D:2043:GLY:N	2.79	0.56
1:A:491:ILE:O	1:A:495:ASN:CB	2.52	0.56
1:B:21:VAL:O	1:B:202:MET:HA	2.06	0.56
1:C:120:CYS:HB3	1:C:145:ALA:HB1	1.87	0.56
1:A:313:SER:HB3	1:A:351:VAL:HB	1.87	0.56
1:B:3780:LEU:HD11	1:B:3816:MET:HG3	1.87	0.56
1:C:4178:LEU:HD11	1:C:4194:TYR:HB3	1.87	0.56
1:D:792:LEU:HB3	1:D:798:GLY:HA2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1240:LYS:HE3	1:D:1242:LEU:HB3	1.87	0.56
1:A:3780:LEU:HD11	1:A:3816:MET:HG3	1.87	0.56
1:B:2318:TYR:HH	1:B:2414:ASN:N	2.04	0.56
1:C:1716:ILE:O	1:C:1720:LEU:HB3	2.05	0.56
1:C:1743:ARG:O	1:C:1964:ARG:NH2	2.38	0.56
1:C:2265:LEU:HD21	1:C:2273:LEU:HD13	1.88	0.56
1:D:181:HIS:CE1	1:D:195:PHE:HB2	2.41	0.56
1:A:21:VAL:O	1:A:202:MET:HA	2.05	0.55
1:A:460:GLN:HG2	1:A:462:GLU:H	1.70	0.55
1:A:2095:GLN:HA	1:A:2127:GLN:HE22	1.70	0.55
1:C:460:GLN:HG2	1:C:462:GLU:H	1.70	0.55
1:C:491:ILE:O	1:C:495:ASN:CB	2.52	0.55
1:C:3780:LEU:HD11	1:C:3816:MET:HG3	1.87	0.55
1:D:16:THR:O	1:D:98:HIS:ND1	2.38	0.55
1:D:278:GLN:N	1:D:315:CYS:SG	2.79	0.55
1:A:2318:TYR:HH	1:A:2414:ASN:N	2.03	0.55
1:B:460:GLN:HG2	1:B:462:GLU:H	1.70	0.55
1:C:1099:GLU:OE2	1:C:1127:HIS:ND1	2.39	0.55
1:C:4674:GLU:HB3	1:C:4715:TYR:HB2	1.87	0.55
1:D:460:GLN:HG2	1:D:462:GLU:H	1.70	0.55
1:D:2254:LEU:O	1:D:2258:LEU:N	2.35	0.55
1:D:2420:HIS:HA	1:D:2423:MET:HG3	1.89	0.55
1:A:16:THR:O	1:A:98:HIS:ND1	2.38	0.55
1:A:395:GLN:NE2	1:A:397:GLU:OE1	2.40	0.55
1:D:952:LYS:HB3	1:D:968:ALA:HB1	1.89	0.55
1:A:278:GLN:N	1:A:315:CYS:SG	2.79	0.55
1:B:395:GLN:NE2	1:B:397:GLU:OE1	2.40	0.55
1:B:2420:HIS:HA	1:B:2423:MET:HG3	1.89	0.55
1:C:614:VAL:HG22	1:C:616:SER:H	1.71	0.55
1:D:120:CYS:HB3	1:D:145:ALA:HB1	1.87	0.55
1:B:315:CYS:SG	1:B:316:PHE:N	2.73	0.55
1:C:395:GLN:NE2	1:C:397:GLU:OE1	2.40	0.55
1:C:2420:HIS:HA	1:C:2423:MET:HG3	1.89	0.55
1:D:1246:GLU:O	1:D:1599:MET:N	2.40	0.55
1:D:2318:TYR:OH	1:D:2414:ASN:N	2.40	0.55
1:A:181:HIS:CE1	1:A:195:PHE:HB2	2.41	0.55
1:A:952:LYS:HB3	1:A:968:ALA:HB1	1.89	0.55
1:A:2318:TYR:OH	1:A:2414:ASN:N	2.40	0.55
1:B:181:HIS:CE1	1:B:195:PHE:HB2	2.41	0.55
1:B:1649:ASP:HB3	1:B:1652:GLU:HG2	1.88	0.55
1:C:111:HIS:HD2	1:C:114:SER:H	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:HIS:HD2	1:D:114:SER:H	1.55	0.55
1:A:426:ARG:HB2	1:A:506:TYR:HA	1.89	0.55
1:B:120:CYS:HB3	1:B:145:ALA:HB1	1.87	0.55
1:C:952:LYS:HB3	1:C:968:ALA:HB1	1.89	0.55
1:D:1833:SER:HG	1:D:1836:PHE:H	1.52	0.55
1:A:1240:LYS:HE3	1:A:1242:LEU:HB3	1.87	0.55
1:A:2042:CYS:SG	1:A:2043:GLY:N	2.79	0.55
1:A:2420:HIS:HA	1:A:2423:MET:HG3	1.89	0.55
1:A:4182:GLU:HB2	1:A:4983:HIS:HE1	1.72	0.55
1:B:1079:LYS:NZ	1:B:1107:PRO:O	2.38	0.55
1:B:2104:ARG:HA	1:B:2107:GLN:HG2	1.88	0.55
1:C:181:HIS:CE1	1:C:195:PHE:HB2	2.41	0.55
1:C:2318:TYR:OH	1:C:2414:ASN:N	2.40	0.55
1:A:1808:ARG:NH1	1:A:1853:ILE:O	2.38	0.55
1:B:426:ARG:HB2	1:B:506:TYR:HA	1.89	0.55
1:B:614:VAL:HG22	1:B:616:SER:H	1.71	0.55
1:B:3817:LEU:HA	1:B:3820:LEU:HD12	1.89	0.55
1:B:3817:LEU:HD13	1:B:3899:PHE:HD1	1.72	0.55
1:C:278:GLN:N	1:C:315:CYS:SG	2.79	0.55
1:C:1079:LYS:NZ	1:C:1107:PRO:O	2.39	0.55
1:C:1238:PHE:O	1:C:1606:SER:N	2.37	0.55
1:D:426:ARG:HB2	1:D:506:TYR:HA	1.89	0.55
1:D:3817:LEU:HA	1:D:3820:LEU:HD12	1.89	0.55
1:A:25:SER:O	1:A:32:GLN:NE2	2.40	0.55
1:B:952:LYS:HB3	1:B:968:ALA:HB1	1.89	0.55
1:C:426:ARG:HB2	1:C:506:TYR:HA	1.89	0.55
1:D:25:SER:O	1:D:32:GLN:NE2	2.40	0.55
1:D:614:VAL:HG22	1:D:616:SER:H	1.71	0.55
1:A:1649:ASP:HB3	1:A:1652:GLU:HG2	1.88	0.54
1:A:2551:UNK:O	1:A:2555:UNK:N	2.40	0.54
1:B:1099:GLU:OE2	1:B:1127:HIS:ND1	2.39	0.54
1:C:1738:LEU:HB3	1:C:2146:PRO:HG3	1.89	0.54
1:D:1808:ARG:NH1	1:D:1853:ILE:O	2.38	0.54
1:A:1099:GLU:OE2	1:A:1127:HIS:ND1	2.39	0.54
1:A:2104:ARG:HA	1:A:2107:GLN:HG2	1.89	0.54
1:A:4010:ILE:HD12	1:A:4131:ARG:HD2	1.89	0.54
1:B:3653:PHE:HA	1:B:3656:SER:HB3	1.89	0.54
1:D:313:SER:HB3	1:D:351:VAL:HB	1.87	0.54
1:D:1099:GLU:OE2	1:D:1127:HIS:ND1	2.39	0.54
1:D:1738:LEU:HB3	1:D:2146:PRO:HG3	1.90	0.54
1:D:2265:LEU:HD21	1:D:2273:LEU:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2551:UNK:O	1:D:2555:UNK:N	2.40	0.54
1:B:4010:ILE:HD12	1:B:4131:ARG:HD2	1.89	0.54
1:C:1649:ASP:HB3	1:C:1652:GLU:HG2	1.88	0.54
1:D:491:ILE:O	1:D:495:ASN:CB	2.52	0.54
1:A:1246:GLU:O	1:A:1599:MET:N	2.40	0.54
1:A:3541:UNK:O	1:A:3545:UNK:N	2.41	0.54
1:C:2816:MET:HE3	1:C:2874:MET:HE1	1.89	0.54
1:C:2913:ALA:HA	1:C:2916:LYS:HB2	1.90	0.54
1:C:4010:ILE:HD12	1:C:4131:ARG:HD2	1.90	0.54
1:D:3541:UNK:O	1:D:3545:UNK:N	2.41	0.54
1:D:3653:PHE:HA	1:D:3656:SER:HB3	1.89	0.54
1:D:4010:ILE:HD12	1:D:4131:ARG:HD2	1.90	0.54
1:B:25:SER:O	1:B:32:GLN:NE2	2.41	0.54
1:C:25:SER:O	1:C:32:GLN:NE2	2.40	0.54
1:C:2104:ARG:HA	1:C:2107:GLN:HG2	1.89	0.54
1:A:609:CYS:SG	1:A:610:ASN:N	2.81	0.54
1:A:614:VAL:HG22	1:A:616:SER:H	1.71	0.54
1:B:2913:ALA:HA	1:B:2916:LYS:HB2	1.90	0.54
1:C:609:CYS:SG	1:C:610:ASN:N	2.81	0.54
1:D:4182:GLU:HB2	1:D:4983:HIS:HE1	1.72	0.54
1:D:4183:ILE:O	1:D:4190:ILE:HA	2.08	0.54
1:A:2913:ALA:HA	1:A:2916:LYS:HB2	1.90	0.54
1:B:111:HIS:HD2	1:B:114:SER:H	1.55	0.54
1:B:3541:UNK:O	1:B:3545:UNK:N	2.41	0.54
1:B:4052:SER:O	1:B:4056:GLU:N	2.36	0.54
1:B:4182:GLU:HB2	1:B:4983:HIS:HE1	1.72	0.54
1:B:4183:ILE:O	1:B:4190:ILE:HA	2.08	0.54
1:C:1246:GLU:O	1:C:1599:MET:N	2.40	0.54
1:D:1649:ASP:HB3	1:D:1652:GLU:HG2	1.88	0.54
1:D:399:GLN:HG2	1:D:403:MET:HE3	1.89	0.54
1:D:1465:UNK:N	1:D:1505:UNK:O	2.41	0.54
1:D:2104:ARG:HA	1:D:2107:GLN:HG2	1.89	0.54
1:A:111:HIS:HD2	1:A:114:SER:H	1.55	0.54
1:A:3817:LEU:HA	1:A:3820:LEU:HD12	1.89	0.54
1:C:3817:LEU:HA	1:C:3820:LEU:HD12	1.89	0.54
1:D:2803:GLU:OE2	1:D:2806:ARG:NH1	2.41	0.54
1:A:399:GLN:HG2	1:A:403:MET:HE3	1.89	0.54
1:A:2265:LEU:HD21	1:A:2273:LEU:HD13	1.88	0.54
1:C:463:GLU:OE2	1:C:467:LYS:NZ	2.34	0.54
1:C:3653:PHE:HA	1:C:3656:SER:HB3	1.89	0.54
1:C:4060:LYS:NZ	1:C:4107:GLU:OE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4152:GLU:OE1	1:A:4194:TYR:OH	2.27	0.53
1:B:243:ARG:NH1	1:B:301:VAL:O	2.37	0.53
1:B:2318:TYR:OH	1:B:2414:ASN:N	2.40	0.53
1:B:2551:UNK:O	1:B:2555:UNK:N	2.40	0.53
1:B:2816:MET:HE3	1:B:2874:MET:HE1	1.89	0.53
1:C:104:GLY:N	1:C:150:MET:O	2.38	0.53
1:C:2551:UNK:O	1:C:2555:UNK:N	2.40	0.53
1:D:2913:ALA:HA	1:D:2916:LYS:HB2	1.90	0.53
1:D:3817:LEU:HD13	1:D:3899:PHE:HD1	1.72	0.53
1:A:3653:PHE:HA	1:A:3656:SER:HB3	1.89	0.53
1:B:4687:TYR:OH	1:B:4699:GLY:O	2.22	0.53
1:C:2803:GLU:OE2	1:C:2806:ARG:NH1	2.41	0.53
1:D:2816:MET:HE3	1:D:2874:MET:HE1	1.89	0.53
1:D:4063:ASP:O	1:D:4067:LYS:NZ	2.37	0.53
1:B:609:CYS:SG	1:B:610:ASN:N	2.81	0.53
1:B:2803:GLU:OE2	1:B:2806:ARG:NH1	2.41	0.53
1:C:3817:LEU:HD13	1:C:3899:PHE:HD1	1.72	0.53
1:D:609:CYS:SG	1:D:610:ASN:N	2.81	0.53
1:B:399:GLN:HG2	1:B:403:MET:HE3	1.89	0.53
1:C:399:GLN:HG2	1:C:403:MET:HE3	1.89	0.53
1:C:1465:UNK:N	1:C:1505:UNK:O	2.41	0.53
1:A:3817:LEU:HD13	1:A:3899:PHE:HD1	1.72	0.53
1:A:4183:ILE:O	1:A:4190:ILE:HA	2.08	0.53
1:B:1738:LEU:HB3	1:B:2146:PRO:HG3	1.89	0.53
1:C:606:LEU:O	1:C:617:ASN:ND2	2.42	0.53
1:C:2182:ILE:HD13	1:C:2185:ILE:HD11	1.91	0.53
1:C:3830:GLN:HA	1:C:3833:GLN:HG2	1.91	0.53
1:C:4182:GLU:HB2	1:C:4983:HIS:HE1	1.72	0.53
1:A:1076:ARG:HB3	1:A:1191:VAL:HG23	1.90	0.53
1:A:606:LEU:O	1:A:617:ASN:ND2	2.42	0.53
1:A:2803:GLU:OE2	1:A:2806:ARG:NH1	2.41	0.53
1:B:1076:ARG:HB3	1:B:1191:VAL:HG23	1.90	0.53
1:C:4183:ILE:O	1:C:4190:ILE:HA	2.08	0.53
1:D:606:LEU:O	1:D:617:ASN:ND2	2.42	0.53
1:A:1465:UNK:N	1:A:1505:UNK:O	2.41	0.53
1:A:4584:ASP:HA	1:A:4627:MET:HA	1.91	0.53
1:B:4763:GLY:O	1:B:4766:THR:OG1	2.27	0.53
1:C:1442:UNK:HA	1:C:1457:UNK:HA	1.91	0.53
1:C:3541:UNK:O	1:C:3545:UNK:N	2.41	0.53
1:D:1238:PHE:O	1:D:1606:SER:N	2.37	0.53
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:ILE:O	1:B:495:ASN:CB	2.52	0.53
1:B:1465:UNK:N	1:B:1505:UNK:O	2.41	0.53
1:C:2042:CYS:SG	1:C:2043:GLY:N	2.79	0.53
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.42	0.53
1:C:4152:GLU:OE1	1:C:4194:TYR:OH	2.27	0.53
1:C:4832:HIS:O	1:C:4835:LYS:NZ	2.42	0.53
1:D:3830:GLN:HA	1:D:3833:GLN:HG2	1.91	0.53
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.42	0.53
1:A:2816:MET:HE3	1:A:2874:MET:HE1	1.89	0.53
1:B:606:LEU:O	1:B:617:ASN:ND2	2.42	0.53
1:A:1738:LEU:HB3	1:A:2146:PRO:HG3	1.89	0.52
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.42	0.52
1:C:243:ARG:NH1	1:C:301:VAL:O	2.36	0.52
1:B:1246:GLU:O	1:B:1599:MET:N	2.40	0.52
1:B:1699:GLU:HA	1:B:1814:MET:HE1	1.91	0.52
1:B:2288:LEU:HA	1:B:3849:ARG:HD2	1.91	0.52
1:B:4108:ILE:HA	1:B:4111:LEU:HD12	1.92	0.52
1:B:4584:ASP:HA	1:B:4627:MET:HA	1.91	0.52
1:C:1699:GLU:HA	1:C:1814:MET:HE1	1.91	0.52
1:C:3923:LEU:HD13	1:C:3961:VAL:HG11	1.91	0.52
1:A:4088:ILE:HG23	1:A:4123:ILE:HB	1.92	0.52
1:B:1442:UNK:HA	1:B:1457:UNK:HA	1.91	0.52
1:B:2182:ILE:HD13	1:B:2185:ILE:HD11	1.91	0.52
1:B:2267:MET:HE3	1:B:2268:GLN:HG2	1.92	0.52
1:D:104:GLY:N	1:D:150:MET:O	2.38	0.52
1:D:4584:ASP:HA	1:D:4627:MET:HA	1.91	0.52
1:A:4108:ILE:HA	1:A:4111:LEU:HD12	1.92	0.52
1:B:3830:GLN:HA	1:B:3833:GLN:HG2	1.91	0.52
1:C:2267:MET:HE3	1:C:2268:GLN:HG2	1.92	0.52
1:D:3937:TYR:O	1:D:4002:LYS:NZ	2.39	0.52
1:A:4687:TYR:OH	1:A:4699:GLY:O	2.22	0.52
1:B:886:ARG:HB3	1:B:891:TRP:HB2	1.92	0.52
1:B:3910:THR:HG23	1:B:3911:THR:HG23	1.92	0.52
1:B:4192:ARG:NE	1:B:4194:TYR:OH	2.43	0.52
1:C:1076:ARG:HB3	1:C:1191:VAL:HG23	1.90	0.52
1:D:1076:ARG:HB3	1:D:1191:VAL:HG23	1.90	0.52
1:A:1442:UNK:HA	1:A:1457:UNK:HA	1.91	0.52
1:A:3830:GLN:HA	1:A:3833:GLN:HG2	1.91	0.52
1:B:3923:LEU:HD13	1:B:3961:VAL:HG11	1.91	0.52
1:C:2095:GLN:NE2	1:C:2127:GLN:O	2.43	0.52
1:C:2288:LEU:HA	1:C:3849:ARG:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3910:THR:HG23	1:C:3911:THR:HG23	1.92	0.52
1:D:395:GLN:NE2	1:D:397:GLU:OE1	2.40	0.52
1:D:3910:THR:HG23	1:D:3911:THR:HG23	1.92	0.52
1:D:4108:ILE:HA	1:D:4111:LEU:HD12	1.92	0.52
1:D:4152:GLU:OE1	1:D:4194:TYR:OH	2.27	0.52
1:B:637:LEU:HD23	1:B:1637:MET:HB3	1.92	0.52
1:B:1830:VAL:HB	1:B:1837:GLN:HA	1.92	0.52
1:C:1716:ILE:HG23	1:C:1720:LEU:HD13	1.92	0.52
1:D:2267:MET:HE3	1:D:2268:GLN:HG2	1.92	0.52
1:D:2288:LEU:HA	1:D:3849:ARG:HD2	1.91	0.52
1:A:3808:GLY:O	1:A:3813:GLN:NE2	2.43	0.52
1:A:3910:THR:HG23	1:A:3911:THR:HG23	1.92	0.52
1:C:3808:GLY:O	1:C:3813:GLN:NE2	2.43	0.52
1:C:3937:TYR:O	1:C:4002:LYS:NZ	2.39	0.52
1:D:3808:GLY:O	1:D:3813:GLN:NE2	2.43	0.52
1:D:4687:TYR:OH	1:D:4699:GLY:O	2.22	0.52
1:D:4832:HIS:O	1:D:4835:LYS:NZ	2.42	0.52
1:A:615:ARG:NH1	1:A:618:GLN:OE1	2.40	0.52
1:A:2182:ILE:HD13	1:A:2185:ILE:HD11	1.91	0.52
1:B:4088:ILE:HG23	1:B:4123:ILE:HB	1.92	0.52
1:C:4584:ASP:HA	1:C:4627:MET:HA	1.91	0.52
1:D:463:GLU:OE2	1:D:467:LYS:NZ	2.34	0.52
1:D:572:PRO:HA	1:D:575:LEU:HD13	1.92	0.52
1:D:2095:GLN:NE2	1:D:2127:GLN:O	2.43	0.52
1:D:2182:ILE:HD13	1:D:2185:ILE:HD11	1.91	0.52
1:A:2267:MET:HE3	1:A:2268:GLN:HG2	1.92	0.52
1:A:4052:SER:O	1:A:4056:GLU:N	2.36	0.52
1:A:4958:CYS:SG	1:A:4959:PHE:N	2.83	0.52
1:B:572:PRO:HA	1:B:575:LEU:HD13	1.92	0.52
1:B:1527:UNK:HA	1:B:1534:UNK:HA	1.92	0.52
1:B:3808:GLY:O	1:B:3813:GLN:NE2	2.43	0.52
1:D:1699:GLU:HA	1:D:1814:MET:HE1	1.91	0.52
1:B:615:ARG:NH1	1:B:618:GLN:OE1	2.40	0.51
1:A:886:ARG:HB3	1:A:891:TRP:HB2	1.92	0.51
1:A:4832:HIS:O	1:A:4835:LYS:NZ	2.42	0.51
1:B:4152:GLU:OE1	1:B:4194:TYR:OH	2.26	0.51
1:B:4958:CYS:SG	1:B:4959:PHE:N	2.83	0.51
1:C:889:GLN:O	1:C:902:ARG:NH1	2.43	0.51
1:C:1830:VAL:HB	1:C:1837:GLN:HA	1.92	0.51
1:C:4108:ILE:HA	1:C:4111:LEU:HD12	1.92	0.51
1:D:116:MET:HB2	1:D:137:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:889:GLN:O	1:D:902:ARG:NH1	2.44	0.51
1:A:572:PRO:HA	1:A:575:LEU:HD13	1.92	0.51
1:A:889:GLN:O	1:A:902:ARG:NH1	2.43	0.51
1:A:1245:PHE:HD1	1:A:1600:LEU:HB3	1.76	0.51
1:A:1699:GLU:HA	1:A:1814:MET:HE1	1.91	0.51
1:A:2288:LEU:HA	1:A:3849:ARG:HD2	1.91	0.51
1:B:776:LEU:HG	1:B:848:HIS:HA	1.92	0.51
1:A:637:LEU:HD23	1:A:1637:MET:HB3	1.92	0.51
1:A:3923:LEU:HD13	1:A:3961:VAL:HG11	1.91	0.51
1:C:615:ARG:NH1	1:C:618:GLN:OE1	2.41	0.51
1:D:1442:UNK:HA	1:D:1457:UNK:HA	1.91	0.51
1:D:4025:VAL:HA	1:D:4028:LEU:HD12	1.93	0.51
1:D:5029:ARG:O	1:D:5033:GLU:CB	2.58	0.51
1:A:1716:ILE:HG23	1:A:1720:LEU:HD13	1.92	0.51
1:A:3937:TYR:O	1:A:4002:LYS:NZ	2.39	0.51
1:B:116:MET:HB2	1:B:137:LEU:HD12	1.92	0.51
1:C:1527:UNK:HA	1:C:1534:UNK:HA	1.92	0.51
1:D:1716:ILE:HG23	1:D:1720:LEU:HD13	1.92	0.51
1:D:4088:ILE:HG23	1:D:4123:ILE:HB	1.92	0.51
1:B:2095:GLN:NE2	1:B:2127:GLN:O	2.43	0.51
1:C:886:ARG:HB3	1:C:891:TRP:HB2	1.92	0.51
1:D:886:ARG:HB3	1:D:891:TRP:HB2	1.92	0.51
1:D:4958:CYS:SG	1:D:4959:PHE:N	2.83	0.51
1:A:1938:GLN:HA	1:A:1941:ASN:HD22	1.76	0.51
1:B:3963:ASN:O	1:B:3966:THR:OG1	2.29	0.51
1:C:637:LEU:HD23	1:C:1637:MET:HB3	1.92	0.51
1:A:2095:GLN:NE2	1:A:2127:GLN:O	2.43	0.51
1:C:281:ARG:HG2	1:C:312:THR:HG21	1.93	0.51
1:C:572:PRO:HA	1:C:575:LEU:HD13	1.92	0.51
1:C:4025:VAL:HA	1:C:4028:LEU:HD12	1.93	0.51
1:C:4958:CYS:SG	1:C:4959:PHE:N	2.83	0.51
1:D:776:LEU:HG	1:D:848:HIS:HA	1.92	0.51
1:D:1830:VAL:HB	1:D:1837:GLN:HA	1.92	0.51
1:B:281:ARG:HG2	1:B:312:THR:HG21	1.93	0.51
1:B:1245:PHE:HD1	1:B:1600:LEU:HB3	1.76	0.51
1:B:4738:ALA:HA	1:B:4743:MET:HE3	1.92	0.51
1:C:116:MET:HB2	1:C:137:LEU:HD12	1.92	0.51
1:C:977:LEU:HD23	1:C:1044:ARG:HG3	1.93	0.51
1:C:1938:GLN:HA	1:C:1941:ASN:HD22	1.76	0.51
1:C:2271:THR:HG22	1:C:2273:LEU:H	1.76	0.51
1:C:4738:ALA:HA	1:C:4743:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1245:PHE:HD1	1:D:1600:LEU:HB3	1.76	0.51
1:A:116:MET:HB2	1:A:137:LEU:HD12	1.92	0.51
1:A:4025:VAL:HA	1:A:4028:LEU:HD12	1.93	0.51
1:A:4957:LYS:HG2	1:A:4964:GLY:HA2	1.93	0.51
1:B:889:GLN:O	1:B:902:ARG:NH1	2.44	0.51
1:B:1716:ILE:HG23	1:B:1720:LEU:HD13	1.92	0.51
1:C:206:CYS:SG	1:C:207:SER:N	2.84	0.51
1:C:233:ILE:HG22	1:C:245:VAL:HA	1.92	0.51
1:C:2121:PHE:O	1:C:3725:TYR:OH	2.28	0.51
1:C:4088:ILE:HG23	1:C:4123:ILE:HB	1.92	0.51
1:D:233:ILE:HG22	1:D:245:VAL:HA	1.92	0.51
1:D:281:ARG:HG2	1:D:312:THR:HG21	1.93	0.51
1:D:348:VAL:H	1:D:388:LEU:HD12	1.76	0.51
1:D:4060:LYS:NZ	1:D:4107:GLU:OE2	2.40	0.51
1:A:463:GLU:OE2	1:A:467:LYS:NZ	2.34	0.50
1:A:2359:ARG:NH2	1:B:179:TYR:OH	2.44	0.50
1:C:281:ARG:HH21	1:C:309:THR:HG1	1.57	0.50
1:C:4052:SER:O	1:C:4056:GLU:N	2.36	0.50
1:D:637:LEU:HD23	1:D:1637:MET:HB3	1.92	0.50
1:D:4208:PRO:HA	1:D:4211:LYS:HB3	1.93	0.50
1:A:1527:UNK:HA	1:A:1534:UNK:HA	1.92	0.50
1:A:2152:THR:O	1:A:2156:LEU:HB2	2.11	0.50
1:C:3905:THR:HA	1:C:3912:THR:HG23	1.93	0.50
1:C:4957:LYS:HG2	1:C:4964:GLY:HA2	1.93	0.50
1:D:206:CYS:SG	1:D:207:SER:N	2.84	0.50
1:D:4738:ALA:HA	1:D:4743:MET:HE3	1.92	0.50
1:D:4957:LYS:HG2	1:D:4964:GLY:HA2	1.93	0.50
1:A:235:ALA:O	1:A:238:SER:OG	2.28	0.50
1:A:281:ARG:HG2	1:A:312:THR:HG21	1.93	0.50
1:A:2271:THR:HG22	1:A:2273:LEU:H	1.76	0.50
1:B:206:CYS:SG	1:B:207:SER:N	2.84	0.50
1:B:2152:THR:O	1:B:2156:LEU:HB2	2.12	0.50
1:B:2271:THR:HG22	1:B:2273:LEU:H	1.76	0.50
1:B:4208:PRO:HA	1:B:4211:LYS:HB3	1.93	0.50
1:A:1218:GLY:HA2	1:A:1223:PHE:HB2	1.93	0.50
1:A:4192:ARG:NE	1:A:4194:TYR:OH	2.43	0.50
1:B:1938:GLN:HA	1:B:1941:ASN:HD22	1.76	0.50
1:C:2359:ARG:NH2	1:D:179:TYR:OH	2.45	0.50
1:D:235:ALA:O	1:D:238:SER:OG	2.28	0.50
1:A:257:ARG:HA	1:A:284:HIS:HE2	1.77	0.50
1:A:776:LEU:HG	1:A:848:HIS:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:HIS:CD2	1:B:114:SER:H	2.30	0.50
1:B:4025:VAL:HA	1:B:4028:LEU:HD12	1.93	0.50
1:B:4232:GLU:OE2	1:B:5017:ARG:NH1	2.45	0.50
1:B:4957:LYS:HG2	1:B:4964:GLY:HA2	1.93	0.50
1:C:111:HIS:CD2	1:C:114:SER:H	2.30	0.50
1:C:776:LEU:HG	1:C:848:HIS:HA	1.93	0.50
1:C:2152:THR:O	1:C:2156:LEU:HB2	2.12	0.50
1:D:3829:PHE:HA	1:D:3832:ILE:HD12	1.93	0.50
1:D:3923:LEU:HD13	1:D:3961:VAL:HG11	1.91	0.50
1:A:1830:VAL:HB	1:A:1837:GLN:HA	1.92	0.50
1:B:977:LEU:HD23	1:B:1044:ARG:HG3	1.93	0.50
1:B:3905:THR:HA	1:B:3912:THR:HG23	1.93	0.50
1:B:4671:PHE:HE1	1:B:4715:TYR:HA	1.77	0.50
1:C:348:VAL:H	1:C:388:LEU:HD12	1.76	0.50
1:D:684:VAL:HA	1:D:781:VAL:HA	1.93	0.50
1:A:233:ILE:HG22	1:A:245:VAL:HA	1.92	0.50
1:A:348:VAL:H	1:A:388:LEU:HD12	1.77	0.50
1:A:2243:SER:HG	1:A:2246:ASN:H	1.59	0.50
1:B:348:VAL:H	1:B:388:LEU:HD12	1.76	0.50
1:B:1679:ASN:ND2	1:B:1798:LEU:O	2.45	0.50
1:C:2243:SER:OG	1:C:2246:ASN:N	2.45	0.50
1:C:4208:PRO:HA	1:C:4211:LYS:HB3	1.93	0.50
1:D:977:LEU:HD23	1:D:1044:ARG:HG3	1.93	0.50
1:D:4192:ARG:NE	1:D:4194:TYR:OH	2.43	0.50
1:B:646:PRO:HD2	1:B:779:PRO:HB2	1.94	0.50
1:B:2121:PHE:O	1:B:3725:TYR:OH	2.28	0.50
1:C:1679:ASN:ND2	1:C:1798:LEU:O	2.45	0.50
1:C:4232:GLU:OE2	1:C:5017:ARG:NH1	2.45	0.50
1:D:1938:GLN:HA	1:D:1941:ASN:HD22	1.76	0.50
1:B:233:ILE:HG22	1:B:245:VAL:HA	1.92	0.50
1:B:257:ARG:HA	1:B:284:HIS:HE2	1.77	0.50
1:B:4832:HIS:O	1:B:4835:LYS:NZ	2.42	0.50
1:D:1679:ASN:ND2	1:D:1798:LEU:O	2.44	0.50
1:A:4671:PHE:HE1	1:A:4715:TYR:HA	1.77	0.49
1:C:4671:PHE:HE1	1:C:4715:TYR:HA	1.77	0.49
1:C:4707:ASN:OD1	1:C:4742:GLY:N	2.42	0.49
1:D:1218:GLY:HA2	1:D:1223:PHE:HB2	1.93	0.49
1:A:280:LEU:HD21	1:A:316:PHE:HE2	1.77	0.49
1:A:646:PRO:HD2	1:A:779:PRO:HB2	1.94	0.49
1:A:733:PRO:HG2	1:A:763:PRO:HD2	1.94	0.49
1:A:3829:PHE:HA	1:A:3832:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4208:PRO:HA	1:A:4211:LYS:HB3	1.93	0.49
1:A:4738:ALA:HA	1:A:4743:MET:HE3	1.92	0.49
1:B:3937:TYR:O	1:B:4002:LYS:NZ	2.39	0.49
1:D:111:HIS:CD2	1:D:114:SER:H	2.30	0.49
1:D:243:ARG:NH1	1:D:301:VAL:O	2.37	0.49
1:D:1527:UNK:HA	1:D:1534:UNK:HA	1.92	0.49
1:D:2152:THR:O	1:D:2156:LEU:HB2	2.11	0.49
1:D:4682:GLU:O	1:D:4727:LYS:NZ	2.40	0.49
1:A:4232:GLU:OE2	1:A:5017:ARG:NH1	2.45	0.49
1:B:281:ARG:HH21	1:B:309:THR:HG1	1.57	0.49
1:B:1739:THR:H	1:B:1742:THR:HB	1.78	0.49
1:C:257:ARG:HA	1:C:284:HIS:HE2	1.77	0.49
1:C:3733:CYS:HB2	1:C:3803:SER:HB3	1.94	0.49
1:A:1679:ASN:ND2	1:A:1798:LEU:O	2.45	0.49
1:A:2346:VAL:HG22	1:A:2348:GLU:H	1.77	0.49
1:B:2927:LEU:HA	1:B:2930:LEU:HD12	1.94	0.49
1:B:3733:CYS:HB2	1:B:3803:SER:HB3	1.94	0.49
1:C:184:THR:HB	1:C:189:LEU:HG	1.94	0.49
1:C:684:VAL:HA	1:C:781:VAL:HA	1.93	0.49
1:D:2271:THR:HG22	1:D:2273:LEU:H	1.76	0.49
1:A:977:LEU:HD23	1:A:1044:ARG:HG3	1.93	0.49
1:A:4707:ASN:OD1	1:A:4742:GLY:N	2.42	0.49
1:B:2346:VAL:HG22	1:B:2348:GLU:H	1.78	0.49
1:B:3948:LYS:NZ	1:B:4008:SER:O	2.46	0.49
1:C:1245:PHE:HD1	1:C:1600:LEU:HB3	1.76	0.49
1:C:2346:VAL:HG22	1:C:2348:GLU:H	1.77	0.49
1:D:257:ARG:HA	1:D:284:HIS:HE2	1.77	0.49
1:D:2002:PRO:HA	1:D:2005:GLN:HB3	1.95	0.49
1:D:3905:THR:HA	1:D:3912:THR:HG23	1.93	0.49
1:B:3761:GLN:HG2	1:B:3765:TYR:HB2	1.95	0.49
1:C:4192:ARG:NE	1:C:4194:TYR:OH	2.43	0.49
1:C:5029:ARG:O	1:C:5033:GLU:CB	2.58	0.49
1:D:184:THR:HB	1:D:189:LEU:HG	1.94	0.49
1:D:646:PRO:HD2	1:D:779:PRO:HB2	1.94	0.49
1:A:684:VAL:HA	1:A:781:VAL:HA	1.93	0.49
1:A:2002:PRO:HA	1:A:2005:GLN:HB3	1.95	0.49
1:A:4060:LYS:NZ	1:A:4107:GLU:OE2	2.40	0.49
1:B:1218:GLY:HA2	1:B:1223:PHE:HB2	1.94	0.49
1:B:1838:PHE:HB3	1:B:1842:LEU:HD11	1.95	0.49
1:C:2927:LEU:HA	1:C:2930:LEU:HD12	1.93	0.49
1:D:346:CYS:N	1:D:388:LEU:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1838:PHE:HB3	1:A:1842:LEU:HD11	1.95	0.49
1:A:3948:LYS:NZ	1:A:4008:SER:O	2.46	0.49
1:B:184:THR:HB	1:B:189:LEU:HG	1.94	0.49
1:B:684:VAL:HA	1:B:781:VAL:HA	1.93	0.49
1:C:1739:THR:H	1:C:1742:THR:HB	1.78	0.49
1:D:1838:PHE:HB3	1:D:1842:LEU:HD11	1.95	0.49
1:A:215:THR:HG22	1:A:273:HIS:HA	1.94	0.49
1:A:1739:THR:H	1:A:1742:THR:HB	1.78	0.49
1:A:1778:SER:N	1:A:1799:SER:O	2.37	0.49
1:A:3905:THR:HA	1:A:3912:THR:HG23	1.93	0.49
1:B:215:THR:HG22	1:B:273:HIS:HA	1.94	0.49
1:B:733:PRO:HG2	1:B:763:PRO:HD2	1.94	0.49
1:B:4712:PRO:HG2	1:B:4718:LYS:HG2	1.95	0.49
1:B:5029:ARG:O	1:B:5033:GLU:CB	2.58	0.49
1:C:646:PRO:HD2	1:C:779:PRO:HB2	1.94	0.49
1:C:3761:GLN:HG2	1:C:3765:TYR:HB2	1.95	0.49
1:D:633:LEU:HB3	1:D:1639:LEU:HD22	1.95	0.49
1:D:3948:LYS:NZ	1:D:4008:SER:O	2.46	0.49
1:A:4104:THR:HG22	1:A:4106:PRO:HD2	1.95	0.49
1:B:3737:GLU:O	1:B:3741:ASN:N	2.46	0.49
1:C:220:LEU:HD11	1:C:390:LEU:HD13	1.95	0.49
1:C:346:CYS:N	1:C:388:LEU:O	2.44	0.49
1:D:4104:THR:HG22	1:D:4106:PRO:HD2	1.95	0.49
1:D:2243:SER:HG	1:D:2246:ASN:H	1.61	0.48
1:A:3733:CYS:HB2	1:A:3803:SER:HB3	1.94	0.48
1:C:215:THR:HG22	1:C:273:HIS:HA	1.94	0.48
1:C:1838:PHE:HB3	1:C:1842:LEU:HD11	1.95	0.48
1:C:3817:LEU:HD22	1:C:3899:PHE:HB2	1.94	0.48
1:C:3948:LYS:NZ	1:C:4008:SER:O	2.46	0.48
1:D:2927:LEU:HA	1:D:2930:LEU:HD12	1.93	0.48
1:D:3737:GLU:O	1:D:3741:ASN:N	2.46	0.48
1:A:281:ARG:HH21	1:A:309:THR:HG1	1.57	0.48
1:A:2927:LEU:HA	1:A:2930:LEU:HD12	1.93	0.48
1:A:4217:PHE:HE2	1:A:4234:PHE:HD1	1.61	0.48
1:A:4712:PRO:HG2	1:A:4718:LYS:HG2	1.95	0.48
1:B:280:LEU:HD21	1:B:316:PHE:HE2	1.77	0.48
1:B:2243:SER:OG	1:B:2246:ASN:N	2.45	0.48
1:B:3829:PHE:HA	1:B:3832:ILE:HD12	1.93	0.48
1:C:164:ARG:N	1:C:167:ASP:OD2	2.46	0.48
1:C:3737:GLU:O	1:C:3741:ASN:N	2.46	0.48
1:C:4104:THR:HG22	1:C:4106:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:683:ARG:NH1	1:D:707:VAL:O	2.40	0.48
1:D:1247:PRO:HA	1:D:1598:GLN:HA	1.96	0.48
1:D:2121:PHE:O	1:D:3725:TYR:OH	2.28	0.48
1:D:3733:CYS:HB2	1:D:3803:SER:HB3	1.94	0.48
1:D:4671:PHE:HE1	1:D:4715:TYR:HA	1.77	0.48
1:A:220:LEU:HD11	1:A:390:LEU:HD13	1.95	0.48
1:A:1247:PRO:HA	1:A:1598:GLN:HA	1.96	0.48
1:B:4060:LYS:NZ	1:B:4107:GLU:OE2	2.40	0.48
1:C:3829:PHE:HA	1:C:3832:ILE:HD12	1.93	0.48
1:D:280:LEU:HD21	1:D:316:PHE:HE2	1.77	0.48
1:A:633:LEU:HB3	1:A:1639:LEU:HD22	1.95	0.48
1:A:1812:LEU:HD21	1:A:1861:GLN:HG2	1.95	0.48
1:A:3761:GLN:HG2	1:A:3765:TYR:HB2	1.95	0.48
1:A:3817:LEU:HD22	1:A:3899:PHE:HB2	1.94	0.48
1:B:1247:PRO:HA	1:B:1598:GLN:HA	1.95	0.48
1:B:4091:LYS:HG2	1:B:4120:ASN:HD21	1.79	0.48
1:D:733:PRO:HG2	1:D:763:PRO:HD2	1.94	0.48
1:A:3737:GLU:O	1:A:3741:ASN:N	2.46	0.48
1:B:220:LEU:HD11	1:B:390:LEU:HD13	1.95	0.48
1:B:2208:MET:HE1	1:B:2253:HIS:HB3	1.96	0.48
1:B:4707:ASN:OD1	1:B:4742:GLY:N	2.42	0.48
1:C:733:PRO:HG2	1:C:763:PRO:HD2	1.94	0.48
1:C:1247:PRO:HA	1:C:1598:GLN:HA	1.95	0.48
1:D:215:THR:HG22	1:D:273:HIS:HA	1.94	0.48
1:D:1739:THR:H	1:D:1742:THR:HB	1.78	0.48
1:A:164:ARG:N	1:A:167:ASP:OD2	2.46	0.48
1:A:448:LEU:HA	1:A:451:TYR:HB3	1.95	0.48
1:A:526:LEU:HA	1:A:529:LEU:HD12	1.96	0.48
1:A:671:VAL:HG22	1:A:740:PRO:HG3	1.96	0.48
1:A:3927:GLN:NE2	1:A:3988:ALA:O	2.47	0.48
1:B:235:ALA:O	1:B:238:SER:OG	2.28	0.48
1:B:683:ARG:NH1	1:B:707:VAL:O	2.40	0.48
1:B:1976:ARG:NH1	1:B:1997:GLU:OE2	2.47	0.48
1:B:3927:GLN:NE2	1:B:3988:ALA:O	2.47	0.48
1:B:4217:PHE:HE2	1:B:4234:PHE:HD1	1.61	0.48
1:C:1218:GLY:HA2	1:C:1223:PHE:HB2	1.93	0.48
1:C:1271:ARG:HA	1:C:1479:UNK:HA	1.96	0.48
1:C:4091:LYS:HG2	1:C:4120:ASN:HD21	1.79	0.48
1:C:4713:SER:OG	1:C:4775:TYR:OH	2.29	0.48
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.96	0.48
1:D:3761:GLN:HG2	1:D:3765:TYR:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4586:PRO:HA	1:D:4628:VAL:HG11	1.96	0.48
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.96	0.48
1:A:4791:TYR:OH	1:A:4815:ASP:O	2.32	0.48
1:B:1154:ASP:O	1:B:1158:ASN:N	2.47	0.48
1:B:2121:PHE:HA	1:B:2124:LEU:HB3	1.95	0.48
1:B:3817:LEU:HD22	1:B:3899:PHE:HB2	1.94	0.48
1:C:235:ALA:O	1:C:238:SER:OG	2.28	0.48
1:C:1812:LEU:HD21	1:C:1861:GLN:HG2	1.95	0.48
1:D:229:GLU:HA	1:D:249:GLY:HA2	1.95	0.48
1:D:241:GLN:O	1:D:289:ARG:NH1	2.47	0.48
1:D:526:LEU:HA	1:D:529:LEU:HD12	1.96	0.48
1:D:615:ARG:NH1	1:D:618:GLN:OE1	2.40	0.48
1:D:671:VAL:HG22	1:D:740:PRO:HG3	1.96	0.48
1:D:2208:MET:HE1	1:D:2253:HIS:HB3	1.96	0.48
1:D:2346:VAL:HG22	1:D:2348:GLU:H	1.77	0.48
1:D:4232:GLU:OE2	1:D:5017:ARG:NH1	2.45	0.48
1:A:118:LEU:HA	1:A:137:LEU:HB3	1.96	0.48
1:A:1238:PHE:O	1:A:1606:SER:N	2.37	0.48
1:A:2208:MET:HE1	1:A:2253:HIS:HB3	1.96	0.48
1:A:4091:LYS:HG2	1:A:4120:ASN:HD21	1.79	0.48
1:B:57:ASN:HD22	1:B:308:HIS:HB2	1.79	0.48
1:B:4848:VAL:O	1:B:4852:THR:OG1	2.30	0.48
1:D:448:LEU:HA	1:D:451:TYR:HB3	1.95	0.48
1:D:1663:HIS:O	1:D:1667:LEU:N	2.47	0.48
1:D:4091:LYS:HG2	1:D:4120:ASN:HD21	1.79	0.48
1:D:4707:ASN:OD1	1:D:4742:GLY:N	2.42	0.48
1:A:179:TYR:OH	1:D:2359:ARG:NH2	2.47	0.48
1:A:184:THR:HB	1:A:189:LEU:HG	1.94	0.48
1:A:1271:ARG:HA	1:A:1479:UNK:HA	1.96	0.48
1:A:2159:LEU:HA	1:A:2162:ILE:HD12	1.96	0.48
1:A:2243:SER:OG	1:A:2246:ASN:N	2.45	0.48
1:B:2002:PRO:HA	1:B:2005:GLN:HB3	1.95	0.48
1:B:4104:THR:HG22	1:B:4106:PRO:HD2	1.95	0.48
1:B:4837:LEU:HG	1:B:4932:ILE:HD12	1.96	0.48
1:B:4883:TYR:HA	1:B:4886:HIS:HD2	1.79	0.48
1:C:2208:MET:HE1	1:C:2253:HIS:HB3	1.96	0.48
1:D:220:LEU:HD11	1:D:390:LEU:HD13	1.95	0.48
1:D:1154:ASP:O	1:D:1158:ASN:N	2.47	0.48
1:A:1865:MET:HB3	1:A:1926:LEU:HB2	1.96	0.47
1:B:671:VAL:HG22	1:B:740:PRO:HG3	1.96	0.47
1:B:1078:GLU:HB3	1:B:1081:TYR:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1663:HIS:O	1:B:1667:LEU:N	2.47	0.47
1:C:671:VAL:HG22	1:C:740:PRO:HG3	1.96	0.47
1:C:793:LEU:HD12	1:C:797:HIS:H	1.79	0.47
1:C:2868:SER:O	1:C:2872:GLN:CB	2.62	0.47
1:D:519:VAL:HG12	1:D:555:GLU:HG3	1.96	0.47
1:D:3817:LEU:HD22	1:D:3899:PHE:HB2	1.94	0.47
1:D:4712:PRO:HG2	1:D:4718:LYS:HG2	1.95	0.47
1:B:241:GLN:O	1:B:289:ARG:NH1	2.47	0.47
1:B:1812:LEU:HD21	1:B:1861:GLN:HG2	1.95	0.47
1:B:1865:MET:HB3	1:B:1926:LEU:HB2	1.96	0.47
1:B:2874:MET:HA	1:B:2877:GLN:HB3	1.96	0.47
1:C:118:LEU:HA	1:C:137:LEU:HB3	1.96	0.47
1:C:633:LEU:HB3	1:C:1639:LEU:HD22	1.95	0.47
1:C:1976:ARG:NH1	1:C:1997:GLU:OE2	2.47	0.47
1:D:1078:GLU:HB3	1:D:1081:TYR:HD2	1.79	0.47
1:D:2868:SER:O	1:D:2872:GLN:CB	2.62	0.47
1:D:2874:MET:HA	1:D:2877:GLN:HB3	1.96	0.47
1:A:184:THR:HA	1:A:189:LEU:HA	1.97	0.47
1:A:519:VAL:HG12	1:A:555:GLU:HG3	1.96	0.47
1:A:1976:ARG:NH1	1:A:1997:GLU:OE2	2.47	0.47
1:A:2874:MET:HA	1:A:2877:GLN:HB3	1.96	0.47
1:B:229:GLU:HA	1:B:249:GLY:HA2	1.95	0.47
1:B:2042:CYS:SG	1:B:2043:GLY:N	2.79	0.47
1:C:241:GLN:O	1:C:289:ARG:NH1	2.47	0.47
1:C:4217:PHE:HE2	1:C:4234:PHE:HD1	1.61	0.47
1:C:4586:PRO:HA	1:C:4628:VAL:HG11	1.96	0.47
1:C:4712:PRO:HG2	1:C:4718:LYS:HG2	1.95	0.47
1:C:4909:TYR:HA	1:C:4912:TYR:HD2	1.79	0.47
1:D:164:ARG:N	1:D:167:ASP:OD2	2.46	0.47
1:D:1976:ARG:NH1	1:D:1997:GLU:OE2	2.47	0.47
1:D:4791:TYR:OH	1:D:4815:ASP:O	2.32	0.47
1:A:4583:SER:O	1:A:4628:VAL:N	2.39	0.47
1:A:5029:ARG:O	1:A:5033:GLU:CB	2.58	0.47
1:B:633:LEU:HB3	1:B:1639:LEU:HD22	1.95	0.47
1:C:118:LEU:HD12	1:C:137:LEU:HB3	1.96	0.47
1:C:229:GLU:HA	1:C:249:GLY:HA2	1.95	0.47
1:C:1154:ASP:O	1:C:1158:ASN:N	2.47	0.47
1:C:4883:TYR:HA	1:C:4886:HIS:HD2	1.79	0.47
1:B:1170:MET:HE1	1:B:1176:GLU:HG3	1.97	0.47
1:B:4586:PRO:HA	1:B:4628:VAL:HG11	1.96	0.47
1:C:57:ASN:HD22	1:C:308:HIS:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:LEU:HD21	1:C:316:PHE:HE2	1.77	0.47
1:C:448:LEU:HA	1:C:451:TYR:HB3	1.95	0.47
1:C:3777:GLU:HA	1:C:3780:LEU:HD13	1.97	0.47
1:D:57:ASN:HD22	1:D:308:HIS:HB2	1.79	0.47
1:D:1812:LEU:HD21	1:D:1861:GLN:HG2	1.95	0.47
1:D:4822:THR:O	1:D:4825:THR:OG1	2.30	0.47
1:D:4919:THR:HA	1:D:4922:PHE:HD2	1.80	0.47
1:D:4960:ILE:HG12	1:D:4983:HIS:HB3	1.97	0.47
1:A:206:CYS:SG	1:A:207:SER:N	2.84	0.47
1:A:2121:PHE:HA	1:A:2124:LEU:HB3	1.95	0.47
1:A:4919:THR:HA	1:A:4922:PHE:HD2	1.80	0.47
1:B:1100:MET:HE2	1:B:1198:GLN:HB3	1.97	0.47
1:B:4190:ILE:HD12	1:B:5031:GLN:HE21	1.80	0.47
1:B:4791:TYR:OH	1:B:4815:ASP:O	2.32	0.47
1:D:793:LEU:HD12	1:D:797:HIS:H	1.79	0.47
1:A:111:HIS:CD2	1:A:114:SER:H	2.30	0.47
1:A:229:GLU:HA	1:A:249:GLY:HA2	1.95	0.47
1:A:241:GLN:O	1:A:289:ARG:NH1	2.47	0.47
1:A:583:ILE:HA	1:A:586:ILE:HD12	1.97	0.47
1:A:1078:GLU:HB3	1:A:1081:TYR:HD2	1.79	0.47
1:A:1154:ASP:O	1:A:1158:ASN:N	2.47	0.47
1:A:1849:LEU:HD22	1:A:1942:LEU:HD12	1.97	0.47
1:A:2868:SER:O	1:A:2872:GLN:CB	2.62	0.47
1:A:4763:GLY:O	1:A:4766:THR:OG1	2.27	0.47
1:B:448:LEU:HA	1:B:451:TYR:HB3	1.95	0.47
1:B:3501:UNK:O	1:B:3505:UNK:N	2.48	0.47
1:B:4863:TYR:HA	1:B:4901:ILE:HG23	1.97	0.47
1:C:583:ILE:HA	1:C:586:ILE:HD12	1.97	0.47
1:C:1078:GLU:HB3	1:C:1081:TYR:HD2	1.79	0.47
1:C:1170:MET:HE1	1:C:1176:GLU:HG3	1.97	0.47
1:C:2002:PRO:HA	1:C:2005:GLN:HB3	1.95	0.47
1:C:2159:LEU:HA	1:C:2162:ILE:HD12	1.96	0.47
1:C:4190:ILE:HD12	1:C:5031:GLN:HE21	1.80	0.47
1:C:4837:LEU:HG	1:C:4932:ILE:HD12	1.96	0.47
1:C:4919:THR:HA	1:C:4922:PHE:HD2	1.80	0.47
1:C:4960:ILE:HG12	1:C:4983:HIS:HB3	1.97	0.47
1:D:118:LEU:HD12	1:D:137:LEU:HB3	1.96	0.47
1:D:660:GLY:HA2	1:D:750:LEU:HD12	1.97	0.47
1:D:1271:ARG:HA	1:D:1479:UNK:HA	1.96	0.47
1:D:2159:LEU:HA	1:D:2162:ILE:HD12	1.96	0.47
1:D:2251:PHE:HA	1:D:2254:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4217:PHE:HE2	1:D:4234:PHE:HD1	1.61	0.47
1:A:793:LEU:HD12	1:A:797:HIS:H	1.79	0.47
1:A:2121:PHE:O	1:A:3725:TYR:OH	2.28	0.47
1:A:2448:GLY:HA2	1:A:2451:LEU:HD12	1.97	0.47
1:A:4837:LEU:HG	1:A:4932:ILE:HD12	1.96	0.47
1:B:164:ARG:N	1:B:167:ASP:OD2	2.46	0.47
1:B:793:LEU:HD12	1:B:797:HIS:H	1.79	0.47
1:B:1778:SER:N	1:B:1799:SER:O	2.37	0.47
1:C:893:TYR:HD1	1:C:907:LEU:HB2	1.80	0.47
1:C:2874:MET:HA	1:C:2877:GLN:HB3	1.96	0.47
1:C:3802:ILE:O	1:C:3806:ASN:CB	2.57	0.47
1:C:4039:MET:HG2	1:C:4042:ARG:NH1	2.30	0.47
1:D:649:PHE:HB3	1:D:776:LEU:HB3	1.97	0.47
1:D:3927:GLN:NE2	1:D:3988:ALA:O	2.47	0.47
1:A:57:ASN:HD22	1:A:308:HIS:HB2	1.79	0.47
1:A:346:CYS:N	1:A:388:LEU:O	2.44	0.47
1:A:1170:MET:HE1	1:A:1176:GLU:HG3	1.97	0.47
1:A:4883:TYR:HA	1:A:4886:HIS:HD2	1.79	0.47
1:A:4909:TYR:HA	1:A:4912:TYR:HD2	1.79	0.47
1:A:5019:TRP:HB3	1:A:5022:PHE:CE2	2.50	0.47
1:B:118:LEU:HA	1:B:137:LEU:HB3	1.96	0.47
1:B:893:TYR:HD1	1:B:907:LEU:HB2	1.80	0.47
1:B:1849:LEU:HD22	1:B:1942:LEU:HD12	1.97	0.47
1:B:2359:ARG:NH2	1:C:179:TYR:OH	2.47	0.47
1:C:519:VAL:HG12	1:C:555:GLU:HG3	1.96	0.47
1:C:2121:PHE:HA	1:C:2124:LEU:HB3	1.95	0.47
1:C:3927:GLN:NE2	1:C:3988:ALA:O	2.47	0.47
1:C:4863:TYR:HA	1:C:4901:ILE:HG23	1.97	0.47
1:D:2006:ILE:HD11	1:D:3641:LEU:HD13	1.97	0.47
1:A:118:LEU:HD12	1:A:137:LEU:HB3	1.96	0.47
1:A:636:ASN:HD22	1:A:702:TRP:HB3	1.80	0.47
1:B:184:THR:HA	1:B:189:LEU:HA	1.97	0.47
1:B:224:HIS:N	1:B:229:GLU:O	2.46	0.47
1:B:526:LEU:HA	1:B:529:LEU:HD12	1.96	0.47
1:B:583:ILE:HA	1:B:586:ILE:HD12	1.97	0.47
1:C:1105:ALA:HB1	1:C:1109:LEU:HD21	1.97	0.47
1:D:4005:GLN:HE21	1:D:4110:PHE:HE1	1.63	0.47
1:D:4763:GLY:O	1:D:4766:THR:OG1	2.27	0.47
1:A:649:PHE:HB3	1:A:776:LEU:HB3	1.97	0.46
1:B:118:LEU:HD12	1:B:137:LEU:HB3	1.96	0.46
1:B:232:THR:HB	1:B:252:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2251:PHE:HA	1:B:2254:LEU:HB2	1.96	0.46
1:B:2739:PRO:HB3	1:B:2884:ASN:HB3	1.97	0.46
1:B:3777:GLU:HA	1:B:3780:LEU:HD13	1.97	0.46
1:B:5019:TRP:HB3	1:B:5022:PHE:CE2	2.50	0.46
1:C:1100:MET:HE2	1:C:1198:GLN:HB3	1.97	0.46
1:C:1663:HIS:O	1:C:1667:LEU:N	2.47	0.46
1:C:4791:TYR:OH	1:C:4815:ASP:O	2.32	0.46
1:D:2739:PRO:HB3	1:D:2884:ASN:HB3	1.97	0.46
1:D:3777:GLU:HA	1:D:3780:LEU:HD13	1.97	0.46
1:D:5019:TRP:HB3	1:D:5022:PHE:CE2	2.50	0.46
1:A:4586:PRO:HA	1:A:4628:VAL:HG11	1.96	0.46
1:B:2159:LEU:HA	1:B:2162:ILE:HD12	1.96	0.46
1:B:2868:SER:O	1:B:2872:GLN:CB	2.62	0.46
1:C:2448:GLY:HA2	1:C:2451:LEU:HD12	1.97	0.46
1:C:3501:UNK:O	1:C:3505:UNK:N	2.48	0.46
1:C:4063:ASP:O	1:C:4067:LYS:NZ	2.37	0.46
1:D:583:ILE:HA	1:D:586:ILE:HD12	1.97	0.46
1:D:893:TYR:HD1	1:D:907:LEU:HB2	1.80	0.46
1:A:2758:PHE:HD2	1:A:2809:ILE:HG12	1.81	0.46
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.96	0.46
1:B:649:PHE:HB3	1:B:776:LEU:HB3	1.97	0.46
1:C:2251:PHE:HA	1:C:2254:LEU:HB2	1.96	0.46
1:C:4005:GLN:HE21	1:C:4110:PHE:HE1	1.63	0.46
1:D:1170:MET:HE1	1:D:1176:GLU:HG3	1.97	0.46
1:D:2121:PHE:HA	1:D:2124:LEU:HB3	1.95	0.46
1:D:3501:UNK:O	1:D:3505:UNK:N	2.48	0.46
1:D:3963:ASN:O	1:D:3966:THR:OG1	2.29	0.46
1:D:4039:MET:HG2	1:D:4042:ARG:NH1	2.30	0.46
1:D:4583:SER:O	1:D:4628:VAL:N	2.39	0.46
1:D:4837:LEU:HG	1:D:4932:ILE:HD12	1.96	0.46
1:A:2739:PRO:HB3	1:A:2884:ASN:HB3	1.97	0.46
1:A:4863:TYR:HA	1:A:4901:ILE:HG23	1.97	0.46
1:B:4960:ILE:HG12	1:B:4983:HIS:HB3	1.97	0.46
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.96	0.46
1:C:526:LEU:HA	1:C:529:LEU:HD12	1.96	0.46
1:C:649:PHE:HB3	1:C:776:LEU:HB3	1.97	0.46
1:C:1849:LEU:HD22	1:C:1942:LEU:HD12	1.97	0.46
1:C:3582:UNK:O	1:C:3586:UNK:CB	2.64	0.46
1:D:3582:UNK:O	1:D:3586:UNK:CB	2.64	0.46
1:A:627:PRO:O	1:A:629:ARG:NH1	2.49	0.46
1:A:660:GLY:HA2	1:A:750:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:ILE:HD12	1:A:870:ILE:HA	1.82	0.46
1:A:4960:ILE:HG12	1:A:4983:HIS:HB3	1.97	0.46
1:B:3582:UNK:O	1:B:3586:UNK:CB	2.64	0.46
1:B:4039:MET:HG2	1:B:4042:ARG:NH1	2.30	0.46
1:C:652:ARG:HD3	1:C:773:LEU:HD13	1.98	0.46
1:C:2868:SER:O	1:C:2872:GLN:HB2	2.16	0.46
1:C:5030:LYS:HA	1:C:5033:GLU:HB2	1.98	0.46
1:D:184:THR:HA	1:D:189:LEU:HA	1.97	0.46
1:A:106:ALA:HA	1:A:149:THR:HA	1.98	0.46
1:A:2251:PHE:HA	1:A:2254:LEU:HB2	1.96	0.46
1:A:3501:UNK:O	1:A:3505:UNK:N	2.48	0.46
1:B:519:VAL:HG12	1:B:555:GLU:HG3	1.96	0.46
1:B:636:ASN:HD22	1:B:702:TRP:HB3	1.80	0.46
1:B:652:ARG:HD3	1:B:773:LEU:HD13	1.98	0.46
1:B:4909:TYR:HA	1:B:4912:TYR:HD2	1.79	0.46
1:C:232:THR:HB	1:C:252:VAL:HG11	1.97	0.46
1:C:1865:MET:HB3	1:C:1926:LEU:HB2	1.96	0.46
1:D:1100:MET:HE2	1:D:1198:GLN:HB3	1.97	0.46
1:D:1849:LEU:HD22	1:D:1942:LEU:HD12	1.97	0.46
1:D:1865:MET:HB3	1:D:1926:LEU:HB2	1.96	0.46
1:D:2868:SER:O	1:D:2872:GLN:HB2	2.16	0.46
1:D:4190:ILE:HD12	1:D:5031:GLN:HE21	1.80	0.46
1:A:1203:ASN:ND2	1:A:1210:SER:O	2.49	0.46
1:A:2004:GLU:HA	1:A:2007:ASN:HD22	1.81	0.46
1:A:3663:LEU:H	1:A:3663:LEU:HG	1.59	0.46
1:B:5030:LYS:HA	1:B:5033:GLU:HB2	1.98	0.46
1:C:5019:TRP:HB3	1:C:5022:PHE:CE2	2.50	0.46
1:D:232:THR:HB	1:D:252:VAL:HG11	1.97	0.46
1:D:4863:TYR:HA	1:D:4901:ILE:HG23	1.97	0.46
1:D:4909:TYR:HA	1:D:4912:TYR:HD2	1.79	0.46
1:A:221:ARG:NE	1:A:253:CYS:O	2.49	0.46
1:A:3802:ILE:O	1:A:3806:ASN:CB	2.57	0.46
1:A:4005:GLN:HE21	1:A:4110:PHE:HE1	1.63	0.46
1:B:2448:GLY:HA2	1:B:2451:LEU:HD12	1.97	0.46
1:C:660:GLY:HA2	1:C:750:LEU:HD12	1.97	0.46
1:C:1124:PHE:HA	1:C:1131:ARG:HA	1.98	0.46
1:D:1105:ALA:HB1	1:D:1109:LEU:HD21	1.97	0.46
1:D:4582:VAL:HG23	1:D:4629:TYR:HA	1.98	0.46
1:D:5030:LYS:HA	1:D:5033:GLU:HB2	1.98	0.46
1:A:893:TYR:HD1	1:A:907:LEU:HB2	1.80	0.46
1:A:3777:GLU:HA	1:A:3780:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ALA:HA	1:B:149:THR:HA	1.98	0.46
1:C:2006:ILE:HD11	1:C:3641:LEU:HD13	1.97	0.46
1:D:134:ASP:N	1:D:134:ASP:OD1	2.49	0.46
1:D:870:ILE:HD12	1:D:870:ILE:HA	1.82	0.46
1:D:1124:PHE:HA	1:D:1131:ARG:HA	1.98	0.46
1:A:650:VAL:H	1:A:777:PHE:H	1.64	0.46
1:A:3963:ASN:O	1:A:3966:THR:OG1	2.29	0.46
1:A:4039:MET:HG2	1:A:4042:ARG:NH1	2.30	0.46
1:B:144:GLU:HG2	1:B:175:SER:HB3	1.98	0.46
1:B:346:CYS:N	1:B:388:LEU:O	2.44	0.46
1:B:1271:ARG:HA	1:B:1479:UNK:HA	1.96	0.46
1:B:4919:THR:HA	1:B:4922:PHE:HD2	1.80	0.46
1:C:13:PHE:HA	1:C:164:ARG:HA	1.98	0.46
1:C:1152:MET:HE1	1:C:1217:CYS:HB3	1.98	0.46
1:D:13:PHE:HA	1:D:164:ARG:HA	1.98	0.46
1:D:118:LEU:HA	1:D:137:LEU:HB3	1.96	0.46
1:D:627:PRO:O	1:D:629:ARG:NH1	2.49	0.46
1:D:650:VAL:H	1:D:777:PHE:H	1.64	0.46
1:D:1152:MET:HE1	1:D:1217:CYS:HB3	1.98	0.46
1:D:2004:GLU:HA	1:D:2007:ASN:HD22	1.81	0.46
1:D:3658:LYS:HA	1:D:3661:TRP:CD2	2.51	0.46
1:D:4063:ASP:OD2	1:D:4067:LYS:NZ	2.45	0.46
1:A:1124:PHE:HA	1:A:1131:ARG:HA	1.98	0.45
1:A:2868:SER:O	1:A:2872:GLN:HB2	2.16	0.45
1:A:3582:UNK:O	1:A:3586:UNK:CB	2.63	0.45
1:B:2758:PHE:HD2	1:B:2809:ILE:HG12	1.81	0.45
1:C:144:GLU:HG2	1:C:175:SER:HB3	1.98	0.45
1:C:184:THR:HA	1:C:189:LEU:HA	1.97	0.45
1:C:2755:ILE:HD13	1:C:2810:LYS:HG2	1.98	0.45
1:C:3658:LYS:HA	1:C:3661:TRP:CD2	2.51	0.45
1:C:4583:SER:O	1:C:4628:VAL:N	2.39	0.45
1:D:395:GLN:HG3	1:D:397:GLU:H	1.81	0.45
1:D:2758:PHE:HD2	1:D:2809:ILE:HG12	1.81	0.45
1:A:2006:ILE:HD11	1:A:3641:LEU:HD13	1.97	0.45
1:B:1238:PHE:O	1:B:1606:SER:N	2.37	0.45
1:B:1284:VAL:HA	1:B:1471:UNK:HA	1.99	0.45
1:B:2868:SER:O	1:B:2872:GLN:HB2	2.16	0.45
1:B:4005:GLN:HE21	1:B:4110:PHE:HE1	1.63	0.45
1:B:4682:GLU:O	1:B:4727:LYS:NZ	2.40	0.45
1:C:939:VAL:HA	1:C:1052:ASN:O	2.17	0.45
1:C:4582:VAL:HG23	1:C:4629:TYR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4848:VAL:O	1:C:4852:THR:OG1	2.30	0.45
1:D:594:GLY:HA3	1:D:1594:ARG:HD3	1.99	0.45
1:D:652:ARG:HD3	1:D:773:LEU:HD13	1.98	0.45
1:D:717:ASP:OD1	1:D:720:HIS:ND1	2.50	0.45
1:D:4826:ILE:O	1:D:4829:SER:OG	2.33	0.45
1:A:594:GLY:HA3	1:A:1594:ARG:HD3	1.99	0.45
1:A:1663:HIS:O	1:A:1667:LEU:N	2.47	0.45
1:A:1663:HIS:NE2	1:A:1711:TYR:OH	2.44	0.45
1:A:3658:LYS:HA	1:A:3661:TRP:CD2	2.51	0.45
1:B:131:LEU:H	1:B:131:LEU:HG	1.63	0.45
1:B:463:GLU:OE2	1:B:467:LYS:NZ	2.34	0.45
1:B:594:GLY:HA3	1:B:1594:ARG:HD3	1.99	0.45
1:B:627:PRO:O	1:B:629:ARG:NH1	2.49	0.45
1:B:1124:PHE:HA	1:B:1131:ARG:HA	1.98	0.45
1:B:2006:ILE:HD11	1:B:3641:LEU:HD13	1.97	0.45
1:C:636:ASN:HD22	1:C:702:TRP:HB3	1.80	0.45
1:C:694:PRO:HA	1:C:696:PRO:HG3	1.98	0.45
1:C:1096:THR:HG23	1:C:1199:VAL:HG22	1.99	0.45
1:C:2739:PRO:HB3	1:C:2884:ASN:HB3	1.97	0.45
1:C:4048:LEU:HD23	1:C:4048:LEU:HA	1.84	0.45
1:D:2448:GLY:HA2	1:D:2451:LEU:HD12	1.97	0.45
1:A:939:VAL:HA	1:A:1052:ASN:O	2.17	0.45
1:A:1100:MET:HE2	1:A:1198:GLN:HB3	1.97	0.45
1:A:1105:ALA:HB1	1:A:1109:LEU:HD21	1.97	0.45
1:A:4063:ASP:OD2	1:A:4067:LYS:NZ	2.45	0.45
1:A:5019:TRP:HB3	1:A:5022:PHE:HE2	1.82	0.45
1:B:13:PHE:HA	1:B:164:ARG:HA	1.98	0.45
1:B:660:GLY:HA2	1:B:750:LEU:HD12	1.97	0.45
1:B:2004:GLU:HA	1:B:2007:ASN:HD22	1.81	0.45
1:B:4063:ASP:OD2	1:B:4067:LYS:NZ	2.45	0.45
1:C:221:ARG:NE	1:C:253:CYS:O	2.49	0.45
1:C:395:GLN:HG3	1:C:397:GLU:H	1.81	0.45
1:C:650:VAL:H	1:C:777:PHE:H	1.64	0.45
1:C:717:ASP:OD1	1:C:720:HIS:ND1	2.50	0.45
1:C:1284:VAL:HA	1:C:1471:UNK:HA	1.99	0.45
1:D:939:VAL:HA	1:D:1052:ASN:O	2.16	0.45
1:D:4883:TYR:HA	1:D:4886:HIS:HD2	1.79	0.45
1:A:2755:ILE:HD13	1:A:2810:LYS:HG2	1.98	0.45
1:A:4190:ILE:HD12	1:A:5031:GLN:HE21	1.80	0.45
1:B:717:ASP:OD1	1:B:720:HIS:ND1	2.50	0.45
1:B:939:VAL:HA	1:B:1052:ASN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1203:ASN:ND2	1:B:1210:SER:O	2.49	0.45
1:B:3948:LYS:HE3	1:B:4012:LEU:HD22	1.98	0.45
1:B:5019:TRP:HB3	1:B:5022:PHE:HE2	1.82	0.45
1:C:5019:TRP:HB3	1:C:5022:PHE:HE2	1.82	0.45
1:D:636:ASN:HD22	1:D:702:TRP:HB3	1.80	0.45
1:D:1096:THR:HG23	1:D:1199:VAL:HG22	1.99	0.45
1:A:224:HIS:N	1:A:229:GLU:O	2.46	0.45
1:A:232:THR:HB	1:A:252:VAL:HG11	1.97	0.45
1:A:652:ARG:HD3	1:A:773:LEU:HD13	1.98	0.45
1:A:1101:ARG:NE	1:A:1115:LEU:HB3	2.29	0.45
1:A:4582:VAL:HG23	1:A:4629:TYR:HA	1.98	0.45
1:A:4848:VAL:O	1:A:4852:THR:OG1	2.30	0.45
1:A:5030:LYS:HA	1:A:5033:GLU:HB2	1.98	0.45
1:B:104:GLY:N	1:B:150:MET:O	2.38	0.45
1:B:1163:THR:HA	1:B:1168:VAL:HA	1.98	0.45
1:C:500:ALA:H	1:C:503:PHE:HB3	1.82	0.45
1:C:627:PRO:O	1:C:629:ARG:NH1	2.49	0.45
1:C:650:VAL:N	1:C:777:PHE:H	2.15	0.45
1:C:709:ASP:HB3	1:C:725:HIS:CE1	2.52	0.45
1:C:4563:ARG:HH11	1:C:4819:GLY:HA3	1.82	0.45
1:D:106:ALA:HA	1:D:149:THR:HA	1.98	0.45
1:D:694:PRO:HA	1:D:696:PRO:HG3	1.98	0.45
1:D:891:TRP:HA	1:D:902:ARG:HB3	1.98	0.45
1:A:709:ASP:HB3	1:A:725:HIS:CE1	2.52	0.45
1:A:1163:THR:HA	1:A:1168:VAL:HA	1.98	0.45
1:A:2165:LEU:HA	1:A:2168:VAL:HB	1.99	0.45
1:B:709:ASP:HB3	1:B:725:HIS:CE1	2.52	0.45
1:B:4563:ARG:HH11	1:B:4819:GLY:HA3	1.82	0.45
1:C:106:ALA:HA	1:C:149:THR:HA	1.98	0.45
1:C:594:GLY:HA3	1:C:1594:ARG:HD3	1.99	0.45
1:C:663:TYR:HB2	1:C:808:TYR:HB3	1.99	0.45
1:C:1778:SER:N	1:C:1799:SER:O	2.37	0.45
1:D:1101:ARG:NE	1:D:1115:LEU:HB3	2.29	0.45
1:A:395:GLN:HG3	1:A:397:GLU:H	1.81	0.45
1:A:717:ASP:OD1	1:A:720:HIS:ND1	2.50	0.45
1:A:1096:THR:HG23	1:A:1199:VAL:HG22	1.99	0.45
1:B:221:ARG:NE	1:B:253:CYS:O	2.49	0.45
1:B:395:GLN:HG3	1:B:397:GLU:H	1.81	0.45
1:B:650:VAL:H	1:B:777:PHE:H	1.64	0.45
1:B:1152:MET:HE1	1:B:1217:CYS:HB3	1.98	0.45
1:B:1263:THR:N	1:B:1266:THR:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1863:LEU:HB3	1:B:1870:VAL:HG11	1.98	0.45
1:B:2165:LEU:HA	1:B:2168:VAL:HB	1.99	0.45
1:D:650:VAL:N	1:D:777:PHE:H	2.15	0.45
1:D:717:ASP:OD1	1:D:717:ASP:N	2.49	0.45
1:D:1863:LEU:HB3	1:D:1870:VAL:HG11	1.98	0.45
1:D:2243:SER:OG	1:D:2246:ASN:N	2.45	0.45
1:A:1263:THR:N	1:A:1266:THR:O	2.50	0.45
1:B:500:ALA:H	1:B:503:PHE:HB3	1.82	0.45
1:B:1096:THR:HG23	1:B:1199:VAL:HG22	1.99	0.45
1:D:37:LEU:HD13	1:D:191:VAL:HG21	1.99	0.45
1:A:564:LEU:HA	1:A:567:VAL:HG22	1.99	0.45
1:A:1285:GLU:N	1:A:1470:UNK:O	2.50	0.45
1:A:4563:ARG:HH11	1:A:4819:GLY:HA3	1.82	0.45
1:B:564:LEU:HA	1:B:567:VAL:HG22	1.99	0.45
1:B:1148:VAL:HB	1:B:1165:ASN:HA	1.99	0.45
1:B:1285:GLU:N	1:B:1470:UNK:O	2.50	0.45
1:C:504:ALA:HB3	1:C:512:ALA:HB2	1.99	0.45
1:C:1285:GLU:N	1:C:1470:UNK:O	2.50	0.45
1:D:71:GLN:O	1:D:108:LEU:N	2.50	0.45
1:D:221:ARG:NE	1:D:253:CYS:O	2.49	0.45
1:D:564:LEU:HA	1:D:567:VAL:HG22	1.99	0.45
1:D:709:ASP:HB3	1:D:725:HIS:CE1	2.52	0.45
1:D:1163:THR:HA	1:D:1168:VAL:HA	1.98	0.45
1:D:1203:ASN:ND2	1:D:1210:SER:O	2.49	0.45
1:D:3948:LYS:HE3	1:D:4012:LEU:HD22	1.98	0.45
1:D:5019:TRP:HB3	1:D:5022:PHE:HE2	1.82	0.45
1:A:4924:VAL:HA	1:A:4928:LEU:HB2	1.99	0.44
1:B:663:TYR:HB2	1:B:808:TYR:HB3	1.99	0.44
1:B:3960:GLN:HA	1:B:3963:ASN:HD22	1.82	0.44
1:C:891:TRP:HA	1:C:902:ARG:HB3	1.98	0.44
1:C:975:VAL:O	1:C:1044:ARG:NE	2.50	0.44
1:C:2004:GLU:HA	1:C:2007:ASN:HD22	1.81	0.44
1:A:449:ILE:HG13	1:A:525:LEU:HD12	1.99	0.44
1:A:717:ASP:OD1	1:A:717:ASP:N	2.49	0.44
1:A:1650:ILE:HG23	1:A:1651:LEU:HG	1.99	0.44
1:B:37:LEU:HD13	1:B:191:VAL:HG21	1.99	0.44
1:B:54:ASN:O	1:B:58:VAL:N	2.46	0.44
1:B:134:ASP:N	1:B:134:ASP:OD1	2.49	0.44
1:B:3700:GLN:HA	1:B:3703:LEU:HD12	2.00	0.44
1:B:4583:SER:O	1:B:4628:VAL:N	2.39	0.44
1:B:4826:ILE:O	1:B:4829:SER:OG	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:LEU:HB3	1:C:472:ARG:NH1	2.32	0.44
1:C:2165:LEU:HA	1:C:2168:VAL:HB	1.99	0.44
1:C:2243:SER:OG	1:C:2245:GLN:N	2.46	0.44
1:C:3700:GLN:HA	1:C:3703:LEU:HD12	2.00	0.44
1:D:468:LEU:HB3	1:D:472:ARG:NH1	2.32	0.44
1:A:689:THR:HA	1:A:778:PHE:HE2	1.83	0.44
1:A:975:VAL:O	1:A:1044:ARG:NE	2.50	0.44
1:A:1152:MET:HE1	1:A:1217:CYS:HB3	1.98	0.44
1:A:2243:SER:OG	1:A:2245:GLN:N	2.46	0.44
1:A:3700:GLN:HA	1:A:3703:LEU:HD12	2.00	0.44
1:B:650:VAL:N	1:B:777:PHE:H	2.15	0.44
1:B:1650:ILE:HG23	1:B:1651:LEU:HG	1.99	0.44
1:B:1663:HIS:NE2	1:B:1711:TYR:OH	2.44	0.44
1:B:3658:LYS:HA	1:B:3661:TRP:CD2	2.51	0.44
1:B:4063:ASP:O	1:B:4067:LYS:NZ	2.37	0.44
1:C:15:ARG:HA	1:C:100:THR:HA	2.00	0.44
1:C:449:ILE:HG13	1:C:525:LEU:HD12	1.99	0.44
1:C:721:LEU:HD22	1:C:768:PHE:HZ	1.83	0.44
1:C:2758:PHE:HD2	1:C:2809:ILE:HG12	1.81	0.44
1:D:3700:GLN:HA	1:D:3703:LEU:HD12	2.00	0.44
1:D:3802:ILE:O	1:D:3806:ASN:CB	2.57	0.44
1:A:104:GLY:N	1:A:150:MET:O	2.38	0.44
1:A:650:VAL:N	1:A:777:PHE:H	2.15	0.44
1:A:694:PRO:HA	1:A:696:PRO:HG3	1.98	0.44
1:A:1072:VAL:HG22	1:A:1195:GLY:HA2	1.99	0.44
1:A:1284:VAL:HA	1:A:1471:UNK:HA	1.99	0.44
1:A:4885:PHE:O	1:A:4889:VAL:HB	2.18	0.44
1:B:1240:LYS:HG3	1:B:1242:LEU:H	1.83	0.44
1:B:2806:ARG:HA	1:B:2809:ILE:HD12	2.00	0.44
1:B:4582:VAL:HG23	1:B:4629:TYR:HA	1.98	0.44
1:C:1263:THR:N	1:C:1266:THR:O	2.50	0.44
1:D:15:ARG:HA	1:D:100:THR:HA	2.00	0.44
1:D:144:GLU:HG2	1:D:175:SER:HB3	1.98	0.44
1:D:2093:SER:O	1:D:2097:LEU:CB	2.65	0.44
1:D:2806:ARG:HA	1:D:2809:ILE:HD12	2.00	0.44
1:D:4563:ARG:HH11	1:D:4819:GLY:HA3	1.82	0.44
1:D:4973:HIS:CD2	1:D:4976:GLU:HB3	2.53	0.44
1:A:575:LEU:HD22	1:A:609:CYS:HB3	2.00	0.44
1:A:1240:LYS:HG3	1:A:1242:LEU:H	1.83	0.44
1:A:1720:LEU:HD23	1:A:1721:GLU:HA	2.00	0.44
1:A:3875:MET:HE3	1:A:3877:ASP:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4978:HIS:HA	1:A:4982:GLU:HB2	2.00	0.44
1:B:468:LEU:HB3	1:B:472:ARG:NH1	2.32	0.44
1:B:1105:ALA:HB1	1:B:1109:LEU:HD21	1.97	0.44
1:B:2755:ILE:HD13	1:B:2810:LYS:HG2	1.98	0.44
1:B:5029:ARG:O	1:B:5033:GLU:CA	2.66	0.44
1:C:224:HIS:N	1:C:229:GLU:O	2.46	0.44
1:C:4873:ASP:OD1	1:C:4875:LYS:NZ	2.48	0.44
1:C:5029:ARG:O	1:C:5033:GLU:CA	2.66	0.44
1:D:1263:THR:N	1:D:1266:THR:O	2.50	0.44
1:D:2165:LEU:HA	1:D:2168:VAL:HB	1.99	0.44
1:D:2755:ILE:HD13	1:D:2810:LYS:HG2	1.98	0.44
1:A:144:GLU:HG2	1:A:175:SER:HB3	1.98	0.44
1:A:1815:LEU:HD22	1:A:1845:VAL:HG21	2.00	0.44
1:B:891:TRP:HA	1:B:902:ARG:HB3	1.98	0.44
1:B:1720:LEU:HD23	1:B:1721:GLU:HA	2.00	0.44
1:B:3875:MET:HE3	1:B:3877:ASP:HB3	2.00	0.44
1:C:689:THR:HA	1:C:778:PHE:HE2	1.83	0.44
1:D:1072:VAL:HG22	1:D:1195:GLY:HA2	1.99	0.44
1:D:1285:GLU:N	1:D:1470:UNK:O	2.50	0.44
1:D:3875:MET:HE3	1:D:3877:ASP:HB3	2.00	0.44
1:D:4558:ASN:OD1	1:D:4558:ASN:N	2.50	0.44
1:D:4978:HIS:HA	1:D:4982:GLU:HB2	2.00	0.44
1:A:468:LEU:HB3	1:A:472:ARG:NH1	2.32	0.44
1:A:1148:VAL:HB	1:A:1165:ASN:HA	1.99	0.44
1:A:4063:ASP:O	1:A:4067:LYS:NZ	2.37	0.44
1:B:2287:ALA:O	1:B:3849:ARG:NH1	2.51	0.44
1:B:4130:ASN:HA	1:B:4133:GLN:HB2	2.00	0.44
1:C:71:GLN:O	1:C:108:LEU:N	2.50	0.44
1:C:342:GLY:HA2	1:C:389:PHE:HD2	1.83	0.44
1:C:564:LEU:HA	1:C:567:VAL:HG22	2.00	0.44
1:C:1101:ARG:N	1:C:1193:SER:OG	2.51	0.44
1:C:1650:ILE:HG23	1:C:1651:LEU:HG	1.99	0.44
1:C:3948:LYS:HE3	1:C:4012:LEU:HD22	1.98	0.44
1:C:3960:GLN:HA	1:C:3963:ASN:HD22	1.82	0.44
1:C:3963:ASN:O	1:C:3966:THR:OG1	2.29	0.44
1:D:500:ALA:H	1:D:503:PHE:HB3	1.82	0.44
1:D:721:LEU:HD22	1:D:768:PHE:HZ	1.83	0.44
1:D:2287:ALA:O	1:D:3849:ARG:NH1	2.51	0.44
1:A:13:PHE:HA	1:A:164:ARG:HA	1.98	0.44
1:A:645:ARG:N	1:A:824:GLU:O	2.51	0.44
1:A:663:TYR:HB2	1:A:808:TYR:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:GLN:HG2	1:A:1187:GLY:HA3	2.00	0.44
1:A:1659:LEU:HA	1:A:1662:PHE:HB3	2.00	0.44
1:A:1863:LEU:HB3	1:A:1870:VAL:HG11	1.98	0.44
1:A:2131:LEU:HD23	1:A:3662:ILE:HB	2.00	0.44
1:A:2287:ALA:O	1:A:3849:ARG:NH1	2.51	0.44
1:B:575:LEU:HD22	1:B:609:CYS:HB3	2.00	0.44
1:B:645:ARG:N	1:B:824:GLU:O	2.51	0.44
1:B:975:VAL:O	1:B:1044:ARG:NE	2.50	0.44
1:B:4885:PHE:O	1:B:4889:VAL:HB	2.17	0.44
1:C:1240:LYS:HG3	1:C:1242:LEU:H	1.83	0.44
1:D:689:THR:HA	1:D:778:PHE:HE2	1.83	0.44
1:D:700:GLU:HA	1:D:1646:ARG:HA	1.99	0.44
1:D:975:VAL:O	1:D:1044:ARG:NE	2.50	0.44
1:D:1154:ASP:HB3	1:D:1157:GLU:HB3	2.00	0.44
1:D:1715:LEU:HA	1:D:1718:ILE:HG12	2.00	0.44
1:A:1715:LEU:HA	1:A:1718:ILE:HG12	2.00	0.44
1:A:4072:VAL:HG11	1:A:4125:PHE:HB2	2.00	0.44
1:A:4973:HIS:CD2	1:A:4976:GLU:HB3	2.53	0.44
1:B:721:LEU:HD22	1:B:768:PHE:HZ	1.83	0.44
1:B:1577:ALA:HB2	1:B:1587:PRO:HA	2.00	0.44
1:B:2203:MET:O	1:B:2206:THR:OG1	2.33	0.44
1:B:3915:ILE:H	1:B:3915:ILE:HG13	1.63	0.44
1:B:4924:VAL:HA	1:B:4928:LEU:HB2	1.99	0.44
1:C:37:LEU:HD13	1:C:191:VAL:HG21	1.99	0.44
1:C:134:ASP:OD1	1:C:134:ASP:N	2.49	0.44
1:C:1123:VAL:O	1:C:1132:TRP:N	2.35	0.44
1:C:1863:LEU:HB3	1:C:1870:VAL:HG11	1.98	0.44
1:C:2093:SER:O	1:C:2097:LEU:CB	2.65	0.44
1:C:3575:UNK:O	1:C:3579:UNK:N	2.51	0.44
1:D:504:ALA:HB3	1:D:512:ALA:HB2	1.99	0.44
1:D:551:LEU:HD22	1:D:585:SER:HB2	2.00	0.44
1:D:1284:VAL:HA	1:D:1471:UNK:HA	1.99	0.44
1:D:2203:MET:O	1:D:2206:THR:OG1	2.33	0.44
1:A:15:ARG:HA	1:A:100:THR:HA	2.00	0.43
1:A:37:LEU:HD13	1:A:191:VAL:HG21	1.99	0.43
1:A:504:ALA:HB3	1:A:512:ALA:HB2	1.99	0.43
1:A:891:TRP:HA	1:A:902:ARG:HB3	1.98	0.43
1:A:1658:ASP:OD1	1:A:1658:ASP:N	2.51	0.43
1:A:1735:ILE:HG23	1:A:1771:LEU:HD23	2.00	0.43
1:B:449:ILE:HG13	1:B:525:LEU:HD12	1.99	0.43
1:B:694:PRO:HA	1:B:696:PRO:HG3	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1101:ARG:NE	1:B:1115:LEU:HB3	2.29	0.43
1:B:2131:LEU:HD23	1:B:3662:ILE:HB	2.00	0.43
1:B:4674:GLU:HG3	1:B:4714:ASN:HB3	2.00	0.43
1:C:551:LEU:HD22	1:C:585:SER:HB2	2.00	0.43
1:C:1577:ALA:HB2	1:C:1587:PRO:HA	2.00	0.43
1:C:3875:MET:HE3	1:C:3877:ASP:HB3	2.00	0.43
1:C:4864:ASN:ND2	1:C:4871:GLU:OE1	2.42	0.43
1:D:1815:LEU:HD22	1:D:1845:VAL:HG21	2.00	0.43
1:D:2243:SER:OG	1:D:2245:GLN:N	2.46	0.43
1:D:4885:PHE:O	1:D:4889:VAL:HB	2.17	0.43
1:A:134:ASP:OD1	1:A:134:ASP:N	2.49	0.43
1:A:500:ALA:H	1:A:503:PHE:HB3	1.82	0.43
1:A:4130:ASN:HA	1:A:4133:GLN:HB2	2.00	0.43
1:A:4826:ILE:O	1:A:4829:SER:OG	2.33	0.43
1:B:232:THR:HG23	1:B:246:TYR:HB2	2.01	0.43
1:B:1715:LEU:HA	1:B:1718:ILE:HG12	2.00	0.43
1:B:1735:ILE:HG23	1:B:1771:LEU:HD23	2.00	0.43
1:B:3575:UNK:O	1:B:3579:UNK:N	2.51	0.43
1:B:4973:HIS:CD2	1:B:4976:GLU:HB3	2.53	0.43
1:C:232:THR:HG23	1:C:246:TYR:HB2	2.01	0.43
1:C:1148:VAL:HB	1:C:1165:ASN:HA	1.99	0.43
1:C:1715:LEU:HA	1:C:1718:ILE:HG12	2.00	0.43
1:C:1815:LEU:HD22	1:C:1845:VAL:HG21	2.00	0.43
1:C:4973:HIS:CD2	1:C:4976:GLU:HB3	2.53	0.43
1:D:1084:GLN:HG2	1:D:1187:GLY:HA3	2.00	0.43
1:D:2131:LEU:HD23	1:D:3662:ILE:HB	2.00	0.43
1:D:3783:ILE:HB	1:D:3828:PHE:HE1	1.83	0.43
1:D:4873:ASP:OD1	1:D:4875:LYS:NZ	2.48	0.43
1:D:4924:VAL:HA	1:D:4928:LEU:HB2	1.99	0.43
1:A:700:GLU:HA	1:A:1646:ARG:HA	1.99	0.43
1:B:2093:SER:O	1:B:2097:LEU:CB	2.65	0.43
1:B:3973:CYS:SG	1:B:3976:ASN:ND2	2.92	0.43
1:C:218:HIS:HB3	1:C:392:ARG:HD3	2.01	0.43
1:C:3783:ILE:HB	1:C:3828:PHE:HE1	1.83	0.43
1:C:4072:VAL:HG11	1:C:4125:PHE:HB2	2.00	0.43
1:C:4885:PHE:O	1:C:4889:VAL:HB	2.18	0.43
1:C:4924:VAL:HA	1:C:4928:LEU:HB2	1.99	0.43
1:D:1101:ARG:N	1:D:1193:SER:OG	2.51	0.43
1:D:2927:LEU:HD23	1:D:2930:LEU:HD12	2.01	0.43
1:D:5029:ARG:O	1:D:5033:GLU:CA	2.66	0.43
1:A:71:GLN:O	1:A:108:LEU:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4063:ASP:OD1	1:B:4169:SER:OG	2.37	0.43
1:C:700:GLU:HA	1:C:1646:ARG:HA	1.99	0.43
1:C:1154:ASP:HB3	1:C:1157:GLU:HB3	2.00	0.43
1:C:1720:LEU:HD23	1:C:1721:GLU:HA	2.00	0.43
1:D:449:ILE:HG13	1:D:525:LEU:HD12	1.99	0.43
1:D:663:TYR:HB2	1:D:808:TYR:HB3	1.99	0.43
1:D:1148:VAL:HB	1:D:1165:ASN:HA	1.99	0.43
1:D:4236:SER:O	1:D:4675:LYS:NZ	2.52	0.43
1:A:342:GLY:HA2	1:A:389:PHE:HD2	1.83	0.43
1:A:1106:ARG:HD2	1:A:1120:LEU:HD12	2.00	0.43
1:A:3948:LYS:HE3	1:A:4012:LEU:HD22	1.99	0.43
1:A:3973:CYS:SG	1:A:3976:ASN:ND2	2.92	0.43
1:A:4674:GLU:HG3	1:A:4714:ASN:HB3	2.00	0.43
1:B:15:ARG:HA	1:B:100:THR:HA	2.00	0.43
1:B:342:GLY:HA2	1:B:389:PHE:HD2	1.83	0.43
1:B:1659:LEU:HA	1:B:1662:PHE:HB3	2.00	0.43
1:B:2243:SER:HG	1:B:2245:GLN:H	1.64	0.43
1:C:379:HIS:CD2	1:C:381:GLU:H	2.37	0.43
1:D:204:PRO:HG2	1:D:268:SER:HB3	2.01	0.43
1:D:379:HIS:CD2	1:D:381:GLU:H	2.37	0.43
1:D:1106:ARG:HD2	1:D:1120:LEU:HD12	2.00	0.43
1:D:4674:GLU:HG3	1:D:4714:ASN:HB3	2.00	0.43
1:A:54:ASN:O	1:A:58:VAL:N	2.46	0.43
1:A:218:HIS:HB3	1:A:392:ARG:HD3	2.01	0.43
1:A:2093:SER:O	1:A:2097:LEU:CB	2.65	0.43
1:A:4236:SER:O	1:A:4675:LYS:NZ	2.52	0.43
1:B:2243:SER:HG	1:B:2245:GLN:N	2.17	0.43
1:C:1072:VAL:HG22	1:C:1195:GLY:HA2	1.99	0.43
1:C:1163:THR:HA	1:C:1168:VAL:HA	1.98	0.43
1:C:1735:ILE:HG23	1:C:1771:LEU:HD23	2.00	0.43
1:C:2927:LEU:HD23	1:C:2930:LEU:HD12	2.01	0.43
1:C:3973:CYS:SG	1:C:3976:ASN:ND2	2.92	0.43
1:D:575:LEU:HD22	1:D:609:CYS:HB3	2.00	0.43
1:D:939:VAL:HG22	1:D:1053:ILE:HG12	2.01	0.43
1:D:1735:ILE:HG23	1:D:1771:LEU:HD23	2.00	0.43
1:A:683:ARG:NH1	1:A:707:VAL:O	2.40	0.43
1:A:2121:PHE:HD1	1:A:2124:LEU:HD22	1.84	0.43
1:A:3575:UNK:O	1:A:3579:UNK:N	2.51	0.43
1:A:3761:GLN:HG2	1:A:3762:ARG:H	1.84	0.43
1:A:4671:PHE:CE1	1:A:4715:TYR:HA	2.54	0.43
1:A:5029:ARG:O	1:A:5033:GLU:CA	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:GLN:O	1:B:108:LEU:N	2.50	0.43
1:B:504:ALA:HB3	1:B:512:ALA:HB2	1.99	0.43
1:B:621:ILE:O	1:B:625:LEU:CB	2.66	0.43
1:B:700:GLU:HA	1:B:1646:ARG:HA	2.00	0.43
1:B:939:VAL:HG22	1:B:1053:ILE:HG12	2.01	0.43
1:B:1072:VAL:HG22	1:B:1195:GLY:HA2	1.99	0.43
1:C:1101:ARG:NE	1:C:1115:LEU:HB3	2.29	0.43
1:C:1111:PRO:HD3	1:C:1605:TRP:HE1	1.84	0.43
1:D:232:THR:HG23	1:D:246:TYR:HB2	2.01	0.43
1:D:1659:LEU:HA	1:D:1662:PHE:HB3	2.00	0.43
1:D:3575:UNK:O	1:D:3579:UNK:N	2.51	0.43
1:D:4072:VAL:HG11	1:D:4125:PHE:HB2	2.00	0.43
1:D:4671:PHE:CE1	1:D:4715:TYR:HA	2.54	0.43
1:A:2806:ARG:HA	1:A:2809:ILE:HD12	2.00	0.43
1:A:3960:GLN:HA	1:A:3963:ASN:HD22	1.82	0.43
1:B:218:HIS:HB3	1:B:392:ARG:HD3	2.01	0.43
1:B:689:THR:HA	1:B:778:PHE:HE2	1.83	0.43
1:B:4567:LEU:HD12	1:B:4816:ILE:HD12	2.00	0.43
1:B:4978:HIS:HA	1:B:4982:GLU:HB2	2.00	0.43
1:C:345:LEU:HD22	1:C:387:ALA:HB1	2.01	0.43
1:C:4034:ASN:HD21	1:C:4040:ILE:HB	1.84	0.43
1:C:4674:GLU:HG3	1:C:4714:ASN:HB3	2.00	0.43
1:D:218:HIS:HB3	1:D:392:ARG:HD3	2.01	0.43
1:D:345:LEU:HD22	1:D:387:ALA:HB1	2.01	0.43
1:D:621:ILE:O	1:D:625:LEU:CB	2.66	0.43
1:D:1658:ASP:OD1	1:D:1658:ASP:N	2.51	0.43
1:A:131:LEU:H	1:A:131:LEU:HG	1.63	0.43
1:A:204:PRO:HG2	1:A:268:SER:HB3	2.01	0.43
1:A:4034:ASN:HD21	1:A:4040:ILE:HB	1.84	0.43
1:B:379:HIS:CD2	1:B:381:GLU:H	2.37	0.43
1:B:717:ASP:OD1	1:B:717:ASP:N	2.49	0.43
1:B:1154:ASP:HB3	1:B:1157:GLU:HB3	2.00	0.43
1:B:2927:LEU:HD23	1:B:2930:LEU:HD12	2.01	0.43
1:C:4130:ASN:HA	1:C:4133:GLN:HB2	2.00	0.43
1:C:4978:HIS:HA	1:C:4982:GLU:HB2	1.99	0.43
1:D:1720:LEU:HD23	1:D:1721:GLU:HA	2.00	0.43
1:D:2121:PHE:HD1	1:D:2124:LEU:HD22	1.84	0.43
1:D:2381:GLU:HA	1:D:2384:ILE:HD12	2.01	0.43
1:D:3960:GLN:HA	1:D:3963:ASN:HD22	1.82	0.43
1:D:3980:LEU:HD23	1:D:3980:LEU:HA	1.87	0.43
1:D:4130:ASN:HA	1:D:4133:GLN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:THR:HG23	1:A:246:TYR:HB2	2.01	0.43
1:A:769:GLU:O	1:A:1523:UNK:N	2.52	0.43
1:A:3783:ILE:HB	1:A:3828:PHE:HE1	1.83	0.43
1:B:1084:GLN:HG2	1:B:1187:GLY:HA3	2.00	0.43
1:B:4021:LYS:HA	1:B:4024:VAL:HG12	2.01	0.43
1:C:331:VAL:HG12	1:C:333:GLY:H	1.84	0.43
1:C:575:LEU:HD22	1:C:609:CYS:HB3	2.00	0.43
1:C:3663:LEU:H	1:C:3663:LEU:HG	1.59	0.43
1:C:4161:ARG:HA	1:C:4164:LEU:HD12	2.01	0.43
1:D:1240:LYS:HG3	1:D:1242:LEU:H	1.83	0.43
1:D:1577:ALA:HB2	1:D:1587:PRO:HA	2.00	0.43
1:D:3973:CYS:SG	1:D:3976:ASN:ND2	2.92	0.43
1:A:1154:ASP:HB3	1:A:1157:GLU:HB3	2.00	0.42
1:A:1577:ALA:HB2	1:A:1587:PRO:HA	2.00	0.42
1:A:2123:LEU:HD12	1:A:2126:ARG:HD3	2.01	0.42
1:A:4063:ASP:OD1	1:A:4169:SER:OG	2.37	0.42
1:B:1815:LEU:HD22	1:B:1845:VAL:HG21	2.00	0.42
1:B:3121:UNK:O	1:B:3124:UNK:N	2.52	0.42
1:B:4034:ASN:HD21	1:B:4040:ILE:HB	1.84	0.42
1:C:204:PRO:HG2	1:C:268:SER:HB3	2.01	0.42
1:C:379:HIS:NE2	1:C:381:GLU:OE1	2.52	0.42
1:C:1663:HIS:NE2	1:C:1711:TYR:OH	2.44	0.42
1:C:2806:ARG:HA	1:C:2809:ILE:HD12	2.00	0.42
1:D:2030:ASP:OD1	1:D:2031:LEU:N	2.52	0.42
1:D:4034:ASN:HD21	1:D:4040:ILE:HB	1.84	0.42
1:D:4848:VAL:O	1:D:4852:THR:OG1	2.30	0.42
1:A:379:HIS:NE2	1:A:381:GLU:OE1	2.52	0.42
1:A:721:LEU:HD22	1:A:768:PHE:HZ	1.83	0.42
1:A:1101:ARG:N	1:A:1193:SER:OG	2.51	0.42
1:B:894:GLY:HA3	1:B:903:LEU:HB3	2.02	0.42
1:B:1660:GLN:O	1:B:1664:SER:N	2.48	0.42
1:C:629:ARG:NH2	1:C:1688:HIS:HA	2.34	0.42
1:C:645:ARG:N	1:C:824:GLU:O	2.51	0.42
1:D:342:GLY:HA2	1:D:389:PHE:HD2	1.83	0.42
1:D:894:GLY:HA3	1:D:903:LEU:HB3	2.02	0.42
1:D:1105:ALA:N	1:D:1189:LEU:O	2.52	0.42
1:D:1650:ILE:HG23	1:D:1651:LEU:HG	1.99	0.42
1:D:2776:SER:O	1:D:2788:HIS:N	2.53	0.42
1:D:3121:UNK:O	1:D:3124:UNK:N	2.52	0.42
1:A:629:ARG:NH2	1:A:1688:HIS:HA	2.34	0.42
1:A:2776:SER:N	1:A:2786:LYS:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ASP:OD1	1:B:330:ASP:N	2.52	0.42
1:B:629:ARG:NH2	1:B:1688:HIS:HA	2.34	0.42
1:B:842:PRO:HD3	1:B:1073:ARG:HG3	2.02	0.42
1:B:1101:ARG:N	1:B:1193:SER:OG	2.51	0.42
1:B:3761:GLN:HG2	1:B:3762:ARG:H	1.84	0.42
1:C:1084:GLN:HG2	1:C:1187:GLY:HA3	2.00	0.42
1:C:1203:ASN:ND2	1:C:1210:SER:O	2.49	0.42
1:C:2121:PHE:HD1	1:C:2124:LEU:HD22	1.84	0.42
1:C:2287:ALA:O	1:C:3849:ARG:NH1	2.51	0.42
1:C:4063:ASP:OD1	1:C:4169:SER:OG	2.37	0.42
1:C:4701:TRP:CZ2	1:C:4781:GLY:HA3	2.55	0.42
1:C:4826:ILE:O	1:C:4829:SER:OG	2.33	0.42
1:D:379:HIS:NE2	1:D:381:GLU:OE1	2.52	0.42
1:D:3761:GLN:HG2	1:D:3762:ARG:H	1.84	0.42
1:D:4063:ASP:OD1	1:D:4169:SER:OG	2.37	0.42
1:A:894:GLY:HA3	1:A:903:LEU:HB3	2.01	0.42
1:A:939:VAL:HG22	1:A:1053:ILE:HG12	2.01	0.42
1:A:4650:HIS:HA	1:A:4653:VAL:HG22	2.02	0.42
1:B:345:LEU:HD22	1:B:387:ALA:HB1	2.01	0.42
1:B:551:LEU:HD22	1:B:585:SER:HB2	2.00	0.42
1:B:1123:VAL:O	1:B:1132:TRP:N	2.35	0.42
1:B:2776:SER:O	1:B:2788:HIS:N	2.53	0.42
1:C:2131:LEU:HD23	1:C:3662:ILE:HB	2.00	0.42
1:C:4236:SER:O	1:C:4675:LYS:NZ	2.52	0.42
1:D:3891:LEU:HB3	1:D:3899:PHE:CZ	2.55	0.42
1:A:379:HIS:CD2	1:A:381:GLU:H	2.37	0.42
1:A:551:LEU:HD22	1:A:585:SER:HB2	2.00	0.42
1:A:842:PRO:HD3	1:A:1073:ARG:HG3	2.02	0.42
1:A:3121:UNK:O	1:A:3124:UNK:N	2.52	0.42
1:B:119:SER:OG	1:B:136:GLY:O	2.36	0.42
1:B:204:PRO:HG2	1:B:268:SER:HB3	2.01	0.42
1:B:3150:UNK:O	1:B:3154:UNK:N	2.53	0.42
1:B:4207:MET:HA	1:B:4208:PRO:HD3	1.92	0.42
1:B:4720:VAL:HA	1:B:4723:LYS:HD3	2.02	0.42
1:C:683:ARG:NH1	1:C:707:VAL:O	2.40	0.42
1:C:769:GLU:O	1:C:1523:UNK:N	2.52	0.42
1:C:3761:GLN:HG2	1:C:3762:ARG:H	1.84	0.42
1:D:645:ARG:N	1:D:824:GLU:O	2.51	0.42
1:D:2829:GLY:HA2	1:D:2932:MET:HA	2.02	0.42
1:D:4650:HIS:HA	1:D:4653:VAL:HG22	2.01	0.42
1:A:345:LEU:HD22	1:A:387:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:PRO:HD3	1:A:1605:TRP:HE1	1.84	0.42
1:A:4021:LYS:HA	1:A:4024:VAL:HG12	2.01	0.42
1:A:4567:LEU:HD12	1:A:4816:ILE:HD12	2.01	0.42
1:B:331:VAL:HG12	1:B:333:GLY:H	1.84	0.42
1:B:3783:ILE:HB	1:B:3828:PHE:HE1	1.83	0.42
1:B:4236:SER:O	1:B:4675:LYS:NZ	2.52	0.42
1:B:4650:HIS:HA	1:B:4653:VAL:HG22	2.02	0.42
1:B:4701:TRP:CZ2	1:B:4781:GLY:HA3	2.55	0.42
1:C:1171:SER:OG	1:C:1175:SER:N	2.51	0.42
1:C:1659:LEU:HA	1:C:1662:PHE:HB3	2.00	0.42
1:C:2776:SER:N	1:C:2786:LYS:O	2.49	0.42
1:C:2829:GLY:HA2	1:C:2932:MET:HA	2.02	0.42
1:C:4567:LEU:HD12	1:C:4816:ILE:HD12	2.01	0.42
1:C:4822:THR:O	1:C:4825:THR:OG1	2.30	0.42
1:D:842:PRO:HD3	1:D:1073:ARG:HG3	2.02	0.42
1:D:4567:LEU:HD12	1:D:4816:ILE:HD12	2.00	0.42
1:D:4720:VAL:HA	1:D:4723:LYS:HD3	2.02	0.42
1:A:3150:UNK:O	1:A:3154:UNK:N	2.53	0.42
1:A:4207:MET:HA	1:A:4208:PRO:HD3	1.92	0.42
1:B:1106:ARG:HD2	1:B:1120:LEU:HD12	2.00	0.42
1:B:2030:ASP:OD1	1:B:2031:LEU:N	2.52	0.42
1:B:2829:GLY:HA2	1:B:2932:MET:HA	2.02	0.42
1:B:4671:PHE:CE1	1:B:4715:TYR:HA	2.54	0.42
1:C:894:GLY:HA3	1:C:903:LEU:HB3	2.01	0.42
1:C:939:VAL:HG22	1:C:1053:ILE:HG12	2.01	0.42
1:C:2030:ASP:OD1	1:C:2031:LEU:N	2.52	0.42
1:C:4001:MET:HE3	1:C:4057:MET:HG3	2.01	0.42
1:C:4671:PHE:CE1	1:C:4715:TYR:HA	2.54	0.42
1:C:4720:VAL:HA	1:C:4723:LYS:HD3	2.02	0.42
1:C:4724:VAL:O	1:C:4729:GLY:N	2.46	0.42
1:C:4763:GLY:O	1:C:4766:THR:OG1	2.27	0.42
1:D:214:VAL:HG12	1:D:274:LEU:HD12	2.02	0.42
1:D:331:VAL:HG12	1:D:333:GLY:H	1.84	0.42
1:D:3150:UNK:O	1:D:3154:UNK:N	2.53	0.42
1:D:4001:MET:HE3	1:D:4057:MET:HG3	2.01	0.42
1:A:621:ILE:O	1:A:625:LEU:CB	2.66	0.42
1:B:468:LEU:HB3	1:B:472:ARG:HH12	1.85	0.42
1:B:520:ASN:ND2	1:B:555:GLU:HG2	2.35	0.42
1:B:580:GLU:HG2	1:B:583:ILE:HD11	2.02	0.42
1:B:1111:PRO:HD3	1:B:1605:TRP:HE1	1.84	0.42
1:B:4072:VAL:HG11	1:B:4125:PHE:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4161:ARG:HA	1:B:4164:LEU:HD12	2.01	0.42
1:C:2381:GLU:HA	1:C:2384:ILE:HD12	2.01	0.42
1:C:3121:UNK:O	1:C:3124:UNK:N	2.52	0.42
1:C:3891:LEU:HB3	1:C:3899:PHE:CZ	2.55	0.42
1:D:330:ASP:OD1	1:D:330:ASP:N	2.52	0.42
1:D:580:GLU:HG2	1:D:583:ILE:HD11	2.02	0.42
1:D:838:HIS:HA	1:D:1201:HIS:HB3	2.02	0.42
1:D:1123:VAL:O	1:D:1132:TRP:N	2.35	0.42
1:A:915:GLU:O	1:A:919:ASN:ND2	2.53	0.42
1:A:2927:LEU:HD23	1:A:2930:LEU:HD12	2.01	0.42
1:A:4720:VAL:HA	1:A:4723:LYS:HD3	2.02	0.42
1:B:1659:LEU:O	1:B:1663:HIS:N	2.49	0.42
1:B:3891:LEU:HB3	1:B:3899:PHE:CZ	2.55	0.42
1:B:4001:MET:HE3	1:B:4057:MET:HG3	2.01	0.42
1:C:842:PRO:HD3	1:C:1073:ARG:HG3	2.02	0.42
1:C:1105:ALA:N	1:C:1189:LEU:O	2.52	0.42
1:C:1106:ARG:HD2	1:C:1120:LEU:HD12	2.00	0.42
1:C:2123:LEU:HD12	1:C:2126:ARG:HD3	2.01	0.42
1:D:224:HIS:N	1:D:229:GLU:O	2.46	0.42
1:D:4161:ARG:HA	1:D:4164:LEU:HD12	2.01	0.42
1:A:331:VAL:HG12	1:A:333:GLY:H	1.84	0.42
1:A:468:LEU:HB3	1:A:472:ARG:HH12	1.85	0.42
1:A:580:GLU:HG2	1:A:583:ILE:HD11	2.02	0.42
1:A:866:HIS:O	1:A:1051:TYR:OH	2.37	0.42
1:B:2121:PHE:HD1	1:B:2124:LEU:HD22	1.84	0.42
1:B:2381:GLU:HA	1:B:2384:ILE:HD12	2.01	0.42
1:B:4151:SER:HA	1:B:4160:LEU:HD21	2.02	0.42
1:C:580:GLU:HG2	1:C:583:ILE:HD11	2.02	0.42
1:C:4021:LYS:HA	1:C:4024:VAL:HG12	2.01	0.42
1:C:4151:SER:HA	1:C:4160:LEU:HD21	2.02	0.42
1:D:3522:UNK:O	1:D:3526:UNK:CB	2.68	0.42
1:D:4875:LYS:HG3	1:D:4885:PHE:CG	2.55	0.42
1:A:273:HIS:CD2	1:A:334:MET:HB3	2.55	0.41
1:A:2290:LEU:HD21	1:A:2295:LEU:HD21	2.02	0.41
1:A:2829:GLY:HA2	1:A:2932:MET:HA	2.02	0.41
1:B:379:HIS:NE2	1:B:381:GLU:OE1	2.53	0.41
1:B:769:GLU:O	1:B:1523:UNK:N	2.52	0.41
1:B:2123:LEU:HD12	1:B:2126:ARG:HD3	2.01	0.41
1:B:3696:ASP:HB2	1:B:3699:HIS:H	1.86	0.41
1:C:520:ASN:ND2	1:C:555:GLU:HG2	2.35	0.41
1:D:273:HIS:CD2	1:D:334:MET:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:ARG:NH2	1:D:1688:HIS:HA	2.34	0.41
1:A:73:LEU:O	1:A:106:ALA:N	2.53	0.41
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.88	0.41
1:A:2776:SER:O	1:A:2788:HIS:N	2.53	0.41
1:A:3696:ASP:HB2	1:A:3699:HIS:H	1.86	0.41
1:B:915:GLU:O	1:B:919:ASN:ND2	2.53	0.41
1:B:4701:TRP:CZ2	1:B:4778:TRP:HA	2.56	0.41
1:C:3150:UNK:O	1:C:3154:UNK:N	2.53	0.41
1:C:3522:UNK:O	1:C:3526:UNK:CB	2.68	0.41
1:C:4701:TRP:CZ2	1:C:4778:TRP:HA	2.56	0.41
1:D:769:GLU:O	1:D:1523:UNK:N	2.52	0.41
1:D:887:ILE:HG21	1:D:959:TYR:HA	2.03	0.41
1:D:1111:PRO:HD3	1:D:1605:TRP:HE1	1.84	0.41
1:D:1659:LEU:O	1:D:1663:HIS:N	2.49	0.41
1:D:2290:LEU:HD21	1:D:2295:LEU:HD21	2.02	0.41
1:A:2459:SER:HB2	1:B:133:PHE:HZ	1.86	0.41
1:A:3891:LEU:HB3	1:A:3899:PHE:CZ	2.55	0.41
1:B:635:THR:HA	1:B:1639:LEU:HA	2.03	0.41
1:B:646:PRO:HA	1:B:823:LEU:HA	2.02	0.41
1:B:1094:ALA:HB3	1:B:1147:ASP:HB3	2.02	0.41
1:B:2290:LEU:HD21	1:B:2295:LEU:HD21	2.02	0.41
1:B:4875:LYS:HG3	1:B:4885:PHE:CG	2.55	0.41
1:C:717:ASP:OD1	1:C:717:ASP:N	2.49	0.41
1:C:915:GLU:O	1:C:919:ASN:ND2	2.53	0.41
1:C:1658:ASP:OD1	1:C:1658:ASP:N	2.51	0.41
1:C:1707:LEU:HD12	1:C:1707:LEU:HA	1.93	0.41
1:C:2776:SER:O	1:C:2788:HIS:N	2.53	0.41
1:C:4875:LYS:HG3	1:C:4885:PHE:CG	2.55	0.41
1:D:393:CYS:SG	1:D:395:GLN:NE2	2.94	0.41
1:D:520:ASN:ND2	1:D:555:GLU:HG2	2.35	0.41
1:D:618:GLN:O	1:D:622:THR:OG1	2.32	0.41
1:D:915:GLU:O	1:D:919:ASN:ND2	2.53	0.41
1:A:887:ILE:HG21	1:A:959:TYR:HA	2.03	0.41
1:A:2381:GLU:HA	1:A:2384:ILE:HD12	2.01	0.41
1:B:273:HIS:CD2	1:B:334:MET:HB3	2.55	0.41
1:B:393:CYS:SG	1:B:395:GLN:NE2	2.94	0.41
1:B:479:GLN:HE21	1:B:536:ASN:ND2	2.19	0.41
1:B:1478:UNK:HA	1:B:1495:UNK:HA	2.02	0.41
1:C:468:LEU:HB3	1:C:472:ARG:HH12	1.85	0.41
1:D:73:LEU:O	1:D:106:ALA:N	2.53	0.41
1:D:2123:LEU:HD12	1:D:2126:ARG:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4052:SER:HA	1:D:4055:VAL:HB	2.02	0.41
1:D:4151:SER:HA	1:D:4160:LEU:HD21	2.02	0.41
1:D:4701:TRP:CZ2	1:D:4778:TRP:HA	2.55	0.41
1:D:4701:TRP:CZ2	1:D:4781:GLY:HA3	2.55	0.41
1:A:4701:TRP:CZ2	1:A:4778:TRP:HA	2.56	0.41
1:B:73:LEU:O	1:B:106:ALA:N	2.53	0.41
1:B:641:VAL:HG11	1:B:705:ASN:HA	2.03	0.41
1:B:2870:GLU:OE2	1:B:2939:ARG:N	2.54	0.41
1:C:54:ASN:O	1:C:58:VAL:N	2.46	0.41
1:C:214:VAL:HG12	1:C:274:LEU:HD12	2.02	0.41
1:C:273:HIS:CD2	1:C:334:MET:HB3	2.55	0.41
1:C:1802:ILE:HG21	1:C:1807:LEU:HD22	2.02	0.41
1:C:4650:HIS:HA	1:C:4653:VAL:HG22	2.02	0.41
1:D:2793:PRO:O	1:D:2796:THR:OG1	2.37	0.41
1:D:3796:SER:O	1:D:3800:LEU:N	2.48	0.41
1:A:393:CYS:SG	1:A:395:GLN:NE2	2.94	0.41
1:A:635:THR:HA	1:A:1639:LEU:HA	2.03	0.41
1:A:641:VAL:HG11	1:A:705:ASN:HA	2.03	0.41
1:A:1659:LEU:O	1:A:1663:HIS:N	2.49	0.41
1:A:4161:ARG:HA	1:A:4164:LEU:HD12	2.01	0.41
1:A:4701:TRP:CZ2	1:A:4781:GLY:HA3	2.54	0.41
1:B:744:VAL:HG22	1:B:759:ILE:HG12	2.03	0.41
1:B:1657:LEU:HD13	1:B:1657:LEU:HA	1.94	0.41
1:C:108:LEU:HB2	1:C:147:TRP:CH2	2.56	0.41
1:C:119:SER:OG	1:C:136:GLY:O	2.36	0.41
1:C:4063:ASP:OD2	1:C:4067:LYS:NZ	2.45	0.41
1:D:1660:GLN:O	1:D:1664:SER:N	2.48	0.41
1:D:3698:LEU:HD23	1:D:3771:HIS:HD2	1.86	0.41
1:D:4048:LEU:HD23	1:D:4048:LEU:HA	1.84	0.41
1:D:4973:HIS:O	1:D:4977:THR:OG1	2.28	0.41
1:A:108:LEU:HB2	1:A:147:TRP:CH2	2.56	0.41
1:A:652:ARG:HD2	1:A:750:LEU:HB3	2.03	0.41
1:A:744:VAL:HG22	1:A:759:ILE:HG12	2.03	0.41
1:A:3522:UNK:O	1:A:3526:UNK:CB	2.68	0.41
1:A:4001:MET:HE3	1:A:4057:MET:HG3	2.01	0.41
1:A:4091:LYS:HA	1:A:4091:LYS:HD3	1.88	0.41
1:A:4875:LYS:HG3	1:A:4885:PHE:CG	2.55	0.41
1:B:108:LEU:HB2	1:B:147:TRP:CH2	2.56	0.41
1:B:652:ARG:HD2	1:B:750:LEU:HB3	2.03	0.41
1:B:867:LEU:HA	1:B:870:ILE:HG22	2.03	0.41
1:B:887:ILE:HG21	1:B:959:TYR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:CYS:SG	1:C:395:GLN:NE2	2.94	0.41
1:C:838:HIS:HA	1:C:1201:HIS:HB3	2.02	0.41
1:C:870:ILE:HD12	1:C:870:ILE:HA	1.82	0.41
1:C:887:ILE:HG21	1:C:959:TYR:HA	2.03	0.41
1:C:1094:ALA:HB3	1:C:1147:ASP:HB3	2.02	0.41
1:C:1651:LEU:HD23	1:C:1651:LEU:HA	1.92	0.41
1:C:2793:PRO:O	1:C:2796:THR:OG1	2.37	0.41
1:D:479:GLN:HE21	1:D:536:ASN:ND2	2.19	0.41
1:D:646:PRO:HA	1:D:823:LEU:HA	2.02	0.41
1:D:1778:SER:N	1:D:1799:SER:O	2.37	0.41
1:D:2862:LEU:HB3	1:D:2928:LYS:HB3	2.03	0.41
1:D:3696:ASP:HB2	1:D:3699:HIS:H	1.85	0.41
1:D:4021:LYS:HA	1:D:4024:VAL:HG12	2.01	0.41
1:A:101:LEU:HB3	1:A:150:MET:HE1	2.03	0.41
1:A:1802:ILE:HG21	1:A:1807:LEU:HD22	2.02	0.41
1:A:2870:GLU:OE2	1:A:2939:ARG:N	2.54	0.41
1:B:1297:PHE:N	1:B:1460:UNK:O	2.47	0.41
1:B:3522:UNK:O	1:B:3526:UNK:CB	2.68	0.41
1:C:519:VAL:HA	1:C:522:LEU:HD12	2.03	0.41
1:C:1716:ILE:HD13	1:C:1716:ILE:HA	1.91	0.41
1:D:1651:LEU:HD23	1:D:1651:LEU:HA	1.92	0.41
1:A:520:ASN:ND2	1:A:555:GLU:HG2	2.35	0.41
1:A:702:TRP:HD1	1:A:1640:HIS:CD2	2.39	0.41
1:A:733:PRO:HD2	1:A:762:CYS:HA	2.03	0.41
1:A:838:HIS:HA	1:A:1201:HIS:HB3	2.02	0.41
1:A:2030:ASP:OD1	1:A:2031:LEU:N	2.52	0.41
1:B:615:ARG:NH2	1:B:1676:LEU:O	2.51	0.41
1:B:1658:ASP:OD1	1:B:1658:ASP:N	2.51	0.41
1:B:1671:ARG:NH2	1:B:1713:ASP:HB3	2.36	0.41
1:B:2466:LEU:HA	1:B:2469:ILE:HD12	2.03	0.41
1:B:3805:LEU:H	1:B:3805:LEU:HG	1.77	0.41
1:B:4052:SER:HA	1:B:4055:VAL:HB	2.02	0.41
1:B:4219:PHE:HA	1:B:4950:VAL:HG11	2.03	0.41
1:C:1671:ARG:NH2	1:C:1713:ASP:HB3	2.36	0.41
1:C:2862:LEU:HB3	1:C:2928:LYS:HB3	2.03	0.41
1:C:3696:ASP:HB2	1:C:3699:HIS:H	1.86	0.41
1:D:468:LEU:HB3	1:D:472:ARG:HH12	1.85	0.41
1:D:1478:UNK:HA	1:D:1495:UNK:HA	2.02	0.41
1:D:2460:LEU:HD23	1:D:2460:LEU:HA	1.93	0.41
1:D:2870:GLU:OE2	1:D:2939:ARG:N	2.54	0.41
1:D:3810:ALA:HA	1:D:3813:GLN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:GLN:HE21	1:A:536:ASN:ND2	2.19	0.41
1:A:646:PRO:HA	1:A:823:LEU:HA	2.02	0.41
1:A:1094:ALA:HB3	1:A:1147:ASP:HB3	2.02	0.41
1:A:1297:PHE:N	1:A:1460:UNK:O	2.47	0.41
1:A:1685:LEU:HA	1:A:1688:HIS:CD2	2.53	0.41
1:A:3796:SER:HA	1:A:3799:LYS:HE3	2.03	0.41
1:B:101:LEU:HB3	1:B:150:MET:HE1	2.03	0.41
1:B:1089:TYR:N	1:B:1224:GLU:O	2.54	0.41
1:B:1105:ALA:N	1:B:1189:LEU:O	2.52	0.41
1:C:73:LEU:O	1:C:106:ALA:N	2.53	0.41
1:C:151:HIS:HB2	1:C:170:ILE:HB	2.03	0.41
1:C:2290:LEU:HD21	1:C:2295:LEU:HD21	2.02	0.41
1:C:3810:ALA:HA	1:C:3813:GLN:HB2	2.02	0.41
1:D:108:LEU:HB2	1:D:147:TRP:CH2	2.56	0.41
1:D:702:TRP:HD1	1:D:1640:HIS:CD2	2.39	0.41
1:D:2466:LEU:HA	1:D:2469:ILE:HD12	2.03	0.41
1:A:658:GLN:O	1:A:662:TRP:NE1	2.48	0.40
1:A:1478:UNK:HA	1:A:1495:UNK:HA	2.02	0.40
1:A:2466:LEU:HA	1:A:2469:ILE:HD12	2.03	0.40
1:A:3842:LEU:HD12	1:A:3930:ILE:HG12	2.03	0.40
1:A:4052:SER:HA	1:A:4055:VAL:HB	2.02	0.40
1:A:4151:SER:HA	1:A:4160:LEU:HD21	2.02	0.40
1:B:82:LEU:HD23	1:B:82:LEU:HA	1.88	0.40
1:B:668:VAL:O	1:B:741:GLU:N	2.53	0.40
1:B:2457:LEU:HD23	1:B:2457:LEU:HA	1.90	0.40
1:B:2874:MET:HE2	1:B:2874:MET:HB3	2.01	0.40
1:C:82:LEU:HD23	1:C:82:LEU:HA	1.88	0.40
1:C:131:LEU:H	1:C:131:LEU:HG	1.63	0.40
1:C:330:ASP:OD1	1:C:330:ASP:N	2.52	0.40
1:C:635:THR:HA	1:C:1639:LEU:HA	2.03	0.40
1:C:2110:TYR:HE2	1:C:2112:GLN:HE21	1.69	0.40
1:C:2297:LYS:HA	1:C:2297:LYS:HD2	1.91	0.40
1:C:4219:PHE:HA	1:C:4950:VAL:HG11	2.03	0.40
1:D:113:HIS:CE1	1:D:402:ARG:HB3	2.56	0.40
1:D:1639:LEU:HD12	1:D:1653:LEU:HD21	2.03	0.40
1:A:1089:TYR:N	1:A:1224:GLU:O	2.54	0.40
1:A:2238:TYR:O	1:A:2242:ILE:HG12	2.21	0.40
1:B:214:VAL:HG22	1:B:341:TYR:CE1	2.57	0.40
1:B:519:VAL:HA	1:B:522:LEU:HD12	2.03	0.40
1:B:2243:SER:OG	1:B:2245:GLN:N	2.46	0.40
1:C:479:GLN:HE21	1:C:536:ASN:ND2	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:GLU:HG3	1:C:620:LEU:HD22	2.03	0.40
1:C:2238:TYR:O	1:C:2242:ILE:HG12	2.21	0.40
1:D:635:THR:HA	1:D:1639:LEU:HA	2.03	0.40
1:D:2238:TYR:O	1:D:2242:ILE:HG12	2.21	0.40
1:A:151:HIS:HB2	1:A:170:ILE:HB	2.03	0.40
1:A:214:VAL:HG22	1:A:341:TYR:CE1	2.57	0.40
1:A:1171:SER:OG	1:A:1175:SER:N	2.51	0.40
1:A:2207:VAL:HG11	1:A:2236:LEU:HD22	2.04	0.40
1:B:113:HIS:CE1	1:B:402:ARG:HB3	2.56	0.40
1:B:214:VAL:HG12	1:B:274:LEU:HD12	2.02	0.40
1:B:838:HIS:HA	1:B:1201:HIS:HB3	2.02	0.40
1:B:2862:LEU:HB3	1:B:2928:LYS:HB3	2.03	0.40
1:B:3698:LEU:HD23	1:B:3771:HIS:HD2	1.86	0.40
1:B:3810:ALA:HA	1:B:3813:GLN:HB2	2.03	0.40
1:B:4815:ASP:OD1	1:B:4815:ASP:N	2.54	0.40
1:C:214:VAL:HG22	1:C:341:TYR:CE1	2.57	0.40
1:C:445:LEU:HD23	1:C:521:LEU:HB3	2.04	0.40
1:C:870:ILE:HD11	1:C:1049:TYR:CG	2.56	0.40
1:C:2466:LEU:HA	1:C:2469:ILE:HD12	2.03	0.40
1:C:3698:LEU:HD23	1:C:3771:HIS:HD2	1.86	0.40
1:C:4052:SER:HA	1:C:4055:VAL:HB	2.02	0.40
1:D:1089:TYR:N	1:D:1224:GLU:O	2.54	0.40
1:D:1671:ARG:NH2	1:D:1713:ASP:HB3	2.36	0.40
1:A:113:HIS:CE1	1:A:402:ARG:HB3	2.56	0.40
1:A:670:GLU:HG3	1:A:787:VAL:HA	2.03	0.40
1:A:4219:PHE:HA	1:A:4950:VAL:HG11	2.03	0.40
1:B:2297:LYS:HD2	1:B:2297:LYS:HA	1.91	0.40
1:B:4091:LYS:HA	1:B:4091:LYS:HD3	1.88	0.40
1:C:1639:LEU:HD12	1:C:1653:LEU:HD21	2.03	0.40
1:C:3819:TYR:HA	1:C:3822:ASP:HB3	2.04	0.40
1:D:101:LEU:HB3	1:D:150:MET:HE1	2.03	0.40
1:D:870:ILE:HD11	1:D:1049:TYR:CG	2.56	0.40
1:D:1802:ILE:HG21	1:D:1807:LEU:HD22	2.02	0.40
1:D:3842:LEU:HD12	1:D:3930:ILE:HG12	2.02	0.40
1:D:4219:PHE:HA	1:D:4950:VAL:HG11	2.03	0.40
1:A:214:VAL:HG12	1:A:274:LEU:HD12	2.02	0.40
1:A:1657:LEU:HD13	1:A:1657:LEU:HA	1.94	0.40
1:A:3810:ALA:HA	1:A:3813:GLN:HB2	2.02	0.40
1:B:151:HIS:HB2	1:B:170:ILE:HB	2.03	0.40
1:B:3796:SER:HA	1:B:3799:LYS:HE3	2.03	0.40
1:C:652:ARG:HD2	1:C:750:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1505:UNK:HA	1:C:1543:UNK:HA	2.04	0.40
1:C:4696:ASP:O	1:C:4699:GLY:N	2.40	0.40
1:D:214:VAL:HG22	1:D:341:TYR:CE1	2.57	0.40
1:D:733:PRO:HD2	1:D:762:CYS:HA	2.03	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	3256/5037 (65%)	2890 (89%)	361 (11%)	5 (0%)	43	78
1	B	3256/5037 (65%)	2891 (89%)	360 (11%)	5 (0%)	43	78
1	C	3256/5037 (65%)	2890 (89%)	361 (11%)	5 (0%)	43	78
1	D	3256/5037 (65%)	2892 (89%)	359 (11%)	5 (0%)	43	78
All	All	13024/20148 (65%)	11563 (89%)	1441 (11%)	20 (0%)	44	78

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1708	ARG
1	B	1708	ARG
1	C	1708	ARG
1	D	1708	ARG
1	A	1293	LEU
1	A	1840	PRO
1	B	1293	LEU
1	B	1840	PRO
1	C	1293	LEU
1	C	1840	PRO
1	D	1293	LEU

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Mol	Chain	Res	Type
1	D	1840	PRO
1	A	1932	PRO
1	B	1932	PRO
1	C	1932	PRO
1	D	1932	PRO
1	C	1839	VAL
1	A	1839	VAL
1	B	1839	VAL
1	D	1839	VAL

### 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	2493/3230 (77%)	2478 (99%)	15 (1%)	78	83
1	B	2493/3230 (77%)	2478 (99%)	15 (1%)	78	83
1	C	2493/3230 (77%)	2478 (99%)	15 (1%)	78	83
1	D	2493/3230 (77%)	2479 (99%)	14 (1%)	78	83
All	All	9972/12920 (77%)	9913 (99%)	59 (1%)	76	83

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LEU
1	A	688	LEU
1	A	719	LEU
1	A	781	VAL
1	A	978	THR
1	A	1839	VAL
1	A	2010	LEU
1	A	2339	VAL
1	A	3663	LEU
1	A	3805	LEU
1	A	4036	VAL
1	A	4154	VAL

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Mol	Chain	Res	Type
1	A	4792	LEU
1	A	4813	LEU
1	A	4985	LEU
1	B	131	LEU
1	B	688	LEU
1	B	719	LEU
1	B	781	VAL
1	B	978	THR
1	B	1839	VAL
1	B	2010	LEU
1	B	2339	VAL
1	B	3663	LEU
1	B	3805	LEU
1	B	4036	VAL
1	B	4154	VAL
1	B	4792	LEU
1	B	4813	LEU
1	B	4985	LEU
1	C	131	LEU
1	C	688	LEU
1	C	719	LEU
1	C	781	VAL
1	C	978	THR
1	C	1839	VAL
1	C	2010	LEU
1	C	2339	VAL
1	C	3663	LEU
1	C	3805	LEU
1	C	4036	VAL
1	C	4154	VAL
1	C	4792	LEU
1	C	4813	LEU
1	C	4985	LEU
1	D	131	LEU
1	D	688	LEU
1	D	719	LEU
1	D	781	VAL
1	D	978	THR
1	D	1839	VAL
1	D	2010	LEU
1	D	2339	VAL
1	D	3663	LEU

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Mol	Chain	Res	Type
1	D	3805	LEU
1	D	4154	VAL
1	D	4792	LEU
1	D	4813	LEU
1	D	4985	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (191) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	105	HIS
1	A	113	HIS
1	A	273	HIS
1	A	379	HIS
1	A	395	GLN
1	A	582	HIS
1	A	593	HIS
1	A	634	GLN
1	A	678	GLN
1	A	765	GLN
1	A	838	HIS
1	A	1206	GLN
1	A	1611	HIS
1	A	1679	ASN
1	A	1693	GLN
1	A	1719	HIS
1	A	1775	HIS
1	A	1861	GLN
1	A	1941	ASN
1	A	1949	GLN
1	A	1953	HIS
1	A	2005	GLN
1	A	2007	ASN
1	A	2011	HIS
1	A	2112	GLN
1	A	2127	GLN
1	A	2773	ASN
1	A	3700	GLN
1	A	3809	ASN
1	A	3814	GLN
1	A	3896	ASN
1	A	3960	GLN

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Mol	Chain	Res	Type
1	A	3963	ASN
1	A	3970	GLN
1	A	3976	ASN
1	A	3994	HIS
1	A	4034	ASN
1	A	4054	ASN
1	A	4120	ASN
1	A	4142	ASN
1	A	4209	GLN
1	A	4246	GLN
1	A	4864	ASN
1	A	4886	HIS
1	A	4933	GLN
1	A	4949	GLN
1	A	4983	HIS
1	A	4997	ASN
1	A	5031	GLN
1	B	57	ASN
1	B	84	ASN
1	B	105	HIS
1	B	113	HIS
1	B	273	HIS
1	B	379	HIS
1	B	395	GLN
1	B	582	HIS
1	B	593	HIS
1	B	634	GLN
1	B	725	HIS
1	B	765	GLN
1	B	838	HIS
1	B	1206	GLN
1	B	1679	ASN
1	B	1693	GLN
1	B	1719	HIS
1	B	1775	HIS
1	B	1861	GLN
1	B	1941	ASN
1	B	1949	GLN
1	B	1953	HIS
1	B	2005	GLN
1	B	2007	ASN
1	B	2011	HIS

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Mol	Chain	Res	Type
1	B	2112	GLN
1	B	2127	GLN
1	B	2441	HIS
1	B	3700	GLN
1	B	3809	ASN
1	B	3814	GLN
1	B	3896	ASN
1	B	3960	GLN
1	B	3963	ASN
1	B	3970	GLN
1	B	3976	ASN
1	B	3994	HIS
1	B	4034	ASN
1	B	4054	ASN
1	B	4120	ASN
1	B	4142	ASN
1	B	4209	GLN
1	B	4246	GLN
1	B	4864	ASN
1	B	4933	GLN
1	B	4949	GLN
1	B	4983	HIS
1	B	4997	ASN
1	B	5031	GLN
1	C	57	ASN
1	C	105	HIS
1	C	113	HIS
1	C	151	HIS
1	C	273	HIS
1	C	379	HIS
1	C	395	GLN
1	C	582	HIS
1	C	593	HIS
1	C	634	GLN
1	C	765	GLN
1	C	838	HIS
1	C	1206	GLN
1	C	1611	HIS
1	C	1679	ASN
1	C	1693	GLN
1	C	1719	HIS
1	C	1775	HIS

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Mol	Chain	Res	Type
1	C	1861	GLN
1	C	1941	ASN
1	C	1949	GLN
1	C	1953	HIS
1	C	2005	GLN
1	C	2007	ASN
1	C	2112	GLN
1	C	2127	GLN
1	C	2441	HIS
1	C	3700	GLN
1	C	3809	ASN
1	C	3814	GLN
1	C	3896	ASN
1	C	3960	GLN
1	C	3963	ASN
1	C	3970	GLN
1	C	3976	ASN
1	C	3994	HIS
1	C	4034	ASN
1	C	4054	ASN
1	C	4120	ASN
1	C	4142	ASN
1	C	4209	GLN
1	C	4246	GLN
1	C	4933	GLN
1	C	4949	GLN
1	C	4983	HIS
1	C	4997	ASN
1	C	5031	GLN
1	D	57	ASN
1	D	105	HIS
1	D	113	HIS
1	D	273	HIS
1	D	379	HIS
1	D	395	GLN
1	D	582	HIS
1	D	593	HIS
1	D	634	GLN
1	D	765	GLN
1	D	838	HIS
1	D	1206	GLN
1	D	1679	ASN

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Mol	Chain	Res	Type
1	D	1693	GLN
1	D	1719	HIS
1	D	1775	HIS
1	D	1861	GLN
1	D	1941	ASN
1	D	1949	GLN
1	D	1953	HIS
1	D	2005	GLN
1	D	2007	ASN
1	D	2112	GLN
1	D	2127	GLN
1	D	3700	GLN
1	D	3809	ASN
1	D	3814	GLN
1	D	3896	ASN
1	D	3960	GLN
1	D	3963	ASN
1	D	3970	GLN
1	D	3976	ASN
1	D	3994	HIS
1	D	4034	ASN
1	D	4054	ASN
1	D	4120	ASN
1	D	4142	ASN
1	D	4209	GLN
1	D	4246	GLN
1	D	4864	ASN
1	D	4933	GLN
1	D	4949	GLN
1	D	4983	HIS
1	D	4997	ASN
1	D	5031	GLN

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	9
1	B	9
1	C	9
1	D	9

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3638:UNK	C	3639:THR	N	46.30
1	B	3638:UNK	C	3639:THR	N	46.30
1	C	3638:UNK	C	3639:THR	N	46.30
1	D	3638:UNK	C	3639:THR	N	46.30
1	A	2733:UNK	C	2734:ASN	N	16.65
1	B	2733:UNK	C	2734:ASN	N	16.65
1	C	2733:UNK	C	2734:ASN	N	16.65
1	D	2733:UNK	C	2734:ASN	N	16.65
1	A	3246:UNK	C	3247:UNK	N	16.59

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3246:UNK	C	3247:UNK	N	16.59
1	C	3246:UNK	C	3247:UNK	N	16.59
1	D	3246:UNK	C	3247:UNK	N	16.58
1	A	3216:UNK	C	3217:UNK	N	15.16
1	B	3216:UNK	C	3217:UNK	N	15.16
1	C	3216:UNK	C	3217:UNK	N	15.16
1	D	3216:UNK	C	3217:UNK	N	15.16
1	A	3535:UNK	C	3536:UNK	N	13.86
1	B	3535:UNK	C	3536:UNK	N	13.86
1	C	3535:UNK	C	3536:UNK	N	13.86
1	D	3535:UNK	C	3536:UNK	N	13.86
1	A	3313:UNK	C	3314:UNK	N	13.77
1	B	3313:UNK	C	3314:UNK	N	13.77
1	C	3313:UNK	C	3314:UNK	N	13.77
1	D	3313:UNK	C	3314:UNK	N	13.77
1	A	3147:UNK	C	3148:UNK	N	13.39
1	B	3147:UNK	C	3148:UNK	N	13.39
1	C	3147:UNK	C	3148:UNK	N	13.39
1	D	3147:UNK	C	3148:UNK	N	13.39
1	A	1572:UNK	C	1573:MET	N	12.12
1	B	1572:UNK	C	1573:MET	N	12.12
1	C	1572:UNK	C	1573:MET	N	12.12
1	D	1572:UNK	C	1573:MET	N	12.12
1	A	3327:UNK	C	3328:UNK	N	7.22
1	B	3327:UNK	C	3328:UNK	N	7.22
1	C	3327:UNK	C	3328:UNK	N	7.22
1	D	3327:UNK	C	3328:UNK	N	7.22

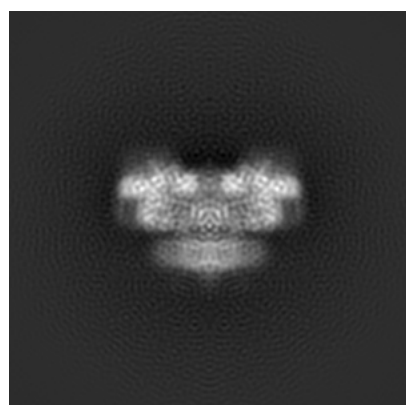
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4295. These allow visual inspection of the internal detail of the map and identification of artifacts.

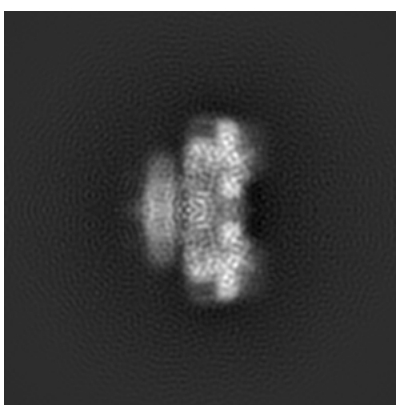
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

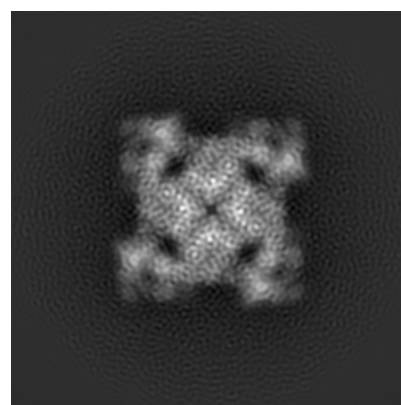
#### 6.1.1 Primary map



X



Y

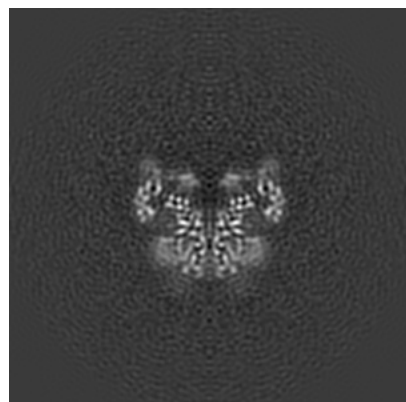


Z

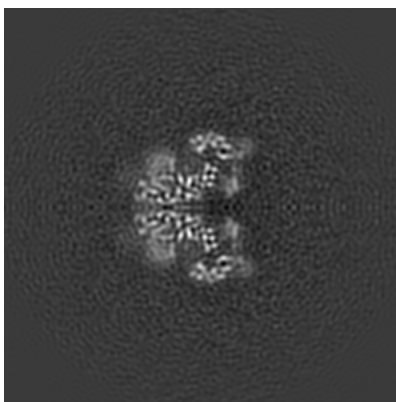
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

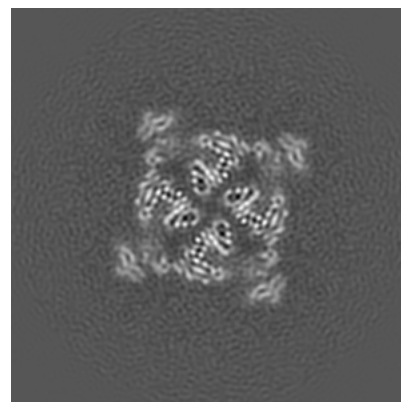
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

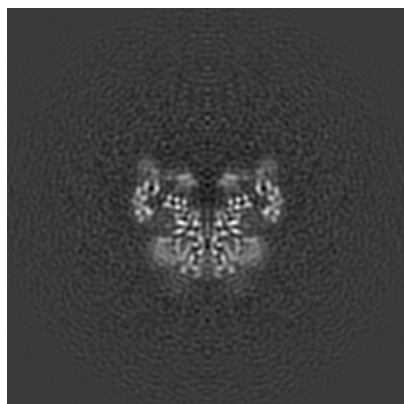


Z Index: 180

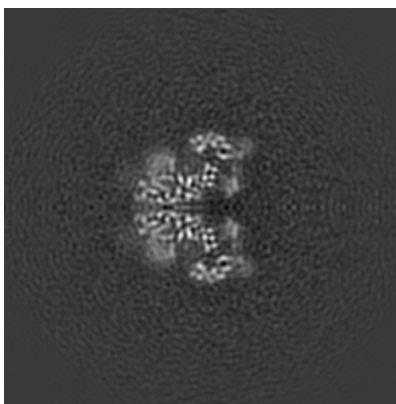
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

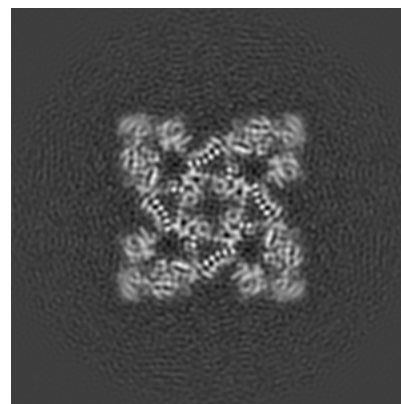
### 6.3.1 Primary map



X Index: 180



Y Index: 180

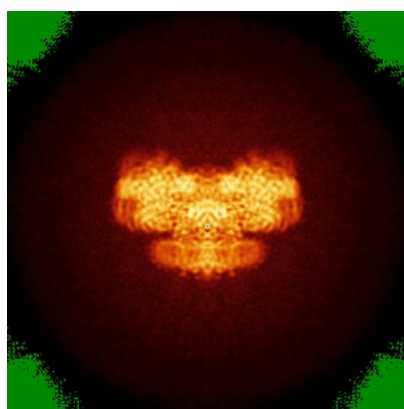


Z Index: 198

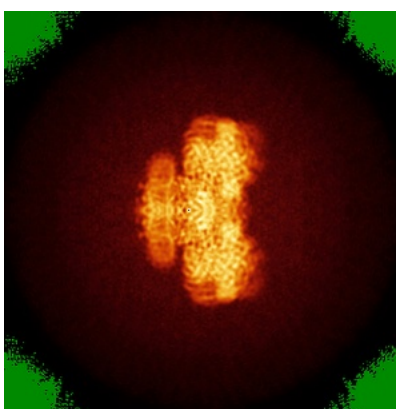
The images above show the largest variance slices of the map in three orthogonal directions.

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

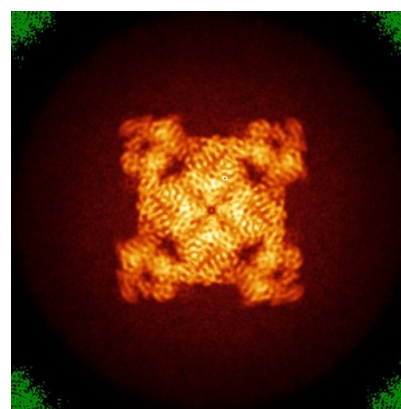
### 6.4.1 Primary map



X



Y



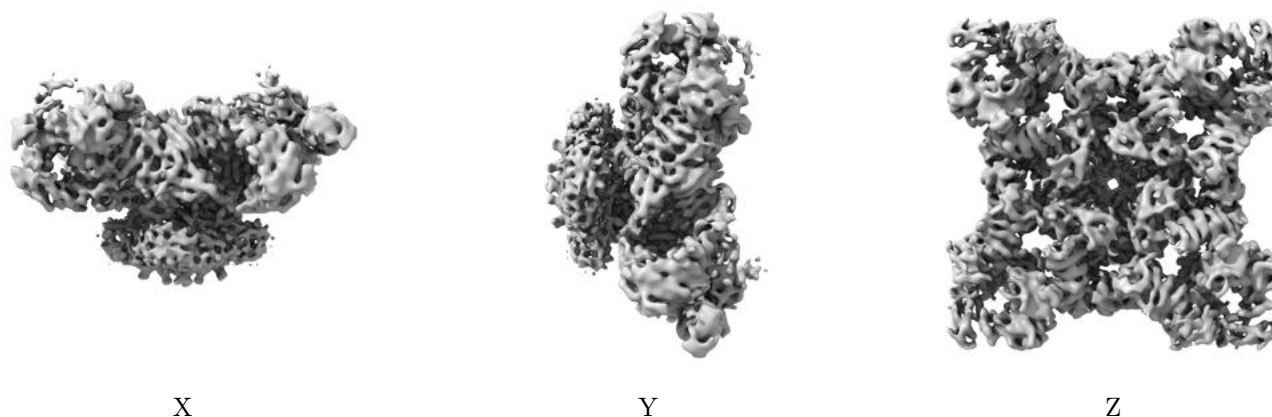
Z

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



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

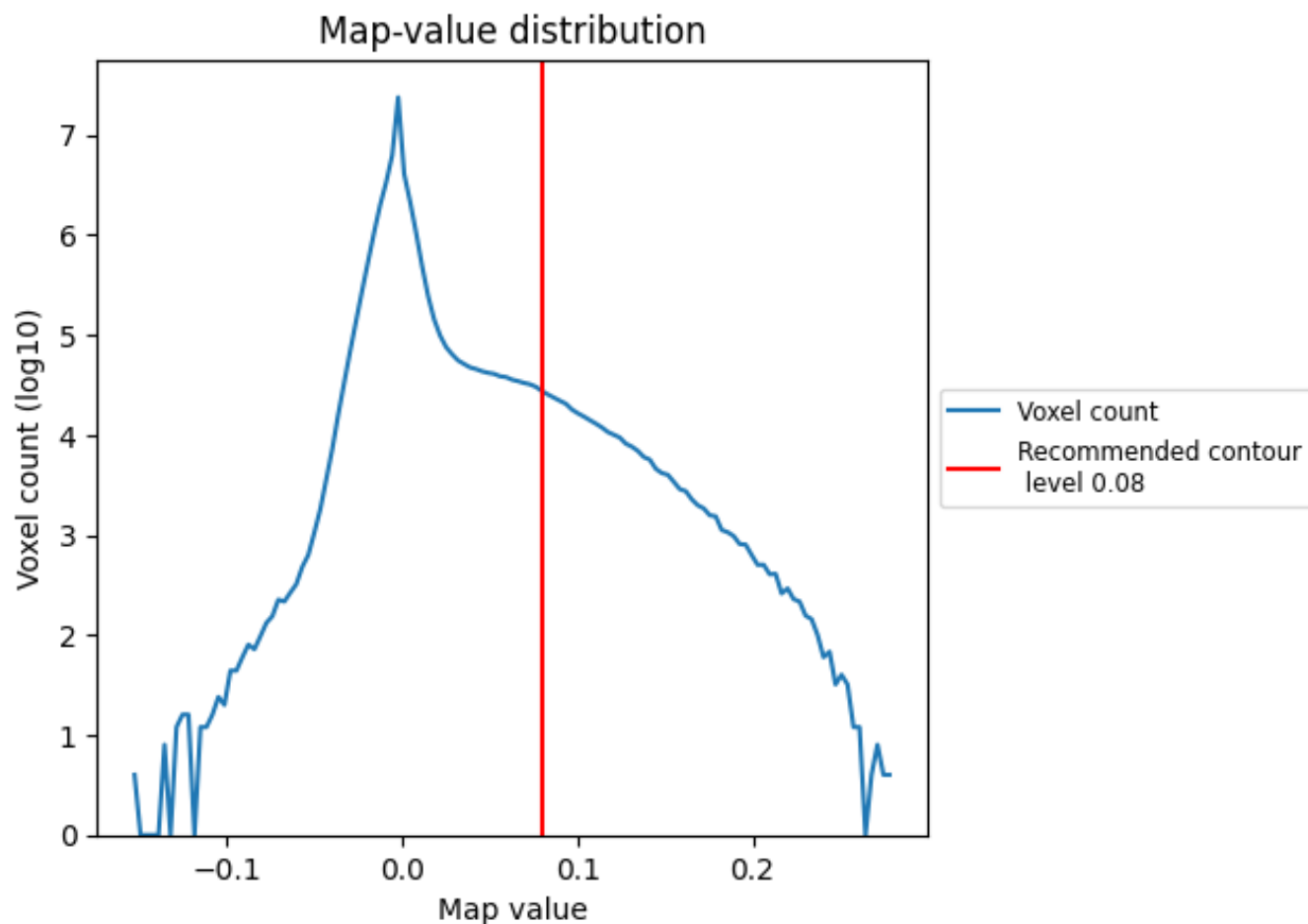
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

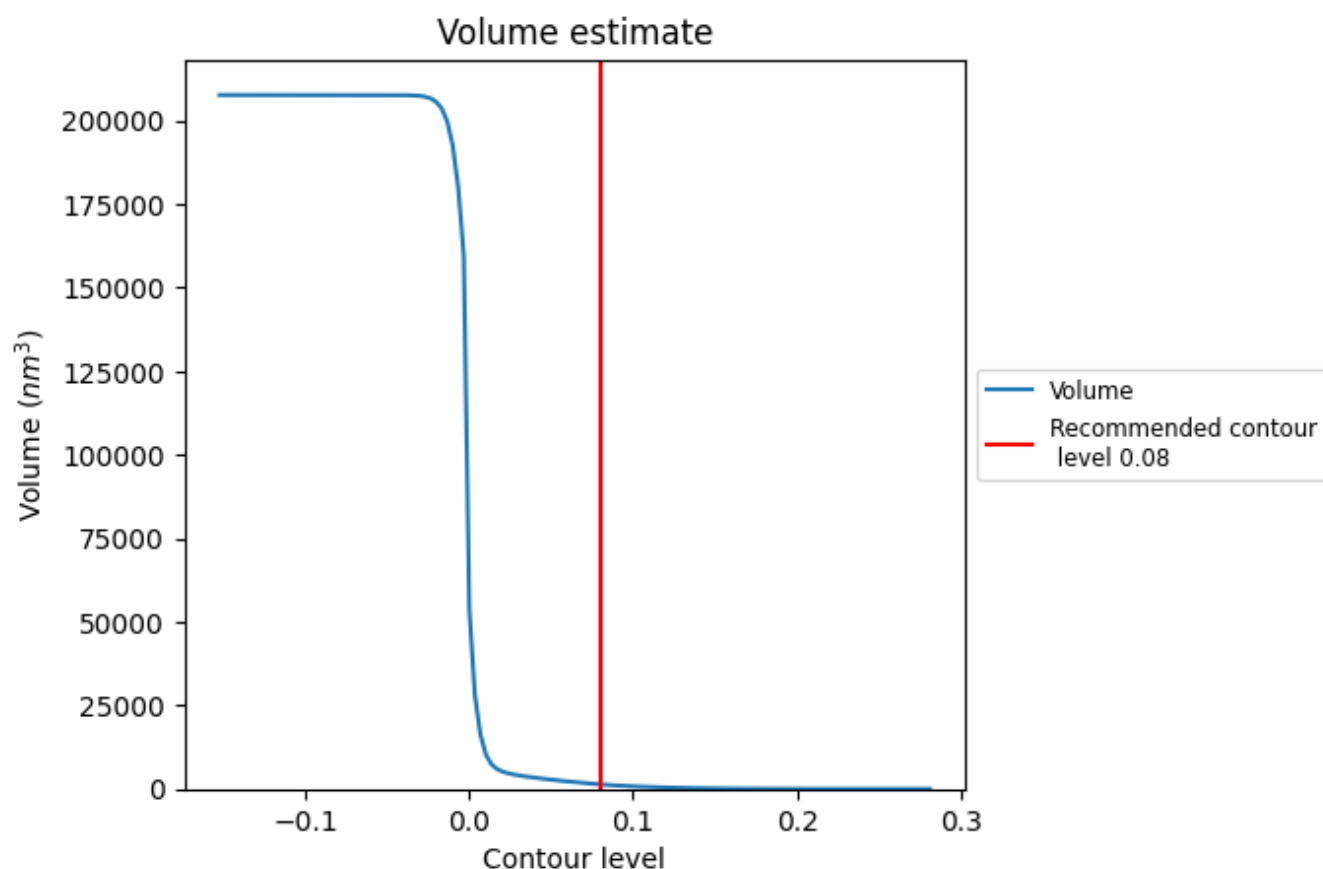
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

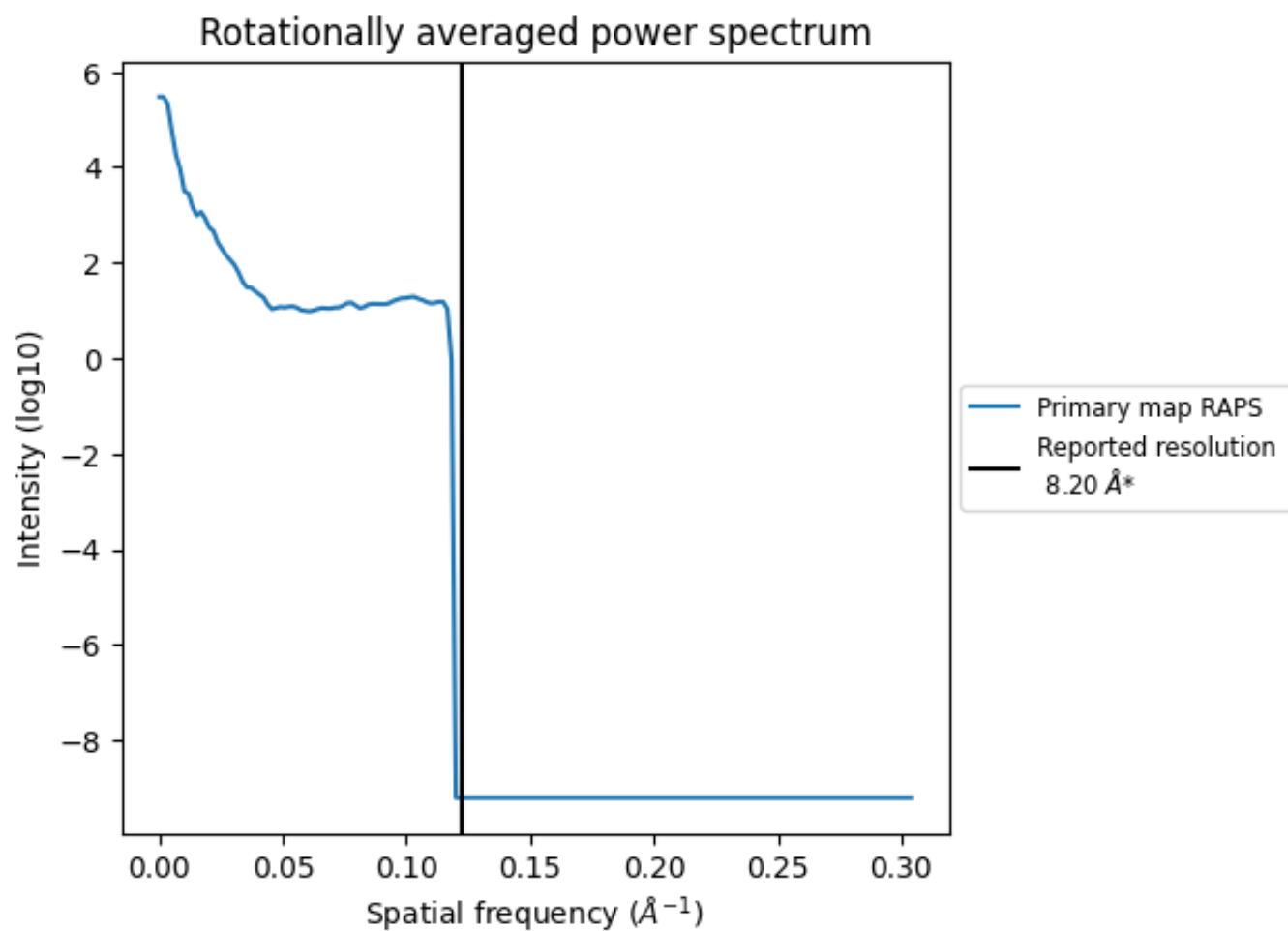
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1382 nm<sup>3</sup>; this corresponds to an approximate mass of 1248 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 ⓘ

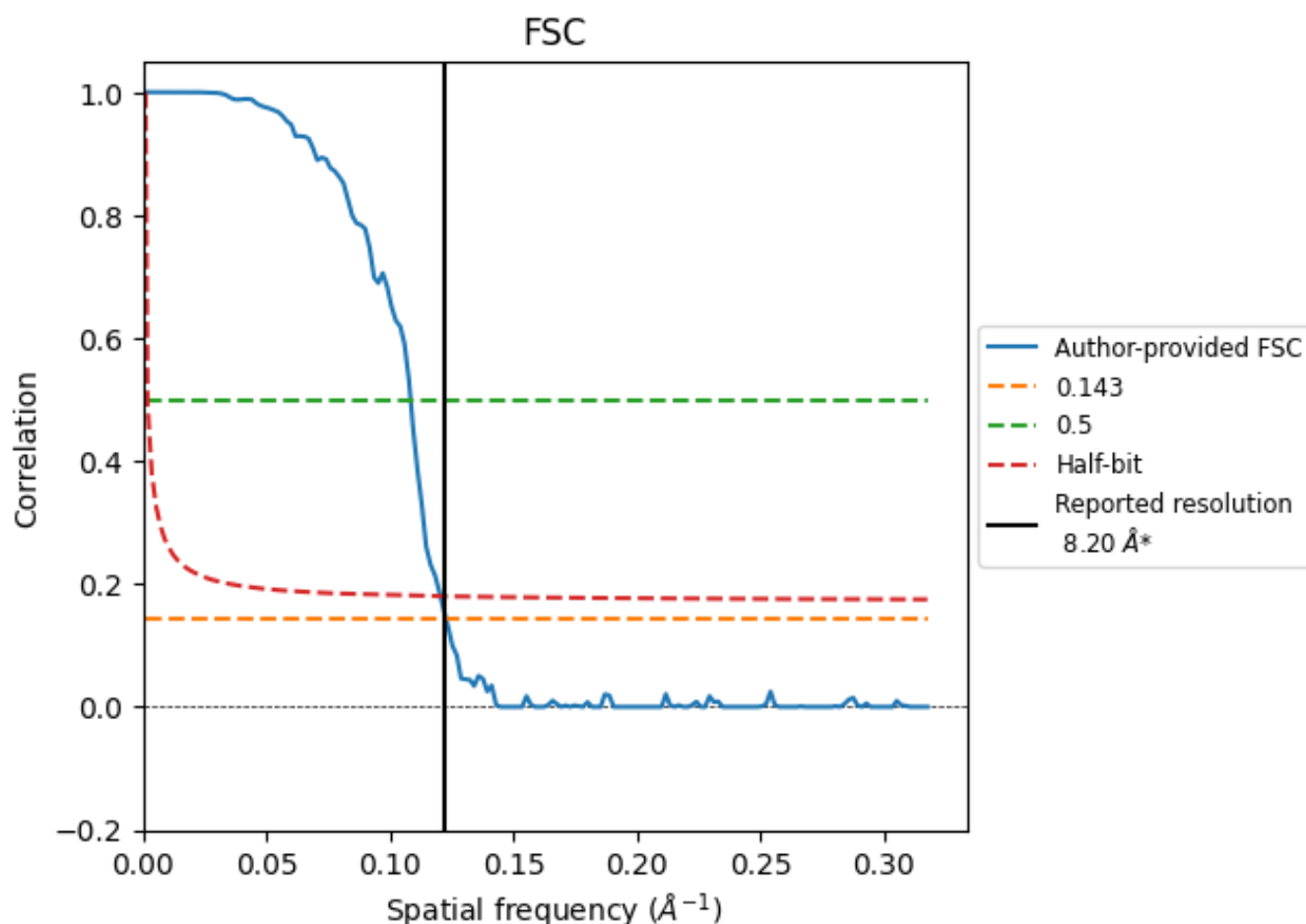


\*Reported resolution corresponds to spatial frequency of 0.122 Å<sup>-1</sup>

## 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 0.122 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

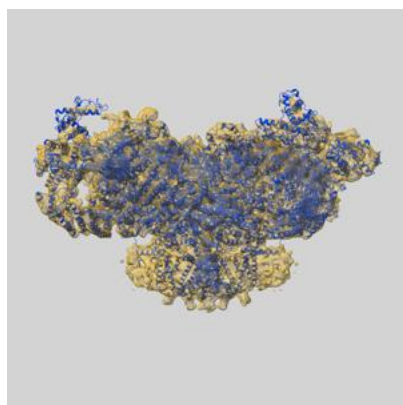
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.20	-	-
Author-provided FSC curve	8.16	9.23	8.31
Unmasked-calculated*	-	-	-

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

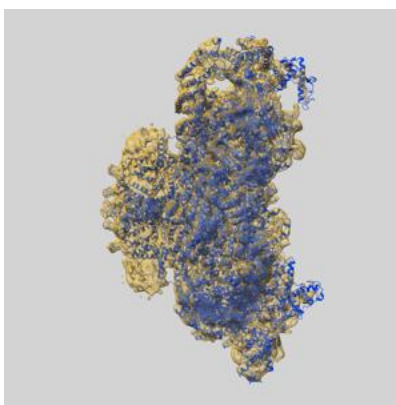
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4295 and PDB model 6FOO. Per-residue inclusion information can be found in section [3](#) on page [4](#).

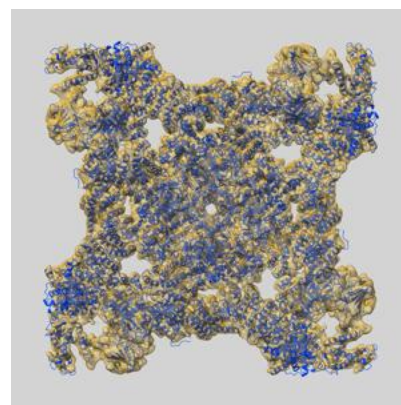
### 9.1 Map-model overlay [i](#)



X



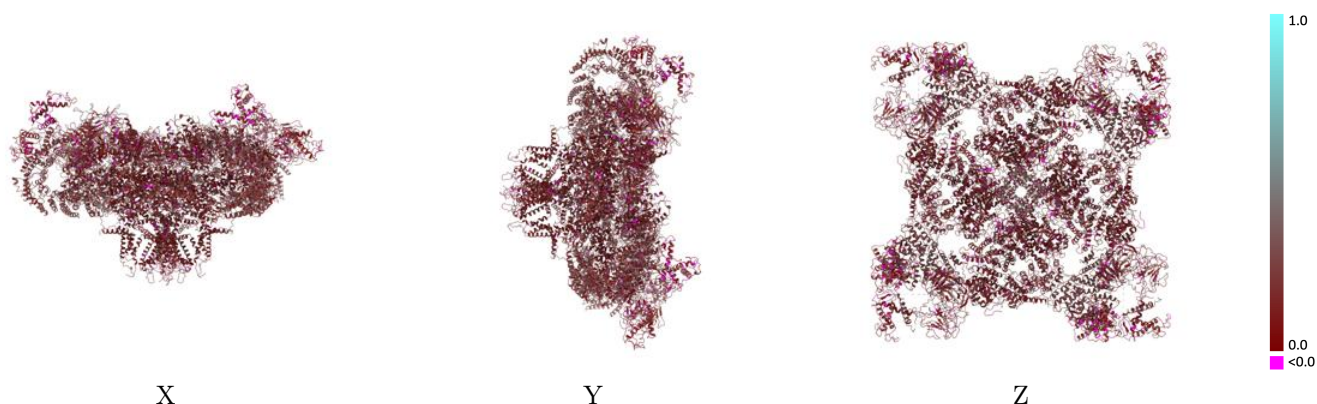
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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](#)



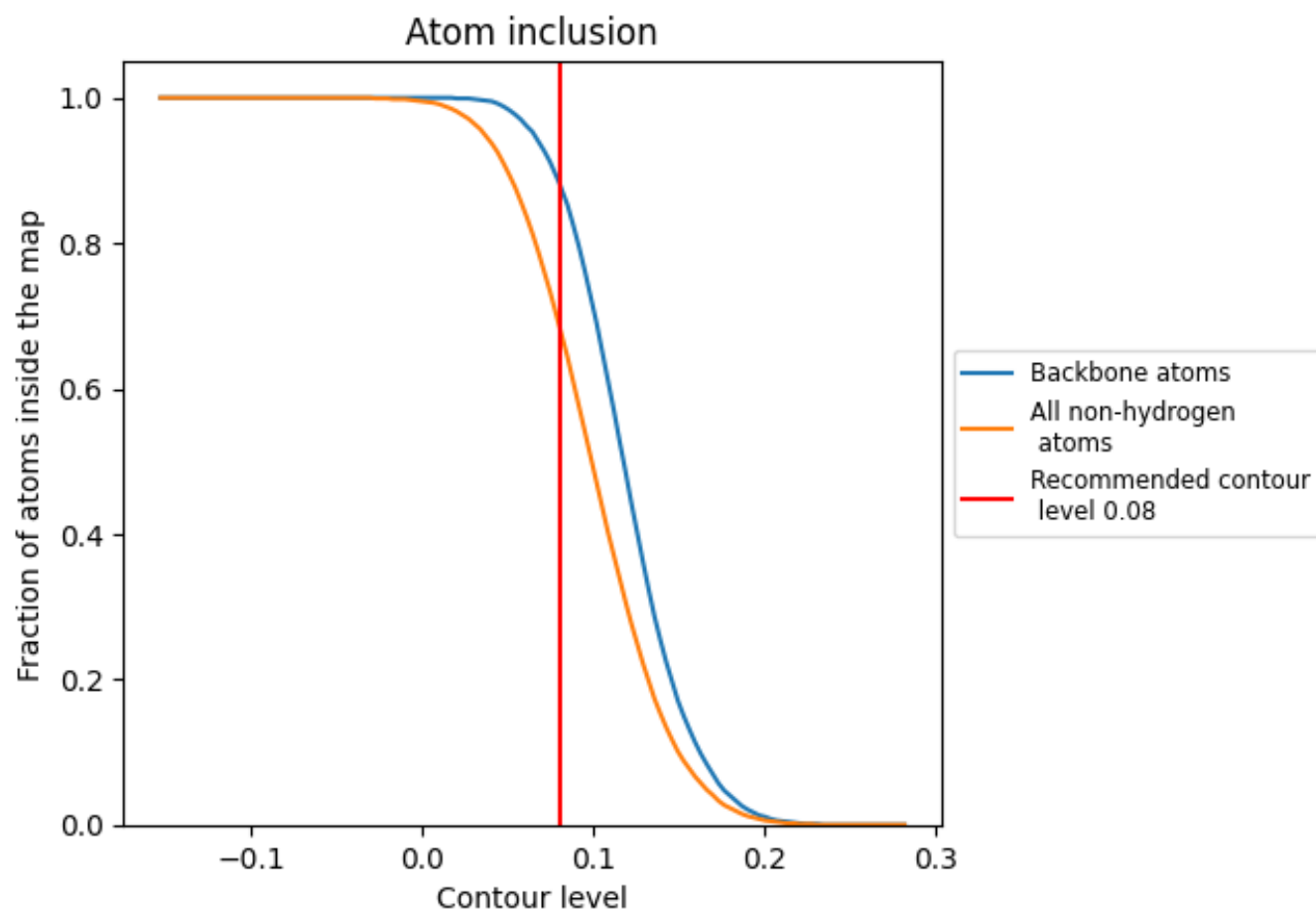
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 69% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6860	<div></div> 0.1800
A	<div></div> 0.6860	<div></div> 0.1800
B	<div></div> 0.6860	<div></div> 0.1800
C	<div></div> 0.6870	<div></div> 0.1800
D	<div></div> 0.6870	<div></div> 0.1800

