



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:17 PM UTC

PDB ID : 8ZJK / pdb_00008zjk
EMDB ID : EMD-60148
Title : Structure of DOCK5/ELMO1/Rac1 core (RhoG/DOCK5/ELMO1/Rac1 dataset, class 3)
Authors : Kukimoto-Niino, M.; Katsura, K.; Ishizuka-Katsura, Y.; Mishima-Tsumagari, C.; Yonemochi, M.; Inoue, M.; Nakagawa, R.; Kaushik, R.; Zhang, K.Y.J.; Shirouzu, M.
Deposited on : 2024-05-15
Resolution : 4.23 Å(reported)
Based on initial model : 7DPA

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

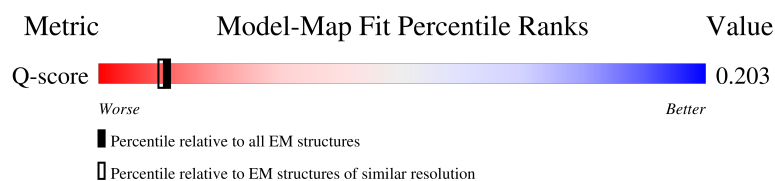
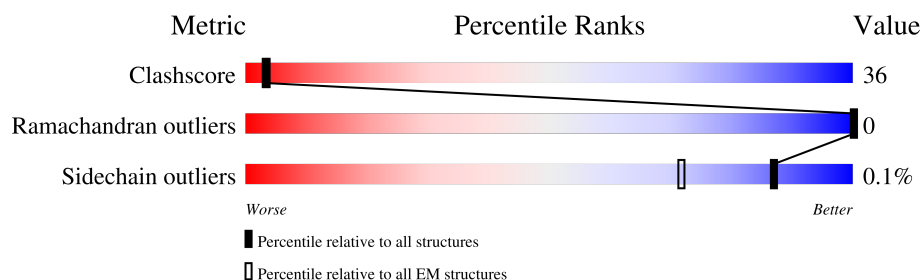
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.23 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.



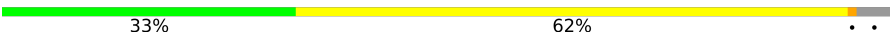
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4685 (3.74 - 4.73)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	733	 10% 17% 73%
1	D	733	 10% 17% 73%
2	B	1648	 7% 40% 60%
2	E	1648	 6% 39% 60%

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Mol	Chain	Length	Quality of chain
3	C	184	 34% 61% . .
3	F	184	 33% 62% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32858 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 Engulfment and cell motility protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	198	Total	C	N	O	S	0	0
			1608	1018	277	303	10		
1	D	198	Total	C	N	O	S	0	0
			1608	1018	277	303	10		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q92556
A	-4	GLY	-	expression tag	UNP Q92556
A	-3	SER	-	expression tag	UNP Q92556
A	-2	GLY	-	expression tag	UNP Q92556
A	-1	GLY	-	expression tag	UNP Q92556
A	0	SER	-	expression tag	UNP Q92556
D	-5	GLY	-	expression tag	UNP Q92556
D	-4	GLY	-	expression tag	UNP Q92556
D	-3	SER	-	expression tag	UNP Q92556
D	-2	GLY	-	expression tag	UNP Q92556
D	-1	GLY	-	expression tag	UNP Q92556
D	0	SER	-	expression tag	UNP Q92556

- Molecule 2 is a protein called Deducator of cytokinesis protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		
2	E	1642	Total	C	N	O	S	0	0
			13436	8618	2264	2484	70		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP Q9H7D0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP Q9H7D0
B	-3	SER	-	expression tag	UNP Q9H7D0
B	-2	GLY	-	expression tag	UNP Q9H7D0
B	-1	GLY	-	expression tag	UNP Q9H7D0
B	0	SER	-	expression tag	UNP Q9H7D0
B	1285	ARG	LYS	variant	UNP Q9H7D0
E	-5	GLY	-	expression tag	UNP Q9H7D0
E	-4	GLY	-	expression tag	UNP Q9H7D0
E	-3	SER	-	expression tag	UNP Q9H7D0
E	-2	GLY	-	expression tag	UNP Q9H7D0
E	-1	GLY	-	expression tag	UNP Q9H7D0
E	0	SER	-	expression tag	UNP Q9H7D0
E	1285	ARG	LYS	variant	UNP Q9H7D0

- Molecule 3 is a protein called Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		
3	F	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	expression tag	UNP P63000
C	-5	SER	-	expression tag	UNP P63000
C	-4	SER	-	expression tag	UNP P63000
C	-3	GLY	-	expression tag	UNP P63000
C	-2	SER	-	expression tag	UNP P63000
C	-1	SER	-	expression tag	UNP P63000
C	0	GLY	-	expression tag	UNP P63000
C	15	ALA	GLY	engineered mutation	UNP P63000
F	-6	GLY	-	expression tag	UNP P63000
F	-5	SER	-	expression tag	UNP P63000
F	-4	SER	-	expression tag	UNP P63000
F	-3	GLY	-	expression tag	UNP P63000
F	-2	SER	-	expression tag	UNP P63000
F	-1	SER	-	expression tag	UNP P63000
F	0	GLY	-	expression tag	UNP P63000
F	15	ALA	GLY	engineered mutation	UNP P63000

[illegible]

Chain B:

7%

40%

60%

GLY
GLY
SER
GLY
GLY
SER

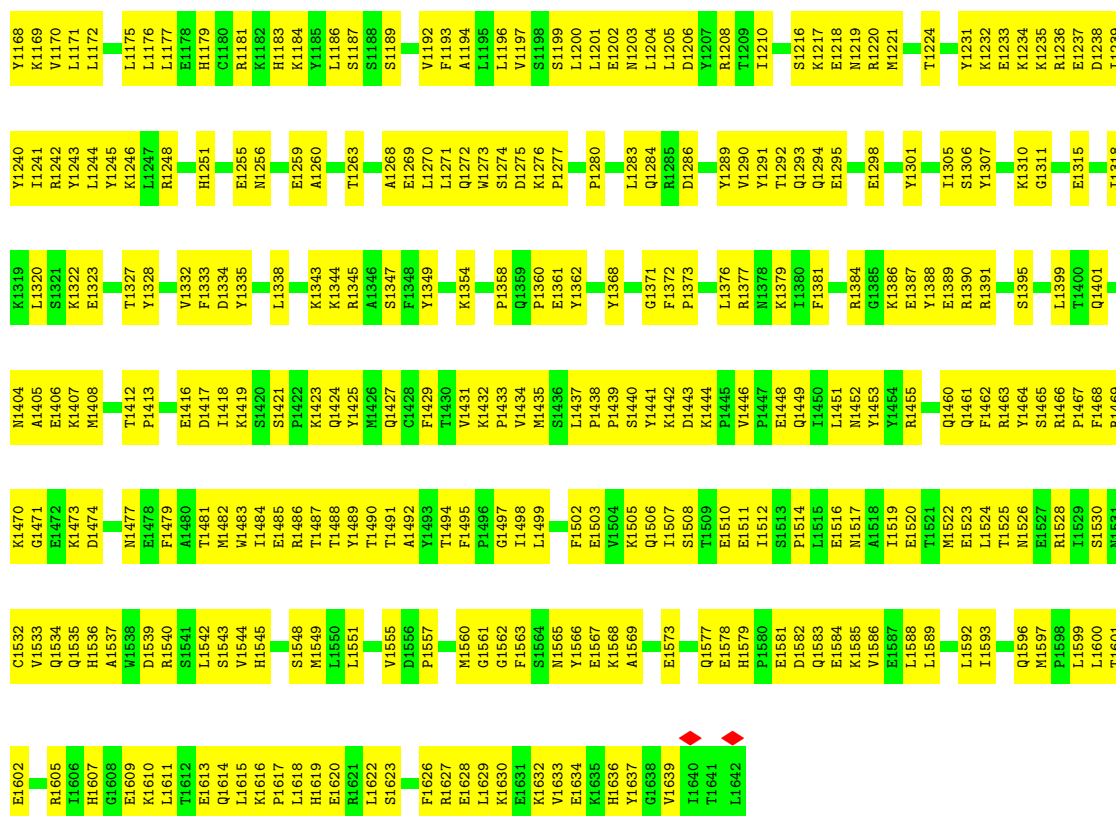
M1
A2
R3
W4
I5
F6
T7
R8
Q10
K11
Y12
V14
A15
I16
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N18
Y19

Q23
D24
V25
E26
L27
S28
L29
Q30
I31
C32
D33
T34
V35
R36
I37
L38
E39
M40
Y41
E42
G43
W44
Y45
R46
G47
Y48
T49
L50
Q51
N52
K55
K56
Q57

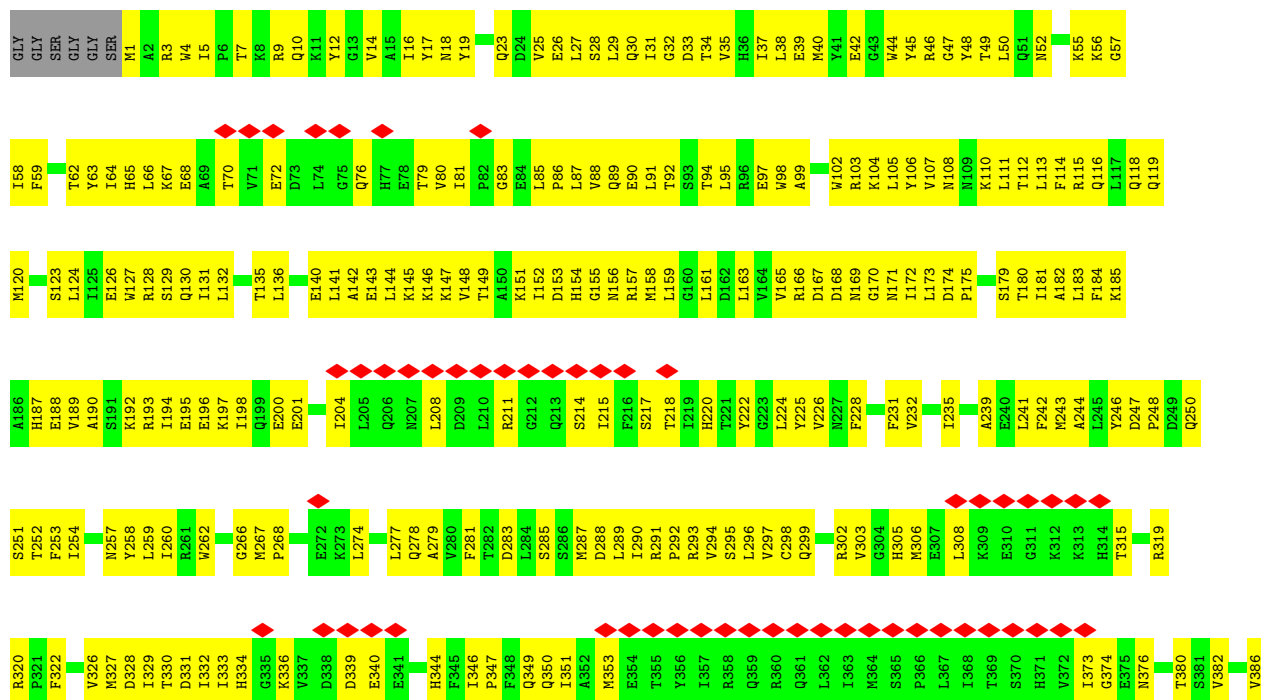
T58
F59
T62
Y63
T64
H65
L66
T67
E68
A69
T70
V71
E72
D73
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G75
H76
T77
E78
T79
W80
L81
P82
G83
E84
P86
L87
H88
G89
E90
L91
M95
T92
S93
T94
L95
R96
E97
W98
A99

M120
S123
L124
I125
A126
W127
L128
S129
Q130
I131
L132
T135
L136
E140
L141
A142
E143
L144
K145
K146
L147
V148
T149
A150
K151
I152
D153
H154
G155
M156
R157
M158
L159
G160
L161
D162
L163
V164
V165
L166
D167
D168
M169
G170
M171
I172
L173
D174
P175
S179
T180
I181
A182
L183
F184
K185

I1099	K1100	F1101	I1102	V1106	G1107	F1108	I1109	L1110	E1111	L1114	T1115	P1116	E1117	V1118	E1119	L1120	R1121	K1122	A1123	T1124	I1125	P1126	I1127	F1128	F1129	D1130	M1131	M1132	Q1133	C1134	E1135	F1136	N1137	F1138	S1139	M1143	F1144	H1145	M1149	E1150	L1151	I1152	T1153	K1154	L1155	D1156	Q1157	V1158	R1159	R1163	G1164	D1165	E1166	Q1167		
V1027	F1031	F1032	F1033	D1034	Q1035	F1038	E1039	L1040	Q1041	L1042	V1043	N1044	N1045	H1048	F1053	L1054	T1055	H1056	E1057	S1058	L1059	Q1060	L1061	E1062	T1063	F1064	S1065	Q1066	A1067	K1068	R1069	N1070	K1071	I1072	K1075	Y1076	G1077	D1078	M1079	R1080	K1081	E1082	I1083	R1086	I1087	R1088	D1089	M1090	G1095	P1096	H1097	K1098				
L886	S887	Q888	Q889	L890	D891	D892	K893	S894	K895	L896	H899	S902	S903	Q904	L905	L906	S907	N908	L909	L910	E911	L912	L913	D914	N917	L918	N919	V921	A922	V923	H924	L925	Q926	L927	N929	E930	R931	L932	L933	R934	M1010	M1011	T1012	T939	V940	I941	G942	N943	N944	L945	I1021	Q946	S947	L950	T950	V954
I958	Q962	Q963	Q964	D965	D966	S967	H968	L969	Y970	H971	Y972	L973	S974	T975	F976	R979	I982	F985	L986	M987	E988	L989	F990	L991	T1063	M992	F993	K994	D995	L996	I997	Y1002	A1003	D1004	D1005	V1008	M1009	M1010	M1011	T1012	R1015	V1016	F1017	L1018	R1019	A1020	I1021	N1022	Q1023	F1024	A1025	E1026				
L820	P821	S822	L823	L824	N825	D826	V827	K828	L829	V830	F831	D832	P833	H834	E835	L839	F840	G841	K842	F843	L844	Q845	S846	L847	Q851	L852	H853	R854	Q855	L856	L857	N858	C859	M860	T863	S866	T867	L868	F869	R870	Q871	S872	E873	C874	R875	E876	V877	L878	L879	R880	P881	L882	D883	Q885		
L8678	L8679	N880	N881	N882	N883	N884	Y8689	L8692	L8693	F8694	L8697	L700	L701	S702	L703	L704	G705	L706	L707	L708	F709	Q710	H711	F712	N713	L716	E717	L718	Y719	L720	Y721	C722	H723	T727	L728	A729	Y730	Y731	K732	K735	V736	L737	N738	F739	Y740	V741	A742	N743	A744	D745	D746	K749				
L763	F764	L765	L766	L767	S770	R771	V772	L773	Y774	L775	R776	S781	K782	D783	G784	D785	F786	F787	N788	N789	S790	L791	R792	Q793	L794	F795	L796	A797	F798	N799	M800	L801	M802	D803	P805	L806	E807	E808	A809	L812	K813	C814	A815	A816	L817	K818	Y819									
L820	P821	S822	L823	L824	N825	D826	V827	K828	L829	V830	F831	D832	P833	H834	E835	L839	F840	G841	K842	F843	L844	Q845	S846	L847	Q851	L852	H853	R854	Q855	L856	L857	N858	C859	M860	T863	S866	T867	L868	F869	R870	Q871	S872	E873	C874	R875	E876	V877	L878	L879	R880	P881	L882	D883	Q885		
L886	S887	Q888	Q889	L890	D891	D892	K893	S894	K895	L896	H899	S902	S903	Q904	L905	L906	S907	N908	L909	L910	E911	L912	L913	D914	N917	L918	N919	V921	A922	V923	H924	L925	Q926	L927	N929	E930	R931	L932	L933	R934	M1010	M1011	T1012	T939	V940	I941	G942	N943	N944	L945	I1021	Q946	S947	L950	T950	V954
I958	Q962	Q963	Q964	D965	D966	S967	H968	L969	Y970	H971	Y972	L973	S974	T975	F976	R979	I982	F985	L986	M987	E988	L989	F990	L991	T1063	M992	F993	K994	D995	L996	I997	Y1002	A1003	D1004	D1005	V1008	M1009	M1010	M1011	T1012	R1015	V1016	F1017	L1018	R1019	A1020	I1021	N1022	Q1023	F1024	A1025	E1026				
V1027	F1031	F1032	F1033	D1034	Q1035	F1038	E1039	L1040	Q1041	L1042	V1043	N1044	N1045	H1048	F1053	L1054	T1055	H1056	E1057	S1058	L1059	Q1060	L1061	E1062	T1063	F1064	S1065	Q1066	A1067	K1068	R1069	N1070	K1071	I1072	K1075	Y1076	G1077	D1078	M1079	R1080	K1081	E1082	I1083	R1086	I1087	R1088	D1089	M1090	G1095	P1096	H1097	K1098				



● Molecule 2: Dedicator of cytokinesis protein 5

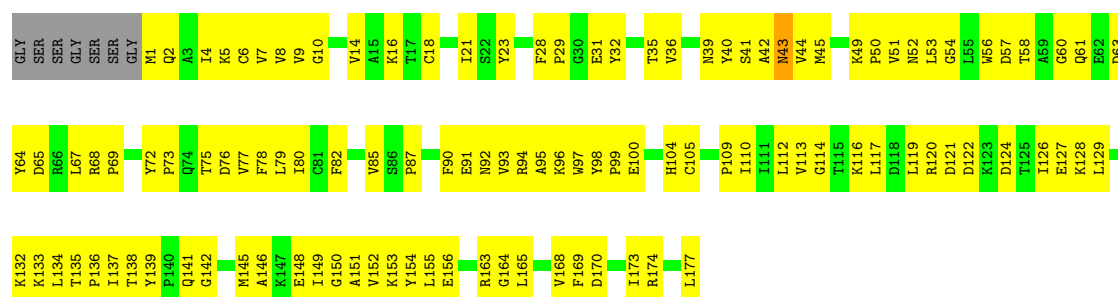


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K1232	E1233	K1234	R1235	G1163	R1236	E1237	D1238	I1239	Y1240	K1168	F1101	I1102	V1106	G1107	L1175	L1176	L1177	E1178	H1179	C1180	K1181	K1182	H1183	K1184	Y1185	L1186	S1187	S1188	S1189	V1192	F1193	L1194	L1195	L1196	V1197	S1198	S1199	L1200	L1201	E1202	N1203	L1204	L1205	D1206	R1208	Y1209	I1210	S1216	K1217	E1218	N1219	L1220	M1221	T1224	Y1231	
D1089	M1090	G1095	K1096	H1097	K1098	I1099	K1100	F1101	I1102	V1106	G1107	P1108	L1176	L1177	E1178	H1179	C1180	K1181	K1182	H1183	K1184	Y1185	L1186	S1187	S1188	S1189	V1192	F1193	L1194	L1195	L1196	V1197	S1198	S1199	L1200	L1201	E1202	N1203	L1204	L1205	D1206	R1208	Y1209	I1210	S1216	K1217	E1218	N1219	L1220	M1221	T1224	Y1231				
Q1023	F1024	A1025	E1026	V1027	I1028	T1029	R1030	N964	D965	F1031	F1032	M1033	D1034	Q1035	F1038	E1039	L1040	Q1041	L1042	M1043	N1044	M1045	H1048	V1051	A1052	F1053	L1054	T1055	H1056	E1057	P1126	L1059	Q1060	L1061	E1062	T1063	S1065	Q1066	A1067	K1068	R1069	M1070	K1071	I1072	Y1076	D1078	M1079	R1080	K1081	E1082	I1083	R1086	I1087	H1088		
D884	Q885	L886	S887	G888	Q889	L890	D891	D892	N893	S894	K896	H899	S902	Q903	Q904	L905	L906	S907	N908	I909	F943	I944	Q945	E946	E947	V918	T921	V923	H924	I925	Q926	L927	I928	N929	E930	A1003	K1004	D1005	V1008	M1009	N1010	M1011	T1012	R1015	G942	M943	F1017	L1018	R945	Q946	S947	I950				
K818	Y819	L820	P821	S822	I823	I824	R825	D826	K828	L829	V830	F831	P833	E835	L839	L905	F840	C841	K842	I843	I844	Q845	S846	I847	Q851	L852	R853	Q854	Q855	L856	L857	N858	C859	M860	I863	S866	L868	F869	Q870	R871	R872	E873	C874	R875	E876	V877	L878	L879	P880	L881	L882	T883				
K749	L753	F754	L757	L760	K761	F764	R765	F766	I767	S770	R771	V772	L773	L774	L775	R776	S781	K782	D783	G784	D785	E786	F787	N788	N789	S790	T791	R792	N793	L794	F795	L796	A797	N798	N799	M800	L801	M802	R803	P804	P805	L806	E807	F808	A809	I812	K813	G814	A815	L816	L817					
T462	P463	K464	M465	V466	E467	V468	T469	M470	S471	V472	H473	D474	G477	K478	L479	H485	A488	G489	Y490	T493	Y496	S498	V499	V500	Q503	C508	M509	Y510	K514	V515	S516	I517	A518	I519	E520	E521	V522	T523	R524	C525	H526	G529	I527	R528	F529	T530	F531	R532	H533	R534	S535					
S536	Q537	E538	T539	R540	D541	K542	S543	E544	F547	G548	V549	A550	F551	V552	K553	L554	M555	N556	P557	D558	G559	T560	T561	L562	L569	V570	V571	Y572	K573	G574	D575	N576	K577	K578	H579	E580	D581	F584	T585	L586	T587	L588	P589	Q590	K591	K592	M593	E594	M595	E596	E597	K598	E599	L600	Q601	A602
S603	K604	N605	L606	V607	T608	F609	T610	P611	S612	K613	D614	K617	F620	Q621	L622	A623	T624	L625	I626	G627	S628	G629	K630	L631	Q633	V634	L637	L638	G639	L640	L641	N642	Q643	R644	S645	N646	S647	Q648	N649	L650	H651	H652	N653	L654	K655	K656	E659	V660	D661	T665	F668	L669				
Q670	N678	I679	M680	M681	E682	M683	Y689	L692	V693	F694	L697	I700	I701	S702	L703	I704	G705	D706	I707	K708	F709	G784	H711	F712	N713	L716	E717	T718	I719	I720	N721	K722	H723	T727	L728	A729	Y730	K731	K732	K735	V736	L737	N738	F739	G740	L741	A742	N743	A744	D745	D746					
K749	L753	F754	L757	L760	K761	F764	R765	F766	I767	S770	R771	V772	L773	L774	L775	R776	S781	K782	D783	G784	D785	E786	F787	N788	N789	S790	T791	R792	N793	L794	F795	L796	A797	N798	N799	M800	L801	M802	R803	P804	P805	L806	E807	F808	A809	I812	K813	G814	A815	L816	L817					
Y819	L820	P821	S822	I823	I824	R825	D826	K828	L829	V830	F831	P833	E835	L839	L905	F840	C841	K842	I843	I844	Q845	S846	I847	Q851	L852	R853	Q854	Q855	L856	L857	N858	C859	M860	I863	S866	L868	F869	Q870	R871	R872	E873	C874	R875	E876	V877	L878	L879	P880	L881	L882	T883					
D884	Q885	L886	S887	G888	Q889	L890	D891	D892	N893	S894	K896	H899	S902	Q903	Q904	L905	L906	S907	N908	I909	F943	I944	Q945	E946	E947	V918	T921	V923	H924	I925	Q926	L927	I928	N929	E930	A1003	K1004	D1005	V1008	M1009	N1010	M1011	T1012	R1015	G942	M943	F1017	L1018	R945	Q946	S947	I950				
V954	I958	Q962	Q963	N964	D965	F1031	F1032	M1033	D1034	Q1035	F1038	E1039	L1040	Q1041	S974	T975	F976	R979	I982	F985	L986	N987	E988	T989	F990	I991	M992	F993	L1127	L1059	Q1060	L1061	E1062	T1063	S1065	Q1066	A1067	K1068	R1069	M1070	K1071	I1072	Y1076	D1078	M1079	R1080	K1081	E1082	I1083	R1086	I1087	H1088				
Q1023	F1024	A1025	E1026	V1027	I1028	T1029	R1030	N964	D965	F1031	F1032	M1033	D1034	Q1035	F1038	E1039	L1040	Q1041	L1042	M1043	N1044	M1045	H1048	V1051	A1052	F1053	L1054	T1055	H1056	E1057	P1126	L1059	Q1060	L1061	E1062	T1063	S1065	Q1066	A1067	K1068	R1069	M1070	K1071	I1072	Y1076	D1078	M1079	R1080	K1081	E1082	I1083	R1086	I1087	H1088		
D1089	M1090	G1095	K1096	H1097	K1098	I1099	K1100	F1101	I1102	V1106	G1107	P1108	L1176	L1177	E1178	H1179	C1180	K1181	K1182	H1183	K1184	Y1185	L1186	S1187	S1188	S1189	V1192	F1193	L1194	L1195	L1196	V1197	S1198	S1199	L1200	L1201	E1202	N1203	L1204	L1205	D1206	R1208	Y1209	I1210	S1216	K1217	E1218	N1219	L1220	M1221	T1224	Y1231				
E1158	V1159	R1163	G1164	D1165	E1166	Q1167	L1168	K1169	F1170	L1171	L1172	L1175	L1176	L1177	E1178	H1179	C1180	K1181	K1182	H1183	K1184	Y1185	L1186	S1187	S1188	S1189	V1192	F1193	L1194	L1195	L1196	V1197	S1198	S1199	L1200	L1201	E1202	N1203	L1204	L1205	D1206	R1208	Y1209	I1210	S1216	K1217	E1218	N1219	L1220	M1221	T1224	Y1231				
K1232	E1233	K1234	R1235	G1163	R1236	E1237	D1238	I1239	Y1240	K1168	F1101	I1102	V1106	G1107	L1175	L1176	L1177	E1178	H1179	C1180	K1181	K1182	H1183	K1184	Y1185	L1186	S1187	S1188	S1189	V1192	F1193	L1194	L1195	L1196	V1197	S1198	S1199	L1200	L1201	E1202	N1203	L1204	L1205	D1206	R1208	Y1209	I1210	S1216	K1217	E1218	N1219	L1220	M1221	T1224	Y1231	
I1305	S1306	Y1307	K1310	E1311	E1315	I1318	K1319	F1401	F1402	P1403	M1404	A1405	K1322	E1323	Y1327	V1332	F1333	D1334	Y1335	L1338	K1344	R1345	A1346	S1347	F1348	Y1349	I1353	P1358	Q1359	P1360	E1361	Y1362	Y1368	G1371	F1372	P1373	L1376	R1377	K1378	K1379	F1381	I1450	M1451	N1452	Y1453	R1454	Y1455		E1389							



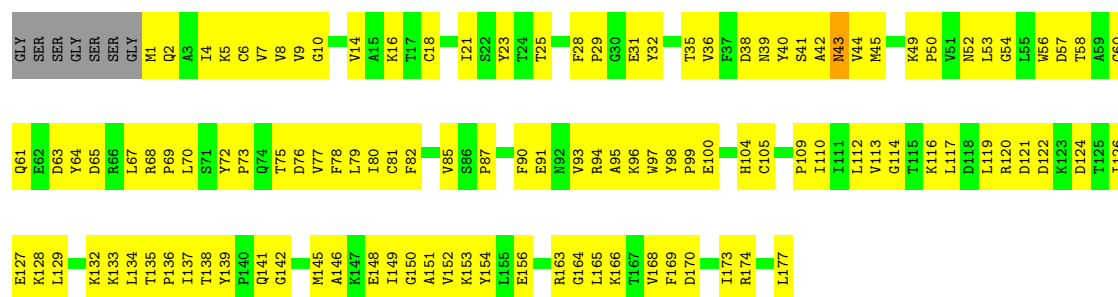
• Molecule 3: Ras-related C3 botulinum toxin substrate 1

Chain C: 34% 61%



• Molecule 3: Ras-related C3 botulinum toxin substrate 1

Chain F: 33% 62%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	120707	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	452.2, 452.2, 452.2	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/1641	0.48	0/2218
1	D	0.23	0/1641	0.48	0/2218
2	B	0.32	1/13722 (0.0%)	0.51	4/18514 (0.0%)
2	E	0.32	1/13722 (0.0%)	0.51	4/18514 (0.0%)
3	C	0.26	0/1415	0.46	0/1924
3	F	0.26	0/1415	0.46	0/1924
All	All	0.31	2/33556 (0.0%)	0.51	8/45312 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	463	PRO	CG-CD	-13.93	1.03	1.50
2	B	463	PRO	CG-CD	-13.90	1.03	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	463	PRO	N-CD-CG	-17.32	77.21	103.20
2	E	463	PRO	N-CD-CG	-17.30	77.25	103.20
2	B	463	PRO	CA-CB-CG	-11.88	81.93	104.50
2	E	463	PRO	CA-CB-CG	-11.87	81.96	104.50
2	B	463	PRO	CB-CG-CD	8.19	132.31	106.10
2	E	463	PRO	CB-CG-CD	8.18	132.28	106.10
2	B	463	PRO	CA-N-CD	-8.07	100.70	112.00
2	E	463	PRO	CA-N-CD	-8.05	100.73	112.00

There are no chirality outliers.

There are no planarity outliers.

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	1608	0	1617	142	0
1	D	1608	0	1617	145	0
2	B	13436	0	13516	954	0
2	E	13436	0	13516	986	0
3	C	1385	0	1407	109	0
3	F	1385	0	1407	120	0
All	All	32858	0	33080	2379	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 36.

All (2379) 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:D:697:ARG:HH21	2:E:30:GLN:HB2	1.33	0.91
1:D:670:ASN:ND2	1:D:676:ASP:O	2.06	0.88
2:E:1579:HIS:HB3	2:E:1582:ASP:HB2	1.56	0.88
1:A:670:ASN:ND2	1:A:676:ASP:O	2.06	0.87
1:A:697:ARG:HH21	2:B:30:GLN:HB2	1.42	0.85
2:B:1579:HIS:HB3	2:B:1582:ASP:HB2	1.56	0.85
2:B:904:GLN:O	2:B:908:ASN:ND2	2.10	0.84
2:E:144:LEU:HD13	2:E:147:LYS:HE2	1.60	0.84
2:E:241:LEU:HB2	2:E:260:ILE:HB	1.59	0.84
2:B:144:LEU:HD13	2:B:147:LYS:HE2	1.60	0.83
2:E:904:GLN:O	2:E:908:ASN:ND2	2.10	0.83
2:E:1393:ASP:OD1	3:F:166:LYS:NZ	2.11	0.83
2:E:115:ARG:HA	2:E:118:GLN:HG3	1.62	0.82
2:B:589:PRO:HB3	2:B:594:GLU:HB3	1.62	0.82
2:E:589:PRO:HB3	2:E:594:GLU:HB3	1.62	0.82
2:B:241:LEU:HB2	2:B:260:ILE:HB	1.59	0.81
2:B:115:ARG:HA	2:B:118:GLN:HG3	1.61	0.81
2:B:530:THR:HA	2:B:549:VAL:HG22	1.63	0.80
2:E:1372:PHE:O	2:E:1377:ARG:NH2	2.15	0.80
2:B:1372:PHE:O	2:B:1377:ARG:NH2	2.15	0.79
2:B:104:LYS:O	2:B:108:ASN:ND2	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:104:LYS:O	2:E:108:ASN:ND2	2.16	0.79
2:E:530:THR:HA	2:E:549:VAL:HG22	1.63	0.79
2:E:1536:HIS:O	2:E:1540:ARG:NH2	2.16	0.79
2:B:890:LEU:HD22	2:B:935:ARG:HG3	1.65	0.79
3:C:87:PRO:HD2	3:C:134:LEU:HD13	1.65	0.79
2:E:890:LEU:HD22	2:E:935:ARG:HG3	1.65	0.78
2:B:1536:HIS:O	2:B:1540:ARG:NH2	2.16	0.78
2:E:556:ASN:N	2:E:560:THR:O	2.15	0.78
2:B:556:ASN:N	2:B:560:THR:O	2.15	0.78
2:B:153:ASP:HA	2:B:156:ASN:HD22	1.49	0.77
2:E:1543:SER:OG	2:E:1545:HIS:ND1	2.17	0.77
3:F:87:PRO:HD2	3:F:134:LEU:HD13	1.65	0.77
3:F:93:VAL:HA	3:F:97:TRP:HB2	1.66	0.77
2:B:589:PRO:HB2	2:B:595:MET:HE2	1.66	0.77
2:B:1390:ARG:NH2	3:C:23:TYR:O	2.18	0.77
2:B:278:GLN:HB2	2:B:425:THR:HG23	1.66	0.77
1:A:563:ARG:HB3	1:A:573:LYS:HE3	1.66	0.77
2:B:879:LEU:HD23	2:B:931:ARG:HH22	1.50	0.77
2:E:4:TRP:HB3	2:E:39:GLU:HB3	1.68	0.76
1:D:563:ARG:HB3	1:D:573:LYS:HE3	1.66	0.76
2:B:749:LYS:HG2	2:B:753:LEU:HD23	1.67	0.76
2:B:902:SER:HA	2:B:905:LEU:HD12	1.66	0.76
2:E:351:ILE:HG12	2:E:382:VAL:HG21	1.66	0.76
2:E:278:GLN:HB2	2:E:425:THR:HG23	1.66	0.76
2:E:749:LYS:HG2	2:E:753:LEU:HD23	1.67	0.76
3:C:93:VAL:HA	3:C:97:TRP:HB2	1.67	0.76
2:E:589:PRO:HB2	2:E:595:MET:HE2	1.66	0.76
2:E:153:ASP:HA	2:E:156:ASN:HD22	1.49	0.75
2:E:1165:ASP:OD2	2:E:1168:TYR:N	2.20	0.75
2:B:4:TRP:HB3	2:B:39:GLU:HB3	1.68	0.75
2:E:879:LEU:HD23	2:E:931:ARG:HH22	1.50	0.75
2:E:46:ARG:HB3	2:E:58:ILE:HG13	1.69	0.75
2:B:351:ILE:HG12	2:B:382:VAL:HG21	1.66	0.75
2:B:740:TYR:HA	2:B:749:LYS:HD3	1.69	0.75
1:D:701:LEU:HD23	2:E:31:ILE:HG23	1.69	0.75
2:E:740:TYR:HA	2:E:749:LYS:HD3	1.69	0.75
1:A:589:GLY:HA3	1:A:604:LEU:HB2	1.69	0.75
2:B:1328:TYR:HA	2:B:1332:VAL:HG12	1.69	0.75
2:E:902:SER:HA	2:E:905:LEU:HD12	1.66	0.74
2:B:166:ARG:NH1	2:B:167:ASP:OD1	2.20	0.74
2:B:1117:GLU:OE1	2:B:1119:GLU:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1465:SER:HA	2:E:1486:ARG:HG2	1.69	0.74
2:E:166:ARG:NH1	2:E:167:ASP:OD1	2.20	0.74
1:A:576:TYR:HB2	1:A:598:GLU:HG2	1.69	0.74
2:B:964:MET:O	2:B:1019:ARG:NH2	2.20	0.74
2:B:242:PHE:HB2	2:B:299:GLN:HB2	1.69	0.74
2:B:1165:ASP:OD2	2:B:1168:TYR:N	2.20	0.73
2:E:1117:GLU:OE1	2:E:1119:GLU:N	2.20	0.73
2:B:23:GLN:HG2	2:B:58:ILE:HB	1.70	0.73
2:B:851:GLN:O	2:B:856:LYS:NZ	2.21	0.73
2:E:964:MET:O	2:E:1019:ARG:NH2	2.20	0.73
1:A:530:SER:HA	1:A:533:ILE:HD12	1.69	0.73
2:B:46:ARG:HB3	2:B:58:ILE:HG13	1.69	0.73
1:D:625:MET:HE1	1:D:638:LEU:HA	1.71	0.73
2:E:242:PHE:HB2	2:E:299:GLN:HB2	1.69	0.73
2:B:244:ALA:HB2	2:B:257:ASN:HA	1.69	0.73
2:B:828:LYS:HE2	2:B:833:PRO:HG3	1.70	0.73
1:D:530:SER:HA	1:D:533:ILE:HD12	1.69	0.73
3:F:7:VAL:HG23	3:F:75:THR:HG21	1.70	0.73
2:B:1543:SER:OG	2:B:1545:HIS:ND1	2.17	0.73
2:E:244:ALA:HB2	2:E:257:ASN:HA	1.69	0.73
2:E:1328:TYR:HA	2:E:1332:VAL:HG12	1.69	0.73
2:B:1466:ARG:NH1	2:B:1467:PRO:O	2.22	0.73
1:D:589:GLY:HA3	1:D:604:LEU:HB2	1.69	0.73
2:E:1277:PRO:HG3	2:E:1292:THR:HA	1.70	0.73
2:B:12:TYR:HB2	2:B:67:LYS:HB2	1.70	0.73
2:B:941:ILE:O	2:B:944:ASN:ND2	2.20	0.73
2:B:1277:PRO:HG3	2:B:1292:THR:HA	1.70	0.73
2:E:1466:ARG:NH1	2:E:1467:PRO:O	2.21	0.73
2:B:1465:SER:HA	2:B:1486:ARG:HG2	1.70	0.73
2:E:851:GLN:O	2:E:856:LYS:NZ	2.21	0.73
2:E:828:LYS:HE2	2:E:833:PRO:HG3	1.70	0.73
2:E:1562:GLY:HA3	3:F:36:VAL:HB	1.70	0.73
2:E:1245:TYR:HD2	2:E:1248:ARG:HH21	1.37	0.72
1:A:625:MET:HE1	1:A:638:LEU:HA	1.71	0.72
2:B:444:ASN:ND2	2:B:517:ILE:O	2.22	0.72
2:B:1034:ASP:OD1	2:B:1097:HIS:NE2	2.21	0.72
1:D:576:TYR:HB2	1:D:598:GLU:HG2	1.69	0.72
2:E:23:GLN:HG2	2:E:58:ILE:HB	1.70	0.72
3:F:61:GLN:O	3:F:68:ARG:NH2	2.22	0.72
2:E:893:ASN:O	2:E:896:LYS:NZ	2.22	0.72
2:E:1549:MET:SD	3:F:54:GLY:HA3	2.30	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:LEU:HD23	2:B:98:TRP:HD1	1.55	0.72
2:E:441:ASP:O	2:E:629:THR:OG1	2.07	0.72
2:E:444:ASN:ND2	2:E:517:ILE:O	2.23	0.72
3:C:7:VAL:HG23	3:C:75:THR:HG21	1.70	0.72
2:E:1292:THR:HG23	2:E:1295:GLU:H	1.54	0.72
2:B:1462:PHE:O	2:B:1489:TYR:N	2.23	0.72
2:B:1292:THR:HG23	2:B:1295:GLU:H	1.54	0.72
1:D:717:PRO:HD2	2:E:1:MET:HE2	1.71	0.72
2:E:941:ILE:O	2:E:944:ASN:ND2	2.20	0.72
2:B:1245:TYR:HD2	2:B:1248:ARG:HH21	1.37	0.71
3:C:61:GLN:O	3:C:68:ARG:NH2	2.22	0.71
1:D:637:VAL:HG12	1:D:640:LEU:HD12	1.72	0.71
1:A:637:VAL:HG12	1:A:640:LEU:HD12	1.72	0.71
2:E:12:TYR:HB2	2:E:67:LYS:HB2	1.70	0.71
3:F:23:TYR:HB2	3:F:165:LEU:HD21	1.70	0.71
2:B:441:ASP:O	2:B:629:THR:OG1	2.07	0.71
2:B:893:ASN:O	2:B:896:LYS:NZ	2.23	0.71
2:B:1216:SER:OG	2:B:1401:GLN:NE2	2.24	0.71
1:A:550:GLN:HE22	2:B:107:VAL:HG12	1.56	0.71
3:C:23:TYR:HB2	3:C:165:LEU:HD21	1.70	0.71
2:E:1462:PHE:O	2:E:1489:TYR:N	2.23	0.71
2:E:1034:ASP:OD1	2:E:1097:HIS:NE2	2.21	0.71
2:B:970:SER:O	2:B:974:SER:OG	2.09	0.70
1:D:550:GLN:HE22	2:E:107:VAL:HG12	1.55	0.70
2:E:472:VAL:HG22	2:E:527:ILE:HG12	1.73	0.70
2:B:1015:ARG:HH21	2:B:1076:TYR:HE1	1.38	0.70
1:D:561:CYS:SG	1:D:594:SER:OG	2.49	0.70
2:E:95:LEU:HD23	2:E:98:TRP:HD1	1.55	0.70
2:B:1143:ASN:OD1	2:B:1145:HIS:ND1	2.25	0.70
1:A:561:CYS:SG	1:A:594:SER:OG	2.49	0.70
2:B:1078:ASP:OD1	2:B:1081:LYS:N	2.25	0.70
2:E:1057:GLU:HA	2:E:1061:LEU:HD23	1.74	0.70
2:E:1062:GLU:OE2	2:E:1080:ARG:NH1	2.25	0.70
2:E:1272:GLN:OE1	2:E:1293:GLN:NE2	2.25	0.69
2:B:1272:GLN:OE1	2:B:1293:GLN:NE2	2.25	0.69
2:B:472:VAL:HG22	2:B:527:ILE:HG12	1.73	0.69
2:B:1259:GLU:OE1	2:B:1259:GLU:N	2.23	0.69
2:E:1216:SER:OG	2:E:1401:GLN:NE2	2.24	0.69
2:E:1432:LYS:HZ1	2:E:1464:TYR:HA	1.58	0.69
2:B:1432:LYS:HZ1	2:B:1464:TYR:HA	1.57	0.69
3:C:98:TYR:HE1	3:C:149:ILE:HD13	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1143:ASN:OD1	2:E:1145:HIS:ND1	2.25	0.69
3:F:116:LYS:HB3	3:F:119:LEU:HB2	1.74	0.69
2:B:518:ALA:HB3	2:B:521:GLU:HB2	1.74	0.69
2:B:1067:ALA:O	2:B:1071:LYS:N	2.17	0.69
3:C:116:LYS:HB3	3:C:119:LEU:HB2	1.74	0.69
2:E:883:THR:HG21	2:E:931:ARG:HB3	1.75	0.69
2:B:1062:GLU:OE2	2:B:1080:ARG:NH1	2.25	0.69
2:E:49:THR:OG1	2:E:52:ASN:OD1	2.11	0.69
2:E:1276:LYS:NZ	2:E:1277:PRO:O	2.26	0.69
2:B:819:TYR:O	2:B:822:SER:OG	2.10	0.69
2:E:879:LEU:HD12	2:E:882:LEU:HB2	1.74	0.69
2:E:939:THR:O	2:E:943:MET:N	2.17	0.69
2:E:970:SER:O	2:E:974:SER:OG	2.09	0.69
2:E:1335:TYR:HA	2:E:1338:LEU:HD23	1.75	0.69
1:A:724:TYR:HB3	2:B:4:TRP:HB2	1.74	0.69
2:E:1015:ARG:HH21	2:E:1076:TYR:HE1	1.38	0.69
2:E:1391:ARG:NH2	3:F:29:PRO:HD3	2.08	0.69
2:B:1057:GLU:HA	2:B:1061:LEU:HD23	1.74	0.69
2:B:1284:GLN:HE21	2:B:1286:ASP:HB2	1.58	0.69
1:A:607:LYS:NZ	1:A:608:LEU:O	2.26	0.68
2:B:49:THR:OG1	2:B:52:ASN:OD1	2.11	0.68
2:B:1149:ASN:HA	2:B:1236:ARG:HH12	1.58	0.68
1:D:551:GLN:HA	1:D:554:ASN:HD22	1.58	0.68
1:D:700:ASP:HB2	2:E:32:GLY:HA2	1.75	0.68
2:E:518:ALA:HB3	2:E:521:GLU:HB2	1.74	0.68
2:B:879:LEU:HD12	2:B:882:LEU:HB2	1.74	0.68
1:D:580:SER:HB2	1:D:585:VAL:HG22	1.76	0.68
2:B:473:HIS:ND1	2:B:477:GLY:O	2.26	0.68
2:E:1:MET:HE1	2:E:44:TRP:CD1	2.28	0.68
2:E:1018:LEU:HD21	2:E:1083:ILE:HG12	1.74	0.68
2:B:154:HIS:HE1	2:B:201:GLU:OE2	1.76	0.68
2:B:226:VAL:HB	2:B:279:ALA:HB3	1.76	0.68
2:E:473:HIS:ND1	2:E:477:GLY:O	2.26	0.68
2:E:1284:GLN:HE21	2:E:1286:ASP:HB2	1.58	0.68
3:F:98:TYR:HE1	3:F:149:ILE:HD13	1.57	0.68
2:B:834:VAL:HB	2:B:873:GLU:HG2	1.74	0.68
2:B:883:THR:HG21	2:B:931:ARG:HB3	1.75	0.68
2:E:154:HIS:HE1	2:E:201:GLU:OE2	1.76	0.68
2:E:226:VAL:HB	2:E:279:ALA:HB3	1.75	0.68
2:B:1241:ILE:HA	2:B:1244:LEU:HD12	1.75	0.68
2:E:7:THR:HG22	2:E:9:ARG:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:607:LYS:NZ	1:D:608:LEU:O	2.26	0.68
2:B:469:THR:O	2:B:530:THR:OG1	2.12	0.68
2:B:1018:LEU:HD21	2:B:1083:ILE:HG12	1.74	0.68
2:B:1276:LYS:NZ	2:B:1277:PRO:O	2.26	0.68
2:B:1:MET:HE1	2:B:44:TRP:CD1	2.29	0.68
2:B:70:THR:HG23	2:B:72:GLU:H	1.58	0.68
2:E:1552:SER:HB3	3:F:39:ASN:HD22	1.59	0.68
2:E:1615:LEU:O	2:E:1619:HIS:N	2.24	0.68
2:E:7:THR:O	2:E:10:GLN:NE2	2.20	0.67
2:E:38:LEU:H	2:E:47:GLY:HA3	1.58	0.67
2:E:70:THR:HG23	2:E:72:GLU:H	1.58	0.67
2:B:7:THR:HG22	2:B:9:ARG:H	1.59	0.67
2:B:562:LEU:O	2:B:633:GLN:NE2	2.27	0.67
2:B:1120:LEU:O	2:B:1124:THR:OG1	2.06	0.67
2:E:445:ASP:HB2	2:E:627:CYS:HB2	1.76	0.67
2:B:1335:TYR:HA	2:B:1338:LEU:HD23	1.75	0.67
1:A:551:GLN:HA	1:A:554:ASN:HD22	1.58	0.67
2:E:1078:ASP:OD1	2:E:1081:LYS:N	2.25	0.67
2:E:1241:ILE:HA	2:E:1244:LEU:HD12	1.75	0.67
1:D:596:GLN:NE2	1:D:597:GLY:O	2.28	0.67
2:E:1032:PHE:HB3	2:E:1043:TRP:HH2	1.59	0.67
2:E:1120:LEU:O	2:E:1124:THR:OG1	2.06	0.67
2:B:38:LEU:H	2:B:47:GLY:HA3	1.58	0.67
2:E:1390:ARG:NH2	3:F:23:TYR:O	2.26	0.67
2:B:1630:LYS:O	2:B:1634:GLU:HG2	1.95	0.67
1:A:580:SER:HB2	1:A:585:VAL:HG22	1.76	0.67
2:B:283:ASP:HB2	2:B:430:LYS:HB3	1.77	0.67
2:B:1043:TRP:H	2:B:1043:TRP:HE3	1.42	0.67
2:E:283:ASP:HB2	2:E:430:LYS:HB3	1.77	0.67
2:E:834:VAL:HB	2:E:873:GLU:HG2	1.74	0.67
2:B:445:ASP:HB2	2:B:627:CYS:HB2	1.76	0.66
3:C:1:MET:HE3	3:C:2:GLN:H	1.60	0.66
3:C:45:MET:HA	3:C:50:PRO:HA	1.77	0.66
2:E:1043:TRP:H	2:E:1043:TRP:HE3	1.42	0.66
2:E:1149:ASN:HA	2:E:1236:ARG:HH12	1.58	0.66
2:E:1630:LYS:O	2:E:1634:GLU:HG2	1.95	0.66
1:A:550:GLN:O	1:A:554:ASN:ND2	2.28	0.66
1:A:596:GLN:NE2	1:A:597:GLY:O	2.28	0.66
2:B:939:THR:O	2:B:943:MET:N	2.17	0.66
2:E:449:THR:HB	2:E:623:ALA:HB3	1.78	0.66
2:B:1516:GLU:HA	2:B:1519:ILE:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:170:ASP:HB3	3:C:174:ARG:HH21	1.61	0.66
2:E:562:LEU:O	2:E:633:GLN:NE2	2.27	0.66
2:E:1628:GLU:O	2:E:1632:LYS:HG2	1.95	0.66
3:F:170:ASP:HB3	3:F:174:ARG:HH21	1.61	0.66
1:A:535:GLU:O	1:A:539:LYS:HB3	1.96	0.66
2:E:1516:GLU:HA	2:E:1519:ILE:HD12	1.77	0.66
2:B:87:LEU:HD23	2:B:91:LEU:HD23	1.78	0.66
2:B:1111:GLU:OE1	2:B:1111:GLU:N	2.27	0.66
2:B:1218:GLU:OE1	2:B:1218:GLU:N	2.26	0.66
2:B:1536:HIS:HA	2:B:1542:LEU:HD13	1.78	0.66
2:B:1615:LEU:O	2:B:1619:HIS:N	2.24	0.66
2:B:1628:GLU:O	2:B:1632:LYS:HG2	1.95	0.66
3:C:120:ARG:HH12	3:C:139:TYR:HB2	1.61	0.66
1:D:535:GLU:O	1:D:539:LYS:HB3	1.96	0.66
2:E:1479:PHE:HE2	2:E:1560:MET:HE1	1.61	0.66
1:A:573:LYS:N	1:A:593:GLU:OE2	2.29	0.66
2:B:1539:ASP:HB3	2:B:1542:LEU:HD12	1.78	0.66
3:F:1:MET:HE3	3:F:2:GLN:H	1.60	0.66
3:F:45:MET:HA	3:F:50:PRO:HA	1.77	0.66
3:F:120:ARG:HH12	3:F:139:TYR:HB2	1.61	0.66
2:B:842:LYS:O	2:B:845:GLN:NE2	2.30	0.66
2:B:1032:PHE:HB3	2:B:1043:TRP:HH2	1.59	0.66
2:E:1259:GLU:OE1	2:E:1259:GLU:N	2.23	0.66
2:B:163:LEU:HD23	2:B:1005:ASP:HB3	1.78	0.65
2:B:680:MET:HE3	2:B:693:VAL:HG21	1.78	0.65
2:B:973:ILE:HA	2:B:976:PHE:CE1	2.31	0.65
2:E:469:THR:O	2:E:530:THR:OG1	2.12	0.65
2:E:883:THR:OG1	2:E:931:ARG:NH1	2.29	0.65
2:E:842:LYS:O	2:E:845:GLN:NE2	2.29	0.65
2:E:1216:SER:OG	2:E:1219:ASN:OD1	2.15	0.65
2:E:1536:HIS:HA	2:E:1542:LEU:HD13	1.78	0.65
2:B:1479:PHE:HE2	2:B:1560:MET:HE1	1.61	0.65
1:D:550:GLN:O	1:D:554:ASN:ND2	2.28	0.65
2:E:166:ARG:O	2:E:171:ASN:HA	1.97	0.65
2:E:228:PHE:HB3	2:E:277:LEU:HB3	1.79	0.65
1:A:551:GLN:OE1	1:A:552:ARG:NH2	2.26	0.65
2:E:966:ASP:HA	2:E:969:TYR:HD2	1.62	0.65
2:E:1539:ASP:HB3	2:E:1542:LEU:HD12	1.78	0.65
2:B:228:PHE:HB3	2:B:277:LEU:HB3	1.79	0.65
1:D:573:LYS:N	1:D:593:GLU:OE2	2.29	0.65
2:E:246:TYR:HA	2:E:253:PHE:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:883:THR:OG1	2:B:931:ARG:NH1	2.29	0.65
2:B:1219:ASN:OD1	2:B:1401:GLN:NE2	2.30	0.65
1:D:707:PRO:HD2	2:E:16:ILE:HG21	1.79	0.65
2:E:973:ILE:HA	2:E:976:PHE:CE1	2.31	0.65
1:A:575:TRP:HZ3	1:A:588:TYR:HB2	1.61	0.65
3:F:100:GLU:O	3:F:104:HIS:ND1	2.25	0.65
2:B:129:SER:HA	2:B:132:LEU:HD12	1.79	0.65
2:B:1328:TYR:HB3	2:B:1338:LEU:HD22	1.79	0.65
1:D:551:GLN:OE1	1:D:552:ARG:NH2	2.26	0.65
2:E:680:MET:HE3	2:E:693:VAL:HG21	1.78	0.65
2:E:1107:GLY:HA2	2:E:1110:LEU:HD13	1.79	0.65
2:E:1399:LEU:HD22	2:E:1405:ALA:HB1	1.79	0.65
2:B:166:ARG:O	2:B:171:ASN:HA	1.97	0.65
2:E:204:ILE:HG13	2:E:211:ARG:HB3	1.79	0.65
2:E:1633:VAL:HA	2:E:1637:TYR:HB2	1.79	0.65
3:F:129:LEU:HA	3:F:132:LYS:HG2	1.79	0.65
2:B:204:ILE:HG13	2:B:211:ARG:HB3	1.79	0.64
2:B:966:ASP:HA	2:B:969:TYR:HD2	1.62	0.64
2:E:1328:TYR:HB3	2:E:1338:LEU:HD22	1.79	0.64
2:B:18:ASN:HB3	2:B:28:SER:HB2	1.79	0.64
2:B:569:LEU:N	2:B:620:PHE:O	2.30	0.64
2:E:87:LEU:HD23	2:E:91:LEU:HD23	1.78	0.64
2:E:910:LEU:HA	2:E:913:LEU:HD12	1.79	0.64
2:E:1368:TYR:O	2:E:1425:TYR:N	2.22	0.64
2:B:1107:GLY:HA2	2:B:1110:LEU:HD13	1.79	0.64
3:C:100:GLU:O	3:C:104:HIS:ND1	2.25	0.64
2:E:876:GLU:OE1	2:E:876:GLU:N	2.31	0.64
2:E:1067:ALA:O	2:E:1071:LYS:N	2.18	0.64
2:B:1434:VAL:HB	2:B:1461:GLN:HB2	1.78	0.64
3:C:129:LEU:HA	3:C:132:LYS:HG2	1.79	0.64
2:E:1219:ASN:OD1	2:E:1401:GLN:NE2	2.30	0.64
3:F:8:VAL:O	3:F:58:THR:OG1	2.15	0.64
2:B:555:MET:HA	2:B:561:THR:HA	1.79	0.64
2:B:569:LEU:O	2:B:592:LYS:NZ	2.30	0.64
2:B:1216:SER:OG	2:B:1219:ASN:OD1	2.15	0.64
1:D:575:TRP:HZ3	1:D:588:TYR:HB2	1.61	0.64
2:E:1434:VAL:HB	2:E:1461:GLN:HB2	1.78	0.64
2:B:843:PHE:O	2:B:846:SER:OG	2.16	0.64
2:E:1618:LEU:O	2:E:1622:LEU:HG	1.98	0.64
2:B:1368:TYR:O	2:B:1425:TYR:N	2.22	0.64
2:B:1399:LEU:HD22	2:B:1405:ALA:HB1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:ARG:HH22	1:D:601:HIS:H	1.46	0.64
2:E:163:LEU:HD23	2:E:1005:ASP:HB3	1.78	0.64
2:E:634:ASN:OD1	2:E:637:LEU:N	2.26	0.64
2:E:819:TYR:O	2:E:822:SER:OG	2.10	0.64
3:F:49:LYS:NZ	3:F:50:PRO:O	2.30	0.64
3:F:77:VAL:HG12	3:F:109:PRO:HG2	1.78	0.64
2:B:449:THR:HB	2:B:623:ALA:HB3	1.78	0.64
2:B:554:LEU:O	2:B:562:LEU:N	2.28	0.64
2:B:1059:LEU:O	2:B:1063:THR:OG1	2.12	0.64
2:B:1284:GLN:HG2	2:B:1286:ASP:H	1.63	0.64
2:E:1506:GLN:NE2	2:E:1507:ILE:O	2.31	0.64
1:A:532:PRO:HG3	1:A:708:ASP:HA	1.80	0.64
2:B:1506:GLN:NE2	2:B:1507:ILE:O	2.31	0.64
3:C:77:VAL:HG12	3:C:109:PRO:HG2	1.78	0.64
2:E:1115:THR:O	2:E:1121:ARG:NH2	2.31	0.64
1:A:670:ASN:HA	1:A:673:LEU:HB2	1.79	0.64
2:B:30:GLN:N	2:B:33:ASP:OD2	2.31	0.64
2:B:1618:LEU:O	2:B:1622:LEU:HG	1.98	0.64
1:D:532:PRO:HG3	1:D:708:ASP:HA	1.80	0.64
1:D:670:ASN:HA	1:D:673:LEU:HB2	1.80	0.64
2:E:485:HIS:HB2	2:E:514:LYS:HB3	1.79	0.64
2:E:569:LEU:O	2:E:592:LYS:NZ	2.30	0.64
2:E:1059:LEU:O	2:E:1063:THR:OG1	2.12	0.64
2:B:239:ALA:HB3	2:B:262:TRP:HB3	1.80	0.63
2:B:246:TYR:HA	2:B:253:PHE:HA	1.79	0.63
1:D:697:ARG:NH2	2:E:30:GLN:HB2	2.10	0.63
2:E:18:ASN:HB3	2:E:28:SER:HB2	1.79	0.63
2:E:129:SER:HA	2:E:132:LEU:HD12	1.79	0.63
2:E:555:MET:HA	2:E:561:THR:HA	1.79	0.63
2:E:1111:GLU:OE1	2:E:1111:GLU:N	2.27	0.63
2:B:910:LEU:HA	2:B:913:LEU:HD12	1.79	0.63
2:B:1115:THR:O	2:B:1121:ARG:NH2	2.31	0.63
1:D:536:LEU:HD11	2:E:17:TYR:HD2	1.63	0.63
2:E:1159:VAL:O	2:E:1208:ARG:NH1	2.32	0.63
2:E:1307:TYR:O	2:E:1311:GLY:N	2.31	0.63
2:B:1633:VAL:HA	2:B:1637:TYR:HB2	1.79	0.63
3:C:8:VAL:O	3:C:58:THR:OG1	2.15	0.63
2:E:843:PHE:O	2:E:846:SER:OG	2.16	0.63
2:E:1602:GLU:HA	2:E:1605:ARG:HG2	1.81	0.63
2:B:932:LEU:HA	2:B:935:ARG:HE	1.64	0.63
2:B:1307:TYR:O	2:B:1311:GLY:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:373:ILE:HG23	2:B:376:ASN:HD22	1.64	0.63
2:B:1280:PRO:HA	2:B:1283:LEU:HD23	1.80	0.63
2:B:1440:SER:H	2:B:1442:LYS:NZ	1.97	0.63
2:B:1460:GLN:NE2	2:B:1491:THR:O	2.28	0.63
2:B:1388:TYR:OH	2:B:1390:ARG:NH1	2.29	0.63
3:C:9:VAL:HG22	3:C:78:PHE:HZ	1.64	0.63
2:E:239:ALA:HB3	2:E:262:TRP:HB3	1.80	0.63
2:E:569:LEU:N	2:E:620:PHE:O	2.30	0.63
2:E:1284:GLN:HG2	2:E:1286:ASP:H	1.63	0.63
2:B:485:HIS:HB2	2:B:514:LYS:HB3	1.79	0.62
2:B:1388:TYR:OH	3:C:44:VAL:HG22	1.99	0.62
2:E:741:VAL:HG21	2:E:798:PHE:HD1	1.64	0.62
3:F:9:VAL:HG22	3:F:78:PHE:HZ	1.65	0.62
2:B:165:VAL:HG23	2:B:175:PRO:HD3	1.81	0.62
2:B:193:ARG:NH1	2:B:196:GLU:OE2	2.31	0.62
2:B:1159:VAL:O	2:B:1208:ARG:NH1	2.32	0.62
2:E:932:LEU:N	2:E:935:ARG:HH21	1.97	0.62
2:E:1623:SER:HB3	2:E:1627:ARG:HH12	1.64	0.62
2:B:556:ASN:ND2	2:B:561:THR:O	2.33	0.62
2:B:1623:SER:HB3	2:B:1627:ARG:HH12	1.64	0.62
2:E:1388:TYR:OH	2:E:1390:ARG:NH1	2.29	0.62
1:A:578:ARG:HH22	1:A:601:HIS:H	1.46	0.62
1:D:561:CYS:HA	1:D:576:TYR:HA	1.82	0.62
2:E:154:HIS:HA	2:E:157:ARG:HG2	1.82	0.62
2:E:373:ILE:HG23	2:E:376:ASN:HD22	1.64	0.62
2:E:554:LEU:O	2:E:562:LEU:N	2.28	0.62
2:E:1440:SER:H	2:E:1442:LYS:NZ	1.97	0.62
2:B:3:ARG:HH22	2:B:42:GLU:H	1.46	0.62
2:B:1117:GLU:OE2	2:B:1121:ARG:N	2.26	0.62
2:E:1280:PRO:HA	2:E:1283:LEU:HD23	1.80	0.62
3:F:98:TYR:CE1	3:F:149:ILE:HD13	2.35	0.62
2:B:523:THR:OG1	2:B:524:ARG:NH1	2.33	0.62
2:B:932:LEU:N	2:B:935:ARG:HH21	1.97	0.62
3:C:98:TYR:CE1	3:C:149:ILE:HD13	2.35	0.62
2:E:30:GLN:N	2:E:33:ASP:OD2	2.31	0.62
2:E:193:ARG:NH1	2:E:196:GLU:OE2	2.31	0.62
2:E:556:ASN:ND2	2:E:561:THR:O	2.33	0.62
2:E:1117:GLU:OE2	2:E:1121:ARG:N	2.26	0.62
2:E:1460:GLN:NE2	2:E:1491:THR:O	2.28	0.62
2:B:154:HIS:HA	2:B:157:ARG:HG2	1.82	0.62
2:B:1404:ASN:OD1	2:B:1424:GLN:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:879:LEU:HG	2:E:931:ARG:HH12	1.65	0.62
2:B:85:LEU:O	2:B:88:VAL:HG22	1.99	0.62
2:B:879:LEU:HG	2:B:931:ARG:HH12	1.65	0.62
2:E:1391:ARG:HH22	3:F:29:PRO:HD3	1.65	0.62
2:E:932:LEU:HA	2:E:935:ARG:HE	1.64	0.61
2:E:1404:ASN:OD1	2:E:1424:GLN:HB2	2.00	0.61
2:B:1231:TYR:O	2:B:1235:LYS:N	2.33	0.61
2:E:1548:SER:HB2	3:F:56:TRP:HH2	1.64	0.61
1:A:536:LEU:HD21	2:B:17:TYR:HB2	1.80	0.61
2:B:1602:GLU:HA	2:B:1605:ARG:HG2	1.81	0.61
2:E:569:LEU:HB2	2:E:620:PHE:HB3	1.82	0.61
2:E:1218:GLU:OE1	2:E:1218:GLU:N	2.26	0.61
2:E:1231:TYR:O	2:E:1235:LYS:N	2.33	0.61
2:E:3:ARG:HH22	2:E:42:GLU:H	1.46	0.61
2:E:85:LEU:O	2:E:88:VAL:HG22	1.99	0.61
2:E:523:THR:OG1	2:E:524:ARG:NH1	2.33	0.61
1:A:561:CYS:HA	1:A:576:TYR:HA	1.82	0.61
2:B:80:VAL:HG22	2:B:85:LEU:HD11	1.83	0.61
2:B:443:ARG:NH2	2:B:445:ASP:OD2	2.34	0.61
2:B:853:VAL:O	2:B:857:LEU:HG	2.01	0.61
2:E:876:GLU:HG2	2:E:877:VAL:HG13	1.83	0.61
2:E:1545:HIS:O	2:E:1548:SER:OG	2.14	0.61
1:D:701:LEU:HD11	2:E:16:ILE:HA	1.83	0.61
2:E:165:VAL:HG23	2:E:175:PRO:HD3	1.81	0.61
2:B:254:ILE:HD12	2:B:294:VAL:HG13	1.83	0.61
2:B:741:VAL:HG21	2:B:798:PHE:HD1	1.64	0.61
2:B:771:ARG:NH2	2:B:781:SER:OG	2.34	0.61
2:B:1488:THR:N	2:B:1508:SER:O	2.33	0.61
1:D:724:TYR:HB3	2:E:4:TRP:HB2	1.82	0.61
2:E:37:ILE:HG21	2:E:45:TYR:HB3	1.83	0.61
2:E:925:ILE:HA	2:E:928:ILE:HD12	1.82	0.61
2:E:1167:GLN:CD	2:E:1167:GLN:H	2.09	0.61
2:E:892:ASP:OD1	2:E:895:ASN:ND2	2.34	0.61
2:E:1315:GLU:OE1	2:E:1315:GLU:N	2.28	0.61
2:B:1294:GLN:O	2:B:1298:GLU:HG3	2.01	0.60
2:E:197:LYS:HA	2:E:200:GLU:HG2	1.83	0.60
2:E:771:ARG:NH2	2:E:781:SER:OG	2.34	0.60
2:E:772:VAL:HA	2:E:775:LEU:HD12	1.83	0.60
3:F:141:GLN:OE1	3:F:141:GLN:N	2.27	0.60
1:A:599:VAL:HG23	1:A:601:HIS:CD2	2.37	0.60
2:B:1135:GLU:O	2:B:1139:SER:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1448:GLU:OE1	2:B:1452:ASN:ND2	2.33	0.60
2:E:1589:LEU:HA	2:E:1592:LEU:HD12	1.83	0.60
2:B:166:ARG:HH22	2:B:168:ASP:HB2	1.65	0.60
2:B:569:LEU:HB2	2:B:620:PHE:HB3	1.82	0.60
2:B:892:ASP:OD1	2:B:895:ASN:ND2	2.34	0.60
2:B:1479:PHE:CZ	3:C:36:VAL:HG12	2.35	0.60
2:E:1283:LEU:HD11	2:E:1291:TYR:HB2	1.83	0.60
2:B:351:ILE:HB	2:B:353:MET:HE2	1.83	0.60
2:B:534:ARG:NE	2:B:541:ASP:OD1	2.27	0.60
2:B:1167:GLN:CD	2:B:1167:GLN:H	2.09	0.60
2:E:166:ARG:HH22	2:E:168:ASP:HB2	1.65	0.60
2:E:853:VAL:O	2:E:857:LEU:HG	2.01	0.60
2:E:1135:GLU:O	2:E:1139:SER:N	2.34	0.60
2:E:1448:GLU:OE1	2:E:1452:ASN:ND2	2.33	0.60
2:B:1315:GLU:OE1	2:B:1315:GLU:N	2.28	0.60
2:E:1066:GLN:HA	2:E:1069:ARG:NH1	2.17	0.60
1:A:562:PHE:N	1:A:575:TRP:O	2.34	0.60
2:B:37:ILE:HG21	2:B:45:TYR:HB3	1.83	0.60
2:E:254:ILE:HD12	2:E:294:VAL:HG13	1.83	0.60
3:F:39:ASN:H	3:F:57:ASP:HB3	1.66	0.60
2:B:7:THR:O	2:B:10:GLN:NE2	2.20	0.60
2:B:772:VAL:HA	2:B:775:LEU:HD12	1.83	0.60
2:B:1545:HIS:O	2:B:1548:SER:OG	2.14	0.60
3:C:126:ILE:HG23	3:C:136:PRO:HG2	1.84	0.60
1:D:599:VAL:HG23	1:D:601:HIS:CD2	2.37	0.60
2:E:1099:ILE:HD13	2:E:1138:PHE:HB2	1.83	0.60
2:E:1063:THR:HA	2:E:1069:ARG:HH11	1.67	0.60
2:E:1294:GLN:O	2:E:1298:GLU:HG3	2.01	0.60
1:A:576:TYR:CD1	1:A:591:LEU:HG	2.36	0.60
2:B:730:TYR:OH	2:B:771:ARG:NH1	2.35	0.60
1:D:576:TYR:CD1	1:D:591:LEU:HG	2.36	0.60
2:E:351:ILE:HB	2:E:353:MET:HE2	1.83	0.60
2:B:1283:LEU:HD11	2:B:1291:TYR:HB2	1.83	0.59
2:E:809:ALA:HB1	2:E:812:ILE:HB	1.84	0.59
1:A:695:LYS:HD2	2:B:125:ILE:HD12	1.83	0.59
2:E:649:ASN:O	2:E:653:ASN:N	2.24	0.59
2:B:232:VAL:O	2:B:398:GLY:N	2.35	0.59
2:B:925:ILE:HA	2:B:928:ILE:HD12	1.82	0.59
2:B:1563:PHE:HA	2:B:1566:TYR:CD2	2.37	0.59
2:E:14:VAL:HB	2:E:65:HIS:HB3	1.84	0.59
2:E:1549:MET:HA	3:F:39:ASN:ND2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:LYS:HA	2:B:200:GLU:HG2	1.83	0.59
2:B:1063:THR:HA	2:B:1069:ARG:HH11	1.67	0.59
2:B:1589:LEU:HA	2:B:1592:LEU:HD12	1.83	0.59
3:C:39:ASN:H	3:C:57:ASP:HB3	1.66	0.59
2:E:80:VAL:HG22	2:E:85:LEU:HD11	1.83	0.59
2:E:443:ARG:NH2	2:E:445:ASP:OD2	2.34	0.59
3:F:126:ILE:HG23	3:F:136:PRO:HG2	1.84	0.59
2:B:1066:GLN:HA	2:B:1069:ARG:NH1	2.17	0.59
2:B:1099:ILE:HD13	2:B:1138:PHE:HB2	1.83	0.59
2:E:887:SER:O	2:E:890:LEU:HB3	2.02	0.59
2:E:1460:GLN:HB2	2:E:1494:THR:HG22	1.84	0.59
2:B:37:ILE:HD13	2:B:45:TYR:HB3	1.85	0.59
2:B:809:ALA:HB1	2:B:812:ILE:HB	1.84	0.59
2:B:876:GLU:HG2	2:B:877:VAL:HG13	1.83	0.59
2:E:147:LYS:O	2:E:151:LYS:HG2	2.03	0.59
2:E:465:ASN:OD1	2:E:503:GLN:N	2.27	0.59
1:A:608:LEU:HD23	1:A:609:PRO:HD2	1.85	0.59
2:B:1460:GLN:HB2	2:B:1494:THR:HG22	1.84	0.59
2:E:27:LEU:HD23	2:E:28:SER:H	1.68	0.59
1:A:588:TYR:HE1	1:A:608:LEU:HB2	1.68	0.59
2:B:1196:LEU:O	2:B:1199:SER:OG	2.19	0.59
2:B:1446:VAL:HG12	2:E:1333:PHE:CZ	2.37	0.59
2:E:297:VAL:HG22	2:E:326:VAL:HG22	1.85	0.59
1:A:643:SER:OG	1:A:653:ASN:ND2	2.35	0.59
3:C:21:ILE:HD11	3:C:35:THR:HG23	1.85	0.59
2:E:156:ASN:HA	2:E:161:LEU:HD12	1.85	0.59
2:E:730:TYR:OH	2:E:771:ARG:NH1	2.35	0.59
2:E:1328:TYR:HB3	2:E:1338:LEU:CD2	2.33	0.59
2:E:1563:PHE:HA	2:E:1566:TYR:CD2	2.37	0.59
2:B:1328:TYR:HB3	2:B:1338:LEU:CD2	2.33	0.59
3:C:174:ARG:HA	3:C:177:LEU:HB2	1.85	0.59
1:D:673:LEU:HB3	1:D:675:LYS:NZ	2.18	0.59
2:E:641:LEU:O	2:E:644:ARG:NH1	2.36	0.59
2:E:1196:LEU:O	2:E:1199:SER:OG	2.19	0.59
2:E:1462:PHE:HB2	2:E:1489:TYR:HB2	1.85	0.59
2:B:757:LEU:HD11	2:B:812:ILE:HG23	1.85	0.58
2:B:1080:ARG:HA	2:B:1083:ILE:HD12	1.85	0.58
1:D:643:SER:OG	1:D:653:ASN:ND2	2.35	0.58
2:E:1002:TYR:HB2	2:E:1010:ASN:HD21	1.68	0.58
3:F:174:ARG:HA	3:F:177:LEU:HB2	1.85	0.58
3:C:5:LYS:N	3:C:76:ASP:OD2	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:562:PHE:N	1:D:575:TRP:O	2.34	0.58
2:B:887:SER:O	2:B:890:LEU:HB3	2.02	0.58
2:E:19:TYR:O	2:E:28:SER:HA	2.03	0.58
3:C:138:THR:H	3:C:141:GLN:NE2	2.01	0.58
2:B:641:LEU:O	2:B:644:ARG:NH1	2.36	0.58
2:B:876:GLU:N	2:B:876:GLU:OE1	2.31	0.58
2:E:1080:ARG:HA	2:E:1083:ILE:HD12	1.85	0.58
1:A:723:VAL:HB	2:B:3:ARG:H	1.68	0.58
2:B:19:TYR:O	2:B:28:SER:HA	2.03	0.58
2:B:156:ASN:HA	2:B:161:LEU:HD12	1.85	0.58
3:F:21:ILE:HD11	3:F:35:THR:HG23	1.85	0.58
2:B:14:VAL:HB	2:B:65:HIS:HB3	1.84	0.58
2:B:569:LEU:HD12	2:B:620:PHE:HD2	1.67	0.58
2:B:637:LEU:HD12	2:B:665:ILE:HD13	1.86	0.58
2:B:719:TYR:HA	2:B:723:HIS:ND1	2.19	0.58
2:B:814:GLY:HA2	2:B:855:GLN:HG2	1.86	0.58
2:B:860:MET:SD	2:B:885:GLN:NE2	2.77	0.58
1:D:588:TYR:HE1	1:D:608:LEU:HB2	1.67	0.58
1:D:608:LEU:HD23	1:D:609:PRO:HD2	1.85	0.58
2:E:569:LEU:HD12	2:E:620:PHE:HD2	1.67	0.58
2:E:1607:HIS:O	2:E:1611:LEU:N	2.36	0.58
2:B:166:ARG:NH2	2:B:168:ASP:HB2	2.19	0.58
2:B:730:TYR:HB2	2:B:767:ILE:HG23	1.85	0.58
2:B:934:ARG:NH2	2:B:988:GLU:OE1	2.37	0.58
2:B:1106:VAL:O	2:B:1109:ILE:HG22	2.04	0.58
2:B:1417:ASP:O	2:B:1421:SER:N	2.37	0.58
2:B:1607:HIS:O	2:B:1611:LEU:N	2.36	0.58
1:D:544:ILE:HG23	1:D:545:LEU:HD22	1.86	0.58
1:D:548:ILE:O	1:D:552:ARG:HG2	2.04	0.58
2:E:59:PHE:HD2	2:E:64:ILE:HG12	1.67	0.58
2:E:730:TYR:HB2	2:E:767:ILE:HG23	1.84	0.58
1:A:548:ILE:O	1:A:552:ARG:HG2	2.04	0.58
2:B:27:LEU:HD23	2:B:28:SER:H	1.68	0.58
2:B:297:VAL:HG22	2:B:326:VAL:HG22	1.85	0.58
2:B:730:TYR:CE1	2:B:771:ARG:HD3	2.39	0.58
2:E:232:VAL:O	2:E:398:GLY:N	2.35	0.58
2:E:262:TRP:HA	2:E:268:PRO:HA	1.86	0.58
2:E:860:MET:SD	2:E:885:GLN:NE2	2.77	0.58
2:E:1106:VAL:O	2:E:1109:ILE:HG22	2.04	0.58
2:E:1121:ARG:O	2:E:1125:ILE:HD12	2.04	0.58
2:B:27:LEU:HD23	2:B:28:SER:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:992:MET:O	2:B:996:LEU:HD23	2.04	0.58
2:B:1031:PHE:C	2:B:1035:GLN:HE22	2.11	0.58
2:E:27:LEU:HD23	2:E:28:SER:N	2.18	0.58
2:E:1231:TYR:HE2	2:E:1243:TYR:CE1	2.22	0.58
2:B:59:PHE:HD2	2:B:64:ILE:HG12	1.67	0.57
2:B:288:ASP:HA	2:B:291:ARG:HE	1.69	0.57
2:B:721:TYR:OH	2:B:765:ARG:NH1	2.37	0.57
2:B:994:LYS:NZ	2:B:1048:HIS:HB3	2.19	0.57
2:E:37:ILE:HD13	2:E:45:TYR:HB3	1.85	0.57
2:E:246:TYR:N	2:E:295:SER:O	2.37	0.57
2:E:787:PHE:O	2:E:791:ILE:HG12	2.04	0.57
2:E:994:LYS:NZ	2:E:1048:HIS:HB3	2.19	0.57
1:A:697:ARG:NH2	2:B:30:GLN:HB2	2.14	0.57
2:B:147:LYS:O	2:B:151:LYS:HG2	2.03	0.57
2:B:787:PHE:O	2:B:791:ILE:HG12	2.04	0.57
2:E:721:TYR:OH	2:E:765:ARG:NH1	2.37	0.57
3:F:138:THR:H	3:F:141:GLN:NE2	2.01	0.57
1:A:544:ILE:HG23	1:A:545:LEU:HD22	1.86	0.57
2:B:1002:TYR:HB2	2:B:1010:ASN:HD21	1.68	0.57
2:B:1514:PRO:HA	2:B:1517:ASN:HD22	1.70	0.57
2:E:934:ARG:NH2	2:E:988:GLU:OE1	2.37	0.57
2:E:1011:MET:HE2	2:E:1011:MET:HA	1.87	0.57
2:B:1011:MET:HE2	2:B:1011:MET:HA	1.86	0.57
2:B:1121:ARG:O	2:B:1125:ILE:HD12	2.04	0.57
2:B:1231:TYR:HE2	2:B:1243:TYR:CE1	2.22	0.57
2:E:1031:PHE:C	2:E:1035:GLN:HE22	2.11	0.57
2:E:1177:LEU:O	2:E:1181:ARG:HG2	2.05	0.57
1:A:673:LEU:HB3	1:A:675:LYS:NZ	2.18	0.57
2:B:226:VAL:O	2:B:279:ALA:N	2.30	0.57
2:B:465:ASN:OD1	2:B:503:GLN:N	2.27	0.57
2:B:550:ALA:HB1	2:B:569:LEU:HB3	1.86	0.57
2:B:1332:VAL:HG13	2:B:1334:ASP:H	1.69	0.57
2:E:166:ARG:NH2	2:E:168:ASP:HB2	2.19	0.57
2:B:630:LYS:HG2	2:B:668:PHE:HZ	1.70	0.57
2:E:94:THR:HG22	2:E:98:TRP:NE1	2.20	0.57
2:E:550:ALA:HB1	2:E:569:LEU:HB3	1.86	0.57
2:E:630:LYS:HG2	2:E:668:PHE:HZ	1.70	0.57
2:E:678:ASN:HA	2:E:681:MET:HE3	1.87	0.57
2:E:1545:HIS:CD2	3:F:5:LYS:HE3	2.40	0.57
2:B:1462:PHE:HB2	2:B:1489:TYR:HB2	1.85	0.57
2:E:792:ARG:NE	2:E:835:GLU:OE1	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:992:MET:O	2:E:996:LEU:HD23	2.04	0.57
2:B:965:ASP:HB3	2:B:968:HIS:CG	2.40	0.57
2:E:637:LEU:HD12	2:E:665:ILE:HD13	1.86	0.57
2:E:814:GLY:HA2	2:E:855:GLN:HG2	1.86	0.57
2:B:1607:HIS:NE2	2:B:1619:HIS:HB2	2.20	0.57
3:C:91:GLU:O	3:C:95:ALA:HB3	2.05	0.57
1:D:643:SER:HA	1:D:652:LEU:O	2.05	0.57
1:A:551:GLN:HG2	2:B:107:VAL:HA	1.85	0.56
2:B:422:ASP:OD1	2:B:425:THR:OG1	2.23	0.56
2:B:1275:ASP:O	2:B:1292:THR:OG1	2.23	0.56
2:E:72:GLU:O	2:E:76:GLN:NE2	2.38	0.56
2:E:757:LEU:HD11	2:E:812:ILE:HG23	1.85	0.56
2:E:1607:HIS:NE2	2:E:1619:HIS:HB2	2.20	0.56
2:B:1135:GLU:OE1	2:B:1139:SER:OG	2.22	0.56
2:E:534:ARG:NE	2:E:541:ASP:OD1	2.27	0.56
2:E:730:TYR:CE1	2:E:771:ARG:HD3	2.39	0.56
2:B:246:TYR:N	2:B:295:SER:O	2.37	0.56
2:B:262:TRP:HA	2:B:268:PRO:HA	1.86	0.56
2:B:792:ARG:NE	2:B:835:GLU:OE1	2.31	0.56
2:E:526:HIS:CE1	2:E:586:LEU:HD21	2.41	0.56
2:E:719:TYR:HA	2:E:723:HIS:ND1	2.19	0.56
2:E:1135:GLU:OE1	2:E:1139:SER:OG	2.22	0.56
3:F:5:LYS:N	3:F:76:ASP:OD2	2.29	0.56
2:B:130:GLN:NE2	2:B:144:LEU:HD11	2.21	0.56
2:B:1177:LEU:O	2:B:1181:ARG:HG2	2.05	0.56
3:C:69:PRO:HB3	3:C:104:HIS:CD2	2.41	0.56
2:E:131:ILE:HD11	2:E:144:LEU:HG	1.88	0.56
2:E:1102:ILE:HD11	2:E:1134:CYS:HB2	1.88	0.56
2:E:1432:LYS:NZ	2:E:1465:SER:H	2.03	0.56
1:A:643:SER:HA	1:A:652:LEU:O	2.05	0.56
2:B:522:VAL:HG11	2:B:631:LEU:HD21	1.88	0.56
2:B:1432:LYS:NZ	2:B:1465:SER:H	2.03	0.56
2:B:1449:GLN:OE1	2:B:1449:GLN:N	2.25	0.56
2:E:35:VAL:HG23	2:E:37:ILE:HG13	1.88	0.56
2:E:431:MET:HE1	2:E:447:TYR:CG	2.41	0.56
2:E:1117:GLU:OE2	2:E:1120:LEU:HG	2.06	0.56
2:E:1332:VAL:HG13	2:E:1334:ASP:H	1.69	0.56
2:E:1613:GLU:OE2	2:E:1614:GLN:HG3	2.06	0.56
1:A:539:LYS:HZ1	1:A:540:ILE:HD11	1.70	0.56
2:B:820:LEU:O	2:B:823:ILE:HG12	2.04	0.56
2:B:1416:GLU:HA	2:B:1419:LYS:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:THR:HG22	2:B:98:TRP:NE1	2.20	0.56
2:B:431:MET:HE1	2:B:447:TYR:CG	2.41	0.56
2:B:640:LEU:HB2	2:B:653:ASN:HB3	1.88	0.56
1:D:670:ASN:O	1:D:674:GLY:N	2.39	0.56
2:E:130:GLN:NE2	2:E:144:LEU:HD11	2.21	0.56
2:E:288:ASP:HA	2:E:291:ARG:HE	1.69	0.56
3:F:69:PRO:HB3	3:F:104:HIS:CD2	2.41	0.56
2:B:35:VAL:HG23	2:B:37:ILE:HG13	1.88	0.56
2:B:754:PHE:HA	2:B:757:LEU:HD12	1.87	0.56
2:E:64:ILE:HG22	2:E:66:LEU:HD22	1.88	0.56
2:E:754:PHE:HA	2:E:757:LEU:HD12	1.87	0.56
2:E:1056:HIS:ND1	2:E:1057:GLU:OE2	2.39	0.56
3:F:41:SER:HA	3:F:54:GLY:HA2	1.88	0.56
2:B:131:ILE:HD11	2:B:144:LEU:HG	1.88	0.56
2:B:1613:GLU:OE2	2:B:1614:GLN:HG3	2.06	0.56
1:D:599:VAL:HG23	1:D:601:HIS:HD2	1.71	0.56
2:E:248:PRO:HD2	2:E:293:ARG:HG3	1.87	0.56
2:E:820:LEU:O	2:E:823:ILE:HG12	2.04	0.56
2:E:1275:ASP:O	2:E:1292:THR:OG1	2.23	0.56
1:A:670:ASN:O	1:A:674:GLY:N	2.39	0.56
2:B:235:ILE:HB	2:B:262:TRP:HZ3	1.71	0.56
2:B:526:HIS:CE1	2:B:586:LEU:HD21	2.41	0.56
2:B:1102:ILE:HD11	2:B:1134:CYS:HB2	1.88	0.56
2:B:1557:PRO:HB2	2:B:1561:GLY:HA2	1.87	0.56
2:E:793:GLN:HA	2:E:796:LEU:HG	1.87	0.56
2:E:965:ASP:HB3	2:E:968:HIS:CG	2.40	0.56
2:E:1038:PHE:O	2:E:1039:GLU:HG2	2.06	0.56
2:E:1514:PRO:HA	2:E:1517:ASN:HD22	1.70	0.56
2:E:1623:SER:HB3	2:E:1627:ARG:HH22	1.71	0.56
2:B:248:PRO:HD2	2:B:293:ARG:HG3	1.87	0.55
2:B:678:ASN:HA	2:B:681:MET:HE3	1.87	0.55
3:C:49:LYS:NZ	3:C:50:PRO:O	2.30	0.55
1:D:584:LYS:HZ2	2:E:1403:PRO:HA	1.71	0.55
2:E:347:PRO:HB2	2:E:392:VAL:HB	1.88	0.55
2:B:72:GLU:O	2:B:76:GLN:NE2	2.38	0.55
2:B:634:ASN:OD1	2:B:637:LEU:N	2.26	0.55
2:E:422:ASP:OD1	2:E:425:THR:OG1	2.23	0.55
3:F:119:LEU:HA	3:F:122:ASP:HB2	1.88	0.55
2:B:1451:LEU:O	2:B:1455:ARG:N	2.39	0.55
2:B:1623:SER:HB3	2:B:1627:ARG:NH1	2.22	0.55
2:E:790:SER:O	2:E:793:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1416:GLU:HA	2:E:1419:LYS:HG2	1.88	0.55
2:E:1451:LEU:O	2:E:1455:ARG:N	2.39	0.55
2:E:1488:THR:N	2:E:1508:SER:O	2.33	0.55
2:B:64:ILE:HG22	2:B:66:LEU:HD22	1.88	0.55
2:B:225:TYR:HE1	2:B:278:GLN:HB3	1.71	0.55
2:B:556:ASN:HD22	2:B:560:THR:HG1	1.54	0.55
2:B:1056:HIS:ND1	2:B:1057:GLU:OE2	2.39	0.55
2:B:1464:TYR:HB3	2:B:1487:THR:OG1	2.07	0.55
2:E:52:ASN:HD21	2:E:55:LYS:HD2	1.71	0.55
2:E:235:ILE:HB	2:E:262:TRP:HZ3	1.71	0.55
2:E:1417:ASP:O	2:E:1421:SER:N	2.37	0.55
3:F:91:GLU:O	3:F:95:ALA:HB3	2.05	0.55
2:B:95:LEU:HA	2:B:98:TRP:CD1	2.42	0.55
3:C:141:GLN:OE1	3:C:141:GLN:N	2.27	0.55
2:E:281:PHE:HD1	2:E:428:ALA:HB3	1.71	0.55
2:E:640:LEU:HB2	2:E:653:ASN:HB3	1.88	0.55
3:F:87:PRO:HA	3:F:90:PHE:HD2	1.72	0.55
1:A:727:ASN:N	2:B:46:ARG:HH22	2.04	0.55
2:B:52:ASN:HD21	2:B:55:LYS:HD2	1.71	0.55
2:B:281:PHE:HD1	2:B:428:ALA:HB3	1.71	0.55
2:B:793:GLN:HA	2:B:796:LEU:HG	1.87	0.55
2:E:25:VAL:HG23	2:E:57:GLY:HA2	1.89	0.55
1:A:599:VAL:HG23	1:A:601:HIS:HD2	1.70	0.55
2:B:1406:GLU:CD	2:B:1423:LYS:HZ2	2.15	0.55
2:B:1408:MET:HE3	2:B:1425:TYR:HB3	1.89	0.55
3:C:119:LEU:HA	3:C:122:ASP:HB2	1.88	0.55
2:E:192:LYS:O	2:E:195:GLU:HG2	2.07	0.55
2:E:225:TYR:HE1	2:E:278:GLN:HB3	1.71	0.55
2:E:1557:PRO:HB2	2:E:1561:GLY:HA2	1.87	0.55
2:B:972:TYR:O	2:B:975:THR:N	2.39	0.55
2:B:1038:PHE:O	2:B:1039:GLU:HG2	2.06	0.55
2:E:962:GLN:O	2:E:1019:ARG:NH1	2.37	0.55
2:E:1117:GLU:OE1	2:E:1118:VAL:N	2.40	0.55
2:B:257:ASN:O	2:B:488:ALA:N	2.31	0.55
2:B:1117:GLU:OE2	2:B:1120:LEU:HG	2.06	0.55
2:E:1032:PHE:HB3	2:E:1043:TRP:CH2	2.42	0.55
2:E:1205:LEU:HA	2:E:1208:ARG:HD3	1.89	0.55
2:E:1584:GLU:HG3	2:E:1585:LYS:HD3	1.88	0.55
2:E:522:VAL:HG11	2:E:631:LEU:HD21	1.88	0.55
2:B:854:ARG:NH2	2:B:858:ASN:OD1	2.39	0.54
2:B:945:ARG:HD3	2:B:947:SER:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1082:GLU:OE2	2:B:1086:ARG:NE	2.24	0.54
2:B:1584:GLU:HG3	2:B:1585:LYS:HD3	1.88	0.54
3:C:87:PRO:HA	3:C:90:PHE:HD2	1.72	0.54
2:E:879:LEU:HA	2:E:882:LEU:HD12	1.90	0.54
2:E:945:ARG:HD3	2:E:947:SER:H	1.72	0.54
2:B:1127:ILE:HG22	2:B:1131:MET:HE3	1.88	0.54
3:C:90:PHE:CE2	3:C:137:ILE:HB	2.42	0.54
2:E:95:LEU:HA	2:E:98:TRP:CD1	2.42	0.54
2:E:412:GLN:HA	2:E:415:LYS:HE2	1.90	0.54
2:E:869:PHE:O	2:E:918:VAL:HG13	2.08	0.54
2:E:1408:MET:HE3	2:E:1425:TYR:HB3	1.89	0.54
1:A:567:ALA:HA	1:A:571:GLN:HB2	1.89	0.54
2:B:89:GLN:O	2:B:92:THR:OG1	2.23	0.54
2:B:591:THR:H	2:B:594:GLU:HB2	1.72	0.54
2:B:1585:LYS:HA	2:B:1588:LEU:HD12	1.90	0.54
2:E:1516:GLU:O	2:E:1519:ILE:N	2.41	0.54
3:F:90:PHE:CE2	3:F:137:ILE:HB	2.42	0.54
1:A:548:ILE:HB	1:A:549:LYS:NZ	2.23	0.54
2:B:446:ILE:HB	2:B:515:VAL:HB	1.90	0.54
2:B:790:SER:O	2:B:793:GLN:HG2	2.06	0.54
3:C:41:SER:HA	3:C:54:GLY:HA2	1.88	0.54
2:E:81:ILE:HD13	2:E:141:LEU:HD21	1.90	0.54
2:E:226:VAL:O	2:E:279:ALA:N	2.30	0.54
2:E:287:MET:HA	2:E:290:ILE:HG12	1.89	0.54
2:B:431:MET:HE3	2:B:625:LEU:HD23	1.89	0.54
2:B:945:ARG:HH11	2:B:946:GLN:H	1.56	0.54
2:B:962:GLN:O	2:B:1019:ARG:NH1	2.37	0.54
2:B:1095:GLY:H	2:B:1098:LYS:HE3	1.72	0.54
2:B:1626:PHE:HD2	2:B:1627:ARG:HD3	1.72	0.54
1:A:544:ILE:HD11	1:A:689:LEU:HB2	1.90	0.54
1:A:693:GLU:O	1:A:696:LEU:HG	2.08	0.54
2:B:854:ARG:HH11	2:B:854:ARG:HA	1.73	0.54
2:B:1205:LEU:HA	2:B:1208:ARG:HD3	1.89	0.54
2:B:1516:GLU:O	2:B:1519:ILE:N	2.40	0.54
2:B:1563:PHE:HA	2:B:1566:TYR:HD2	1.72	0.54
3:C:5:LYS:HB3	3:C:75:THR:HG23	1.89	0.54
3:C:7:VAL:HB	3:C:78:PHE:HD2	1.73	0.54
2:E:1435:MET:SD	2:E:1455:ARG:HA	2.48	0.54
2:B:646:ASN:ND2	2:B:653:ASN:HD21	2.06	0.54
2:B:1623:SER:HB3	2:B:1627:ARG:HH22	1.71	0.54
2:E:155:GLY:HA2	2:E:158:MET:SD	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:854:ARG:HH11	2:E:854:ARG:HA	1.73	0.54
2:E:917:ASP:N	2:E:917:ASP:OD1	2.41	0.54
2:B:155:GLY:HA2	2:B:158:MET:SD	2.48	0.54
2:B:192:LYS:O	2:B:195:GLU:HG2	2.07	0.54
3:C:64:TYR:HD2	3:C:67:LEU:HD12	1.73	0.54
1:D:548:ILE:HB	1:D:549:LYS:NZ	2.23	0.54
2:E:771:ARG:HH21	2:E:784:GLY:HA2	1.72	0.54
2:E:854:ARG:NH2	2:E:858:ASN:OD1	2.39	0.54
2:E:1563:PHE:HA	2:E:1566:TYR:HD2	1.73	0.54
1:A:555:ARG:NH2	2:B:109:ASN:OD1	2.40	0.54
2:B:1387:GLU:HG2	2:B:1388:TYR:N	2.22	0.54
2:B:1435:MET:SD	2:B:1455:ARG:HA	2.48	0.54
1:D:544:ILE:HD11	1:D:689:LEU:HB2	1.90	0.54
1:D:564:LYS:HZ1	1:D:590:ASP:HA	1.71	0.54
1:D:567:ALA:HA	1:D:571:GLN:HB2	1.89	0.54
2:E:19:TYR:HB2	2:E:59:PHE:HE1	1.73	0.54
2:E:561:THR:HG21	2:E:631:LEU:HB3	1.90	0.54
2:E:1406:GLU:CD	2:E:1423:LYS:HZ2	2.15	0.54
2:E:1464:TYR:HB3	2:E:1487:THR:OG1	2.07	0.54
1:A:603:SER:N	1:A:606:ASP:OD1	2.41	0.54
2:B:81:ILE:HD13	2:B:141:LEU:HD21	1.90	0.54
2:B:287:MET:HA	2:B:290:ILE:HG12	1.89	0.54
2:B:1202:GLU:OE2	2:B:1203:ASN:ND2	2.41	0.54
2:B:1440:SER:H	2:B:1442:LYS:HZ1	1.56	0.54
2:E:584:PHE:O	2:E:587:THR:OG1	2.22	0.54
3:F:5:LYS:HB3	3:F:75:THR:HG23	1.89	0.54
2:B:589:PRO:CB	2:B:594:GLU:HB3	2.36	0.53
2:E:1127:ILE:HG22	2:E:1131:MET:HE3	1.89	0.53
2:E:1344:LYS:O	2:E:1347:SER:OG	2.21	0.53
2:E:1623:SER:HB3	2:E:1627:ARG:NH1	2.22	0.53
2:B:172:ILE:HG13	2:B:173:LEU:HD12	1.90	0.53
2:B:353:MET:HG3	2:B:374:GLY:O	2.08	0.53
2:B:471:SER:N	2:B:528:ARG:O	2.36	0.53
1:D:552:ARG:NH1	1:D:664:ILE:HG12	2.23	0.53
2:E:172:ILE:HG13	2:E:173:LEU:HD12	1.90	0.53
2:E:302:ARG:HD3	2:E:322:PHE:HD1	1.72	0.53
2:E:431:MET:HE3	2:E:625:LEU:HD23	1.89	0.53
2:E:1040:LEU:HD12	2:E:1097:HIS:CE1	2.44	0.53
1:A:544:ILE:CD1	1:A:689:LEU:HB2	2.38	0.53
2:B:25:VAL:HG23	2:B:57:GLY:HA2	1.89	0.53
2:B:181:ILE:HG22	2:B:185:LYS:NZ	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:PRO:HB2	2:B:392:VAL:HB	1.88	0.53
2:B:412:GLN:HA	2:B:415:LYS:HE2	1.90	0.53
2:B:732:LYS:HA	2:B:735:LYS:HD3	1.91	0.53
2:B:1060:GLN:OE1	2:B:1060:GLN:N	2.32	0.53
1:D:603:SER:N	1:D:606:ASP:OD1	2.41	0.53
2:B:771:ARG:HH21	2:B:784:GLY:HA2	1.72	0.53
2:B:869:PHE:O	2:B:918:VAL:HG13	2.08	0.53
2:B:1117:GLU:OE1	2:B:1118:VAL:N	2.40	0.53
2:B:1168:TYR:O	2:B:1172:LEU:HD23	2.08	0.53
2:B:1470:LYS:HB3	2:B:1483:TRP:CD1	2.43	0.53
2:B:1536:HIS:CG	2:B:1542:LEU:HD22	2.44	0.53
2:E:446:ILE:HB	2:E:515:VAL:HB	1.90	0.53
2:E:945:ARG:HH11	2:E:946:GLN:H	1.55	0.53
2:E:1202:GLU:OE2	2:E:1203:ASN:ND2	2.41	0.53
2:E:1387:GLU:HG2	2:E:1388:TYR:N	2.23	0.53
2:E:1418:ILE:HA	2:E:1421:SER:HB3	1.91	0.53
1:A:557:VAL:HA	1:A:579:LEU:HB3	1.91	0.53
2:B:972:TYR:HA	2:B:975:THR:OG1	2.09	0.53
2:B:1418:ILE:HA	2:B:1421:SER:HB3	1.91	0.53
2:B:1449:GLN:HA	2:B:1452:ASN:ND2	2.24	0.53
1:D:693:GLU:O	1:D:696:LEU:HG	2.08	0.53
2:E:130:GLN:HE21	2:E:144:LEU:HD11	1.73	0.53
2:E:471:SER:N	2:E:528:ARG:O	2.36	0.53
2:E:646:ASN:ND2	2:E:653:ASN:HD21	2.06	0.53
2:E:973:ILE:HA	2:E:976:PHE:CZ	2.43	0.53
2:E:1205:LEU:HD13	2:E:1208:ARG:HD3	1.91	0.53
2:E:1477:ASN:HB3	2:E:1568:LYS:NZ	2.23	0.53
1:A:548:ILE:HB	1:A:549:LYS:HZ2	1.74	0.53
2:B:302:ARG:HD3	2:B:322:PHE:HD1	1.72	0.53
2:B:1232:LYS:HB2	2:B:1240:TYR:CE2	2.44	0.53
2:B:1477:ASN:HB3	2:B:1568:LYS:NZ	2.24	0.53
2:E:591:THR:H	2:E:594:GLU:HB2	1.72	0.53
2:E:972:TYR:HA	2:E:975:THR:OG1	2.09	0.53
2:E:1585:LYS:HA	2:E:1588:LEU:HD12	1.90	0.53
2:B:52:ASN:ND2	2:B:55:LYS:HD2	2.24	0.53
2:B:327:MET:HB2	2:B:346:ILE:HG23	1.91	0.53
2:B:529:PHE:HE2	2:B:552:VAL:HG12	1.73	0.53
2:B:883:THR:CG2	2:B:931:ARG:HB3	2.39	0.53
2:B:917:ASP:N	2:B:917:ASP:OD1	2.41	0.53
3:C:141:GLN:H	3:C:141:GLN:CD	2.15	0.53
2:E:353:MET:HG3	2:E:374:GLY:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:529:PHE:HE2	2:E:552:VAL:HG12	1.73	0.53
2:E:589:PRO:CB	2:E:594:GLU:HB3	2.36	0.53
2:E:670:GLN:HG3	2:E:719:TYR:CD1	2.44	0.53
2:E:1024:PHE:HA	2:E:1027:VAL:HG22	1.91	0.53
1:A:541:GLN:O	1:A:544:ILE:HG22	2.09	0.53
1:A:552:ARG:NH1	1:A:664:ILE:HG12	2.23	0.53
1:A:679:SER:HB3	1:A:681:LEU:HG	1.91	0.53
2:B:561:THR:HG21	2:B:631:LEU:HB3	1.90	0.53
2:B:670:GLN:HG3	2:B:719:TYR:CD1	2.44	0.53
2:B:882:LEU:HA	2:B:885:GLN:HE21	1.73	0.53
2:B:973:ILE:HA	2:B:976:PHE:CZ	2.44	0.53
2:B:1017:PHE:O	2:B:1021:ILE:HG12	2.09	0.53
2:B:1551:LEU:HB3	2:B:1622:LEU:HD13	1.91	0.53
2:E:89:GLN:O	2:E:92:THR:OG1	2.23	0.53
2:E:181:ILE:HG22	2:E:185:LYS:NZ	2.23	0.53
2:E:906:LEU:HD12	2:E:909:ILE:HD11	1.91	0.53
2:E:1232:LYS:HB2	2:E:1240:TYR:CE2	2.44	0.53
1:A:578:ARG:HB3	1:A:587:HIS:HB2	1.91	0.53
1:D:536:LEU:HD21	2:E:17:TYR:HB2	1.91	0.53
2:E:1391:ARG:HD2	2:E:1429:PHE:HA	1.91	0.53
3:F:7:VAL:HB	3:F:78:PHE:HD2	1.73	0.53
1:A:584:LYS:O	1:A:607:LYS:NZ	2.42	0.53
2:B:649:ASN:O	2:B:653:ASN:N	2.24	0.53
1:D:544:ILE:CD1	1:D:689:LEU:HB2	2.38	0.53
2:E:327:MET:HB2	2:E:346:ILE:HG23	1.91	0.53
2:E:875:ARG:HE	2:E:924:HIS:CD2	2.26	0.53
2:E:882:LEU:HA	2:E:885:GLN:HE21	1.73	0.53
2:E:1059:LEU:HD12	2:E:1116:PRO:HB2	1.90	0.53
2:E:1189:SER:O	2:E:1192:VAL:HG22	2.09	0.53
2:E:1237:GLU:O	2:E:1240:TYR:HB3	2.09	0.53
2:E:1536:HIS:CG	2:E:1542:LEU:HD22	2.44	0.53
2:E:1558:ALA:N	3:F:38:ASP:OD2	2.42	0.53
2:E:1626:PHE:HD2	2:E:1627:ARG:HD3	1.72	0.53
3:F:28:PHE:HB3	3:F:31:GLU:HG3	1.91	0.53
3:F:64:TYR:HD2	3:F:67:LEU:HD12	1.73	0.53
2:B:630:LYS:HG2	2:B:668:PHE:CZ	2.44	0.52
2:B:1205:LEU:HD13	2:B:1208:ARG:HD3	1.91	0.52
2:B:1601:THR:HG1	2:B:1626:PHE:HZ	1.56	0.52
1:D:677:MET:HE2	1:D:677:MET:HA	1.91	0.52
2:E:52:ASN:ND2	2:E:55:LYS:HD2	2.24	0.52
2:E:1168:TYR:O	2:E:1172:LEU:HD23	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1362:TYR:CE1	2:E:1384:ARG:HG3	2.44	0.52
2:E:1449:GLN:HA	2:E:1452:ASN:ND2	2.24	0.52
2:E:1470:LYS:HB3	2:E:1483:TRP:CD1	2.43	0.52
2:B:710:GLN:HA	2:B:713:ASN:OD1	2.09	0.52
2:B:879:LEU:HA	2:B:882:LEU:HD12	1.90	0.52
2:B:1059:LEU:HD12	2:B:1116:PRO:HB2	1.90	0.52
2:B:1175:LEU:O	2:B:1179:HIS:ND1	2.43	0.52
1:D:557:VAL:HA	1:D:579:LEU:HB3	1.91	0.52
2:E:630:LYS:HG2	2:E:668:PHE:CZ	2.44	0.52
2:E:1095:GLY:H	2:E:1098:LYS:HE3	1.72	0.52
2:B:1322:LYS:HG2	2:B:1345:ARG:NH1	2.24	0.52
2:B:1470:LYS:HD3	2:B:1483:TRP:CG	2.45	0.52
3:C:1:MET:HE3	3:C:2:GLN:N	2.23	0.52
2:E:826:ASP:HA	2:E:829:LEU:HB2	1.91	0.52
2:E:1238:ASP:HA	2:E:1241:ILE:HD12	1.92	0.52
2:E:1277:PRO:HA	2:E:1293:GLN:HG3	1.91	0.52
2:E:1322:LYS:HG2	2:E:1345:ARG:NH1	2.24	0.52
2:E:1551:LEU:HB3	2:E:1622:LEU:HD13	1.91	0.52
3:F:1:MET:HE3	3:F:2:GLN:N	2.23	0.52
3:F:87:PRO:HA	3:F:90:PHE:CD2	2.44	0.52
2:B:473:HIS:HB2	2:B:526:HIS:CE1	2.45	0.52
2:B:875:ARG:HE	2:B:924:HIS:CD2	2.26	0.52
2:B:1032:PHE:HB3	2:B:1043:TRP:CH2	2.42	0.52
1:D:536:LEU:HD21	2:E:18:ASN:H	1.73	0.52
1:D:714:PRO:HG2	2:E:44:TRP:CZ2	2.44	0.52
2:E:852:LEU:HB3	2:E:855:GLN:HB3	1.91	0.52
2:E:1449:GLN:OE1	2:E:1449:GLN:N	2.25	0.52
1:A:665:TRP:O	1:A:669:LEU:HG	2.09	0.52
2:B:19:TYR:HB2	2:B:59:PHE:HE1	1.73	0.52
2:B:906:LEU:HD12	2:B:909:ILE:HD11	1.91	0.52
2:B:923:VAL:O	2:B:927:LEU:HG	2.10	0.52
2:B:1362:TYR:HD2	2:B:1462:PHE:CE2	2.27	0.52
3:C:28:PHE:HB3	3:C:31:GLU:HG3	1.91	0.52
1:D:679:SER:HB3	1:D:681:LEU:HG	1.91	0.52
2:E:226:VAL:N	2:E:279:ALA:O	2.34	0.52
2:E:883:THR:CG2	2:E:931:ARG:HB3	2.39	0.52
2:E:923:VAL:O	2:E:927:LEU:HG	2.10	0.52
2:E:1017:PHE:O	2:E:1021:ILE:HG12	2.09	0.52
2:B:220:HIS:CE1	2:B:436:ILE:HD12	2.45	0.52
2:B:800:MET:O	2:B:804:ARG:HG3	2.10	0.52
2:B:914:ASP:HB2	2:B:963:GLN:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1040:LEU:HD12	2:B:1097:HIS:CE1	2.44	0.52
2:B:1361:GLU:OE2	2:B:1388:TYR:HA	2.10	0.52
3:C:90:PHE:CD2	3:C:137:ILE:HD12	2.44	0.52
2:E:220:HIS:CE1	2:E:436:ILE:HD12	2.45	0.52
2:E:450:LEU:HB3	2:E:620:PHE:HZ	1.75	0.52
2:E:1395:SER:O	2:E:1399:LEU:HG	2.10	0.52
2:B:654:LEU:HB3	2:B:692:LEU:HB3	1.92	0.52
2:B:826:ASP:HA	2:B:829:LEU:HB2	1.91	0.52
2:E:800:MET:O	2:E:804:ARG:HG3	2.10	0.52
2:B:267:MET:SD	2:B:274:LEU:HD22	2.50	0.52
2:B:1238:ASP:HA	2:B:1241:ILE:HD12	1.92	0.52
2:E:267:MET:SD	2:E:274:LEU:HD22	2.50	0.52
2:E:654:LEU:HB3	2:E:692:LEU:HB3	1.92	0.52
2:E:710:GLN:HA	2:E:713:ASN:OD1	2.09	0.52
2:E:965:ASP:OD1	2:E:966:ASP:N	2.42	0.52
2:E:1145:HIS:O	2:E:1149:ASN:ND2	2.43	0.52
2:E:1582:ASP:HA	2:E:1585:LYS:HZ3	1.74	0.52
3:F:43:ASN:HA	3:F:52:ASN:HA	1.91	0.52
2:B:37:ILE:HA	2:B:47:GLY:HA3	1.92	0.52
2:B:115:ARG:HE	2:B:118:GLN:HE21	1.57	0.52
2:B:771:ARG:O	2:B:775:LEU:HG	2.09	0.52
2:B:1024:PHE:HA	2:B:1027:VAL:HG22	1.91	0.52
2:B:1217:LYS:HG2	2:B:1220:ARG:NH2	2.25	0.52
2:B:1391:ARG:HH22	3:C:29:PRO:HD3	1.74	0.52
2:B:1578:GLU:HG3	2:B:1579:HIS:ND1	2.25	0.52
3:C:87:PRO:HA	3:C:90:PHE:CD2	2.44	0.52
1:D:564:LYS:HG3	1:D:575:TRP:NE1	2.25	0.52
2:E:532:ARG:NE	2:E:544:GLU:O	2.42	0.52
2:E:732:LYS:HA	2:E:735:LYS:HD3	1.91	0.52
2:E:771:ARG:O	2:E:775:LEU:HG	2.08	0.52
3:F:90:PHE:CD2	3:F:137:ILE:HD12	2.44	0.52
1:A:609:PRO:HB2	1:A:612:ASP:OD1	2.10	0.52
2:B:285:SER:N	2:B:288:ASP:OD2	2.38	0.52
2:B:965:ASP:OD1	2:B:966:ASP:N	2.42	0.52
2:B:1277:PRO:HA	2:B:1293:GLN:HG3	1.91	0.52
2:B:1362:TYR:CE1	2:B:1384:ARG:HG3	2.44	0.52
2:E:62:THR:HG23	2:E:63:TYR:HD1	1.74	0.52
2:E:257:ASN:O	2:E:488:ALA:N	2.31	0.52
2:E:554:LEU:HA	2:E:562:LEU:HB2	1.91	0.52
2:E:914:ASP:HB2	2:E:963:GLN:NE2	2.25	0.52
2:E:1362:TYR:HD2	2:E:1462:PHE:CE2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LYS:HG3	1:A:575:TRP:NE1	2.25	0.51
2:B:474:ASP:OD1	2:B:478:LYS:N	2.43	0.51
2:B:1023:GLN:O	2:B:1027:VAL:HG13	2.11	0.51
2:B:1145:HIS:O	2:B:1149:ASN:ND2	2.43	0.51
3:C:137:ILE:HG23	3:C:141:GLN:HE21	1.75	0.51
2:E:1290:VAL:HG23	2:E:1291:TYR:H	1.76	0.51
2:E:1439:PRO:HA	2:E:1442:LYS:HZ3	1.75	0.51
2:E:1632:LYS:O	2:E:1637:TYR:N	2.27	0.51
2:B:34:THR:O	2:B:50:LEU:HB2	2.10	0.51
2:B:856:LYS:O	2:B:860:MET:HE3	2.10	0.51
2:B:1099:ILE:C	2:B:1101:PHE:H	2.18	0.51
2:B:1189:SER:O	2:B:1192:VAL:HG22	2.09	0.51
3:C:69:PRO:HA	3:C:72:TYR:CD2	2.45	0.51
2:E:115:ARG:HE	2:E:118:GLN:HE21	1.58	0.51
2:E:1217:LYS:O	2:E:1221:MET:HG3	2.11	0.51
2:E:1305:ILE:HD11	2:E:1320:LEU:HB2	1.92	0.51
2:E:1406:GLU:OE1	2:E:1423:LYS:NZ	2.43	0.51
2:E:1470:LYS:HD3	2:E:1483:TRP:CG	2.45	0.51
2:B:130:GLN:HE21	2:B:144:LEU:HD11	1.73	0.51
2:B:853:VAL:HA	2:B:856:LYS:HG2	1.93	0.51
2:B:1301:TYR:HE2	2:B:1320:LEU:HD22	1.74	0.51
1:D:563:ARG:HA	1:D:573:LYS:O	2.11	0.51
2:E:474:ASP:OD1	2:E:478:LYS:N	2.43	0.51
2:E:853:VAL:HA	2:E:856:LYS:HG2	1.93	0.51
2:E:1361:GLU:OE2	2:E:1388:TYR:HA	2.10	0.51
3:F:146:ALA:O	3:F:150:GLY:N	2.43	0.51
2:E:856:LYS:O	2:E:860:MET:HE3	2.10	0.51
2:E:972:TYR:O	2:E:975:THR:N	2.39	0.51
2:E:1217:LYS:HG2	2:E:1220:ARG:NH2	2.25	0.51
3:F:69:PRO:HA	3:F:72:TYR:CD2	2.45	0.51
3:F:137:ILE:HG23	3:F:141:GLN:HE21	1.75	0.51
1:A:677:MET:HA	1:A:677:MET:HE2	1.91	0.51
2:B:62:THR:HG23	2:B:63:TYR:HD1	1.74	0.51
2:B:450:LEU:HB3	2:B:620:PHE:HZ	1.75	0.51
2:B:1391:ARG:HD2	2:B:1429:PHE:HA	1.91	0.51
2:B:1468:PHE:CE2	2:B:1470:LYS:HB2	2.45	0.51
3:C:146:ALA:O	3:C:150:GLY:N	2.43	0.51
1:D:541:GLN:O	1:D:544:ILE:HG22	2.09	0.51
1:D:665:TRP:O	1:D:669:LEU:HG	2.09	0.51
1:D:714:PRO:HG2	2:E:44:TRP:CE2	2.46	0.51
2:E:473:HIS:HB2	2:E:526:HIS:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:795:PHE:O	2:E:798:PHE:HB2	2.10	0.51
2:E:1175:LEU:O	2:E:1179:HIS:ND1	2.43	0.51
2:E:1468:PHE:HB3	2:E:1483:TRP:O	2.10	0.51
2:E:1578:GLU:HG3	2:E:1579:HIS:ND1	2.25	0.51
2:B:678:ASN:O	2:B:682:GLU:HG2	2.11	0.51
2:B:1065:SER:OG	2:B:1068:LYS:HB2	2.10	0.51
2:B:1237:GLU:O	2:B:1240:TYR:HB3	2.09	0.51
2:B:1562:GLY:HA3	3:C:36:VAL:HB	1.92	0.51
2:B:1586:VAL:HA	2:B:1589:LEU:HD12	1.93	0.51
1:D:578:ARG:HB3	1:D:587:HIS:HB2	1.91	0.51
2:E:157:ARG:HH21	2:E:194:ILE:HD13	1.76	0.51
2:E:1301:TYR:HE2	2:E:1320:LEU:HD22	1.74	0.51
2:B:1439:PRO:HA	2:B:1442:LYS:HZ3	1.75	0.51
3:C:43:ASN:HA	3:C:52:ASN:HA	1.91	0.51
3:C:153:LYS:NZ	3:C:154:TYR:O	2.44	0.51
2:E:288:ASP:OD1	2:E:291:ARG:NH2	2.33	0.51
2:E:493:ILE:HD11	2:E:496:TYR:HD1	1.75	0.51
2:E:882:LEU:O	2:E:886:LEU:HD23	2.11	0.51
2:E:1358:PRO:HB2	2:E:1387:GLU:HB2	1.93	0.51
2:E:1627:ARG:HA	2:E:1630:LYS:HB2	1.93	0.51
1:A:563:ARG:HA	1:A:573:LYS:O	2.11	0.51
2:B:380:THR:HG21	2:B:510:TYR:CD2	2.46	0.51
2:B:554:LEU:HA	2:B:562:LEU:HB2	1.91	0.51
2:B:719:TYR:CD1	2:B:723:HIS:HB2	2.45	0.51
1:D:588:TYR:N	1:D:603:SER:OG	2.44	0.51
2:E:215:ILE:O	2:E:218:THR:OG1	2.27	0.51
2:E:285:SER:N	2:E:288:ASP:OD2	2.38	0.51
2:E:1197:VAL:O	2:E:1201:LEU:HD23	2.11	0.51
1:A:723:VAL:HG23	2:B:2:ALA:HB1	1.93	0.51
2:B:46:ARG:HA	2:B:57:GLY:O	2.11	0.51
2:B:226:VAL:N	2:B:279:ALA:O	2.34	0.51
2:B:764:PHE:HA	2:B:767:ILE:HB	1.93	0.51
2:B:1358:PRO:HB2	2:B:1387:GLU:HB2	1.93	0.51
2:B:1406:GLU:OE1	2:B:1423:LYS:NZ	2.43	0.51
2:E:380:THR:HG21	2:E:510:TYR:CD2	2.46	0.51
2:E:1066:GLN:OE1	2:E:1069:ARG:NH1	2.40	0.51
2:E:1468:PHE:CE2	2:E:1470:LYS:HB2	2.45	0.51
2:E:1492:ALA:HB2	2:E:1505:LYS:HE3	1.93	0.51
1:A:596:GLN:NE2	1:A:599:VAL:HG13	2.26	0.51
2:B:157:ARG:HH21	2:B:194:ILE:HD13	1.76	0.51
2:B:288:ASP:OD1	2:B:291:ARG:NH2	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:493:ILE:HD11	2:B:496:TYR:HD1	1.75	0.51
2:B:965:ASP:O	2:B:969:TYR:N	2.42	0.51
2:B:1395:SER:O	2:B:1399:LEU:HG	2.10	0.51
3:C:164:GLY:O	3:C:168:VAL:N	2.39	0.51
1:D:609:PRO:HB2	1:D:612:ASP:OD1	2.10	0.51
1:D:688:THR:O	1:D:692:MET:HG2	2.11	0.51
2:E:1586:VAL:HA	2:E:1589:LEU:HD12	1.93	0.51
2:B:795:PHE:O	2:B:798:PHE:HB2	2.10	0.50
2:B:1305:ILE:HD11	2:B:1320:LEU:HB2	1.92	0.50
1:D:536:LEU:HG	2:E:18:ASN:OD1	2.10	0.50
1:D:596:GLN:NE2	1:D:599:VAL:HG13	2.26	0.50
2:E:760:LEU:HD22	2:E:764:PHE:CZ	2.46	0.50
2:E:1065:SER:OG	2:E:1068:LYS:HB2	2.10	0.50
1:A:588:TYR:CE1	1:A:608:LEU:HB2	2.46	0.50
1:A:659:LYS:NZ	1:A:680:ASP:OD2	2.39	0.50
2:B:180:THR:O	2:B:183:LEU:HB2	2.11	0.50
2:B:790:SER:HA	2:B:793:GLN:CD	2.36	0.50
2:B:1217:LYS:O	2:B:1221:MET:HG3	2.11	0.50
2:B:1492:ALA:HB2	2:B:1505:LYS:HE3	1.93	0.50
2:E:37:ILE:HA	2:E:47:GLY:HA3	1.92	0.50
2:E:259:LEU:HD23	2:E:490:TYR:CG	2.46	0.50
2:E:262:TRP:CZ2	2:E:266:GLY:HA2	2.46	0.50
2:E:990:PHE:CD2	2:E:1042:LEU:HD11	2.47	0.50
2:E:1466:ARG:O	2:E:1484:ILE:HA	2.11	0.50
2:B:215:ILE:O	2:B:218:THR:OG1	2.27	0.50
2:B:450:LEU:O	2:B:510:TYR:N	2.44	0.50
2:B:584:PHE:O	2:B:587:THR:OG1	2.22	0.50
2:B:760:LEU:HD22	2:B:764:PHE:CZ	2.46	0.50
2:B:852:LEU:HB3	2:B:855:GLN:HB3	1.92	0.50
2:E:180:THR:O	2:E:183:LEU:HB2	2.11	0.50
2:E:308:LEU:HG	2:E:320:ARG:HH22	1.77	0.50
2:E:678:ASN:O	2:E:682:GLU:HG2	2.11	0.50
2:E:1023:GLN:O	2:E:1027:VAL:HG13	2.11	0.50
3:F:80:ILE:HG23	3:F:112:LEU:HD12	1.93	0.50
1:A:688:THR:O	1:A:692:MET:HG2	2.11	0.50
1:A:701:LEU:HD23	2:B:31:ILE:HG23	1.93	0.50
2:B:308:LEU:HG	2:B:320:ARG:HH22	1.77	0.50
2:B:532:ARG:NE	2:B:544:GLU:O	2.42	0.50
2:B:656:LYS:O	2:B:659:GLU:HG2	2.12	0.50
2:B:1582:ASP:HA	2:B:1585:LYS:HZ3	1.76	0.50
2:E:46:ARG:HA	2:E:57:GLY:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:683:MET:HE1	2:E:689:TYR:CG	2.46	0.50
2:E:719:TYR:CD1	2:E:723:HIS:HB2	2.45	0.50
1:A:578:ARG:NH2	1:A:601:HIS:H	2.09	0.50
1:A:695:LYS:O	1:A:698:LEU:HG	2.12	0.50
2:B:259:LEU:HD23	2:B:490:TYR:CG	2.46	0.50
2:B:306:MET:HA	2:B:306:MET:HE3	1.94	0.50
2:B:471:SER:HB2	2:B:479:LEU:HD13	1.93	0.50
2:B:809:ALA:HB3	2:B:813:LYS:HZ2	1.77	0.50
2:B:1468:PHE:HB3	2:B:1483:TRP:O	2.10	0.50
2:E:225:TYR:N	2:E:404:LYS:O	2.43	0.50
2:E:680:MET:HE3	2:E:693:VAL:CG2	2.41	0.50
2:E:796:LEU:HA	2:E:799:ASN:ND2	2.27	0.50
2:E:991:ILE:HG22	2:E:1045:ASN:HD21	1.77	0.50
2:E:1371:GLY:C	2:E:1424:GLN:HE21	2.20	0.50
2:E:1484:ILE:HB	2:E:1512:ILE:HD12	1.94	0.50
1:A:588:TYR:N	1:A:603:SER:OG	2.44	0.50
2:B:1098:LYS:O	2:B:1102:ILE:HG13	2.12	0.50
2:B:1197:VAL:O	2:B:1201:LEU:HD23	2.11	0.50
2:B:1239:ILE:O	2:B:1243:TYR:HD1	1.95	0.50
2:B:1290:VAL:HG23	2:B:1291:TYR:H	1.76	0.50
2:B:1484:ILE:HB	2:B:1512:ILE:HD12	1.94	0.50
2:B:1627:ARG:HA	2:B:1630:LYS:HB2	1.92	0.50
1:D:707:PRO:HD2	2:E:16:ILE:CG2	2.41	0.50
2:E:306:MET:HA	2:E:306:MET:HE3	1.93	0.50
2:E:741:VAL:HG21	2:E:798:PHE:CD1	2.46	0.50
2:E:790:SER:HA	2:E:793:GLN:CD	2.36	0.50
2:E:797:ALA:HA	2:E:800:MET:HE2	1.94	0.50
2:E:1549:MET:HE1	3:F:56:TRP:CE2	2.47	0.50
2:B:157:ARG:HH12	2:B:197:LYS:HD3	1.77	0.50
2:B:296:LEU:HB2	2:B:329:ILE:HD13	1.94	0.50
2:B:997:ILE:HD13	2:B:1053:PHE:HB2	1.94	0.50
2:E:656:LYS:O	2:E:659:GLU:HG2	2.12	0.50
2:E:997:ILE:HD13	2:E:1053:PHE:HB2	1.94	0.50
2:E:1099:ILE:C	2:E:1101:PHE:H	2.18	0.50
3:F:169:PHE:O	3:F:173:ILE:HG12	2.12	0.50
2:B:499:VAL:O	2:B:509:TRP:NE1	2.43	0.50
2:B:796:LEU:HA	2:B:799:ASN:ND2	2.27	0.50
2:B:921:THR:OG1	2:B:924:HIS:HB3	2.12	0.50
2:B:1042:LEU:HD12	2:B:1045:ASN:HB3	1.94	0.50
2:B:1183:HIS:CG	2:B:1184:LYS:H	2.30	0.50
2:B:1388:TYR:CE2	3:C:44:VAL:HA	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:584:LYS:O	1:D:607:LYS:NZ	2.42	0.50
2:E:450:LEU:O	2:E:510:TYR:N	2.44	0.50
2:E:471:SER:HB2	2:E:479:LEU:HD13	1.93	0.50
2:E:570:VAL:HG22	2:E:592:LYS:HD3	1.94	0.50
2:E:1066:GLN:HA	2:E:1069:ARG:CZ	2.42	0.50
1:A:564:LYS:HZ3	1:A:575:TRP:CG	2.30	0.50
1:A:617:VAL:O	1:A:642:PHE:HA	2.12	0.50
2:B:683:MET:HE1	2:B:689:TYR:CG	2.46	0.50
2:B:1156:ASP:OD1	2:B:1243:TYR:OH	2.30	0.50
2:B:1408:MET:SD	2:B:1427:GLN:HB3	2.52	0.50
2:B:1464:TYR:N	2:B:1487:THR:O	2.45	0.50
2:E:189:VAL:HG13	2:E:193:ARG:NH2	2.27	0.50
2:E:466:VAL:HG22	2:E:547:PHE:HZ	1.77	0.50
2:E:474:ASP:O	2:E:526:HIS:NE2	2.45	0.50
2:E:994:LYS:HZ2	2:E:1048:HIS:HB3	1.75	0.50
2:E:1042:LEU:HD12	2:E:1045:ASN:HB3	1.94	0.50
2:E:1561:GLY:O	2:E:1565:ASN:ND2	2.31	0.50
2:B:99:ALA:O	2:B:103:ARG:HG2	2.12	0.49
2:B:225:TYR:N	2:B:404:LYS:O	2.43	0.49
2:B:1012:THR:HG22	2:B:1015:ARG:NH2	2.27	0.49
2:B:1066:GLN:HA	2:B:1069:ARG:CZ	2.42	0.49
2:B:1117:GLU:CD	2:B:1120:LEU:HG	2.37	0.49
3:C:80:ILE:HG23	3:C:112:LEU:HD12	1.93	0.49
2:E:840:PHE:O	2:E:844:ILE:HG12	2.12	0.49
2:E:1183:HIS:CG	2:E:1184:LYS:H	2.30	0.49
2:E:1408:MET:SD	2:E:1427:GLN:HB3	2.52	0.49
2:E:1464:TYR:N	2:E:1487:THR:O	2.45	0.49
2:E:1479:PHE:HA	2:E:1482:MET:HG2	1.94	0.49
2:B:882:LEU:O	2:B:886:LEU:HD23	2.11	0.49
2:B:990:PHE:CD2	2:B:1042:LEU:HD11	2.47	0.49
2:B:1466:ARG:O	2:B:1484:ILE:HA	2.11	0.49
1:D:548:ILE:HB	1:D:549:LYS:HZ2	1.76	0.49
2:E:34:THR:O	2:E:50:LEU:HB2	2.10	0.49
2:E:99:ALA:O	2:E:103:ARG:HG2	2.12	0.49
2:E:1388:TYR:CE2	3:F:44:VAL:HG13	2.46	0.49
1:A:657:PRO:HB2	1:A:661:GLU:OE2	2.12	0.49
2:B:4:TRP:CE3	2:B:46:ARG:HG2	2.47	0.49
2:B:474:ASP:O	2:B:526:HIS:NE2	2.45	0.49
2:B:1372:PHE:CZ	2:B:1424:GLN:HB3	2.48	0.49
2:B:1597:MET:HA	2:B:1600:LEU:HD12	1.95	0.49
2:E:921:THR:OG1	2:E:924:HIS:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1372:PHE:CZ	2:E:1424:GLN:HB3	2.48	0.49
2:E:1386:LYS:HG3	2:E:1387:GLU:OE1	2.12	0.49
3:F:52:ASN:OD1	3:F:53:LEU:N	2.45	0.49
1:A:531:ARG:HH21	1:A:534:LEU:HD12	1.77	0.49
2:B:189:VAL:HG13	2:B:193:ARG:NH2	2.27	0.49
2:B:262:TRP:CZ2	2:B:266:GLY:HA2	2.47	0.49
2:B:1623:SER:HB3	2:B:1627:ARG:NH2	2.27	0.49
3:C:170:ASP:HB3	3:C:174:ARG:NH2	2.26	0.49
1:D:586:LEU:HB2	1:D:608:LEU:HB2	1.94	0.49
2:E:4:TRP:CE3	2:E:46:ARG:HG2	2.47	0.49
2:E:764:PHE:HA	2:E:767:ILE:HB	1.93	0.49
2:E:1098:LYS:O	2:E:1102:ILE:HG13	2.12	0.49
3:F:137:ILE:HG23	3:F:141:GLN:HG3	1.94	0.49
1:A:586:LEU:HB2	1:A:608:LEU:HB2	1.94	0.49
2:B:840:PHE:O	2:B:844:ILE:HG12	2.12	0.49
2:B:882:LEU:HD23	2:B:885:GLN:NE2	2.27	0.49
2:B:943:MET:HG3	2:B:950:ILE:HD13	1.94	0.49
2:B:1581:GLU:OE1	2:B:1581:GLU:N	2.44	0.49
1:D:541:GLN:HG3	1:D:545:LEU:HD23	1.94	0.49
2:E:190:ALA:O	2:E:194:ILE:HG12	2.13	0.49
2:E:296:LEU:HB2	2:E:329:ILE:HD13	1.94	0.49
2:E:414:GLN:HG2	2:E:421:VAL:HG12	1.95	0.49
2:E:882:LEU:HD23	2:E:885:GLN:NE2	2.28	0.49
2:E:1082:GLU:OE2	2:E:1086:ARG:NE	2.24	0.49
2:E:1117:GLU:CD	2:E:1120:LEU:HG	2.37	0.49
2:E:1221:MET:HA	2:E:1224:THR:HG22	1.95	0.49
3:F:153:LYS:NZ	3:F:154:TYR:O	2.44	0.49
2:B:570:VAL:HG22	2:B:592:LYS:HD3	1.94	0.49
2:B:694:PHE:HZ	2:B:737:LEU:HD13	1.77	0.49
2:B:730:TYR:HB3	2:B:770:SER:HB3	1.95	0.49
2:B:741:VAL:HG21	2:B:798:PHE:CD1	2.46	0.49
1:D:531:ARG:HH21	1:D:534:LEU:HD12	1.77	0.49
1:D:548:ILE:HD13	2:E:106:TYR:CE1	2.48	0.49
1:D:617:VAL:O	1:D:642:PHE:HA	2.12	0.49
1:D:657:PRO:HB2	1:D:661:GLU:OE2	2.12	0.49
2:E:157:ARG:HH12	2:E:197:LYS:HD3	1.77	0.49
3:F:35:THR:OG1	3:F:40:TYR:OH	2.28	0.49
1:A:541:GLN:HG3	1:A:545:LEU:HD23	1.94	0.49
2:B:414:GLN:HG2	2:B:421:VAL:HG12	1.95	0.49
2:B:508:CYS:HB3	2:B:510:TYR:HE2	1.78	0.49
2:B:788:ASN:HA	2:B:831:PHE:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1371:GLY:C	2:B:1424:GLN:HE21	2.20	0.49
2:B:1534:GLN:HA	2:B:1537:ALA:HB3	1.95	0.49
2:E:4:TRP:CZ3	2:E:46:ARG:HG2	2.48	0.49
2:E:18:ASN:HA	2:E:29:LEU:O	2.13	0.49
2:E:166:ARG:HB3	2:E:171:ASN:HA	1.95	0.49
2:E:467:GLU:HB2	2:E:500:VAL:HG22	1.95	0.49
2:E:753:LEU:HD11	2:E:812:ILE:HG12	1.93	0.49
2:E:809:ALA:HB3	2:E:813:LYS:HZ2	1.77	0.49
2:E:1068:LYS:O	2:E:1072:ILE:HG12	2.13	0.49
2:E:1110:LEU:HD21	2:E:1151:LEU:HD12	1.94	0.49
2:E:1156:ASP:OD1	2:E:1243:TYR:OH	2.30	0.49
3:F:139:TYR:O	3:F:142:GLY:N	2.46	0.49
2:B:941:ILE:HD13	2:B:988:GLU:HB3	1.95	0.49
2:B:1068:LYS:O	2:B:1072:ILE:HG12	2.13	0.49
2:B:1386:LYS:HG3	2:B:1387:GLU:OE1	2.12	0.49
2:B:1479:PHE:HA	2:B:1482:MET:HG2	1.94	0.49
3:C:2:GLN:O	3:C:52:ASN:N	2.40	0.49
3:C:18:CYS:SG	3:C:32:TYR:OH	2.68	0.49
3:C:124:ASP:O	3:C:127:GLU:HG2	2.13	0.49
2:E:508:CYS:HB3	2:E:510:TYR:HE2	1.77	0.49
2:E:572:TYR:OH	2:E:589:PRO:O	2.17	0.49
2:E:1623:SER:HB3	2:E:1627:ARG:NH2	2.27	0.49
2:B:4:TRP:CZ3	2:B:46:ARG:HG2	2.48	0.49
2:B:190:ALA:O	2:B:194:ILE:HG12	2.13	0.49
2:B:466:VAL:HG22	2:B:547:PHE:HZ	1.77	0.49
2:B:680:MET:HE3	2:B:693:VAL:CG2	2.41	0.49
2:B:753:LEU:HD11	2:B:812:ILE:HG12	1.93	0.49
1:D:551:GLN:HG2	2:E:107:VAL:HA	1.95	0.49
2:E:868:LEU:HD23	2:E:912:VAL:HG11	1.94	0.49
2:E:943:MET:HG3	2:E:950:ILE:HD13	1.93	0.49
1:A:537:LYS:HG3	1:A:694:ILE:HG21	1.95	0.49
1:A:564:LYS:HZ1	1:A:590:ASP:HA	1.77	0.49
2:B:991:ILE:HG22	2:B:1045:ASN:HD21	1.77	0.49
2:B:1495:PHE:HE1	2:B:1502:PHE:HD2	1.60	0.49
2:E:788:ASN:HA	2:E:831:PHE:HE1	1.78	0.49
2:E:1242:ARG:O	2:E:1246:LYS:HG2	2.13	0.49
2:B:529:PHE:CE2	2:B:552:VAL:HG12	2.48	0.48
2:B:570:VAL:HG21	2:B:595:MET:HE3	1.94	0.48
2:B:1485:GLU:HG3	2:B:1511:GLU:OE1	2.13	0.48
1:D:695:LYS:O	1:D:698:LEU:HG	2.12	0.48
2:E:349:GLN:NE2	2:E:350:GLN:O	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1544:VAL:HG12	2:E:1610:LYS:HB3	1.95	0.48
2:E:1633:VAL:O	2:E:1639:VAL:HG22	2.13	0.48
1:A:579:LEU:HA	1:A:586:LEU:HD13	1.96	0.48
2:B:18:ASN:HA	2:B:29:LEU:O	2.13	0.48
2:B:467:GLU:HB2	2:B:500:VAL:HG22	1.95	0.48
2:B:1242:ARG:O	2:B:1246:LYS:HG2	2.13	0.48
3:C:61:GLN:HB2	3:C:64:TYR:HD1	1.78	0.48
1:D:587:HIS:HA	1:D:606:ASP:HA	1.94	0.48
1:D:588:TYR:CE1	1:D:608:LEU:HB2	2.46	0.48
2:E:718:THR:O	2:E:722:LYS:HE2	2.13	0.48
2:E:1063:THR:HA	2:E:1069:ARG:CD	2.43	0.48
2:E:1486:ARG:NE	2:E:1510:GLU:OE1	2.46	0.48
2:B:288:ASP:HA	2:B:291:ARG:NE	2.27	0.48
2:B:467:GLU:OE2	2:B:534:ARG:NH1	2.46	0.48
2:B:718:THR:O	2:B:722:LYS:HE2	2.13	0.48
2:B:797:ALA:HA	2:B:800:MET:HE2	1.94	0.48
2:B:1344:LYS:O	2:B:1347:SER:OG	2.21	0.48
2:B:1544:VAL:HG12	2:B:1610:LYS:HB3	1.95	0.48
2:B:1626:PHE:CD2	2:B:1627:ARG:HD3	2.48	0.48
2:E:467:GLU:OE2	2:E:534:ARG:NH1	2.46	0.48
2:E:694:PHE:HZ	2:E:737:LEU:HD13	1.77	0.48
2:E:1012:THR:HG22	2:E:1015:ARG:NH2	2.28	0.48
2:E:1440:SER:H	2:E:1442:LYS:HZ1	1.61	0.48
2:E:1514:PRO:HA	2:E:1517:ASN:HB2	1.94	0.48
2:E:1534:GLN:HA	2:E:1537:ALA:HB3	1.95	0.48
2:B:792:ARG:HA	2:B:795:PHE:HD2	1.79	0.48
2:B:868:LEU:HD23	2:B:912:VAL:HG11	1.94	0.48
2:B:1062:GLU:O	2:B:1069:ARG:HD3	2.13	0.48
2:B:1066:GLN:OE1	2:B:1069:ARG:NH1	2.41	0.48
3:C:53:LEU:HD22	3:C:173:ILE:HD11	1.95	0.48
2:E:288:ASP:HA	2:E:291:ARG:NE	2.27	0.48
2:E:303:VAL:HG22	2:E:319:ARG:HG2	1.95	0.48
2:E:451:ILE:HD12	2:E:621:GLN:HG2	1.96	0.48
2:E:529:PHE:CE2	2:E:552:VAL:HG12	2.48	0.48
1:A:536:LEU:HD11	2:B:17:TYR:HD2	1.78	0.48
2:B:12:TYR:HB3	2:B:67:LYS:HD3	1.95	0.48
2:B:143:GLU:HG3	2:B:147:LYS:NZ	2.28	0.48
2:B:187:HIS:CE1	2:B:1009:MET:HB2	2.49	0.48
2:B:1072:ILE:O	2:B:1076:TYR:N	2.40	0.48
3:C:137:ILE:HG23	3:C:141:GLN:HG3	1.94	0.48
2:E:929:MET:HE3	2:E:964:MET:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1256:ASN:HB3	2:E:1259:GLU:OE1	2.14	0.48
2:E:1495:PHE:HE1	2:E:1502:PHE:HD2	1.60	0.48
1:A:548:ILE:HD13	2:B:106:TYR:CE1	2.48	0.48
2:B:135:THR:HG23	2:B:136:LEU:HD22	1.95	0.48
2:B:1033:MET:HG3	2:B:1034:ASP:H	1.78	0.48
2:B:1166:GLU:O	2:B:1170:VAL:HG23	2.14	0.48
2:B:1514:PRO:HA	2:B:1517:ASN:HB2	1.94	0.48
3:C:14:VAL:HB	3:C:16:LYS:HZ2	1.79	0.48
2:E:143:GLU:HG3	2:E:147:LYS:NZ	2.28	0.48
2:E:145:LYS:O	2:E:149:THR:OG1	2.26	0.48
2:E:1239:ILE:O	2:E:1243:TYR:HD1	1.95	0.48
2:E:1418:ILE:HG21	2:E:1425:TYR:HB2	1.95	0.48
2:E:1597:MET:HA	2:E:1600:LEU:HD12	1.95	0.48
3:F:124:ASP:O	3:F:127:GLU:HG2	2.13	0.48
3:F:129:LEU:HB3	3:F:134:LEU:O	2.14	0.48
2:B:208:LEU:HD23	2:B:211:ARG:HH21	1.78	0.48
2:B:1012:THR:HG22	2:B:1015:ARG:HH22	1.79	0.48
2:B:1102:ILE:O	2:B:1106:VAL:HG23	2.14	0.48
2:B:1633:VAL:O	2:B:1639:VAL:HG22	2.13	0.48
3:C:129:LEU:HB3	3:C:134:LEU:O	2.14	0.48
2:E:208:LEU:HD23	2:E:211:ARG:HH21	1.78	0.48
2:E:721:TYR:HB2	2:E:722:LYS:HZ3	1.77	0.48
2:E:785:ASP:N	2:E:785:ASP:OD1	2.47	0.48
2:E:824:ILE:HD13	2:E:863:ILE:HD13	1.96	0.48
2:E:1012:THR:HG22	2:E:1015:ARG:HH22	1.79	0.48
2:E:1485:GLU:HG3	2:E:1511:GLU:OE1	2.13	0.48
2:E:1588:LEU:O	2:E:1592:LEU:HG	2.14	0.48
3:F:61:GLN:HB2	3:F:64:TYR:HD1	1.78	0.48
3:F:72:TYR:HD2	3:F:104:HIS:HB3	1.79	0.48
2:B:1110:LEU:HD21	2:B:1151:LEU:HD12	1.94	0.48
2:B:1632:LYS:O	2:B:1637:TYR:N	2.27	0.48
3:C:72:TYR:HD2	3:C:104:HIS:HB3	1.79	0.48
3:C:129:LEU:HA	3:C:132:LYS:HE3	1.96	0.48
2:E:187:HIS:CE1	2:E:1009:MET:HB2	2.49	0.48
2:E:228:PHE:HE2	2:E:399:LEU:HD12	1.78	0.48
2:E:660:VAL:HB	2:E:665:ILE:HD11	1.96	0.48
2:E:1062:GLU:O	2:E:1069:ARG:HD3	2.13	0.48
1:A:545:LEU:O	1:A:549:LYS:HG2	2.14	0.48
1:A:587:HIS:HA	1:A:606:ASP:HA	1.94	0.48
2:B:744:ALA:HA	2:B:753:LEU:HD22	1.96	0.48
2:B:987:MET:CE	2:B:1042:LEU:HD13	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1129:PHE:HA	2:B:1132:MET:HG3	1.96	0.48
2:B:1199:SER:O	2:B:1202:GLU:HG3	2.14	0.48
2:E:112:THR:OG1	2:E:113:LEU:N	2.45	0.48
2:E:744:ALA:HA	2:E:753:LEU:HD22	1.96	0.48
2:E:1060:GLN:OE1	2:E:1060:GLN:N	2.32	0.48
2:E:1301:TYR:O	2:E:1305:ILE:HG12	2.14	0.48
2:E:1373:PRO:HD2	2:E:1376:LEU:HD12	1.95	0.48
2:E:1474:ASP:N	2:E:1474:ASP:OD1	2.47	0.48
2:E:1632:LYS:HA	2:E:1636:HIS:HB3	1.96	0.48
3:F:5:LYS:HE2	3:F:56:TRP:HZ2	1.79	0.48
2:B:112:THR:OG1	2:B:113:LEU:N	2.45	0.48
2:B:166:ARG:HB3	2:B:171:ASN:HA	1.95	0.48
2:B:1221:MET:HA	2:B:1224:THR:HG22	1.95	0.48
2:B:1251:HIS:O	2:B:1255:GLU:N	2.47	0.48
2:B:1273:TRP:CE2	2:B:1327:THR:HG21	2.49	0.48
2:E:135:THR:HG23	2:E:136:LEU:HD22	1.95	0.48
2:E:1129:PHE:HA	2:E:1132:MET:HG3	1.96	0.48
2:E:1486:ARG:O	2:E:1510:GLU:N	2.47	0.48
2:E:1621:ARG:CZ	3:F:70:LEU:HD13	2.44	0.48
3:F:129:LEU:HA	3:F:132:LYS:HE3	1.96	0.48
2:B:340:GLU:CD	2:B:420:LEU:HD21	2.39	0.47
2:B:419:HIS:CD2	2:B:420:LEU:HG	2.50	0.47
2:B:824:ILE:HD13	2:B:863:ILE:HD13	1.96	0.47
2:B:929:MET:HE3	2:B:964:MET:CE	2.43	0.47
2:B:1256:ASN:HB3	2:B:1259:GLU:OE1	2.14	0.47
2:B:1486:ARG:NE	2:B:1510:GLU:OE1	2.46	0.47
3:C:65:ASP:HA	3:C:68:ARG:HG2	1.96	0.47
3:C:139:TYR:O	3:C:142:GLY:N	2.46	0.47
1:D:545:LEU:O	1:D:549:LYS:HG2	2.14	0.47
1:D:578:ARG:NH2	1:D:601:HIS:H	2.09	0.47
2:E:340:GLU:CD	2:E:420:LEU:HD21	2.39	0.47
2:E:730:TYR:HB3	2:E:770:SER:HB3	1.95	0.47
3:F:65:ASP:HA	3:F:68:ARG:HG2	1.96	0.47
3:F:170:ASP:HB3	3:F:174:ARG:NH2	2.26	0.47
2:B:88:VAL:O	2:B:91:LEU:HG	2.14	0.47
2:B:1109:ILE:HG21	2:B:1131:MET:HE1	1.96	0.47
2:B:1200:LEU:O	2:B:1204:LEU:HD23	2.14	0.47
2:B:1301:TYR:O	2:B:1305:ILE:HG12	2.14	0.47
2:B:1470:LYS:HD3	2:B:1483:TRP:CD1	2.49	0.47
3:C:5:LYS:HE2	3:C:56:TRP:HZ2	1.79	0.47
1:D:537:LYS:HG3	1:D:694:ILE:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:987:MET:CE	2:E:1042:LEU:HD13	2.44	0.47
2:E:1516:GLU:O	2:E:1517:ASN:C	2.57	0.47
2:B:166:ARG:HG2	2:B:173:LEU:HB2	1.96	0.47
2:B:228:PHE:HE2	2:B:399:LEU:HD12	1.78	0.47
2:B:785:ASP:OD1	2:B:785:ASP:N	2.47	0.47
2:B:990:PHE:CE2	2:B:1042:LEU:HD21	2.49	0.47
2:B:1063:THR:HA	2:B:1069:ARG:CD	2.43	0.47
2:B:1418:ILE:HG21	2:B:1425:TYR:HB2	1.95	0.47
1:D:584:LYS:NZ	2:E:1403:PRO:HA	2.29	0.47
2:E:570:VAL:HG21	2:E:595:MET:HE3	1.94	0.47
2:E:941:ILE:HD13	2:E:988:GLU:HB3	1.95	0.47
2:E:1062:GLU:O	2:E:1068:LYS:HB3	2.15	0.47
2:E:1102:ILE:O	2:E:1106:VAL:HG23	2.14	0.47
2:E:1251:HIS:O	2:E:1255:GLU:N	2.47	0.47
2:E:1273:TRP:CE2	2:E:1327:THR:HG21	2.49	0.47
2:E:1621:ARG:HD3	3:F:67:LEU:HD22	1.95	0.47
3:F:2:GLN:O	3:F:52:ASN:N	2.40	0.47
3:F:164:GLY:O	3:F:168:VAL:HG23	2.14	0.47
1:A:564:LYS:O	1:A:573:LYS:NZ	2.32	0.47
2:B:572:TYR:OH	2:B:589:PRO:O	2.17	0.47
3:C:96:LYS:C	3:C:99:PRO:HD2	2.40	0.47
3:C:169:PHE:O	3:C:173:ILE:HG12	2.12	0.47
2:E:792:ARG:HA	2:E:795:PHE:HD2	1.79	0.47
2:E:868:LEU:HD13	2:E:878:LEU:HD21	1.96	0.47
2:E:965:ASP:O	2:E:969:TYR:N	2.42	0.47
2:E:1166:GLU:O	2:E:1170:VAL:HG23	2.14	0.47
2:E:1452:ASN:HA	2:E:1455:ARG:HB2	1.96	0.47
2:E:1485:GLU:OE1	2:E:1485:GLU:N	2.47	0.47
2:B:154:HIS:O	2:B:157:ARG:HG2	2.14	0.47
2:B:303:VAL:HG22	2:B:319:ARG:HG2	1.95	0.47
2:B:436:ILE:HG22	2:B:438:LEU:HD22	1.97	0.47
2:B:661:ASP:O	2:B:665:ILE:HG12	2.15	0.47
2:B:859:CYS:O	2:B:863:ILE:HG12	2.13	0.47
2:B:1060:GLN:HG2	2:B:1061:LEU:N	2.30	0.47
2:B:1485:GLU:OE1	2:B:1485:GLU:N	2.47	0.47
3:C:164:GLY:O	3:C:168:VAL:HG23	2.14	0.47
1:D:578:ARG:O	1:D:587:HIS:N	2.24	0.47
1:D:698:LEU:HA	2:E:31:ILE:HG21	1.95	0.47
2:E:154:HIS:O	2:E:157:ARG:HG2	2.14	0.47
2:E:661:ASP:O	2:E:665:ILE:HG12	2.15	0.47
2:E:1060:GLN:HG2	2:E:1061:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1200:LEU:O	2:E:1204:LEU:HD23	2.14	0.47
2:E:1470:LYS:HD3	2:E:1483:TRP:CD1	2.49	0.47
2:B:578:LYS:HB3	2:B:584:PHE:CE2	2.49	0.47
2:B:1083:ILE:O	2:B:1087:ILE:HG12	2.15	0.47
2:B:1127:ILE:O	2:B:1131:MET:HG3	2.15	0.47
2:B:1474:ASP:N	2:B:1474:ASP:OD1	2.47	0.47
1:D:579:LEU:HA	1:D:586:LEU:HD13	1.96	0.47
2:E:119:GLN:HE22	2:E:120:MET:HE3	1.80	0.47
2:E:170:GLY:O	2:E:172:ILE:HG23	2.14	0.47
2:E:809:ALA:HB3	2:E:813:LYS:NZ	2.30	0.47
2:E:866:SER:C	2:E:868:LEU:H	2.21	0.47
2:E:882:LEU:HA	2:E:885:GLN:NE2	2.30	0.47
3:F:121:ASP:HA	3:F:126:ILE:HD11	1.97	0.47
3:F:163:ARG:C	3:F:165:LEU:H	2.23	0.47
1:A:700:ASP:HB2	2:B:32:GLY:HA2	1.96	0.47
2:B:119:GLN:HE22	2:B:120:MET:HE3	1.80	0.47
2:B:328:ASP:OD1	2:B:328:ASP:N	2.47	0.47
2:B:382:VAL:O	2:B:386:VAL:HG23	2.15	0.47
2:B:451:ILE:HD12	2:B:621:GLN:HG2	1.96	0.47
2:B:743:ASN:HB3	2:B:749:LYS:HD2	1.95	0.47
2:B:783:ASP:HB3	2:B:786:GLU:HB2	1.97	0.47
2:B:816:ALA:O	2:B:820:LEU:HD23	2.15	0.47
2:B:1121:ARG:HG2	2:B:1125:ILE:HD11	1.96	0.47
2:B:1452:ASN:OD1	2:B:1453:TYR:N	2.48	0.47
2:B:1530:SER:O	2:B:1534:GLN:OE1	2.33	0.47
2:B:1555:VAL:HG21	2:B:1622:LEU:HD22	1.97	0.47
2:B:1588:LEU:O	2:B:1592:LEU:HG	2.14	0.47
3:C:6:CYS:SG	3:C:79:LEU:HD23	2.55	0.47
3:C:163:ARG:C	3:C:165:LEU:H	2.22	0.47
2:E:12:TYR:HB3	2:E:67:LYS:HD3	1.95	0.47
2:E:105:LEU:HD23	2:E:105:LEU:HA	1.73	0.47
2:E:382:VAL:O	2:E:386:VAL:HG23	2.15	0.47
2:E:471:SER:OG	2:E:528:ARG:HB3	2.15	0.47
2:E:499:VAL:O	2:E:509:TRP:NE1	2.43	0.47
2:E:783:ASP:HB3	2:E:786:GLU:HB2	1.97	0.47
2:E:859:CYS:O	2:E:863:ILE:HG12	2.13	0.47
2:E:1033:MET:HG3	2:E:1034:ASP:H	1.78	0.47
2:E:1199:SER:O	2:E:1202:GLU:HG3	2.14	0.47
2:E:1231:TYR:CE2	2:E:1239:ILE:HD12	2.49	0.47
2:E:1432:LYS:HZ1	2:E:1465:SER:H	1.61	0.47
2:B:533:HIS:HB3	2:B:544:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1125:ILE:N	2:B:1126:PRO:HD2	2.29	0.47
1:D:547:LEU:O	1:D:550:GLN:NE2	2.48	0.47
1:D:687:ASP:OD1	1:D:688:THR:N	2.47	0.47
2:E:38:LEU:HD23	2:E:48:TYR:H	1.80	0.47
2:E:88:VAL:O	2:E:91:LEU:HG	2.14	0.47
2:E:468:VAL:HB	2:E:498:SER:HB3	1.97	0.47
2:E:533:HIS:HB3	2:E:544:GLU:HG2	1.96	0.47
2:E:1042:LEU:O	2:E:1045:ASN:N	2.48	0.47
2:E:1127:ILE:O	2:E:1131:MET:HG3	2.15	0.47
2:E:1154:LYS:HA	2:E:1157:GLN:OE1	2.15	0.47
2:E:1483:TRP:NE1	2:E:1514:PRO:HD3	2.30	0.47
2:E:1626:PHE:CD2	2:E:1627:ARG:HD3	2.48	0.47
3:F:64:TYR:HB2	3:F:68:ARG:NH2	2.30	0.47
1:A:687:ASP:OD1	1:A:688:THR:N	2.48	0.47
2:B:170:GLY:O	2:B:172:ILE:HG23	2.14	0.47
2:B:287:MET:SD	2:B:291:ARG:NH2	2.88	0.47
2:B:1386:LYS:HB3	2:B:1389:GLU:HG3	1.97	0.47
2:B:1632:LYS:HA	2:B:1636:HIS:HB3	1.96	0.47
1:D:697:ARG:HH21	2:E:30:GLN:CB	2.16	0.47
2:E:287:MET:SD	2:E:291:ARG:NH2	2.88	0.47
2:E:419:HIS:CD2	2:E:420:LEU:HG	2.49	0.47
2:E:578:LYS:HB3	2:E:584:PHE:CE2	2.49	0.47
2:E:816:ALA:O	2:E:820:LEU:HD23	2.15	0.47
2:E:987:MET:SD	2:E:1042:LEU:HD13	2.54	0.47
2:E:1125:ILE:N	2:E:1126:PRO:HD2	2.29	0.47
2:B:113:LEU:HA	2:B:116:GLN:CD	2.41	0.47
2:B:166:ARG:NH1	2:B:168:ASP:H	2.13	0.47
2:B:327:MET:HE1	2:B:344:HIS:ND1	2.30	0.47
2:B:868:LEU:HD13	2:B:878:LEU:HD21	1.96	0.47
2:B:1042:LEU:O	2:B:1045:ASN:N	2.48	0.47
2:B:1075:LYS:HE3	2:B:1075:LYS:HB3	1.58	0.47
2:B:1406:GLU:HG3	2:B:1425:TYR:CE1	2.50	0.47
2:B:1452:ASN:HA	2:B:1455:ARG:HB2	1.96	0.47
2:B:1486:ARG:O	2:B:1510:GLU:N	2.47	0.47
2:E:305:HIS:HA	2:E:315:THR:O	2.15	0.47
3:F:53:LEU:HD22	3:F:173:ILE:HD11	1.95	0.47
2:B:706:ASP:O	2:B:710:GLN:N	2.48	0.46
2:B:871:GLN:HB3	2:B:875:ARG:HB2	1.97	0.46
2:B:1373:PRO:HD2	2:B:1376:LEU:HD12	1.95	0.46
3:C:35:THR:HG1	3:C:40:TYR:HH	1.52	0.46
1:D:688:THR:O	1:D:691:SER:OG	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1557:PRO:HB2	2:E:1560:MET:O	2.15	0.46
2:B:660:VAL:HB	2:B:665:ILE:HD11	1.96	0.46
2:B:931:ARG:C	2:B:932:LEU:HD22	2.41	0.46
2:B:1388:TYR:HE2	3:C:44:VAL:HG13	1.80	0.46
2:E:59:PHE:CD2	2:E:64:ILE:HG12	2.50	0.46
2:E:79:THR:HA	2:E:85:LEU:HD22	1.98	0.46
2:E:706:ASP:O	2:E:710:GLN:N	2.48	0.46
2:E:743:ASN:HB3	2:E:749:LYS:HD2	1.95	0.46
2:E:990:PHE:CE2	2:E:1042:LEU:HD21	2.49	0.46
2:E:1109:ILE:HG21	2:E:1131:MET:HE1	1.96	0.46
2:E:1452:ASN:OD1	2:E:1453:TYR:N	2.48	0.46
2:E:1573:GLU:O	2:E:1577:GLN:NE2	2.48	0.46
3:F:14:VAL:HB	3:F:16:LYS:HZ2	1.80	0.46
3:F:96:LYS:C	3:F:99:PRO:HD2	2.40	0.46
2:B:258:TYR:HA	2:B:488:ALA:HB3	1.98	0.46
2:B:349:GLN:NE2	2:B:350:GLN:O	2.43	0.46
2:B:866:SER:C	2:B:868:LEU:H	2.22	0.46
2:B:994:LYS:HZ2	2:B:1048:HIS:HB3	1.79	0.46
2:B:1231:TYR:CE2	2:B:1239:ILE:HD12	2.49	0.46
1:D:724:TYR:HB2	2:E:4:TRP:O	2.15	0.46
2:E:59:PHE:CE2	2:E:63:TYR:HB3	2.50	0.46
2:E:166:ARG:HG2	2:E:173:LEU:HB2	1.96	0.46
2:E:700:ILE:O	2:E:703:LEU:HG	2.16	0.46
2:E:1233:GLU:HG3	2:E:1234:LYS:HD2	1.97	0.46
3:F:132:LYS:HD2	3:F:134:LEU:HD12	1.98	0.46
2:B:59:PHE:CE2	2:B:63:TYR:HB3	2.50	0.46
2:B:806:LEU:HD12	2:B:813:LYS:HE3	1.97	0.46
2:B:817:LEU:HB2	2:B:855:GLN:HG3	1.98	0.46
2:B:882:LEU:HA	2:B:885:GLN:NE2	2.30	0.46
2:B:1154:LYS:HA	2:B:1157:GLN:OE1	2.15	0.46
2:B:1470:LYS:O	2:B:1481:THR:HA	2.15	0.46
2:B:1536:HIS:CD2	2:B:1542:LEU:HB3	2.50	0.46
2:B:1557:PRO:HB2	2:B:1560:MET:O	2.15	0.46
2:B:1573:GLU:O	2:B:1577:GLN:NE2	2.48	0.46
2:E:327:MET:HE1	2:E:344:HIS:ND1	2.30	0.46
2:E:436:ILE:HG22	2:E:438:LEU:HD22	1.97	0.46
2:E:594:GLU:HA	2:E:597:GLU:HG3	1.97	0.46
2:E:871:GLN:HB3	2:E:875:ARG:HB2	1.97	0.46
2:E:879:LEU:O	2:E:882:LEU:N	2.49	0.46
2:E:1015:ARG:N	2:E:1079:MET:HE1	2.31	0.46
2:E:1386:LYS:HB3	2:E:1389:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1406:GLU:HG3	2:E:1425:TYR:CE1	2.50	0.46
2:E:1470:LYS:O	2:E:1481:THR:HA	2.15	0.46
2:E:1470:LYS:N	2:E:1481:THR:O	2.46	0.46
2:E:1530:SER:O	2:E:1534:GLN:OE1	2.33	0.46
1:A:543:GLU:H	1:A:543:GLU:CD	2.24	0.46
1:A:693:GLU:O	1:A:697:ARG:HG2	2.15	0.46
2:B:111:LEU:O	2:B:115:ARG:HG2	2.16	0.46
2:B:127:TRP:O	2:B:130:GLN:HG2	2.16	0.46
2:B:809:ALA:HB3	2:B:813:LYS:NZ	2.30	0.46
2:B:1125:ILE:HD13	2:B:1171:LEU:HD22	1.98	0.46
2:B:1483:TRP:NE1	2:B:1514:PRO:HD3	2.30	0.46
3:C:64:TYR:HB2	3:C:68:ARG:NH2	2.30	0.46
1:D:536:LEU:HA	1:D:539:LYS:HE3	1.98	0.46
1:D:544:ILE:O	1:D:548:ILE:HG12	2.15	0.46
2:E:931:ARG:C	2:E:932:LEU:HD22	2.41	0.46
2:E:932:LEU:CA	2:E:935:ARG:HE	2.28	0.46
2:E:1083:ILE:O	2:E:1087:ILE:HG12	2.15	0.46
3:F:82:PHE:HE1	3:F:112:LEU:HG	1.80	0.46
1:A:544:ILE:O	1:A:548:ILE:HG12	2.15	0.46
2:B:38:LEU:HD23	2:B:48:TYR:H	1.80	0.46
2:B:189:VAL:O	2:B:193:ARG:HG2	2.16	0.46
2:B:647:SER:HA	2:B:650:ILE:HG13	1.97	0.46
2:B:700:ILE:O	2:B:703:LEU:HG	2.16	0.46
2:B:1015:ARG:N	2:B:1079:MET:HE1	2.31	0.46
2:B:1561:GLY:O	2:B:1565:ASN:ND2	2.31	0.46
1:A:547:LEU:O	1:A:550:GLN:NE2	2.48	0.46
1:A:727:ASN:H	2:B:46:ARG:HH22	1.62	0.46
2:B:987:MET:SD	2:B:1042:LEU:HD13	2.54	0.46
2:B:1406:GLU:C	2:B:1407:LYS:HD3	2.40	0.46
2:B:1516:GLU:O	2:B:1517:ASN:C	2.57	0.46
2:B:1530:SER:O	2:B:1533:VAL:HB	2.15	0.46
3:C:52:ASN:OD1	3:C:53:LEU:N	2.45	0.46
2:E:10:GLN:HG3	2:E:37:ILE:HB	1.98	0.46
2:E:1406:GLU:C	2:E:1407:LYS:HD3	2.40	0.46
3:F:164:GLY:O	3:F:168:VAL:N	2.39	0.46
1:A:622:CYS:HB3	1:A:624:HIS:ND1	2.31	0.46
2:B:127:TRP:O	2:B:131:ILE:HG12	2.16	0.46
2:B:979:ARG:O	2:B:982:ILE:HG22	2.16	0.46
2:B:1611:LEU:HD12	2:B:1615:LEU:HB2	1.96	0.46
2:E:113:LEU:HA	2:E:116:GLN:CD	2.40	0.46
2:E:267:MET:SD	2:E:268:PRO:HD2	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:679:ILE:HG22	2:E:680:MET:HE2	1.98	0.46
2:E:757:LEU:HD13	2:E:815:ALA:HB3	1.98	0.46
2:E:966:ASP:HA	2:E:969:TYR:CD2	2.48	0.46
2:E:1536:HIS:CD2	2:E:1542:LEU:HB3	2.50	0.46
3:F:6:CYS:SG	3:F:79:LEU:HD23	2.55	0.46
2:B:79:THR:HA	2:B:85:LEU:HD22	1.98	0.46
2:B:195:GLU:HA	2:B:198:ILE:HG12	1.97	0.46
2:B:679:ILE:HG22	2:B:680:MET:HE2	1.98	0.46
2:B:1062:GLU:O	2:B:1068:LYS:HB3	2.15	0.46
1:D:562:PHE:CE1	1:D:577:CYS:HB3	2.51	0.46
2:E:127:TRP:O	2:E:130:GLN:HG2	2.16	0.46
2:E:127:TRP:O	2:E:131:ILE:HG12	2.16	0.46
2:E:979:ARG:O	2:E:982:ILE:HG22	2.16	0.46
2:E:1555:VAL:HG21	2:E:1622:LEU:HD22	1.97	0.46
2:B:319:ARG:HB2	2:B:499:VAL:HA	1.98	0.46
2:B:468:VAL:HB	2:B:498:SER:HB3	1.97	0.46
1:D:591:LEU:HD22	1:D:604:LEU:HD13	1.98	0.46
2:E:166:ARG:NH1	2:E:168:ASP:H	2.13	0.46
2:E:732:LYS:O	2:E:736:VAL:HG23	2.15	0.46
2:E:817:LEU:HB2	2:E:855:GLN:HG3	1.98	0.46
2:E:1306:SER:O	2:E:1310:LYS:HG2	2.16	0.46
2:E:1530:SER:O	2:E:1533:VAL:HB	2.15	0.46
2:E:1611:LEU:HD12	2:E:1615:LEU:HB2	1.96	0.46
2:B:115:ARG:HE	2:B:118:GLN:NE2	2.14	0.45
2:B:1306:SER:O	2:B:1310:LYS:HG2	2.16	0.45
3:C:121:ASP:HA	3:C:126:ILE:HD11	1.97	0.45
3:C:135:THR:HB	3:C:137:ILE:HG13	1.98	0.45
1:D:629:GLY:O	1:D:632:LYS:HG3	2.16	0.45
2:E:195:GLU:HA	2:E:198:ILE:HG12	1.97	0.45
2:E:258:TYR:HA	2:E:488:ALA:HB3	1.97	0.45
2:E:473:HIS:CE1	2:E:479:LEU:HB2	2.51	0.45
2:E:647:SER:HA	2:E:650:ILE:HG13	1.97	0.45
2:E:806:LEU:HD12	2:E:813:LYS:HE3	1.97	0.45
2:E:908:ASN:O	2:E:912:VAL:HG23	2.16	0.45
2:E:964:MET:SD	2:E:965:ASP:N	2.87	0.45
2:E:1545:HIS:HD2	3:F:5:LYS:HE3	1.79	0.45
2:E:1549:MET:HA	3:F:39:ASN:HD21	1.79	0.45
3:F:135:THR:HB	3:F:137:ILE:HG13	1.98	0.45
1:A:536:LEU:HA	1:A:539:LYS:HE3	1.98	0.45
1:A:550:GLN:HA	1:A:553:LEU:HD12	1.98	0.45
1:A:562:PHE:CE1	1:A:577:CYS:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:GLN:HG3	2:B:37:ILE:HB	1.97	0.45
2:B:188:GLU:O	2:B:192:LYS:HG3	2.16	0.45
2:B:594:GLU:HA	2:B:597:GLU:HG3	1.97	0.45
2:B:879:LEU:O	2:B:882:LEU:N	2.49	0.45
2:B:964:MET:SD	2:B:965:ASP:N	2.87	0.45
2:B:1233:GLU:HG3	2:B:1234:LYS:HD2	1.97	0.45
3:C:82:PHE:HE1	3:C:112:LEU:HG	1.81	0.45
3:C:132:LYS:HD2	3:C:134:LEU:HD12	1.98	0.45
2:E:26:GLU:OE1	2:E:29:LEU:HD11	2.16	0.45
2:E:188:GLU:O	2:E:192:LYS:HG3	2.16	0.45
2:E:243:MET:HA	2:E:298:CYS:HA	1.99	0.45
2:E:1153:THR:HG22	2:E:1157:GLN:HE22	1.81	0.45
2:E:1251:HIS:NE2	2:E:1498:ILE:O	2.49	0.45
2:E:1268:ALA:HA	2:E:1271:LEU:HD13	1.98	0.45
2:E:1581:GLU:OE1	2:E:1581:GLU:N	2.44	0.45
2:B:243:MET:HA	2:B:298:CYS:HA	1.99	0.45
2:B:305:HIS:HA	2:B:315:THR:O	2.16	0.45
2:B:471:SER:OG	2:B:528:ARG:HB3	2.15	0.45
2:B:732:LYS:O	2:B:736:VAL:HG23	2.15	0.45
2:B:795:PHE:CE2	2:B:839:LEU:HD13	2.52	0.45
2:B:1111:GLU:O	2:B:1163:ARG:NH1	2.42	0.45
2:B:1183:HIS:HB3	2:B:1187:SER:OG	2.16	0.45
3:C:49:LYS:HZ2	3:C:51:VAL:HG12	1.81	0.45
2:E:896:LYS:HA	2:E:899:HIS:CE1	2.51	0.45
2:E:945:ARG:HH11	2:E:946:GLN:N	2.14	0.45
2:E:1125:ILE:HD13	2:E:1171:LEU:HD22	1.98	0.45
1:A:557:VAL:O	1:A:578:ARG:HG3	2.16	0.45
1:A:591:LEU:HD22	1:A:604:LEU:HD13	1.98	0.45
1:A:717:PRO:HD2	2:B:1:MET:HE2	1.98	0.45
2:B:267:MET:SD	2:B:268:PRO:HD2	2.56	0.45
2:B:927:LEU:CB	2:B:931:ARG:HH21	2.29	0.45
2:B:1153:THR:HG22	2:B:1157:GLN:HE22	1.81	0.45
2:B:1463:ARG:HA	2:B:1488:THR:HA	1.98	0.45
2:E:474:ASP:OD2	2:E:478:LYS:HE3	2.17	0.45
2:E:772:VAL:O	2:E:776:ARG:HG2	2.16	0.45
2:E:1201:LEU:O	2:E:1205:LEU:HD23	2.17	0.45
1:A:640:LEU:O	1:A:655:ILE:HA	2.16	0.45
2:B:757:LEU:HD13	2:B:815:ALA:HB3	1.98	0.45
2:B:896:LYS:HA	2:B:899:HIS:CE1	2.51	0.45
2:B:1032:PHE:O	2:B:1040:LEU:HD22	2.17	0.45
2:B:1201:LEU:O	2:B:1205:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:95:ALA:O	3:C:99:PRO:HG2	2.16	0.45
1:D:693:GLU:O	1:D:697:ARG:HG2	2.15	0.45
1:D:701:LEU:HD23	2:E:31:ILE:CG2	2.43	0.45
2:E:115:ARG:HE	2:E:118:GLN:NE2	2.14	0.45
2:E:1033:MET:N	2:E:1035:GLN:HE21	2.14	0.45
2:E:1121:ARG:HG2	2:E:1125:ILE:HD11	1.96	0.45
2:B:181:ILE:HG22	2:B:185:LYS:HZ1	1.79	0.45
2:B:184:PHE:O	2:B:188:GLU:OE1	2.35	0.45
2:B:473:HIS:CE1	2:B:479:LEU:HB2	2.51	0.45
3:C:18:CYS:HG	3:C:32:TYR:HH	1.56	0.45
1:D:550:GLN:HA	1:D:553:LEU:HD12	1.98	0.45
1:D:663:CYS:HB3	1:D:679:SER:HA	1.99	0.45
2:E:302:ARG:HD3	2:E:322:PHE:CD1	2.52	0.45
2:E:727:THR:O	2:E:774:TYR:HB2	2.17	0.45
2:E:1473:LYS:HD3	2:E:1481:THR:HG21	1.99	0.45
2:B:930:GLU:O	2:B:935:ARG:NH2	2.50	0.45
2:B:1193:PHE:O	2:B:1196:LEU:HB3	2.17	0.45
2:B:1251:HIS:NE2	2:B:1498:ILE:O	2.49	0.45
1:D:532:PRO:O	1:D:536:LEU:HD13	2.17	0.45
2:E:111:LEU:O	2:E:115:ARG:HG2	2.16	0.45
2:E:166:ARG:HB2	2:E:174:ASP:H	1.82	0.45
2:E:189:VAL:O	2:E:193:ARG:HG2	2.16	0.45
2:E:1072:ILE:O	2:E:1076:TYR:N	2.40	0.45
2:E:1183:HIS:HB3	2:E:1187:SER:OG	2.16	0.45
3:F:95:ALA:O	3:F:99:PRO:HG2	2.16	0.45
1:A:625:MET:HE3	1:A:638:LEU:HD12	1.99	0.45
2:B:332:ILE:HD13	2:B:403:LEU:HD12	1.99	0.45
2:B:697:LEU:O	2:B:701:ILE:HG12	2.17	0.45
2:B:945:ARG:HH11	2:B:946:GLN:N	2.14	0.45
2:E:876:GLU:HA	2:E:924:HIS:HE2	1.82	0.45
2:E:927:LEU:CB	2:E:931:ARG:HH21	2.29	0.45
2:E:930:GLU:O	2:E:935:ARG:NH2	2.50	0.45
2:E:1193:PHE:O	2:E:1196:LEU:HB3	2.17	0.45
1:A:646:TYR:CE1	1:A:652:LEU:HG	2.52	0.45
1:A:716:GLU:HG3	2:B:44:TRP:CZ2	2.52	0.45
2:B:142:ALA:O	2:B:146:LYS:HG3	2.16	0.45
2:B:339:ASP:OD1	2:B:339:ASP:N	2.50	0.45
2:B:908:ASN:O	2:B:912:VAL:HG23	2.16	0.45
2:B:1611:LEU:HD13	2:B:1619:HIS:HB2	1.99	0.45
1:D:622:CYS:HB3	1:D:624:HIS:ND1	2.31	0.45
2:E:102:TRP:CH2	2:E:118:GLN:HG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:179:SER:OG	2:E:182:ALA:HB3	2.17	0.45
2:E:584:PHE:CE2	2:E:588:LEU:HD11	2.51	0.45
2:E:764:PHE:HD2	2:E:767:ILE:HD12	1.82	0.45
2:E:870:ARG:HH12	2:E:874:CYS:N	2.15	0.45
2:E:1412:THR:HB	2:E:1413:PRO:HD3	1.99	0.45
1:A:572:ASP:CG	1:A:592:GLU:HA	2.42	0.45
1:A:629:GLY:O	1:A:632:LYS:HG3	2.16	0.45
1:A:663:CYS:HB3	1:A:679:SER:HA	1.99	0.45
1:A:708:ASP:N	1:A:708:ASP:OD1	2.50	0.45
2:B:26:GLU:HG3	2:B:58:ILE:O	2.17	0.45
2:B:98:TRP:HZ3	2:B:159:LEU:HD12	1.82	0.45
2:B:166:ARG:HB2	2:B:174:ASP:H	1.82	0.45
2:B:294:VAL:N	2:B:330:THR:OG1	2.26	0.45
2:B:727:THR:O	2:B:774:TYR:HB2	2.17	0.45
2:B:789:ASN:HA	2:B:792:ARG:HD2	1.98	0.45
2:B:1033:MET:N	2:B:1035:GLN:HE21	2.14	0.45
2:B:1043:TRP:CE3	2:B:1043:TRP:N	2.83	0.45
2:B:1058:SER:HA	2:B:1080:ARG:NH1	2.32	0.45
2:B:1122:LYS:HD2	2:B:1171:LEU:HD11	1.99	0.45
2:B:1361:GLU:C	2:B:1362:TYR:HD1	2.25	0.45
2:B:1417:ASP:N	2:B:1417:ASP:OD1	2.50	0.45
2:B:1469:ARG:NH1	2:B:1473:LYS:HG3	2.33	0.45
3:C:149:ILE:HG23	3:C:151:ALA:H	1.82	0.45
2:E:877:VAL:O	2:E:880:PRO:HD2	2.17	0.45
2:E:1058:SER:HA	2:E:1080:ARG:NH1	2.32	0.45
2:E:1087:ILE:HA	2:E:1090:MET:HG2	1.99	0.45
2:E:1361:GLU:C	2:E:1362:TYR:HD1	2.25	0.45
3:F:149:ILE:HG23	3:F:151:ALA:H	1.82	0.45
2:B:146:LYS:HE2	2:B:146:LYS:HB2	1.78	0.44
2:B:854:ARG:HA	2:B:854:ARG:HD2	1.72	0.44
1:D:640:LEU:O	1:D:655:ILE:HA	2.16	0.44
2:E:37:ILE:HD13	2:E:45:TYR:CB	2.48	0.44
2:E:87:LEU:O	2:E:90:GLU:HG3	2.17	0.44
2:E:332:ILE:HD13	2:E:403:LEU:HD12	1.99	0.44
2:E:1391:ARG:CD	2:E:1429:PHE:HA	2.47	0.44
2:B:772:VAL:O	2:B:776:ARG:HG2	2.16	0.44
2:B:870:ARG:NH1	2:B:874:CYS:SG	2.91	0.44
2:B:1206:ASP:O	2:B:1210:ILE:HG12	2.17	0.44
2:B:1473:LYS:HD3	2:B:1481:THR:HG21	1.99	0.44
2:B:1482:MET:HA	2:B:1482:MET:HE3	1.99	0.44
2:B:1617:PRO:O	2:B:1620:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:557:VAL:O	1:D:578:ARG:HG3	2.16	0.44
1:D:708:ASP:OD1	1:D:708:ASP:N	2.50	0.44
1:D:721:ASP:OD1	1:D:721:ASP:N	2.50	0.44
2:E:802:MET:HE1	2:E:846:SER:C	2.43	0.44
2:E:879:LEU:O	2:E:880:PRO:C	2.61	0.44
2:E:1022:ASN:HB3	2:E:1086:ARG:HH12	1.83	0.44
2:E:1054:LEU:HD11	2:E:1080:ARG:HB3	1.99	0.44
3:F:110:ILE:O	3:F:152:VAL:HG12	2.17	0.44
1:A:549:LYS:HE3	1:A:677:MET:HG2	2.00	0.44
2:B:204:ILE:CG1	2:B:211:ARG:HB3	2.46	0.44
2:B:870:ARG:HH12	2:B:874:CYS:N	2.15	0.44
2:B:875:ARG:HG2	2:B:924:HIS:CE1	2.52	0.44
2:B:923:VAL:O	2:B:926:GLN:HB2	2.17	0.44
2:B:1372:PHE:N	2:B:1424:GLN:HG2	2.33	0.44
2:B:1391:ARG:CD	2:B:1429:PHE:HA	2.47	0.44
3:C:72:TYR:HB3	3:C:105:CYS:SG	2.58	0.44
3:C:85:VAL:O	3:C:129:LEU:HD21	2.17	0.44
1:D:625:MET:HE3	1:D:638:LEU:HD12	1.99	0.44
2:E:10:GLN:NE2	2:E:37:ILE:O	2.34	0.44
2:E:25:VAL:HB	2:E:56:LYS:O	2.18	0.44
2:E:204:ILE:CG1	2:E:211:ARG:HB3	2.46	0.44
2:E:328:ASP:OD1	2:E:328:ASP:N	2.47	0.44
2:E:761:LYS:HE2	2:E:765:ARG:NE	2.32	0.44
2:E:795:PHE:CE2	2:E:839:LEU:HD13	2.52	0.44
2:E:854:ARG:HA	2:E:854:ARG:HD2	1.72	0.44
2:E:857:LEU:HD13	2:E:905:LEU:HD11	2.00	0.44
2:E:870:ARG:NH1	2:E:874:CYS:SG	2.91	0.44
2:E:875:ARG:HG2	2:E:924:HIS:CE1	2.52	0.44
2:E:1125:ILE:HD12	2:E:1125:ILE:H	1.82	0.44
2:E:1259:GLU:HG3	2:E:1497:GLY:O	2.17	0.44
2:B:140:GLU:O	2:B:144:LEU:HD23	2.17	0.44
2:B:652:HIS:CD2	2:B:656:LYS:HD3	2.53	0.44
2:B:761:LYS:HE2	2:B:765:ARG:NE	2.32	0.44
2:B:764:PHE:HD2	2:B:767:ILE:HD12	1.82	0.44
2:B:1236:ARG:HD3	2:B:1236:ARG:HA	1.80	0.44
2:E:142:ALA:O	2:E:146:LYS:HG3	2.16	0.44
2:E:642:ASN:HA	2:E:644:ARG:NH1	2.32	0.44
2:E:775:LEU:CD2	2:E:781:SER:HB2	2.48	0.44
2:E:1469:ARG:NH1	2:E:1473:LYS:HG3	2.32	0.44
2:B:87:LEU:O	2:B:90:GLU:HG3	2.17	0.44
2:B:166:ARG:HA	2:B:166:ARG:HD2	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:SER:OG	2:B:182:ALA:HB3	2.16	0.44
2:B:877:VAL:O	2:B:880:PRO:HD2	2.17	0.44
2:B:1125:ILE:HD12	2:B:1125:ILE:H	1.82	0.44
2:E:184:PHE:O	2:E:188:GLU:OE1	2.35	0.44
2:E:697:LEU:O	2:E:701:ILE:HG12	2.17	0.44
2:E:1320:LEU:HA	2:E:1323:GLU:OE1	2.17	0.44
2:E:1360:PRO:HG2	2:E:1362:TYR:HE1	1.83	0.44
2:E:1535:GLN:OE1	2:E:1542:LEU:HD11	2.18	0.44
3:F:72:TYR:HB3	3:F:105:CYS:SG	2.58	0.44
1:A:721:ASP:N	1:A:721:ASP:OD1	2.50	0.44
2:B:120:MET:SD	2:B:151:LYS:HE3	2.58	0.44
2:B:519:ILE:HG22	2:B:630:LYS:HE3	2.00	0.44
2:B:642:ASN:HA	2:B:644:ARG:NH1	2.32	0.44
2:B:775:LEU:CD2	2:B:781:SER:HB2	2.48	0.44
2:B:821:PRO:O	2:B:824:ILE:HG12	2.18	0.44
2:B:1114:LEU:HB3	2:B:1163:ARG:HG2	2.00	0.44
2:B:1412:THR:HB	2:B:1413:PRO:HD3	2.00	0.44
3:C:90:PHE:HA	3:C:93:VAL:HG12	2.00	0.44
3:C:110:ILE:O	3:C:152:VAL:HG12	2.17	0.44
2:E:581:ASP:HB3	2:E:584:PHE:HB3	2.00	0.44
2:E:738:ASN:HA	2:E:741:VAL:HG12	2.00	0.44
2:E:1032:PHE:O	2:E:1040:LEU:HD22	2.17	0.44
2:E:1328:TYR:O	2:E:1333:PHE:N	2.43	0.44
2:E:1372:PHE:N	2:E:1424:GLN:HG2	2.33	0.44
2:E:1490:THR:OG1	2:E:1506:GLN:HB3	2.18	0.44
2:E:1532:CYS:HA	2:E:1535:GLN:CG	2.48	0.44
2:E:1617:PRO:O	2:E:1620:GLU:HG3	2.18	0.44
3:F:63:ASP:OD1	3:F:64:TYR:N	2.51	0.44
1:A:627:GLU:HG2	1:A:631:LEU:HB2	2.00	0.44
2:B:102:TRP:CH2	2:B:118:GLN:HG2	2.52	0.44
2:B:102:TRP:HH2	2:B:118:GLN:HA	1.83	0.44
2:B:584:PHE:CE2	2:B:588:LEU:HD11	2.52	0.44
2:B:1232:LYS:HB2	2:B:1240:TYR:HE2	1.82	0.44
2:B:1268:ALA:HA	2:B:1271:LEU:HD13	1.98	0.44
2:B:1320:LEU:HA	2:B:1323:GLU:OE1	2.17	0.44
2:B:1535:GLN:OE1	2:B:1542:LEU:HD11	2.18	0.44
1:D:646:TYR:CE1	1:D:652:LEU:HG	2.52	0.44
1:D:678:MET:HA	1:D:683:ARG:HH12	1.83	0.44
2:E:319:ARG:HB2	2:E:499:VAL:HA	1.98	0.44
2:E:745:ASP:OD1	2:E:745:ASP:N	2.49	0.44
2:E:1024:PHE:O	2:E:1027:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1232:LYS:HB2	2:E:1240:TYR:HE2	1.82	0.44
2:E:1599:LEU:HA	2:E:1602:GLU:OE1	2.18	0.44
1:A:674:GLY:C	1:A:675:LYS:HD3	2.43	0.44
2:B:129:SER:O	2:B:132:LEU:HB2	2.18	0.44
2:B:746:ASP:HB3	2:B:749:LYS:HB3	2.00	0.44
2:B:799:ASN:HA	2:B:802:MET:HG3	2.00	0.44
2:B:904:GLN:OE1	2:B:908:ASN:ND2	2.26	0.44
2:B:1087:ILE:HA	2:B:1090:MET:HG2	1.99	0.44
2:B:1175:LEU:HB3	2:B:1179:HIS:CE1	2.53	0.44
2:B:1532:CYS:HA	2:B:1535:GLN:HG3	1.99	0.44
1:D:674:GLY:C	1:D:675:LYS:HD3	2.43	0.44
2:E:1125:ILE:HG12	2:E:1172:LEU:HD22	2.00	0.44
2:E:1240:TYR:CE1	2:E:1244:LEU:HD11	2.53	0.44
2:E:1264:LEU:HD12	2:E:1264:LEU:HA	1.81	0.44
2:E:1463:ARG:HA	2:E:1488:THR:HA	1.98	0.44
2:E:1532:CYS:HA	2:E:1535:GLN:HG3	1.99	0.44
3:F:18:CYS:HG	3:F:32:TYR:HH	1.56	0.44
2:B:26:GLU:OE1	2:B:29:LEU:HD11	2.16	0.44
2:B:228:PHE:HA	2:B:401:VAL:HG12	2.00	0.44
2:B:738:ASN:HA	2:B:741:VAL:HG12	2.00	0.44
2:B:1024:PHE:O	2:B:1027:VAL:HG22	2.18	0.44
2:B:1545:HIS:O	2:B:1549:MET:HG2	2.18	0.44
3:C:93:VAL:O	3:C:98:TYR:HB3	2.18	0.44
1:D:549:LYS:HE3	1:D:677:MET:HG2	2.00	0.44
1:D:659:LYS:NZ	1:D:680:ASP:OD2	2.39	0.44
2:E:26:GLU:HG3	2:E:58:ILE:O	2.17	0.44
2:E:98:TRP:HZ3	2:E:159:LEU:HD12	1.82	0.44
2:E:102:TRP:HH2	2:E:118:GLN:HA	1.83	0.44
2:E:152:ILE:O	2:E:156:ASN:ND2	2.51	0.44
2:E:166:ARG:HB2	2:E:174:ASP:HB2	1.99	0.44
2:E:738:ASN:ND2	2:E:793:GLN:HG3	2.33	0.44
2:E:799:ASN:HA	2:E:802:MET:HG3	2.00	0.44
2:E:923:VAL:O	2:E:926:GLN:HB2	2.17	0.44
2:E:1114:LEU:HB3	2:E:1163:ARG:HG2	2.00	0.44
2:E:1417:ASP:N	2:E:1417:ASP:OD1	2.50	0.44
2:E:1516:GLU:O	2:E:1520:GLU:OE1	2.36	0.44
2:B:123:SER:O	2:B:126:GLU:HG3	2.18	0.43
2:B:166:ARG:HB2	2:B:174:ASP:HB2	1.99	0.43
2:B:474:ASP:OD2	2:B:478:LYS:HE3	2.16	0.43
2:B:654:LEU:HB2	2:B:692:LEU:HD13	2.00	0.43
2:B:874:CYS:HA	2:B:877:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:932:LEU:CA	2:B:935:ARG:HE	2.28	0.43
2:B:1155:LEU:HD21	2:B:1201:LEU:HD21	2.00	0.43
1:D:567:ALA:HB3	1:D:573:LYS:HD3	2.00	0.43
2:E:120:MET:SD	2:E:151:LYS:HE3	2.58	0.43
2:E:123:SER:O	2:E:126:GLU:HG3	2.18	0.43
2:E:331:ASP:HB3	2:E:336:LYS:HD2	2.00	0.43
2:E:556:ASN:HD22	2:E:560:THR:HG1	1.59	0.43
2:E:1097:HIS:HA	2:E:1100:LYS:NZ	2.33	0.43
2:E:1111:GLU:O	2:E:1163:ARG:NH1	2.42	0.43
2:E:1122:LYS:HD2	2:E:1171:LEU:HD11	2.00	0.43
2:E:1206:ASP:O	2:E:1210:ILE:HG12	2.17	0.43
2:E:1231:TYR:CZ	2:E:1239:ILE:HD12	2.53	0.43
2:E:1611:LEU:HD13	2:E:1619:HIS:HB2	1.99	0.43
1:A:678:MET:HA	1:A:683:ARG:HH12	1.83	0.43
2:B:439:PRO:HA	2:B:712:PHE:CE2	2.53	0.43
2:B:466:VAL:HG13	2:B:531:PHE:HB3	2.00	0.43
2:B:1022:ASN:HB3	2:B:1086:ARG:HH12	1.83	0.43
2:B:1523:GLU:O	2:B:1526:ASN:N	2.51	0.43
2:E:339:ASP:N	2:E:339:ASP:OD1	2.50	0.43
2:E:746:ASP:HB3	2:E:749:LYS:HB3	2.00	0.43
2:E:826:ASP:O	2:E:830:VAL:HG22	2.19	0.43
2:E:874:CYS:HA	2:E:877:VAL:HG22	2.00	0.43
2:E:1066:GLN:CD	2:E:1069:ARG:HH12	2.26	0.43
2:E:1545:HIS:O	2:E:1549:MET:HG2	2.18	0.43
1:A:562:PHE:CD1	1:A:577:CYS:HB3	2.54	0.43
1:A:707:PRO:HD2	2:B:16:ILE:HG21	2.00	0.43
2:B:25:VAL:HB	2:B:56:LYS:O	2.18	0.43
2:B:248:PRO:HB3	2:B:387:ILE:HG21	2.01	0.43
2:B:302:ARG:HD3	2:B:322:PHE:CD1	2.52	0.43
2:B:802:MET:HE1	2:B:846:SER:C	2.43	0.43
2:B:826:ASP:O	2:B:830:VAL:HG22	2.19	0.43
2:B:857:LEU:HD13	2:B:905:LEU:HD11	2.00	0.43
2:B:979:ARG:NH1	2:B:1031:PHE:O	2.52	0.43
2:B:1063:THR:HA	2:B:1069:ARG:HD3	1.99	0.43
1:D:572:ASP:CG	1:D:592:GLU:HA	2.42	0.43
1:D:575:TRP:HB2	1:D:591:LEU:H	1.82	0.43
2:E:248:PRO:HB3	2:E:387:ILE:HG21	2.01	0.43
2:E:789:ASN:HA	2:E:792:ARG:HD2	1.98	0.43
2:E:991:ILE:HG13	2:E:992:MET:N	2.33	0.43
2:E:1512:ILE:HA	2:E:1516:GLU:OE1	2.18	0.43
2:E:1583:GLN:O	2:E:1586:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:451:ILE:HD11	2:B:623:ALA:HB2	2.00	0.43
2:B:738:ASN:ND2	2:B:793:GLN:HG3	2.33	0.43
2:B:745:ASP:OD1	2:B:745:ASP:N	2.49	0.43
2:B:1054:LEU:HD11	2:B:1080:ARG:HB3	1.99	0.43
2:B:1240:TYR:CE1	2:B:1244:LEU:HD11	2.53	0.43
2:B:1259:GLU:HG3	2:B:1497:GLY:O	2.17	0.43
2:B:1490:THR:OG1	2:B:1506:GLN:HB3	2.18	0.43
2:B:1532:CYS:HA	2:B:1535:GLN:CG	2.48	0.43
1:D:652:LEU:HB3	1:D:654:PHE:CZ	2.53	0.43
1:D:661:GLU:HA	1:D:664:ILE:HB	2.00	0.43
1:D:701:LEU:CD2	2:E:31:ILE:HG23	2.44	0.43
2:E:439:PRO:HA	2:E:712:PHE:CE2	2.53	0.43
2:E:716:LEU:O	2:E:720:ILE:HG13	2.19	0.43
2:E:1630:LYS:O	2:E:1633:VAL:HG22	2.18	0.43
1:A:532:PRO:O	1:A:536:LEU:HD13	2.17	0.43
1:A:575:TRP:HB2	1:A:591:LEU:H	1.82	0.43
2:B:163:LEU:HD11	2:B:194:ILE:HD11	2.01	0.43
3:C:63:ASP:OD1	3:C:64:TYR:N	2.51	0.43
1:D:562:PHE:CD1	1:D:577:CYS:HB3	2.54	0.43
2:E:140:GLU:O	2:E:144:LEU:HD23	2.18	0.43
2:E:228:PHE:HA	2:E:401:VAL:HG12	2.00	0.43
2:E:519:ILE:HG22	2:E:630:LYS:HE3	2.00	0.43
2:E:652:HIS:CD2	2:E:656:LYS:HD3	2.53	0.43
1:A:661:GLU:HA	1:A:664:ILE:HB	2.00	0.43
2:B:9:ARG:HD2	2:B:68:GLU:HG2	2.01	0.43
2:B:879:LEU:O	2:B:880:PRO:C	2.61	0.43
2:B:1193:PHE:O	2:B:1197:VAL:HG23	2.18	0.43
2:B:1231:TYR:CE2	2:B:1243:TYR:CE1	3.06	0.43
2:B:1381:PHE:CZ	2:B:1503:GLU:HB3	2.53	0.43
2:B:1486:ARG:NE	2:B:1512:ILE:HD11	2.34	0.43
2:B:1512:ILE:HA	2:B:1516:GLU:OE1	2.18	0.43
1:D:678:MET:SD	1:D:678:MET:N	2.92	0.43
2:E:5:ILE:O	2:E:40:MET:HG2	2.19	0.43
2:E:294:VAL:N	2:E:330:THR:OG1	2.26	0.43
2:E:319:ARG:O	2:E:500:VAL:N	2.52	0.43
2:E:654:LEU:HB2	2:E:692:LEU:HD13	2.00	0.43
2:E:707:ILE:HA	2:E:710:GLN:CD	2.44	0.43
2:E:969:TYR:CD2	2:E:1023:GLN:HG3	2.54	0.43
2:E:1165:ASP:O	2:E:1168:TYR:HB3	2.19	0.43
2:E:1482:MET:HE3	2:E:1482:MET:HA	1.99	0.43
2:E:1621:ARG:NH1	3:F:70:LEU:HD13	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ALA:HB3	1:A:573:LYS:HD3	1.99	0.43
1:A:578:ARG:HB2	1:A:598:GLU:OE1	2.19	0.43
1:A:616:VAL:HG23	1:A:643:SER:C	2.43	0.43
1:A:678:MET:N	1:A:678:MET:SD	2.92	0.43
2:B:127:TRP:HD1	2:B:130:GLN:NE2	2.17	0.43
2:B:152:ILE:O	2:B:156:ASN:ND2	2.51	0.43
2:B:319:ARG:O	2:B:500:VAL:N	2.52	0.43
2:B:876:GLU:HA	2:B:924:HIS:HE2	1.82	0.43
1:D:543:GLU:H	1:D:543:GLU:CD	2.24	0.43
1:D:578:ARG:HB2	1:D:598:GLU:OE1	2.19	0.43
1:D:627:GLU:HG2	1:D:631:LEU:HB2	2.00	0.43
2:E:860:MET:HE2	2:E:860:MET:HB3	1.77	0.43
1:A:552:ARG:HH12	1:A:664:ILE:HG12	1.84	0.43
2:B:331:ASP:HA	2:B:334:HIS:HB2	2.01	0.43
2:B:394:HIS:HB2	2:B:397:GLN:O	2.19	0.43
2:B:985:PHE:HA	2:B:988:GLU:OE1	2.19	0.43
2:B:1118:VAL:O	2:B:1122:LYS:HG2	2.19	0.43
2:B:1231:TYR:CZ	2:B:1239:ILE:HD12	2.53	0.43
3:C:129:LEU:O	3:C:133:LYS:N	2.52	0.43
2:E:9:ARG:HD3	2:E:9:ARG:HA	1.70	0.43
2:E:950:ILE:O	2:E:954:VAL:HG23	2.19	0.43
2:E:1175:LEU:HB3	2:E:1179:HIS:CE1	2.53	0.43
2:E:1438:PRO:HB2	2:E:1441:TYR:CD2	2.54	0.43
2:E:1522:MET:HE3	2:E:1526:ASN:OD1	2.19	0.43
2:E:1566:TYR:OH	3:F:36:VAL:HG11	2.18	0.43
3:F:69:PRO:HA	3:F:72:TYR:CG	2.54	0.43
3:F:69:PRO:O	3:F:73:PRO:HD3	2.19	0.43
3:F:93:VAL:O	3:F:98:TYR:HB3	2.18	0.43
2:B:5:ILE:O	2:B:40:MET:HG2	2.19	0.43
2:B:59:PHE:CD2	2:B:64:ILE:HG12	2.50	0.43
2:B:102:TRP:CH2	2:B:118:GLN:HA	2.54	0.43
2:B:761:LYS:HE2	2:B:765:ARG:HE	1.83	0.43
2:B:991:ILE:HG13	2:B:992:MET:N	2.33	0.43
2:B:1136:PHE:HB2	2:B:1186:LEU:HD23	2.00	0.43
2:B:1613:GLU:HA	2:B:1616:LYS:HD2	2.01	0.43
2:E:591:THR:N	2:E:594:GLU:OE2	2.51	0.43
2:E:1381:PHE:CZ	2:E:1503:GLU:HB3	2.53	0.43
3:F:91:GLU:O	3:F:95:ALA:CB	2.66	0.43
2:B:86:PRO:HA	2:B:89:GLN:OE1	2.19	0.43
2:B:700:ILE:O	2:B:704:ILE:HG13	2.19	0.43
2:B:707:ILE:HA	2:B:710:GLN:CD	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1260:ALA:O	2:B:1263:THR:OG1	2.35	0.43
3:C:124:ASP:O	3:C:128:LYS:HD3	2.19	0.43
2:E:94:THR:HG22	2:E:98:TRP:CE2	2.54	0.43
2:E:111:LEU:HA	2:E:114:PHE:HB3	2.01	0.43
2:E:129:SER:O	2:E:132:LEU:HB2	2.18	0.43
2:E:728:LEU:HA	2:E:730:TYR:CE2	2.54	0.43
2:E:821:PRO:O	2:E:824:ILE:HG12	2.18	0.43
2:E:985:PHE:HA	2:E:988:GLU:OE1	2.19	0.43
2:E:1136:PHE:HB2	2:E:1186:LEU:HD23	2.00	0.43
2:E:1379:LYS:HA	2:E:1379:LYS:HD2	1.74	0.43
3:F:85:VAL:O	3:F:129:LEU:HD21	2.17	0.43
3:F:90:PHE:HA	3:F:93:VAL:HG12	2.00	0.43
1:A:689:LEU:HD22	2:B:102:TRP:HE1	1.84	0.42
2:B:91:LEU:HD11	2:B:128:ARG:HG3	2.00	0.42
2:B:250:GLN:HB3	2:B:252:THR:HG22	2.01	0.42
2:B:331:ASP:HB3	2:B:336:LYS:HD2	2.00	0.42
2:B:581:ASP:HB3	2:B:584:PHE:HB3	2.00	0.42
2:B:591:THR:N	2:B:594:GLU:OE2	2.51	0.42
2:B:1022:ASN:O	2:B:1026:GLU:OE1	2.37	0.42
2:B:1360:PRO:HG2	2:B:1362:TYR:HE1	1.83	0.42
2:B:1499:LEU:HD23	2:B:1499:LEU:HA	1.86	0.42
2:B:1516:GLU:O	2:B:1520:GLU:OE1	2.36	0.42
3:C:87:PRO:HG2	3:C:134:LEU:HD22	2.01	0.42
1:D:563:ARG:HB2	1:D:655:ILE:O	2.18	0.42
2:E:9:ARG:HD2	2:E:68:GLU:HG2	2.01	0.42
2:E:182:ALA:HA	2:E:185:LYS:HG2	2.01	0.42
2:E:451:ILE:HD11	2:E:623:ALA:HB2	2.00	0.42
2:E:1114:LEU:HD22	2:E:1168:TYR:OH	2.19	0.42
2:E:1193:PHE:O	2:E:1197:VAL:HG23	2.18	0.42
2:E:1523:GLU:O	2:E:1526:ASN:N	2.51	0.42
3:F:41:SER:OG	3:F:53:LEU:O	2.29	0.42
1:A:652:LEU:HB3	1:A:654:PHE:CZ	2.53	0.42
2:B:16:ILE:HD12	2:B:63:TYR:HA	2.00	0.42
2:B:37:ILE:HD13	2:B:45:TYR:CB	2.47	0.42
2:B:553:LYS:HE3	2:B:586:LEU:HD22	2.01	0.42
2:B:707:ILE:HD13	2:B:710:GLN:OE1	2.19	0.42
2:B:716:LEU:O	2:B:720:ILE:HG13	2.19	0.42
2:B:1114:LEU:HD22	2:B:1168:TYR:OH	2.19	0.42
2:B:1176:LEU:HD22	2:B:1194:ALA:HB2	2.00	0.42
2:B:1599:LEU:HA	2:B:1602:GLU:OE1	2.18	0.42
2:B:1605:ARG:O	2:B:1609:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:GLU:O	3:C:95:ALA:CB	2.66	0.42
2:E:102:TRP:CH2	2:E:118:GLN:HA	2.54	0.42
2:E:231:PHE:HD2	2:E:262:TRP:CG	2.37	0.42
2:E:331:ASP:HA	2:E:334:HIS:HB2	2.01	0.42
2:E:707:ILE:HD13	2:E:710:GLN:OE1	2.19	0.42
2:E:1008:VAL:O	2:E:1012:THR:HG23	2.19	0.42
2:E:1063:THR:HA	2:E:1069:ARG:HD3	2.00	0.42
2:E:1155:LEU:HD21	2:E:1201:LEU:HD21	2.00	0.42
2:E:1486:ARG:NE	2:E:1512:ILE:HD11	2.34	0.42
2:E:1605:ARG:O	2:E:1609:GLU:HG3	2.19	0.42
2:B:182:ALA:HA	2:B:185:LYS:HG2	2.01	0.42
2:B:594:GLU:O	2:B:597:GLU:HG3	2.19	0.42
2:B:727:THR:O	2:B:730:TYR:HE2	2.03	0.42
1:D:616:VAL:HG23	1:D:643:SER:C	2.43	0.42
2:E:98:TRP:CH2	2:E:155:GLY:HA3	2.55	0.42
2:E:700:ILE:O	2:E:704:ILE:HG13	2.19	0.42
2:E:1022:ASN:O	2:E:1026:GLU:OE1	2.37	0.42
2:E:1499:LEU:HD23	2:E:1499:LEU:HA	1.86	0.42
2:B:94:THR:HG22	2:B:98:TRP:CE2	2.54	0.42
2:B:111:LEU:HA	2:B:114:PHE:HB3	2.01	0.42
2:B:889:GLN:O	2:B:895:ASN:ND2	2.52	0.42
2:B:1125:ILE:HG12	2:B:1172:LEU:HD22	2.00	0.42
3:C:69:PRO:HA	3:C:72:TYR:CG	2.54	0.42
2:E:86:PRO:HA	2:E:89:GLN:OE1	2.19	0.42
2:E:95:LEU:HA	2:E:98:TRP:HD1	1.84	0.42
2:E:144:LEU:O	2:E:148:VAL:HG22	2.20	0.42
2:E:1135:GLU:HG3	2:E:1144:PHE:HA	2.02	0.42
2:E:1613:GLU:HA	2:E:1616:LYS:HD2	2.01	0.42
3:F:42:ALA:O	3:F:53:LEU:HG	2.20	0.42
3:F:117:LEU:HD13	3:F:156:GLU:HB3	2.01	0.42
1:A:547:LEU:O	1:A:550:GLN:HG3	2.20	0.42
1:A:564:LYS:HE3	1:A:590:ASP:CG	2.45	0.42
1:A:607:LYS:HE3	1:A:609:PRO:HA	2.00	0.42
2:B:95:LEU:HA	2:B:98:TRP:HD1	1.84	0.42
2:B:1056:HIS:HD1	2:B:1057:GLU:CD	2.27	0.42
2:B:1166:GLU:O	2:B:1169:LYS:HG2	2.20	0.42
2:B:1318:ILE:HD13	2:B:1349:TYR:CZ	2.55	0.42
2:E:127:TRP:HD1	2:E:130:GLN:NE2	2.17	0.42
2:E:761:LYS:HE2	2:E:765:ARG:HE	1.83	0.42
2:E:1176:LEU:HD22	2:E:1194:ALA:HB2	2.00	0.42
3:F:2:GLN:HE22	3:F:4:ILE:HD11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:124:ASP:O	3:F:128:LYS:HD3	2.19	0.42
3:F:129:LEU:O	3:F:133:LYS:N	2.52	0.42
2:B:88:VAL:O	2:B:92:THR:HG23	2.20	0.42
2:B:225:TYR:CE1	2:B:278:GLN:HB3	2.54	0.42
2:B:927:LEU:HB3	2:B:931:ARG:HH21	1.85	0.42
2:B:1289:TYR:O	2:B:1290:VAL:C	2.63	0.42
2:B:1630:LYS:O	2:B:1633:VAL:HG22	2.18	0.42
3:C:2:GLN:HE22	3:C:4:ILE:HD11	1.84	0.42
3:C:145:MET:O	3:C:148:GLU:HB3	2.20	0.42
1:D:563:ARG:NH2	1:D:573:LYS:HE2	2.35	0.42
2:E:165:VAL:C	2:E:171:ASN:HD22	2.22	0.42
2:E:551:PHE:CE2	2:E:586:LEU:HD23	2.55	0.42
2:E:979:ARG:NH1	2:E:1031:PHE:O	2.52	0.42
2:E:1166:GLU:O	2:E:1169:LYS:HG2	2.20	0.42
2:E:1488:THR:OG1	2:E:1508:SER:HB2	2.20	0.42
1:A:563:ARG:NH2	1:A:573:LYS:HE2	2.35	0.42
2:B:140:GLU:N	2:B:140:GLU:OE1	2.53	0.42
2:B:950:ILE:O	2:B:954:VAL:HG23	2.19	0.42
2:B:1086:ARG:HA	2:B:1089:ASP:OD2	2.19	0.42
2:B:1165:ASP:O	2:B:1168:TYR:HB3	2.19	0.42
2:B:1168:TYR:CZ	2:B:1172:LEU:HD21	2.55	0.42
2:B:1388:TYR:CE2	3:C:44:VAL:HG13	2.54	0.42
2:B:1438:PRO:HB2	2:B:1441:TYR:CD2	2.54	0.42
3:C:153:LYS:HD2	3:C:153:LYS:HA	1.85	0.42
1:A:563:ARG:HB2	1:A:655:ILE:O	2.19	0.42
2:B:95:LEU:HD23	2:B:98:TRP:CD1	2.45	0.42
2:B:143:GLU:O	2:B:147:LYS:HG2	2.20	0.42
2:B:189:VAL:HA	2:B:192:LYS:HE2	2.02	0.42
2:B:590:GLY:H	2:B:594:GLU:CD	2.28	0.42
2:B:1568:LYS:HD2	2:B:1569:ALA:N	2.35	0.42
1:D:652:LEU:HD23	1:D:652:LEU:HA	1.87	0.42
2:E:88:VAL:O	2:E:92:THR:HG23	2.20	0.42
2:E:466:VAL:HG13	2:E:531:PHE:HB3	2.00	0.42
2:E:1079:MET:O	2:E:1083:ILE:HG13	2.20	0.42
2:E:1168:TYR:CZ	2:E:1172:LEU:HD21	2.55	0.42
2:E:1318:ILE:HD13	2:E:1349:TYR:CZ	2.55	0.42
2:E:1548:SER:HB2	3:F:56:TRP:CH2	2.49	0.42
1:A:624:HIS:CD2	1:A:633:GLN:HG3	2.55	0.42
1:A:627:GLU:HG3	1:A:629:GLY:H	1.84	0.42
1:A:652:LEU:HD23	1:A:652:LEU:HA	1.87	0.42
2:B:231:PHE:HD2	2:B:262:TRP:CG	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:728:LEU:HA	2:B:730:TYR:CE2	2.54	0.42
2:B:1003:ALA:C	2:B:1005:ASP:H	2.28	0.42
2:B:1379:LYS:HD2	2:B:1379:LYS:HA	1.74	0.42
3:C:42:ALA:O	3:C:53:LEU:HG	2.20	0.42
1:D:564:LYS:HE3	1:D:590:ASP:CG	2.45	0.42
1:D:608:LEU:HD21	1:D:644:ILE:HG21	2.02	0.42
2:E:163:LEU:HD11	2:E:194:ILE:HD11	2.00	0.42
2:E:594:GLU:O	2:E:597:GLU:HG3	2.19	0.42
2:E:738:ASN:HD21	2:E:793:GLN:HG3	1.85	0.42
2:E:1059:LEU:HA	2:E:1062:GLU:OE1	2.19	0.42
2:E:1418:ILE:HG21	2:E:1425:TYR:CD2	2.55	0.42
2:E:1524:LEU:HD12	2:E:1528:ARG:HH12	1.85	0.42
2:B:98:TRP:CH2	2:B:155:GLY:HA3	2.55	0.42
2:B:105:LEU:HA	2:B:105:LEU:HD23	1.74	0.42
2:B:522:VAL:HA	2:B:525:CYS:HB2	2.02	0.42
2:B:806:LEU:HD12	2:B:813:LYS:CE	2.49	0.42
2:B:1269:GLU:OE1	2:B:1270:LEU:HD22	2.20	0.42
2:B:1443:ASP:OD1	2:B:1444:LYS:HD3	2.20	0.42
2:B:1583:GLN:O	2:B:1586:VAL:HG12	2.19	0.42
2:B:1596:GLN:O	2:B:1600:LEU:HG	2.20	0.42
1:D:607:LYS:HE3	1:D:609:PRO:HA	2.00	0.42
1:D:627:GLU:HG3	1:D:629:GLY:H	1.84	0.42
2:E:247:ASP:O	2:E:251:SER:N	2.53	0.42
2:E:1127:ILE:HA	2:E:1130:ASP:OD2	2.20	0.42
1:A:661:GLU:HA	1:A:664:ILE:HD12	2.01	0.41
2:B:1418:ILE:HG21	2:B:1425:TYR:CD2	2.55	0.41
2:B:1522:MET:HE3	2:B:1526:ASN:OD1	2.19	0.41
2:B:1611:LEU:HD11	2:B:1616:LYS:HA	2.02	0.41
3:C:82:PHE:CZ	3:C:114:GLY:HA2	2.55	0.41
1:D:552:ARG:HH12	1:D:664:ILE:HG12	1.84	0.41
1:D:624:HIS:CD2	1:D:633:GLN:HG3	2.55	0.41
2:E:250:GLN:HB3	2:E:252:THR:HG22	2.01	0.41
2:E:806:LEU:HD12	2:E:813:LYS:CE	2.49	0.41
2:E:929:MET:HE1	2:E:968:HIS:O	2.19	0.41
2:E:1287:SER:HG	2:E:1289:TYR:HE1	1.67	0.41
3:F:82:PHE:CZ	3:F:114:GLY:HA2	2.55	0.41
3:F:87:PRO:HG2	3:F:134:LEU:HD22	2.01	0.41
1:A:715:LYS:HA	1:A:715:LYS:HD3	1.87	0.41
2:B:165:VAL:C	2:B:171:ASN:HD22	2.22	0.41
2:B:247:ASP:O	2:B:251:SER:N	2.53	0.41
2:B:435:GLU:O	2:B:708:LYS:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:593:MET:O	2:B:596:GLU:HG2	2.20	0.41
2:B:921:THR:O	2:B:925:ILE:N	2.41	0.41
2:B:969:TYR:CD2	2:B:1023:GLN:HG3	2.54	0.41
2:B:1008:VAL:O	2:B:1012:THR:HG23	2.19	0.41
2:B:1097:HIS:HA	2:B:1100:LYS:NZ	2.34	0.41
2:B:1127:ILE:HA	2:B:1130:ASP:OD2	2.20	0.41
2:B:1135:GLU:HG3	2:B:1144:PHE:HA	2.02	0.41
2:B:1432:LYS:HB2	2:B:1463:ARG:HG3	2.02	0.41
3:C:69:PRO:O	3:C:73:PRO:HD3	2.19	0.41
3:C:92:ASN:O	3:C:96:LYS:N	2.40	0.41
3:C:117:LEU:HD13	3:C:156:GLU:HB3	2.01	0.41
2:E:149:THR:HA	2:E:152:ILE:HG12	2.03	0.41
2:E:258:TYR:HE1	2:E:489:GLY:HA3	1.85	0.41
2:E:394:HIS:HB2	2:E:397:GLN:O	2.19	0.41
2:E:802:MET:HE1	2:E:847:ILE:HA	2.03	0.41
2:E:879:LEU:O	2:E:882:LEU:HB2	2.20	0.41
2:E:1431:VAL:HG12	2:E:1464:TYR:HB2	2.03	0.41
1:A:578:ARG:NH1	1:A:600:PRO:HA	2.35	0.41
2:B:144:LEU:O	2:B:148:VAL:HG22	2.20	0.41
2:B:224:LEU:HD13	2:B:333:ILE:HG12	2.02	0.41
2:B:1628:GLU:HG2	2:B:1629:LEU:HD22	2.02	0.41
2:E:91:LEU:HD11	2:E:128:ARG:HG3	2.01	0.41
2:E:889:GLN:O	2:E:895:ASN:ND2	2.52	0.41
2:E:927:LEU:HB3	2:E:931:ARG:HH21	1.85	0.41
2:E:1043:TRP:CE3	2:E:1043:TRP:N	2.83	0.41
2:E:1095:GLY:N	2:E:1098:LYS:HE3	2.35	0.41
2:E:1568:LYS:HD2	2:E:1569:ALA:N	2.35	0.41
2:B:9:ARG:HA	2:B:9:ARG:HD3	1.70	0.41
2:B:287:MET:N	2:B:435:GLU:OE2	2.43	0.41
2:B:757:LEU:HA	2:B:760:LEU:HG	2.01	0.41
2:B:802:MET:HE1	2:B:847:ILE:HA	2.02	0.41
2:B:892:ASP:OD1	2:B:892:ASP:N	2.52	0.41
2:B:1059:LEU:HA	2:B:1062:GLU:OE1	2.19	0.41
2:B:1274:SER:O	2:B:1294:GLN:HG3	2.21	0.41
2:B:1381:PHE:HA	2:B:1503:GLU:HA	2.02	0.41
2:B:1524:LEU:HD12	2:B:1525:THR:N	2.36	0.41
3:C:80:ILE:O	3:C:113:VAL:HG22	2.21	0.41
1:D:661:GLU:HA	1:D:664:ILE:HD12	2.01	0.41
2:E:140:GLU:N	2:E:140:GLU:OE1	2.53	0.41
2:E:590:GLY:H	2:E:594:GLU:CD	2.28	0.41
2:E:740:TYR:HD1	2:E:749:LYS:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:757:LEU:HA	2:E:760:LEU:HG	2.01	0.41
2:E:1095:GLY:HA3	2:E:1096:PRO:HD3	1.91	0.41
2:E:1118:VAL:O	2:E:1122:LYS:HG2	2.19	0.41
2:E:1381:PHE:HA	2:E:1503:GLU:HA	2.02	0.41
2:E:1443:ASP:OD1	2:E:1444:LYS:HD3	2.20	0.41
2:E:1471:GLY:C	2:E:1481:THR:HG22	2.46	0.41
3:F:10:GLY:O	3:F:60:GLY:HA3	2.21	0.41
3:F:39:ASN:HA	3:F:57:ASP:H	1.86	0.41
1:A:711:PRO:HG2	2:B:16:ILE:HD12	2.03	0.41
2:B:551:PHE:CE2	2:B:586:LEU:HD23	2.55	0.41
2:B:1079:MET:O	2:B:1083:ILE:HG13	2.20	0.41
2:B:1343:LYS:HE3	2:B:1343:LYS:HB2	1.81	0.41
2:B:1488:THR:OG1	2:B:1508:SER:HB2	2.20	0.41
3:C:10:GLY:O	3:C:60:GLY:HA3	2.21	0.41
1:D:564:LYS:O	1:D:573:LYS:NZ	2.32	0.41
2:E:16:ILE:HD12	2:E:63:TYR:HA	2.00	0.41
2:E:904:GLN:OE1	2:E:908:ASN:ND2	2.26	0.41
2:E:1236:ARG:HD3	2:E:1236:ARG:HA	1.80	0.41
2:E:1289:TYR:O	2:E:1290:VAL:C	2.63	0.41
1:A:608:LEU:HD21	1:A:644:ILE:HG21	2.02	0.41
2:B:124:LEU:HD21	2:B:151:LYS:HB2	2.02	0.41
2:B:929:MET:HE1	2:B:968:HIS:O	2.19	0.41
1:D:685:ASP:HA	1:D:688:THR:HG22	2.02	0.41
2:E:124:LEU:HD21	2:E:151:LYS:HB2	2.02	0.41
2:E:166:ARG:HH21	2:E:169:ASN:HD21	1.69	0.41
2:E:472:VAL:O	2:E:479:LEU:HD12	2.21	0.41
2:E:727:THR:O	2:E:730:TYR:HE2	2.03	0.41
2:E:1086:ARG:HA	2:E:1089:ASP:OD2	2.19	0.41
3:F:80:ILE:O	3:F:113:VAL:HG22	2.21	0.41
2:B:94:THR:O	2:B:97:GLU:HG3	2.21	0.41
2:B:166:ARG:HH21	2:B:169:ASN:HD21	1.69	0.41
2:B:868:LEU:O	2:B:871:GLN:HG3	2.21	0.41
2:B:965:ASP:O	2:B:968:HIS:HB2	2.21	0.41
2:B:1354:LYS:HE3	2:B:1354:LYS:HB3	1.87	0.41
3:C:39:ASN:HA	3:C:57:ASP:H	1.85	0.41
1:D:578:ARG:NH1	1:D:600:PRO:HA	2.35	0.41
2:E:718:THR:HG22	2:E:723:HIS:HE1	1.86	0.41
2:E:868:LEU:O	2:E:871:GLN:HG3	2.21	0.41
2:E:1276:LYS:HD2	2:E:1277:PRO:HD2	2.03	0.41
3:F:21:ILE:O	3:F:25:THR:OG1	2.32	0.41
3:F:145:MET:O	3:F:148:GLU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:LEU:HD23	1:A:609:PRO:CD	2.51	0.41
2:B:877:VAL:C	2:B:880:PRO:HD2	2.46	0.41
2:B:1126:PRO:HD3	2:B:1175:LEU:HD13	2.03	0.41
2:B:1328:TYR:O	2:B:1333:PHE:N	2.43	0.41
2:B:1431:VAL:HG12	2:B:1464:TYR:HB2	2.02	0.41
2:B:1536:HIS:NE2	2:B:1542:LEU:HB3	2.36	0.41
2:E:113:LEU:O	2:E:116:GLN:HG2	2.20	0.41
2:E:143:GLU:O	2:E:147:LYS:HG2	2.20	0.41
2:E:220:HIS:O	2:E:285:SER:HA	2.21	0.41
2:E:258:TYR:CE1	2:E:489:GLY:HA3	2.56	0.41
2:E:522:VAL:HA	2:E:525:CYS:HB2	2.02	0.41
2:E:593:MET:O	2:E:596:GLU:HG2	2.20	0.41
2:E:1051:VAL:O	2:E:1055:THR:OG1	2.36	0.41
1:A:560:THR:O	1:A:576:TYR:HA	2.21	0.41
1:A:685:ASP:HA	1:A:688:THR:HG22	2.02	0.41
2:B:113:LEU:O	2:B:116:GLN:HG2	2.20	0.41
2:B:149:THR:HA	2:B:152:ILE:HG12	2.03	0.41
2:B:258:TYR:HE1	2:B:489:GLY:HA3	1.85	0.41
2:B:472:VAL:O	2:B:479:LEU:HD12	2.21	0.41
2:B:738:ASN:HD21	2:B:793:GLN:HG3	1.85	0.41
2:B:987:MET:HE1	2:B:1042:LEU:HD13	2.02	0.41
2:B:1095:GLY:N	2:B:1098:LYS:HE3	2.35	0.41
2:B:1320:LEU:HA	2:B:1320:LEU:HD23	1.85	0.41
2:B:1384:ARG:HD2	2:B:1495:PHE:HB3	2.03	0.41
2:B:1432:LYS:HE2	2:B:1463:ARG:O	2.21	0.41
2:B:1437:LEU:HD21	2:B:1442:LYS:NZ	2.36	0.41
2:B:1464:TYR:O	2:B:1486:ARG:HA	2.21	0.41
2:B:1519:ILE:O	2:B:1523:GLU:HG3	2.21	0.41
2:B:1524:LEU:HD12	2:B:1528:ARG:HH12	1.85	0.41
2:B:1536:HIS:ND1	2:B:1542:LEU:HD22	2.36	0.41
2:B:1563:PHE:O	2:B:1567:GLU:HG2	2.21	0.41
1:D:547:LEU:O	1:D:550:GLN:HG3	2.20	0.41
2:E:70:THR:H	2:E:76:GLN:NE2	2.19	0.41
2:E:189:VAL:HA	2:E:192:LYS:HE2	2.02	0.41
2:E:214:SER:O	2:E:217:SER:OG	2.39	0.41
2:E:225:TYR:CE1	2:E:278:GLN:HB3	2.54	0.41
2:E:905:LEU:O	2:E:909:ILE:HG12	2.21	0.41
2:E:954:VAL:O	2:E:958:ILE:HG12	2.21	0.41
2:E:1260:ALA:O	2:E:1263:THR:OG1	2.35	0.41
2:E:1269:GLU:OE1	2:E:1270:LEU:HD22	2.20	0.41
2:E:1432:LYS:HE2	2:E:1463:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1432:LYS:HB2	2:E:1463:ARG:HG3	2.02	0.41
2:E:1433:PRO:HA	2:E:1462:PHE:CD2	2.56	0.41
2:E:1464:TYR:O	2:E:1486:ARG:HA	2.21	0.41
2:E:1524:LEU:HD12	2:E:1525:THR:N	2.36	0.41
2:E:1563:PHE:O	2:E:1567:GLU:HG2	2.21	0.41
2:E:1611:LEU:HD11	2:E:1616:LYS:HA	2.02	0.41
2:E:1628:GLU:HG2	2:E:1629:LEU:HD22	2.02	0.41
3:F:8:VAL:HG13	3:F:81:CYS:SG	2.61	0.41
1:A:579:LEU:HD12	1:A:585:VAL:O	2.21	0.41
1:A:679:SER:HB2	1:A:682:THR:OG1	2.21	0.41
2:B:83:GLY:O	2:B:145:LYS:NZ	2.54	0.41
2:B:220:HIS:NE2	2:B:436:ILE:HB	2.36	0.41
2:B:258:TYR:CE1	2:B:489:GLY:HA3	2.56	0.41
2:B:966:ASP:HA	2:B:969:TYR:CD2	2.48	0.41
2:E:105:LEU:HD22	2:E:110:LYS:HB2	2.03	0.41
2:E:146:LYS:HB2	2:E:146:LYS:HE2	1.78	0.41
2:E:228:PHE:HZ	2:E:231:PHE:HB2	1.86	0.41
2:E:435:GLU:O	2:E:708:LYS:HD3	2.20	0.41
2:E:638:LEU:O	2:E:642:ASN:N	2.54	0.41
2:E:1003:ALA:C	2:E:1005:ASP:H	2.28	0.41
2:E:1018:LEU:HD23	2:E:1018:LEU:HA	1.89	0.41
2:E:1026:GLU:O	2:E:1029:THR:OG1	2.33	0.41
2:E:1276:LYS:HD2	2:E:1276:LYS:HA	1.81	0.41
2:E:1437:LEU:HD21	2:E:1442:LYS:HD2	2.02	0.41
2:E:1551:LEU:HD23	2:E:1551:LEU:HA	1.86	0.41
2:E:1596:GLN:O	2:E:1600:LEU:HG	2.20	0.41
2:E:1621:ARG:CD	3:F:67:LEU:HD22	2.50	0.41
2:B:224:LEU:HD23	2:B:281:PHE:CD2	2.56	0.40
2:B:638:LEU:O	2:B:642:ASN:N	2.54	0.40
2:B:905:LEU:O	2:B:909:ILE:HG12	2.21	0.40
2:B:931:ARG:O	2:B:932:LEU:HD22	2.21	0.40
2:B:1386:LYS:CB	2:B:1389:GLU:HG3	2.51	0.40
2:E:80:VAL:H	2:E:85:LEU:HD11	1.86	0.40
2:E:166:ARG:HA	2:E:166:ARG:HD2	1.80	0.40
2:E:220:HIS:NE2	2:E:436:ILE:HB	2.36	0.40
2:E:224:LEU:HD23	2:E:281:PHE:CD2	2.56	0.40
2:E:634:ASN:O	2:E:638:LEU:HD23	2.21	0.40
2:E:877:VAL:C	2:E:880:PRO:HD2	2.46	0.40
2:E:931:ARG:O	2:E:932:LEU:HD22	2.21	0.40
2:E:987:MET:HE1	2:E:1042:LEU:HD13	2.02	0.40
2:E:1274:SER:O	2:E:1294:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1386:LYS:CB	2:E:1389:GLU:HG3	2.51	0.40
2:E:1437:LEU:HD21	2:E:1442:LYS:NZ	2.36	0.40
2:B:1122:LYS:HB3	2:B:1122:LYS:HE2	1.88	0.40
2:B:1437:LEU:HD21	2:B:1442:LYS:HD2	2.02	0.40
2:B:1471:GLY:C	2:B:1481:THR:HG22	2.46	0.40
2:B:1593:ILE:O	2:B:1596:GLN:HB3	2.22	0.40
2:E:964:MET:HE2	2:E:964:MET:HB2	1.70	0.40
2:E:1056:HIS:HD1	2:E:1057:GLU:CD	2.27	0.40
2:E:1143:ASN:HD21	2:E:1145:HIS:CE1	2.40	0.40
2:E:1384:ARG:HD2	2:E:1495:PHE:HB3	2.03	0.40
3:F:153:LYS:HA	3:F:153:LYS:HD2	1.85	0.40
2:B:116:GLN:O	2:B:120:MET:HG2	2.21	0.40
2:B:166:ARG:O	2:B:167:ASP:C	2.64	0.40
2:B:166:ARG:HH21	2:B:169:ASN:ND2	2.19	0.40
2:B:701:ILE:HD12	2:B:716:LEU:HD21	2.03	0.40
2:B:718:THR:HA	2:B:722:LYS:HZ3	1.86	0.40
2:B:879:LEU:O	2:B:882:LEU:HB2	2.20	0.40
3:C:113:VAL:HA	3:C:155:LEU:O	2.22	0.40
1:D:541:GLN:N	1:D:542:PRO:HD3	2.36	0.40
2:E:94:THR:O	2:E:97:GLU:HG3	2.21	0.40
2:E:116:GLN:O	2:E:120:MET:HG2	2.21	0.40
2:E:222:TYR:CE2	2:E:289:LEU:HD11	2.57	0.40
2:E:553:LYS:HE3	2:E:586:LEU:HD22	2.01	0.40
2:E:701:ILE:HD12	2:E:716:LEU:HD21	2.03	0.40
2:E:965:ASP:O	2:E:968:HIS:HB2	2.21	0.40
2:E:1486:ARG:HB2	2:E:1510:GLU:HB2	2.04	0.40
2:E:1519:ILE:O	2:E:1523:GLU:HG3	2.21	0.40
2:E:1536:HIS:NE2	2:E:1542:LEU:HB3	2.36	0.40
2:E:1593:ILE:O	2:E:1596:GLN:HB3	2.22	0.40
2:B:10:GLN:CG	2:B:37:ILE:HB	2.52	0.40
2:B:220:HIS:O	2:B:285:SER:HA	2.21	0.40
2:B:256:GLU:OE1	2:B:429:ARG:N	2.47	0.40
2:B:718:THR:HG22	2:B:723:HIS:HE1	1.86	0.40
2:B:964:MET:HE2	2:B:964:MET:HB2	1.70	0.40
2:B:1276:LYS:HD2	2:B:1277:PRO:HD2	2.03	0.40
2:B:1483:TRP:CE2	2:B:1514:PRO:HD3	2.56	0.40
3:C:120:ARG:NH2	3:C:139:TYR:H	2.20	0.40
1:D:560:THR:O	1:D:576:TYR:HA	2.21	0.40
1:D:698:LEU:HA	2:E:31:ILE:CG2	2.52	0.40
1:D:715:LYS:HA	1:D:715:LYS:HD3	1.87	0.40
2:E:292:PRO:O	2:E:330:THR:HG21	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:997:ILE:HG21	2:E:1053:PHE:HA	2.04	0.40
2:E:1113:THR:HG21	2:E:1128:PHE:HE2	1.87	0.40
2:E:1126:PRO:HD3	2:E:1175:LEU:HD13	2.03	0.40
2:E:1353:ILE:HD12	2:E:1353:ILE:HA	1.87	0.40
2:E:1466:ARG:H	2:E:1484:ILE:HG23	1.86	0.40
3:F:93:VAL:HG13	3:F:94:ARG:N	2.37	0.40
2:B:80:VAL:H	2:B:85:LEU:HD11	1.86	0.40
2:B:740:TYR:HD1	2:B:749:LYS:HG3	1.86	0.40
2:B:954:VAL:O	2:B:958:ILE:HG12	2.21	0.40
2:B:990:PHE:HD2	2:B:1042:LEU:HD11	1.84	0.40
2:B:1433:PRO:HA	2:B:1462:PHE:CD2	2.56	0.40
3:C:93:VAL:HG13	3:C:94:ARG:N	2.37	0.40
2:E:14:VAL:O	2:E:64:ILE:HA	2.22	0.40
2:E:83:GLY:O	2:E:145:LYS:NZ	2.54	0.40
2:E:224:LEU:HD13	2:E:333:ILE:HG12	2.02	0.40
2:E:712:PHE:O	2:E:716:LEU:N	2.52	0.40
2:E:821:PRO:HA	2:E:824:ILE:HG23	2.04	0.40
2:E:870:ARG:NH1	2:E:873:GLU:HB3	2.37	0.40
2:E:958:ILE:HB	2:E:1016:VAL:HG21	2.03	0.40
2:E:999:LYS:HE2	2:E:999:LYS:HB3	1.90	0.40
3:F:21:ILE:HD12	3:F:40:TYR:CZ	2.57	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	196/733 (27%)	179 (91%)	17 (9%)	0	100	100
1	D	196/733 (27%)	179 (91%)	17 (9%)	0	100	100
2	B	1640/1648 (100%)	1512 (92%)	128 (8%)	0	100	100
2	E	1640/1648 (100%)	1512 (92%)	128 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	175/184 (95%)	164 (94%)	11 (6%)	0	100	100
3	F	175/184 (95%)	165 (94%)	10 (6%)	0	100	100
All	All	4022/5130 (78%)	3711 (92%)	311 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/664 (28%)	183 (100%)	0	100	100
1	D	183/664 (28%)	183 (100%)	0	100	100
2	B	1495/1497 (100%)	1495 (100%)	0	100	100
2	E	1495/1497 (100%)	1495 (100%)	0	100	100
3	C	153/157 (98%)	152 (99%)	1 (1%)	76	78
3	F	153/157 (98%)	152 (99%)	1 (1%)	76	78
All	All	3662/4636 (79%)	3660 (100%)	2 (0%)	87	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	43	ASN
3	F	43	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	550	GLN
1	A	554	ASN
1	A	596	GLN
2	B	130	GLN
2	B	156	ASN

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Mol	Chain	Res	Type
2	B	187	HIS
2	B	257	ASN
2	B	376	ASN
2	B	556	ASN
2	B	653	ASN
2	B	738	ASN
2	B	769	GLN
2	B	885	GLN
2	B	926	GLN
2	B	963	GLN
2	B	1023	GLN
2	B	1035	GLN
2	B	1203	ASN
2	B	1427	GLN
2	B	1531	ASN
2	B	1619	HIS
3	C	2	GLN
1	D	550	GLN
1	D	554	ASN
1	D	596	GLN
2	E	65	HIS
2	E	130	GLN
2	E	156	ASN
2	E	187	HIS
2	E	257	ASN
2	E	376	ASN
2	E	414	GLN
2	E	556	ASN
2	E	576	ASN
2	E	653	ASN
2	E	738	ASN
2	E	769	GLN
2	E	885	GLN
2	E	926	GLN
2	E	963	GLN
2	E	1023	GLN
2	E	1035	GLN
2	E	1203	ASN
2	E	1293	GLN
2	E	1531	ASN
2	E	1614	GLN
2	E	1619	HIS

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Mol	Chain	Res	Type
3	F	2	GLN
3	F	39	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

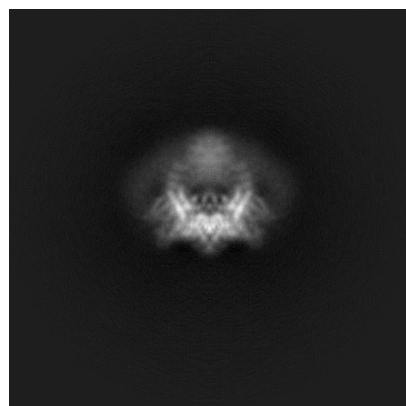
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60148. These allow visual inspection of the internal detail of the map and identification of artifacts.

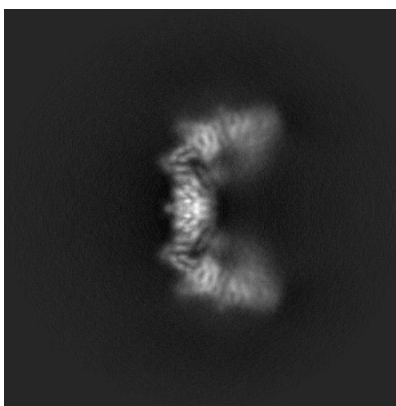
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

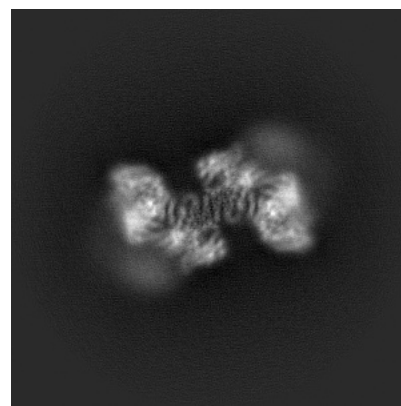
6.1.1 Primary map



X

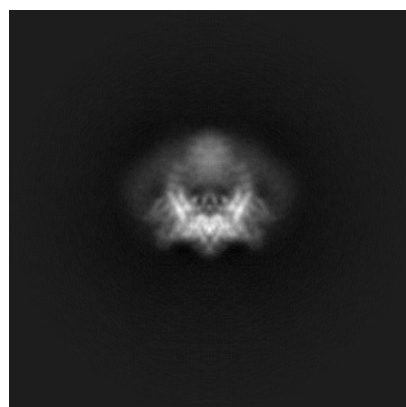


Y

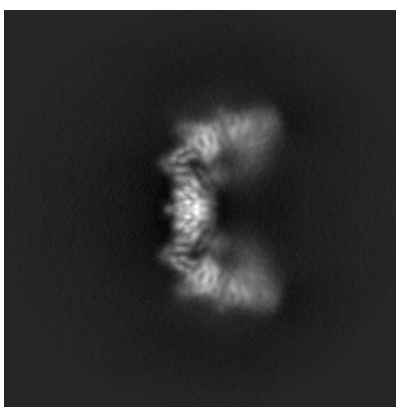


Z

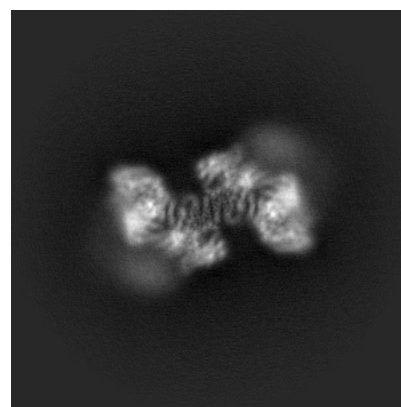
6.1.2 Raw map



X



Y

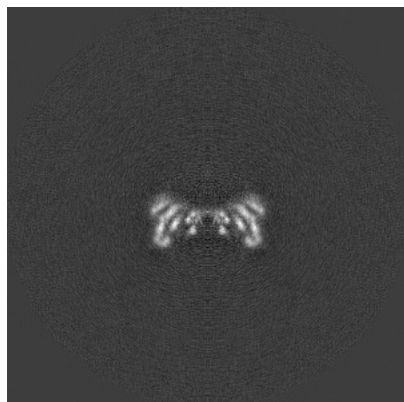


Z

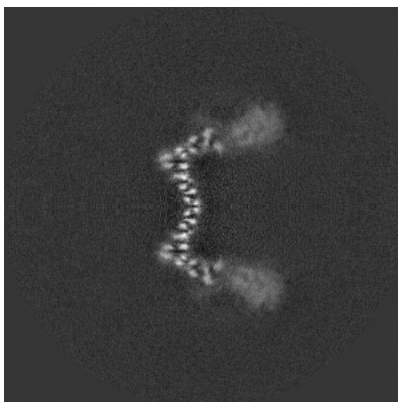
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

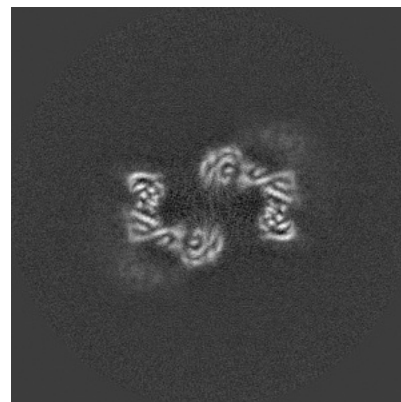
6.2.1 Primary map



X Index: 170

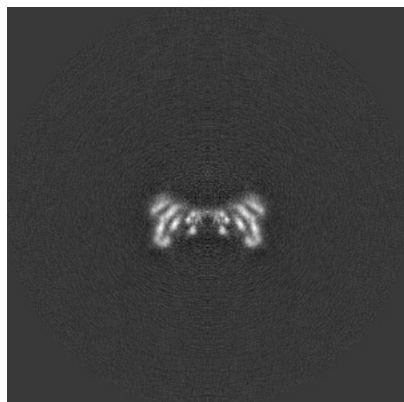


Y Index: 170

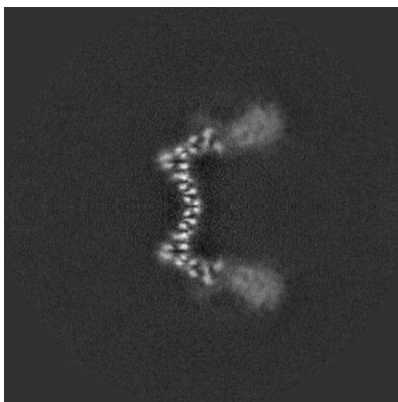


Z Index: 170

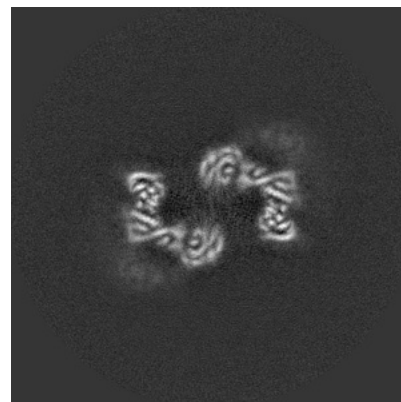
6.2.2 Raw map



X Index: 170



Y Index: 170

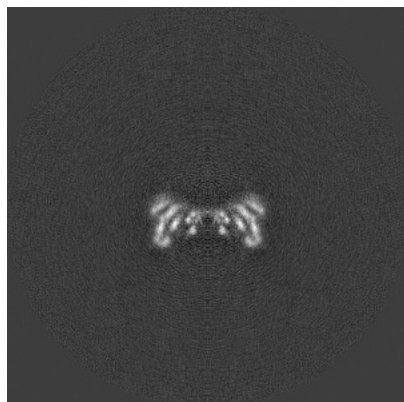


Z Index: 170

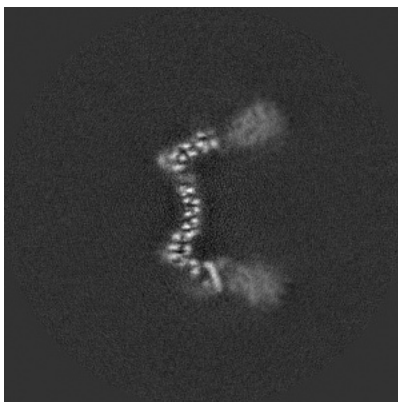
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

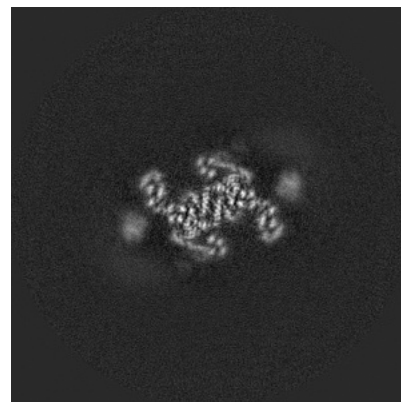
6.3.1 Primary map



X Index: 170

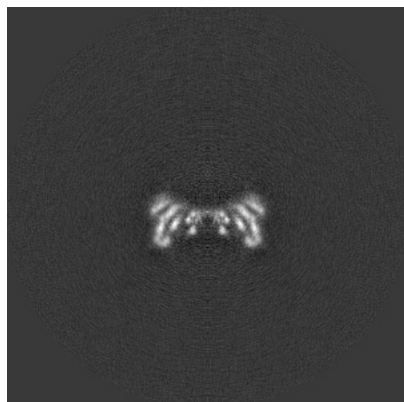


Y Index: 166

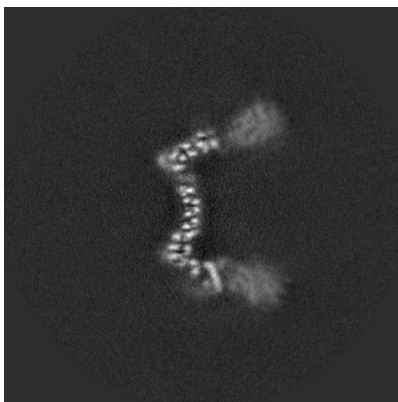


Z Index: 155

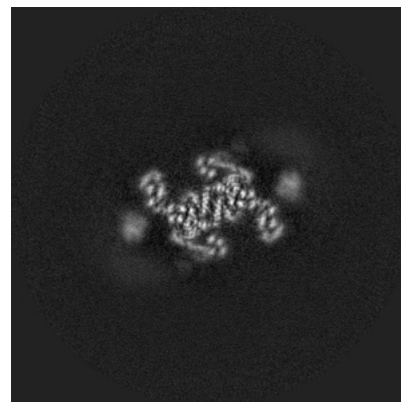
6.3.2 Raw map



X Index: 170



Y Index: 166

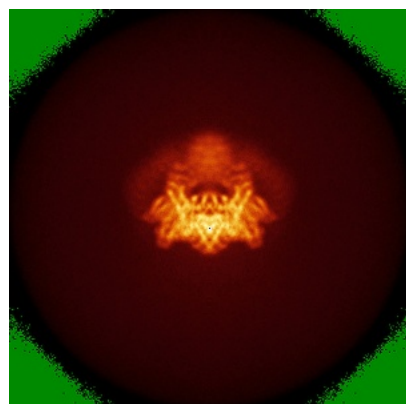


Z Index: 155

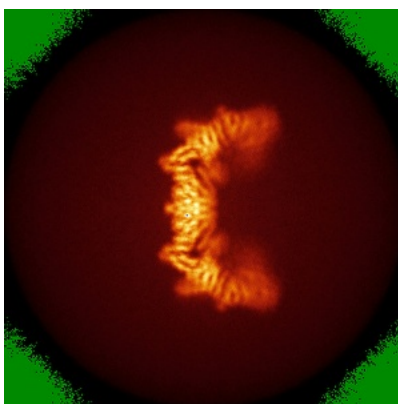
The images above show the largest variance slices of the map in three orthogonal directions.

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

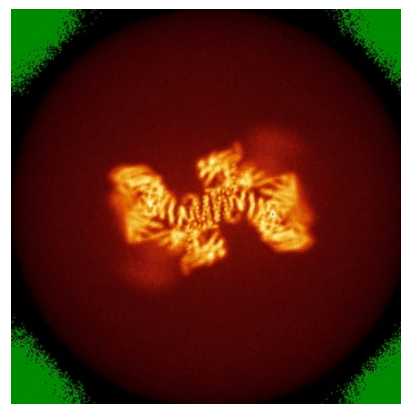
6.4.1 Primary map



X



Y



Z

6.4.2 Raw map



X



Y

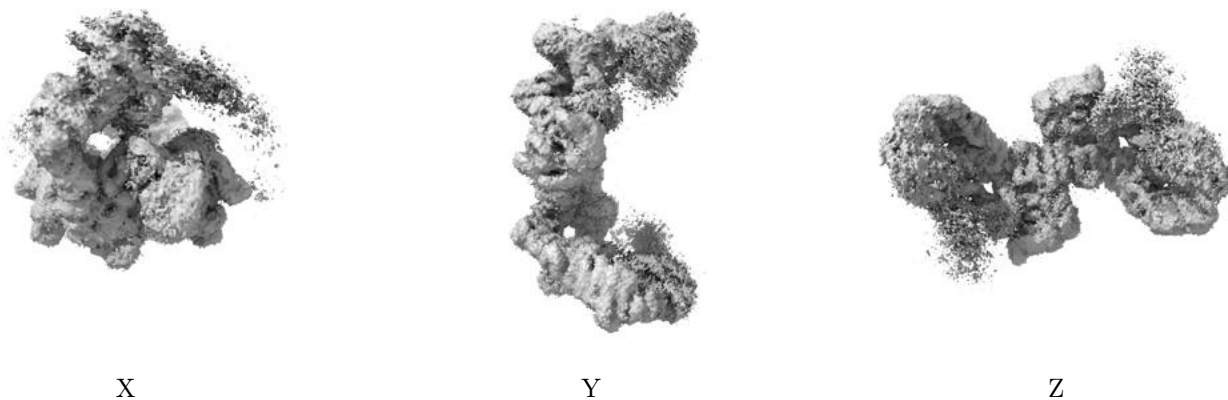


Z

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

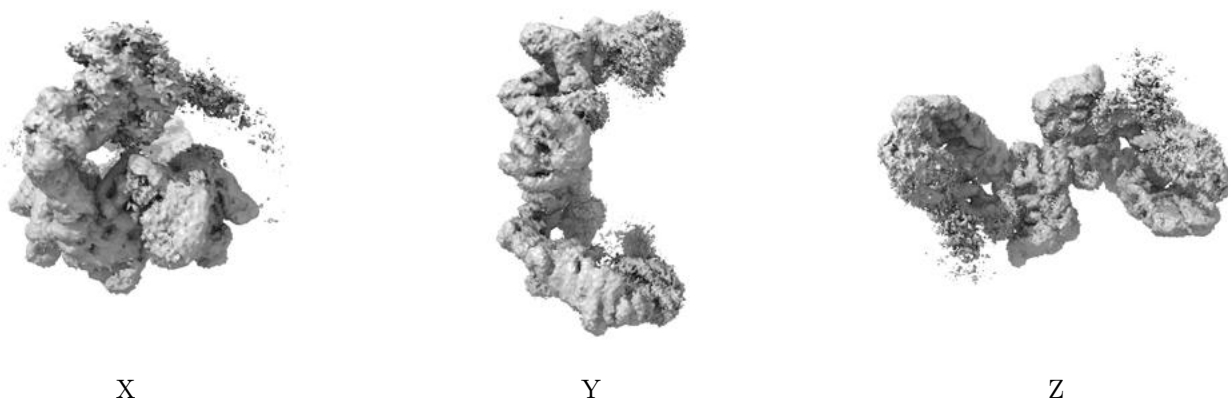
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

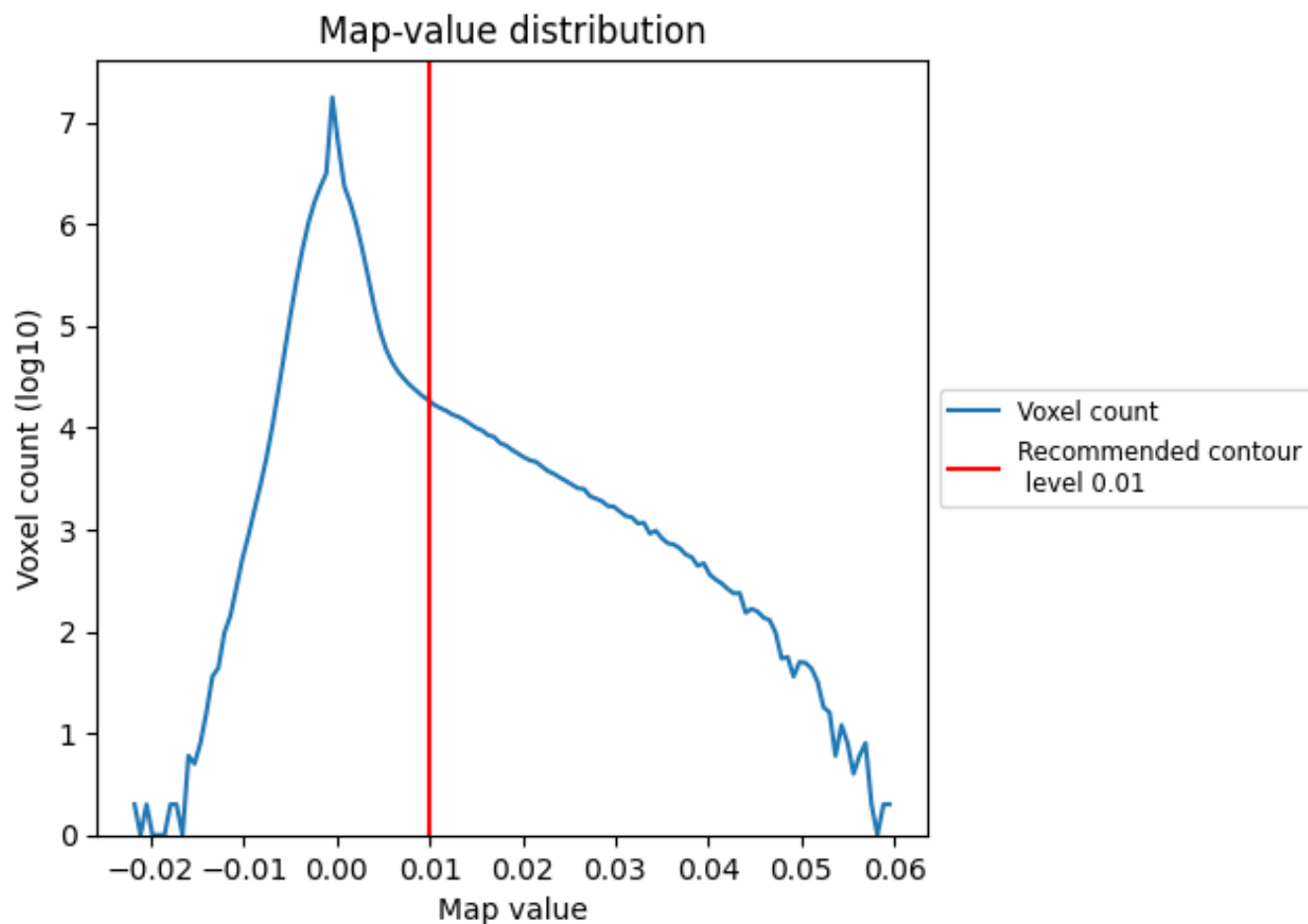
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

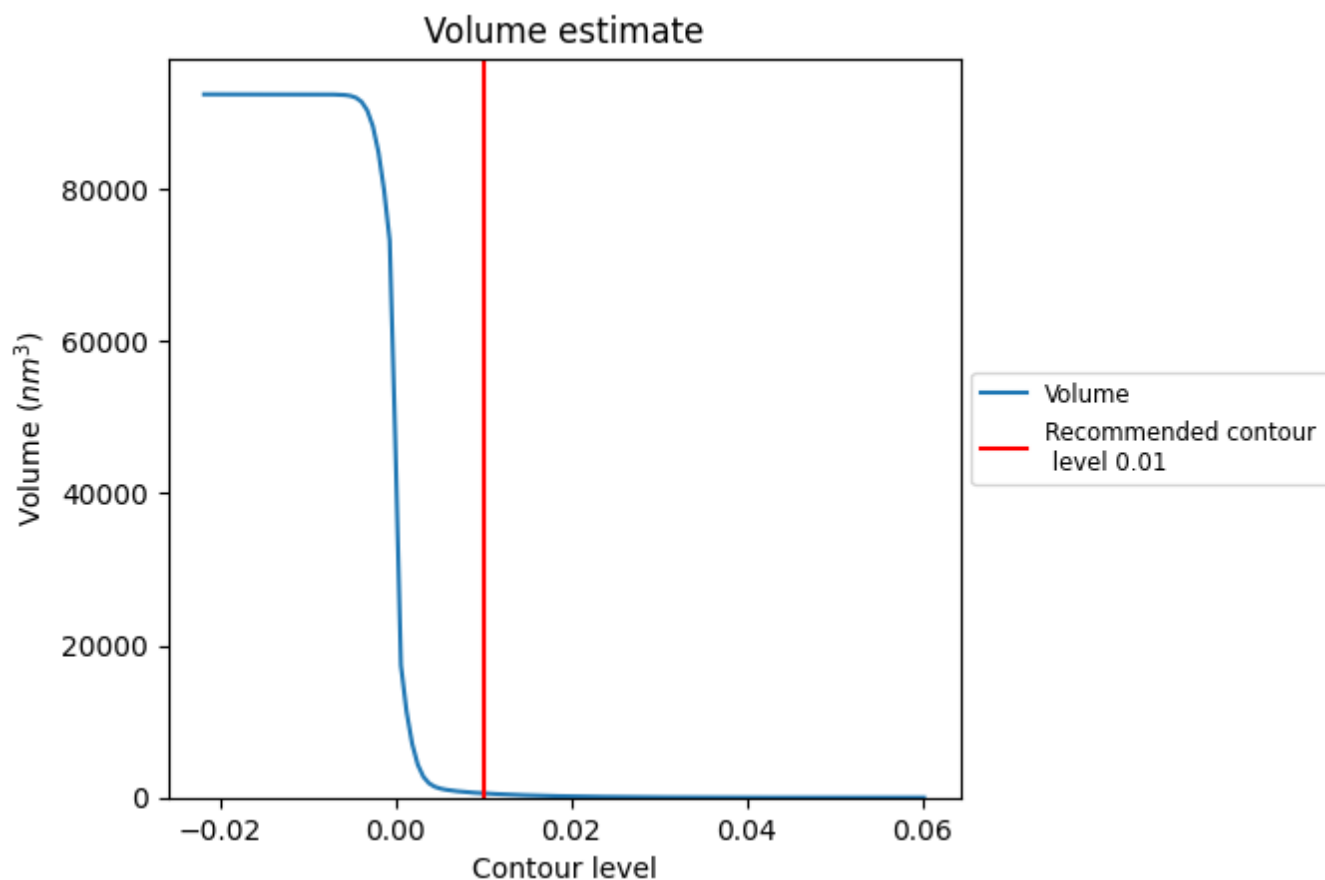
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

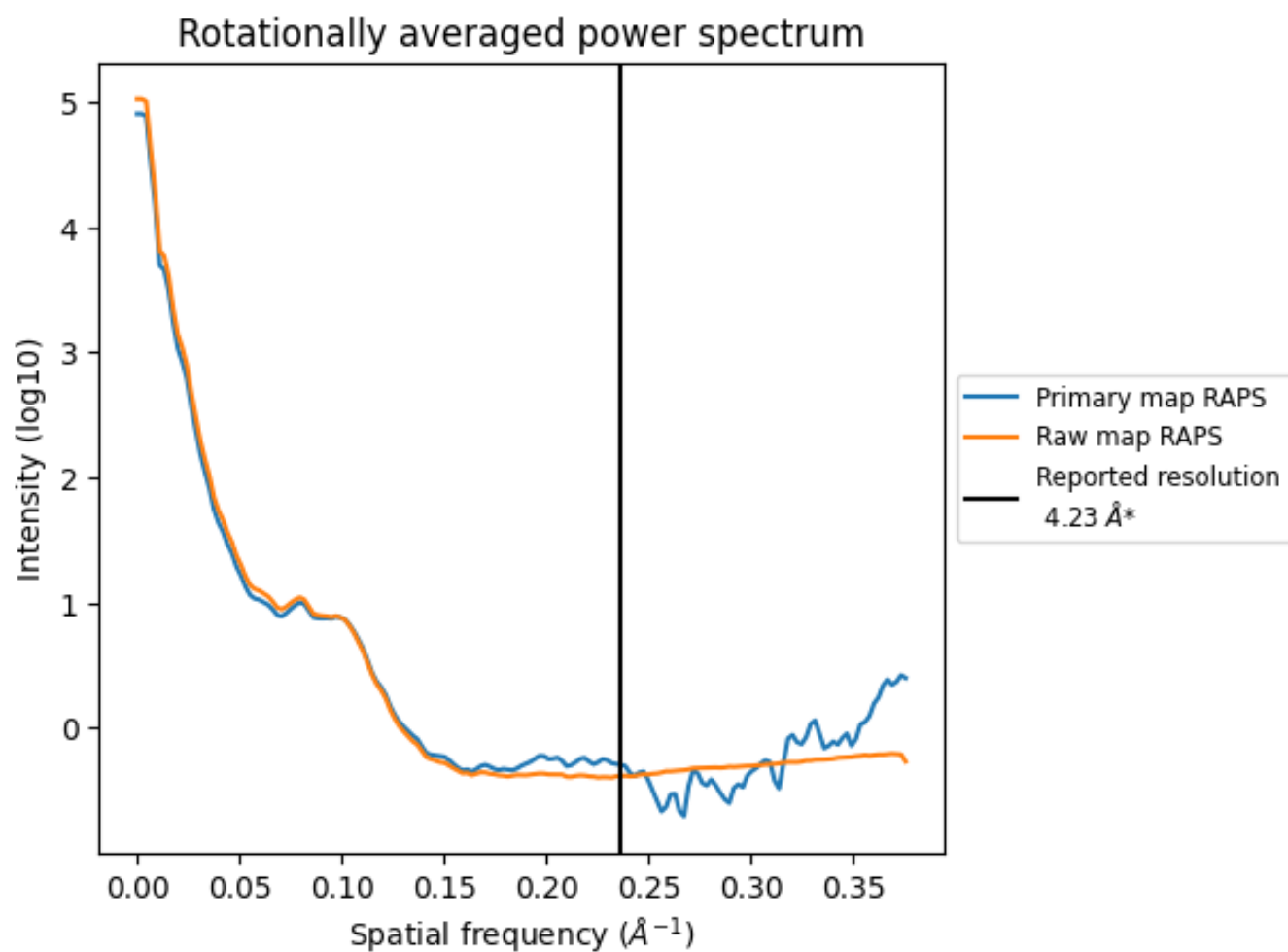
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 558 nm^3 ; this corresponds to an approximate mass of 504 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 ⓘ

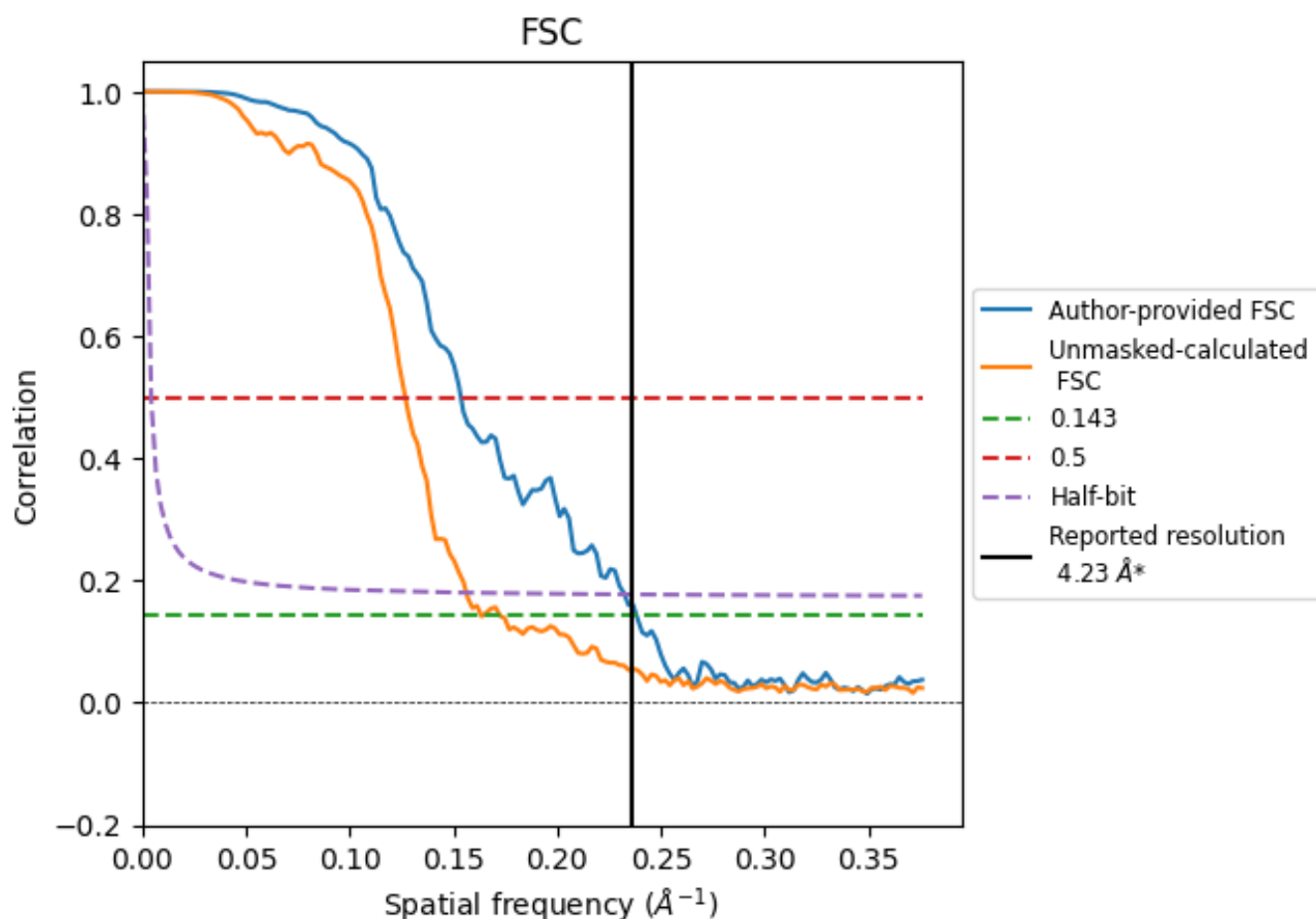


*Reported resolution corresponds to spatial frequency of 0.236 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.236 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

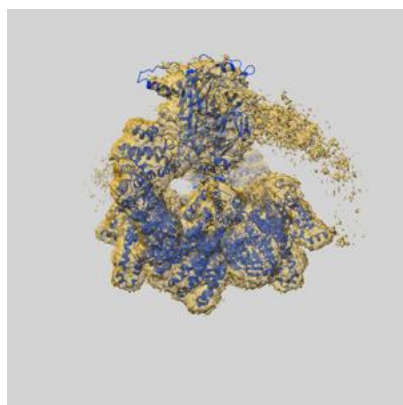
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.23	-	-
Author-provided FSC curve	4.20	6.51	4.30
Unmasked-calculated*	6.12	7.89	6.40

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.12 differs from the reported value 4.23 by more than 10 %

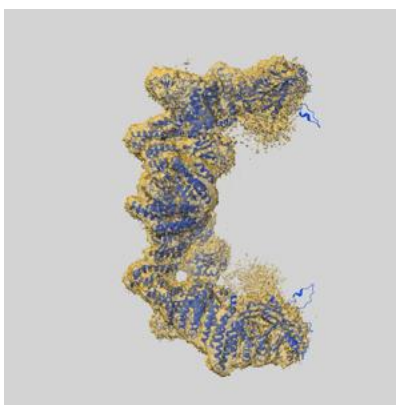
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60148 and PDB model 8ZJK. Per-residue inclusion information can be found in section [3](#) on page [6](#).

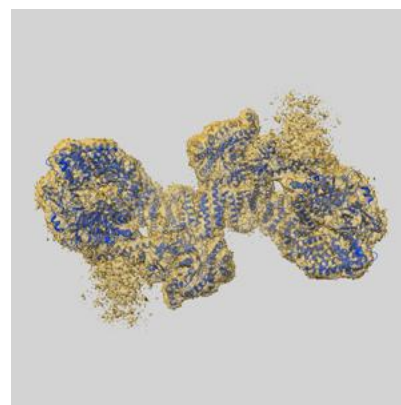
9.1 Map-model overlay [i](#)



X



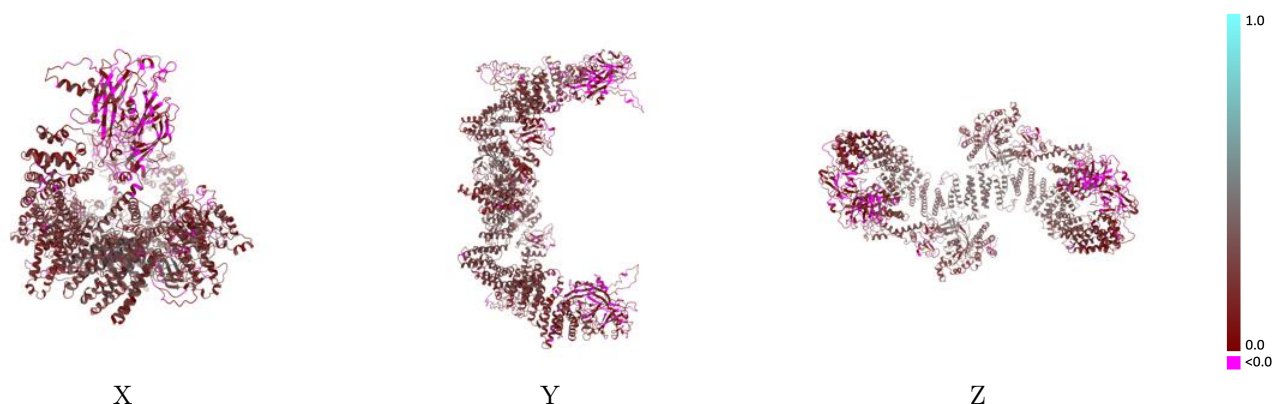
Y



Z

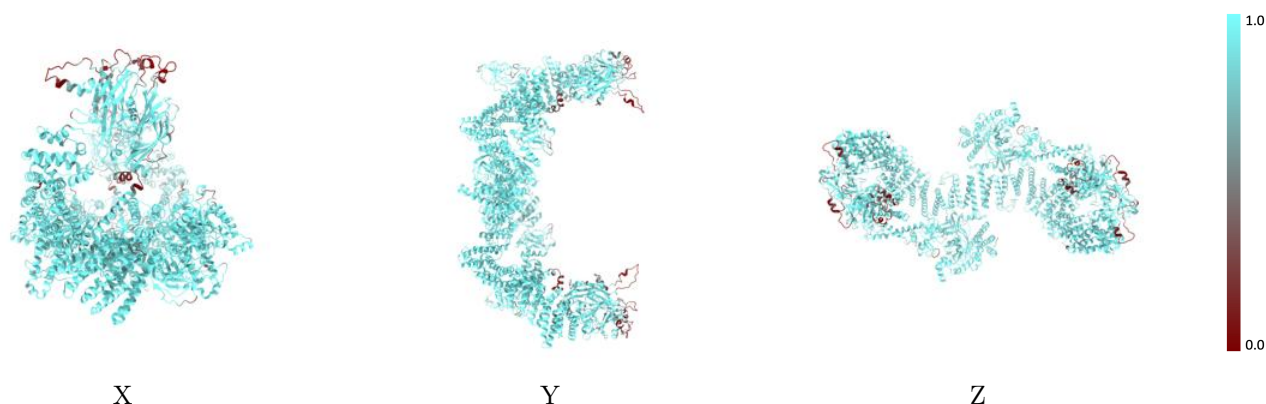
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



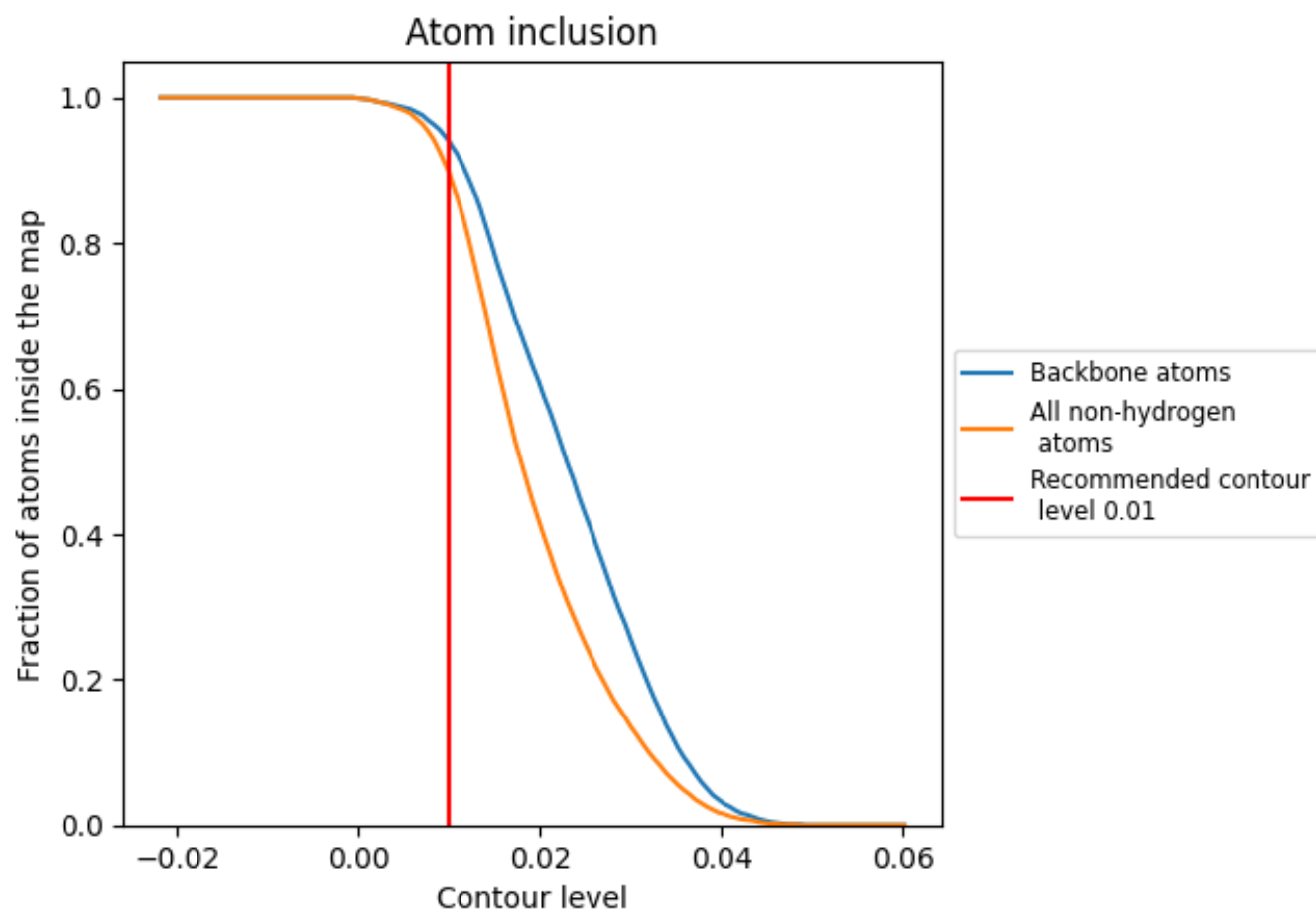
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8970	0.2030
A	0.8970	0.1680
B	0.8870	0.2030
C	0.9560	0.2450
D	0.9070	0.1610
E	0.8930	0.2040
F	0.9600	0.2420

1.0

0.0

<0.0