



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:21 PM UTC

PDB ID : 6CNF / pdb_00006cnf
EMDB ID : EMD-7533
Title : Yeast RNA polymerase III elongation complex
Authors : Han, Y.; He, Y.
Deposited on : 2018-03-08
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

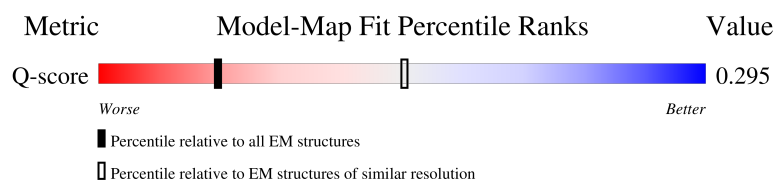
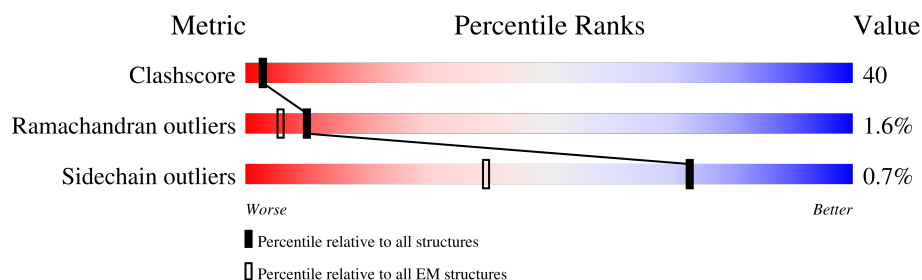
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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.



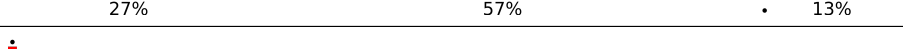
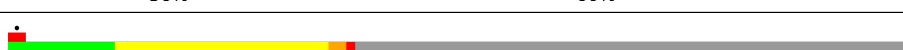
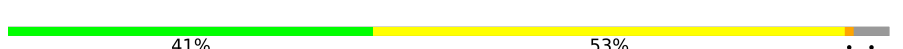
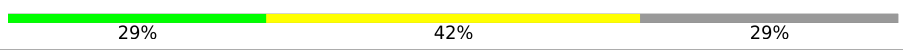
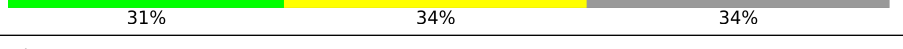
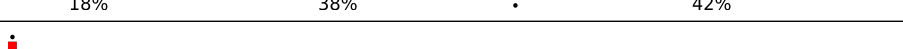
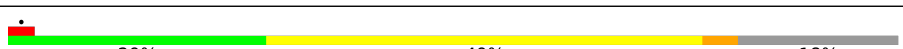
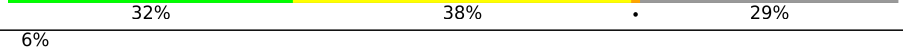
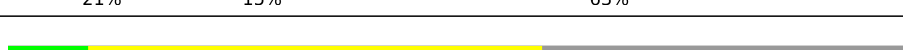
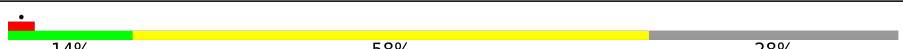
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	1460	 38% 57% . .
2	B	1149	 35% 59% . .
3	C	335	 39% 56% .
4	D	161	 30% 41% . 26%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	212	
8	H	146	
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	251	
18	R	736	
19	S	594	
20	X	79	
21	Y	79	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 47675 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 DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1428	Total	C	N	O	S	0	0
			11159	7029	1972	2099	59		

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8788	5558	1516	1654	60		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	119	Total	C	N	O	S	0	0
			977	628	156	187	6		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1759	1116	310	321	12		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			671	429	114	125	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	184	Total	C	N	O	S	0	0
			1484	972	239	267	6		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	703	188	224	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	42	Total	C	N	O	S	0	0
			321	204	47	64	6		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			363	224	72	63	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	164	Total	C	N	O	S	0	0
			1338	857	227	253	1		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	110	Total	C	N	O	S	0	0
			845	536	152	154	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	539	Total	C	N	O	S	0	0
			4329	2756	741	813	19		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	277	Total	C	N	O	S	0	0
			2242	1438	368	425	11		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	54	Total	C	N	O	0	0
			368	238	64	66		

- Molecule 18 is a protein called Transcription factor IIIB 70 kDa subunit,TATA-box-binding protein,Transcription factor IIIB 70 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	522	Total	C	N	O	S	0	0
			4131	2621	733	757	20		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	383	ALA	-	linker	UNP P29056
R	384	MET	-	linker	UNP P29056
R	385	PRO	-	linker	UNP P29056
R	386	TRP	-	linker	UNP P29056
R	567	GLY	-	linker	UNP P13393
R	568	SER	-	linker	UNP P13393
R	569	GLY	-	linker	UNP P13393
R	570	SER	-	linker	UNP P13393
R	571	GLY	-	linker	UNP P13393

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Chain	Residue	Modelled	Actual	Comment	Reference
R	572	SER	-	linker	UNP P13393
R	573	GLY	-	linker	UNP P13393
R	574	SER	-	linker	UNP P13393
R	575	GLY	-	linker	UNP P13393
R	576	SER	-	linker	UNP P13393
R	577	GLY	-	linker	UNP P13393
R	578	SER	CYS	engineered mutation	UNP P29056

- Molecule 19 is a protein called Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B".

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	217	Total	C	N	O	S	0	0
			1649	1035	286	321	7		

- Molecule 20 is a DNA chain called DNA (79-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	47	Total	C	N	O	P	0	0
			959	463	164	286	46		

- Molecule 21 is a DNA chain called DNA (79-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	57	Total	C	N	O	P	0	0
			1169	560	220	333	56		

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	A	2	Total	Zn	0
			2	2	
22	B	1	Total	Zn	0
			1	1	
22	I	1	Total	Zn	0
			1	1	
22	J	1	Total	Zn	0
			1	1	
22	L	1	Total	Zn	0
			1	1	

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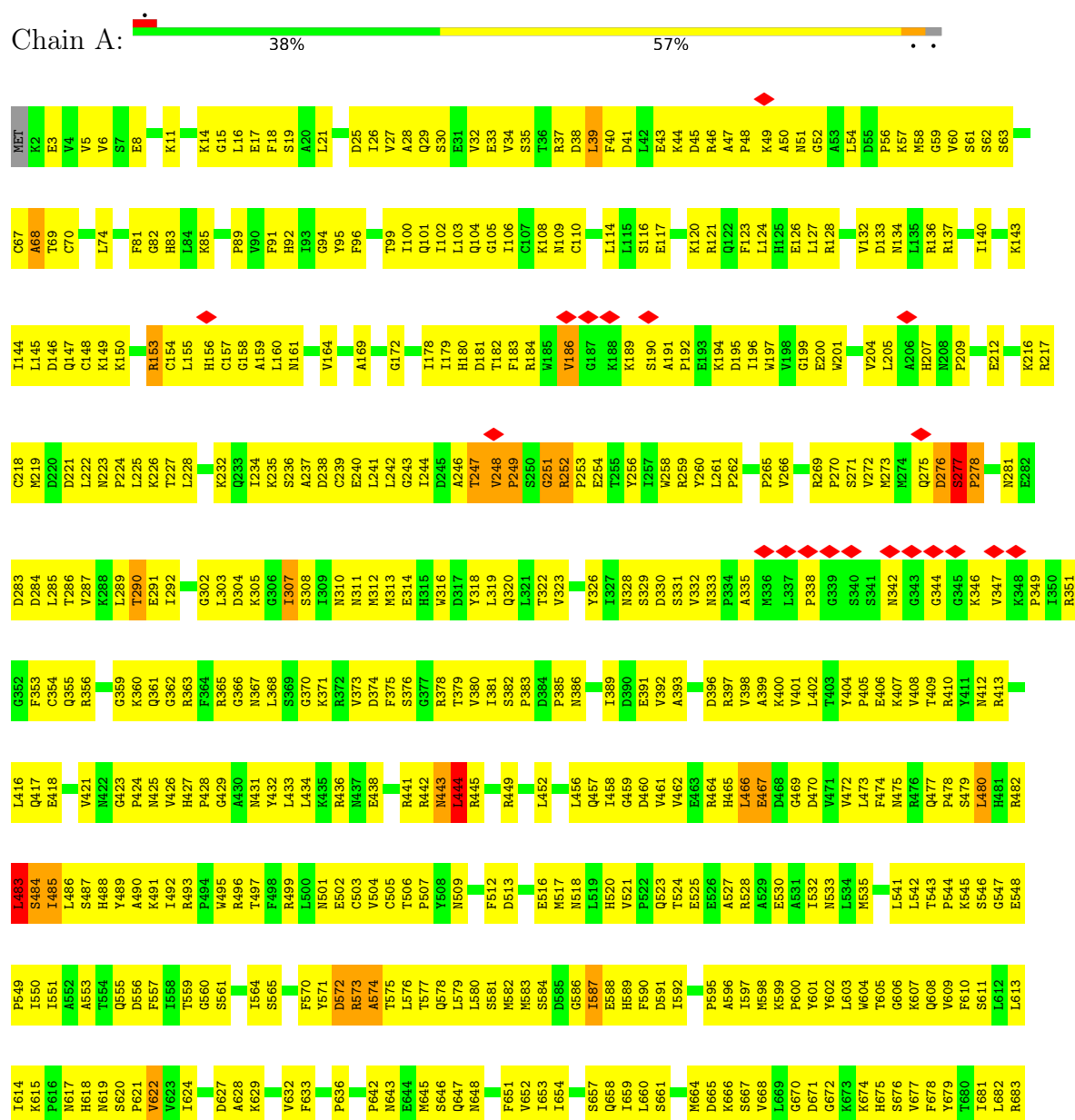
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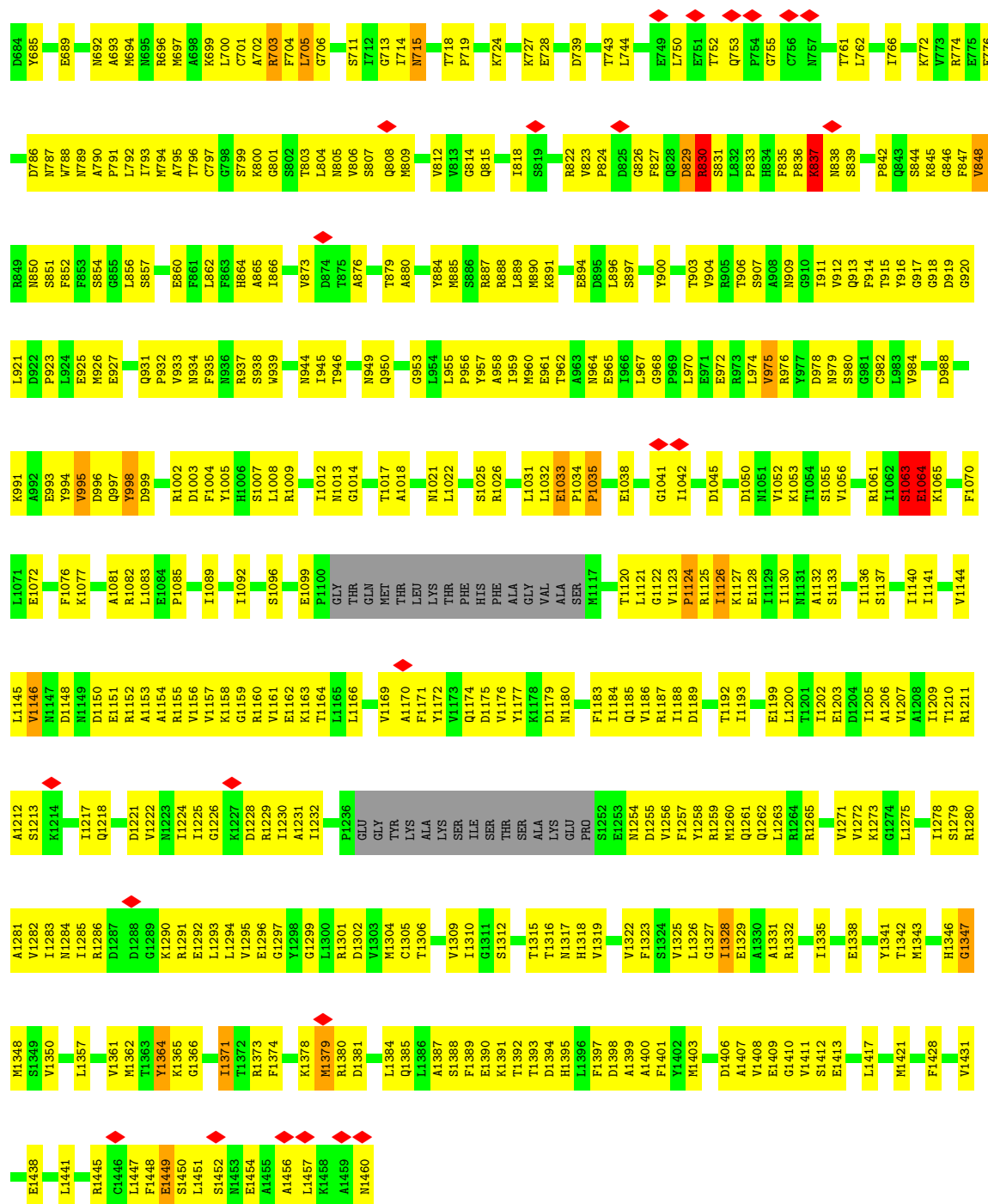
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
22	R	1	1	1	0

3 Residue-property plots

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

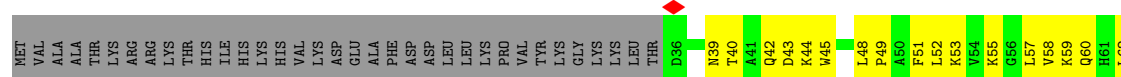
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1



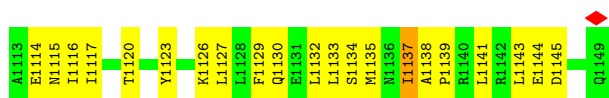


• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

Chain B: 35% 59%

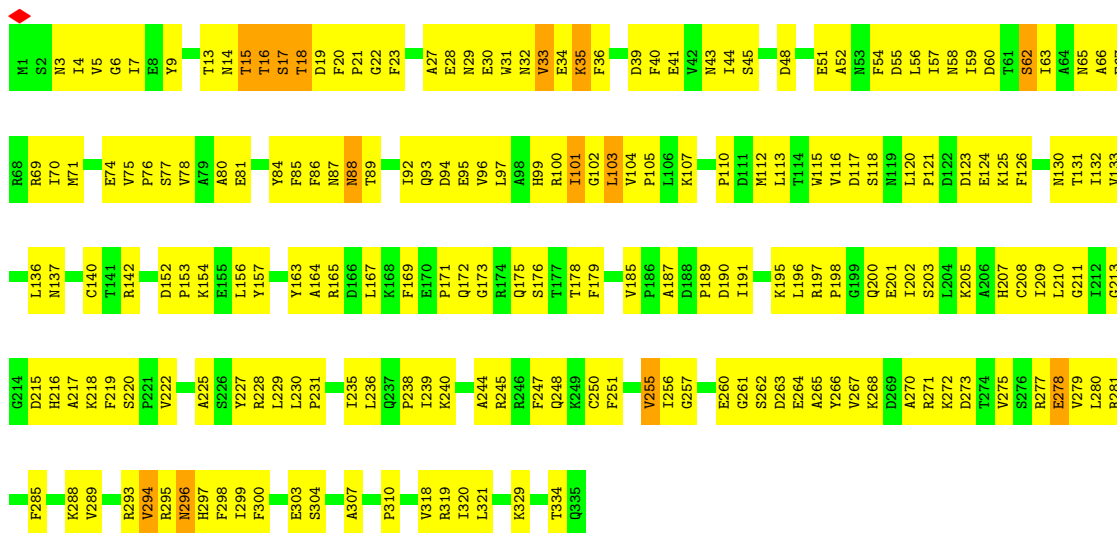


L1046	E974	R904	Q822	D747	L681	R610	D545	S480	K408	E338	E267	N203	G138	D63
Q1049	Y975	R905	S823	P750	G882	P611	S546	R481	K409	A339	I268	R204	R139	S4
P1050	G976	G909	L824	G884	V684	I613	L549	S484	N410	L340	L271	I205	I140	F85
R1054	G981	K911	G825	N754	G886	I614	L550	G485	R412	D341	G274	V207	I141	M66
S1055	S982	F912	V832	A755	G887	V615	L551	P486	A413	F342	E267	E208	I142	Y67
R1056	D986	S913	V832	T756	G888	S616	G553	A488	M414	E344	E267	A209	M143	F68
D1057	S914	S914	T841	V757	G889	Q619	G554	A489	E415	K345	S277	D210	H144	D72
G1058	N987	R915	Y842	A758	G890	S620	G555	L489	Y416	A346	S278	E211	K145	D72
G1059	S988	H916	R943	V759	G891	S621	V555	Q490	D417	L347	Q279	K212	E146	I76
L1060	K990	G917	N844	M760	H692	V622	V556	Q490	D417	Y348	Q280	K213	E147	I77
R1061	R993	Q918	N844	S761	H693	V623	L557	Q493	A418	I349	I282	G214	E148	
L1062	L991	K919	V847	Y762	N894	K623	N558	Q493	L419		I282	I215	G150	Q81
G1063	V992	G920	P848	S763	N894	D624	G559	F494	L420	M552	F283	V216	R151	L82
E1064	D993	V921	P848	S764	G895	I625	T560	G495	A284	T953	A284	Q217	M152	L83
M1065	Q994	G922	N850	G764	S696	H626	L561	M496	R354	R354	V285		P153	L84
E1066		G923	N851	Y765	G697	L627	V562	L497	R355	R355	N287	V220	I154	S85
R1067	K1001	I924	S851	I767	N698	R628	G563	C498	N362		E288	S222	L156	D86
D1068	D1002	I925	P855	E768	N699	L630	S564	A500	P363		E289	S223	R157	D88
C1069	M1003	V926		G769	Q702	L631	I565	D501	M364		K292	H225	S158	D89
I1070	L1004	Q927	N858	A770	M705	L635	F567	F503	I366		I295	F226	E90	F91
Y1071	Y1005	Q928	N859	L771	M705	L635	P568	E504	D367		Y296	H226	Y163	Y92
A1072	S1006	E929	V860	V772	A709	F637	T569	A507	R435		R227	R227	L164	Y93
Y1073	G1007	D930	N861	L773	I710	D638	F571	C508	S438		R228	R228	Y164	Y94
	D1008	M931		N774	I710			G509	T439		Y297	S229	D165	Y95
S1076	T1009	P932	Q863	K775	I713	F640	Q574	G509	S438		Q298	Y232	A166	
Q1077	G1010	F933	Y864	S777	A714	L510	F575	G509	T439		Q299	V233	D167	V96
L1078	E1011	N934	Y715	S777	A714	L510	R576	G509	T439		Q300	I234	E168	D97
L1079	C1012	D935	Q865	Y778	N716	G644	H577	G509	T439		Q301	I235	S169	I98
L1080	L1013		Y866	Y779	Q717	L645	L578	G509	T439		Q302	I236	K170	R99
E1081	I1017	I938	R867	R780	F718	L645	L578	G509	T439		Q303	I237	M171	V100
K1082	F1018	V939	E868	G781	R719	L645	L578	G509	T439		Q304	I238	A172	G101
L1083	F1019	P940	A869	F782	R720	E647	R580	G509	T439		Q305	I239	K173	K102
M1084	D941	I942	P870	F782	R720	E647	R580	G509	T439		Q306	I240	L174	G103
I1085	I1022	I943	I872	E786	I721	L649	K583	G509	T439		Q307	I241	N175	N107
S1086	Y1023	I944	Y873	T787	D722	D650	V584	G509	T439		Q308	I242	E176	S107
S1087	Y1024	N945		R788	D723	V651	S585	G509	T439		Q309	I243	G177	T108
D1088	Q1025	H947	E877	K789	L725	N652	E586	G509	T439		Q310	I244	L179	K109
E1091	K1026	H947	P878	L795	L726	N655	S588	G509	T439		Q311	I245	D180	D110
V1092	L1027	H947	H880	L796	Y726	N656	S589	G509	T439		Q312	I246	P181	Y111
D1093	K1028	H947	H880	K796	M728	N657	S591	G509	T439		Q313	I247	Y184	H116
V1094	H1029	S951	H880	K797	M729	N658	S592	G509	T439		Q314	I248	F185	D122
C1095	M1030	D882	D882	Y796	Y730	L658	S592	G509	T439		Q315	I249	I186	M123
	V1031	Q883	Q883	A799	Y731	L659	S593	G509	T439		Q316	I250	V187	T124
G1099	L1032	M886	M886	H801	Q732	A660	N593	G509	T439		Q317	I251	N188	Y125
L1100	D1033	S887	S887	H801	Q733	V667	Q596	G509	T439		Q318	I252	G189	T126
M1101	K1034	S887	S887	H801	Q734	P668	M597	G509	T439		Q319	I253	T190	A127
G1102	M1035	S887	S887	H801	Q735	P668	A598	G509	T439		Q320	I254	E191	P128
Y1103	H1036	S887	S887	H801	Q736	P668	A598	G509	T439		Q321	I255	K192	I129
S1104	A1037	S887	S887	H801	Q737	P668	A598	G509	T439		Q322	I256	E191	Y130
G1105	R1038	S887	S887	H801	Q738	P668	A598	G509	T439		Q323	I257	K192	V131
W1106	A1039	S887	S887	H801	Q739	P668	A598	G509	T439		Q324	I258	E191	D132
C1107	R1040	S887	S887	H801	Q740	P668	A598	G509	T439		Q325	I259	K192	I133
T1108	G1041	S887	S887	H801	Q741	P668	A598	G509	T439		Q326	I260	E191	E134
T1109	F1042	S887	S887	H801	Q742	P668	A598	G509	T439		Q327	I261	K192	Y136
C1110	A1043	S887	S887	H801	Q743	P668	A598	G509	T439		Q328	I262	E191	S201
S1112	V1045	S887	S887	H801	Q744	P668	A598	G509	T439		Q329	I263	K192	K202
		S887	S887	H801	Q745	P668	A598	G509	T439		Q330	I264	E191	
		S887	S887	H801	Q746	P668	A598	G509	T439		Q331	I265	E191	
		S887	S887	H801	Q747	P668	A598	G509	T439		Q332	I266	E191	
		S887	S887	H801	Q748	P668	A598	G509	T439		Q333	I267	E191	
		S887	S887	H801	Q749	P668	A598	G509	T439		Q334	I268	E191	
		S887	S887	H801	Q750	P668	A598	G509	T439		Q335	I269	E191	
		S887	S887	H801	Q751	P668	A598	G509	T439		Q336	I270	E191	
		S887	S887	H801	Q752	P668	A598	G509	T439		Q337	I271	E191	
		S887	S887	H801	Q753	P668	A598	G509	T439		Q338	I272	E191	
		S887	S887	H801	Q754	P668	A598	G509	T439		Q339	I273	E191	
		S887	S887	H801	Q755	P668	A598	G509	T439		Q340	I274	E191	
		S887	S887	H801	Q756	P668	A598	G509	T439		Q341	I275	E191	
		S887	S887	H801	Q757	P668	A598	G509	T439		Q342	I276	E191	
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		S887	S887	H801	Q759	P668	A598	G509	T439		Q344	I278	E191	
		S887	S887	H801	Q760	P668	A598	G509	T439		Q345	I279	E191	
		S887	S887	H801	Q761	P668	A598	G509	T439		Q346	I280	E191	
		S887	S887	H801	Q762	P668	A598	G509	T439		Q347	I281	E191	
		S887	S887	H801	Q763	P668	A598	G509	T439		Q348	I282	E191	
		S887	S887	H801	Q764	P668	A598	G509	T439		Q349	I283	E191	
		S887	S887	H801	Q765	P668	A598	G509	T439		Q350	I284	E191	
		S887	S887	H801	Q766	P668	A598	G509	T439		Q351	I285	E191	
		S887	S887	H801	Q767	P668	A598	G509	T439		Q352	I286	E191	
		S887	S887	H801	Q768	P668	A598	G509	T439		Q353	I287	E191	
		S887	S887	H801	Q769	P668	A598	G509	T439		Q354	I288	E191	
		S887	S887	H801	Q770	P668	A598	G509	T439		Q355	I289	E191	
		S887	S887	H801	Q771	P668	A598	G509	T439		Q356	I290	E191	
		S887	S887	H801	Q772	P668	A598	G509	T439		Q357	I291	E191	
		S887	S887	H801	Q773	P668	A598	G509	T439		Q358	I292	E191	
		S887	S887	H801	Q774	P668	A598	G509	T439		Q359	I293	E191	
		S887	S887	H801	Q775	P668	A598	G509	T439		Q360	I294	E191	
		S887	S887	H801	Q776	P668	A598	G509	T439		Q361	I295	E191	
		S887	S887	H801	Q777	P668	A598	G509	T439		Q362	I296	E191	
		S887	S887	H801	Q778	P668	A598	G509	T439		Q363	I297	E191	
		S887	S887	H801	Q779	P668	A598	G509	T439		Q364	I298	E191	
		S887	S887	H801	Q780	P668	A598	G509	T439		Q365	I299	E191	
		S887	S887	H801	Q781	P668	A598	G509	T439		Q366	I300	E191	
		S887	S887	H801	Q782	P668	A598	G509	T439		Q367	I301	E191	
		S887	S887	H801	Q783	P668	A598	G509	T439		Q368	I302	E191	
		S887	S887	H801	Q784	P668	A598	G509	T439		Q369	I303	E191	
		S887	S887	H801	Q785	P668	A598	G509	T439		Q370	I304	E191	
		S887	S887	H801	Q786	P668	A598	G509	T439		Q371	I305	E191	
		S887	S887	H801	Q787	P668	A598	G509	T439		Q372	I306	E191	
		S887	S887	H801	Q788	P668	A598	G509	T439		Q373	I307	E191	
		S887	S887	H801	Q789	P668	A598	G509	T439		Q374	I308	E191	
		S887	S887	H801	Q790	P668	A598	G509	T439		Q375	I309	E191	
		S887	S887	H801	Q791	P668	A598	G509	T439					



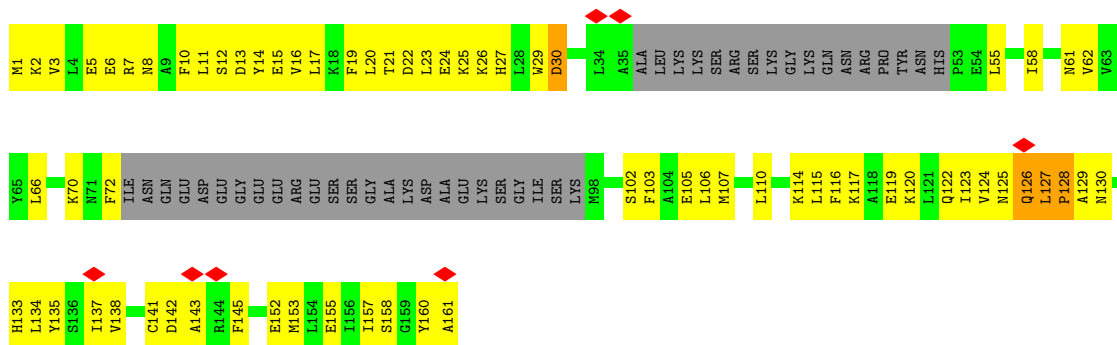
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 39% 56%



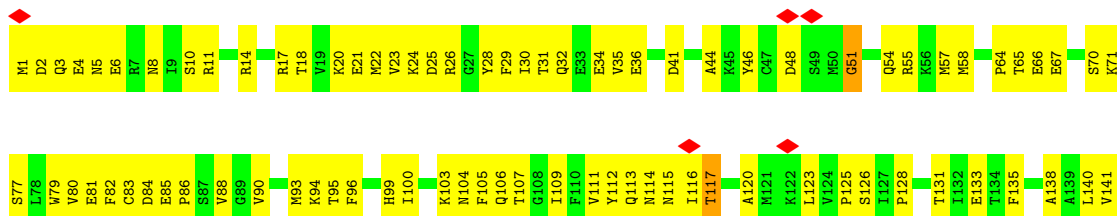
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

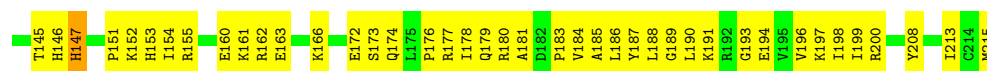
Chain D: 30% 41% 26%



• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

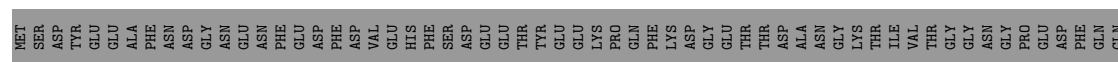
Chain E: 42% 57%





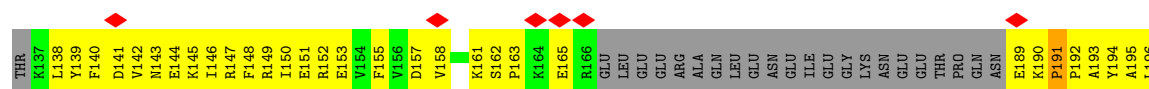
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 21% 30% 46%



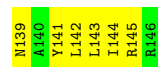
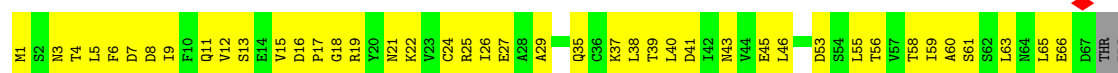
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8

Chain G: 6% 27% 57% 13%

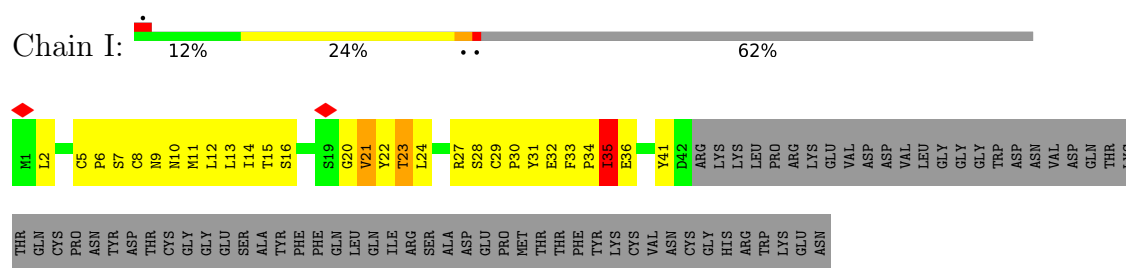


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

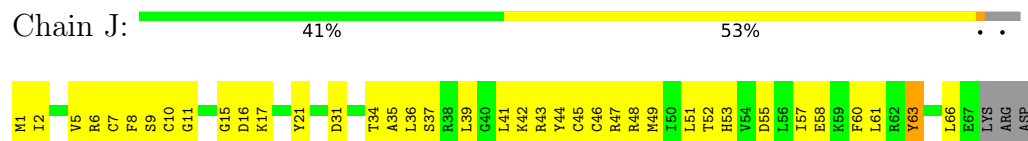
Chain H: 36% 60%



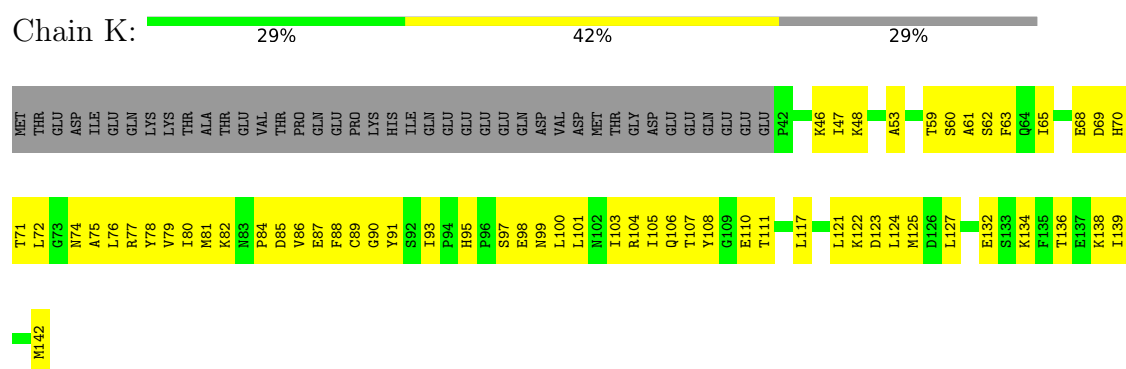
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



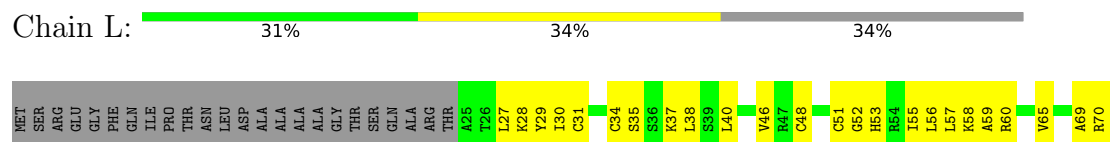
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



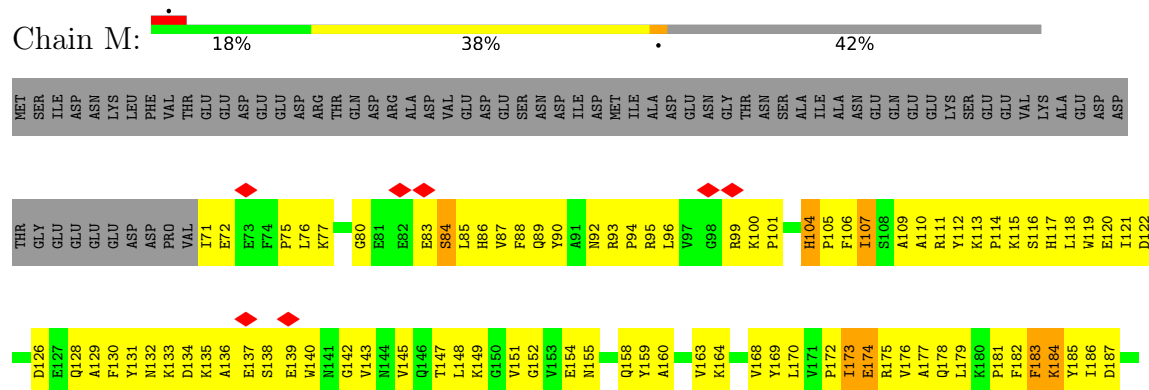
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

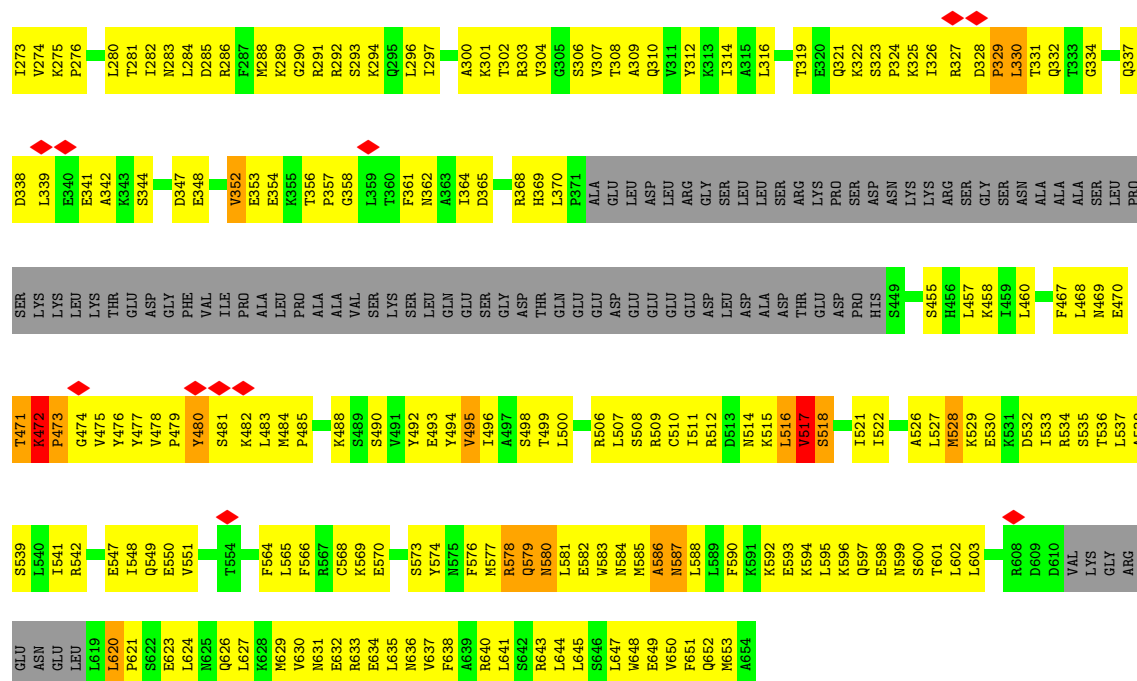


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

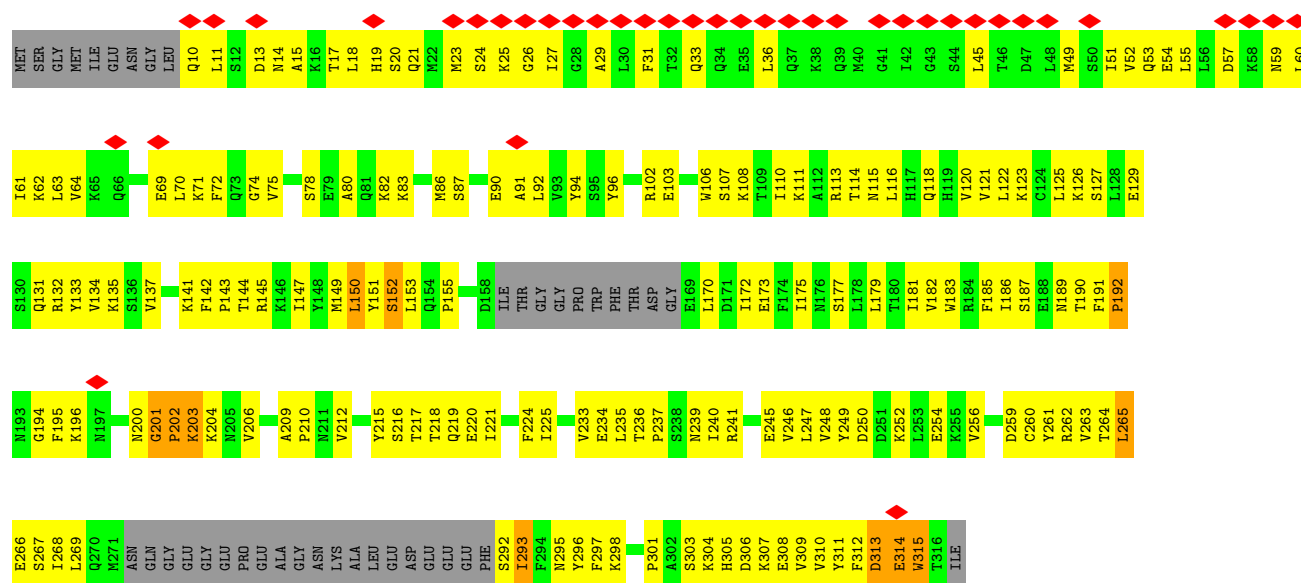


- Molecule 13: DNA-directed RNA polymerase III subunit RPC5



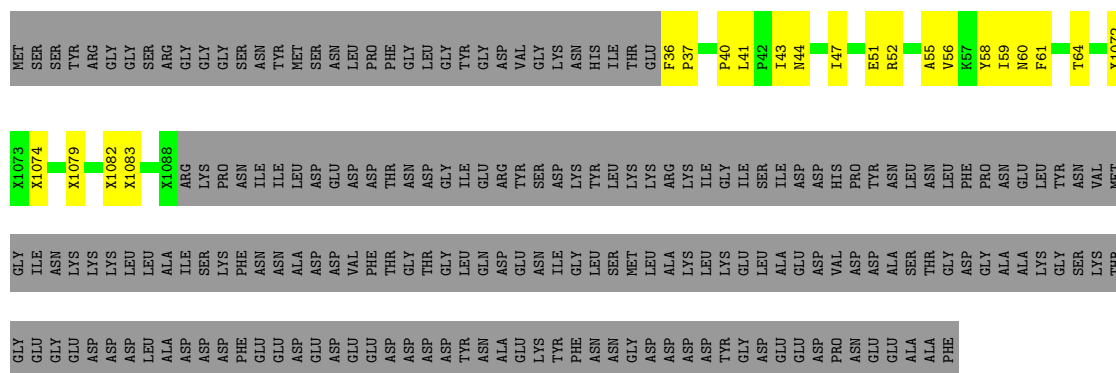


• Molecule 16: DNA-directed RNA polymerase III subunit RPC6

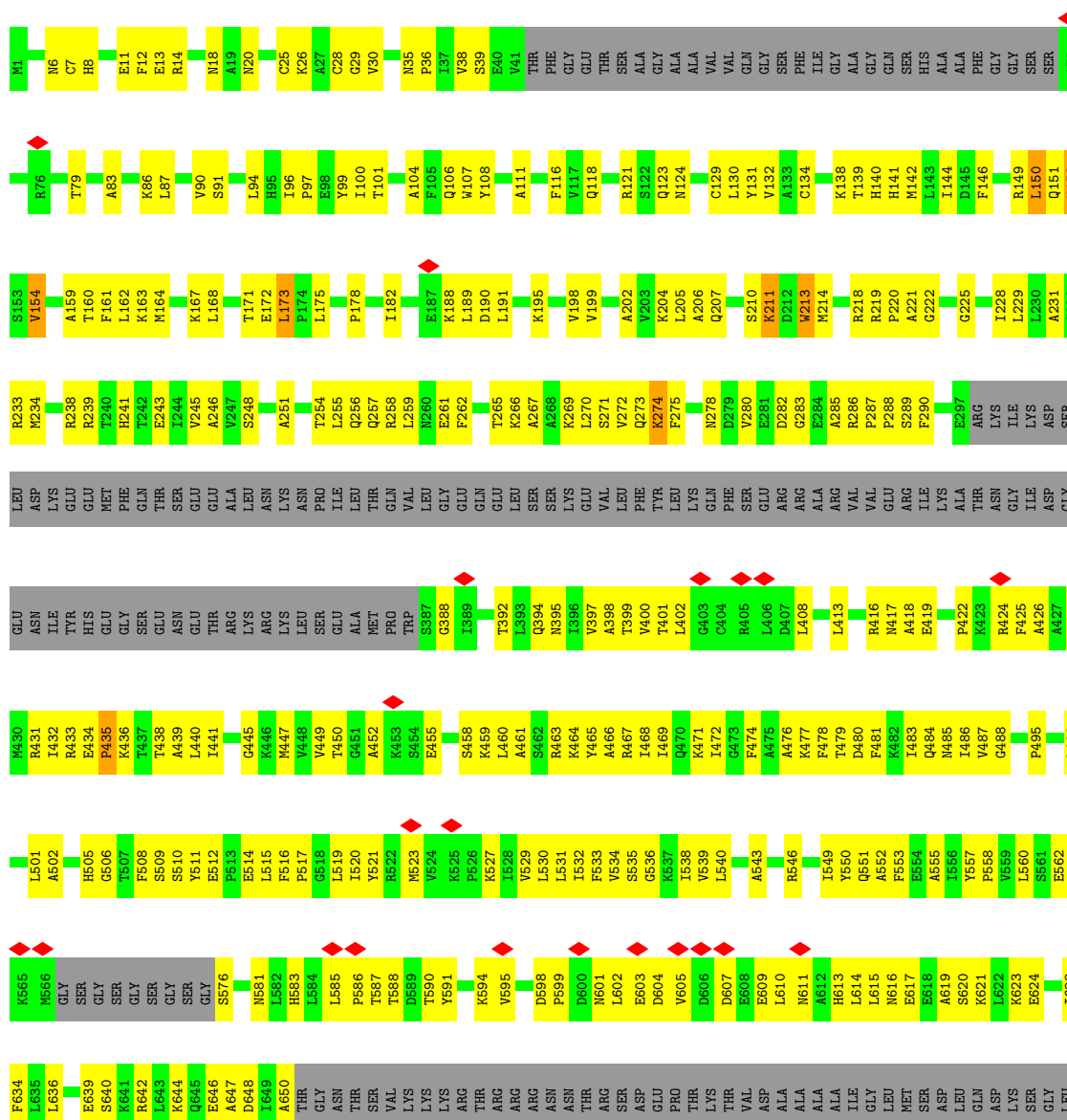


• Molecule 17: DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7





- Molecule 18: Transcription factor IIIB 70 kDa subunit, TATA-box-binding protein, Transcription factor IIIB 70 kDa subunit



• Molecule 19: Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B"

- Molecule 20: DNA (79-MER)

- Molecule 21: DNA (79-MER)



A64
C65
T66
A67
A68
T69
A70
T71
A72
T73
G74
T75
T76
G77
A78
A79

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	47141	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF amplitude correction was performed following 3D auto refinement in relion.	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	68.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.197	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	339.84, 339.84, 339.84	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.18, 1.18, 1.18	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	2/11358 (0.0%)	0.79	30/15345 (0.2%)
2	B	0.35	2/8943 (0.0%)	0.81	24/12068 (0.2%)
3	C	0.32	0/2711	0.78	7/3676 (0.2%)
4	D	0.20	0/991	0.69	2/1328 (0.2%)
5	E	0.28	0/1795	0.71	4/2416 (0.2%)
6	F	0.29	0/683	0.66	0/923
7	G	0.24	0/1523	0.65	2/2066 (0.1%)
8	H	0.28	0/1138	0.69	0/1540
9	I	0.30	0/328	0.89	0/445
10	J	0.44	1/558 (0.2%)	0.72	0/750
11	K	0.31	0/803	0.70	0/1083
12	L	0.28	0/365	0.75	1/485 (0.2%)
13	M	0.26	0/1369	0.84	9/1851 (0.5%)
14	N	0.24	0/855	0.77	3/1149 (0.3%)
15	O	0.30	0/4394	0.83	14/5928 (0.2%)
16	P	0.25	0/2282	0.70	5/3075 (0.2%)
17	Q	0.28	0/281	0.63	0/381
18	R	0.27	2/4200 (0.0%)	0.63	7/5659 (0.1%)
19	S	0.23	0/1464	0.60	2/1971 (0.1%)
20	X	0.30	0/1072	0.56	0/1651
21	Y	0.26	0/1313	0.47	0/2022
All	All	0.31	7/48426 (0.0%)	0.75	110/65812 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	151	GLN	CA-C	7.58	1.63	1.52
18	R	173	LEU	C-N	7.15	1.50	1.33
10	J	63	TYR	C-N	-6.36	1.25	1.33
2	B	550	HIS	CA-C	6.29	1.60	1.52
1	A	829	ASP	CA-C	6.08	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	SER	C-N	-6.01	1.25	1.33
2	B	558	ASN	CA-C	5.55	1.60	1.52

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	587	ASN	N-CA-C	12.08	124.44	111.03
15	O	472	LYS	CA-C-N	9.37	131.55	119.84
15	O	472	LYS	C-N-CA	9.37	131.55	119.84
2	B	824	LEU	N-CA-C	9.32	119.21	108.49
18	R	211	LYS	N-CA-C	9.19	121.30	111.28
3	C	35	LYS	N-CA-C	-9.02	101.45	111.28
3	C	279	VAL	N-CA-C	-8.87	100.17	112.50
1	A	573	ARG	N-CA-C	8.84	121.72	111.11
1	A	1126	ILE	N-CA-C	-8.64	101.81	110.62
13	M	184	LYS	N-CA-C	-8.51	101.99	112.38
18	R	151	GLN	CA-C-O	8.20	129.38	120.20
18	R	188	LYS	N-CA-C	8.14	122.47	112.54
1	A	574	ALA	N-CA-C	7.89	120.65	111.02
13	M	104	HIS	CA-C-N	7.88	129.69	119.84
13	M	104	HIS	C-N-CA	7.88	129.69	119.84
13	M	238	ASP	N-CA-C	7.78	120.74	111.33
15	O	471	THR	N-CA-C	7.72	120.15	109.18
3	C	17	SER	N-CA-C	7.68	120.39	111.02
2	B	501	ASP	N-CA-C	7.58	120.43	108.67
19	S	447	PRO	N-CA-C	7.42	123.67	113.65
18	R	150	LEU	N-CA-C	7.37	119.65	109.18
1	A	1449	GLU	N-CA-C	7.29	118.87	111.07
15	O	164	ILE	N-CA-C	7.24	121.16	111.17
15	O	482	LYS	N-CA-C	-7.11	104.24	113.12
1	A	830	ARG	N-CA-C	7.05	117.81	107.88
15	O	579	GLN	N-CA-C	-7.03	103.61	111.28
2	B	558	ASN	CA-C-O	7.02	127.29	119.78
2	B	177	CYS	N-CA-C	6.94	118.45	109.64
16	P	265	LEU	N-CA-C	-6.87	103.45	112.24
2	B	944	MET	CA-C-N	6.87	130.65	120.83
2	B	944	MET	C-N-CA	6.87	130.65	120.83
4	D	126	GLN	N-CA-C	6.71	119.22	110.43
15	O	34	ILE	N-CA-C	6.60	118.15	110.62
2	B	551	LEU	N-CA-C	6.57	119.75	109.96
2	B	575	PHE	N-CA-C	6.57	118.10	111.07
1	A	702	ALA	N-CA-C	6.48	120.05	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	296	ASN	N-CA-C	6.47	120.64	112.87
1	A	1124	PRO	N-CA-C	6.42	122.32	113.65
13	M	174	GLU	N-CA-C	6.38	119.33	108.67
5	E	117	THR	CA-C-N	6.23	125.79	119.19
5	E	117	THR	C-N-CA	6.23	125.79	119.19
1	A	1146	VAL	N-CA-C	6.19	122.22	109.34
1	A	466	LEU	N-CA-C	6.17	119.58	107.98
1	A	443	ASN	N-CA-C	6.06	119.51	109.46
4	D	30	ASP	CB-CA-C	-6.03	108.62	115.79
14	N	399	ILE	N-CA-C	-6.00	100.92	108.84
3	C	15	THR	N-CA-C	5.99	123.55	110.80
1	A	1126	ILE	N-CA-CB	5.98	118.67	110.54
15	O	528	MET	CB-CA-C	-5.95	109.72	116.63
2	B	576	ARG	N-CA-CB	5.94	118.80	109.94
16	P	201	GLY	CA-C-N	5.93	127.25	119.84
16	P	201	GLY	C-N-CA	5.93	127.25	119.84
18	R	152	VAL	N-CA-C	5.92	121.66	109.34
2	B	974	GLU	N-CA-C	5.91	118.37	108.02
1	A	1364	TYR	CA-C-N	-5.88	114.58	121.64
1	A	1364	TYR	C-N-CA	-5.88	114.58	121.64
3	C	18	THR	N-CA-C	5.88	119.76	112.24
15	O	580	ASN	N-CA-C	-5.86	104.58	110.97
2	B	550	HIS	CA-C-O	5.77	126.76	119.78
1	A	480	LEU	N-CA-CB	5.73	120.17	110.49
18	R	151	GLN	N-CA-C	5.73	119.08	111.75
1	A	1063	SER	N-CA-C	5.72	118.81	108.69
1	A	601	TYR	CB-CA-C	-5.71	108.35	116.34
2	B	569	THR	N-CA-C	5.71	122.95	110.80
1	A	153	ARG	N-CA-C	5.68	118.73	109.24
15	O	480	TYR	N-CA-C	5.65	119.76	111.34
18	R	213	TRP	N-CA-C	5.64	119.46	112.24
5	E	51	GLY	CA-C-N	5.59	128.42	120.49
5	E	51	GLY	C-N-CA	5.59	128.42	120.49
2	B	300	GLN	N-CA-C	5.58	122.69	110.80
1	A	248	VAL	N-CA-C	5.58	120.92	108.88
1	A	703	ARG	N-CA-C	5.57	120.06	112.04
1	A	248	VAL	CA-C-N	5.56	126.79	119.84
1	A	248	VAL	C-N-CA	5.56	126.79	119.84
1	A	495	TRP	CB-CA-C	-5.54	108.58	115.89
7	G	122	THR	CA-C-N	5.54	126.76	119.84
7	G	122	THR	C-N-CA	5.54	126.76	119.84
12	L	52	GLY	N-CA-C	-5.51	108.10	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	934	ASN	CB-CA-C	-5.50	108.63	116.34
14	N	399	ILE	N-CA-CB	5.46	116.88	110.82
2	B	934	ASN	N-CA-C	5.45	116.06	108.00
2	B	544	ILE	CA-C-N	5.44	129.39	120.63
2	B	544	ILE	C-N-CA	5.44	129.39	120.63
3	C	278	GLU	CB-CA-C	-5.42	102.30	111.02
1	A	1347	GLY	N-CA-C	5.40	119.49	111.76
1	A	572	ASP	N-CA-C	5.38	118.30	110.17
19	S	448	TYR	CA-C-O	5.34	127.46	119.23
1	A	715	ASN	N-CA-C	5.29	118.53	111.75
1	A	829	ASP	CA-C-O	5.29	128.08	120.51
16	P	152	SER	N-CA-CB	5.29	119.42	110.49
16	P	314	GLU	N-CA-C	-5.28	106.02	113.20
13	M	173	ILE	N-CA-C	5.27	120.31	109.34
1	A	169	ALA	CA-C-O	5.26	120.99	117.94
14	N	398	SER	N-CA-C	5.25	117.98	109.06
1	A	1379	MET	N-CA-C	-5.24	106.01	112.72
2	B	635	LEU	CA-C-N	5.24	133.09	122.04
2	B	635	LEU	C-N-CA	5.24	133.09	122.04
1	A	467	GLU	N-CA-CB	5.20	117.56	110.38
2	B	297	THR	N-CA-C	5.17	117.45	110.06
13	M	183	PHE	N-CA-C	5.14	117.45	108.76
15	O	40	ARG	N-CA-C	5.14	121.75	110.80
1	A	1041	GLY	N-CA-C	-5.14	107.45	114.64
2	B	576	ARG	N-CA-C	-5.14	104.94	111.11
2	B	863	GLN	N-CA-C	-5.12	105.51	112.26
2	B	580	ARG	N-CA-C	5.11	118.98	112.34
15	O	578	ARG	N-CA-C	5.09	117.57	111.71
13	M	174	GLU	CB-CA-C	-5.09	110.31	117.23
15	O	166	LEU	N-CA-CB	5.07	117.52	110.07
13	M	104	HIS	N-CA-C	5.05	116.75	109.48
2	B	507	ALA	CB-CA-C	-5.05	109.27	116.34

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	11159	0	11285	1043	0
2	B	8788	0	8901	797	0
3	C	2655	0	2628	227	0
4	D	977	0	983	92	0
5	E	1759	0	1788	122	0
6	F	671	0	692	57	0
7	G	1484	0	1485	144	0
8	H	1120	0	1089	95	0
9	I	321	0	303	41	0
10	J	549	0	559	53	0
11	K	792	0	790	80	0
12	L	363	0	387	26	0
13	M	1338	0	1307	144	0
14	N	845	0	891	77	0
15	O	4329	0	4497	456	0
16	P	2242	0	2265	239	0
17	Q	368	0	308	28	0
18	R	4131	0	4230	280	0
19	S	1649	0	1455	111	0
20	X	959	0	539	59	0
21	Y	1169	0	645	66	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
22	R	1	0	0	0	0
All	All	47675	0	47027	3766	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 40.

All (3766) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:SER:HB2	2:B:1069:CYS:SG	1.40	1.58
15:O:330:LEU:CD1	15:O:331:THR:HG23	1.27	1.58
15:O:330:LEU:CD1	15:O:331:THR:H	1.20	1.54
1:A:1145:LEU:CD1	1:A:1146:VAL:H	1.20	1.52
2:B:590:ILE:HA	2:B:601:ILE:CD1	1.45	1.45
1:A:1145:LEU:HD12	1:A:1146:VAL:N	1.23	1.42
15:O:330:LEU:HD12	15:O:331:THR:N	1.13	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:115:THR:CG2	6:F:116:ASP:H	1.16	1.32
16:P:203:LYS:CG	16:P:206:VAL:HA	1.57	1.32
15:O:182:SER:O	15:O:187:ILE:HG12	1.13	1.28
15:O:182:SER:HB2	15:O:187:ILE:CG2	1.63	1.27
1:A:1032:LEU:O	1:A:1033:GLU:HG3	1.25	1.26
1:A:154:CYS:HB3	1:A:157:CYS:SG	1.77	1.24
16:P:135:LYS:HB3	16:P:151:TYR:CD1	1.73	1.23
19:S:516:ILE:O	19:S:520:LYS:HG3	1.38	1.23
1:A:18:PHE:CE1	2:B:1139:PRO:HB3	1.73	1.22
15:O:472:LYS:HB3	15:O:475:VAL:CG1	1.68	1.22
7:G:59:LEU:HD11	7:G:64:GLY:CA	1.70	1.21
15:O:182:SER:CB	15:O:187:ILE:CG2	2.18	1.21
2:B:590:ILE:CA	2:B:601:ILE:HD11	1.67	1.21
18:R:222:GLY:HA3	18:R:258:ARG:NH2	1.55	1.21
6:F:115:THR:HG22	6:F:116:ASP:N	1.32	1.20
15:O:330:LEU:CD1	15:O:331:THR:CG2	2.18	1.20
2:B:600:HIS:O	2:B:601:ILE:HD13	1.03	1.19
13:M:85:LEU:O	13:M:173:ILE:HD12	1.40	1.19
18:R:91:SER:OG	18:R:96:ILE:HD11	1.44	1.18
16:P:264:THR:O	16:P:265:LEU:HG	1.44	1.17
15:O:182:SER:CB	15:O:187:ILE:HG23	1.72	1.17
13:M:84:SER:O	13:M:85:LEU:HD12	1.45	1.16
15:O:583:TRP:HH2	16:P:312:PHE:CD1	1.63	1.15
15:O:328:ASP:OD1	15:O:329:PRO:HD3	1.44	1.15
1:A:484:SER:CB	2:B:1069:CYS:SG	2.35	1.14
15:O:330:LEU:HD11	15:O:331:THR:HG23	1.16	1.14
1:A:953:GLY:HA2	1:A:1063:SER:CB	1.78	1.13
2:B:170:LYS:O	2:B:174:LEU:HB2	1.47	1.13
1:A:33:GLU:HG3	1:A:83:HIS:NE2	1.63	1.12
1:A:424:PRO:HD3	1:A:444:LEU:HD23	1.28	1.11
2:B:600:HIS:O	2:B:601:ILE:CD1	1.98	1.11
16:P:203:LYS:HG3	16:P:206:VAL:CA	1.79	1.11
2:B:418:ALA:HB1	2:B:421:SER:HB2	1.18	1.10
18:R:7:CYS:SG	18:R:28:CYS:HB3	1.91	1.10
1:A:402:LEU:HD23	1:A:466:LEU:HD11	1.10	1.10
1:A:402:LEU:HD23	1:A:466:LEU:CD1	1.80	1.09
15:O:182:SER:HB3	15:O:187:ILE:HG23	1.18	1.09
2:B:558:ASN:HA	2:B:602:ALA:HB1	1.35	1.08
1:A:622:VAL:HA	1:A:685:TYR:CE2	1.88	1.08
1:A:1064:GLU:HG2	1:A:1065:LYS:H	0.95	1.08
4:D:14:TYR:OH	4:D:124:VAL:HG21	1.51	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:330:LEU:HD13	15:O:331:THR:HG23	1.32	1.08
1:A:402:LEU:CD2	1:A:466:LEU:HD11	1.83	1.08
1:A:18:PHE:CE1	2:B:1139:PRO:CB	2.38	1.06
2:B:299:GLN:HG2	2:B:322:GLU:HB2	1.09	1.06
1:A:953:GLY:HA2	1:A:1063:SER:HB2	1.36	1.06
1:A:153:ARG:HD3	15:O:339:LEU:HG	1.36	1.05
7:G:87:GLY:O	7:G:146:ILE:HB	1.57	1.05
18:R:222:GLY:CA	18:R:258:ARG:HH21	1.69	1.05
19:S:483:GLU:O	19:S:487:GLU:HB2	1.54	1.05
15:O:583:TRP:CH2	16:P:312:PHE:CD1	2.44	1.04
15:O:584:ASN:ND2	16:P:310:VAL:HG22	1.72	1.04
1:A:18:PHE:HE1	2:B:1139:PRO:CB	1.71	1.04
2:B:525:GLU:O	2:B:603:THR:HG21	1.57	1.04
3:C:228:ARG:O	3:C:299:ILE:HB	1.57	1.04
1:A:1448:PHE:CE1	4:D:14:TYR:HD2	1.75	1.03
2:B:795:LEU:HB2	2:B:894:ALA:O	1.56	1.03
15:O:182:SER:HB2	15:O:187:ILE:HG21	1.09	1.02
3:C:17:SER:O	3:C:18:THR:HG22	1.60	1.02
16:P:152:SER:O	19:S:520:LYS:HE2	1.59	1.02
1:A:1064:GLU:HG2	1:A:1065:LYS:N	1.74	1.01
2:B:590:ILE:HA	2:B:601:ILE:HD12	1.41	1.01
15:O:583:TRP:HH2	16:P:312:PHE:CE1	1.77	1.01
2:B:590:ILE:HA	2:B:601:ILE:HD11	1.03	1.01
15:O:182:SER:O	15:O:187:ILE:CG1	2.09	1.00
16:P:152:SER:O	19:S:520:LYS:HG2	1.60	1.00
2:B:415:GLU:O	2:B:416:TYR:C	2.04	1.00
2:B:579:ARG:HH12	2:B:647:GLU:HG3	1.24	1.00
3:C:84:TYR:HB2	3:C:205:LYS:O	1.61	0.99
16:P:203:LYS:HG3	16:P:206:VAL:HA	1.01	0.99
1:A:1009:ARG:O	1:A:1013:ASN:HB2	1.60	0.99
2:B:558:ASN:HA	2:B:602:ALA:CB	1.92	0.99
1:A:482:ARG:HD3	1:A:544:PRO:HG3	1.40	0.99
18:R:222:GLY:CA	18:R:258:ARG:NH2	2.25	0.99
15:O:517:VAL:HG22	15:O:518:SER:N	1.76	0.99
16:P:135:LYS:HB3	16:P:151:TYR:HD1	0.85	0.99
2:B:558:ASN:H	2:B:602:ALA:CB	1.74	0.98
2:B:590:ILE:HG13	2:B:601:ILE:HD11	1.44	0.98
18:R:620:SER:O	18:R:624:GLU:HB3	1.61	0.98
4:D:119:GLU:OE2	4:D:127:LEU:HD11	1.64	0.98
14:N:290:ILE:O	14:N:294:LEU:HB2	1.64	0.98
16:P:135:LYS:CB	16:P:151:TYR:HD1	1.76	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:472:LYS:HB3	15:O:475:VAL:HG12	0.99	0.98
1:A:483:LEU:HD13	1:A:507:PRO:HB3	1.43	0.98
2:B:415:GLU:HG3	2:B:416:TYR:H	1.28	0.98
7:G:59:LEU:CD1	7:G:64:GLY:C	2.37	0.97
1:A:30:SER:HB3	1:A:82:GLY:O	1.63	0.97
1:A:277:SER:HB3	1:A:278:PRO:CD	1.91	0.97
15:O:573:SER:HA	15:O:576:PHE:CD2	1.99	0.97
1:A:953:GLY:HA2	1:A:1063:SER:OG	1.65	0.96
2:B:558:ASN:N	2:B:602:ALA:HB2	1.80	0.96
6:F:135:ARG:HH12	7:G:58:GLN:NE2	1.61	0.96
15:O:330:LEU:HD12	15:O:331:THR:CA	1.93	0.96
15:O:472:LYS:CB	15:O:475:VAL:HG12	1.95	0.96
2:B:549:LEU:HD23	2:B:549:LEU:O	1.66	0.96
2:B:590:ILE:CA	2:B:601:ILE:CD1	2.32	0.95
1:A:1256:VAL:O	1:A:1260:MET:HB2	1.66	0.95
3:C:239:ILE:HG22	3:C:288:LYS:HD3	1.48	0.95
1:A:1032:LEU:O	1:A:1033:GLU:CG	2.13	0.95
2:B:587:PHE:CD2	2:B:588:ILE:N	2.34	0.95
7:G:59:LEU:HD11	7:G:64:GLY:C	1.89	0.95
16:P:293:ILE:H	16:P:293:ILE:HD13	1.32	0.95
15:O:471:THR:O	15:O:473:PRO:HD3	1.66	0.95
1:A:1064:GLU:CG	1:A:1065:LYS:H	1.80	0.95
16:P:152:SER:C	19:S:520:LYS:HE2	1.91	0.94
9:I:8:CYS:HB3	9:I:29:CYS:SG	2.08	0.94
13:M:84:SER:C	13:M:85:LEU:HD12	1.92	0.94
1:A:474:PHE:O	1:A:485:ILE:HD13	1.66	0.94
15:O:297:ILE:O	15:O:301:LYS:HB2	1.68	0.94
19:S:458:PHE:O	19:S:462:GLU:HB2	1.68	0.93
2:B:590:ILE:CG1	2:B:601:ILE:HD11	1.97	0.93
7:G:83:GLU:O	7:G:149:ARG:HA	1.67	0.93
18:R:257:GLN:O	18:R:261:GLU:HB2	1.69	0.93
1:A:277:SER:HB3	1:A:278:PRO:HD2	1.49	0.93
18:R:400:VAL:HA	18:R:480:ASP:O	1.69	0.92
1:A:1448:PHE:HE1	4:D:14:TYR:HD2	1.17	0.92
2:B:600:HIS:C	2:B:601:ILE:HD13	1.95	0.92
1:A:18:PHE:CD1	2:B:1139:PRO:HA	2.04	0.92
1:A:178:ILE:HD11	1:A:222:LEU:HB2	1.50	0.92
15:O:200:LEU:HB3	15:O:280:LEU:HB3	1.50	0.92
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.51	0.92
13:M:154:GLU:HA	13:M:174:GLU:O	1.69	0.91
19:S:516:ILE:HG22	19:S:520:LYS:HE3	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:62:DC:H4'	20:X:63:DC:OP1	1.69	0.91
16:P:152:SER:CA	19:S:520:LYS:HE2	2.01	0.91
19:S:517:GLU:HA	19:S:520:LYS:HD2	1.52	0.91
2:B:558:ASN:N	2:B:602:ALA:CB	2.33	0.91
2:B:1106:TRP:HE1	7:G:162:SER:HA	1.35	0.91
2:B:590:ILE:CB	2:B:601:ILE:HD11	1.99	0.91
19:S:470:GLU:O	19:S:474:ARG:HB3	1.69	0.91
2:B:776:SER:HB2	2:B:928:GLN:HE21	1.36	0.90
1:A:520:HIS:HE1	2:B:1062:LEU:HD21	1.34	0.90
1:A:590:PHE:HB2	11:K:106:GLN:HE22	1.36	0.90
1:A:1145:LEU:HB2	1:A:1309:VAL:HA	1.51	0.90
18:R:558:PRO:O	18:R:562:GLU:HB2	1.71	0.90
1:A:483:LEU:CD1	1:A:507:PRO:HB3	2.02	0.89
7:G:59:LEU:HD11	7:G:64:GLY:N	1.86	0.89
18:R:418:ALA:HA	18:R:429:ILE:O	1.71	0.89
1:A:232:LYS:HD3	16:P:315:TRP:CZ2	2.07	0.89
2:B:1094:VAL:O	2:B:1116:ILE:HA	1.73	0.89
16:P:201:GLY:N	16:P:202:PRO:HD3	1.88	0.89
1:A:277:SER:CB	1:A:278:PRO:CD	2.49	0.88
1:A:251:GLY:O	1:A:252:ARG:O	1.91	0.88
1:A:363:ARG:HA	1:A:367:ASN:HB2	1.53	0.88
15:O:573:SER:HA	15:O:576:PHE:HD2	1.35	0.88
16:P:203:LYS:CG	16:P:206:VAL:CA	2.44	0.88
1:A:424:PRO:HD3	1:A:444:LEU:CD2	2.03	0.88
1:A:829:ASP:O	1:A:830:ARG:HG2	1.73	0.88
5:E:99:HIS:O	5:E:103:LYS:HB2	1.72	0.88
15:O:182:SER:HB3	15:O:187:ILE:CG2	1.94	0.88
1:A:946:THR:OG1	1:A:1065:LYS:HB3	1.72	0.87
15:O:588:LEU:HG	15:O:637:VAL:HG23	1.55	0.87
15:O:330:LEU:HD11	15:O:331:THR:CG2	1.97	0.87
1:A:248:VAL:N	1:A:249:PRO:HD3	1.89	0.87
2:B:772:VAL:HG13	2:B:943:ILE:HG23	1.56	0.87
1:A:18:PHE:HD1	2:B:1139:PRO:HA	1.37	0.87
14:N:395:ILE:HD12	14:N:411:ARG:HA	1.56	0.87
15:O:636:ASN:O	15:O:640:ARG:HB2	1.75	0.87
2:B:418:ALA:CB	2:B:421:SER:HB2	2.02	0.87
2:B:129:ILE:HD11	2:B:152:MET:HB2	1.57	0.86
2:B:376:ARG:HH21	2:B:607:ARG:HH12	1.22	0.86
1:A:1176:VAL:O	1:A:1183:PHE:HB2	1.74	0.86
2:B:589:SER:O	2:B:590:ILE:HB	1.76	0.86
2:B:992:VAL:HG21	3:C:278:GLU:OE1	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1448:PHE:CE1	4:D:14:TYR:CD2	2.64	0.86
1:A:988:ASP:HA	1:A:991:LYS:HB3	1.58	0.86
15:O:583:TRP:CH2	16:P:312:PHE:CE1	2.61	0.86
1:A:1145:LEU:HD12	1:A:1146:VAL:CA	2.06	0.86
15:O:328:ASP:O	15:O:329:PRO:O	1.94	0.86
19:S:434:MET:HE3	19:S:479:PRO:HA	1.58	0.86
1:A:579:LEU:HD21	1:A:704:PHE:HD1	1.41	0.85
3:C:70:ILE:HG13	3:C:74:GLU:HB2	1.57	0.85
7:G:59:LEU:CD1	7:G:64:GLY:CA	2.54	0.85
2:B:590:ILE:HG13	2:B:601:ILE:CD1	2.06	0.85
6:F:115:THR:CG2	6:F:116:ASP:N	1.95	0.85
1:A:1378:LYS:HG3	1:A:1379:MET:H	1.41	0.85
2:B:558:ASN:CA	2:B:602:ALA:CB	2.54	0.85
18:R:222:GLY:HA3	18:R:258:ARG:HH21	1.30	0.85
1:A:424:PRO:CD	1:A:444:LEU:HD23	2.06	0.85
2:B:418:ALA:HB1	2:B:421:SER:CB	2.06	0.85
16:P:33:GLN:NE2	16:P:49:MET:SD	2.50	0.85
16:P:311:TYR:HA	17:Q:40:PRO:HA	1.59	0.85
2:B:555:VAL:HG12	2:B:564:SER:H	1.42	0.84
1:A:232:LYS:HD3	16:P:315:TRP:CH2	2.13	0.84
16:P:134:VAL:C	16:P:151:TYR:HB2	2.02	0.84
3:C:33:VAL:O	3:C:34:GLU:HB2	1.74	0.84
1:A:201:TRP:HB3	1:A:205:LEU:HD13	1.60	0.83
2:B:529:ILE:HD11	2:B:575:PHE:HE1	1.42	0.83
1:A:49:LYS:HD2	1:A:54:LEU:HB3	1.60	0.83
2:B:558:ASN:CA	2:B:602:ALA:HB1	2.08	0.83
1:A:573:ARG:HH21	11:K:87:GLU:HB3	1.40	0.83
1:A:579:LEU:HD21	1:A:704:PHE:CD1	2.14	0.83
4:D:110:LEU:HB3	4:D:120:LYS:HE3	1.60	0.83
15:O:324:PRO:HB3	15:O:327:ARG:HB3	1.60	0.83
15:O:328:ASP:OD1	15:O:329:PRO:CD	2.26	0.83
1:A:1145:LEU:HA	1:A:1310:ILE:H	1.44	0.82
3:C:256:ILE:HD13	3:C:265:ALA:HB1	1.60	0.82
11:K:88:PHE:HB3	11:K:106:GLN:HG2	1.60	0.82
1:A:582:MET:HE2	1:A:703:ARG:HB3	1.61	0.82
2:B:934:ASN:HB3	2:B:1004:LEU:HD23	1.59	0.82
13:M:112:TYR:HD1	13:M:119:TRP:HE1	1.27	0.82
15:O:125:GLU:HB2	15:O:128:HIS:HB2	1.61	0.82
1:A:181:ASP:HB2	1:A:219:MET:HB3	1.61	0.82
1:A:1184:ILE:HB	1:A:1232:ILE:HB	1.61	0.82
1:A:724:LYS:O	1:A:728:GLU:HB2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:PRO:O	1:A:837:LYS:O	1.97	0.82
2:B:299:GLN:HG2	2:B:322:GLU:CB	2.03	0.82
1:A:962:THR:O	1:A:965:GLU:HB3	1.79	0.82
1:A:247:THR:C	1:A:249:PRO:HD3	2.05	0.82
1:A:1145:LEU:O	1:A:1310:ILE:HG22	1.80	0.82
18:R:121:ARG:HB2	18:R:124:ASN:HD22	1.45	0.82
1:A:30:SER:CB	1:A:82:GLY:C	2.52	0.81
1:A:482:ARG:HD2	1:A:1092:ILE:HG12	1.61	0.81
18:R:467:ARG:HG3	18:R:610:LEU:HD22	1.62	0.81
2:B:731:PRO:HB2	2:B:750:PRO:HG2	1.60	0.81
1:A:329:SER:HB3	1:A:355:GLN:HE21	1.45	0.81
1:A:393:ALA:HB3	1:A:499:ARG:HB2	1.60	0.81
1:A:794:MET:HA	1:A:797:CYS:HB2	1.59	0.81
10:J:10:CYS:SG	10:J:43:ARG:NE	2.52	0.81
15:O:517:VAL:HG22	15:O:518:SER:H	1.46	0.81
15:O:221:LYS:H	15:O:224:LYS:HB3	1.44	0.81
15:O:330:LEU:CG	15:O:331:THR:H	1.90	0.81
16:P:31:PHE:HD2	16:P:72:PHE:HB2	1.46	0.81
2:B:298:GLN:HB2	13:M:186:ILE:HG21	1.62	0.81
15:O:171:VAL:O	15:O:175:LEU:HB3	1.80	0.81
15:O:573:SER:O	15:O:576:PHE:CD2	2.33	0.81
2:B:364:LYS:HG3	2:B:365:MET:H	1.46	0.81
7:G:119:CYS:HB2	7:G:128:TRP:HB3	1.63	0.81
18:R:94:LEU:HD23	18:R:149:ARG:HH21	1.45	0.81
4:D:64:ASN:HD21	7:G:102:LEU:HB3	1.44	0.80
5:E:29:PHE:HB2	5:E:65:THR:HB	1.63	0.80
8:H:58:THR:HB	8:H:143:LEU:HB3	1.61	0.80
15:O:297:ILE:O	15:O:301:LYS:CB	2.29	0.80
16:P:152:SER:O	19:S:520:LYS:CG	2.29	0.80
3:C:137:ASN:HA	3:C:202:ILE:O	1.82	0.80
7:G:59:LEU:HG	7:G:60:LYS:N	1.94	0.80
16:P:152:SER:O	19:S:520:LYS:CE	2.29	0.80
2:B:667:VAL:HG12	2:B:669:SER:H	1.45	0.80
16:P:195:PHE:HB3	16:P:201:GLY:O	1.81	0.80
15:O:578:ARG:HG2	15:O:648:TRP:HH2	1.46	0.80
1:A:45:ASP:OD1	1:A:46:ARG:N	2.13	0.80
2:B:473:ILE:O	2:B:511:VAL:HA	1.81	0.80
1:A:30:SER:HB2	1:A:82:GLY:C	2.07	0.80
1:A:814:GLY:H	1:A:848:VAL:HG13	1.46	0.80
15:O:105:LYS:HB2	15:O:121:TYR:HB2	1.62	0.80
1:A:269:ARG:NH2	1:A:286:THR:H	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:ARG:NH2	11:K:87:GLU:HB3	1.97	0.79
2:B:609:CYS:HB3	2:B:648:TYR:HB3	1.62	0.79
19:S:483:GLU:O	19:S:487:GLU:CB	2.31	0.79
1:A:30:SER:HB2	1:A:82:GLY:HA2	1.64	0.79
1:A:829:ASP:O	1:A:830:ARG:CG	2.30	0.79
2:B:320:LEU:HA	2:B:324:ILE:HG13	1.64	0.79
19:S:506:GLN:O	19:S:510:LYS:HB2	1.82	0.79
1:A:399:ALA:HA	1:A:466:LEU:HD12	1.65	0.79
6:F:76:LYS:HD3	6:F:79:ARG:HH21	1.45	0.79
15:O:330:LEU:HD12	15:O:331:THR:CB	2.13	0.79
16:P:33:GLN:NE2	19:S:372:MET:SD	2.56	0.79
13:M:94:PRO:HB3	14:N:391:LEU:HA	1.65	0.79
15:O:172:GLU:O	15:O:176:SER:HB2	1.83	0.79
1:A:571:TYR:HB3	1:A:575:THR:HG23	1.64	0.79
16:P:152:SER:HA	19:S:520:LYS:HE2	1.62	0.79
2:B:124:THR:HA	2:B:187:VAL:HA	1.65	0.78
5:E:152:LYS:HE2	5:E:154:ILE:HD11	1.65	0.78
1:A:622:VAL:HA	1:A:685:TYR:CD2	2.17	0.78
1:A:654:ILE:HG12	1:A:659:ILE:HA	1.65	0.78
2:B:1012:CYS:SG	3:C:293:ARG:NH2	2.56	0.78
16:P:201:GLY:N	16:P:202:PRO:CD	2.45	0.78
16:P:252:LYS:HD2	16:P:266:GLU:HG2	1.62	0.78
12:L:48:CYS:SG	12:L:51:CYS:O	2.41	0.78
16:P:203:LYS:CB	16:P:206:VAL:HA	2.12	0.78
1:A:1305:CYS:SG	5:E:11:ARG:NH1	2.57	0.78
15:O:48:LEU:HD22	15:O:581:LEU:HD11	1.65	0.78
13:M:89:GLN:HE21	13:M:178:GLN:HE22	1.29	0.78
14:N:290:ILE:O	14:N:294:LEU:CB	2.31	0.78
18:R:521:TYR:HB3	18:R:530:LEU:HB2	1.64	0.78
1:A:109:ASN:OD1	1:A:110:CYS:N	2.15	0.78
15:O:134:GLY:H	17:Q:58:TYR:HD1	1.31	0.78
1:A:30:SER:HA	1:A:81:PHE:O	1.84	0.78
1:A:49:LYS:HG3	1:A:56:PRO:HD3	1.65	0.78
1:A:549:PRO:HG3	1:A:679:TYR:HB2	1.66	0.78
1:A:829:ASP:C	1:A:830:ARG:CG	2.56	0.78
15:O:60:ARG:HB2	15:O:90:SER:OG	1.83	0.78
16:P:52:VAL:HG13	16:P:61:ILE:HD11	1.66	0.78
16:P:252:LYS:CD	16:P:266:GLU:HG2	2.13	0.78
1:A:29:GLN:HE22	2:B:1133:LEU:HD21	1.49	0.78
1:A:1448:PHE:HE1	4:D:14:TYR:CD2	2.01	0.78
7:G:59:LEU:HD11	7:G:64:GLY:HA2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:SER:HB2	1:A:664:MET:HE2	1.67	0.77
1:A:957:TYR:HB2	1:A:1033:GLU:O	1.83	0.77
15:O:338:ASP:HB3	15:O:341:GLU:HB3	1.66	0.77
5:E:123:LEU:HD21	5:E:126:SER:HB2	1.64	0.77
18:R:469:ILE:HG21	18:R:476:ALA:HB3	1.66	0.77
3:C:43:ASN:HB2	3:C:55:ASP:HB3	1.66	0.77
12:L:31:CYS:HB2	12:L:35:SER:H	1.48	0.77
20:X:77:DC:O2	21:Y:3:DG:N2	2.17	0.77
1:A:1145:LEU:CB	1:A:1309:VAL:HA	2.15	0.77
1:A:953:GLY:CA	1:A:1063:SER:OG	2.31	0.77
2:B:299:GLN:CG	2:B:322:GLU:HB2	2.04	0.77
2:B:698:ARG:HH21	2:B:952:ARG:HG2	1.50	0.77
15:O:41:THR:HA	16:P:315:TRP:HD1	1.47	0.77
1:A:1380:ARG:HH11	1:A:1385:GLN:HE22	1.31	0.77
16:P:195:PHE:CB	16:P:201:GLY:O	2.32	0.77
16:P:203:LYS:HD3	16:P:203:LYS:H	1.49	0.77
2:B:267:GLU:O	2:B:271:LEU:HB2	1.84	0.77
1:A:502:GLU:HG2	2:B:767:ILE:HG13	1.65	0.77
16:P:11:LEU:O	16:P:15:ALA:HB2	1.85	0.77
2:B:186:ILE:HA	2:B:191:GLU:HA	1.67	0.77
2:B:728:MET:SD	2:B:753:GLN:NE2	2.58	0.77
1:A:483:LEU:HD11	1:A:550:ILE:HG21	1.66	0.76
1:A:621:PRO:HG2	1:A:689:GLU:OE1	1.85	0.76
2:B:198:GLU:HA	2:B:377:LEU:HA	1.65	0.76
2:B:613:ILE:HA	2:B:646:VAL:HG12	1.65	0.76
5:E:155:ARG:HB2	5:E:188:LEU:HD21	1.66	0.76
11:K:89:CYS:HA	11:K:104:ARG:O	1.85	0.76
1:A:1186:VAL:H	1:A:1230:ILE:HG12	1.51	0.76
16:P:90:GLU:O	16:P:94:TYR:HB3	1.86	0.76
4:D:127:LEU:HB2	4:D:133:HIS:HB3	1.67	0.76
1:A:1033:GLU:HB3	1:A:1034:PRO:HD2	1.68	0.76
2:B:741:ILE:HG23	2:B:746:TYR:HB3	1.68	0.76
3:C:248:GLN:HB3	3:C:256:ILE:HD11	1.66	0.76
2:B:797:ARG:HG2	2:B:803:GLN:HG2	1.67	0.76
3:C:17:SER:O	3:C:18:THR:CG2	2.34	0.76
15:O:577:MET:O	15:O:580:ASN:HB3	1.85	0.76
19:S:443:SER:HB2	19:S:451:ARG:HB3	1.66	0.76
1:A:116:SER:HA	1:A:120:LYS:HE3	1.68	0.76
1:A:353:PHE:O	1:A:356:ARG:HG2	1.85	0.76
2:B:583:LYS:HG2	2:B:584:VAL:HG13	1.67	0.76
1:A:1151:GLU:HG3	1:A:1152:ARG:HG3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:92:ILE:HD11	10:J:2:ILE:HD13	1.67	0.76
7:G:189:GLU:HG3	7:G:191:PRO:HD3	1.67	0.76
18:R:258:ARG:HA	18:R:261:GLU:HB3	1.66	0.75
14:N:400:ALA:HB3	14:N:405:SER:HA	1.68	0.75
15:O:124:GLU:HG3	15:O:126:GLY:H	1.50	0.75
1:A:1124:PRO:O	1:A:1127:LYS:HB2	1.87	0.75
15:O:584:ASN:HD21	16:P:310:VAL:HG22	1.52	0.75
16:P:133:TYR:O	16:P:151:TYR:N	2.19	0.75
1:A:974:LEU:HD21	1:A:998:TYR:HB3	1.68	0.75
2:B:735:MET:HB2	2:B:754:ASN:HD21	1.51	0.75
18:R:222:GLY:HA2	18:R:258:ARG:HH21	1.51	0.75
14:N:287:HIS:O	14:N:291:LEU:HB2	1.86	0.75
18:R:392:THR:O	18:R:488:GLY:HA2	1.87	0.75
15:O:517:VAL:CG2	15:O:521:ILE:HB	2.16	0.75
15:O:629:MET:O	15:O:633:ARG:CB	2.34	0.75
1:A:1441:LEU:HD21	7:G:54:VAL:HG12	1.67	0.75
15:O:516:LEU:HD12	15:O:565:LEU:HD23	1.69	0.75
15:O:648:TRP:NE1	15:O:652:GLN:OE1	2.20	0.75
7:G:124:GLU:O	7:G:125:GLU:HB3	1.85	0.75
15:O:629:MET:O	15:O:633:ARG:HB2	1.86	0.75
18:R:222:GLY:HA3	18:R:258:ARG:CZ	2.17	0.75
1:A:479:SER:O	2:B:1065:MET:HE3	1.87	0.74
2:B:976:GLY:HA2	2:B:981:GLY:HA3	1.67	0.74
7:G:129:ILE:HG23	7:G:138:LEU:HA	1.67	0.74
1:A:402:LEU:CG	1:A:466:LEU:HD11	2.18	0.74
15:O:620:LEU:HD12	15:O:621:PRO:HD2	1.67	0.74
1:A:410:ARG:HH12	6:F:106:PRO:HA	1.52	0.74
19:S:516:ILE:O	19:S:520:LYS:CG	2.29	0.74
1:A:1034:PRO:O	1:A:1035:PRO:C	2.29	0.74
1:A:829:ASP:C	1:A:830:ARG:HG3	2.12	0.74
8:H:129:TYR:O	8:H:131:ASN:N	2.20	0.74
15:O:517:VAL:CG2	15:O:518:SER:N	2.50	0.74
2:B:454:VAL:HG13	2:B:455:THR:HG23	1.69	0.74
18:R:650:ALA:HB2	19:S:517:GLU:CD	2.13	0.74
1:A:332:VAL:HG13	1:A:333:ASN:H	1.51	0.74
2:B:496:MET:HE2	2:B:608:ILE:HG22	1.69	0.74
15:O:213:ASP:O	15:O:216:GLN:N	2.21	0.74
1:A:1174:GLN:H	1:A:1186:VAL:HG12	1.53	0.74
2:B:337:VAL:CG2	2:B:345:LYS:HB3	2.17	0.74
4:D:14:TYR:CE1	4:D:124:VAL:HG11	2.23	0.74
1:A:805:ASN:ND2	2:B:950:PRO:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1034:PRO:O	1:A:1035:PRO:O	2.06	0.74
2:B:337:VAL:HG21	2:B:345:LYS:HB3	1.70	0.74
15:O:200:LEU:HA	15:O:281:THR:O	1.88	0.74
11:K:93:ILE:HG22	11:K:95:HIS:H	1.53	0.73
15:O:212:GLU:HG2	15:O:334:GLY:HA2	1.70	0.73
18:R:239:ARG:NH1	19:S:291:UNK:O	2.21	0.73
2:B:590:ILE:HG13	2:B:601:ILE:CG1	2.17	0.73
16:P:45:LEU:HG	19:S:372:MET:HG2	1.70	0.73
16:P:216:SER:OG	16:P:261:TYR:N	2.21	0.73
16:P:221:ILE:O	16:P:225:ILE:N	2.20	0.73
1:A:30:SER:HB2	1:A:82:GLY:CA	2.16	0.73
1:A:850:ASN:HB3	1:A:854:SER:OG	1.87	0.73
2:B:125:TYR:HB3	2:B:186:ILE:HG23	1.71	0.73
2:B:332:ILE:HG13	2:B:333:ALA:H	1.51	0.73
1:A:475:ASN:HB2	1:A:485:ILE:HD11	1.70	0.73
3:C:19:ASP:HB3	3:C:29:ASN:HD22	1.52	0.73
1:A:221:ASP:O	1:A:226:LYS:NZ	2.22	0.73
1:A:632:VAL:O	1:A:648:ASN:ND2	2.22	0.73
2:B:97:ASP:HB3	2:B:132:ASP:HB2	1.71	0.73
3:C:107:LYS:HB3	3:C:185:VAL:HG23	1.70	0.73
12:L:27:LEU:HD11	12:L:37:LYS:HB2	1.70	0.73
15:O:289:LYS:HE2	15:O:323:SER:HB3	1.70	0.73
2:B:87:VAL:HG11	2:B:407:LEU:HD13	1.69	0.73
2:B:780:ARG:NH1	10:J:9:SER:O	2.22	0.73
8:H:21:ASN:OD1	8:H:22:LYS:N	2.22	0.73
2:B:496:MET:HG2	2:B:610:ARG:HD2	1.70	0.73
13:M:236:VAL:O	13:M:240:GLU:HB2	1.89	0.73
1:A:429:GLY:C	1:A:465:HIS:HD1	1.97	0.73
1:A:789:ASN:HD21	1:A:792:LEU:HD13	1.53	0.73
1:A:1163:LYS:HG3	1:A:1164:THR:H	1.53	0.73
16:P:172:ILE:HG22	16:P:173:GLU:H	1.54	0.73
4:D:103:PHE:O	4:D:106:LEU:HB3	1.88	0.72
1:A:1140:ILE:HA	1:A:1295:VAL:O	1.88	0.72
18:R:124:ASN:HB3	18:R:160:THR:HG21	1.71	0.72
1:A:573:ARG:HH12	1:A:592:ILE:HG12	1.54	0.72
2:B:227:ARG:HH11	2:B:449:MET:HG3	1.54	0.72
16:P:69:GLU:HG3	16:P:70:LEU:H	1.54	0.72
2:B:844:ASN:HA	2:B:870:PRO:HB3	1.72	0.72
3:C:140:CYS:HB2	3:C:196:LEU:HD13	1.71	0.72
1:A:402:LEU:HB3	1:A:466:LEU:HD11	1.70	0.72
1:A:1122:GLY:O	1:A:1125:ARG:HG2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1332:ARG:NH2	5:E:200:ARG:HE	1.87	0.72
5:E:28:TYR:HA	5:E:64:PRO:HA	1.71	0.72
8:H:131:ASN:HA	8:H:134:ASN:HD22	1.54	0.72
1:A:3:GLU:HB3	7:G:37:LYS:HG3	1.72	0.72
1:A:33:GLU:CG	1:A:83:HIS:NE2	2.47	0.72
1:A:328:ASN:OD1	1:A:329:SER:N	2.21	0.72
2:B:89:PRO:HA	19:S:383:ARG:HH11	1.54	0.72
2:B:325:GLU:O	2:B:329:THR:N	2.22	0.72
1:A:470:ASP:O	1:A:489:TYR:HA	1.90	0.72
2:B:109:LYS:NZ	2:B:111:TYR:O	2.20	0.72
2:B:415:GLU:HG3	2:B:416:TYR:N	2.03	0.72
2:B:524:ASP:HB3	2:B:588:ILE:HD11	1.71	0.72
7:G:203:ASP:HB3	7:G:211:TRP:HE1	1.54	0.72
15:O:570:GLU:HA	15:O:573:SER:HB3	1.72	0.72
1:A:30:SER:HB3	1:A:82:GLY:C	2.15	0.72
10:J:9:SER:OG	10:J:45:CYS:SG	2.45	0.72
19:S:458:PHE:O	19:S:462:GLU:CB	2.37	0.72
1:A:33:GLU:N	1:A:83:HIS:CE1	2.58	0.72
15:O:182:SER:O	15:O:183:MET:C	2.31	0.72
18:R:202:ALA:O	18:R:205:LEU:HB3	1.88	0.72
1:A:34:VAL:HG13	1:A:35:SER:H	1.55	0.71
1:A:181:ASP:OD1	1:A:182:THR:N	2.22	0.71
15:O:182:SER:O	15:O:183:MET:O	2.08	0.71
18:R:79:THR:O	18:R:83:ALA:HB2	1.89	0.71
2:B:558:ASN:CA	2:B:602:ALA:HB2	2.19	0.71
5:E:77:SER:O	5:E:105:PHE:HB3	1.90	0.71
5:E:86:PRO:HA	5:E:113:GLN:HB3	1.72	0.71
7:G:59:LEU:HD13	7:G:64:GLY:C	2.13	0.71
15:O:52:LEU:HB3	15:O:127:ILE:HG21	1.70	0.71
15:O:472:LYS:CB	15:O:475:VAL:CG1	2.61	0.71
1:A:109:ASN:HD22	1:A:159:ALA:HB3	1.53	0.71
1:A:464:ARG:NH1	1:A:467:GLU:OE1	2.23	0.71
1:A:483:LEU:HD13	1:A:507:PRO:CB	2.18	0.71
1:A:632:VAL:HG11	1:A:796:THR:HA	1.72	0.71
18:R:398:ALA:HB3	18:R:449:VAL:HB	1.71	0.71
20:X:77:DC:N3	21:Y:3:DG:N1	2.38	0.71
2:B:234:ILE:HB	2:B:240:ILE:HG22	1.72	0.71
16:P:131:GLN:HB3	16:P:133:TYR:HD2	1.55	0.71
15:O:578:ARG:HG2	15:O:648:TRP:CH2	2.25	0.71
16:P:191:PHE:HB2	16:P:192:PRO:HD2	1.72	0.71
15:O:365:ASP:N	15:O:476:TYR:OH	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:132:ARG:O	16:P:151:TYR:CD2	2.44	0.71
18:R:91:SER:OG	18:R:96:ILE:CD1	2.34	0.71
1:A:38:ASP:O	1:A:40:PHE:N	2.24	0.71
5:E:172:GLU:HG2	5:E:173:SER:H	1.55	0.71
7:G:104:ILE:HG23	7:G:105:PHE:H	1.54	0.71
18:R:138:LYS:NZ	18:R:173:LEU:O	2.20	0.71
18:R:191:LEU:HB2	18:R:195:LYS:HD2	1.73	0.71
1:A:1328:ILE:O	1:A:1331:ALA:N	2.23	0.71
2:B:201:SER:OG	2:B:376:ARG:NH1	2.24	0.71
2:B:412:ARG:NH1	2:B:413:ALA:O	2.24	0.71
16:P:203:LYS:HG3	16:P:206:VAL:CB	2.21	0.71
21:Y:1:DA:H2''	21:Y:2:DC:H5'	1.71	0.71
1:A:1406:ASP:CG	1:A:1407:ALA:H	1.99	0.70
2:B:610:ARG:O	2:B:648:TYR:HA	1.90	0.70
13:M:182:PHE:O	13:M:183:PHE:HD1	1.74	0.70
2:B:228:LYS:HD3	2:B:244:HIS:HE2	1.55	0.70
2:B:615:VAL:HA	2:B:620:SER:HA	1.72	0.70
12:L:31:CYS:SG	12:L:34:CYS:HB2	2.31	0.70
18:R:467:ARG:HA	18:R:602:LEU:HD21	1.73	0.70
1:A:431:ASN:OD1	1:A:432:TYR:N	2.23	0.70
1:A:921:LEU:HD23	1:A:932:PRO:HG2	1.73	0.70
3:C:275:VAL:HG21	3:C:293:ARG:HD3	1.73	0.70
15:O:636:ASN:O	15:O:640:ARG:CB	2.39	0.70
16:P:92:LEU:O	16:P:96:TYR:CB	2.39	0.70
18:R:628:ILE:HG21	19:S:499:ASN:HD21	1.55	0.70
1:A:363:ARG:HH21	2:B:1046:LEU:HD21	1.56	0.70
8:H:1:MET:HG3	8:H:3:ASN:H	1.55	0.70
15:O:53:VAL:O	15:O:57:LEU:N	2.20	0.70
16:P:92:LEU:O	16:P:96:TYR:HB3	1.92	0.70
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.72	0.70
16:P:64:VAL:HB	16:P:71:LYS:HB2	1.73	0.70
1:A:330:ASP:OD1	1:A:331:SER:N	2.25	0.70
1:A:900:TYR:CE1	6:F:136:ARG:HD3	2.27	0.70
5:E:95:THR:O	5:E:99:HIS:ND1	2.24	0.70
15:O:328:ASP:O	15:O:329:PRO:C	2.34	0.70
15:O:573:SER:HG	15:O:576:PHE:HE2	1.39	0.70
16:P:264:THR:C	16:P:265:LEU:HG	2.15	0.70
18:R:189:LEU:O	18:R:191:LEU:HG	1.91	0.70
1:A:269:ARG:HH22	1:A:283:ASP:C	1.99	0.70
1:A:286:THR:O	1:A:290:THR:HB	1.92	0.70
8:H:60:ALA:O	8:H:141:TYR:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:234:ASP:O	15:O:238:ARG:N	2.25	0.70
16:P:236:THR:HG23	16:P:239:ASN:H	1.57	0.70
18:R:195:LYS:O	18:R:199:VAL:N	2.24	0.70
18:R:257:GLN:O	18:R:261:GLU:CB	2.38	0.70
1:A:81:PHE:CD2	1:A:265:PRO:HD3	2.27	0.70
2:B:816:ASP:OD1	2:B:822:GLN:NE2	2.25	0.70
6:F:115:THR:HG23	6:F:116:ASP:H	1.48	0.70
13:M:117:HIS:HB2	13:M:119:TRP:NE1	2.07	0.70
1:A:668:VAL:HB	1:A:677:VAL:HG23	1.72	0.70
1:A:1329:GLU:OE2	1:A:1332:ARG:NH2	2.24	0.70
3:C:231:PRO:HA	3:C:293:ARG:HG2	1.73	0.70
8:H:116:TYR:O	8:H:122:LEU:HA	1.92	0.70
15:O:517:VAL:O	15:O:518:SER:HB3	1.91	0.70
18:R:519:LEU:HB3	18:R:532:ILE:HB	1.74	0.70
1:A:277:SER:CB	1:A:278:PRO:HD3	2.21	0.69
2:B:760:MET:HG2	2:B:762:TYR:H	1.57	0.69
9:I:9:ASN:HD22	13:M:92:ASN:HA	1.56	0.69
12:L:51:CYS:SG	12:L:53:HIS:HB3	2.32	0.69
15:O:583:TRP:HZ3	17:Q:41:LEU:CD2	2.05	0.69
1:A:67:CYS:HB3	1:A:70:CYS:O	1.92	0.69
2:B:514:LEU:HB3	2:B:518:THR:HG21	1.74	0.69
2:B:529:ILE:HD11	2:B:575:PHE:CE1	2.26	0.69
2:B:579:ARG:NH1	2:B:647:GLU:HG3	2.04	0.69
2:B:612:LEU:HD21	2:B:649:LEU:HD12	1.74	0.69
3:C:153:PRO:HA	3:C:156:LEU:HB2	1.74	0.69
4:D:7:ARG:HE	4:D:10:PHE:HZ	1.39	0.69
7:G:39:ILE:HD12	7:G:40:PRO:HD2	1.74	0.69
11:K:117:LEU:O	11:K:121:LEU:HB2	1.92	0.69
15:O:80:VAL:HG11	15:O:87:ASP:HB2	1.74	0.69
15:O:547:GLU:HG2	15:O:548:ILE:H	1.55	0.69
2:B:197:GLN:NE2	2:B:476:GLN:OE1	2.25	0.69
2:B:756:THR:N	10:J:48:ARG:HH12	1.89	0.69
2:B:1004:LEU:HB2	2:B:1013:LEU:HD12	1.74	0.69
15:O:40:ARG:HG2	15:O:587:ASN:OD1	1.92	0.69
15:O:140:ILE:HD11	15:O:160:VAL:HG21	1.74	0.69
18:R:255:LEU:O	18:R:258:ARG:N	2.25	0.69
1:A:432:TYR:HE1	1:A:443:ASN:ND2	1.89	0.69
1:A:1254:ASN:ND2	9:I:15:THR:OG1	2.25	0.69
2:B:263:LEU:HD12	2:B:297:THR:HG22	1.74	0.69
2:B:534:TYR:HA	2:B:538:VAL:HG22	1.74	0.69
4:D:126:GLN:O	4:D:127:LEU:HG	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:41:LEU:O	17:Q:44:ASN:ND2	2.25	0.69
18:R:225:GLY:HA2	18:R:228:ILE:HD12	1.74	0.69
1:A:272:VAL:HG11	1:A:281:ASN:HD22	1.57	0.69
2:B:244:HIS:CE1	2:B:333:ALA:HB2	2.27	0.69
8:H:99:GLY:HA3	8:H:118:PHE:HD1	1.57	0.69
14:N:371:LEU:HD23	14:N:382:ILE:HB	1.74	0.69
7:G:112:GLN:HG2	7:G:115:LEU:HD13	1.75	0.69
13:M:85:LEU:O	13:M:173:ILE:CD1	2.31	0.69
16:P:254:GLU:HB3	16:P:262:ARG:HB2	1.72	0.69
2:B:616:SER:N	2:B:619:GLN:O	2.25	0.69
10:J:52:THR:HG22	10:J:53:HIS:H	1.56	0.69
16:P:11:LEU:O	16:P:15:ALA:CB	2.39	0.69
18:R:463:ARG:NH1	18:R:601:ASN:O	2.23	0.69
1:A:172:GLY:HA3	1:A:331:SER:HB3	1.75	0.69
1:A:374:ASP:OD1	2:B:1038:ARG:NE	2.24	0.69
1:A:386:ASN:HA	1:A:699:LYS:HG2	1.73	0.69
1:A:444:LEU:HD21	1:A:449:ARG:HD3	1.74	0.69
2:B:765:TYR:CD1	2:B:924:ILE:HG13	2.27	0.69
2:B:771:LEU:O	2:B:923:GLY:N	2.22	0.69
2:B:987:MET:HA	2:B:990:ILE:HB	1.73	0.69
3:C:165:ARG:N	3:C:189:PRO:O	2.22	0.69
5:E:54:GLN:HE21	5:E:57:MET:HE2	1.58	0.69
6:F:115:THR:HG22	6:F:116:ASP:H	0.52	0.69
16:P:206:VAL:HG11	16:P:210:PRO:HB3	1.75	0.69
18:R:632:ALA:O	18:R:636:LEU:HB2	1.92	0.69
1:A:615:LYS:HG3	1:A:620:SER:OG	1.91	0.69
1:A:622:VAL:CA	1:A:685:TYR:CE2	2.72	0.69
1:A:955:LEU:HB2	1:A:958:ALA:HB3	1.75	0.69
2:B:167:ASP:O	2:B:169:SER:N	2.24	0.69
2:B:591:TYR:HB3	2:B:653:GLU:HA	1.75	0.69
2:B:1006:SER:HB3	2:B:1010:GLY:H	1.58	0.69
1:A:99:THR:HA	1:A:102:ILE:HG22	1.74	0.69
15:O:41:THR:HA	16:P:315:TRP:CD1	2.28	0.69
19:S:460:ASN:OD1	19:S:464:LYS:NZ	2.23	0.69
2:B:1095:CYS:HB2	2:B:1107:CYS:SG	2.33	0.68
18:R:171:THR:OG1	18:R:172:GLU:OE1	2.11	0.68
5:E:178:ILE:N	5:E:213:ILE:O	2.26	0.68
7:G:84:ILE:HA	7:G:148:PHE:O	1.93	0.68
7:G:112:GLN:HE22	7:G:128:TRP:CD1	2.11	0.68
7:G:124:GLU:O	7:G:125:GLU:CB	2.41	0.68
15:O:79:LEU:HD22	15:O:91:VAL:HG13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:126:PHE:HB3	3:C:131:THR:HG21	1.74	0.68
15:O:110:THR:HA	15:O:116:LYS:HA	1.75	0.68
1:A:590:PHE:HB2	11:K:106:GLN:NE2	2.07	0.68
2:B:587:PHE:CG	2:B:588:ILE:N	2.53	0.68
15:O:51:GLU:O	15:O:55:ALA:N	2.21	0.68
16:P:151:TYR:OH	18:R:647:ALA:O	2.12	0.68
5:E:180:ARG:HH12	5:E:191:LYS:HA	1.57	0.68
7:G:59:LEU:CD1	7:G:65:SER:N	2.56	0.68
13:M:83:GLU:O	13:M:84:SER:O	2.11	0.68
1:A:520:HIS:CE1	2:B:1062:LEU:HD21	2.24	0.68
2:B:1132:LEU:HD22	2:B:1137:ILE:HD13	1.74	0.68
4:D:115:LEU:HA	4:D:138:VAL:HG21	1.76	0.68
9:I:8:CYS:CB	9:I:29:CYS:SG	2.81	0.68
15:O:46:LEU:HA	15:O:49:TYR:HD2	1.59	0.68
15:O:166:LEU:HB3	15:O:169:LEU:HD11	1.75	0.68
15:O:471:THR:O	15:O:473:PRO:CD	2.40	0.68
13:M:77:LYS:HA	14:N:360:VAL:HG22	1.76	0.68
13:M:182:PHE:O	13:M:183:PHE:CD1	2.47	0.68
18:R:189:LEU:HB2	18:R:195:LYS:NZ	2.09	0.68
21:Y:12:DA:H2"	21:Y:13:DA:C8	2.28	0.68
1:A:406:GLU:HB3	1:A:462:VAL:O	1.94	0.68
3:C:35:LYS:O	3:C:39:ASP:CB	2.42	0.68
4:D:13:ASP:OD1	4:D:17:LEU:N	2.22	0.68
7:G:16:ASP:O	7:G:19:HIS:ND1	2.25	0.68
15:O:163:VAL:O	15:O:167:GLY:N	2.27	0.68
16:P:189:ASN:HD21	16:P:216:SER:HA	1.58	0.68
1:A:18:PHE:CD1	2:B:1139:PRO:CA	2.76	0.68
1:A:958:ALA:O	1:A:961:GLU:HB2	1.94	0.68
1:A:1038:GLU:HB3	1:A:1042:ILE:HD11	1.75	0.68
2:B:622:VAL:HG12	2:B:624:ASP:H	1.58	0.68
4:D:119:GLU:HA	4:D:122:GLN:HB3	1.75	0.68
7:G:59:LEU:HD11	7:G:64:GLY:H	1.57	0.68
15:O:517:VAL:HG21	15:O:521:ILE:HB	1.76	0.68
18:R:266:LYS:HG2	18:R:283:GLY:HA3	1.76	0.68
2:B:587:PHE:HD2	2:B:588:ILE:H	1.33	0.67
7:G:49:TYR:HB2	7:G:75:VAL:HG23	1.75	0.67
1:A:273:MET:HG3	1:A:275:GLN:HB3	1.76	0.67
1:A:1213:SER:HB2	1:A:1217:ILE:HB	1.75	0.67
2:B:298:GLN:HG2	13:M:186:ILE:HG21	1.73	0.67
6:F:115:THR:HG23	6:F:116:ASP:N	2.07	0.67
18:R:144:ILE:HD12	18:R:154:VAL:HG11	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:14:DC:H1'	21:Y:15:DT:H5'	1.76	0.67
1:A:485:ILE:HG22	1:A:535:MET:SD	2.34	0.67
2:B:1002:ASP:OD1	2:B:1003:MET:N	2.27	0.67
3:C:116:VAL:HA	3:C:130:ASN:HD21	1.59	0.67
16:P:149:MET:O	16:P:150:LEU:O	2.12	0.67
1:A:572:ASP:OD1	1:A:575:THR:HG22	1.94	0.67
18:R:245:VAL:HA	18:R:248:SER:HB3	1.75	0.67
11:K:47:ILE:HG12	11:K:65:ILE:HG12	1.77	0.67
1:A:41:ASP:OD2	1:A:50:ALA:N	2.28	0.67
2:B:43:ASP:OD1	2:B:44:LYS:N	2.26	0.67
2:B:864:THR:OG1	2:B:865:GLN:N	2.27	0.67
16:P:96:TYR:OH	16:P:113:ARG:NH1	2.27	0.67
1:A:269:ARG:CZ	1:A:286:THR:H	2.07	0.67
2:B:49:PRO:O	2:B:53:LYS:N	2.28	0.67
2:B:769:ASP:OD2	2:B:952:ARG:NH2	2.28	0.67
15:O:195:CYS:SG	15:O:196:GLU:N	2.64	0.67
1:A:400:LYS:HA	1:A:465:HIS:CD2	2.30	0.67
15:O:573:SER:CA	15:O:576:PHE:CD2	2.78	0.67
2:B:552:ASN:OD1	2:B:553:TYR:HD2	1.78	0.67
2:B:902:GLN:HE21	2:B:904:ARG:HE	1.43	0.67
11:K:136:THR:HA	11:K:139:ILE:HG22	1.75	0.67
16:P:21:GLN:O	16:P:26:GLY:N	2.27	0.67
20:X:23:DT:H2'	20:X:24:DT:C6	2.28	0.67
7:G:122:THR:O	7:G:124:GLU:N	2.28	0.67
13:M:95:ARG:HB3	13:M:101:PRO:HB3	1.77	0.67
1:A:572:ASP:H	1:A:575:THR:CG2	2.08	0.66
1:A:1272:VAL:HG13	1:A:1273:LYS:H	1.59	0.66
10:J:7:CYS:SG	10:J:11:GLY:N	2.65	0.66
18:R:581:ASN:ND2	18:R:583:HIS:O	2.28	0.66
2:B:342:PHE:O	2:B:346:ALA:HB2	1.95	0.66
2:B:1028:LYS:HG2	2:B:1029:HIS:H	1.60	0.66
5:E:6:GLU:O	5:E:10:SER:CB	2.43	0.66
18:R:397:VAL:HG12	18:R:484:GLN:HB2	1.77	0.66
2:B:141:ILE:HG23	2:B:142:ILE:H	1.61	0.66
2:B:169:SER:O	2:B:173:LYS:N	2.27	0.66
4:D:14:TYR:CZ	4:D:124:VAL:HG21	2.30	0.66
1:A:15:GLY:H	1:A:1408:VAL:HG12	1.61	0.66
1:A:1409:GLU:H	1:A:1413:GLU:HG2	1.59	0.66
1:A:1445:ARG:HG3	1:A:1447:LEU:HD12	1.78	0.66
13:M:85:LEU:HG	14:N:398:SER:HB3	1.78	0.66
15:O:125:GLU:OE1	15:O:128:HIS:ND1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:470:GLU:H	15:O:479:PRO:HD3	1.60	0.66
1:A:432:TYR:HE1	1:A:443:ASN:CG	2.03	0.66
1:A:1148:ASP:HB2	1:A:1290:LYS:HA	1.76	0.66
1:A:535:MET:HE2	2:B:1073:TYR:HD2	1.60	0.66
1:A:676:SER:HB2	1:A:679:TYR:HB3	1.77	0.66
1:A:957:TYR:HD1	1:A:1031:LEU:HD13	1.60	0.66
3:C:30:GLU:HG3	11:K:84:PRO:HG3	1.77	0.66
13:M:111:ARG:HB3	13:M:243:ILE:HG23	1.77	0.66
13:M:154:GLU:CA	13:M:174:GLU:O	2.44	0.66
5:E:24:LYS:HB2	5:E:30:ILE:HD11	1.77	0.66
9:I:2:LEU:HA	9:I:11:MET:HE1	1.78	0.66
15:O:190:LEU:HG	15:O:193:GLN:HB3	1.77	0.66
1:A:999:ASP:OD1	1:A:1002:ARG:NH1	2.29	0.66
11:K:62:SER:OG	11:K:104:ARG:NH1	2.28	0.66
15:O:206:LEU:HD22	15:O:252:ILE:HG23	1.78	0.66
1:A:425:ASN:OD1	1:A:426:VAL:N	2.25	0.66
1:A:595:PRO:HA	1:A:604:TRP:NE1	2.10	0.66
2:B:247:ILE:HD12	2:B:309:VAL:HA	1.78	0.66
5:E:22:MET:HE3	5:E:187:TYR:HA	1.76	0.66
16:P:49:MET:HE2	19:S:364:LEU:HD11	1.76	0.66
16:P:61:ILE:HA	16:P:74:GLY:HA2	1.78	0.66
16:P:102:ARG:HD2	16:P:155:PRO:HG3	1.78	0.66
3:C:35:LYS:O	3:C:39:ASP:HB2	1.95	0.66
4:D:135:TYR:HD1	4:D:141:CYS:HB3	1.61	0.66
2:B:303:GLU:O	2:B:307:ALA:N	2.26	0.65
16:P:293:ILE:HD13	16:P:293:ILE:N	2.07	0.65
19:S:494:THR:HB	19:S:497:ASP:HB2	1.78	0.65
2:B:660:ALA:HB3	2:B:673:LEU:HB3	1.77	0.65
11:K:59:THR:O	11:K:106:GLN:HA	1.96	0.65
13:M:117:HIS:HB2	13:M:119:TRP:HE1	1.59	0.65
15:O:516:LEU:HA	15:O:566:PHE:O	1.95	0.65
15:O:288:MET:SD	15:O:291:ARG:NH2	2.69	0.65
15:O:314:ILE:HG21	15:O:369:HIS:CD2	2.32	0.65
1:A:353:PHE:N	1:A:355:GLN:OE1	2.29	0.65
2:B:234:ILE:HA	2:B:240:ILE:HA	1.77	0.65
11:K:88:PHE:HB3	11:K:106:GLN:CG	2.25	0.65
15:O:242:LYS:O	15:O:246:LYS:N	2.20	0.65
18:R:206:ALA:O	18:R:210:SER:N	2.25	0.65
18:R:394:GLN:HB3	21:Y:67:DA:H5"	1.77	0.65
1:A:95:TYR:O	1:A:99:THR:N	2.26	0.65
1:A:921:LEU:HA	1:A:1082:ARG:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:GLN:HG2	2:B:82:LEU:HG	1.78	0.65
3:C:255:VAL:HG22	3:C:256:ILE:H	1.61	0.65
5:E:88:VAL:HG23	5:E:117:THR:HG22	1.77	0.65
13:M:96:LEU:H	13:M:101:PRO:HA	1.62	0.65
16:P:149:MET:C	16:P:150:LEU:O	2.36	0.65
18:R:118:GLN:HE21	20:X:24:DT:H4'	1.61	0.65
5:E:32:GLN:HA	5:E:35:VAL:HG12	1.79	0.65
5:E:55:ARG:NH1	5:E:113:GLN:OE1	2.29	0.65
13:M:152:GLY:HA3	13:M:177:ALA:HA	1.77	0.65
13:M:164:LYS:HE3	13:M:259:ILE:HD11	1.79	0.65
15:O:573:SER:HA	15:O:576:PHE:CE2	2.31	0.65
15:O:643:ARG:HH21	17:Q:43:ILE:HA	1.60	0.65
16:P:135:LYS:NZ	16:P:153:LEU:O	2.27	0.65
18:R:152:VAL:HG22	18:R:154:VAL:H	1.61	0.65
1:A:1170:ALA:HA	1:A:1188:ILE:HG12	1.78	0.65
3:C:19:ASP:HB3	3:C:29:ASN:ND2	2.10	0.65
3:C:56:LEU:HB3	3:C:298:PHE:HB2	1.76	0.65
16:P:215:TYR:OH	16:P:262:ARG:NE	2.30	0.65
1:A:232:LYS:CD	16:P:315:TRP:CZ2	2.80	0.65
2:B:541:ILE:HA	2:B:544:ILE:HD12	1.79	0.65
4:D:126:GLN:NE2	4:D:127:LEU:H	1.95	0.65
5:E:185:ALA:O	5:E:189:GLY:N	2.29	0.65
8:H:6:PHE:CE2	8:H:8:ASP:HB2	2.31	0.65
11:K:69:ASP:OD1	11:K:70:HIS:N	2.25	0.65
1:A:793:ILE:O	1:A:797:CYS:N	2.29	0.65
13:M:135:LYS:HE3	13:M:140:TRP:HE1	1.61	0.65
15:O:467:PHE:HD1	15:O:468:LEU:HD13	1.62	0.65
16:P:152:SER:O	19:S:520:LYS:CD	2.45	0.65
2:B:84:LEU:HD21	19:S:383:ARG:HH12	1.61	0.65
1:A:366:GLY:O	2:B:1061:ARG:NH1	2.22	0.64
1:A:1050:ASP:O	1:A:1053:LYS:N	2.29	0.64
1:A:1145:LEU:O	1:A:1310:ILE:CG2	2.44	0.64
3:C:76:PRO:HB2	3:C:210:LEU:HD11	1.79	0.64
7:G:5:SER:O	7:G:73:ARG:HA	1.97	0.64
8:H:95:TYR:N	8:H:144:ILE:O	2.29	0.64
16:P:263:VAL:HG12	16:P:265:LEU:H	1.60	0.64
1:A:224:PRO:HA	1:A:227:THR:HG22	1.79	0.64
1:A:434:LEU:HB3	1:A:461:VAL:HB	1.79	0.64
1:A:583:MET:HG3	1:A:700:LEU:HB2	1.78	0.64
1:A:645:MET:HE2	8:H:122:LEU:HB3	1.80	0.64
2:B:298:GLN:CB	13:M:186:ILE:HG21	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:ARG:NH2	2:B:367:ASP:OD2	2.30	0.64
16:P:107:SER:O	16:P:110:ILE:N	2.30	0.64
1:A:479:SER:HB2	2:B:1066:GLU:HA	1.78	0.64
2:B:694:ASN:OD1	2:B:916:HIS:NE2	2.30	0.64
2:B:849:THR:N	2:B:865:GLN:O	2.30	0.64
4:D:129:ALA:HB1	4:D:153:MET:HB3	1.80	0.64
6:F:86:THR:HB	6:F:89:GLU:H	1.60	0.64
6:F:136:ARG:HB2	6:F:144:GLU:HB3	1.79	0.64
8:H:95:TYR:HB3	8:H:144:ILE:HB	1.79	0.64
1:A:1166:LEU:O	1:A:1170:ALA:N	2.30	0.64
1:A:1332:ARG:HH22	5:E:200:ARG:HE	1.43	0.64
2:B:210:ASP:HB3	2:B:213:LYS:HD2	1.79	0.64
11:K:80:ILE:HG22	11:K:86:VAL:HG11	1.80	0.64
15:O:330:LEU:HD12	15:O:331:THR:CG2	2.05	0.64
16:P:203:LYS:CE	16:P:206:VAL:HG22	2.27	0.64
2:B:376:ARG:HH21	2:B:607:ARG:NH1	1.93	0.64
3:C:164:ALA:HA	3:C:167:LEU:HD13	1.78	0.64
4:D:6:GLU:HG3	7:G:42:VAL:HG23	1.80	0.64
15:O:184:LYS:HA	15:O:187:ILE:HD11	1.78	0.64
18:R:289:SER:HB2	18:R:535:SER:HB3	1.78	0.64
1:A:18:PHE:CE1	2:B:1139:PRO:CA	2.80	0.64
1:A:1145:LEU:HD12	1:A:1146:VAL:H	0.50	0.64
1:A:1448:PHE:HZ	4:D:16:VAL:HG23	1.62	0.64
2:B:369:ARG:HG3	2:B:369:ARG:O	1.97	0.64
12:L:48:CYS:SG	12:L:53:HIS:O	2.56	0.64
15:O:172:GLU:O	15:O:176:SER:CB	2.45	0.64
15:O:352:VAL:HG13	15:O:353:GLU:H	1.63	0.64
1:A:484:SER:HB2	2:B:1069:CYS:CB	2.28	0.64
1:A:572:ASP:H	1:A:575:THR:HG22	1.62	0.64
1:A:675:HIS:HB3	1:A:937:ARG:HH22	1.61	0.64
1:A:1092:ILE:O	1:A:1096:SER:HB2	1.98	0.64
2:B:143:MET:SD	19:S:399:GLU:HB2	2.37	0.64
2:B:1002:ASP:HB3	2:B:1019:PHE:HE1	1.61	0.64
5:E:6:GLU:O	5:E:10:SER:HB2	1.97	0.64
13:M:164:LYS:HG3	14:N:300:LYS:HD3	1.79	0.64
11:K:95:HIS:HE1	11:K:98:GLU:HB3	1.63	0.64
14:N:394:VAL:HB	14:N:412:VAL:HB	1.78	0.64
15:O:141:ILE:HA	15:O:144:MET:HB2	1.79	0.64
15:O:307:VAL:HG13	15:O:308:THR:H	1.63	0.64
1:A:183:PHE:CD2	1:A:184:ARG:HG3	2.32	0.64
1:A:222:LEU:HG	1:A:226:LYS:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:ALA:HA	3:C:208:CYS:HA	1.80	0.64
3:C:228:ARG:HE	3:C:299:ILE:HD13	1.62	0.64
14:N:363:ILE:HA	14:N:373:VAL:HG22	1.79	0.64
16:P:10:GLN:HB3	16:P:13:ASP:HB3	1.80	0.64
18:R:211:LYS:NZ	18:R:280:VAL:O	2.27	0.64
1:A:109:ASN:ND2	1:A:157:CYS:SG	2.71	0.64
1:A:361:GLN:O	1:A:367:ASN:ND2	2.31	0.64
14:N:287:HIS:O	14:N:291:LEU:CB	2.45	0.64
21:Y:59:DG:H2'	21:Y:60:DT:H71	1.80	0.64
1:A:154:CYS:SG	1:A:155:LEU:N	2.70	0.63
2:B:775:LYS:HB2	2:B:927:LYS:O	1.98	0.63
3:C:45:SER:H	3:C:54:PHE:HA	1.62	0.63
8:H:24:CYS:SG	8:H:25:ARG:N	2.71	0.63
8:H:125:LEU:HD13	8:H:130:ARG:HH11	1.62	0.63
9:I:34:PRO:O	9:I:35:ILE:HG13	1.97	0.63
10:J:17:LYS:HD3	10:J:41:LEU:HD11	1.79	0.63
16:P:108:LYS:HA	16:P:111:LYS:HD3	1.81	0.63
1:A:402:LEU:CB	1:A:466:LEU:HD11	2.28	0.63
1:A:436:ARG:HH11	1:A:459:GLY:HA3	1.62	0.63
2:B:295:ILE:O	2:B:300:GLN:NE2	2.27	0.63
16:P:152:SER:HA	19:S:520:LYS:CE	2.28	0.63
16:P:266:GLU:O	16:P:269:LEU:N	2.30	0.63
16:P:137:VAL:HG11	16:P:149:MET:HE3	1.80	0.63
2:B:259:ALA:HB1	2:B:302:LEU:HD23	1.81	0.63
2:B:481:ARG:O	2:B:487:ARG:NH2	2.31	0.63
2:B:558:ASN:H	2:B:602:ALA:HB2	1.42	0.63
2:B:725:LEU:HD23	2:B:788:ARG:HD2	1.81	0.63
2:B:780:ARG:HA	3:C:103:LEU:HD11	1.80	0.63
15:O:249:PHE:O	15:O:252:ILE:HB	1.97	0.63
18:R:213:TRP:O	18:R:214:MET:HE2	1.99	0.63
20:X:23:DT:H3'	20:X:24:DT:H71	1.81	0.63
1:A:81:PHE:HZ	2:B:1130:GLN:HG2	1.63	0.63
1:A:574:ALA:H	3:C:20:PHE:HZ	1.47	0.63
1:A:848:VAL:HB	1:A:860:GLU:HB2	1.79	0.63
1:A:1156:VAL:O	1:A:1159:GLY:N	2.30	0.63
2:B:887:SER:HA	12:L:46:VAL:HG11	1.81	0.63
8:H:12:VAL:HG13	8:H:26:ILE:HD11	1.81	0.63
13:M:230:SER:O	13:M:234:HIS:N	2.26	0.63
15:O:330:LEU:CD1	15:O:331:THR:CB	2.76	0.63
1:A:313:MET:O	1:A:316:TRP:N	2.31	0.63
1:A:1373:ARG:HD3	1:A:1390:GLU:CD	2.24	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:ARG:HG2	2:B:141:ILE:HG21	1.81	0.63
2:B:553:TYR:HA	2:B:597:MET:HB3	1.81	0.63
2:B:1054:ARG:HG2	2:B:1055:SER:H	1.64	0.63
4:D:125:ASN:OD1	4:D:126:GLN:N	2.27	0.63
13:M:159:TYR:O	14:N:307:PHE:N	2.28	0.63
15:O:159:ILE:O	15:O:163:VAL:HG23	1.98	0.63
16:P:45:LEU:HA	19:S:372:MET:HE2	1.80	0.63
1:A:19:SER:O	2:B:1138:ALA:N	2.32	0.63
1:A:1022:LEU:HA	1:A:1025:SER:HB3	1.79	0.63
2:B:220:VAL:HG12	2:B:229:SER:HA	1.79	0.63
2:B:267:GLU:O	2:B:271:LEU:CB	2.46	0.63
2:B:855:PRO:O	18:R:106:GLN:NE2	2.32	0.63
7:G:9:ASP:OD1	7:G:10:LEU:N	2.29	0.63
12:L:31:CYS:HB2	12:L:35:SER:N	2.14	0.63
15:O:134:GLY:HA2	15:O:137:ILE:HD12	1.80	0.63
16:P:106:TRP:CG	16:P:107:SER:H	2.17	0.63
18:R:551:GLN:O	18:R:555:ALA:HB2	1.98	0.63
19:S:432:LEU:O	19:S:476:LYS:NZ	2.30	0.63
1:A:18:PHE:HA	2:B:1138:ALA:O	1.98	0.63
1:A:791:PRO:O	1:A:795:ALA:N	2.29	0.63
2:B:248:ALA:HB3	2:B:308:LYS:HE2	1.81	0.63
2:B:295:ILE:HD13	9:I:28:SER:HB3	1.80	0.63
2:B:723:THR:HA	2:B:790:LYS:HG2	1.80	0.63
2:B:910:ASP:N	2:B:922:CYS:SG	2.68	0.63
2:B:1008:ILE:O	3:C:65:ASN:ND2	2.32	0.63
4:D:14:TYR:OH	4:D:124:VAL:CG2	2.40	0.63
5:E:141:VAL:HG23	5:E:142:VAL:H	1.64	0.63
15:O:132:TYR:OH	15:O:291:ARG:NH1	2.31	0.63
1:A:606:GLY:HA2	1:A:609:VAL:HG12	1.79	0.63
1:A:864:HIS:HE2	2:B:695:GLN:HA	1.64	0.63
1:A:1099:GLU:OE1	1:A:1099:GLU:N	2.31	0.63
2:B:696:SER:HA	2:B:699:ASN:HD22	1.63	0.63
2:B:775:LYS:HA	2:B:778:ILE:HG22	1.81	0.63
2:B:832:VAL:HB	12:L:60:ARG:HA	1.81	0.63
5:E:83:CYS:SG	5:E:84:ASP:N	2.71	0.63
10:J:17:LYS:O	10:J:21:TYR:N	2.21	0.63
13:M:112:TYR:H	13:M:243:ILE:HG12	1.64	0.63
15:O:73:ARG:HB2	15:O:121:TYR:HE1	1.64	0.63
1:A:354:CYS:SG	1:A:1393:THR:OG1	2.57	0.62
1:A:1304:MET:HE2	5:E:147:HIS:NE2	2.14	0.62
2:B:213:LYS:HD3	2:B:216:VAL:HG23	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:521:THR:OG1	2:B:609:CYS:SG	2.57	0.62
2:B:914:SER:HB3	2:B:918:GLN:HB2	1.81	0.62
15:O:186:THR:O	15:O:187:ILE:C	2.42	0.62
16:P:151:TYR:CD2	16:P:151:TYR:O	2.52	0.62
16:P:203:LYS:HE2	16:P:206:VAL:HG22	1.81	0.62
1:A:61:SER:HB2	1:A:271:SER:HB3	1.79	0.62
1:A:1128:GLU:O	1:A:1132:ALA:N	2.20	0.62
1:A:1411:VAL:HG13	1:A:1412:SER:H	1.64	0.62
2:B:298:GLN:HG2	13:M:186:ILE:CG2	2.28	0.62
2:B:818:ILE:O	2:B:822:GLN:N	2.32	0.62
5:E:79:TRP:HE1	5:E:81:GLU:HB3	1.65	0.62
15:O:127:ILE:O	15:O:131:LEU:N	2.29	0.62
15:O:206:LEU:HA	15:O:209:THR:HB	1.81	0.62
15:O:549:GLN:HB2	15:O:565:LEU:HB2	1.82	0.62
18:R:83:ALA:O	18:R:87:LEU:HB2	1.99	0.62
1:A:572:ASP:N	1:A:575:THR:HG22	2.14	0.62
1:A:1032:LEU:C	1:A:1033:GLU:HG3	2.20	0.62
3:C:239:ILE:CG2	3:C:288:LYS:HD3	2.26	0.62
5:E:153:HIS:HB3	5:E:196:VAL:HG21	1.80	0.62
18:R:246:ALA:HA	19:S:405:LEU:HD11	1.81	0.62
1:A:1003:ASP:O	1:A:1007:SER:CB	2.46	0.62
1:A:1145:LEU:CD1	1:A:1146:VAL:N	2.05	0.62
1:A:1285:ILE:HA	1:A:1291:ARG:HG2	1.80	0.62
3:C:85:PHE:CE2	3:C:94:ASP:HB2	2.34	0.62
7:G:10:LEU:HA	7:G:69:ASN:HA	1.81	0.62
1:A:469:GLY:N	1:A:490:ALA:O	2.32	0.62
15:O:140:ILE:O	15:O:144:MET:N	2.33	0.62
1:A:232:LYS:HD3	16:P:315:TRP:HZ2	1.64	0.62
1:A:303:LEU:HG	15:O:538:ALA:HB1	1.80	0.62
1:A:896:LEU:HD12	1:A:906:THR:HA	1.82	0.62
1:A:1145:LEU:CA	1:A:1310:ILE:HG22	2.30	0.62
3:C:88:ASN:HB3	12:L:60:ARG:NH1	2.14	0.62
15:O:239:SER:HA	15:O:242:LYS:HD3	1.82	0.62
15:O:587:ASN:O	15:O:590:PHE:N	2.32	0.62
18:R:485:ASN:OD1	18:R:486:ILE:N	2.33	0.62
1:A:370:GLY:O	2:B:1061:ARG:NH1	2.32	0.62
1:A:535:MET:HG3	2:B:1073:TYR:CD2	2.35	0.62
1:A:978:ASP:HB2	1:A:984:VAL:N	2.15	0.62
7:G:10:LEU:HD12	7:G:69:ASN:HB3	1.81	0.62
14:N:306:VAL:O	14:N:415:LYS:HA	1.99	0.62
16:P:194:GLY:O	16:P:196:LYS:NZ	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:639:GLU:HG3	18:R:642:ARG:HH21	1.65	0.62
1:A:59:GLY:HA3	1:A:266:VAL:HB	1.81	0.62
1:A:850:ASN:ND2	1:A:860:GLU:OE2	2.31	0.62
2:B:589:SER:OG	2:B:590:ILE:N	2.31	0.62
15:O:328:ASP:O	15:O:330:LEU:HG	1.99	0.62
18:R:94:LEU:HD11	18:R:146:PHE:CD1	2.35	0.62
18:R:189:LEU:HB2	18:R:195:LYS:HZ1	1.65	0.62
1:A:915:THR:HG23	1:A:918:GLY:HA2	1.81	0.62
1:A:1145:LEU:HA	1:A:1310:ILE:HG22	1.82	0.62
1:A:1438:GLU:HA	1:A:1441:LEU:HD13	1.82	0.62
4:D:24:GLU:HG3	4:D:29:TRP:HA	1.82	0.62
15:O:316:LEU:HA	15:O:319:THR:HG22	1.81	0.62
16:P:27:ILE:HB	16:P:31:PHE:HB2	1.82	0.62
1:A:1449:GLU:O	4:D:117:LYS:NZ	2.33	0.62
2:B:1054:ARG:NH2	21:Y:25:DA:OP1	2.33	0.62
2:B:1101:MET:SD	2:B:1126:LYS:HG3	2.40	0.62
3:C:4:ILE:O	3:C:14:ASN:ND2	2.28	0.62
4:D:133:HIS:CE1	7:G:211:TRP:HB3	2.34	0.62
9:I:24:LEU:HG	9:I:33:PHE:HB2	1.82	0.62
14:N:287:HIS:HD2	14:N:384:LYS:HE2	1.65	0.62
15:O:31:VAL:HG12	15:O:32:MET:HG3	1.82	0.62
18:R:94:LEU:HD11	18:R:146:PHE:HD1	1.64	0.62
1:A:232:LYS:CE	16:P:315:TRP:CZ2	2.83	0.61
1:A:482:ARG:CD	1:A:1092:ILE:HG12	2.30	0.61
1:A:1045:ASP:HB2	1:A:1053:LYS:HD3	1.82	0.61
2:B:248:ALA:O	2:B:249:GLU:HG3	2.00	0.61
3:C:121:PRO:HA	3:C:125:LYS:HE3	1.82	0.61
4:D:127:LEU:O	4:D:129:ALA:N	2.31	0.61
14:N:397:LEU:HG	14:N:408:LEU:HA	1.82	0.61
1:A:542:LEU:HA	1:A:549:PRO:HA	1.81	0.61
2:B:204:ARG:HH12	2:B:376:ARG:HH12	1.48	0.61
2:B:536:LEU:HD22	2:B:571:PHE:HD1	1.64	0.61
2:B:1106:TRP:CD1	7:G:163:PRO:HD3	2.35	0.61
5:E:64:PRO:HD3	5:E:77:SER:HA	1.81	0.61
5:E:113:GLN:O	5:E:114:ASN:ND2	2.32	0.61
5:E:200:ARG:HD2	5:E:208:TYR:CZ	2.35	0.61
13:M:228:THR:HA	13:M:232:LEU:HD22	1.81	0.61
15:O:161:GLN:HB2	17:Q:61:PHE:HD1	1.65	0.61
1:A:314:GLU:O	1:A:318:TYR:CB	2.47	0.61
1:A:1009:ARG:O	1:A:1013:ASN:CB	2.43	0.61
6:F:115:THR:HG22	6:F:116:ASP:CA	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:287:HIS:CD2	14:N:384:LYS:HE2	2.34	0.61
1:A:379:THR:HG21	1:A:497:THR:HA	1.81	0.61
2:B:553:TYR:HB3	2:B:598:ALA:N	2.15	0.61
2:B:773:LEU:HD11	2:B:912:PHE:HE2	1.65	0.61
2:B:1112:SER:HB2	2:B:1114:GLU:HG2	1.83	0.61
15:O:102:ARG:NH2	15:O:282:ILE:O	2.31	0.61
1:A:261:LEU:HD12	1:A:262:PRO:HD2	1.83	0.61
1:A:365:ARG:HD3	1:A:887:ARG:HH21	1.66	0.61
6:F:86:THR:OG1	6:F:136:ARG:NH2	2.33	0.61
1:A:502:GLU:CD	1:A:502:GLU:H	2.05	0.61
2:B:77:ILE:HD13	2:B:98:ILE:HG12	1.82	0.61
2:B:588:ILE:O	2:B:588:ILE:HG22	2.00	0.61
2:B:650:ASP:OD1	2:B:651:VAL:N	2.34	0.61
1:A:442:ARG:HG2	18:R:30:VAL:HG22	1.82	0.61
1:A:483:LEU:O	1:A:486:LEU:CD1	2.49	0.61
1:A:907:SER:OG	1:A:1409:GLU:HB3	2.00	0.61
1:A:978:ASP:N	1:A:982:CYS:O	2.30	0.61
1:A:1177:TYR:OH	1:A:1260:MET:SD	2.55	0.61
3:C:277:ARG:O	3:C:277:ARG:HG3	1.99	0.61
19:S:363:GLN:HB2	19:S:378:THR:HG21	1.83	0.61
1:A:790:ALA:HB1	1:A:794:MET:HE2	1.82	0.61
7:G:204:GLY:HA2	7:G:210:TRP:HB2	1.83	0.61
15:O:222:HIS:CE1	15:O:244:ASN:HB3	2.35	0.61
18:R:144:ILE:HA	18:R:154:VAL:HG11	1.82	0.61
18:R:402:LEU:HD11	18:R:441:ILE:HD11	1.80	0.61
1:A:1207:VAL:HA	1:A:1210:THR:HG22	1.83	0.61
2:B:239:LYS:HG2	2:B:241:TYR:CE2	2.35	0.61
7:G:88:TRP:CD1	7:G:143:ASN:H	2.19	0.61
13:M:71:ILE:HG12	14:N:367:LYS:HZ2	1.63	0.61
16:P:145:ARG:HB3	16:P:147:ILE:HG23	1.81	0.61
1:A:184:ARG:O	1:A:189:LYS:NZ	2.31	0.60
1:A:205:LEU:HD12	1:A:212:GLU:HG2	1.83	0.60
1:A:269:ARG:NH1	1:A:285:LEU:HB2	2.15	0.60
1:A:355:GLN:H	1:A:355:GLN:CD	2.09	0.60
2:B:209:ALA:HA	2:B:215:ILE:HG23	1.83	0.60
8:H:128:ASN:CG	8:H:129:TYR:H	2.08	0.60
18:R:91:SER:OG	18:R:101:THR:HG22	2.01	0.60
19:S:418:ASP:HB3	19:S:449:ARG:HH22	1.63	0.60
1:A:1213:SER:O	1:A:1217:ILE:N	2.34	0.60
7:G:46:ILE:HD11	7:G:77:PHE:HB2	1.82	0.60
8:H:93:TYR:HB2	8:H:143:LEU:HG	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:384:LYS:HA	14:N:416:ILE:HD11	1.81	0.60
15:O:599:ASN:O	15:O:603:LEU:N	2.23	0.60
16:P:308:GLU:OE1	16:P:308:GLU:N	2.33	0.60
18:R:28:CYS:SG	18:R:29:GLY:N	2.74	0.60
18:R:633:ASP:HA	18:R:636:LEU:HB3	1.83	0.60
1:A:906:THR:OG1	1:A:907:SER:N	2.35	0.60
1:A:997:GLN:C	1:A:999:ASP:H	2.08	0.60
7:G:10:LEU:HD21	7:G:67:TYR:HB3	1.82	0.60
7:G:207:LEU:HD22	7:G:210:TRP:CD1	2.37	0.60
13:M:134:ASP:O	13:M:138:SER:N	2.34	0.60
18:R:531:LEU:HB2	18:R:539:VAL:HB	1.81	0.60
1:A:385:PRO:HD2	2:B:765:TYR:CD1	2.36	0.60
1:A:1136:ILE:HD12	1:A:1318:HIS:HB3	1.84	0.60
2:B:860:VAL:HG13	2:B:861:ASN:H	1.67	0.60
2:B:934:ASN:OD1	2:B:935:ASP:N	2.35	0.60
18:R:468:ILE:HG23	18:R:472:ILE:HD12	1.81	0.60
1:A:116:SER:OG	1:A:117:GLU:OE1	2.16	0.60
1:A:402:LEU:HB3	1:A:466:LEU:CD1	2.31	0.60
1:A:413:ARG:NH1	1:A:456:LEU:O	2.35	0.60
2:B:667:VAL:HB	2:B:670:MET:HG3	1.82	0.60
2:B:727:LEU:HD11	2:B:786:GLU:HB2	1.83	0.60
3:C:165:ARG:NH1	3:C:190:ASP:OD1	2.35	0.60
7:G:27:THR:HA	7:G:30:LEU:HD12	1.83	0.60
8:H:39:THR:HB	8:H:124:ARG:HB3	1.82	0.60
11:K:85:ASP:O	11:K:107:THR:OG1	2.20	0.60
18:R:398:ALA:HA	18:R:484:GLN:H	1.65	0.60
1:A:11:LYS:HG3	2:B:1117:ILE:HD13	1.84	0.60
1:A:714:ILE:HD12	2:B:958:MET:HE3	1.82	0.60
2:B:247:ILE:HG13	2:B:248:ALA:H	1.66	0.60
2:B:658:TYR:CE2	2:B:670:MET:HG2	2.36	0.60
3:C:66:ALA:O	3:C:70:ILE:HG22	2.01	0.60
15:O:98:LEU:HB3	15:O:103:CYS:HB2	1.84	0.60
15:O:263:LEU:HB3	15:O:272:ARG:HH21	1.67	0.60
16:P:206:VAL:HB	16:P:210:PRO:HD3	1.83	0.60
1:A:248:VAL:HG23	1:A:248:VAL:O	2.01	0.60
1:A:956:PRO:HB2	1:A:1031:LEU:HD11	1.83	0.60
1:A:1120:THR:O	1:A:1125:ARG:HD2	2.02	0.60
2:B:417:ASP:O	2:B:419:LEU:N	2.34	0.60
2:B:544:ILE:HG22	2:B:546:SER:H	1.64	0.60
2:B:589:SER:O	2:B:590:ILE:CB	2.47	0.60
2:B:611:PRO:HG3	2:B:648:TYR:HE1	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:842:TYR:HB2	2:B:881:ILE:HD11	1.82	0.60
3:C:32:ASN:O	3:C:33:VAL:HG23	2.02	0.60
10:J:35:ALA:O	10:J:39:LEU:N	2.34	0.60
15:O:123:ASN:O	15:O:126:GLY:N	2.34	0.60
16:P:107:SER:O	16:P:110:ILE:HG22	2.00	0.60
11:K:88:PHE:O	11:K:105:ILE:HA	2.02	0.60
15:O:327:ARG:C	15:O:329:PRO:HD2	2.27	0.60
18:R:607:ASP:OD1	18:R:610:LEU:N	2.32	0.60
1:A:134:ASN:ND2	1:A:1381:ASP:OD1	2.35	0.60
1:A:1141:ILE:HB	1:A:1295:VAL:HB	1.84	0.60
2:B:166:ALA:HB1	2:B:170:LYS:HB2	1.83	0.60
9:I:16:SER:HA	9:I:22:TYR:HA	1.82	0.60
1:A:553:ALA:HB1	1:A:557:PHE:HB2	1.84	0.60
2:B:717:GLN:HE21	2:B:727:LEU:HD22	1.66	0.60
4:D:58:ILE:O	4:D:62:VAL:N	2.24	0.60
10:J:60:PHE:O	10:J:63:TYR:N	2.35	0.60
15:O:330:LEU:CD1	15:O:331:THR:N	2.02	0.60
18:R:632:ALA:O	18:R:636:LEU:CB	2.50	0.60
1:A:100:ILE:O	1:A:104:GLN:HB2	2.02	0.59
1:A:890:MET:O	1:A:894:GLU:N	2.35	0.59
1:A:1158:LYS:O	1:A:1162:GLU:HB2	2.02	0.59
2:B:48:LEU:HD21	2:B:743:LEU:HD21	1.83	0.59
2:B:489:LEU:HD11	2:B:499:THR:HG22	1.84	0.59
2:B:555:VAL:O	2:B:561:LEU:HA	2.02	0.59
15:O:471:THR:OG1	15:O:477:TYR:N	2.35	0.59
1:A:1202:ILE:O	1:A:1205:ILE:HG13	2.01	0.59
2:B:95:TYR:OH	2:B:396:ASN:ND2	2.34	0.59
2:B:227:ARG:NH1	2:B:449:MET:HG3	2.17	0.59
2:B:300:GLN:N	2:B:300:GLN:OE1	2.35	0.59
4:D:15:GLU:O	4:D:19:PHE:N	2.35	0.59
5:E:66:GLU:HG3	5:E:67:GLU:H	1.66	0.59
14:N:366:HIS:HB3	14:N:370:LYS:HB2	1.85	0.59
15:O:102:ARG:O	15:O:123:ASN:ND2	2.34	0.59
15:O:507:LEU:O	15:O:511:ILE:HG12	2.02	0.59
15:O:583:TRP:HZ3	17:Q:41:LEU:HD21	1.67	0.59
16:P:111:LYS:O	16:P:115:ASN:N	2.33	0.59
18:R:463:ARG:NH1	18:R:598:ASP:O	2.35	0.59
5:E:116:ILE:O	5:E:116:ILE:HG22	2.02	0.59
11:K:68:GLU:HG3	11:K:69:ASP:H	1.67	0.59
15:O:527:LEU:HD12	15:O:528:MET:HG2	1.83	0.59
15:O:584:ASN:HB3	15:O:588:LEU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:402:LEU:HB3	18:R:476:ALA:HB1	1.83	0.59
21:Y:13:DA:C5	21:Y:14:DC:N4	2.70	0.59
3:C:59:ILE:HD12	3:C:60:ASP:O	2.03	0.59
7:G:59:LEU:HD21	7:G:64:GLY:HA2	1.83	0.59
14:N:307:PHE:CD1	14:N:416:ILE:HG22	2.37	0.59
18:R:408:LEU:HB3	18:R:428:VAL:HG23	1.82	0.59
2:B:464:ILE:HG12	2:B:687:LEU:HD11	1.83	0.59
5:E:180:ARG:N	5:E:215:MET:O	2.31	0.59
13:M:134:ASP:HA	13:M:137:GLU:HB2	1.83	0.59
16:P:237:PRO:HA	16:P:240:ILE:HB	1.84	0.59
18:R:213:TRP:CB	18:R:285:ALA:HB1	2.33	0.59
1:A:63:SER:HB2	1:A:74:LEU:HD12	1.84	0.59
2:B:327:ILE:HD11	13:M:231:LEU:HB2	1.84	0.59
2:B:918:GLN:HG3	2:B:944:MET:HE1	1.84	0.59
4:D:17:LEU:HD22	4:D:66:LEU:HB3	1.84	0.59
4:D:126:GLN:C	4:D:127:LEU:HG	2.27	0.59
5:E:25:ASP:OD1	5:E:25:ASP:N	2.35	0.59
8:H:125:LEU:CD1	8:H:130:ARG:HH11	2.15	0.59
15:O:633:ARG:NE	16:P:308:GLU:OE2	2.35	0.59
16:P:312:PHE:HD1	17:Q:41:LEU:HD11	1.66	0.59
19:S:439:PHE:HB2	19:S:451:ARG:HH21	1.68	0.59
19:S:506:GLN:O	19:S:510:LYS:CB	2.49	0.59
1:A:643:ASN:HB2	1:A:651:PHE:CZ	2.37	0.59
1:A:995:VAL:HG23	1:A:996:ASP:H	1.68	0.59
1:A:1160:ARG:HA	1:A:1273:LYS:HE3	1.84	0.59
1:A:1265:ARG:HH21	2:B:285:VAL:HG22	1.66	0.59
2:B:101:GLY:HA2	2:B:109:LYS:HD3	1.83	0.59
15:O:239:SER:O	15:O:243:MET:N	2.28	0.59
15:O:352:VAL:O	15:O:357:PRO:HD2	2.02	0.59
18:R:467:ARG:HD3	18:R:602:LEU:HG	1.84	0.59
1:A:103:LEU:HD11	1:A:222:LEU:HD22	1.84	0.59
1:A:752:THR:HA	1:A:761:THR:HG21	1.83	0.59
14:N:364:ARG:HH11	14:N:365:VAL:H	1.48	0.59
18:R:505:HIS:O	18:R:509:SER:N	2.36	0.59
1:A:18:PHE:HE1	2:B:1139:PRO:HB2	1.65	0.59
1:A:109:ASN:ND2	1:A:159:ALA:HB3	2.18	0.59
1:A:976:ARG:HH22	1:A:995:VAL:N	2.01	0.59
2:B:177:CYS:SG	2:B:714:ALA:HB1	2.42	0.59
2:B:337:VAL:HG23	2:B:345:LYS:HE2	1.84	0.59
2:B:710:ILE:HG12	2:B:1026:LYS:O	2.02	0.59
2:B:1092:VAL:HG22	2:B:1126:LYS:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:147:ARG:NH2	7:G:211:TRP:HB2	2.18	0.59
16:P:187:SER:HA	16:P:263:VAL:HG21	1.85	0.59
16:P:301:PRO:HB2	16:P:303:SER:HB3	1.83	0.59
18:R:646:GLU:OE1	19:S:510:LYS:HE3	2.03	0.59
1:A:1125:ARG:HG3	1:A:1126:ILE:N	2.18	0.59
1:A:1157:VAL:HG12	1:A:1160:ARG:HD2	1.84	0.59
2:B:472:ARG:HH21	2:B:511:VAL:HG11	1.67	0.59
2:B:798:TYR:O	2:B:801:HIS:N	2.28	0.59
13:M:112:TYR:HD1	13:M:119:TRP:NE1	1.97	0.59
15:O:105:LYS:HB3	15:O:210:PRO:HG3	1.84	0.59
18:R:178:PRO:HG3	18:R:220:PRO:HB3	1.84	0.59
18:R:609:GLU:O	18:R:613:HIS:N	2.36	0.59
1:A:277:SER:OG	1:A:278:PRO:HD3	2.03	0.58
1:A:678:PHE:CE2	1:A:694:MET:HG2	2.38	0.58
1:A:1282:VAL:O	1:A:1293:LEU:HA	2.03	0.58
2:B:131:VAL:HG21	2:B:149:ILE:HG23	1.85	0.58
2:B:554:GLY:O	2:B:599:VAL:N	2.27	0.58
3:C:33:VAL:HG12	3:C:34:GLU:N	2.18	0.58
3:C:173:GLY:C	3:C:175:GLN:H	2.10	0.58
5:E:31:THR:HG22	5:E:34:GLU:HG2	1.85	0.58
11:K:95:HIS:ND1	11:K:97:SER:OG	2.31	0.58
11:K:117:LEU:O	11:K:121:LEU:CB	2.51	0.58
1:A:572:ASP:N	1:A:575:THR:CG2	2.66	0.58
1:A:588:GLU:O	11:K:104:ARG:NH2	2.36	0.58
1:A:600:PRO:HD2	8:H:96:VAL:HG22	1.85	0.58
1:A:1153:ALA:HA	1:A:1156:VAL:HB	1.85	0.58
5:E:161:LYS:NZ	5:E:193:GLY:O	2.28	0.58
15:O:364:ILE:HA	15:O:476:TYR:CZ	2.38	0.58
15:O:492:TYR:O	15:O:495:VAL:HG23	2.03	0.58
16:P:149:MET:O	16:P:150:LEU:C	2.46	0.58
16:P:293:ILE:H	16:P:293:ILE:CD1	1.99	0.58
1:A:1421:MET:HE1	2:B:1071:ILE:HD12	1.84	0.58
2:B:1043:ARG:NH1	18:R:35:ASN:OD1	2.36	0.58
3:C:6:GLY:HA3	3:C:13:THR:HB	1.85	0.58
3:C:30:GLU:HG2	11:K:82:LYS:O	2.03	0.58
6:F:147:SER:HB3	6:F:150:GLU:HG3	1.84	0.58
8:H:39:THR:O	8:H:123:MET:HA	2.03	0.58
8:H:61:SER:HB2	8:H:139:ASN:HD22	1.68	0.58
18:R:270:LEU:O	18:R:273:GLN:NE2	2.33	0.58
1:A:577:THR:HG23	11:K:88:PHE:CD1	2.38	0.58
1:A:1449:GLU:OE2	4:D:10:PHE:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:LYS:HZ1	2:B:519:HIS:HA	1.67	0.58
2:B:84:LEU:HD13	2:B:91:PHE:CD2	2.39	0.58
2:B:126:SER:OG	2:B:151:ARG:HB3	2.03	0.58
2:B:257:LEU:HD23	2:B:268:ILE:HG23	1.85	0.58
3:C:216:HIS:HB3	3:C:218:LYS:HG2	1.86	0.58
3:C:227:TYR:HB3	3:C:300:PHE:HD1	1.68	0.58
3:C:294:VAL:HG13	3:C:297:HIS:HB3	1.84	0.58
3:C:303:GLU:HG3	10:J:43:ARG:HH12	1.69	0.58
4:D:11:LEU:HD21	4:D:16:VAL:HG21	1.83	0.58
7:G:88:TRP:HA	7:G:146:ILE:HD12	1.84	0.58
9:I:8:CYS:SG	9:I:29:CYS:HB2	2.43	0.58
15:O:183:MET:O	15:O:187:ILE:CG1	2.52	0.58
15:O:303:ARG:HA	16:P:265:LEU:HD21	1.84	0.58
16:P:221:ILE:O	16:P:225:ILE:HG12	2.03	0.58
18:R:546:ARG:NH1	18:R:586:PRO:O	2.37	0.58
1:A:1448:PHE:CD2	4:D:11:LEU:HG	2.38	0.58
2:B:235:THR:HG22	2:B:236:LYS:HG3	1.85	0.58
15:O:630:VAL:O	15:O:634:GLU:HG2	2.04	0.58
18:R:395:ASN:HB2	21:Y:67:DA:H5'	1.84	0.58
18:R:435:PRO:HD2	18:R:461:ALA:HB2	1.86	0.58
19:S:442:ILE:HG21	19:S:454:VAL:HG11	1.84	0.58
1:A:196:ILE:O	1:A:199:GLY:N	2.36	0.58
1:A:363:ARG:NH2	2:B:1046:LEU:HD21	2.19	0.58
1:A:694:MET:O	1:A:697:MET:HB3	2.04	0.58
2:B:211:GLU:O	2:B:212:LYS:HG2	2.03	0.58
2:B:590:ILE:CB	2:B:601:ILE:CD1	2.72	0.58
2:B:818:ILE:HG13	2:B:821:HIS:H	1.67	0.58
6:F:116:ASP:OD2	6:F:119:ARG:NH1	2.36	0.58
13:M:113:LYS:HE2	13:M:118:LEU:HB2	1.84	0.58
13:M:159:TYR:HE2	14:N:309:LEU:HB2	1.69	0.58
15:O:183:MET:O	15:O:187:ILE:HG12	2.04	0.58
2:B:142:ILE:HG13	19:S:396:LYS:HA	1.84	0.58
2:B:232:TYR:HB2	2:B:242:LEU:HD23	1.85	0.58
2:B:529:ILE:HD12	2:B:532:LEU:HD23	1.85	0.58
2:B:552:ASN:OD1	2:B:553:TYR:CD2	2.56	0.58
7:G:112:GLN:HE22	7:G:128:TRP:HD1	1.50	0.58
15:O:106:TYR:H	15:O:210:PRO:HD3	1.69	0.58
15:O:578:ARG:HA	15:O:648:TRP:CZ3	2.39	0.58
15:O:629:MET:O	15:O:633:ARG:HB3	2.04	0.58
2:B:217:GLN:HE21	2:B:232:TYR:HB3	1.68	0.58
3:C:113:LEU:HD21	3:C:132:ILE:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:14:TYR:CE1	4:D:124:VAL:CG1	2.87	0.58
8:H:102:TYR:CZ	8:H:115:TYR:HB3	2.39	0.58
13:M:104:HIS:ND1	13:M:105:PRO:O	2.36	0.58
15:O:581:LEU:HD22	15:O:648:TRP:CZ2	2.39	0.58
1:A:38:ASP:C	1:A:40:PHE:H	2.11	0.58
1:A:579:LEU:CD2	1:A:704:PHE:CD1	2.86	0.58
1:A:1141:ILE:O	1:A:1294:LEU:HA	2.04	0.58
1:A:1169:VAL:O	1:A:1188:ILE:HG23	2.03	0.58
2:B:610:ARG:NH2	2:B:674:GLU:OE1	2.37	0.58
4:D:130:ASN:OD1	4:D:133:HIS:ND1	2.37	0.58
15:O:597:GLN:HA	15:O:600:SER:HB2	1.85	0.58
16:P:83:LYS:HA	16:P:86:MET:HG2	1.83	0.58
18:R:94:LEU:HB2	18:R:96:ILE:HG23	1.86	0.58
18:R:433:ARG:HD3	19:S:473:LEU:HD23	1.86	0.58
1:A:1064:GLU:CG	1:A:1065:LYS:N	2.47	0.58
2:B:694:ASN:OD1	2:B:954:THR:OG1	2.22	0.58
3:C:257:GLY:N	3:C:266:TYR:O	2.34	0.58
13:M:148:LEU:HD23	13:M:179:LEU:HG	1.86	0.58
15:O:233:SER:O	15:O:236:LYS:HG2	2.04	0.58
1:A:436:ARG:N	1:A:460:ASP:OD1	2.37	0.57
1:A:724:LYS:O	1:A:728:GLU:CB	2.51	0.57
4:D:20:LEU:O	4:D:24:GLU:CB	2.52	0.57
8:H:15:VAL:HG12	8:H:17:PRO:HD3	1.84	0.57
8:H:138:GLU:OE1	8:H:138:GLU:N	2.37	0.57
1:A:123:PHE:CD2	1:A:144:ILE:HD13	2.40	0.57
1:A:668:VAL:HA	1:A:676:SER:HA	1.85	0.57
1:A:1130:ILE:HG22	1:A:1371:ILE:HG21	1.87	0.57
2:B:904:ARG:HH12	2:B:1033:ASP:CG	2.11	0.57
15:O:634:GLU:HA	15:O:637:VAL:HG12	1.87	0.57
1:A:201:TRP:HB3	1:A:205:LEU:CD1	2.33	0.57
1:A:501:ASN:O	1:A:504:VAL:HG22	2.05	0.57
1:A:571:TYR:HB3	1:A:575:THR:CG2	2.34	0.57
2:B:77:ILE:HG21	2:B:98:ILE:HD11	1.85	0.57
2:B:459:SER:N	2:B:469:MET:SD	2.61	0.57
8:H:129:TYR:O	8:H:131:ASN:OD1	2.22	0.57
10:J:55:ASP:OD1	10:J:57:ILE:HG22	2.04	0.57
18:R:439:ALA:HA	18:R:450:THR:H	1.70	0.57
1:A:37:ARG:HG2	1:A:38:ASP:H	1.68	0.57
1:A:653:ILE:HG23	1:A:660:LEU:HB2	1.87	0.57
2:B:298:GLN:CG	13:M:186:ILE:HG21	2.34	0.57
2:B:415:GLU:CG	2:B:416:TYR:H	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:756:THR:H	10:J:48:ARG:HH12	1.51	0.57
4:D:128:PRO:O	4:D:129:ALA:C	2.48	0.57
18:R:123:GLN:HG2	18:R:150:LEU:HD21	1.84	0.57
1:A:997:GLN:O	1:A:999:ASP:N	2.34	0.57
2:B:192:LYS:HG2	2:B:457:VAL:HA	1.85	0.57
3:C:256:ILE:HA	3:C:267:VAL:HA	1.86	0.57
5:E:32:GLN:O	5:E:36:GLU:N	2.38	0.57
7:G:59:LEU:CD1	7:G:64:GLY:HA2	2.29	0.57
14:N:373:VAL:HB	14:N:382:ILE:HG22	1.85	0.57
15:O:365:ASP:H	15:O:476:TYR:HH	1.51	0.57
15:O:578:ARG:HA	15:O:648:TRP:HZ3	1.69	0.57
2:B:64:SER:HB3	2:B:381:GLY:HA3	1.86	0.57
2:B:279:TYR:HA	2:B:282:ILE:HD12	1.86	0.57
2:B:362:ASN:ND2	2:B:365:MET:SD	2.75	0.57
4:D:126:GLN:HE21	4:D:127:LEU:H	1.51	0.57
15:O:105:LYS:HG2	15:O:123:ASN:HA	1.85	0.57
15:O:221:LYS:N	15:O:224:LYS:HB3	2.18	0.57
1:A:584:SER:O	1:A:586:GLY:N	2.37	0.57
4:D:142:ASP:OD1	4:D:143:ALA:N	2.35	0.57
15:O:58:GLY:O	15:O:62:ALA:N	2.37	0.57
15:O:197:MET:HB2	15:O:286:ARG:HG3	1.87	0.57
16:P:132:ARG:O	16:P:151:TYR:HD2	1.87	0.57
18:R:218:ARG:CZ	21:Y:71:DT:H5'	2.35	0.57
1:A:524:THR:HG22	2:B:1081:GLU:HB2	1.86	0.57
1:A:1361:VAL:HA	1:A:1364:TYR:HB2	1.86	0.57
4:D:102:SER:O	4:D:106:LEU:N	2.38	0.57
5:E:93:MET:SD	5:E:120:ALA:HA	2.45	0.57
9:I:30:PRO:HD3	13:M:135:LYS:HE2	1.84	0.57
18:R:79:THR:O	18:R:83:ALA:CB	2.52	0.57
18:R:485:ASN:ND2	20:X:13:DT:O4'	2.38	0.57
1:A:706:GLY:HA2	2:B:762:TYR:HA	1.86	0.57
2:B:882:ASP:OD2	3:C:93:GLN:NE2	2.36	0.57
16:P:203:LYS:HB2	16:P:206:VAL:HA	1.86	0.57
18:R:521:TYR:HE2	18:R:523:MET:HB2	1.69	0.57
6:F:80:ALA:O	6:F:81:THR:OG1	2.21	0.56
15:O:285:ASP:OD1	15:O:286:ARG:N	2.34	0.56
15:O:601:THR:HG23	15:O:602:LEU:H	1.69	0.56
16:P:235:LEU:HD21	16:P:239:ASN:HB3	1.87	0.56
18:R:18:ASN:HD21	18:R:20:ASN:ND2	2.02	0.56
20:X:63:DC:N3	21:Y:18:DG:N2	2.53	0.56
1:A:16:LEU:HD11	1:A:1417:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:LEU:O	1:A:466:LEU:HG	2.05	0.56
1:A:485:ILE:C	1:A:486:LEU:HD12	2.30	0.56
2:B:552:ASN:OD1	2:B:568:PRO:HB3	2.05	0.56
2:B:575:PHE:HE2	2:B:589:SER:O	1.88	0.56
4:D:64:ASN:ND2	7:G:102:LEU:HB3	2.19	0.56
15:O:322:LYS:HG2	15:O:357:PRO:HB3	1.87	0.56
15:O:329:PRO:O	15:O:330:LEU:HG	2.05	0.56
18:R:162:LEU:HD12	18:R:515:LEU:HD21	1.86	0.56
18:R:455:GLU:OE1	18:R:546:ARG:NH2	2.39	0.56
1:A:18:PHE:CE1	2:B:1139:PRO:HA	2.37	0.56
1:A:30:SER:OG	1:A:83:HIS:HB3	2.04	0.56
1:A:32:VAL:C	1:A:83:HIS:CE1	2.83	0.56
1:A:424:PRO:HD3	1:A:444:LEU:CG	2.35	0.56
1:A:611:SER:OG	1:A:658:GLN:HA	2.05	0.56
1:A:666:LYS:HG2	1:A:667:SER:H	1.69	0.56
1:A:703:ARG:HH22	11:K:93:ILE:HB	1.70	0.56
1:A:788:TRP:HA	1:A:793:ILE:HD11	1.86	0.56
1:A:903:THR:HA	1:A:914:PHE:O	2.05	0.56
1:A:1144:VAL:HG12	1:A:1292:GLU:HG3	1.87	0.56
2:B:299:GLN:HE21	2:B:322:GLU:HB3	1.70	0.56
2:B:521:THR:O	2:B:606:GLY:N	2.34	0.56
2:B:915:ARG:NH1	2:B:960:GLU:OE2	2.38	0.56
2:B:916:HIS:CG	2:B:957:LYS:HB2	2.40	0.56
2:B:1038:ARG:NH1	2:B:1050:PRO:HB3	2.20	0.56
2:B:1063:GLY:O	2:B:1067:ARG:N	2.27	0.56
3:C:62:SER:O	3:C:65:ASN:N	2.38	0.56
6:F:79:ARG:NH1	6:F:145:ASP:O	2.39	0.56
16:P:202:PRO:HD2	16:P:204:LYS:HE2	1.87	0.56
18:R:615:LEU:HD13	18:R:619:ALA:HB3	1.87	0.56
1:A:1008:LEU:HD11	1:A:1070:PHE:HE2	1.69	0.56
2:B:198:GLU:OE2	2:B:375:LYS:HB3	2.05	0.56
2:B:343:ARG:O	2:B:346:ALA:HB3	2.06	0.56
3:C:14:ASN:ND2	3:C:295:ARG:HH12	2.03	0.56
15:O:292:ARG:HH22	15:O:650:VAL:HA	1.71	0.56
1:A:216:LYS:HG3	1:A:217:ARG:H	1.69	0.56
1:A:287:VAL:O	1:A:290:THR:HG22	2.04	0.56
2:B:585:SER:O	2:B:586:GLU:HB2	2.04	0.56
15:O:286:ARG:NE	15:O:321:GLN:O	2.38	0.56
15:O:585:MET:HE3	15:O:644:LEU:HG	1.88	0.56
18:R:558:PRO:O	18:R:562:GLU:CB	2.49	0.56
19:S:470:GLU:O	19:S:474:ARG:CB	2.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:TYR:HA	1:A:575:THR:HG21	1.88	0.56
2:B:138:GLY:H	2:B:141:ILE:HG21	1.69	0.56
2:B:658:TYR:HD2	2:B:670:MET:HA	1.71	0.56
2:B:914:SER:OG	2:B:957:LYS:NZ	2.21	0.56
6:F:75:PRO:HG2	6:F:78:GLN:HG2	1.87	0.56
7:G:2:PHE:N	7:G:76:VAL:O	2.39	0.56
18:R:7:CYS:SG	18:R:28:CYS:CB	2.82	0.56
18:R:198:VAL:HG13	18:R:231:ALA:HB3	1.87	0.56
19:S:416:TYR:OH	21:Y:76:DT:H5"	2.05	0.56
1:A:368:LEU:O	1:A:371:LYS:HG3	2.06	0.56
2:B:415:GLU:O	2:B:416:TYR:O	2.21	0.56
3:C:31:TRP:CG	3:C:32:ASN:N	2.72	0.56
15:O:592:LYS:HD2	15:O:638:PHE:CZ	2.41	0.56
15:O:635:LEU:HB3	17:Q:47:ILE:HD13	1.87	0.56
18:R:468:ILE:HG13	18:R:610:LEU:HD11	1.87	0.56
1:A:474:PHE:C	1:A:485:ILE:HD13	2.30	0.56
1:A:559:THR:HG21	2:B:947:HIS:CE1	2.41	0.56
1:A:608:GLN:O	1:A:611:SER:N	2.39	0.56
13:M:136:ALA:HA	13:M:142:GLY:H	1.71	0.56
18:R:620:SER:O	18:R:624:GLU:CB	2.45	0.56
1:A:81:PHE:CZ	2:B:1130:GLN:HG2	2.40	0.56
1:A:555:GLN:HE22	2:B:768:GLU:HG3	1.68	0.56
1:A:1323:PHE:HA	1:A:1327:GLY:HA2	1.88	0.56
2:B:136:THR:HG22	2:B:142:ILE:HG22	1.88	0.56
2:B:873:TYR:OH	2:B:877:GLU:O	2.23	0.56
7:G:53:THR:HG21	7:G:71:THR:HG22	1.88	0.56
10:J:45:CYS:O	10:J:48:ARG:HG2	2.06	0.56
16:P:31:PHE:O	16:P:72:PHE:N	2.39	0.56
1:A:81:PHE:CD2	1:A:265:PRO:CD	2.89	0.56
1:A:196:ILE:O	1:A:200:GLU:HG3	2.06	0.56
1:A:575:THR:HG23	1:A:576:LEU:N	2.21	0.56
1:A:1072:GLU:O	1:A:1076:PHE:HB2	2.05	0.56
1:A:1304:MET:HE2	5:E:147:HIS:HE2	1.71	0.56
1:A:1315:THR:HG22	1:A:1316:THR:H	1.71	0.56
3:C:67:PHE:O	3:C:71:MET:HB2	2.06	0.56
5:E:20:LYS:O	5:E:23:VAL:HG12	2.06	0.56
9:I:23:THR:HA	9:I:35:ILE:HG22	1.87	0.56
15:O:640:ARG:O	15:O:643:ARG:HB2	2.06	0.56
16:P:313:ASP:OD1	16:P:313:ASP:N	2.37	0.56
1:A:57:LYS:HA	1:A:68:ALA:HB3	1.88	0.55
1:A:786:ASP:OD1	1:A:787:ASN:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:ALA:HA	10:J:63:TYR:CE1	2.42	0.55
2:B:525:GLU:HG3	2:B:528:PRO:HD2	1.87	0.55
2:B:782:PHE:HA	10:J:8:PHE:CZ	2.41	0.55
8:H:8:ASP:OD1	8:H:9:ILE:N	2.39	0.55
11:K:76:LEU:HG	11:K:80:ILE:HD11	1.88	0.55
13:M:85:LEU:O	13:M:173:ILE:O	2.25	0.55
15:O:467:PHE:CD1	15:O:468:LEU:HD13	2.41	0.55
18:R:397:VAL:O	18:R:484:GLN:N	2.39	0.55
1:A:238:ASP:HA	1:A:241:LEU:HD12	1.88	0.55
1:A:400:LYS:HA	1:A:465:HIS:HD2	1.67	0.55
1:A:412:ASN:HB3	1:A:416:LEU:HD22	1.88	0.55
1:A:427:HIS:O	1:A:429:GLY:N	2.38	0.55
1:A:475:ASN:HB3	1:A:518:ASN:HB2	1.87	0.55
1:A:582:MET:HE2	1:A:703:ARG:CB	2.34	0.55
1:A:598:MET:C	8:H:96:VAL:HG21	2.31	0.55
2:B:97:ASP:OD2	2:B:99:ARG:NH1	2.39	0.55
2:B:378:GLU:OE2	2:B:382:GLN:HB2	2.06	0.55
2:B:493:GLN:HG3	2:B:497:LEU:HD12	1.88	0.55
2:B:909:GLY:HA2	2:B:921:VAL:HG13	1.88	0.55
3:C:80:ALA:HB3	3:C:102:GLY:HA2	1.88	0.55
3:C:229:LEU:HB3	3:C:293:ARG:NH1	2.20	0.55
8:H:110:ASP:O	8:H:128:ASN:HA	2.06	0.55
15:O:190:LEU:HD11	15:O:199:TYR:HE2	1.71	0.55
19:S:430:LYS:O	19:S:434:MET:HG2	2.06	0.55
5:E:21:GLU:HB3	5:E:35:VAL:HG21	1.87	0.55
7:G:59:LEU:HD11	7:G:65:SER:N	2.19	0.55
7:G:98:LYS:HE2	7:G:106:ASP:HB2	1.88	0.55
14:N:306:VAL:HG23	14:N:415:LYS:HD3	1.88	0.55
18:R:164:MET:HE3	18:R:168:LEU:HD12	1.87	0.55
18:R:401:THR:N	18:R:479:THR:O	2.35	0.55
1:A:17:GLU:O	2:B:1138:ALA:O	2.25	0.55
1:A:147:GLN:NE2	1:A:150:LYS:HD2	2.21	0.55
1:A:314:GLU:O	1:A:318:TYR:HB3	2.07	0.55
1:A:621:PRO:HD2	1:A:689:GLU:OE2	2.07	0.55
1:A:1003:ASP:O	1:A:1007:SER:HB3	2.05	0.55
1:A:1145:LEU:CG	1:A:1146:VAL:H	2.02	0.55
2:B:228:LYS:HD3	2:B:244:HIS:NE2	2.20	0.55
3:C:101:ILE:O	3:C:104:VAL:HG12	2.07	0.55
7:G:87:GLY:HA3	7:G:148:PHE:HE2	1.71	0.55
8:H:114:VAL:HB	8:H:125:LEU:HG	1.87	0.55
11:K:106:GLN:HG3	11:K:106:GLN:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:498:SER:HB3	16:P:296:TYR:CD1	2.42	0.55
1:A:581:SER:HB2	11:K:90:GLY:HA3	1.88	0.55
1:A:1260:MET:HA	1:A:1263:LEU:HD12	1.89	0.55
2:B:205:ILE:HG22	2:B:355:ARG:HH11	1.71	0.55
2:B:264:SER:C	2:B:266:LEU:H	2.14	0.55
3:C:84:TYR:CE2	3:C:207:HIS:HE1	2.25	0.55
3:C:215:ASP:OD2	12:L:70:ARG:NH2	2.40	0.55
6:F:135:ARG:HH12	7:G:58:GLN:HE21	1.45	0.55
18:R:172:GLU:HG3	18:R:506:GLY:HA3	1.89	0.55
20:X:23:DT:O4	21:Y:56:DA:N6	2.40	0.55
1:A:81:PHE:CD2	1:A:265:PRO:CG	2.89	0.55
1:A:504:VAL:O	1:A:507:PRO:HD2	2.07	0.55
1:A:921:LEU:HG	1:A:1081:ALA:O	2.06	0.55
1:A:1456:ALA:O	1:A:1460:ASN:ND2	2.39	0.55
2:B:1088:ASP:OD2	2:B:1123:TYR:N	2.40	0.55
3:C:59:ILE:HD13	3:C:63:ILE:HD11	1.89	0.55
3:C:105:PRO:HB2	3:C:187:ALA:HB2	1.89	0.55
8:H:38:LEU:HD21	8:H:40:LEU:HB2	1.88	0.55
9:I:29:CYS:HA	13:M:183:PHE:HE2	1.71	0.55
15:O:89:ASP:O	15:O:93:THR:N	2.33	0.55
16:P:200:ASN:C	16:P:202:PRO:HD3	2.31	0.55
2:B:989:LYS:HA	2:B:992:VAL:HG12	1.89	0.55
4:D:17:LEU:HB2	4:D:66:LEU:HD23	1.87	0.55
10:J:36:LEU:HD22	10:J:47:ARG:HG3	1.89	0.55
14:N:364:ARG:HG3	14:N:365:VAL:N	2.21	0.55
15:O:538:ALA:O	15:O:541:ILE:HG22	2.06	0.55
18:R:12:PHE:HD1	18:R:25:CYS:HB3	1.72	0.55
1:A:1451:LEU:HB3	4:D:107:MET:HB3	1.87	0.55
2:B:993:ASP:OD1	2:B:994:GLN:N	2.40	0.55
8:H:5:LEU:HG	8:H:133:ASN:HB3	1.87	0.55
13:M:72:GLU:HB2	14:N:364:ARG:HE	1.72	0.55
15:O:133:SER:O	15:O:137:ILE:N	2.35	0.55
15:O:579:GLN:HG2	16:P:315:TRP:CZ3	2.42	0.55
18:R:459:LYS:HD2	18:R:595:VAL:HB	1.89	0.55
1:A:432:TYR:OH	18:R:20:ASN:ND2	2.40	0.55
2:B:848:PRO:HB2	2:B:851:SER:HB3	1.89	0.55
3:C:154:LYS:HA	3:C:157:TYR:O	2.07	0.55
4:D:155:GLU:O	4:D:158:SER:OG	2.24	0.55
9:I:14:ILE:HD13	9:I:24:LEU:HB3	1.88	0.55
12:L:29:TYR:O	12:L:38:LEU:N	2.38	0.55
15:O:356:THR:HB	15:O:357:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:133:TYR:C	16:P:151:TYR:HB3	2.32	0.55
18:R:455:GLU:HG2	18:R:588:THR:HG23	1.88	0.55
1:A:457:GLN:N	1:A:460:ASP:OD2	2.40	0.55
1:A:632:VAL:HG21	1:A:796:THR:HG23	1.88	0.55
1:A:827:PHE:HB3	2:B:655:ASN:OD1	2.07	0.55
1:A:988:ASP:OD1	1:A:993:GLU:N	2.33	0.55
2:B:574:GLN:HE22	14:N:422:ILE:HG12	1.71	0.55
3:C:136:LEU:HD12	3:C:167:LEU:HA	1.88	0.55
1:A:1072:GLU:O	1:A:1076:PHE:CB	2.55	0.54
1:A:1347:GLY:O	1:A:1348:MET:HG2	2.07	0.54
2:B:611:PRO:HG3	2:B:648:TYR:CE1	2.42	0.54
2:B:687:LEU:O	2:B:915:ARG:NH2	2.40	0.54
7:G:92:CYS:SG	7:G:98:LYS:N	2.63	0.54
8:H:11:GLN:O	8:H:29:ALA:N	2.39	0.54
13:M:159:TYR:HD1	13:M:172:PRO:HA	1.72	0.54
13:M:160:ALA:HA	14:N:306:VAL:HA	1.89	0.54
15:O:46:LEU:HA	15:O:49:TYR:CD2	2.42	0.54
18:R:402:LEU:HD12	18:R:445:GLY:HA2	1.88	0.54
18:R:510:SER:N	18:R:520:ILE:O	2.31	0.54
1:A:11:LYS:HG3	2:B:1117:ILE:HG21	1.87	0.54
1:A:418:GLU:O	1:A:421:VAL:HG12	2.07	0.54
1:A:541:LEU:HG	1:A:551:ILE:HD11	1.88	0.54
1:A:911:ILE:HG22	5:E:174:GLN:O	2.07	0.54
2:B:207:VAL:H	2:B:355:ARG:HH22	1.54	0.54
2:B:887:SER:HB3	12:L:55:ILE:HG22	1.88	0.54
3:C:58:ASN:N	3:C:296:ASN:O	2.39	0.54
11:K:138:LYS:O	11:K:142:MET:N	2.40	0.54
14:N:307:PHE:CG	14:N:416:ILE:HG22	2.41	0.54
15:O:171:VAL:O	15:O:175:LEU:CB	2.53	0.54
15:O:203:ILE:HG22	15:O:207:HIS:CD2	2.41	0.54
15:O:570:GLU:O	15:O:574:TYR:N	2.40	0.54
16:P:183:TRP:HD1	16:P:247:LEU:HD23	1.72	0.54
16:P:203:LYS:HD3	16:P:203:LYS:N	2.20	0.54
19:S:291:UNK:O	19:S:293:UNK:N	2.41	0.54
1:A:114:LEU:HD11	1:A:148:CYS:HB2	1.89	0.54
1:A:356:ARG:HE	1:A:363:ARG:HH22	1.55	0.54
1:A:1189:ASP:OD2	1:A:1192:THR:N	2.41	0.54
6:F:76:LYS:HD2	6:F:79:ARG:HE	1.72	0.54
10:J:53:HIS:ND1	10:J:53:HIS:O	2.41	0.54
13:M:90:TYR:HE2	13:M:93:ARG:H	1.56	0.54
13:M:187:ASP:O	13:M:191:VAL:N	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:170:THR:OG1	15:O:173:ASP:N	2.28	0.54
15:O:650:VAL:HG13	15:O:651:PHE:H	1.72	0.54
1:A:409:THR:H	1:A:412:ASN:HD22	1.54	0.54
1:A:1034:PRO:C	1:A:1035:PRO:O	2.49	0.54
1:A:1053:LYS:O	1:A:1056:VAL:N	2.40	0.54
1:A:1150:ASP:OD1	1:A:1291:ARG:HD2	2.06	0.54
1:A:1203:GLU:HA	1:A:1206:ALA:HB3	1.89	0.54
2:B:141:ILE:HG23	2:B:142:ILE:N	2.22	0.54
5:E:188:LEU:HD23	5:E:190:LEU:HD11	1.90	0.54
11:K:65:ILE:N	11:K:101:LEU:O	2.36	0.54
13:M:90:TYR:HB3	13:M:179:LEU:HB3	1.89	0.54
15:O:133:SER:HB2	17:Q:58:TYR:CE1	2.41	0.54
15:O:576:PHE:CD1	15:O:576:PHE:C	2.86	0.54
1:A:925:GLU:CD	1:A:1081:ALA:HA	2.31	0.54
2:B:552:ASN:OD1	2:B:553:TYR:N	2.40	0.54
3:C:33:VAL:HG12	3:C:34:GLU:H	1.73	0.54
3:C:48:ASP:HB2	3:C:51:GLU:H	1.71	0.54
15:O:517:VAL:O	15:O:565:LEU:HG	2.08	0.54
16:P:54:GLU:HA	16:P:57:ASP:HB3	1.89	0.54
18:R:424:ARG:HH12	21:Y:64:DA:H4'	1.72	0.54
19:S:446:TYR:O	19:S:449:ARG:HB3	2.06	0.54
1:A:200:GLU:HG2	15:O:515:LYS:HD3	1.90	0.54
1:A:533:ASN:HD22	6:F:94:LEU:HD22	1.73	0.54
1:A:683:ARG:HH22	1:A:925:GLU:HA	1.72	0.54
1:A:714:ILE:HG23	1:A:715:ASN:N	2.21	0.54
1:A:1222:VAL:HA	1:A:1231:ALA:O	2.07	0.54
2:B:244:HIS:HB3	2:B:247:ILE:HG22	1.89	0.54
2:B:1079:LEU:O	2:B:1083:LEU:N	2.31	0.54
7:G:104:ILE:HG12	7:G:105:PHE:CD1	2.43	0.54
13:M:92:ASN:HD21	13:M:181:PRO:HD3	1.73	0.54
13:M:93:ARG:HH21	13:M:105:PRO:HB3	1.73	0.54
15:O:471:THR:OG1	15:O:477:TYR:HB3	2.07	0.54
16:P:241:ARG:O	16:P:245:GLU:HG2	2.07	0.54
18:R:204:LYS:HA	18:R:207:GLN:HB2	1.90	0.54
1:A:92:HIS:CD2	1:A:94:GLY:H	2.26	0.54
2:B:757:VAL:HG11	2:B:1022:ILE:HD12	1.90	0.54
2:B:990:ILE:HG22	2:B:991:LEU:HD12	1.90	0.54
10:J:16:ASP:OD1	10:J:17:LYS:HG3	2.07	0.54
13:M:121:ILE:N	13:M:148:LEU:O	2.36	0.54
14:N:389:THR:HG23	14:N:390:PHE:H	1.73	0.54
15:O:472:LYS:O	15:O:475:VAL:N	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:537:LEU:HD11	15:O:566:PHE:CE2	2.42	0.54
18:R:505:HIS:O	18:R:508:PHE:N	2.40	0.54
1:A:124:LEU:HD22	1:A:128:ARG:HH12	1.71	0.54
2:B:192:LYS:HZ3	2:B:438:SER:C	2.14	0.54
2:B:558:ASN:H	2:B:602:ALA:CA	2.20	0.54
15:O:125:GLU:CB	15:O:128:HIS:HB2	2.34	0.54
15:O:573:SER:OG	15:O:576:PHE:HE2	1.89	0.54
1:A:407:LYS:HG2	1:A:461:VAL:HG22	1.89	0.54
1:A:475:ASN:HB2	1:A:485:ILE:CD1	2.38	0.54
1:A:542:LEU:HD13	1:A:682:LEU:HD23	1.90	0.54
1:A:800:LYS:HB3	2:B:951:SER:OG	2.07	0.54
1:A:1145:LEU:C	1:A:1310:ILE:HG22	2.32	0.54
2:B:337:VAL:HG23	2:B:338:GLU:H	1.73	0.54
2:B:533:CYS:SG	2:B:538:VAL:HG11	2.48	0.54
2:B:612:LEU:HD13	2:B:672:HIS:HB3	1.90	0.54
2:B:782:PHE:HD1	10:J:8:PHE:CD2	2.26	0.54
7:G:88:TRP:O	7:G:99:VAL:HA	2.08	0.54
1:A:432:TYR:CE1	1:A:443:ASN:CG	2.86	0.54
1:A:1161:VAL:HG22	1:A:1275:LEU:HD13	1.89	0.54
1:A:1180:ASN:HB3	9:I:21:VAL:H	1.72	0.54
3:C:256:ILE:HG22	3:C:267:VAL:HG22	1.90	0.54
3:C:278:GLU:O	3:C:281:ARG:HG2	2.08	0.54
4:D:127:LEU:O	4:D:127:LEU:HD12	2.07	0.54
7:G:104:ILE:HG12	7:G:105:PHE:HD1	1.73	0.54
7:G:150:ILE:HG21	7:G:196:LEU:HD23	1.90	0.54
9:I:5:CYS:HB3	9:I:10:ASN:H	1.73	0.54
15:O:196:GLU:HG3	15:O:197:MET:H	1.73	0.54
15:O:516:LEU:HD12	15:O:565:LEU:CD2	2.36	0.54
16:P:266:GLU:OE2	16:P:269:LEU:HD13	2.07	0.54
19:S:420:TRP:CE3	19:S:424:GLU:HG2	2.43	0.54
1:A:1163:LYS:HB2	1:A:1279:SER:O	2.07	0.53
2:B:883:GLN:HE21	12:L:57:LEU:HD21	1.72	0.53
2:B:903:ASN:ND2	3:C:95:GLU:OE2	2.42	0.53
2:B:1026:LYS:NZ	2:B:1030:MET:SD	2.79	0.53
4:D:126:GLN:HG3	4:D:127:LEU:N	2.24	0.53
1:A:114:LEU:HD22	1:A:161:ASN:HD21	1.72	0.53
1:A:153:ARG:HD3	15:O:339:LEU:CG	2.24	0.53
1:A:513:ASP:OD1	2:B:911:LYS:NZ	2.41	0.53
1:A:636:PRO:HA	1:A:647:GLN:HE22	1.73	0.53
2:B:296:TYR:CD2	13:M:186:ILE:HD11	2.43	0.53
2:B:722:ASP:OD1	2:B:723:THR:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:73:ALA:HA	6:F:143:PHE:CD2	2.43	0.53
14:N:371:LEU:HD13	14:N:384:LYS:HD3	1.90	0.53
15:O:197:MET:HB3	15:O:321:GLN:OE1	2.07	0.53
18:R:211:LYS:HE2	18:R:282:ASP:HB3	1.89	0.53
1:A:262:PRO:HG2	2:B:1134:SER:O	2.08	0.53
1:A:543:THR:N	1:A:548:GLU:O	2.38	0.53
2:B:131:VAL:HG23	2:B:147:VAL:HB	1.90	0.53
2:B:1095:CYS:SG	2:B:1115:ASN:HB3	2.49	0.53
3:C:60:ASP:HB3	11:K:78:TYR:CZ	2.44	0.53
10:J:6:ARG:HB3	10:J:11:GLY:HA2	1.91	0.53
13:M:93:ARG:NH2	13:M:105:PRO:HB3	2.23	0.53
13:M:246:THR:OG1	14:N:404:SER:HA	2.07	0.53
15:O:255:LYS:HB3	15:O:256:PRO:HD3	1.90	0.53
15:O:492:TYR:CZ	15:O:495:VAL:HB	2.43	0.53
16:P:175:ILE:HG22	16:P:179:LEU:HD13	1.90	0.53
16:P:268:ILE:HD12	16:P:297:PHE:HZ	1.72	0.53
1:A:85:LYS:NZ	1:A:260:TYR:OH	2.39	0.53
1:A:147:GLN:HE22	1:A:150:LYS:HD2	1.72	0.53
1:A:232:LYS:NZ	16:P:315:TRP:CZ2	2.75	0.53
1:A:627:ASP:HA	1:A:652:VAL:O	2.09	0.53
1:A:1391:LYS:O	1:A:1395:HIS:ND1	2.38	0.53
1:A:1448:PHE:CD1	4:D:14:TYR:CD2	2.95	0.53
3:C:97:LEU:O	3:C:101:ILE:HD12	2.08	0.53
9:I:33:PHE:CD1	9:I:34:PRO:HD2	2.43	0.53
13:M:84:SER:C	13:M:85:LEU:CD1	2.75	0.53
15:O:164:ILE:HG12	15:O:282:ILE:HG12	1.91	0.53
1:A:218:CYS:SG	15:O:551:VAL:HA	2.48	0.53
1:A:703:ARG:NH2	11:K:93:ILE:HB	2.23	0.53
1:A:1284:ASN:N	1:A:1292:GLU:O	2.27	0.53
2:B:623:LYS:O	2:B:625:ILE:N	2.37	0.53
3:C:77:SER:O	3:C:211:GLY:N	2.33	0.53
7:G:141:ASP:OD1	7:G:142:VAL:N	2.42	0.53
14:N:309:LEU:HD23	14:N:418:VAL:HG21	1.89	0.53
16:P:92:LEU:O	16:P:96:TYR:HB2	2.09	0.53
18:R:239:ARG:HD2	18:R:243:GLU:OE1	2.09	0.53
1:A:38:ASP:CG	1:A:39:LEU:H	2.17	0.53
1:A:126:GLU:OE2	1:A:136:ARG:NH2	2.42	0.53
1:A:441:ARG:HH12	2:B:1040:ARG:NH1	2.06	0.53
1:A:968:GLY:O	1:A:972:GLU:HG2	2.07	0.53
1:A:1387:ALA:O	1:A:1392:THR:HG22	2.08	0.53
2:B:523:ASP:O	2:B:523:ASP:OD1	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:914:SER:O	2:B:915:ARG:HG2	2.08	0.53
3:C:88:ASN:O	12:L:60:ARG:HD3	2.09	0.53
13:M:163:VAL:HG22	13:M:168:VAL:HG22	1.90	0.53
15:O:326:ILE:O	15:O:329:PRO:HD2	2.08	0.53
15:O:590:PHE:O	15:O:594:LYS:N	2.33	0.53
19:S:382:ASP:HB3	19:S:385:LYS:HG2	1.90	0.53
1:A:396:ASP:OD1	1:A:397:ARG:N	2.41	0.53
2:B:328:ALA:O	2:B:332:ILE:HG23	2.09	0.53
2:B:502:THR:HG23	2:B:510:LEU:HD11	1.90	0.53
2:B:1092:VAL:HG12	2:B:1094:VAL:HG13	1.91	0.53
3:C:84:TYR:HE2	3:C:207:HIS:HE1	1.55	0.53
3:C:88:ASN:CG	3:C:202:ILE:HG12	2.34	0.53
13:M:226:ARG:HG3	13:M:227:LEU:H	1.74	0.53
16:P:55:LEU:O	16:P:60:LEU:N	2.35	0.53
16:P:106:TRP:CG	16:P:107:SER:N	2.76	0.53
16:P:218:THR:HG21	16:P:259:ASP:HB3	1.90	0.53
18:R:132:VAL:HG12	18:R:161:PHE:HE1	1.74	0.53
18:R:214:MET:HE1	18:R:286:ARG:C	2.33	0.53
1:A:81:PHE:CE2	1:A:265:PRO:CG	2.91	0.53
1:A:427:HIS:HB3	1:A:428:PRO:HD3	1.90	0.53
1:A:559:THR:HG21	2:B:947:HIS:HE1	1.74	0.53
1:A:885:MET:HE3	1:A:1130:ILE:HD12	1.91	0.53
1:A:964:ASN:HA	1:A:967:LEU:HB2	1.90	0.53
1:A:1329:GLU:HG2	5:E:198:ILE:HG21	1.89	0.53
2:B:265:ASP:HA	2:B:268:ILE:HD12	1.90	0.53
2:B:590:ILE:HG13	2:B:601:ILE:HG12	1.91	0.53
2:B:1106:TRP:NE1	7:G:163:PRO:HD3	2.24	0.53
7:G:111:PRO:O	7:G:199:SER:OG	2.27	0.53
8:H:43:ASN:OD1	8:H:45:GLU:N	2.42	0.53
15:O:155:LEU:O	15:O:159:ILE:HG12	2.09	0.53
15:O:211:ILE:HD13	15:O:214:LEU:HD21	1.91	0.53
18:R:486:ILE:N	18:R:543:ALA:O	2.42	0.53
1:A:41:ASP:OD1	1:A:49:LYS:N	2.42	0.53
1:A:818:ILE:HD11	1:A:824:PRO:HD2	1.89	0.53
2:B:1003:MET:SD	3:C:293:ARG:NH2	2.82	0.53
3:C:222:VAL:HA	3:C:304:SER:HA	1.91	0.53
5:E:135:PHE:HB3	5:E:140:LEU:HD13	1.91	0.53
16:P:51:ILE:O	16:P:55:LEU:HG	2.09	0.53
18:R:234:MET:HE1	18:R:274:LYS:HA	1.90	0.53
1:A:1391:LYS:NZ	21:Y:17:DG:OP1	2.42	0.53
3:C:240:LYS:HD2	3:C:262:SER:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:255:VAL:HG13	3:C:256:ILE:N	2.24	0.53
13:M:113:LYS:HZ1	13:M:237:ALA:HB1	1.74	0.53
15:O:470:GLU:N	15:O:479:PRO:HD3	2.24	0.53
18:R:483:ILE:HD13	18:R:486:ILE:HD11	1.91	0.53
1:A:302:GLY:C	1:A:304:ASP:H	2.17	0.52
1:A:622:VAL:O	1:A:657:SER:OG	2.23	0.52
2:B:52:LEU:HD13	2:B:743:LEU:HD23	1.90	0.52
2:B:426:SER:C	2:B:428:ASN:H	2.16	0.52
4:D:20:LEU:O	4:D:24:GLU:HB2	2.09	0.52
15:O:249:PHE:CE2	15:O:330:LEU:HD13	2.43	0.52
15:O:509:ARG:O	15:O:512:ARG:HB3	2.08	0.52
16:P:218:THR:OG1	16:P:219:GLN:OE1	2.20	0.52
18:R:195:LYS:HA	18:R:198:VAL:HB	1.90	0.52
20:X:26:DT:H2'	20:X:27:DC:C6	2.44	0.52
1:A:383:PRO:HG3	1:A:512:PHE:CZ	2.43	0.52
1:A:513:ASP:OD1	2:B:919:LYS:HG2	2.09	0.52
2:B:915:ARG:HD2	2:B:1023:TYR:HD2	1.73	0.52
3:C:238:PRO:O	3:C:239:ILE:HG13	2.09	0.52
7:G:190:LYS:C	7:G:192:PRO:HD3	2.34	0.52
13:M:231:LEU:HA	13:M:235:LYS:H	1.73	0.52
15:O:104:VAL:HA	15:O:122:TYR:HA	1.91	0.52
15:O:248:ASP:O	15:O:252:ILE:HG12	2.10	0.52
15:O:626:GLN:HA	15:O:629:MET:HB2	1.92	0.52
18:R:273:GLN:HB2	19:S:277:UNK:H	1.74	0.52
1:A:108:LYS:HE2	1:A:180:HIS:CD2	2.45	0.52
2:B:178:PRO:HD3	10:J:63:TYR:OH	2.09	0.52
2:B:306:GLY:O	2:B:309:VAL:HG12	2.09	0.52
2:B:531:LYS:O	2:B:535:VAL:HG23	2.09	0.52
3:C:84:TYR:CB	3:C:205:LYS:O	2.47	0.52
3:C:229:LEU:HD23	3:C:293:ARG:HH12	1.75	0.52
4:D:72:PHE:O	7:G:145:LYS:NZ	2.42	0.52
6:F:115:THR:O	6:F:116:ASP:OD1	2.27	0.52
8:H:16:ASP:O	8:H:18:GLY:N	2.37	0.52
10:J:41:LEU:HD23	10:J:47:ARG:HA	1.91	0.52
13:M:255:PHE:O	13:M:259:ILE:HG12	2.09	0.52
14:N:316:PHE:HA	14:N:377:ASN:ND2	2.25	0.52
15:O:105:LYS:HE3	15:O:123:ASN:HA	1.91	0.52
15:O:549:GLN:HB2	15:O:565:LEU:CB	2.39	0.52
18:R:256:GLN:HA	18:R:259:LEU:HB3	1.91	0.52
1:A:238:ASP:OD1	1:A:239:CYS:N	2.41	0.52
2:B:458:LEU:HG	2:B:469:MET:SD	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:558:ASN:N	2:B:602:ALA:HB1	2.19	0.52
3:C:197:ARG:HE	10:J:61:LEU:HB3	1.74	0.52
7:G:59:LEU:HG	7:G:60:LYS:H	1.72	0.52
7:G:88:TRP:HB3	7:G:144:GLU:O	2.10	0.52
8:H:56:THR:HB	8:H:145:ARG:HG2	1.92	0.52
14:N:371:LEU:HD22	14:N:384:LYS:HD3	1.92	0.52
15:O:529:LYS:HG3	15:O:532:ASP:H	1.75	0.52
16:P:221:ILE:O	16:P:224:PHE:HB3	2.10	0.52
17:Q:56:VAL:HA	17:Q:59:ILE:HD12	1.92	0.52
18:R:478:PHE:O	18:R:599:PRO:HB3	2.07	0.52
19:S:312:UNK:O	19:S:316:UNK:N	2.43	0.52
1:A:912:VAL:HG12	1:A:1364:TYR:CD1	2.45	0.52
2:B:607:ARG:NH2	2:B:650:ASP:OD2	2.39	0.52
2:B:858:ASN:OD1	2:B:859:ASN:N	2.43	0.52
2:B:864:THR:O	2:B:865:GLN:C	2.51	0.52
2:B:1106:TRP:C	2:B:1116:ILE:HD11	2.34	0.52
3:C:85:PHE:HE2	3:C:94:ASP:HB2	1.72	0.52
3:C:260:GLU:HB3	3:C:263:ASP:HB2	1.91	0.52
7:G:115:LEU:H	7:G:199:SER:HB3	1.74	0.52
8:H:103:LYS:HB3	8:H:115:TYR:HD2	1.74	0.52
15:O:152:HIS:HA	15:O:155:LEU:HD12	1.90	0.52
16:P:78:SER:O	16:P:82:LYS:HB2	2.09	0.52
16:P:90:GLU:OE2	16:P:127:SER:OG	2.22	0.52
18:R:395:ASN:OD1	18:R:452:ALA:N	2.43	0.52
1:A:314:GLU:O	1:A:318:TYR:HB2	2.08	0.52
1:A:338:PRO:HG2	1:A:342:ASN:HB2	1.91	0.52
1:A:999:ASP:HA	1:A:1002:ARG:HB2	1.92	0.52
2:B:343:ARG:HE	2:B:541:ILE:HG12	1.74	0.52
15:O:199:TYR:O	15:O:283:ASN:N	2.41	0.52
16:P:62:LYS:HG2	16:P:75:VAL:HB	1.92	0.52
16:P:153:LEU:HB3	16:P:155:PRO:HD3	1.90	0.52
16:P:252:LYS:HD3	16:P:266:GLU:HG2	1.91	0.52
1:A:310:ASN:HA	15:O:564:PHE:CE2	2.44	0.52
1:A:856:LEU:HD13	2:B:692:HIS:O	2.10	0.52
1:A:916:TYR:CE1	1:A:1089:ILE:HG21	2.44	0.52
1:A:1456:ALA:HB2	4:D:116:PHE:HA	1.92	0.52
2:B:177:CYS:SG	2:B:179:LEU:N	2.83	0.52
2:B:347:LEU:HD22	2:B:561:LEU:HD22	1.91	0.52
2:B:824:LEU:HA	2:B:831:GLU:OE1	2.10	0.52
9:I:32:GLU:HG3	13:M:132:ASN:HB2	1.91	0.52
10:J:31:ASP:HB2	10:J:34:THR:OG1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:133:LYS:O	13:M:137:GLU:N	2.42	0.52
15:O:640:ARG:NH1	17:Q:44:ASN:OD1	2.43	0.52
18:R:395:ASN:H	18:R:487:VAL:HB	1.74	0.52
3:C:52:ALA:HB2	3:C:310:PRO:HG2	1.90	0.52
11:K:93:ILE:HG22	11:K:95:HIS:N	2.23	0.52
15:O:76:VAL:HA	15:O:79:LEU:HD13	1.91	0.52
15:O:590:PHE:O	15:O:593:GLU:N	2.42	0.52
16:P:134:VAL:O	16:P:151:TYR:HB2	2.10	0.52
1:A:46:ARG:HE	1:A:278:PRO:HA	1.74	0.52
1:A:1014:GLY:HA2	1:A:1017:THR:HG22	1.90	0.52
2:B:405:LYS:HA	2:B:408:LYS:HE2	1.91	0.52
15:O:125:GLU:HB2	15:O:128:HIS:CB	2.37	0.52
15:O:517:VAL:HG13	15:O:518:SER:H	1.74	0.52
1:A:1003:ASP:O	1:A:1007:SER:HB2	2.10	0.52
1:A:1164:THR:OG1	1:A:1272:VAL:HG12	2.10	0.52
4:D:114:LYS:HB2	4:D:145:PHE:CZ	2.45	0.52
13:M:76:LEU:HB3	13:M:168:VAL:HB	1.92	0.52
15:O:90:SER:HA	15:O:93:THR:HB	1.92	0.52
15:O:472:LYS:O	15:O:474:GLY:N	2.43	0.52
16:P:53:GLN:NE2	19:S:363:GLN:HA	2.25	0.52
1:A:573:ARG:HH21	11:K:87:GLU:CB	2.15	0.51
1:A:998:TYR:O	1:A:1002:ARG:N	2.32	0.51
1:A:1136:ILE:HG12	1:A:1137:SER:O	2.10	0.51
3:C:40:PHE:HD2	11:K:134:LYS:HG3	1.75	0.51
3:C:100:ARG:HE	10:J:5:VAL:HG13	1.75	0.51
12:L:28:LYS:NZ	12:L:40:LEU:O	2.31	0.51
15:O:568:CYS:SG	15:O:569:LYS:N	2.82	0.51
16:P:31:PHE:HB3	16:P:72:PHE:O	2.09	0.51
18:R:511:TYR:HB2	18:R:519:LEU:HG	1.92	0.51
18:R:619:ALA:O	18:R:623:LYS:HB3	2.10	0.51
1:A:693:ALA:HA	1:A:696:ARG:HH11	1.75	0.51
1:A:1409:GLU:N	1:A:1413:GLU:HG2	2.24	0.51
2:B:112:LEU:HD11	2:B:127:ALA:HA	1.93	0.51
2:B:524:ASP:CB	2:B:588:ILE:HD11	2.38	0.51
2:B:667:VAL:HG23	2:B:670:MET:HE3	1.93	0.51
18:R:213:TRP:HB3	18:R:285:ALA:HB1	1.92	0.51
1:A:528:ARG:HH12	6:F:118:LEU:HB2	1.75	0.51
1:A:1259:ARG:O	1:A:1263:LEU:HG	2.09	0.51
2:B:45:TRP:CE2	2:B:739:LYS:HD3	2.44	0.51
2:B:615:VAL:HG22	2:B:671:THR:C	2.35	0.51
2:B:776:SER:HB2	2:B:928:GLN:NE2	2.16	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:153:GLU:OE2	7:G:194:TYR:HA	2.10	0.51
12:L:53:HIS:NE2	12:L:55:ILE:HG12	2.25	0.51
18:R:214:MET:HE1	18:R:287:PRO:N	2.25	0.51
20:X:11:DA:C8	20:X:12:DT:H73	2.45	0.51
1:A:815:GLN:HG2	1:A:847:PHE:HD1	1.75	0.51
1:A:1161:VAL:HG13	1:A:1275:LEU:HB2	1.92	0.51
2:B:137:ARG:HG2	2:B:141:ILE:HG12	1.93	0.51
2:B:204:ARG:NH1	2:B:376:ARG:HH22	2.07	0.51
2:B:932:PRO:HB2	2:B:1004:LEU:HB3	1.93	0.51
11:K:63:PHE:O	11:K:103:ILE:HG22	2.10	0.51
13:M:178:GLN:OE1	14:N:392:GLN:NE2	2.43	0.51
16:P:306:ASP:HB2	16:P:308:GLU:OE1	2.10	0.51
1:A:32:VAL:HG11	1:A:57:LYS:HD2	1.92	0.51
1:A:482:ARG:O	1:A:482:ARG:HG2	2.09	0.51
1:A:595:PRO:HD3	8:H:79:TRP:CD2	2.45	0.51
1:A:931:GLN:O	1:A:933:VAL:N	2.38	0.51
1:A:974:LEU:HD11	1:A:998:TYR:CG	2.45	0.51
1:A:1448:PHE:CE2	4:D:11:LEU:HG	2.46	0.51
2:B:156:LEU:HD22	2:B:184:TYR:CZ	2.46	0.51
2:B:557:LEU:O	2:B:560:THR:HB	2.11	0.51
2:B:587:PHE:HE2	2:B:602:ALA:O	1.93	0.51
2:B:864:THR:HA	2:B:866:TYR:CE2	2.46	0.51
3:C:81:GLU:OE2	12:L:70:ARG:NH1	2.43	0.51
6:F:111:LEU:HD23	6:F:112:GLU:O	2.10	0.51
7:G:203:ASP:HB3	7:G:211:TRP:NE1	2.24	0.51
13:M:88:PHE:HB2	14:N:395:ILE:CG2	2.40	0.51
15:O:547:GLU:OE1	15:O:569:LYS:HG3	2.10	0.51
18:R:219:ARG:HH11	18:R:220:PRO:HD2	1.75	0.51
19:S:420:TRP:CD1	19:S:457:LYS:HD2	2.46	0.51
19:S:421:THR:HG23	19:S:424:GLU:H	1.76	0.51
1:A:186:VAL:HG22	1:A:189:LYS:HD3	1.93	0.51
1:A:389:ILE:HG13	1:A:501:ASN:ND2	2.25	0.51
1:A:789:ASN:OD1	1:A:789:ASN:N	2.43	0.51
1:A:999:ASP:O	1:A:1003:ASP:HB2	2.10	0.51
2:B:129:ILE:HG22	2:B:131:VAL:HG13	1.93	0.51
2:B:429:ILE:HG23	2:B:430:THR:H	1.76	0.51
2:B:738:THR:H	2:B:741:ILE:HD13	1.76	0.51
3:C:321:LEU:HD21	11:K:124:LEU:HD21	1.92	0.51
5:E:88:VAL:HG21	5:E:112:TYR:CE1	2.45	0.51
6:F:103:MET:SD	7:G:65:SER:OG	2.68	0.51
8:H:9:ILE:HA	8:H:55:LEU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:407:ASN:HD21	21:Y:73:DT:H3'	1.75	0.51
1:A:200:GLU:HA	15:O:515:LYS:HD2	1.92	0.51
1:A:307:ILE:HB	1:A:311:ASN:OD1	2.10	0.51
1:A:401:VAL:HG12	18:R:18:ASN:HB2	1.92	0.51
1:A:1209:ILE:O	1:A:1212:ALA:N	2.41	0.51
2:B:128:PRO:HA	2:B:151:ARG:HG2	1.92	0.51
2:B:253:ILE:HG22	2:B:286:ASN:ND2	2.25	0.51
2:B:321:GLN:H	2:B:324:ILE:HB	1.76	0.51
2:B:613:ILE:N	2:B:673:LEU:O	2.33	0.51
2:B:760:MET:HE2	2:B:943:ILE:HD11	1.91	0.51
13:M:86:HIS:CD2	13:M:175:ARG:HB2	2.45	0.51
15:O:123:ASN:CG	15:O:124:GLU:HG2	2.35	0.51
15:O:634:GLU:HA	15:O:637:VAL:CG1	2.40	0.51
16:P:31:PHE:CD2	16:P:72:PHE:HB2	2.36	0.51
16:P:295:ASN:HD21	16:P:298:LYS:HB3	1.75	0.51
18:R:523:MET:O	18:R:527:LYS:HA	2.11	0.51
1:A:25:ASP:HA	1:A:28:ALA:HB3	1.93	0.51
1:A:67:CYS:O	1:A:69:THR:N	2.44	0.51
1:A:222:LEU:HA	1:A:226:LYS:NZ	2.25	0.51
1:A:715:ASN:HA	1:A:718:THR:HB	1.92	0.51
1:A:911:ILE:HG23	5:E:176:PRO:HD3	1.92	0.51
2:B:172:ALA:HA	10:J:63:TYR:HE1	1.76	0.51
2:B:544:ILE:HD11	2:B:563:GLY:HA2	1.93	0.51
3:C:88:ASN:ND2	3:C:202:ILE:HG12	2.26	0.51
5:E:6:GLU:O	5:E:10:SER:HB3	2.11	0.51
5:E:31:THR:HG23	5:E:34:GLU:H	1.75	0.51
6:F:135:ARG:NH1	7:G:58:GLN:NE2	2.45	0.51
7:G:207:LEU:HD23	7:G:209:SER:H	1.74	0.51
10:J:7:CYS:SG	10:J:10:CYS:HB2	2.51	0.51
16:P:265:LEU:HD12	16:P:268:ILE:HG12	1.92	0.51
18:R:540:LEU:HD11	18:R:552:ALA:HB3	1.93	0.51
1:A:124:LEU:HB3	1:A:128:ARG:HH12	1.76	0.51
1:A:464:ARG:HB3	1:A:467:GLU:OE2	2.11	0.51
1:A:557:PHE:HA	1:A:701:CYS:SG	2.51	0.51
1:A:949:ASN:HA	1:A:1061:ARG:NH2	2.26	0.51
1:A:1207:VAL:O	1:A:1211:ARG:HG2	2.11	0.51
2:B:527:GLU:HG3	2:B:531:LYS:HE3	1.92	0.51
2:B:590:ILE:CG1	2:B:601:ILE:CG1	2.89	0.51
2:B:986:ASP:OD1	2:B:987:MET:N	2.43	0.51
5:E:99:HIS:O	5:E:103:LYS:CB	2.54	0.51
15:O:211:ILE:HA	15:O:214:LEU:HG	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:361:PHE:HB3	15:O:480:TYR:CE2	2.46	0.51
16:P:111:LYS:HA	16:P:114:THR:HG22	1.93	0.51
2:B:778:ILE:HD11	2:B:905:ARG:HG2	1.92	0.51
2:B:1036:HIS:NE2	2:B:1054:ARG:HA	2.26	0.51
9:I:21:VAL:C	9:I:23:THR:H	2.19	0.51
15:O:290:GLY:O	15:O:293:SER:HB2	2.11	0.51
20:X:22:DT:H2''	20:X:23:DT:O4'	2.10	0.51
21:Y:11:DC:H1'	21:Y:12:DA:C8	2.46	0.51
1:A:238:ASP:HB2	1:A:241:LEU:HB2	1.92	0.50
1:A:487:SER:OG	1:A:532:ILE:HA	2.10	0.50
1:A:570:PHE:HB3	1:A:603:LEU:HD13	1.93	0.50
1:A:1205:ILE:O	1:A:1209:ILE:HG12	2.11	0.50
2:B:55:LYS:HD2	2:B:59:LYS:HZ2	1.76	0.50
2:B:489:LEU:HG	2:B:493:GLN:OE1	2.10	0.50
2:B:1002:ASP:HB3	2:B:1019:PHE:CE1	2.44	0.50
5:E:11:ARG:O	5:E:14:ARG:N	2.44	0.50
15:O:471:THR:OG1	15:O:475:VAL:O	2.20	0.50
18:R:12:PHE:CD1	18:R:25:CYS:HB3	2.46	0.50
18:R:218:ARG:NH1	21:Y:71:DT:H5'	2.26	0.50
18:R:610:LEU:HA	18:R:613:HIS:CD2	2.46	0.50
18:R:650:ALA:CB	19:S:517:GLU:CD	2.83	0.50
21:Y:57:DA:C6	21:Y:58:DA:C6	3.00	0.50
1:A:124:LEU:HD22	1:A:128:ARG:HH22	1.76	0.50
1:A:815:GLN:HE21	1:A:847:PHE:HB2	1.76	0.50
1:A:1166:LEU:HA	1:A:1169:VAL:HB	1.92	0.50
2:B:914:SER:HA	2:B:1024:TYR:CD2	2.46	0.50
3:C:213:GLY:HA2	3:C:219:PHE:HB2	1.93	0.50
5:E:112:TYR:CG	5:E:116:ILE:HG12	2.45	0.50
6:F:89:GLU:OE1	6:F:90:ARG:N	2.44	0.50
6:F:92:ARG:HH12	7:G:61:PRO:HB3	1.75	0.50
8:H:96:VAL:HA	8:H:142:LEU:O	2.11	0.50
9:I:13:LEU:HD21	9:I:27:ARG:HB2	1.94	0.50
16:P:209:ALA:O	16:P:212:VAL:HG12	2.11	0.50
19:S:406:TYR:HB2	19:S:410:SER:HB2	1.94	0.50
1:A:91:PHE:CE2	1:A:96:PHE:HD1	2.30	0.50
1:A:121:ARG:HA	1:A:124:LEU:HD12	1.92	0.50
1:A:409:THR:H	1:A:412:ASN:ND2	2.10	0.50
1:A:753:GLN:O	1:A:755:GLY:N	2.39	0.50
1:A:822:ARG:NH2	1:A:845:LYS:HB2	2.26	0.50
1:A:1022:LEU:O	1:A:1026:ARG:N	2.43	0.50
3:C:31:TRP:CE2	11:K:123:ASP:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:394:GLN:HE21	21:Y:68:DA:H5'	1.75	0.50
18:R:644:LYS:O	18:R:648:ASP:N	2.40	0.50
1:A:21:LEU:HD11	2:B:1133:LEU:HD11	1.93	0.50
1:A:133:ASP:OD1	1:A:134:ASN:N	2.40	0.50
1:A:194:LYS:HA	1:A:197:TRP:HB3	1.93	0.50
1:A:472:VAL:HG22	1:A:521:VAL:HG12	1.93	0.50
1:A:1225:ILE:H	1:A:1229:ARG:HE	1.58	0.50
2:B:244:HIS:NE2	2:B:333:ALA:HB2	2.25	0.50
2:B:338:GLU:HA	2:B:345:LYS:NZ	2.26	0.50
2:B:1076:SER:OG	2:B:1077:GLN:N	2.44	0.50
4:D:70:LYS:HD2	4:D:160:TYR:CE2	2.46	0.50
13:M:229:GLY:O	13:M:232:LEU:HB3	2.11	0.50
15:O:648:TRP:CZ2	15:O:652:GLN:HB3	2.47	0.50
19:S:384:HIS:HA	19:S:387:ALA:HB3	1.93	0.50
21:Y:18:DG:N7	21:Y:19:DC:C4	2.79	0.50
1:A:43:GLU:O	1:A:44:LYS:HG2	2.11	0.50
1:A:398:VAL:O	1:A:402:LEU:N	2.45	0.50
1:A:628:ALA:O	1:A:651:PHE:HA	2.11	0.50
1:A:857:SER:N	1:A:860:GLU:OE2	2.43	0.50
2:B:205:ILE:HD13	2:B:352:MET:HB2	1.94	0.50
2:B:211:GLU:HG3	2:B:212:LYS:H	1.77	0.50
2:B:639:ASP:OD1	2:B:643:LEU:HD13	2.12	0.50
2:B:880:HIS:N	2:B:901:ARG:O	2.36	0.50
5:E:153:HIS:CD2	5:E:198:ILE:HG12	2.47	0.50
8:H:11:GLN:HA	8:H:53:ASP:O	2.10	0.50
11:K:95:HIS:CE1	11:K:98:GLU:HB3	2.45	0.50
1:A:378:ARG:HH22	1:A:477:GLN:HE21	1.58	0.50
1:A:541:LEU:HD22	1:A:682:LEU:HD22	1.93	0.50
2:B:149:ILE:O	2:B:426:SER:HB2	2.12	0.50
2:B:354:ARG:CZ	2:B:549:LEU:HG	2.42	0.50
2:B:738:THR:O	2:B:741:ILE:N	2.45	0.50
3:C:152:ASP:C	3:C:154:LYS:H	2.19	0.50
3:C:197:ARG:HB3	3:C:198:PRO:HD2	1.93	0.50
4:D:115:LEU:HD23	4:D:138:VAL:HG11	1.92	0.50
5:E:67:GLU:HA	5:E:70:SER:OG	2.11	0.50
5:E:93:MET:HE1	5:E:123:LEU:O	2.11	0.50
5:E:100:ILE:O	5:E:104:ASN:ND2	2.44	0.50
5:E:112:TYR:N	5:E:135:PHE:O	2.23	0.50
13:M:89:GLN:HB3	14:N:394:VAL:HG13	1.93	0.50
14:N:315:ALA:HB1	14:N:376:GLY:HA3	1.94	0.50
16:P:195:PHE:HB2	16:P:201:GLY:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HD11	1:A:259:ARG:HD2	1.94	0.50
1:A:1317:ASN:O	1:A:1318:HIS:ND1	2.45	0.50
2:B:99:ARG:NE	2:B:102:LYS:O	2.31	0.50
2:B:694:ASN:HD21	2:B:916:HIS:CE1	2.30	0.50
3:C:89:THR:CG2	3:C:200:GLN:HA	2.40	0.50
6:F:135:ARG:NE	6:F:143:PHE:HE1	2.10	0.50
7:G:7:ILE:C	7:G:71:THR:HG1	2.17	0.50
10:J:66:LEU:HA	12:L:35:SER:OG	2.12	0.50
15:O:498:SER:HB3	16:P:296:TYR:HD1	1.75	0.50
15:O:527:LEU:HD21	16:P:246:VAL:HG11	1.93	0.50
1:A:533:ASN:ND2	6:F:94:LEU:HD22	2.27	0.50
1:A:933:VAL:HG22	1:A:1004:PHE:HE1	1.76	0.50
4:D:22:ASP:O	4:D:26:LYS:HG2	2.12	0.50
4:D:127:LEU:HD22	4:D:137:ILE:HD11	1.93	0.50
5:E:86:PRO:HB3	5:E:114:ASN:HB2	1.92	0.50
6:F:97:ARG:O	6:F:101:ILE:HG12	2.12	0.50
14:N:283:LEU:O	14:N:286:ASP:HB3	2.11	0.50
15:O:626:GLN:O	15:O:630:VAL:HG12	2.12	0.50
21:Y:23:DG:H2''	21:Y:24:DG:C8	2.46	0.50
1:A:474:PHE:CZ	1:A:517:MET:HG3	2.47	0.50
1:A:1121:LEU:HB3	1:A:1346:HIS:NE2	2.27	0.50
1:A:1136:ILE:CD1	1:A:1318:HIS:HB3	2.42	0.50
2:B:904:ARG:NH2	2:B:1033:ASP:OD1	2.33	0.50
2:B:1057:ASP:OD1	2:B:1058:GLY:N	2.44	0.50
5:E:46:TYR:CZ	5:E:58:MET:HA	2.46	0.50
9:I:20:GLY:C	9:I:22:TYR:H	2.20	0.50
13:M:253:GLU:HA	13:M:256:LYS:HB2	1.93	0.50
15:O:47:PHE:CE2	15:O:586:ALA:HB1	2.46	0.50
15:O:197:MET:O	15:O:283:ASN:ND2	2.45	0.50
15:O:518:SER:O	15:O:522:ILE:HG12	2.12	0.50
15:O:573:SER:CA	15:O:576:PHE:CE2	2.95	0.50
16:P:82:LYS:HG2	16:P:86:MET:HE2	1.93	0.50
18:R:520:ILE:HD11	20:X:11:DA:H4'	1.93	0.50
1:A:133:ASP:CG	1:A:134:ASN:H	2.18	0.49
1:A:133:ASP:O	1:A:137:ARG:N	2.40	0.49
1:A:423:GLY:HA2	1:A:444:LEU:CD2	2.42	0.49
1:A:1188:ILE:HB	1:A:1228:ASP:CB	2.42	0.49
1:A:1188:ILE:HB	1:A:1228:ASP:HB3	1.94	0.49
1:A:1302:ASP:N	1:A:1302:ASP:OD1	2.45	0.49
2:B:205:ILE:HG22	2:B:355:ARG:NH1	2.27	0.49
2:B:613:ILE:HG13	2:B:675:ILE:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:717:GLN:NE2	2:B:727:LEU:HD22	2.27	0.49
4:D:152:GLU:HA	4:D:155:GLU:HG2	1.94	0.49
5:E:90:VAL:O	5:E:94:LYS:HG2	2.11	0.49
5:E:177:ARG:CZ	5:E:215:MET:HE3	2.42	0.49
6:F:83:PRO:O	6:F:151:LEU:HG	2.12	0.49
8:H:11:GLN:HB3	8:H:29:ALA:HB3	1.94	0.49
11:K:60:SER:HA	11:K:106:GLN:HA	1.94	0.49
15:O:69:VAL:HG22	15:O:122:TYR:CD1	2.47	0.49
15:O:573:SER:C	15:O:576:PHE:CD2	2.90	0.49
1:A:483:LEU:CD1	1:A:550:ILE:HG21	2.40	0.49
1:A:994:TYR:O	5:E:197:LYS:NZ	2.35	0.49
2:B:65:PHE:HZ	2:B:154:ILE:HA	1.78	0.49
3:C:21:PRO:HG3	3:C:30:GLU:HB2	1.93	0.49
3:C:86:PHE:N	3:C:203:SER:O	2.41	0.49
3:C:110:PRO:C	3:C:112:MET:H	2.19	0.49
5:E:17:ARG:O	5:E:21:GLU:HG2	2.12	0.49
13:M:113:LYS:HG3	13:M:116:SER:O	2.12	0.49
13:M:154:GLU:CB	13:M:174:GLU:O	2.60	0.49
18:R:467:ARG:O	18:R:471:LYS:CB	2.60	0.49
1:A:81:PHE:HD2	1:A:265:PRO:HD3	1.75	0.49
1:A:252:ARG:HB2	1:A:253:PRO:HD2	1.94	0.49
1:A:423:GLY:HA2	1:A:444:LEU:HD23	1.94	0.49
1:A:434:LEU:O	1:A:461:VAL:N	2.40	0.49
2:B:909:GLY:O	2:B:1031:VAL:HB	2.13	0.49
2:B:961:LEU:HD21	2:B:1019:PHE:C	2.37	0.49
8:H:63:LEU:O	8:H:89:LEU:N	2.40	0.49
8:H:63:LEU:O	8:H:88:SER:HB2	2.12	0.49
9:I:29:CYS:HA	13:M:135:LYS:HE2	1.94	0.49
9:I:32:GLU:N	13:M:130:PHE:O	2.45	0.49
15:O:492:TYR:HB2	15:O:574:TYR:CE1	2.47	0.49
18:R:219:ARG:NH1	18:R:221:ALA:H	2.09	0.49
18:R:477:LYS:HB3	18:R:599:PRO:HB2	1.94	0.49
1:A:94:GLY:HA3	1:A:1397:PHE:CE1	2.47	0.49
1:A:316:TRP:O	1:A:319:LEU:HB3	2.12	0.49
1:A:610:PHE:CE1	1:A:613:LEU:HD23	2.46	0.49
2:B:116:HIS:CD2	2:B:175:ASN:O	2.66	0.49
2:B:143:MET:HE3	19:S:397:VAL:HG13	1.94	0.49
2:B:281:ASP:HA	2:B:284:ALA:HB3	1.95	0.49
2:B:536:LEU:HD23	2:B:536:LEU:O	2.11	0.49
3:C:78:VAL:HG22	3:C:208:CYS:SG	2.53	0.49
5:E:67:GLU:O	5:E:71:LYS:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:110:ALA:HA	13:M:120:GLU:O	2.12	0.49
18:R:502:ALA:O	18:R:506:GLY:N	2.41	0.49
19:S:364:LEU:HB3	19:S:374:ILE:HD12	1.93	0.49
1:A:580:LEU:HB3	11:K:88:PHE:CE1	2.46	0.49
2:B:575:PHE:HZ	2:B:588:ILE:HG22	1.77	0.49
2:B:776:SER:HB3	3:C:217:ALA:HB2	1.94	0.49
5:E:26:ARG:NH1	5:E:188:LEU:O	2.45	0.49
5:E:191:LYS:N	5:E:194:GLU:OE1	2.43	0.49
7:G:52:LEU:HD12	7:G:53:THR:HG22	1.93	0.49
11:K:132:GLU:O	11:K:136:THR:HG22	2.12	0.49
13:M:118:LEU:HB3	13:M:149:LYS:HD2	1.95	0.49
13:M:126:ASP:HB3	13:M:128:GLN:HG2	1.93	0.49
15:O:251:LYS:HA	15:O:254:ASN:HB2	1.93	0.49
15:O:578:ARG:O	15:O:581:LEU:HB3	2.12	0.49
16:P:217:THR:HB	16:P:220:GLU:HB3	1.95	0.49
18:R:213:TRP:HB2	18:R:285:ALA:HB1	1.95	0.49
18:R:425:PHE:HD1	21:Y:63:DT:H1'	1.77	0.49
19:S:423:GLU:O	19:S:426:ILE:HG12	2.13	0.49
20:X:6:DC:H2''	20:X:7:DA:OP2	2.13	0.49
1:A:18:PHE:O	1:A:1403:MET:HA	2.13	0.49
1:A:774:ARG:HH21	1:A:808:GLN:HE21	1.61	0.49
2:B:140:ASN:HB3	19:S:395:GLU:H	1.78	0.49
2:B:234:ILE:CD1	2:B:238:GLY:H	2.25	0.49
2:B:540:ASP:OD1	2:B:541:ILE:N	2.45	0.49
2:B:716:ASN:ND2	2:B:720:ARG:HD2	2.28	0.49
2:B:795:LEU:HA	2:B:804:ASP:OD2	2.12	0.49
2:B:1036:HIS:NE2	2:B:1058:GLY:HA2	2.27	0.49
8:H:112:ILE:O	8:H:126:GLU:HA	2.13	0.49
13:M:106:PHE:O	13:M:107:ILE:HG22	2.13	0.49
15:O:312:TYR:HE1	15:O:468:LEU:HD11	1.78	0.49
15:O:492:TYR:CE1	15:O:495:VAL:HB	2.47	0.49
15:O:581:LEU:HB2	15:O:648:TRP:CZ3	2.48	0.49
16:P:59:ASN:OD1	16:P:80:ALA:HB1	2.12	0.49
18:R:229:LEU:O	18:R:233:ARG:HB2	2.12	0.49
19:S:418:ASP:HB3	19:S:449:ARG:NH2	2.28	0.49
19:S:425:MET:O	19:S:428:PHE:HB3	2.12	0.49
1:A:360:LYS:HA	1:A:365:ARG:NH2	2.28	0.49
1:A:1163:LYS:HD3	1:A:1278:ILE:O	2.12	0.49
1:A:1278:ILE:HG12	1:A:1297:GLY:HA3	1.95	0.49
2:B:97:ASP:OD1	2:B:98:ILE:N	2.46	0.49
2:B:306:GLY:HA3	2:B:324:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:630:LEU:HD13	2:B:635:LEU:HD23	1.95	0.49
2:B:1106:TRP:NE1	7:G:161:LYS:O	2.45	0.49
3:C:256:ILE:HA	3:C:268:LYS:H	1.76	0.49
4:D:119:GLU:HG3	4:D:123:ILE:HG23	1.93	0.49
7:G:155:PHE:HA	7:G:193:ALA:O	2.13	0.49
8:H:61:SER:HA	8:H:141:TYR:CD2	2.48	0.49
14:N:299:ASN:CG	14:N:301:PRO:HD3	2.38	0.49
15:O:291:ARG:HH11	15:O:649:GLU:HG2	1.77	0.49
15:O:507:LEU:O	15:O:511:ILE:N	2.31	0.49
15:O:637:VAL:HG13	15:O:638:PHE:H	1.78	0.49
16:P:313:ASP:C	16:P:315:TRP:H	2.21	0.49
18:R:267:ALA:HB1	18:R:270:LEU:HD22	1.94	0.49
18:R:425:PHE:CD1	21:Y:63:DT:H1'	2.48	0.49
18:R:617:GLU:HG2	18:R:621:LYS:HE2	1.95	0.49
19:S:387:ALA:O	19:S:391:ASN:N	2.38	0.49
1:A:54:LEU:CD1	1:A:286:THR:HG21	2.43	0.49
1:A:101:GLN:HB3	1:A:145:LEU:HD11	1.94	0.49
1:A:619:ASN:O	1:A:621:PRO:HD3	2.12	0.49
1:A:1123:VAL:N	1:A:1124:PRO:HD2	2.27	0.49
1:A:1284:ASN:OD1	1:A:1285:ILE:N	2.36	0.49
2:B:45:TRP:NE1	2:B:739:LYS:HD3	2.27	0.49
2:B:116:HIS:HB2	2:B:176:GLU:HB2	1.94	0.49
2:B:368:ASP:O	2:B:370:ASP:N	2.46	0.49
2:B:575:PHE:CE2	2:B:589:SER:O	2.66	0.49
2:B:811:VAL:HG22	2:B:817:PRO:HD3	1.94	0.49
2:B:1004:LEU:HD12	2:B:1017:ILE:HD12	1.95	0.49
7:G:38:ILE:HD11	7:G:194:TYR:CB	2.43	0.49
13:M:154:GLU:OE1	13:M:175:ARG:HG2	2.13	0.49
13:M:164:LYS:HB3	13:M:169:TYR:HE2	1.78	0.49
14:N:395:ILE:HD11	14:N:408:LEU:HD21	1.94	0.49
15:O:455:SER:HA	15:O:458:LYS:HD3	1.95	0.49
15:O:484:MET:O	15:O:488:LYS:HG2	2.12	0.49
16:P:62:LYS:HD3	16:P:83:LYS:HE2	1.93	0.49
18:R:650:ALA:HB2	19:S:517:GLU:OE2	2.11	0.49
20:X:74:DA:C6	20:X:75:DG:C6	3.01	0.49
1:A:8:GLU:OE1	1:A:8:GLU:N	2.46	0.49
1:A:81:PHE:CE2	1:A:265:PRO:HG2	2.48	0.49
1:A:376:SER:HB2	2:B:1060:LEU:HD12	1.94	0.49
1:A:521:VAL:C	2:B:1082:ARG:HH22	2.20	0.49
1:A:794:MET:HA	1:A:797:CYS:CB	2.36	0.49
1:A:833:PRO:HB2	2:B:659:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:399:PHE:HA	2:B:402:SER:HB3	1.95	0.49
2:B:552:ASN:ND2	2:B:565:ILE:O	2.44	0.49
3:C:69:ARG:NH2	11:K:70:HIS:HB2	2.28	0.49
7:G:59:LEU:CD2	7:G:64:GLY:HA2	2.42	0.49
9:I:6:PRO:C	9:I:7:SER:HG	2.20	0.49
15:O:510:CYS:SG	15:O:514:ASN:ND2	2.86	0.49
1:A:379:THR:HG22	1:A:380:VAL:N	2.27	0.49
1:A:675:HIS:CB	1:A:937:ARG:HH22	2.26	0.49
2:B:756:THR:HG23	2:B:940:PRO:HA	1.95	0.49
3:C:230:LEU:HD13	3:C:297:HIS:CE1	2.47	0.49
4:D:3:VAL:HG13	7:G:7:ILE:HG22	1.94	0.49
5:E:26:ARG:NH2	5:E:187:TYR:O	2.45	0.49
10:J:45:CYS:SG	10:J:46:CYS:N	2.85	0.49
11:K:122:LYS:O	11:K:125:MET:HB2	2.13	0.49
13:M:106:PHE:CD2	13:M:107:ILE:HB	2.47	0.49
16:P:268:ILE:HD12	16:P:297:PHE:CZ	2.48	0.49
18:R:424:ARG:NH1	21:Y:64:DA:OP1	2.46	0.49
18:R:433:ARG:NH1	19:S:470:GLU:OE1	2.46	0.49
18:R:516:PHE:HB2	20:X:11:DA:H5'	1.94	0.49
1:A:57:LYS:HA	1:A:67:CYS:O	2.13	0.48
1:A:485:ILE:CG2	1:A:535:MET:SD	3.00	0.48
1:A:842:PRO:C	1:A:844:SER:H	2.20	0.48
2:B:83:ILE:HG13	2:B:93:LEU:HB3	1.95	0.48
2:B:244:HIS:ND1	2:B:332:ILE:HD12	2.28	0.48
2:B:733:GLN:NE2	2:B:747:ASP:HB2	2.28	0.48
2:B:1081:GLU:HA	2:B:1085:ILE:HB	1.95	0.48
7:G:138:LEU:HD12	7:G:139:TYR:O	2.13	0.48
14:N:286:ASP:OD2	14:N:384:LYS:HB3	2.13	0.48
15:O:190:LEU:HD11	15:O:199:TYR:CE2	2.48	0.48
15:O:500:LEU:HD21	15:O:539:SER:OG	2.13	0.48
15:O:506:ARG:HB3	16:P:250:ASP:OD1	2.13	0.48
18:R:219:ARG:HD2	18:R:220:PRO:HD2	1.95	0.48
1:A:251:GLY:C	1:A:252:ARG:O	2.55	0.48
1:A:666:LYS:HA	1:A:670:GLY:HA3	1.94	0.48
1:A:873:VAL:HG21	2:B:487:ARG:HG2	1.95	0.48
1:A:957:TYR:CD1	1:A:1031:LEU:HD13	2.46	0.48
1:A:1172:TYR:OH	1:A:1187:ARG:HD3	2.13	0.48
2:B:158:SER:O	2:B:164:TYR:HB2	2.12	0.48
2:B:590:ILE:CA	2:B:601:ILE:HD12	2.21	0.48
8:H:61:SER:HB2	8:H:139:ASN:ND2	2.27	0.48
13:M:88:PHE:HB2	14:N:395:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:121:ILE:HG21	13:M:179:LEU:HD21	1.95	0.48
13:M:158:GLN:HG2	14:N:308:GLN:HG2	1.96	0.48
15:O:297:ILE:O	15:O:301:LYS:HB3	2.12	0.48
15:O:347:ASP:OD1	15:O:348:GLU:N	2.45	0.48
16:P:63:LEU:HD11	16:P:70:LEU:HD13	1.95	0.48
16:P:106:TRP:CZ3	16:P:108:LYS:HB3	2.48	0.48
1:A:808:GLN:HB3	1:A:852:PHE:HE2	1.78	0.48
2:B:734:PRO:HB3	2:B:1023:TYR:CD2	2.48	0.48
2:B:916:HIS:CD2	2:B:957:LYS:HB2	2.48	0.48
3:C:35:LYS:O	3:C:39:ASP:HB3	2.11	0.48
4:D:6:GLU:OE2	7:G:42:VAL:HA	2.13	0.48
7:G:34:PHE:O	7:G:37:LYS:HB2	2.13	0.48
12:L:30:ILE:O	12:L:56:LEU:HB2	2.13	0.48
15:O:35:SER:O	15:O:36:SER:HB3	2.13	0.48
15:O:52:LEU:HD11	15:O:131:LEU:HD12	1.95	0.48
15:O:623:GLU:O	15:O:627:LEU:HG	2.13	0.48
16:P:106:TRP:CD1	16:P:145:ARG:HA	2.49	0.48
18:R:636:LEU:HD22	19:S:502:LEU:HD21	1.94	0.48
20:X:21:DC:H42	21:Y:58:DA:N6	2.12	0.48
1:A:373:VAL:HG11	2:B:1082:ARG:HD3	1.95	0.48
1:A:602:TYR:N	3:C:23:PHE:O	2.47	0.48
1:A:822:ARG:CZ	1:A:845:LYS:HB2	2.43	0.48
1:A:1224:ILE:HG12	1:A:1226:GLY:N	2.28	0.48
1:A:1406:ASP:CG	1:A:1407:ALA:N	2.69	0.48
2:B:430:THR:O	2:B:434:ASN:ND2	2.47	0.48
2:B:494:PHE:CE1	2:B:680:ILE:HD12	2.49	0.48
2:B:601:ILE:HG22	2:B:601:ILE:O	2.13	0.48
2:B:657:SER:OG	2:B:671:THR:OG1	2.32	0.48
3:C:36:PHE:HE1	3:C:59:ILE:HG22	1.77	0.48
3:C:113:LEU:HD11	3:C:132:ILE:HD11	1.95	0.48
3:C:165:ARG:HB2	3:C:189:PRO:HB2	1.94	0.48
15:O:580:ASN:O	15:O:581:LEU:C	2.57	0.48
15:O:583:TRP:CZ3	17:Q:41:LEU:HD21	2.46	0.48
16:P:245:GLU:O	16:P:248:VAL:HB	2.14	0.48
18:R:419:GLU:HB2	18:R:429:ILE:HD13	1.94	0.48
18:R:521:TYR:HD2	18:R:530:LEU:HD13	1.77	0.48
1:A:378:ARG:NH2	1:A:477:GLN:HE21	2.11	0.48
1:A:803:THR:HA	1:A:806:VAL:HG12	1.94	0.48
1:A:896:LEU:HD21	1:A:912:VAL:HG21	1.95	0.48
1:A:949:ASN:OD1	1:A:950:GLN:N	2.47	0.48
2:B:163:LEU:HD22	2:B:171:MET:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:VAL:HG21	2:B:438:SER:HB3	1.95	0.48
2:B:556:TYR:CE2	2:B:561:LEU:HB2	2.48	0.48
2:B:591:TYR:CZ	2:B:600:HIS:HB2	2.49	0.48
2:B:779:ASP:CG	3:C:216:HIS:HD1	2.21	0.48
2:B:1094:VAL:HG21	2:B:1143:LEU:HD11	1.95	0.48
3:C:30:GLU:OE2	11:K:84:PRO:HD3	2.13	0.48
3:C:163:TYR:HA	3:C:191:ILE:O	2.13	0.48
13:M:83:GLU:OE1	14:N:400:ALA:HA	2.13	0.48
13:M:109:ALA:HB3	13:M:122:ASP:HB2	1.95	0.48
13:M:148:LEU:HA	13:M:181:PRO:HA	1.95	0.48
15:O:45:ASP:N	15:O:582:GLU:OE2	2.47	0.48
16:P:55:LEU:HD22	16:P:60:LEU:HD12	1.95	0.48
16:P:83:LYS:HA	16:P:86:MET:CG	2.44	0.48
16:P:122:LEU:HD23	16:P:125:LEU:HD12	1.96	0.48
16:P:190:THR:HA	16:P:215:TYR:CE1	2.48	0.48
1:A:351:ARG:HB2	1:A:355:GLN:CD	2.39	0.48
1:A:408:VAL:HA	1:A:412:ASN:HD22	1.79	0.48
1:A:1077:LYS:O	1:A:1081:ALA:N	2.46	0.48
1:A:1447:LEU:HB3	1:A:1450:SER:HB3	1.96	0.48
2:B:140:ASN:HD22	19:S:394:LYS:HA	1.78	0.48
2:B:435:ARG:O	2:B:439:THR:CB	2.62	0.48
15:O:58:GLY:HA2	15:O:62:ALA:HB2	1.95	0.48
16:P:264:THR:O	16:P:265:LEU:CG	2.38	0.48
18:R:397:VAL:N	18:R:485:ASN:O	2.46	0.48
18:R:483:ILE:HG21	18:R:486:ILE:HG13	1.95	0.48
20:X:24:DT:C6	20:X:25:DT:H72	2.49	0.48
1:A:26:ILE:HG23	1:A:262:PRO:HB3	1.94	0.48
1:A:225:LEU:HD21	15:O:541:ILE:O	2.14	0.48
1:A:580:LEU:HB3	11:K:88:PHE:HE1	1.77	0.48
1:A:830:ARG:NH2	2:B:655:ASN:O	2.47	0.48
1:A:896:LEU:HD23	1:A:1357:LEU:HD11	1.96	0.48
1:A:1171:PHE:CE2	1:A:1172:TYR:HD2	2.32	0.48
2:B:135:TYR:CZ	2:B:143:MET:HB3	2.48	0.48
2:B:152:MET:SD	2:B:153:PRO:HD2	2.54	0.48
2:B:554:GLY:HA2	2:B:564:SER:CB	2.43	0.48
2:B:930:ASP:O	2:B:931:MET:HG2	2.12	0.48
2:B:1009:THR:O	11:K:74:ASN:ND2	2.47	0.48
3:C:107:LYS:HG3	3:C:307:ALA:O	2.13	0.48
13:M:89:GLN:HG3	14:N:392:GLN:HE21	1.78	0.48
15:O:202:GLN:N	15:O:280:LEU:HG	2.28	0.48
15:O:239:SER:O	15:O:242:LYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:484:MET:HB2	15:O:485:PRO:HD3	1.96	0.48
16:P:116:LEU:HB3	16:P:120:VAL:HG21	1.95	0.48
18:R:107:TRP:O	18:R:111:ALA:N	2.38	0.48
18:R:140:HIS:ND1	18:R:140:HIS:O	2.47	0.48
18:R:275:PHE:HD1	18:R:278:ASN:H	1.60	0.48
18:R:640:SER:OG	19:S:506:GLN:NE2	2.45	0.48
19:S:444:GLN:NE2	19:S:490:LYS:HE3	2.29	0.48
1:A:15:GLY:C	1:A:16:LEU:HD12	2.39	0.48
1:A:103:LEU:HD21	1:A:108:LYS:HE3	1.96	0.48
1:A:189:LYS:HE2	1:A:191:ALA:HB2	1.95	0.48
1:A:251:GLY:O	1:A:252:ARG:C	2.57	0.48
1:A:794:MET:SD	2:B:947:HIS:ND1	2.86	0.48
2:B:435:ARG:O	2:B:439:THR:OG1	2.28	0.48
2:B:891:ASN:HD21	2:B:893:GLN:CD	2.22	0.48
3:C:17:SER:C	3:C:18:THR:HG22	2.33	0.48
5:E:86:PRO:CB	5:E:114:ASN:HB2	2.43	0.48
5:E:88:VAL:HG21	5:E:112:TYR:HE1	1.79	0.48
8:H:104:PHE:HE1	8:H:114:VAL:HG13	1.79	0.48
10:J:36:LEU:CD2	10:J:47:ARG:HG3	2.44	0.48
13:M:83:GLU:C	13:M:84:SER:O	2.57	0.48
15:O:261:GLN:O	15:O:275:LYS:HB2	2.14	0.48
18:R:472:ILE:HD11	18:R:614:LEU:HB3	1.96	0.48
1:A:51:ASN:OD1	1:A:52:GLY:N	2.46	0.48
1:A:192:PRO:HA	1:A:195:ASP:HB2	1.96	0.48
1:A:240:GLU:N	1:A:244:ILE:O	2.47	0.48
1:A:427:HIS:NE2	1:A:492:ILE:HG13	2.28	0.48
1:A:491:LYS:HD3	1:A:493:ARG:NH2	2.29	0.48
1:A:790:ALA:HB3	1:A:791:PRO:HD3	1.94	0.48
1:A:1199:GLU:H	1:A:1273:LYS:HE2	1.78	0.48
1:A:1325:VAL:HG23	1:A:1326:LEU:H	1.78	0.48
1:A:1332:ARG:O	1:A:1335:ILE:HG22	2.13	0.48
2:B:191:GLU:HG3	2:B:458:LEU:HB3	1.96	0.48
2:B:1026:LYS:C	2:B:1027:LEU:HD12	2.39	0.48
5:E:79:TRP:NE1	5:E:81:GLU:HB3	2.27	0.48
5:E:107:THR:HB	5:E:131:THR:HG22	1.95	0.48
8:H:6:PHE:CZ	8:H:8:ASP:HB2	2.49	0.48
8:H:41:ASP:CG	8:H:122:LEU:H	2.21	0.48
15:O:168:SER:C	15:O:169:LEU:HD12	2.39	0.48
15:O:183:MET:O	15:O:187:ILE:HG13	2.14	0.48
15:O:353:GLU:HB2	15:O:481:SER:HB3	1.96	0.48
16:P:185:PHE:HE2	16:P:217:THR:HG21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:60:ASN:O	17:Q:64:THR:OG1	2.22	0.48
19:S:307:UNK:O	19:S:311:UNK:CB	2.61	0.48
1:A:32:VAL:CG1	1:A:57:LYS:HD2	2.44	0.48
1:A:489:TYR:CE1	1:A:532:ILE:HG12	2.49	0.48
1:A:600:PRO:HD2	8:H:96:VAL:CG2	2.44	0.48
1:A:939:TRP:HA	1:A:1070:PHE:CD1	2.48	0.48
1:A:1373:ARG:NH1	1:A:1390:GLU:OE2	2.47	0.48
2:B:129:ILE:O	2:B:148:GLU:HA	2.14	0.48
2:B:241:TYR:HB3	2:B:250:GLU:HA	1.95	0.48
2:B:614:ILE:HA	2:B:672:HIS:CD2	2.49	0.48
2:B:702:GLN:HA	2:B:705:MET:HE3	1.95	0.48
3:C:260:GLU:O	3:C:264:GLU:N	2.47	0.48
5:E:5:ASN:O	5:E:8:ASN:N	2.47	0.48
15:O:517:VAL:HG21	15:O:521:ILE:CB	2.44	0.48
16:P:203:LYS:HG3	16:P:206:VAL:HG13	1.96	0.48
18:R:229:LEU:O	18:R:233:ARG:CB	2.62	0.48
1:A:560:GLY:HA3	1:A:705:LEU:HD22	1.95	0.47
1:A:1193:ILE:HG12	1:A:1200:LEU:HD11	1.96	0.47
2:B:458:LEU:HA	2:B:469:MET:HE1	1.95	0.47
2:B:519:HIS:HB3	2:B:609:CYS:HB2	1.96	0.47
2:B:909:GLY:N	2:B:922:CYS:SG	2.86	0.47
3:C:231:PRO:HB3	3:C:275:VAL:HG22	1.96	0.47
3:C:256:ILE:HG22	3:C:267:VAL:HA	1.96	0.47
5:E:96:PHE:O	5:E:100:ILE:HG12	2.14	0.47
7:G:63:ASP:OD2	7:G:65:SER:HB2	2.14	0.47
7:G:203:ASP:OD1	7:G:204:GLY:N	2.42	0.47
8:H:35:GLN:O	8:H:126:GLU:HG3	2.14	0.47
8:H:107:VAL:O	8:H:111:LEU:HB2	2.14	0.47
15:O:38:GLU:C	15:O:40:ARG:H	2.22	0.47
15:O:496:ILE:HA	15:O:499:THR:HB	1.96	0.47
18:R:274:LYS:O	18:R:275:PHE:CG	2.67	0.47
20:X:76:DG:C5	20:X:77:DC:C4	3.01	0.47
1:A:404:TYR:CD1	1:A:405:PRO:HD2	2.48	0.47
1:A:561:SER:HB3	1:A:664:MET:HE3	1.95	0.47
1:A:1332:ARG:CZ	5:E:200:ARG:HH21	2.26	0.47
2:B:579:ARG:HH12	2:B:647:GLU:CG	2.11	0.47
4:D:21:THR:O	4:D:25:LYS:HB2	2.14	0.47
7:G:162:SER:HB3	7:G:165:GLU:HB2	1.95	0.47
13:M:96:LEU:N	13:M:101:PRO:HA	2.26	0.47
13:M:140:TRP:HB2	13:M:185:TYR:CD1	2.48	0.47
15:O:300:ALA:O	15:O:304:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:292:SER:HB2	16:P:293:ILE:HD13	1.95	0.47
18:R:452:ALA:HB1	18:R:458:SER:HB2	1.95	0.47
1:A:81:PHE:CD2	1:A:265:PRO:HG3	2.49	0.47
1:A:1454:GLU:HA	1:A:1457:LEU:HD12	1.96	0.47
2:B:132:ASP:HA	2:B:145:LYS:O	2.14	0.47
2:B:693:HIS:HB3	2:B:955:VAL:HG23	1.95	0.47
2:B:1067:ARG:O	2:B:1070:VAL:HG22	2.14	0.47
7:G:153:GLU:HG2	7:G:195:ALA:H	1.79	0.47
9:I:7:SER:OG	9:I:8:CYS:N	2.45	0.47
18:R:86:LYS:O	18:R:90:VAL:HG12	2.15	0.47
1:A:308:SER:O	1:A:312:MET:HB2	2.15	0.47
1:A:1256:VAL:O	1:A:1260:MET:CB	2.50	0.47
1:A:1281:ALA:HB2	1:A:1295:VAL:HG22	1.95	0.47
2:B:735:MET:HE1	10:J:51:LEU:HD22	1.97	0.47
2:B:934:ASN:CG	2:B:935:ASP:H	2.23	0.47
7:G:22:THR:O	7:G:26:ILE:HG12	2.14	0.47
13:M:112:TYR:OH	13:M:114:PRO:HA	2.15	0.47
15:O:126:GLY:C	15:O:128:HIS:N	2.71	0.47
15:O:310:GLN:HE21	15:O:314:ILE:HG23	1.79	0.47
18:R:131:TYR:HA	18:R:134:CYS:SG	2.53	0.47
19:S:381:VAL:HG22	19:S:383:ARG:H	1.79	0.47
20:X:65:DA:H2''	20:X:66:DG:H8	1.79	0.47
1:A:212:GLU:H	1:A:212:GLU:CD	2.22	0.47
1:A:433:LEU:HD13	1:A:452:LEU:HD21	1.96	0.47
1:A:483:LEU:HD12	1:A:507:PRO:HB3	1.90	0.47
1:A:664:MET:O	1:A:667:SER:OG	2.29	0.47
1:A:1285:ILE:HG23	1:A:1291:ARG:HG2	1.96	0.47
2:B:409:LYS:O	2:B:411:ASN:N	2.45	0.47
2:B:568:PRO:O	2:B:571:PHE:HB3	2.15	0.47
2:B:1132:LEU:O	2:B:1135:MET:N	2.48	0.47
3:C:88:ASN:OD1	3:C:89:THR:N	2.48	0.47
3:C:239:ILE:O	3:C:244:ALA:HB2	2.15	0.47
3:C:256:ILE:C	3:C:268:LYS:HG2	2.39	0.47
6:F:99:LEU:HD21	6:F:103:MET:HE3	1.95	0.47
15:O:105:LYS:HE3	15:O:124:GLU:H	1.79	0.47
15:O:239:SER:HA	15:O:242:LYS:HB2	1.96	0.47
15:O:496:ILE:HG12	15:O:499:THR:HG21	1.96	0.47
16:P:203:LYS:HG3	16:P:206:VAL:CG1	2.45	0.47
20:X:13:DT:H2''	20:X:14:DA:O4'	2.14	0.47
20:X:62:DC:C4'	20:X:63:DC:OP1	2.53	0.47
1:A:200:GLU:HA	15:O:515:LYS:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:THR:HG22	1:A:380:VAL:H	1.79	0.47
1:A:727:LYS:HD2	1:A:812:VAL:HB	1.96	0.47
1:A:978:ASP:HB3	1:A:982:CYS:HB2	1.96	0.47
1:A:1005:TYR:O	1:A:1008:LEU:N	2.47	0.47
2:B:467:LEU:HA	2:B:470:MET:HE3	1.96	0.47
5:E:151:PRO:HB2	5:E:199:ILE:O	2.15	0.47
6:F:71:GLU:HA	6:F:141:GLY:O	2.14	0.47
8:H:7:ASP:OD1	8:H:58:THR:OG1	2.24	0.47
15:O:273:ILE:HG12	15:O:274:VAL:N	2.28	0.47
18:R:231:ALA:HA	18:R:234:MET:HB3	1.96	0.47
1:A:351:ARG:HB2	1:A:355:GLN:NE2	2.30	0.47
1:A:478:PRO:O	1:A:480:LEU:HD12	2.14	0.47
1:A:547:GLY:O	1:A:674:LYS:HE2	2.14	0.47
1:A:550:ILE:HG23	1:A:551:ILE:HG23	1.95	0.47
1:A:815:GLN:H	1:A:847:PHE:HA	1.80	0.47
1:A:850:ASN:HD22	1:A:856:LEU:HA	1.80	0.47
1:A:1306:THR:O	1:A:1309:VAL:HG22	2.14	0.47
1:A:1312:SER:OG	5:E:147:HIS:O	2.26	0.47
2:B:134:GLU:OE2	19:S:396:LYS:NZ	2.48	0.47
2:B:392:PHE:O	2:B:395:PHE:HB3	2.15	0.47
2:B:401:LEU:HA	2:B:404:ASP:HB2	1.97	0.47
2:B:420:LEU:HD11	18:R:149:ARG:O	2.15	0.47
2:B:612:LEU:HD11	2:B:649:LEU:CD1	2.45	0.47
2:B:758:ALA:O	2:B:943:ILE:HD12	2.15	0.47
2:B:1106:TRP:CZ3	2:B:1111:LYS:HB2	2.49	0.47
3:C:132:ILE:HG23	3:C:169:PHE:HE1	1.79	0.47
5:E:41:ASP:HA	5:E:44:ALA:HB3	1.97	0.47
5:E:178:ILE:HG21	5:E:185:ALA:HB2	1.96	0.47
7:G:86:THR:HA	7:G:146:ILE:O	2.15	0.47
7:G:89:ILE:HG23	7:G:142:VAL:HG12	1.95	0.47
7:G:121:TYR:HD1	7:G:127:ALA:O	1.98	0.47
8:H:13:SER:HB3	8:H:27:GLU:O	2.15	0.47
13:M:251:THR:OG1	13:M:254:GLN:NE2	2.47	0.47
15:O:174:TYR:CE2	15:O:178:VAL:HG21	2.50	0.47
15:O:584:ASN:O	15:O:588:LEU:N	2.48	0.47
16:P:14:ASN:HA	16:P:17:THR:HG22	1.96	0.47
16:P:177:SER:O	16:P:181:ILE:HG12	2.14	0.47
16:P:203:LYS:HG2	16:P:206:VAL:H	1.79	0.47
18:R:13:GLU:OE1	18:R:25:CYS:HA	2.14	0.47
18:R:198:VAL:HG13	18:R:231:ALA:CB	2.44	0.47
18:R:273:GLN:HB2	19:S:277:UNK:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:78:DG:N2	21:Y:3:DG:N3	2.62	0.47
1:A:477:GLN:HB2	1:A:478:PRO:HD3	1.97	0.47
1:A:483:LEU:CD1	1:A:507:PRO:CB	2.83	0.47
1:A:980:SER:HB3	5:E:163:GLU:HG2	1.97	0.47
2:B:84:LEU:HB2	2:B:91:PHE:HD2	1.80	0.47
2:B:615:VAL:HG22	2:B:671:THR:O	2.15	0.47
2:B:901:ARG:NH2	3:C:94:ASP:OD1	2.47	0.47
3:C:31:TRP:CZ2	11:K:123:ASP:HB3	2.49	0.47
3:C:32:ASN:CG	3:C:33:VAL:H	2.23	0.47
6:F:108:PHE:HE2	6:F:131:PRO:HG3	1.77	0.47
11:K:60:SER:HB3	11:K:104:ARG:HH22	1.79	0.47
13:M:113:LYS:HD3	13:M:241:ALA:HB2	1.97	0.47
15:O:306:SER:HA	15:O:309:ALA:HB3	1.95	0.47
15:O:579:GLN:CG	16:P:315:TRP:CZ3	2.98	0.47
15:O:581:LEU:HD22	15:O:648:TRP:CH2	2.49	0.47
16:P:151:TYR:O	16:P:151:TYR:CG	2.68	0.47
18:R:466:ALA:HA	18:R:469:ILE:HD12	1.96	0.47
19:S:446:TYR:HB2	19:S:449:ARG:HB3	1.96	0.47
20:X:75:DG:O6	21:Y:4:DC:N4	2.48	0.47
1:A:613:LEU:HD11	1:A:696:ARG:HG3	1.97	0.47
1:A:851:SER:O	1:A:854:SER:OG	2.20	0.47
1:A:919:ASP:OD2	1:A:921:LEU:HB2	2.14	0.47
1:A:979:ASN:ND2	5:E:160:GLU:OE2	2.47	0.47
1:A:1136:ILE:HG21	1:A:1318:HIS:ND1	2.30	0.47
2:B:496:MET:CG	2:B:610:ARG:HD2	2.41	0.47
2:B:636:ASP:OD1	2:B:637:PHE:N	2.47	0.47
2:B:724:LEU:HD21	2:B:726:TYR:CE2	2.48	0.47
3:C:33:VAL:O	3:C:34:GLU:CB	2.51	0.47
3:C:270:ALA:O	3:C:271:ARG:HG2	2.14	0.47
3:C:319:ARG:HB2	11:K:132:GLU:OE2	2.14	0.47
8:H:4:THR:HA	8:H:60:ALA:CB	2.45	0.47
9:I:13:LEU:O	9:I:24:LEU:HB2	2.15	0.47
15:O:353:GLU:H	15:O:481:SER:HB3	1.79	0.47
18:R:214:MET:HE1	18:R:287:PRO:HA	1.97	0.47
18:R:440:LEU:O	18:R:447:MET:HB2	2.15	0.47
18:R:615:LEU:HD12	18:R:616:ASN:O	2.14	0.47
21:Y:12:DA:C5	21:Y:13:DA:C6	3.03	0.47
1:A:30:SER:CB	1:A:82:GLY:O	2.42	0.47
1:A:482:ARG:HH11	1:A:544:PRO:HD3	1.80	0.47
1:A:542:LEU:HD21	1:A:679:TYR:CE1	2.50	0.47
1:A:545:LYS:HG3	1:A:546:SER:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1177:TYR:HD1	1:A:1183:PHE:H	1.62	0.47
1:A:1272:VAL:HG13	1:A:1273:LYS:N	2.28	0.47
1:A:1380:ARG:NH1	1:A:1385:GLN:HE22	2.08	0.47
2:B:234:ILE:HD12	2:B:238:GLY:H	1.79	0.47
2:B:710:ILE:HD11	2:B:1026:LYS:HB3	1.97	0.47
2:B:967:GLY:O	2:B:971:GLY:N	2.48	0.47
3:C:15:THR:O	3:C:16:THR:C	2.58	0.47
13:M:139:GLU:HB3	13:M:140:TRP:CE3	2.50	0.47
15:O:106:TYR:N	15:O:210:PRO:HD3	2.30	0.47
15:O:291:ARG:HH12	15:O:652:GLN:NE2	2.13	0.47
15:O:324:PRO:HG3	15:O:327:ARG:HH21	1.79	0.47
15:O:631:ASN:O	15:O:634:GLU:N	2.48	0.47
16:P:246:VAL:O	16:P:250:ASP:N	2.34	0.47
18:R:116:PHE:CZ	18:R:164:MET:HB3	2.50	0.47
18:R:471:LYS:NZ	18:R:611:ASN:OD1	2.40	0.47
20:X:10:DT:H2"	20:X:11:DA:N7	2.30	0.47
1:A:204:VAL:HG21	15:O:517:VAL:HA	1.96	0.46
1:A:212:GLU:O	1:A:216:LYS:HB2	2.14	0.46
1:A:285:LEU:HD21	1:A:353:PHE:HD1	1.80	0.46
1:A:314:GLU:OE1	1:A:314:GLU:N	2.48	0.46
1:A:399:ALA:CA	1:A:466:LEU:HD12	2.42	0.46
1:A:815:GLN:HA	1:A:846:GLY:O	2.15	0.46
1:A:1180:ASN:N	9:I:21:VAL:HA	2.29	0.46
1:A:1255:ASP:O	1:A:1258:TYR:N	2.48	0.46
2:B:760:MET:C	2:B:946:PRO:HD3	2.40	0.46
2:B:776:SER:HA	2:B:779:ASP:HB2	1.96	0.46
2:B:849:THR:HG22	2:B:865:GLN:O	2.14	0.46
3:C:21:PRO:HB2	3:C:27:ALA:HB1	1.96	0.46
5:E:22:MET:HE1	5:E:135:PHE:CZ	2.49	0.46
5:E:107:THR:OG1	5:E:131:THR:HG23	2.16	0.46
7:G:4:LEU:HD11	7:G:73:ARG:HB3	1.96	0.46
15:O:455:SER:HA	15:O:458:LYS:HB2	1.97	0.46
15:O:478:VAL:HG12	15:O:479:PRO:O	2.15	0.46
18:R:6:ASN:O	18:R:8:HIS:ND1	2.42	0.46
18:R:207:GLN:O	18:R:211:LYS:N	2.35	0.46
1:A:269:ARG:HH22	1:A:284:ASP:N	2.13	0.46
1:A:413:ARG:O	1:A:417:GLN:HG2	2.15	0.46
1:A:464:ARG:HH11	1:A:467:GLU:CD	2.24	0.46
1:A:525:GLU:O	1:A:528:ARG:N	2.47	0.46
1:A:1213:SER:HB2	1:A:1218:GLN:H	1.80	0.46
1:A:1452:SER:HB2	4:D:117:LYS:NZ	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ASP:HA	2:B:189:GLY:CA	2.45	0.46
2:B:137:ARG:H	2:B:141:ILE:HG21	1.79	0.46
2:B:490:GLN:OE1	2:B:490:GLN:N	2.44	0.46
2:B:613:ILE:HD12	2:B:673:LEU:HD11	1.97	0.46
3:C:71:MET:HG2	3:C:222:VAL:HG21	1.97	0.46
7:G:110:ILE:HA	7:G:198:GLY:H	1.80	0.46
14:N:396:ALA:C	14:N:397:LEU:HD12	2.41	0.46
15:O:98:LEU:O	15:O:102:ARG:N	2.49	0.46
16:P:134:VAL:CA	16:P:151:TYR:HB2	2.45	0.46
17:Q:36:PHE:N	17:Q:37:PRO:HD2	2.30	0.46
1:A:244:ILE:HD11	1:A:1401:PHE:CZ	2.49	0.46
1:A:418:GLU:O	1:A:421:VAL:N	2.44	0.46
1:A:713:GLY:HA3	2:B:1001:LYS:HD2	1.96	0.46
1:A:885:MET:O	1:A:889:LEU:CB	2.64	0.46
1:A:968:GLY:C	1:A:970:LEU:H	2.23	0.46
1:A:1431:VAL:HG13	7:G:57:GLY:O	2.14	0.46
2:B:240:ILE:HG13	2:B:286:ASN:HD22	1.80	0.46
2:B:321:GLN:O	2:B:324:ILE:HB	2.15	0.46
2:B:385:SER:OG	2:B:386:LEU:N	2.47	0.46
2:B:659:ILE:HG22	2:B:660:ALA:O	2.14	0.46
2:B:934:ASN:HD21	2:B:938:ILE:HD11	1.80	0.46
3:C:84:TYR:CE2	3:C:207:HIS:CE1	3.04	0.46
11:K:124:LEU:O	11:K:127:LEU:HB2	2.15	0.46
13:M:112:TYR:CZ	13:M:114:PRO:HA	2.51	0.46
14:N:286:ASP:O	14:N:290:ILE:HG22	2.16	0.46
14:N:376:GLY:H	14:N:379:VAL:HG12	1.81	0.46
15:O:576:PHE:CD1	15:O:577:MET:N	2.84	0.46
18:R:219:ARG:N	21:Y:72:DA:OP1	2.49	0.46
18:R:551:GLN:O	18:R:555:ALA:CB	2.63	0.46
20:X:72:DT:H2"	20:X:73:DA:C8	2.51	0.46
1:A:197:TRP:HA	1:A:200:GLU:OE1	2.14	0.46
1:A:269:ARG:CZ	1:A:285:LEU:HB2	2.46	0.46
1:A:356:ARG:HG3	1:A:363:ARG:HH12	1.80	0.46
1:A:587:ILE:HA	11:K:53:ALA:HB2	1.96	0.46
1:A:1012:ILE:HD11	1:A:1070:PHE:CE2	2.50	0.46
1:A:1179:ASP:OD1	9:I:35:ILE:HB	2.16	0.46
2:B:72:ASP:O	2:B:76:ILE:HG12	2.14	0.46
2:B:84:LEU:HG	2:B:85:SER:O	2.16	0.46
2:B:95:TYR:CD1	2:B:133:ILE:HG12	2.49	0.46
2:B:345:LYS:HA	2:B:348:TYR:HB3	1.98	0.46
2:B:575:PHE:O	2:B:578:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1082:ARG:O	2:B:1087:SER:OG	2.34	0.46
3:C:62:SER:HB3	11:K:75:ALA:HA	1.98	0.46
10:J:17:LYS:HD3	10:J:41:LEU:CD1	2.46	0.46
14:N:302:GLU:HB3	14:N:410:GLY:HA2	1.98	0.46
15:O:190:LEU:HD21	15:O:199:TYR:CE2	2.49	0.46
15:O:457:LEU:HD21	15:O:476:TYR:OH	2.15	0.46
16:P:131:GLN:HB3	16:P:133:TYR:CD2	2.43	0.46
19:S:439:PHE:HA	19:S:442:ILE:HD12	1.97	0.46
1:A:543:THR:HB	1:A:550:ILE:HB	1.98	0.46
1:A:714:ILE:CG2	1:A:715:ASN:N	2.78	0.46
1:A:804:LEU:O	1:A:807:SER:HB3	2.15	0.46
1:A:1185:GLN:HA	1:A:1230:ILE:HG13	1.96	0.46
1:A:1315:THR:HG22	1:A:1316:THR:N	2.30	0.46
1:A:1395:HIS:O	1:A:1399:ALA:HB2	2.16	0.46
2:B:556:TYR:HA	2:B:560:THR:O	2.16	0.46
2:B:800:ASN:HA	2:B:855:PRO:HB3	1.97	0.46
3:C:172:GLN:H	3:C:175:GLN:HB3	1.81	0.46
6:F:98:ALA:O	6:F:101:ILE:N	2.49	0.46
7:G:55:GLU:N	7:G:55:GLU:OE1	2.49	0.46
13:M:89:GLN:NE2	13:M:178:GLN:HE22	2.06	0.46
15:O:302:THR:O	16:P:265:LEU:HD11	2.16	0.46
15:O:468:LEU:H	15:O:483:LEU:HD13	1.80	0.46
15:O:522:ILE:O	15:O:526:ALA:N	2.21	0.46
18:R:129:CYS:O	18:R:132:VAL:HG22	2.15	0.46
18:R:434:GLU:HA	18:R:436:LYS:H	1.81	0.46
1:A:864:HIS:NE2	2:B:695:GLN:HA	2.29	0.46
1:A:1017:THR:OG1	1:A:1032:LEU:HD22	2.16	0.46
1:A:1342:THR:HG23	1:A:1343:MET:H	1.81	0.46
2:B:338:GLU:OE1	2:B:339:ALA:N	2.48	0.46
2:B:554:GLY:O	2:B:599:VAL:HG12	2.16	0.46
2:B:640:PHE:O	2:B:645:LEU:N	2.36	0.46
2:B:649:LEU:HD13	2:B:653:GLU:OE1	2.16	0.46
3:C:56:LEU:O	3:C:297:HIS:HD2	1.98	0.46
3:C:71:MET:O	3:C:75:VAL:HG22	2.15	0.46
4:D:55:LEU:O	4:D:58:ILE:HG13	2.15	0.46
13:M:183:PHE:C	13:M:185:TYR:N	2.72	0.46
15:O:253:ILE:O	15:O:256:PRO:HD2	2.16	0.46
15:O:263:LEU:HB3	15:O:272:ARG:NH2	2.30	0.46
15:O:595:LEU:HD12	15:O:598:GLU:HG3	1.98	0.46
16:P:141:LYS:HG2	16:P:142:PHE:H	1.81	0.46
19:S:413:ARG:NH1	20:X:9:DA:H3'	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:68:DT:H2''	20:X:69:DG:C8	2.50	0.46
21:Y:69:DT:H73	21:Y:70:DA:N6	2.29	0.46
1:A:223:ASN:HD22	1:A:225:LEU:HB3	1.81	0.46
1:A:228:LEU:HD21	1:A:232:LYS:HE3	1.96	0.46
1:A:542:LEU:HD21	1:A:679:TYR:HE1	1.79	0.46
1:A:665:ASP:CG	1:A:797:CYS:HA	2.40	0.46
1:A:818:ILE:HD11	1:A:823:VAL:HA	1.97	0.46
1:A:1395:HIS:O	1:A:1399:ALA:CB	2.63	0.46
2:B:66:ASN:CG	2:B:159:ASN:H	2.22	0.46
2:B:207:VAL:HG23	2:B:355:ARG:NH1	2.31	0.46
2:B:422:ILE:O	2:B:426:SER:N	2.49	0.46
2:B:702:GLN:OE1	2:B:917:GLY:N	2.48	0.46
2:B:775:LYS:HA	2:B:778:ILE:CG2	2.45	0.46
3:C:171:PRO:HB2	3:C:176:SER:HB2	1.98	0.46
3:C:278:GLU:HB3	3:C:281:ARG:HG2	1.97	0.46
6:F:86:THR:C	6:F:88:TYR:H	2.24	0.46
7:G:51:LEU:HD12	7:G:72:PHE:HB3	1.98	0.46
7:G:124:GLU:OE1	7:G:124:GLU:HA	2.15	0.46
8:H:65:LEU:HG	8:H:66:GLU:H	1.81	0.46
15:O:196:GLU:HG3	15:O:197:MET:N	2.30	0.46
16:P:116:LEU:HB3	16:P:120:VAL:CG2	2.46	0.46
16:P:170:LEU:HD23	16:P:172:ILE:H	1.80	0.46
18:R:439:ALA:HB3	18:R:465:TYR:CZ	2.51	0.46
20:X:16:DT:H2'	20:X:17:DA:C8	2.51	0.46
21:Y:56:DA:H1'	21:Y:57:DA:H5'	1.97	0.46
1:A:885:MET:HA	1:A:888:ARG:HE	1.81	0.46
1:A:1385:GLN:O	1:A:1388:SER:N	2.47	0.46
1:A:1410:GLY:O	1:A:1413:GLU:HB3	2.15	0.46
2:B:81:GLN:OE1	2:B:81:GLN:N	2.49	0.46
2:B:214:GLY:HA3	2:B:234:ILE:CG2	2.46	0.46
2:B:574:GLN:NE2	14:N:422:ILE:HG12	2.31	0.46
2:B:727:LEU:HD21	2:B:786:GLU:HB2	1.96	0.46
2:B:804:ASP:HB2	2:B:847:VAL:HG12	1.98	0.46
2:B:810:ARG:H	2:B:821:HIS:CD2	2.32	0.46
3:C:178:THR:HG23	3:C:179:PHE:CD2	2.51	0.46
3:C:190:ASP:O	3:C:191:ILE:HG13	2.16	0.46
3:C:255:VAL:HG22	3:C:256:ILE:N	2.30	0.46
7:G:2:PHE:CD2	7:G:79:PRO:HB3	2.50	0.46
8:H:115:TYR:HA	8:H:123:MET:O	2.16	0.46
15:O:134:GLY:N	17:Q:58:TYR:HD1	2.07	0.46
20:X:8:DT:H1'	20:X:9:DA:H5'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:11:DC:H2'	21:Y:11:DC:OP2	2.16	0.46
1:A:232:LYS:CD	16:P:315:TRP:CH2	2.92	0.46
2:B:123:MET:HE3	2:B:890:ASP:HB3	1.98	0.46
2:B:155:MET:HB2	2:B:185:PHE:CE1	2.51	0.46
2:B:868:GLU:OE1	2:B:868:GLU:N	2.45	0.46
7:G:99:VAL:O	7:G:108:ILE:HB	2.16	0.46
10:J:7:CYS:SG	10:J:10:CYS:N	2.89	0.46
12:L:29:TYR:CB	12:L:58:LYS:HA	2.45	0.46
15:O:124:GLU:HG3	15:O:126:GLY:N	2.26	0.46
15:O:358:GLY:HA2	15:O:361:PHE:HB2	1.98	0.46
16:P:295:ASN:ND2	16:P:298:LYS:HB3	2.30	0.46
1:A:140:ILE:O	1:A:143:LYS:N	2.49	0.46
1:A:224:PRO:HD2	1:A:316:TRP:HH2	1.80	0.46
1:A:381:ILE:HG22	1:A:382:SER:H	1.81	0.46
1:A:607:LYS:HD2	1:A:659:ILE:HG21	1.97	0.46
1:A:624:ILE:N	1:A:657:SER:OG	2.48	0.46
1:A:1394:ASP:O	1:A:1398:ASP:CB	2.64	0.46
2:B:538:VAL:HG12	2:B:565:ILE:HB	1.98	0.46
2:B:540:ASP:OD1	2:B:541:ILE:HG22	2.16	0.46
2:B:823:SER:O	2:B:823:SER:OG	2.34	0.46
3:C:191:ILE:HG23	10:J:15:GLY:HA3	1.96	0.46
3:C:329:LYS:NZ	11:K:122:LYS:HD2	2.31	0.46
8:H:104:PHE:CE1	8:H:114:VAL:HG13	2.50	0.46
13:M:89:GLN:HE21	13:M:178:GLN:NE2	2.05	0.46
14:N:385:GLY:O	14:N:416:ILE:HA	2.16	0.46
15:O:54:LYS:HA	15:O:58:GLY:CA	2.46	0.46
15:O:583:TRP:CZ3	17:Q:41:LEU:CD2	2.94	0.46
1:A:356:ARG:CG	1:A:363:ARG:HH12	2.29	0.45
1:A:405:PRO:HD3	1:A:523:GLN:NE2	2.31	0.45
1:A:703:ARG:NH2	11:K:93:ILE:O	2.48	0.45
1:A:1278:ILE:HG23	1:A:1297:GLY:HA3	1.98	0.45
2:B:343:ARG:NH2	2:B:546:SER:OG	2.42	0.45
2:B:552:ASN:CG	2:B:553:TYR:H	2.23	0.45
3:C:3:ASN:O	3:C:294:VAL:HA	2.16	0.45
3:C:228:ARG:O	3:C:299:ILE:CB	2.47	0.45
5:E:85:GLU:CD	5:E:86:PRO:HD2	2.41	0.45
6:F:101:ILE:HG13	6:F:120:ILE:HD11	1.98	0.45
15:O:68:LEU:HD21	15:O:121:TYR:C	2.42	0.45
18:R:11:GLU:N	18:R:11:GLU:OE1	2.49	0.45
18:R:214:MET:HE1	18:R:287:PRO:CA	2.46	0.45
1:A:45:ASP:CG	1:A:46:ARG:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:LEU:HA	1:A:487:SER:HA	1.98	0.45
1:A:636:PRO:HA	1:A:647:GLN:NE2	2.31	0.45
1:A:667:SER:OG	1:A:668:VAL:N	2.50	0.45
1:A:864:HIS:HE2	2:B:695:GLN:CB	2.29	0.45
1:A:1262:GLN:HA	1:A:1265:ARG:HB3	1.97	0.45
2:B:204:ARG:CZ	2:B:376:ARG:HH22	2.29	0.45
2:B:660:ALA:N	2:B:672:HIS:O	2.36	0.45
2:B:675:ILE:HG13	2:B:676:GLU:N	2.31	0.45
2:B:916:HIS:CD2	2:B:957:LYS:H	2.35	0.45
2:B:1006:SER:HB3	2:B:1010:GLY:N	2.29	0.45
2:B:1129:PHE:CE2	2:B:1141:LEU:HD11	2.51	0.45
5:E:86:PRO:CA	5:E:113:GLN:HB3	2.42	0.45
10:J:42:LYS:HG3	10:J:43:ARG:H	1.80	0.45
11:K:110:GLU:CD	11:K:111:THR:H	2.23	0.45
12:L:29:TYR:HB3	12:L:59:ALA:H	1.81	0.45
13:M:131:TYR:OH	13:M:143:VAL:HA	2.16	0.45
13:M:135:LYS:HZ2	13:M:140:TRP:HZ2	1.61	0.45
13:M:257:ASP:O	13:M:261:LYS:HG3	2.16	0.45
15:O:468:LEU:HB3	15:O:469:ASN:H	1.55	0.45
16:P:295:ASN:HD21	16:P:298:LYS:HD3	1.81	0.45
16:P:307:LYS:N	16:P:308:GLU:OE1	2.49	0.45
18:R:104:ALA:O	18:R:108:TYR:N	2.33	0.45
18:R:467:ARG:CZ	18:R:603:GLU:HG3	2.46	0.45
18:R:469:ILE:HG22	18:R:474:PHE:O	2.15	0.45
1:A:58:MET:HG2	1:A:266:VAL:HG23	1.98	0.45
1:A:232:LYS:HD3	16:P:315:TRP:HH2	1.73	0.45
1:A:284:ASP:O	1:A:287:VAL:N	2.49	0.45
1:A:629:LYS:HG3	1:A:651:PHE:CE1	2.51	0.45
1:A:1002:ARG:O	1:A:1005:TYR:N	2.50	0.45
1:A:1378:LYS:CG	1:A:1379:MET:H	2.18	0.45
2:B:248:ALA:HB3	2:B:308:LYS:HG2	1.99	0.45
2:B:621:ARG:HG2	2:B:644:GLY:O	2.16	0.45
2:B:772:VAL:HG13	2:B:943:ILE:CG2	2.37	0.45
5:E:181:ALA:HA	5:E:186:LEU:HD21	1.98	0.45
7:G:203:ASP:O	7:G:205:MET:HG2	2.16	0.45
13:M:159:TYR:CG	13:M:170:LEU:HD21	2.52	0.45
14:N:310:PRO:HD3	14:N:418:VAL:HB	1.97	0.45
15:O:202:GLN:HA	15:O:280:LEU:HA	1.99	0.45
15:O:292:ARG:NH2	15:O:653:MET:O	2.49	0.45
16:P:120:VAL:HA	16:P:123:LYS:HE3	1.98	0.45
18:R:132:VAL:HG12	18:R:161:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:478:PHE:HB3	18:R:599:PRO:HA	1.98	0.45
18:R:540:LEU:HD22	18:R:549:ILE:HA	1.98	0.45
18:R:587:THR:O	18:R:590:THR:OG1	2.31	0.45
18:R:610:LEU:HA	18:R:613:HIS:HD2	1.81	0.45
20:X:16:DT:H2''	20:X:17:DA:O4'	2.17	0.45
1:A:48:PRO:C	1:A:49:LYS:HG2	2.42	0.45
1:A:207:HIS:C	1:A:209:PRO:HD3	2.41	0.45
1:A:365:ARG:CD	1:A:887:ARG:HH21	2.29	0.45
1:A:665:ASP:OD1	1:A:797:CYS:HA	2.15	0.45
1:A:1431:VAL:HB	6:F:133:VAL:HG13	1.98	0.45
2:B:241:TYR:HE1	2:B:252:PRO:HG3	1.81	0.45
2:B:349:ILE:HA	2:B:352:MET:HE2	1.97	0.45
2:B:681:LEU:HD21	2:B:691:PRO:HG2	1.98	0.45
4:D:102:SER:HA	4:D:105:GLU:HB2	1.98	0.45
5:E:162:ARG:O	5:E:166:LYS:HG2	2.17	0.45
5:E:200:ARG:HD2	5:E:208:TYR:CE2	2.51	0.45
6:F:84:TYR:HD1	6:F:152:ILE:HG23	1.81	0.45
6:F:133:VAL:HG23	6:F:146:TRP:C	2.41	0.45
15:O:94:THR:O	15:O:98:LEU:HG	2.16	0.45
15:O:338:ASP:O	15:O:342:ALA:N	2.30	0.45
15:O:516:LEU:O	15:O:516:LEU:HG	2.15	0.45
16:P:202:PRO:HD2	16:P:204:LYS:CE	2.45	0.45
1:A:15:GLY:O	1:A:16:LEU:HD12	2.17	0.45
1:A:285:LEU:HD21	1:A:353:PHE:CD1	2.51	0.45
1:A:356:ARG:HE	1:A:363:ARG:NH2	2.14	0.45
1:A:391:GLU:HA	1:A:488:HIS:HB3	1.98	0.45
1:A:580:LEU:HD23	11:K:88:PHE:CE1	2.51	0.45
1:A:864:HIS:HE2	2:B:695:GLN:CA	2.29	0.45
2:B:89:PRO:HA	19:S:383:ARG:HD2	1.99	0.45
2:B:462:SER:HB3	2:B:709:ALA:O	2.16	0.45
2:B:614:ILE:HG12	2:B:672:HIS:CD2	2.52	0.45
3:C:89:THR:HG21	3:C:200:GLN:HA	1.99	0.45
3:C:120:LEU:HA	3:C:121:PRO:HD3	1.77	0.45
11:K:69:ASP:CG	11:K:70:HIS:H	2.22	0.45
15:O:39:GLN:O	15:O:47:PHE:HZ	2.00	0.45
15:O:650:VAL:HG13	15:O:651:PHE:CD2	2.52	0.45
16:P:60:LEU:O	16:P:75:VAL:HG12	2.17	0.45
18:R:121:ARG:HB2	18:R:124:ASN:ND2	2.24	0.45
18:R:422:PRO:HB2	18:R:634:PHE:CZ	2.51	0.45
19:S:517:GLU:HA	19:S:520:LYS:CD	2.35	0.45
21:Y:2:DC:H2''	21:Y:3:DG:OP2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASP:OD1	1:A:147:GLN:N	2.49	0.45
1:A:483:LEU:O	1:A:486:LEU:HD11	2.15	0.45
1:A:598:MET:HB2	8:H:96:VAL:HB	1.99	0.45
1:A:615:LYS:CG	1:A:620:SER:OG	2.64	0.45
1:A:835:PHE:CE2	1:A:844:SER:HA	2.51	0.45
1:A:887:ARG:O	1:A:890:MET:HB3	2.17	0.45
1:A:1221:ASP:OD1	1:A:1222:VAL:N	2.49	0.45
2:B:637:PHE:C	2:B:639:ASP:H	2.25	0.45
2:B:738:THR:HB	2:B:741:ILE:HD12	1.98	0.45
2:B:738:THR:HA	2:B:976:GLY:O	2.16	0.45
2:B:757:VAL:HA	2:B:942:ILE:O	2.17	0.45
2:B:843:ILE:HG22	2:B:871:VAL:HG12	1.98	0.45
4:D:114:LYS:HB2	4:D:145:PHE:CE1	2.52	0.45
5:E:86:PRO:O	5:E:115:ASN:HB3	2.16	0.45
6:F:81:THR:HG22	6:F:82:THR:N	2.31	0.45
7:G:96:GLY:HA2	7:G:112:GLN:HG3	1.97	0.45
7:G:123:PRO:O	7:G:124:GLU:HB2	2.16	0.45
10:J:9:SER:OG	10:J:10:CYS:N	2.50	0.45
12:L:28:LYS:HB3	12:L:29:TYR:CD2	2.51	0.45
13:M:155:ASN:OD1	13:M:155:ASN:N	2.49	0.45
15:O:468:LEU:HG	15:O:478:VAL:CG1	2.47	0.45
15:O:579:GLN:HG2	16:P:315:TRP:CH2	2.52	0.45
16:P:118:GLN:HE21	16:P:122:LEU:HD11	1.80	0.45
21:Y:18:DG:O6	21:Y:19:DC:N4	2.50	0.45
1:A:30:SER:CB	1:A:82:GLY:CA	2.90	0.45
1:A:40:PHE:O	1:A:47:ALA:HA	2.16	0.45
1:A:410:ARG:NE	6:F:104:ASN:OD1	2.49	0.45
2:B:59:LYS:O	2:B:63:ASP:N	2.39	0.45
2:B:76:ILE:HD12	2:B:389:GLU:OE1	2.16	0.45
2:B:95:TYR:HD1	2:B:133:ILE:HG12	1.80	0.45
2:B:1095:CYS:O	2:B:1099:GLY:HA2	2.17	0.45
8:H:1:MET:HG2	8:H:3:ASN:ND2	2.31	0.45
13:M:149:LYS:HB3	13:M:182:PHE:HE1	1.82	0.45
15:O:600:SER:HA	15:O:603:LEU:HD12	1.98	0.45
15:O:623:GLU:OE1	15:O:624:LEU:HD12	2.17	0.45
18:R:262:PHE:O	18:R:265:THR:OG1	2.29	0.45
20:X:67:DT:H2''	20:X:68:DT:OP2	2.16	0.45
21:Y:64:DA:H2'	21:Y:65:DC:C6	2.51	0.45
1:A:289:LEU:HA	1:A:292:ILE:HB	1.99	0.45
1:A:366:GLY:HA3	2:B:1061:ARG:HH22	1.82	0.45
1:A:582:MET:CE	1:A:703:ARG:HB3	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:MET:HA	1:A:700:LEU:HB2	1.98	0.45
1:A:678:PHE:CZ	1:A:694:MET:HG2	2.51	0.45
1:A:968:GLY:O	1:A:970:LEU:N	2.48	0.45
2:B:767:ILE:HG22	2:B:768:GLU:N	2.31	0.45
2:B:911:LYS:HD3	2:B:1029:HIS:HB2	1.97	0.45
7:G:157:ASP:OD1	7:G:158:VAL:N	2.45	0.45
15:O:167:GLY:O	15:O:281:THR:HG23	2.17	0.45
15:O:329:PRO:C	15:O:330:LEU:HG	2.42	0.45
18:R:97:PRO:HD2	18:R:100:ILE:HD12	1.97	0.45
18:R:604:ASP:OD1	18:R:605:VAL:N	2.50	0.45
1:A:14:LYS:HB2	2:B:1144:GLU:OE2	2.17	0.45
1:A:1154:ALA:HB1	1:A:1283:ILE:HD12	1.99	0.45
2:B:59:LYS:HA	2:B:62:LEU:HB2	1.99	0.45
2:B:244:HIS:CE1	2:B:333:ALA:CB	2.97	0.45
2:B:796:LYS:HE2	2:B:798:TYR:CE1	2.52	0.45
3:C:96:VAL:O	3:C:100:ARG:HG2	2.17	0.45
4:D:19:PHE:O	4:D:22:ASP:HB2	2.16	0.45
7:G:201:GLN:OE1	7:G:201:GLN:N	2.42	0.45
13:M:72:GLU:OE1	14:N:364:ARG:NH2	2.43	0.45
15:O:328:ASP:OD1	15:O:328:ASP:N	2.49	0.45
18:R:142:MET:SD	18:R:219:ARG:NH2	2.90	0.45
18:R:397:VAL:HB	18:R:485:ASN:HB3	1.99	0.45
1:A:108:LYS:N	1:A:108:LYS:HD2	2.31	0.45
1:A:679:TYR:OH	1:A:927:GLU:HA	2.16	0.45
1:A:814:GLY:HA2	1:A:848:VAL:H	1.82	0.45
1:A:1448:PHE:HZ	4:D:16:VAL:CG2	2.29	0.45
1:A:1448:PHE:HD1	4:D:14:TYR:CE2	2.35	0.45
2:B:281:ASP:OD1	2:B:282:ILE:N	2.50	0.45
2:B:464:ILE:HD11	2:B:746:TYR:CE1	2.52	0.45
2:B:780:ARG:HE	3:C:217:ALA:HB1	1.81	0.45
7:G:53:THR:CG2	7:G:71:THR:HG22	2.47	0.45
16:P:18:LEU:HD11	16:P:36:LEU:HD11	1.99	0.45
16:P:26:GLY:O	16:P:31:PHE:HB2	2.17	0.45
16:P:60:LEU:O	16:P:75:VAL:N	2.48	0.45
16:P:102:ARG:HB3	16:P:155:PRO:HG2	1.99	0.45
16:P:217:THR:O	16:P:218:THR:OG1	2.35	0.45
21:Y:22:DT:H2"	21:Y:23:DG:H8	1.82	0.45
1:A:654:ILE:HG23	1:A:658:GLN:C	2.43	0.44
1:A:904:VAL:HG13	1:A:912:VAL:HG23	1.99	0.44
1:A:1448:PHE:CD1	4:D:14:TYR:CE2	3.05	0.44
2:B:909:GLY:HA2	2:B:921:VAL:CG1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1091:GLU:HA	2:B:1120:THR:HA	1.99	0.44
3:C:15:THR:HG22	3:C:16:THR:N	2.32	0.44
3:C:20:PHE:CE2	3:C:22:GLY:HA3	2.52	0.44
3:C:222:VAL:HG11	3:C:225:ALA:HB2	1.99	0.44
6:F:143:PHE:O	6:F:144:GLU:HB2	2.17	0.44
15:O:596:LYS:O	15:O:600:SER:N	2.50	0.44
16:P:311:TYR:CD2	17:Q:37:PRO:HG2	2.52	0.44
18:R:130:LEU:HD23	18:R:146:PHE:CE1	2.52	0.44
1:A:128:ARG:NH2	1:A:240:GLU:OE2	2.49	0.44
1:A:484:SER:N	2:B:1069:CYS:SG	2.90	0.44
1:A:801:GLY:N	2:B:951:SER:OG	2.50	0.44
1:A:815:GLN:NE2	1:A:847:PHE:HB2	2.32	0.44
1:A:862:LEU:HD22	2:B:494:PHE:HD1	1.81	0.44
1:A:1171:PHE:CD2	1:A:1172:TYR:HD2	2.36	0.44
1:A:1187:ARG:HA	1:A:1228:ASP:O	2.17	0.44
2:B:539:GLU:OE1	2:B:539:GLU:N	2.50	0.44
2:B:886:MET:HG2	2:B:896:ILE:HG12	1.99	0.44
3:C:211:GLY:HA3	3:C:219:PHE:CE2	2.52	0.44
4:D:5:GLU:OE2	4:D:8:ASN:HA	2.17	0.44
5:E:65:THR:HG23	5:E:66:GLU:HG2	1.99	0.44
6:F:151:LEU:HD23	6:F:152:ILE:N	2.32	0.44
9:I:33:PHE:CE2	9:I:35:ILE:HA	2.52	0.44
15:O:141:ILE:HA	15:O:144:MET:CB	2.45	0.44
15:O:271:LEU:HD23	15:O:272:ARG:N	2.32	0.44
15:O:362:ASN:HD21	15:O:478:VAL:HG23	1.82	0.44
16:P:103:GLU:OE1	16:P:103:GLU:N	2.45	0.44
16:P:126:LYS:O	16:P:129:GLU:HB3	2.17	0.44
16:P:309:VAL:HG21	16:P:311:TYR:CZ	2.52	0.44
18:R:287:PRO:HD2	18:R:290:PHE:HE1	1.83	0.44
18:R:529:VAL:HG11	20:X:12:DT:H4'	1.99	0.44
18:R:601:ASN:HB3	18:R:604:ASP:OD2	2.16	0.44
20:X:65:DA:H2''	20:X:66:DG:C8	2.53	0.44
1:A:291:GLU:OE1	1:A:322:THR:HG21	2.18	0.44
1:A:506:THR:OG1	1:A:507:PRO:HD3	2.18	0.44
1:A:597:ILE:HG12	1:A:603:LEU:HB2	1.99	0.44
1:A:646:SER:O	8:H:25:ARG:NH2	2.51	0.44
1:A:697:MET:O	1:A:700:LEU:HB3	2.17	0.44
1:A:884:TYR:CE2	1:A:888:ARG:HD3	2.52	0.44
1:A:1052:VAL:O	1:A:1055:SER:HB3	2.17	0.44
3:C:78:VAL:HG23	3:C:209:ILE:C	2.42	0.44
3:C:157:TYR:CG	3:C:198:PRO:HD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:42:LYS:HG3	10:J:43:ARG:N	2.32	0.44
13:M:115:LYS:O	13:M:175:ARG:NH2	2.49	0.44
15:O:39:GLN:O	15:O:47:PHE:CZ	2.70	0.44
15:O:507:LEU:HD12	15:O:508:SER:N	2.31	0.44
16:P:87:SER:O	16:P:91:ALA:N	2.50	0.44
16:P:252:LYS:HD3	16:P:266:GLU:CD	2.42	0.44
18:R:598:ASP:HB3	18:R:601:ASN:OD1	2.17	0.44
18:R:636:LEU:HD13	19:S:502:LEU:HD21	1.98	0.44
1:A:57:LYS:HB2	1:A:69:THR:HG23	1.99	0.44
1:A:739:ASP:O	1:A:743:THR:N	2.28	0.44
1:A:920:GLY:O	1:A:1083:LEU:N	2.28	0.44
1:A:1164:THR:CB	1:A:1271:VAL:HA	2.48	0.44
1:A:1175:ASP:OD1	1:A:1184:ILE:HA	2.17	0.44
1:A:1392:THR:OG1	1:A:1393:THR:N	2.50	0.44
2:B:87:VAL:O	19:S:383:ARG:NH1	2.50	0.44
2:B:740:THR:O	2:B:743:LEU:HB2	2.17	0.44
2:B:1103:TYR:C	2:B:1104:SER:HG	2.25	0.44
3:C:235:ILE:C	3:C:236:LEU:HD12	2.43	0.44
4:D:134:LEU:HD12	4:D:135:TYR:N	2.31	0.44
5:E:80:VAL:HG23	5:E:109:ILE:HD11	1.98	0.44
6:F:85:MET:HE3	6:F:153:VAL:HG12	1.99	0.44
7:G:97:ILE:HD13	7:G:140:PHE:CZ	2.53	0.44
8:H:38:LEU:CD2	8:H:40:LEU:HB2	2.47	0.44
8:H:79:TRP:CH2	8:H:81:PRO:HA	2.53	0.44
10:J:52:THR:HG22	10:J:53:HIS:N	2.30	0.44
11:K:61:ALA:HB1	11:K:63:PHE:CE1	2.53	0.44
11:K:68:GLU:HG3	11:K:69:ASP:N	2.31	0.44
15:O:490:SER:O	15:O:493:GLU:HG2	2.18	0.44
15:O:630:VAL:C	15:O:633:ARG:HB3	2.43	0.44
20:X:70:DG:H2"	20:X:71:DT:OP2	2.16	0.44
20:X:73:DA:H2"	20:X:74:DA:H8	1.82	0.44
1:A:216:LYS:HG3	1:A:217:ARG:N	2.32	0.44
1:A:371:LYS:NZ	2:B:1049:GLN:OE1	2.36	0.44
1:A:408:VAL:HG13	1:A:458:ILE:O	2.17	0.44
1:A:923:PRO:HA	1:A:926:MET:HE2	2.00	0.44
2:B:58:VAL:HG12	2:B:62:LEU:HD13	1.99	0.44
2:B:619:GLN:OE1	2:B:619:GLN:N	2.51	0.44
2:B:843:ILE:CG2	2:B:871:VAL:HG12	2.47	0.44
2:B:1040:ARG:HB3	18:R:35:ASN:HD21	1.82	0.44
3:C:195:LYS:NZ	10:J:58:GLU:OE2	2.48	0.44
5:E:115:ASN:OD1	5:E:116:ILE:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:55:GLU:OE2	7:G:69:ASN:N	2.51	0.44
7:G:190:LYS:NZ	7:G:192:PRO:HG3	2.32	0.44
15:O:273:ILE:HG23	15:O:274:VAL:O	2.18	0.44
18:R:432:ILE:HG13	18:R:434:GLU:H	1.81	0.44
1:A:6:VAL:O	7:G:33:LYS:NZ	2.50	0.44
1:A:157:CYS:SG	1:A:158:GLY:N	2.91	0.44
1:A:239:CYS:O	1:A:242:LEU:N	2.51	0.44
1:A:535:MET:HE2	2:B:1073:TYR:CD2	2.45	0.44
1:A:792:LEU:HD21	8:H:19:ARG:NH2	2.33	0.44
1:A:900:TYR:CD1	1:A:1085:PRO:HG2	2.53	0.44
1:A:1257:PHE:O	1:A:1260:MET:HB3	2.17	0.44
2:B:178:PRO:HD2	2:B:715:TYR:HD2	1.83	0.44
2:B:735:MET:HB2	2:B:754:ASN:ND2	2.28	0.44
3:C:216:HIS:NE2	12:L:70:ARG:HB2	2.33	0.44
6:F:117:PRO:O	6:F:120:ILE:HG13	2.18	0.44
8:H:123:MET:HE2	8:H:125:LEU:HD23	1.99	0.44
13:M:253:GLU:O	13:M:257:ASP:N	2.45	0.44
16:P:247:LEU:O	16:P:252:LYS:N	2.50	0.44
18:R:251:ALA:HB3	18:R:254:THR:OG1	2.18	0.44
19:S:413:ARG:CZ	20:X:9:DA:H3'	2.47	0.44
1:A:43:GLU:O	1:A:45:ASP:N	2.51	0.44
1:A:381:ILE:HG22	1:A:382:SER:N	2.33	0.44
1:A:483:LEU:HD22	1:A:486:LEU:HD11	1.99	0.44
2:B:247:ILE:HG13	2:B:248:ALA:N	2.31	0.44
2:B:426:SER:O	2:B:428:ASN:N	2.50	0.44
2:B:647:GLU:OE1	2:B:647:GLU:N	2.51	0.44
2:B:987:MET:CA	2:B:990:ILE:HB	2.47	0.44
3:C:33:VAL:CG1	3:C:34:GLU:H	2.29	0.44
3:C:85:PHE:HB2	12:L:65:VAL:HG13	1.98	0.44
3:C:121:PRO:O	3:C:124:GLU:HB2	2.18	0.44
5:E:17:ARG:HG3	5:E:35:VAL:HG22	2.00	0.44
8:H:65:LEU:HB2	8:H:89:LEU:HB2	1.98	0.44
10:J:34:THR:HA	10:J:37:SER:HB2	1.99	0.44
11:K:81:MET:HE2	11:K:89:CYS:SG	2.57	0.44
13:M:87:VAL:HG13	13:M:176:VAL:HG13	2.00	0.44
18:R:219:ARG:HH11	18:R:220:PRO:CD	2.29	0.44
18:R:219:ARG:HB2	18:R:514:GLU:OE1	2.18	0.44
18:R:546:ARG:HH12	18:R:591:TYR:HE2	1.66	0.44
1:A:60:VAL:HG23	1:A:74:LEU:HD23	1.99	0.44
1:A:865:ALA:HA	2:B:696:SER:OG	2.18	0.44
1:A:891:LYS:HE3	2:B:1064:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:GLY:HA3	5:E:179:GLN:HG3	2.00	0.44
2:B:135:TYR:CD2	2:B:419:LEU:HD11	2.53	0.44
2:B:317:LEU:O	2:B:320:LEU:HG	2.18	0.44
2:B:914:SER:C	2:B:916:HIS:H	2.25	0.44
3:C:5:VAL:HG23	3:C:7:ILE:HD11	1.99	0.44
3:C:67:PHE:CE1	3:C:318:VAL:HG22	2.53	0.44
5:E:153:HIS:CE1	5:E:184:VAL:HG11	2.53	0.44
9:I:30:PRO:HB3	13:M:135:LYS:HD3	1.99	0.44
18:R:583:HIS:NE2	18:R:585:LEU:O	2.51	0.44
20:X:70:DG:H1'	20:X:71:DT:O5'	2.17	0.44
21:Y:3:DG:H1'	21:Y:4:DC:H5'	1.98	0.44
1:A:153:ARG:HA	1:A:160:LEU:HA	1.99	0.44
1:A:323:VAL:O	1:A:326:TYR:HB3	2.18	0.44
1:A:516:GLU:OE2	2:B:1034:LYS:HD3	2.17	0.44
1:A:692:ASN:O	1:A:696:ARG:HG2	2.18	0.44
1:A:949:ASN:HD21	8:H:135:LEU:HD23	1.81	0.44
1:A:1373:ARG:HG3	1:A:1374:PHE:N	2.31	0.44
2:B:410:PRO:HA	2:B:414:MET:SD	2.58	0.44
2:B:901:ARG:NE	3:C:93:GLN:HE21	2.15	0.44
2:B:1003:MET:HE1	3:C:293:ARG:NE	2.32	0.44
3:C:33:VAL:CG1	3:C:34:GLU:N	2.80	0.44
5:E:111:VAL:HG13	5:E:135:PHE:HB2	2.00	0.44
8:H:114:VAL:O	8:H:124:ARG:HA	2.18	0.44
14:N:291:LEU:O	14:N:294:LEU:HB3	2.17	0.44
15:O:220:GLU:HG2	15:O:221:LYS:H	1.83	0.44
15:O:239:SER:O	15:O:243:MET:HG2	2.18	0.44
15:O:602:LEU:HD22	15:O:626:GLN:HE21	1.83	0.44
16:P:14:ASN:HB3	16:P:51:ILE:HD13	2.00	0.44
19:S:422:VAL:O	19:S:426:ILE:HG23	2.18	0.44
19:S:434:MET:HB2	19:S:435:TRP:CE3	2.53	0.44
1:A:51:ASN:CG	1:A:52:GLY:H	2.24	0.43
1:A:205:LEU:O	1:A:209:PRO:HG3	2.18	0.43
1:A:237:ALA:N	15:O:70:ALA:O	2.46	0.43
1:A:320:GLN:HA	1:A:323:VAL:HG12	2.00	0.43
1:A:371:LYS:HE3	2:B:1087:SER:HB3	2.00	0.43
1:A:429:GLY:O	1:A:465:HIS:ND1	2.32	0.43
1:A:524:THR:H	2:B:1081:GLU:HG3	1.82	0.43
1:A:571:TYR:HH	1:A:704:PHE:HZ	1.63	0.43
2:B:185:PHE:CZ	2:B:384:ILE:HD11	2.53	0.43
2:B:385:SER:HG	2:B:386:LEU:H	1.66	0.43
2:B:405:LYS:HG2	2:B:408:LYS:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1006:SER:OG	2:B:1009:THR:N	2.50	0.43
5:E:48:ASP:O	5:E:51:GLY:N	2.50	0.43
5:E:145:THR:HG21	5:E:187:TYR:CZ	2.53	0.43
7:G:88:TRP:HD1	7:G:89:ILE:O	2.01	0.43
7:G:104:ILE:HG23	7:G:105:PHE:N	2.29	0.43
8:H:128:ASN:CG	8:H:129:TYR:N	2.74	0.43
11:K:47:ILE:HG21	11:K:63:PHE:HB3	2.00	0.43
13:M:159:TYR:CE2	14:N:309:LEU:HB2	2.51	0.43
14:N:365:VAL:HG13	14:N:370:LYS:O	2.18	0.43
15:O:73:ARG:CB	15:O:121:TYR:HE1	2.29	0.43
16:P:256:VAL:O	16:P:260:CYS:HB3	2.18	0.43
16:P:314:GLU:O	16:P:315:TRP:HB2	2.18	0.43
18:R:431:ARG:HG3	18:R:438:THR:HA	1.99	0.43
21:Y:61:DA:H5'	21:Y:61:DA:C8	2.52	0.43
21:Y:69:DT:H6	21:Y:69:DT:H2'	1.60	0.43
1:A:43:GLU:C	1:A:45:ASP:H	2.26	0.43
1:A:575:THR:CG2	1:A:576:LEU:N	2.81	0.43
1:A:1261:GLN:HG2	2:B:288:GLU:HG2	1.99	0.43
1:A:1286:ARG:N	1:A:1290:LYS:O	2.31	0.43
2:B:59:LYS:HZ1	2:B:519:HIS:CG	2.35	0.43
2:B:203:ASN:N	2:B:220:VAL:O	2.34	0.43
2:B:629:LYS:O	2:B:635:LEU:HB2	2.18	0.43
3:C:21:PRO:HB3	3:C:28:GLU:N	2.32	0.43
3:C:273:ASP:CG	3:C:275:VAL:H	2.27	0.43
5:E:133:GLU:HG2	5:E:135:PHE:CE2	2.54	0.43
14:N:292:ARG:O	14:N:296:LYS:HG2	2.18	0.43
14:N:304:PHE:HD2	14:N:396:ALA:HB3	1.83	0.43
15:O:620:LEU:HD23	15:O:623:GLU:HB2	2.00	0.43
17:Q:56:VAL:O	17:Q:60:ASN:N	2.35	0.43
20:X:8:DT:H6	20:X:8:DT:H2'	1.68	0.43
21:Y:63:DT:H73	21:Y:64:DA:H62	1.83	0.43
1:A:83:HIS:O	1:A:83:HIS:CG	2.70	0.43
1:A:409:THR:N	1:A:412:ASN:HD22	2.14	0.43
1:A:572:ASP:OD1	1:A:575:THR:CG2	2.65	0.43
1:A:762:LEU:O	1:A:766:ILE:HG22	2.18	0.43
1:A:949:ASN:HA	1:A:1061:ARG:HH21	1.82	0.43
2:B:274:GLY:HA2	2:B:549:LEU:HD13	2.00	0.43
2:B:405:LYS:HA	2:B:408:LYS:HG3	2.00	0.43
2:B:1049:GLN:HB2	2:B:1050:PRO:HD2	1.99	0.43
3:C:239:ILE:HG21	3:C:288:LYS:HB3	1.98	0.43
3:C:278:GLU:HB3	3:C:281:ARG:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:115:LEU:N	7:G:199:SER:HB3	2.33	0.43
13:M:72:GLU:OE1	14:N:364:ARG:NE	2.49	0.43
15:O:127:ILE:HG23	15:O:130:LEU:HB2	2.00	0.43
15:O:218:LEU:HD21	15:O:248:ASP:HB2	2.00	0.43
16:P:191:PHE:HB3	16:P:203:LYS:HD2	2.00	0.43
18:R:159:ALA:O	18:R:163:LYS:HG2	2.17	0.43
1:A:14:LYS:HB2	2:B:1144:GLU:CD	2.43	0.43
1:A:359:GLY:O	1:A:362:GLY:N	2.43	0.43
1:A:380:VAL:O	1:A:497:THR:OG1	2.36	0.43
1:A:661:SER:HB2	8:H:122:LEU:HD11	2.00	0.43
1:A:1145:LEU:HB3	1:A:1309:VAL:HG12	1.99	0.43
2:B:48:LEU:HB3	2:B:49:PRO:HD3	2.00	0.43
2:B:554:GLY:HA2	2:B:564:SER:HB2	1.99	0.43
2:B:933:PHE:CZ	2:B:1005:TYR:HB2	2.54	0.43
3:C:40:PHE:CD2	11:K:134:LYS:HG3	2.52	0.43
3:C:99:HIS:HA	12:L:69:ALA:HB1	2.00	0.43
5:E:93:MET:HE2	5:E:93:MET:HB3	1.78	0.43
8:H:43:ASN:HD21	8:H:46:LEU:HD13	1.83	0.43
10:J:36:LEU:HA	10:J:39:LEU:HB3	2.00	0.43
15:O:53:VAL:HG21	15:O:65:ILE:HD12	2.01	0.43
15:O:532:ASP:O	15:O:536:THR:HG22	2.18	0.43
16:P:142:PHE:HA	16:P:143:PRO:HD3	1.87	0.43
19:S:390:GLU:HG2	19:S:393:TYR:CE2	2.53	0.43
1:A:401:VAL:O	2:B:1039:ALA:HB2	2.19	0.43
1:A:1202:ILE:O	1:A:1205:ILE:N	2.52	0.43
1:A:1445:ARG:HG3	1:A:1447:LEU:H	1.83	0.43
2:B:384:ILE:O	2:B:388:PHE:HB3	2.18	0.43
2:B:498:CYS:SG	2:B:500:ALA:N	2.92	0.43
2:B:781:GLY:HA2	3:C:99:HIS:HE1	1.83	0.43
2:B:841:ILE:HD13	2:B:872:ILE:HG13	2.00	0.43
2:B:849:THR:HG22	2:B:865:GLN:HB3	2.01	0.43
2:B:912:PHE:HE1	2:B:1026:LYS:HG3	1.84	0.43
7:G:115:LEU:HA	7:G:200:CYS:O	2.19	0.43
15:O:312:TYR:CD1	15:O:468:LEU:HD21	2.53	0.43
15:O:579:GLN:O	15:O:583:TRP:CD1	2.71	0.43
15:O:632:GLU:HA	15:O:635:LEU:HD12	2.01	0.43
18:R:533:PHE:CZ	21:Y:69:DT:H1'	2.53	0.43
19:S:446:TYR:CB	19:S:449:ARG:HB3	2.48	0.43
20:X:5:DA:H4'	20:X:6:DC:OP1	2.18	0.43
1:A:897:SER:O	1:A:904:VAL:HG23	2.19	0.43
1:A:997:GLN:C	1:A:999:ASP:N	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:LEU:O	1:A:1033:GLU:CB	2.64	0.43
1:A:1202:ILE:O	1:A:1206:ALA:N	2.31	0.43
2:B:145:LYS:HG3	19:S:399:GLU:HB3	2.01	0.43
2:B:531:LYS:HA	2:B:534:TYR:HD2	1.83	0.43
3:C:247:PHE:CE1	3:C:289:VAL:HG21	2.53	0.43
9:I:5:CYS:SG	9:I:9:ASN:N	2.92	0.43
10:J:44:TYR:HA	10:J:47:ARG:HB3	2.00	0.43
11:K:110:GLU:OE2	11:K:111:THR:HG23	2.18	0.43
13:M:147:THR:C	13:M:148:LEU:HD12	2.44	0.43
14:N:364:ARG:O	14:N:371:LEU:HD12	2.17	0.43
15:O:581:LEU:O	15:O:585:MET:HB2	2.19	0.43
16:P:179:LEU:O	16:P:182:VAL:HG12	2.19	0.43
18:R:402:LEU:HD13	18:R:476:ALA:HB1	2.00	0.43
19:S:466:PRO:O	19:S:470:GLU:HG2	2.18	0.43
1:A:18:PHE:CD1	2:B:1139:PRO:CB	2.97	0.43
1:A:33:GLU:CA	1:A:83:HIS:CE1	3.02	0.43
1:A:126:GLU:OE1	1:A:127:LEU:HD12	2.18	0.43
1:A:374:ASP:CG	1:A:375:PHE:H	2.27	0.43
1:A:505:CYS:O	1:A:509:ASN:N	2.51	0.43
1:A:933:VAL:HG11	1:A:935:PHE:CZ	2.54	0.43
1:A:1338:GLU:O	1:A:1341:TYR:N	2.52	0.43
2:B:58:VAL:HA	2:B:60:GLN:OE1	2.18	0.43
2:B:383:LEU:HB3	2:B:442:TRP:CH2	2.54	0.43
2:B:395:PHE:HE1	2:B:425:HIS:O	2.01	0.43
2:B:476:GLN:HG2	2:B:477:PHE:H	1.84	0.43
2:B:529:ILE:HD13	2:B:584:VAL:HG11	2.00	0.43
3:C:190:ASP:O	10:J:16:ASP:HB3	2.17	0.43
3:C:230:LEU:HD22	3:C:297:HIS:ND1	2.34	0.43
4:D:23:LEU:O	4:D:27:HIS:N	2.47	0.43
7:G:151:GLU:N	7:G:197:LEU:O	2.36	0.43
9:I:5:CYS:HB3	9:I:10:ASN:N	2.34	0.43
9:I:11:MET:HG3	9:I:12:LEU:O	2.19	0.43
13:M:227:LEU:O	13:M:232:LEU:HD13	2.18	0.43
15:O:496:ILE:HA	15:O:499:THR:CB	2.48	0.43
15:O:538:ALA:O	15:O:542:ARG:HG3	2.18	0.43
16:P:14:ASN:O	16:P:18:LEU:CB	2.66	0.43
16:P:142:PHE:CE2	16:P:144:THR:HB	2.53	0.43
16:P:186:ILE:HG22	16:P:263:VAL:HG22	2.00	0.43
19:S:438:ASP:O	19:S:442:ILE:HG13	2.19	0.43
1:A:238:ASP:CG	1:A:239:CYS:H	2.26	0.43
1:A:240:GLU:N	1:A:240:GLU:OE1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:TYR:CE1	1:A:1401:PHE:HD1	2.37	0.43
2:B:39:ASN:HB3	2:B:42:GLN:HB2	2.00	0.43
2:B:649:LEU:HD22	2:B:653:GLU:CD	2.43	0.43
2:B:729:THR:HG22	2:B:730:TYR:CE1	2.54	0.43
2:B:982:SER:HB3	2:B:987:MET:HE2	2.00	0.43
3:C:19:ASP:O	3:C:29:ASN:HB3	2.19	0.43
3:C:89:THR:HG22	3:C:201:GLU:H	1.83	0.43
4:D:12:SER:OG	4:D:14:TYR:CE2	2.72	0.43
4:D:20:LEU:O	4:D:24:GLU:HB3	2.18	0.43
8:H:6:PHE:HE2	8:H:8:ASP:HB2	1.81	0.43
13:M:173:ILE:O	13:M:173:ILE:HG13	2.18	0.43
15:O:262:ILE:O	15:O:274:VAL:HA	2.19	0.43
15:O:517:VAL:O	15:O:518:SER:CB	2.59	0.43
18:R:399:THR:O	18:R:481:PHE:HA	2.19	0.43
19:S:382:ASP:O	19:S:383:ARG:HB3	2.18	0.43
1:A:89:PRO:HB3	1:A:228:LEU:HD13	2.00	0.43
1:A:105:GLY:HA2	1:A:148:CYS:SG	2.58	0.43
1:A:409:THR:O	1:A:410:ARG:C	2.61	0.43
1:A:479:SER:O	2:B:1065:MET:CE	2.64	0.43
1:A:610:PHE:O	1:A:613:LEU:HB3	2.19	0.43
1:A:714:ILE:HG13	1:A:718:THR:OG1	2.19	0.43
1:A:809:MET:HE1	2:B:950:PRO:HA	2.00	0.43
1:A:955:LEU:O	1:A:959:ILE:HG13	2.19	0.43
1:A:1305:CYS:SG	5:E:141:VAL:HG11	2.58	0.43
2:B:536:LEU:HD22	2:B:571:PHE:CD1	2.50	0.43
2:B:947:HIS:C	2:B:950:PRO:HD2	2.44	0.43
3:C:247:PHE:O	3:C:250:CYS:HB3	2.19	0.43
7:G:147:ARG:NH2	7:G:208:VAL:HA	2.33	0.43
7:G:152:ARG:O	7:G:197:LEU:HG	2.19	0.43
13:M:99:ARG:HG3	13:M:100:LYS:N	2.34	0.43
14:N:389:THR:HG23	14:N:390:PHE:N	2.34	0.43
15:O:460:LEU:HD22	15:O:476:TYR:HB2	2.00	0.43
15:O:530:GLU:HA	15:O:533:ILE:HB	2.00	0.43
15:O:645:LEU:O	15:O:649:GLU:HG3	2.19	0.43
18:R:467:ARG:NH1	18:R:603:GLU:HG3	2.34	0.43
19:S:409:GLY:N	21:Y:73:DT:H5"	2.34	0.43
1:A:148:CYS:SG	1:A:149:LYS:N	2.92	0.43
1:A:197:TRP:HA	1:A:200:GLU:CD	2.43	0.43
1:A:578:GLN:HG2	1:A:582:MET:SD	2.59	0.43
1:A:590:PHE:HA	1:A:617:ASN:OD1	2.19	0.43
1:A:629:LYS:HG3	1:A:651:PHE:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018:ALA:O	1:A:1021:ASN:HB2	2.19	0.43
1:A:1397:PHE:CZ	2:B:1135:MET:SD	3.11	0.43
1:A:1448:PHE:HD1	4:D:14:TYR:HE2	1.67	0.43
2:B:55:LYS:HG2	2:B:59:LYS:HD3	2.00	0.43
2:B:246:SER:OG	2:B:247:ILE:N	2.51	0.43
2:B:316:LYS:HD3	13:M:226:ARG:HE	1.84	0.43
2:B:372:VAL:HG11	2:B:608:ILE:HD12	2.00	0.43
2:B:385:SER:O	2:B:389:GLU:HG2	2.18	0.43
2:B:628:ARG:HA	2:B:631:LEU:HG	2.01	0.43
3:C:220:SER:OG	3:C:222:VAL:O	2.33	0.43
4:D:126:GLN:CG	4:D:127:LEU:N	2.82	0.43
5:E:126:SER:O	5:E:128:PRO:HD3	2.18	0.43
7:G:39:ILE:HG23	7:G:42:VAL:HG13	2.01	0.43
10:J:1:MET:HE3	10:J:60:PHE:HE2	1.84	0.43
13:M:72:GLU:H	14:N:364:ARG:HE	1.66	0.43
15:O:124:GLU:CG	15:O:126:GLY:H	2.25	0.43
15:O:199:TYR:C	15:O:200:LEU:HD12	2.44	0.43
15:O:252:ILE:O	15:O:255:LYS:HB3	2.19	0.43
15:O:330:LEU:HD13	15:O:331:THR:CG2	2.20	0.43
15:O:550:GLU:N	15:O:550:GLU:OE1	2.52	0.43
15:O:650:VAL:HG13	15:O:651:PHE:N	2.32	0.43
18:R:171:THR:HG23	18:R:173:LEU:HG	2.01	0.43
19:S:434:MET:SD	19:S:477:LEU:HD11	2.59	0.43
19:S:507:ASN:HA	19:S:510:LYS:HB3	2.00	0.43
20:X:78:DG:C5	20:X:79:DT:C4	3.06	0.43
21:Y:16:DT:H6	21:Y:16:DT:H2'	1.62	0.43
1:A:528:ARG:O	1:A:532:ILE:HG22	2.19	0.42
1:A:826:GLY:H	1:A:831:SER:HA	1.84	0.42
1:A:876:ALA:O	1:A:879:THR:OG1	2.28	0.42
1:A:1033:GLU:HB3	1:A:1034:PRO:CD	2.44	0.42
1:A:1171:PHE:HB3	1:A:1188:ILE:HA	2.00	0.42
1:A:1397:PHE:O	1:A:1400:ALA:N	2.52	0.42
2:B:566:ARG:HG3	2:B:567:PHE:CG	2.54	0.42
2:B:967:GLY:HA2	2:B:974:GLU:OE2	2.19	0.42
3:C:6:GLY:H	3:C:14:ASN:HB3	1.83	0.42
4:D:126:GLN:O	4:D:127:LEU:C	2.62	0.42
13:M:76:LEU:HA	13:M:168:VAL:O	2.19	0.42
13:M:159:TYR:CD2	13:M:170:LEU:HD11	2.54	0.42
14:N:305:MET:HG2	14:N:414:GLY:HA3	2.01	0.42
15:O:56:HIS:CG	15:O:57:LEU:HG	2.54	0.42
15:O:292:ARG:HH12	15:O:650:VAL:CB	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:332:GLN:HE22	15:O:337:GLN:CG	2.32	0.42
15:O:641:LEU:O	15:O:644:LEU:N	2.52	0.42
18:R:96:ILE:HG22	18:R:141:HIS:CE1	2.54	0.42
18:R:550:TYR:HA	18:R:553:PHE:HB3	2.01	0.42
21:Y:77:DG:H1'	21:Y:78:DA:C8	2.54	0.42
1:A:308:SER:HA	15:O:534:ARG:CD	2.49	0.42
1:A:614:ILE:O	1:A:622:VAL:HG21	2.19	0.42
1:A:633:PHE:CZ	1:A:643:ASN:HB3	2.55	0.42
1:A:818:ILE:HG21	1:A:866:ILE:HG22	2.01	0.42
1:A:1380:ARG:HH11	1:A:1385:GLN:NE2	2.08	0.42
1:A:1394:ASP:O	1:A:1398:ASP:HB3	2.18	0.42
2:B:124:THR:OG1	2:B:187:VAL:HG12	2.19	0.42
2:B:516:LEU:HD11	2:B:683:ALA:HA	2.01	0.42
4:D:129:ALA:HB3	4:D:157:ILE:HB	2.00	0.42
5:E:18:THR:O	5:E:22:MET:HB2	2.19	0.42
5:E:111:VAL:HG12	5:E:112:TYR:O	2.18	0.42
5:E:177:ARG:NH1	5:E:215:MET:HE3	2.35	0.42
6:F:131:PRO:C	6:F:132:LEU:HD12	2.44	0.42
8:H:56:THR:O	8:H:144:ILE:HA	2.18	0.42
8:H:101:ALA:HB2	8:H:116:TYR:HE1	1.83	0.42
11:K:46:LYS:HD2	11:K:46:LYS:HA	1.90	0.42
13:M:117:HIS:CG	13:M:118:LEU:H	2.37	0.42
13:M:259:ILE:O	13:M:262:GLU:HG2	2.19	0.42
15:O:133:SER:O	15:O:136:ILE:N	2.52	0.42
15:O:179:THR:OG1	15:O:181:ASP:OD2	2.36	0.42
15:O:506:ARG:O	16:P:249:TYR:HB3	2.18	0.42
16:P:45:LEU:HD22	19:S:366:LEU:HB3	2.01	0.42
16:P:137:VAL:HG21	16:P:149:MET:HG2	2.00	0.42
16:P:190:THR:HA	16:P:215:TYR:CZ	2.54	0.42
16:P:312:PHE:CD1	17:Q:41:LEU:HD11	2.51	0.42
17:Q:52:ARG:O	17:Q:55:ALA:N	2.52	0.42
18:R:419:GLU:HB2	18:R:429:ILE:HB	2.00	0.42
20:X:3:DC:H2''	20:X:4:DA:H2'	2.00	0.42
20:X:66:DG:N1	21:Y:15:DT:O2	2.51	0.42
20:X:73:DA:C6	20:X:74:DA:C6	3.07	0.42
1:A:11:LYS:HE3	2:B:1144:GLU:C	2.44	0.42
1:A:333:ASN:O	1:A:335:ALA:N	2.46	0.42
1:A:595:PRO:HA	1:A:604:TRP:CE2	2.54	0.42
1:A:605:THR:OG1	8:H:119:GLY:O	2.25	0.42
1:A:1325:VAL:HG23	1:A:1326:LEU:N	2.35	0.42
2:B:319:ILE:O	2:B:324:ILE:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:698:ARG:HE	2:B:952:ARG:HB3	1.83	0.42
2:B:763:SER:O	2:B:765:TYR:N	2.52	0.42
3:C:31:TRP:HE3	11:K:82:LYS:HD2	1.83	0.42
3:C:238:PRO:C	3:C:239:ILE:HG13	2.44	0.42
3:C:334:THR:HG23	11:K:48:LYS:HG3	2.01	0.42
7:G:119:CYS:HA	7:G:129:ILE:O	2.20	0.42
7:G:204:GLY:HA3	7:G:211:TRP:CG	2.53	0.42
8:H:37:LYS:H	8:H:126:GLU:HG2	1.84	0.42
15:O:80:VAL:HG21	15:O:87:ASP:OD1	2.18	0.42
15:O:294:LYS:HA	15:O:297:ILE:HD12	2.01	0.42
15:O:353:GLU:N	15:O:481:SER:HB3	2.34	0.42
15:O:478:VAL:HG13	15:O:479:PRO:HD2	1.99	0.42
16:P:215:TYR:O	16:P:216:SER:OG	2.32	0.42
16:P:221:ILE:HA	16:P:224:PHE:HB3	2.00	0.42
18:R:422:PRO:HA	18:R:426:ALA:HA	2.01	0.42
18:R:424:ARG:NH1	21:Y:64:DA:H4'	2.33	0.42
18:R:516:PHE:CD1	18:R:517:PRO:HD2	2.54	0.42
1:A:289:LEU:HA	1:A:292:ILE:HD12	2.00	0.42
1:A:496:ARG:O	1:A:497:THR:HB	2.19	0.42
1:A:527:ALA:O	1:A:530:GLU:HB3	2.20	0.42
1:A:794:MET:CA	1:A:797:CYS:HB2	2.40	0.42
1:A:837:LYS:O	1:A:839:SER:N	2.52	0.42
2:B:60:GLN:H	2:B:60:GLN:CD	2.24	0.42
2:B:60:GLN:HG2	2:B:520:ILE:HD12	2.01	0.42
2:B:680:ILE:HG23	2:B:681:LEU:HD12	2.02	0.42
3:C:78:VAL:HA	3:C:210:LEU:HA	2.01	0.42
5:E:11:ARG:HH21	5:E:138:ALA:HA	1.85	0.42
8:H:63:LEU:HD23	8:H:90:ALA:HB2	2.01	0.42
15:O:54:LYS:HA	15:O:58:GLY:N	2.35	0.42
15:O:259:LEU:HD22	15:O:262:ILE:HD12	2.01	0.42
18:R:512:GLU:HB2	18:R:515:LEU:HB3	2.01	0.42
20:X:5:DA:C5	20:X:6:DC:C4	3.08	0.42
1:A:18:PHE:CD1	2:B:1139:PRO:HB3	2.42	0.42
1:A:668:VAL:O	1:A:677:VAL:N	2.50	0.42
1:A:972:GLU:O	1:A:975:VAL:HG13	2.18	0.42
1:A:1145:LEU:HA	1:A:1310:ILE:N	2.23	0.42
1:A:1172:TYR:CZ	1:A:1187:ARG:HB2	2.54	0.42
2:B:212:LYS:O	2:B:214:GLY:N	2.52	0.42
2:B:325:GLU:O	2:B:328:ALA:N	2.52	0.42
2:B:969:LEU:HB3	2:B:994:GLN:OE1	2.18	0.42
2:B:1045:VAL:HG13	18:R:38:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:GLY:C	3:C:175:GLN:N	2.77	0.42
6:F:90:ARG:O	6:F:94:LEU:HB2	2.20	0.42
8:H:125:LEU:HD13	8:H:130:ARG:NH1	2.31	0.42
13:M:122:ASP:HB3	13:M:145:VAL:CG2	2.49	0.42
15:O:115:LYS:HB3	15:O:116:LYS:H	1.73	0.42
15:O:307:VAL:HG13	15:O:308:THR:N	2.31	0.42
16:P:20:SER:O	16:P:24:SER:CB	2.67	0.42
18:R:182:ILE:HD13	18:R:199:VAL:HG13	2.02	0.42
21:Y:66:DT:H2'	21:Y:67:DA:C8	2.54	0.42
1:A:91:PHE:O	1:A:258:TRP:HD1	2.02	0.42
1:A:389:ILE:HD11	1:A:503:CYS:HB2	2.01	0.42
1:A:493:ARG:HB2	1:A:499:ARG:HH21	1.83	0.42
1:A:572:ASP:H	1:A:575:THR:HG21	1.81	0.42
1:A:904:VAL:CG1	1:A:913:GLN:HB3	2.50	0.42
2:B:192:LYS:NZ	2:B:438:SER:O	2.36	0.42
2:B:682:GLY:H	2:B:685:ALA:HB3	1.85	0.42
3:C:31:TRP:HH2	11:K:127:LEU:HG	1.84	0.42
3:C:51:GLU:C	3:C:310:PRO:HG3	2.45	0.42
3:C:244:ALA:O	3:C:247:PHE:HB3	2.19	0.42
6:F:79:ARG:HB3	6:F:146:TRP:CZ2	2.55	0.42
7:G:21:ASP:HB3	7:G:24:SER:HB2	2.01	0.42
7:G:109:PHE:O	7:G:197:LEU:HA	2.20	0.42
9:I:35:ILE:HD12	9:I:36:GLU:HG2	1.99	0.42
13:M:80:GLY:N	13:M:261:LYS:HE2	2.34	0.42
15:O:41:THR:O	16:P:315:TRP:NE1	2.53	0.42
15:O:94:THR:O	15:O:97:SER:HB2	2.20	0.42
15:O:274:VAL:O	15:O:276:PRO:HD3	2.19	0.42
15:O:494:TYR:O	15:O:496:ILE:N	2.52	0.42
15:O:577:MET:HG3	15:O:651:PHE:CE2	2.54	0.42
17:Q:47:ILE:HG13	17:Q:51:GLU:CD	2.45	0.42
21:Y:62:DT:H6	21:Y:62:DT:H2'	1.59	0.42
1:A:68:ALA:O	1:A:69:THR:C	2.63	0.42
1:A:349:PRO:HA	1:A:351:ARG:NH1	2.35	0.42
1:A:399:ALA:HA	1:A:466:LEU:CD1	2.43	0.42
1:A:472:VAL:HG13	1:A:520:HIS:O	2.20	0.42
1:A:677:VAL:O	1:A:681:ILE:HG13	2.20	0.42
1:A:970:LEU:HD13	1:A:1005:TYR:CZ	2.55	0.42
1:A:1153:ALA:O	1:A:1157:VAL:HG22	2.20	0.42
1:A:1188:ILE:H	1:A:1228:ASP:HB2	1.85	0.42
1:A:1319:VAL:HA	1:A:1322:VAL:HG23	2.02	0.42
2:B:63:ASP:O	2:B:67:TYR:N	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:GLU:O	2:B:292:LYS:HG2	2.19	0.42
4:D:133:HIS:HE1	7:G:212:GLU:H	1.67	0.42
7:G:142:VAL:C	7:G:144:GLU:H	2.27	0.42
11:K:69:ASP:CG	11:K:70:HIS:N	2.77	0.42
13:M:187:ASP:O	13:M:191:VAL:HG23	2.19	0.42
15:O:183:MET:HE2	15:O:183:MET:HA	2.01	0.42
15:O:284:LEU:HD21	15:O:288:MET:HE2	2.01	0.42
15:O:352:VAL:HG13	15:O:353:GLU:N	2.33	0.42
15:O:585:MET:HE1	15:O:648:TRP:CB	2.49	0.42
18:R:269:LYS:HA	18:R:272:VAL:HG12	2.01	0.42
18:R:282:ASP:OD1	18:R:283:GLY:N	2.51	0.42
21:Y:74:DG:C4	21:Y:75:DT:C4	3.08	0.42
1:A:38:ASP:N	1:A:38:ASP:OD1	2.53	0.42
1:A:284:ASP:OD1	1:A:285:LEU:N	2.50	0.42
1:A:891:LYS:NZ	1:A:1389:PHE:HA	2.35	0.42
1:A:925:GLU:OE2	1:A:1081:ALA:HA	2.20	0.42
1:A:934:ASN:ND2	1:A:937:ARG:HE	2.18	0.42
1:A:944:ASN:OD1	1:A:945:ILE:N	2.52	0.42
1:A:1448:PHE:CZ	4:D:16:VAL:HG23	2.49	0.42
2:B:39:ASN:OD1	2:B:40:THR:N	2.53	0.42
2:B:135:TYR:O	2:B:142:ILE:HA	2.19	0.42
2:B:609:CYS:HA	2:B:649:LEU:O	2.20	0.42
2:B:658:TYR:CD2	2:B:670:MET:HA	2.53	0.42
4:D:24:GLU:OE2	4:D:30:ASP:N	2.34	0.42
4:D:157:ILE:O	4:D:161:ALA:N	2.52	0.42
8:H:136:LYS:O	8:H:136:LYS:HG2	2.18	0.42
11:K:68:GLU:HG2	11:K:72:LEU:HD23	2.02	0.42
11:K:71:THR:OG1	11:K:72:LEU:N	2.52	0.42
11:K:99:ASN:O	11:K:100:LEU:HD12	2.19	0.42
15:O:361:PHE:HB3	15:O:480:TYR:HE2	1.84	0.42
15:O:468:LEU:HG	15:O:478:VAL:HG13	2.01	0.42
15:O:527:LEU:HD23	16:P:246:VAL:HG21	2.01	0.42
15:O:601:THR:HG23	15:O:602:LEU:N	2.34	0.42
16:P:108:LYS:HA	16:P:111:LYS:HB2	2.02	0.42
16:P:135:LYS:CB	16:P:151:TYR:CD1	2.67	0.42
19:S:390:GLU:OE1	19:S:394:LYS:HE3	2.19	0.42
1:A:252:ARG:O	1:A:254:GLU:N	2.52	0.42
1:A:378:ARG:HH22	1:A:477:GLN:NE2	2.18	0.42
1:A:378:ARG:NH1	1:A:518:ASN:HD21	2.17	0.42
1:A:404:TYR:CE1	1:A:528:ARG:HD2	2.55	0.42
1:A:493:ARG:HB2	1:A:499:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:SER:C	1:A:586:GLY:H	2.27	0.42
1:A:671:ASP:CG	1:A:672:GLY:H	2.27	0.42
1:A:744:LEU:HB2	1:A:750:LEU:HD11	2.01	0.42
1:A:774:ARG:NH2	1:A:804:LEU:HD11	2.35	0.42
1:A:794:MET:HB3	1:A:799:SER:OG	2.20	0.42
1:A:799:SER:OG	1:A:800:LYS:N	2.53	0.42
1:A:1175:ASP:HB2	9:I:41:TYR:OH	2.20	0.42
2:B:202:LYS:HD3	2:B:222:SER:OG	2.20	0.42
2:B:236:LYS:O	2:B:239:LYS:HB3	2.20	0.42
2:B:252:PRO:O	2:B:256:VAL:HG23	2.20	0.42
2:B:502:THR:CG2	2:B:510:LEU:HD11	2.50	0.42
2:B:556:TYR:HB3	2:B:559:GLY:HA2	2.02	0.42
2:B:558:ASN:H	2:B:602:ALA:HA	1.85	0.42
2:B:652:ASN:O	2:B:655:ASN:HB3	2.20	0.42
2:B:831:GLU:OE1	2:B:831:GLU:N	2.53	0.42
3:C:97:LEU:HD11	3:C:202:ILE:HD13	2.01	0.42
3:C:123:ASP:OD1	3:C:124:GLU:N	2.53	0.42
5:E:54:GLN:NE2	5:E:57:MET:HE2	2.29	0.42
5:E:145:THR:HG23	5:E:146:HIS:N	2.35	0.42
13:M:71:ILE:HG21	14:N:367:LYS:NZ	2.35	0.42
15:O:108:GLN:N	15:O:108:GLN:OE1	2.53	0.42
15:O:471:THR:HB	15:O:477:TYR:O	2.19	0.42
15:O:574:TYR:CD1	15:O:651:PHE:HE1	2.38	0.42
18:R:104:ALA:HA	18:R:107:TRP:HB2	2.01	0.42
18:R:195:LYS:O	18:R:198:VAL:HB	2.19	0.42
18:R:467:ARG:O	18:R:471:LYS:HB3	2.20	0.42
21:Y:8:DA:H2"	21:Y:9:DA:C8	2.55	0.42
21:Y:72:DA:C5	21:Y:73:DT:C4	3.08	0.42
1:A:106:ILE:CD1	1:A:234:ILE:HG12	2.49	0.42
1:A:235:LYS:O	1:A:236:SER:C	2.63	0.42
1:A:238:ASP:O	1:A:239:CYS:C	2.63	0.42
1:A:305:LYS:O	15:O:535:SER:OG	2.37	0.42
1:A:579:LEU:O	1:A:582:MET:N	2.52	0.42
1:A:809:MET:O	1:A:851:SER:HB2	2.20	0.42
1:A:1133:SER:OG	20:X:64:DA:H5"	2.20	0.42
1:A:1144:VAL:HG23	1:A:1310:ILE:CG2	2.50	0.42
1:A:1144:VAL:HA	1:A:1292:GLU:HG3	2.02	0.42
2:B:197:GLN:HE22	2:B:451:ARG:HD2	1.84	0.42
2:B:460:ARG:CZ	2:B:720:ARG:HH12	2.33	0.42
2:B:725:LEU:HB3	2:B:788:ARG:HB2	2.01	0.42
2:B:915:ARG:HD2	2:B:1023:TYR:CD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:22:ASP:O	4:D:26:LYS:N	2.41	0.42
5:E:31:THR:O	5:E:34:GLU:HB2	2.19	0.42
5:E:183:PRO:O	5:E:187:TYR:N	2.48	0.42
6:F:86:THR:HB	6:F:89:GLU:N	2.32	0.42
7:G:38:ILE:HD11	7:G:194:TYR:HB3	2.02	0.42
8:H:65:LEU:HD13	8:H:89:LEU:HD12	2.02	0.42
8:H:100:THR:OG1	8:H:138:GLU:HA	2.20	0.42
15:O:282:ILE:H	15:O:282:ILE:HD12	1.85	0.42
15:O:291:ARG:HG3	15:O:292:ARG:N	2.35	0.42
16:P:86:MET:HB3	16:P:90:GLU:CB	2.49	0.42
16:P:121:VAL:O	16:P:125:LEU:HG	2.20	0.42
16:P:191:PHE:CB	16:P:203:LYS:HD2	2.50	0.42
16:P:304:LYS:HG3	16:P:305:HIS:CD2	2.55	0.42
18:R:238:ARG:HE	19:S:286:UNK:CB	2.33	0.42
18:R:416:ARG:HG2	18:R:613:HIS:O	2.20	0.42
19:S:413:ARG:HG3	20:X:9:DA:OP1	2.20	0.42
21:Y:61:DA:C4	21:Y:62:DT:N3	2.87	0.42
1:A:27:VAL:HA	1:A:30:SER:OG	2.19	0.41
1:A:270:PRO:HG3	2:B:1046:LEU:HD13	2.02	0.41
1:A:399:ALA:CB	1:A:466:LEU:HB2	2.50	0.41
1:A:1092:ILE:O	1:A:1096:SER:CB	2.68	0.41
1:A:1128:GLU:HG2	1:A:1136:ILE:HG13	2.02	0.41
1:A:1144:VAL:HG23	1:A:1310:ILE:HG23	2.02	0.41
1:A:1179:ASP:OD1	9:I:36:GLU:N	2.51	0.41
1:A:1385:GLN:C	1:A:1388:SER:H	2.28	0.41
2:B:340:LEU:HD23	2:B:340:LEU:HA	1.87	0.41
2:B:987:MET:O	2:B:991:LEU:N	2.48	0.41
2:B:1038:ARG:HH11	2:B:1058:GLY:C	2.27	0.41
2:B:1038:ARG:HH21	2:B:1041:GLY:H	1.67	0.41
3:C:229:LEU:HB3	3:C:293:ARG:HH12	1.85	0.41
4:D:5:GLU:HB3	7:G:6:LYS:HB3	2.02	0.41
7:G:4:LEU:HD21	7:G:73:ARG:HE	1.85	0.41
7:G:82:GLY:HA2	7:G:150:ILE:O	2.20	0.41
11:K:77:ARG:HD2	11:K:91:TYR:HE1	1.85	0.41
13:M:75:PRO:HA	14:N:362:SER:OG	2.20	0.41
15:O:92:LYS:NZ	17:Q:1082:UNK:HA	2.35	0.41
16:P:183:TRP:HZ2	16:P:266:GLU:HB3	1.85	0.41
16:P:233:VAL:HG23	16:P:234:GLU:O	2.20	0.41
18:R:195:LYS:O	18:R:199:VAL:HG23	2.20	0.41
19:S:430:LYS:HD3	19:S:482:ASP:OD2	2.20	0.41
1:A:91:PHE:HB2	1:A:224:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:SER:OG	2:B:1017:ILE:HA	2.20	0.41
1:A:919:ASP:CG	1:A:921:LEU:HB2	2.45	0.41
1:A:1130:ILE:HA	1:A:1362:MET:HE1	2.01	0.41
1:A:1305:CYS:HB2	5:E:141:VAL:HG21	2.01	0.41
1:A:1342:THR:HG23	1:A:1343:MET:N	2.35	0.41
1:A:1411:VAL:HG13	1:A:1412:SER:N	2.32	0.41
1:A:1448:PHE:CZ	4:D:16:VAL:CG2	3.03	0.41
2:B:240:ILE:CG1	2:B:286:ASN:HD22	2.33	0.41
2:B:797:ARG:NH1	18:R:99:TYR:HE2	2.18	0.41
2:B:1060:LEU:HD23	2:B:1060:LEU:HA	1.80	0.41
2:B:1135:MET:HE2	2:B:1135:MET:HB3	1.79	0.41
3:C:247:PHE:HD1	3:C:285:PHE:CD2	2.39	0.41
7:G:51:LEU:HD11	7:G:70:VAL:HG21	2.02	0.41
7:G:59:LEU:HD12	7:G:65:SER:C	2.45	0.41
7:G:63:ASP:CG	7:G:65:SER:H	2.28	0.41
8:H:4:THR:HA	8:H:60:ALA:HB1	2.01	0.41
10:J:8:PHE:CG	10:J:49:MET:HE1	2.55	0.41
13:M:122:ASP:HB3	13:M:145:VAL:HG21	2.02	0.41
15:O:47:PHE:CZ	15:O:590:PHE:CE2	3.08	0.41
15:O:101:LEU:HD21	15:O:130:LEU:HD11	2.00	0.41
15:O:203:ILE:HG22	15:O:207:HIS:HD2	1.83	0.41
15:O:341:GLU:HA	15:O:344:SER:HB2	2.02	0.41
15:O:638:PHE:HD1	17:Q:58:TYR:CE2	2.37	0.41
18:R:13:GLU:CD	18:R:26:LYS:HG3	2.45	0.41
18:R:438:THR:HG22	18:R:439:ALA:O	2.20	0.41
19:S:417:THR:HG22	19:S:453:GLN:NE2	2.34	0.41
1:A:29:GLN:HG2	2:B:1109:THR:HB	2.03	0.41
1:A:37:ARG:CG	1:A:38:ASP:H	2.33	0.41
1:A:347:VAL:HG12	1:A:349:PRO:HD2	2.03	0.41
1:A:378:ARG:NH2	1:A:516:GLU:OE1	2.54	0.41
1:A:918:GLY:HA3	5:E:208:TYR:CE1	2.55	0.41
1:A:1260:MET:O	1:A:1263:LEU:HB2	2.21	0.41
1:A:1328:ILE:O	1:A:1329:GLU:C	2.63	0.41
2:B:151:ARG:N	2:B:430:THR:OG1	2.52	0.41
2:B:576:ARG:O	2:B:580:ARG:HG2	2.20	0.41
2:B:593:ASN:ND2	2:B:596:GLN:HB3	2.35	0.41
2:B:736:VAL:HG11	2:B:960:GLU:HG3	2.01	0.41
2:B:1129:PHE:CZ	2:B:1141:LEU:HD21	2.54	0.41
3:C:117:ASP:OD1	3:C:118:SER:N	2.52	0.41
6:F:136:ARG:O	6:F:143:PHE:C	2.64	0.41
7:G:207:LEU:HB3	7:G:210:TRP:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:24:LEU:HG	9:I:33:PHE:CG	2.55	0.41
11:K:85:ASP:OD1	11:K:108:TYR:HB2	2.20	0.41
13:M:184:LYS:HA	13:M:184:LYS:HD2	1.83	0.41
15:O:123:ASN:O	15:O:124:GLU:C	2.62	0.41
15:O:174:TYR:O	15:O:178:VAL:HG23	2.20	0.41
15:O:472:LYS:HB3	15:O:475:VAL:HG11	1.84	0.41
15:O:587:ASN:O	15:O:588:LEU:C	2.63	0.41
17:Q:1079:UNK:O	17:Q:1083:UNK:N	2.54	0.41
18:R:138:LYS:HE3	18:R:175:LEU:O	2.21	0.41
18:R:417:ASN:HA	19:S:437:THR:HG22	2.02	0.41
18:R:495:PRO:HA	18:R:534:VAL:O	2.20	0.41
1:A:269:ARG:NE	1:A:286:THR:OG1	2.38	0.41
1:A:852:PHE:CZ	2:B:953:MET:HE3	2.56	0.41
1:A:1199:GLU:HB3	5:E:3:GLN:HE22	1.85	0.41
2:B:209:ALA:HB2	2:B:366:ILE:HG21	2.01	0.41
2:B:234:ILE:HD11	2:B:237:ASN:N	2.35	0.41
2:B:627:LEU:HD23	2:B:627:LEU:HA	1.88	0.41
2:B:762:TYR:OH	2:B:930:ASP:HB3	2.20	0.41
2:B:860:VAL:HG13	2:B:861:ASN:N	2.33	0.41
3:C:100:ARG:HH12	10:J:2:ILE:HB	1.84	0.41
3:C:133:VAL:HA	3:C:207:HIS:HA	2.03	0.41
3:C:251:PHE:CB	3:C:255:VAL:HG21	2.51	0.41
5:E:82:PHE:CD1	5:E:111:VAL:HB	2.55	0.41
5:E:90:VAL:O	5:E:93:MET:HB2	2.20	0.41
10:J:6:ARG:HB3	10:J:11:GLY:CA	2.49	0.41
15:O:160:VAL:O	15:O:163:VAL:HB	2.19	0.41
15:O:292:ARG:O	15:O:296:LEU:HG	2.21	0.41
15:O:472:LYS:HA	15:O:473:PRO:HD2	1.68	0.41
15:O:632:GLU:O	15:O:635:LEU:HB2	2.20	0.41
20:X:25:DT:C6	20:X:26:DT:H72	2.55	0.41
20:X:29:DG:C8	20:X:29:DG:H5'	2.55	0.41
20:X:74:DA:H2''	20:X:75:DG:H8	1.85	0.41
21:Y:14:DC:C2	21:Y:15:DT:C2	3.08	0.41
1:A:62:SER:OG	1:A:63:SER:N	2.53	0.41
1:A:181:ASP:OD2	1:A:219:MET:HA	2.20	0.41
1:A:378:ARG:NE	1:A:516:GLU:OE1	2.53	0.41
1:A:404:TYR:OH	1:A:525:GLU:OE2	2.26	0.41
1:A:557:PHE:CE1	2:B:767:ILE:HD11	2.55	0.41
1:A:837:LYS:HE2	1:A:837:LYS:HB3	1.39	0.41
1:A:960:MET:O	1:A:964:ASN:N	2.49	0.41
1:A:1229:ARG:HH12	1:A:1231:ALA:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1365:LYS:O	5:E:177:ARG:HB2	2.21	0.41
2:B:549:LEU:O	2:B:549:LEU:CD2	2.54	0.41
2:B:689:PRO:HD3	2:B:915:ARG:CZ	2.50	0.41
2:B:824:LEU:HB2	2:B:825:GLY:H	1.40	0.41
2:B:987:MET:O	2:B:990:ILE:HB	2.20	0.41
3:C:21:PRO:HD3	3:C:29:ASN:O	2.20	0.41
3:C:55:ASP:CG	3:C:297:HIS:HE2	2.29	0.41
7:G:15:PRO:HA	7:G:18:PHE:CE2	2.55	0.41
9:I:6:PRO:HG2	9:I:31:TYR:CZ	2.55	0.41
9:I:23:THR:OG1	9:I:24:LEU:N	2.54	0.41
13:M:142:GLY:HA2	13:M:185:TYR:OH	2.20	0.41
13:M:183:PHE:CD2	13:M:185:TYR:HD2	2.37	0.41
14:N:374:LYS:HD3	14:N:378:VAL:HG23	2.03	0.41
15:O:75:SER:HB2	15:O:119:TYR:CE1	2.55	0.41
15:O:135:LEU:O	15:O:138:ASP:HB3	2.21	0.41
15:O:369:HIS:CG	15:O:370:LEU:N	2.88	0.41
15:O:369:HIS:O	15:O:370:LEU:HB2	2.20	0.41
18:R:190:ASP:O	18:R:191:LEU:HB2	2.19	0.41
18:R:441:ILE:HD12	18:R:447:MET:HB3	2.01	0.41
18:R:455:GLU:HB2	18:R:591:TYR:HB2	2.02	0.41
19:S:382:ASP:C	19:S:384:HIS:H	2.28	0.41
20:X:64:DA:C6	20:X:65:DA:C6	3.09	0.41
21:Y:60:DT:C2	21:Y:61:DA:N7	2.89	0.41
1:A:413:ARG:O	1:A:417:GLN:N	2.39	0.41
1:A:607:LYS:HG3	8:H:120:GLY:HA3	2.02	0.41
1:A:618:HIS:CE1	8:H:77:ARG:HH12	2.39	0.41
1:A:913:GLN:NE2	1:A:917:GLY:H	2.17	0.41
2:B:399:PHE:HA	2:B:402:SER:CB	2.50	0.41
2:B:947:HIS:O	2:B:950:PRO:HD2	2.20	0.41
2:B:957:LYS:NZ	2:B:1022:ILE:HD13	2.36	0.41
2:B:1055:SER:OG	2:B:1056:ARG:N	2.51	0.41
3:C:41:GLU:O	3:C:57:ILE:HG22	2.20	0.41
4:D:61:ASN:OD1	7:G:103:GLY:HA3	2.20	0.41
5:E:1:MET:HG3	5:E:4:GLU:H	1.85	0.41
8:H:99:GLY:HA3	8:H:118:PHE:HA	2.03	0.41
15:O:265:VAL:O	15:O:273:ILE:N	2.26	0.41
15:O:328:ASP:N	15:O:329:PRO:CD	2.83	0.41
15:O:478:VAL:HB	15:O:480:TYR:CZ	2.56	0.41
15:O:638:PHE:CD1	17:Q:58:TYR:HE2	2.38	0.41
18:R:460:LEU:HD23	18:R:464:LYS:HE2	2.02	0.41
19:S:439:PHE:HB2	19:S:451:ARG:NH2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:67:DA:H1'	21:Y:68:DA:C5	2.55	0.41
1:A:11:LYS:HD2	2:B:1145:ASP:HA	2.03	0.41
1:A:240:GLU:C	1:A:243:GLY:H	2.27	0.41
1:A:614:ILE:HG21	1:A:624:ILE:HD12	2.02	0.41
1:A:988:ASP:HA	1:A:991:LYS:CB	2.41	0.41
2:B:68:PHE:CE1	2:B:385:SER:HA	2.56	0.41
2:B:193:VAL:HG12	2:B:194:ILE:N	2.36	0.41
2:B:224:THR:OG1	2:B:225:HIS:N	2.52	0.41
2:B:232:TYR:CE1	2:B:253:ILE:HB	2.56	0.41
2:B:263:LEU:HD21	2:B:296:TYR:CD1	2.55	0.41
2:B:458:LEU:HA	2:B:469:MET:SD	2.61	0.41
2:B:630:LEU:HA	2:B:635:LEU:HB2	2.03	0.41
2:B:718:PHE:HE2	10:J:1:MET:HE1	1.86	0.41
2:B:732:GLN:NE2	10:J:49:MET:HG2	2.35	0.41
3:C:44:ILE:HA	3:C:54:PHE:HB2	2.03	0.41
3:C:70:ILE:HD11	3:C:320:ILE:HB	2.03	0.41
5:E:106:GLN:O	5:E:107:THR:HB	2.20	0.41
5:E:117:THR:HG23	5:E:120:ALA:H	1.86	0.41
7:G:84:ILE:CG2	7:G:147:ARG:HB3	2.51	0.41
8:H:6:PHE:CG	8:H:7:ASP:N	2.88	0.41
9:I:21:VAL:O	9:I:23:THR:N	2.47	0.41
15:O:32:MET:O	15:O:34:ILE:N	2.54	0.41
15:O:289:LYS:HZ2	15:O:325:LYS:HD3	1.85	0.41
15:O:583:TRP:CZ2	16:P:312:PHE:O	2.74	0.41
16:P:19:HIS:O	16:P:23:MET:HG2	2.20	0.41
16:P:87:SER:H	16:P:90:GLU:HB2	1.85	0.41
18:R:402:LEU:HA	18:R:477:LYS:O	2.19	0.41
21:Y:24:DG:H2''	21:Y:25:DA:C8	2.56	0.41
1:A:273:MET:HE2	18:R:39:SER:OG	2.20	0.41
1:A:363:ARG:HD3	2:B:1127:LEU:HD21	2.02	0.41
1:A:438:GLU:O	1:A:438:GLU:HG2	2.19	0.41
1:A:556:ASP:OD1	2:B:947:HIS:NE2	2.53	0.41
1:A:574:ALA:HB1	11:K:77:ARG:HH22	1.85	0.41
1:A:926:MET:HG3	1:A:932:PRO:HG3	2.02	0.41
1:A:1152:ARG:O	1:A:1153:ALA:C	2.63	0.41
1:A:1319:VAL:O	1:A:1322:VAL:N	2.54	0.41
1:A:1451:LEU:HG	4:D:107:MET:SD	2.61	0.41
2:B:52:LEU:HD11	2:B:57:LEU:HD12	2.03	0.41
2:B:879:SER:HA	2:B:902:GLN:HB3	2.02	0.41
3:C:270:ALA:C	3:C:272:LYS:H	2.28	0.41
8:H:5:LEU:HB2	8:H:59:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:75:SER:H	15:O:78:GLU:HB3	1.86	0.41
15:O:220:GLU:HG2	15:O:221:LYS:N	2.35	0.41
16:P:25:LYS:HG3	16:P:26:GLY:N	2.36	0.41
18:R:142:MET:HG3	18:R:144:ILE:HG22	2.03	0.41
18:R:267:ALA:O	18:R:271:SER:N	2.47	0.41
18:R:514:GLU:HG2	19:S:408:TYR:CZ	2.55	0.41
18:R:521:TYR:CE2	18:R:523:MET:HB2	2.51	0.41
18:R:590:THR:O	18:R:594:LYS:HG3	2.21	0.41
19:S:420:TRP:CH2	19:S:449:ARG:HG2	2.56	0.41
20:X:67:DT:H6	20:X:67:DT:H2'	1.65	0.41
1:A:127:LEU:HD11	1:A:140:ILE:HG21	2.02	0.41
1:A:269:ARG:NH2	1:A:283:ASP:C	2.74	0.41
1:A:283:ASP:O	1:A:287:VAL:HG23	2.21	0.41
1:A:402:LEU:HD23	1:A:466:LEU:HD13	1.87	0.41
1:A:589:HIS:HA	11:K:104:ARG:NH2	2.36	0.41
1:A:591:ASP:OD1	1:A:591:ASP:N	2.52	0.41
1:A:927:GLU:H	1:A:932:PRO:HA	1.85	0.41
1:A:1155:ARG:O	1:A:1158:LYS:HB3	2.21	0.41
1:A:1299:GLY:C	1:A:1301:ARG:H	2.29	0.41
2:B:68:PHE:HE1	2:B:385:SER:HA	1.85	0.41
2:B:490:GLN:H	2:B:490:GLN:CD	2.26	0.41
2:B:556:TYR:OH	2:B:561:LEU:HD12	2.20	0.41
2:B:1038:ARG:HD3	2:B:1059:GLY:N	2.35	0.41
2:B:1054:ARG:NE	21:Y:24:DG:OP1	2.42	0.41
3:C:5:VAL:HG12	3:C:14:ASN:O	2.21	0.41
3:C:76:PRO:HB3	3:C:115:TRP:CZ2	2.56	0.41
3:C:216:HIS:CG	3:C:218:LYS:HE3	2.56	0.41
3:C:245:ARG:O	3:C:248:GLN:HG2	2.21	0.41
5:E:2:ASP:O	5:E:5:ASN:HB2	2.21	0.41
5:E:23:VAL:HG22	5:E:28:TYR:HB2	2.03	0.41
8:H:61:SER:CB	8:H:139:ASN:HD22	2.32	0.41
13:M:72:GLU:O	14:N:364:ARG:HG2	2.21	0.41
15:O:132:TYR:OH	15:O:652:GLN:NE2	2.44	0.41
15:O:175:LEU:HA	15:O:178:VAL:HB	2.01	0.41
15:O:291:ARG:HH22	15:O:652:GLN:HE21	1.68	0.41
15:O:314:ILE:HD12	15:O:368:ARG:HB2	2.01	0.41
15:O:354:GLU:OE2	15:O:477:TYR:HE2	2.03	0.41
15:O:529:LYS:O	15:O:533:ILE:HG12	2.20	0.41
15:O:638:PHE:CD1	17:Q:58:TYR:CE2	3.09	0.41
16:P:69:GLU:HG3	16:P:70:LEU:N	2.31	0.41
16:P:133:TYR:C	16:P:151:TYR:CB	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:14:ARG:HH22	18:R:36:PRO:HG2	1.84	0.41
18:R:167:LYS:HA	18:R:167:LYS:HD3	1.90	0.41
18:R:241:HIS:O	18:R:245:VAL:HG22	2.20	0.41
18:R:287:PRO:HA	18:R:288:PRO:HD3	1.96	0.41
18:R:413:LEU:HD22	18:R:624:GLU:CD	2.46	0.41
18:R:439:ALA:HA	18:R:450:THR:N	2.35	0.41
19:S:449:ARG:HD3	19:S:449:ARG:HA	1.87	0.41
20:X:8:DT:C4	20:X:9:DA:N6	2.88	0.41
20:X:63:DC:H2''	20:X:64:DA:N7	2.36	0.41
20:X:79:DT:N3	21:Y:1:DA:N1	2.69	0.41
21:Y:53:DG:H1'	21:Y:54:DA:H5'	2.03	0.41
21:Y:56:DA:C6	21:Y:57:DA:C6	3.08	0.41
1:A:108:LYS:HG2	1:A:180:HIS:NE2	2.36	0.41
1:A:155:LEU:HD11	1:A:156:HIS:HD2	1.85	0.41
1:A:366:GLY:CA	2:B:1061:ARG:HH22	2.34	0.41
1:A:1343:MET:HE3	1:A:1350:VAL:HG21	2.03	0.41
2:B:51:PHE:HD1	2:B:637:PHE:CZ	2.39	0.41
2:B:143:MET:HA	19:S:397:VAL:O	2.21	0.41
2:B:332:ILE:HG13	2:B:333:ALA:N	2.27	0.41
2:B:343:ARG:NE	2:B:541:ILE:HG12	2.36	0.41
2:B:623:LYS:C	2:B:625:ILE:H	2.28	0.41
2:B:969:LEU:HA	10:J:47:ARG:NH1	2.35	0.41
2:B:1114:GLU:HG3	2:B:1115:ASN:N	2.36	0.41
3:C:142:ARG:HB2	3:C:198:PRO:HG3	2.03	0.41
4:D:11:LEU:H	7:G:3:ILE:HG22	1.84	0.41
7:G:148:PHE:CE1	7:G:150:ILE:HD11	2.56	0.41
7:G:207:LEU:HB3	7:G:210:TRP:CD2	2.56	0.41
14:N:304:PHE:HB2	14:N:411:ARG:O	2.21	0.41
15:O:353:GLU:HB3	15:O:361:PHE:HE2	1.86	0.41
15:O:517:VAL:HG21	15:O:521:ILE:CG2	2.51	0.41
18:R:434:GLU:HA	18:R:435:PRO:HA	1.89	0.41
19:S:425:MET:HG2	19:S:429:TYR:CE2	2.56	0.41
20:X:6:DC:C2	20:X:7:DA:C5	3.09	0.41
20:X:77:DC:H2''	20:X:78:DG:C8	2.55	0.41
1:A:5:VAL:HG23	7:G:38:ILE:O	2.20	0.40
1:A:329:SER:OG	1:A:330:ASP:N	2.54	0.40
1:A:907:SER:C	1:A:909:ASN:H	2.29	0.40
1:A:937:ARG:HG3	1:A:938:SER:N	2.36	0.40
1:A:1280:ARG:HG3	1:A:1296:GLU:OE1	2.21	0.40
2:B:101:GLY:O	2:B:109:LYS:HA	2.22	0.40
2:B:140:ASN:HD22	19:S:394:LYS:HG2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:926:VAL:HG13	2:B:930:ASP:HB2	2.03	0.40
3:C:6:GLY:N	3:C:13:THR:O	2.55	0.40
3:C:9:TYR:HB3	3:C:280:LEU:HB3	2.04	0.40
3:C:32:ASN:OD1	3:C:33:VAL:N	2.54	0.40
6:F:135:ARG:HH22	7:G:58:GLN:HE21	1.69	0.40
6:F:143:PHE:CG	6:F:144:GLU:N	2.87	0.40
8:H:12:VAL:HB	8:H:53:ASP:H	1.87	0.40
10:J:42:LYS:HG3	10:J:43:ARG:HG3	2.02	0.40
15:O:185:TYR:CD2	15:O:185:TYR:O	2.74	0.40
15:O:584:ASN:ND2	16:P:310:VAL:CG2	2.63	0.40
18:R:607:ASP:C	18:R:609:GLU:H	2.29	0.40
20:X:13:DT:C4	20:X:14:DA:C6	3.09	0.40
1:A:164:VAL:HA	1:A:179:ILE:O	2.20	0.40
1:A:443:ASN:O	1:A:445:ARG:N	2.55	0.40
1:A:561:SER:HA	1:A:564:ILE:HG22	2.03	0.40
1:A:642:PRO:HG3	8:H:115:TYR:CE2	2.56	0.40
1:A:719:PRO:O	1:A:724:LYS:NZ	2.54	0.40
1:A:934:ASN:CG	1:A:937:ARG:HG2	2.47	0.40
2:B:65:PHE:O	2:B:68:PHE:HB3	2.21	0.40
2:B:138:GLY:O	2:B:141:ILE:HG22	2.21	0.40
2:B:603:THR:O	2:B:603:THR:OG1	2.24	0.40
2:B:961:LEU:HD22	2:B:1018:PHE:CZ	2.57	0.40
2:B:1038:ARG:NH2	2:B:1041:GLY:H	2.20	0.40
3:C:31:TRP:CD1	3:C:32:ASN:N	2.89	0.40
3:C:54:PHE:CZ	3:C:300:PHE:CD2	3.09	0.40
3:C:55:ASP:OD1	3:C:56:LEU:N	2.54	0.40
3:C:240:LYS:HB2	3:C:261:GLY:O	2.21	0.40
11:K:60:SER:HB3	11:K:104:ARG:NH2	2.35	0.40
14:N:365:VAL:HG12	14:N:366:HIS:O	2.21	0.40
15:O:573:SER:O	15:O:576:PHE:CE2	2.74	0.40
16:P:106:TRP:HB2	16:P:147:ILE:HG22	2.04	0.40
16:P:252:LYS:HD3	16:P:266:GLU:CG	2.50	0.40
18:R:96:ILE:HG22	18:R:141:HIS:NE2	2.35	0.40
18:R:557:TYR:HA	18:R:560:LEU:HD12	2.02	0.40
21:Y:10:DC:H2''	21:Y:11:DC:C5	2.56	0.40
21:Y:70:DA:H2''	21:Y:71:DT:O5'	2.19	0.40
1:A:126:GLU:O	1:A:132:VAL:HG21	2.22	0.40
1:A:205:LEU:HA	1:A:212:GLU:HG2	2.03	0.40
1:A:329:SER:HB3	1:A:355:GLN:NE2	2.24	0.40
1:A:392:VAL:HG23	1:A:488:HIS:CD2	2.55	0.40
1:A:571:TYR:CA	1:A:575:THR:HG21	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:PRO:HG2	1:A:689:GLU:CD	2.46	0.40
1:A:633:PHE:HZ	1:A:643:ASN:HB3	1.86	0.40
1:A:714:ILE:CD1	2:B:958:MET:HE3	2.50	0.40
1:A:880:ALA:HA	21:Y:20:DC:O4'	2.22	0.40
1:A:885:MET:O	1:A:889:LEU:HB3	2.22	0.40
1:A:1384:LEU:HD12	1:A:1413:GLU:OE1	2.22	0.40
1:A:1428:PHE:CD1	6:F:134:ILE:HG23	2.57	0.40
2:B:341:ASP:HB3	13:M:151:VAL:HG11	2.02	0.40
2:B:612:LEU:O	2:B:646:VAL:HB	2.21	0.40
2:B:1129:PHE:HE2	2:B:1141:LEU:HD11	1.87	0.40
3:C:70:ILE:O	3:C:75:VAL:HG13	2.20	0.40
3:C:142:ARG:HG3	3:C:157:TYR:HE1	1.87	0.40
8:H:134:ASN:O	8:H:135:LEU:HD12	2.22	0.40
11:K:79:VAL:HG21	11:K:124:LEU:HD12	2.02	0.40
11:K:124:LEU:HA	11:K:127:LEU:HD12	2.03	0.40
13:M:111:ARG:HB3	13:M:243:ILE:CG2	2.46	0.40
13:M:126:ASP:HB2	13:M:129:ALA:HB2	2.03	0.40
15:O:271:LEU:HD23	15:O:272:ARG:H	1.87	0.40
15:O:647:LEU:O	15:O:650:VAL:HG12	2.21	0.40
16:P:29:ALA:O	16:P:71:LYS:HB3	2.21	0.40
17:Q:1072:UNK:O	17:Q:1074:UNK:N	2.54	0.40
18:R:388:GLY:HA3	18:R:576:SER:HB2	2.02	0.40
18:R:514:GLU:HG2	19:S:408:TYR:CE1	2.56	0.40
1:A:433:LEU:O	1:A:442:ARG:N	2.39	0.40
1:A:483:LEU:HD13	1:A:507:PRO:CG	2.51	0.40
1:A:596:ALA:HB2	1:A:608:GLN:OE1	2.21	0.40
1:A:610:PHE:CZ	1:A:697:MET:HE1	2.55	0.40
1:A:772:LYS:O	1:A:776:GLU:HB2	2.21	0.40
1:A:857:SER:O	1:A:860:GLU:HG2	2.21	0.40
2:B:181:PRO:HB2	2:B:470:MET:HE1	2.03	0.40
2:B:241:TYR:CE1	2:B:252:PRO:HG3	2.56	0.40
2:B:325:GLU:HG3	2:B:329:THR:N	2.35	0.40
2:B:379:LEU:HA	2:B:379:LEU:HD23	1.91	0.40
2:B:465:SER:O	2:B:469:MET:N	2.43	0.40
2:B:1013:LEU:HD23	2:B:1013:LEU:HA	1.85	0.40
2:B:1031:VAL:O	2:B:1034:LYS:N	2.54	0.40
4:D:25:LYS:HA	4:D:29:TRP:HB2	2.02	0.40
13:M:89:GLN:HB2	14:N:392:GLN:HB3	2.03	0.40
13:M:160:ALA:HA	14:N:306:VAL:HG12	2.03	0.40
14:N:311:THR:O	14:N:314:PRO:HD3	2.21	0.40
15:O:52:LEU:O	15:O:56:HIS:N	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:515:LYS:HE2	15:O:515:LYS:HB3	1.85	0.40
18:R:134:CYS:HB2	18:R:139:THR:OG1	2.22	0.40
18:R:498:LEU:HA	18:R:501:LEU:HB3	2.03	0.40
1:A:164:VAL:HB	1:A:180:HIS:HB3	2.04	0.40
1:A:246:ALA:O	1:A:247:THR:HG23	2.22	0.40
1:A:344:GLY:C	1:A:346:LYS:H	2.29	0.40
2:B:81:GLN:O	2:B:94:LYS:HA	2.21	0.40
2:B:254:ALA:O	2:B:258:LYS:HG2	2.22	0.40
2:B:736:VAL:HA	2:B:974:GLU:O	2.20	0.40
2:B:795:LEU:CB	2:B:894:ALA:O	2.45	0.40
2:B:824:LEU:HA	2:B:831:GLU:CD	2.46	0.40
3:C:133:VAL:HB	3:C:207:HIS:CD2	2.57	0.40
3:C:153:PRO:HB3	3:C:197:ARG:HH12	1.87	0.40
4:D:1:MET:HG3	4:D:2:LYS:N	2.37	0.40
7:G:87:GLY:CA	7:G:148:PHE:HE2	2.35	0.40
7:G:108:ILE:HG23	7:G:196:LEU:HB2	2.04	0.40
7:G:111:PRO:HD2	7:G:198:GLY:H	1.87	0.40
8:H:5:LEU:HD13	8:H:60:ALA:HA	2.04	0.40
9:I:29:CYS:HB3	13:M:183:PHE:CE2	2.56	0.40
13:M:83:GLU:O	13:M:84:SER:C	2.65	0.40
13:M:147:THR:HB	13:M:182:PHE:O	2.21	0.40
14:N:364:ARG:CG	14:N:365:VAL:N	2.83	0.40
15:O:170:THR:HB	15:O:276:PRO:O	2.22	0.40
15:O:184:LYS:HD3	15:O:187:ILE:HD11	2.03	0.40
15:O:292:ARG:HH12	15:O:650:VAL:HB	1.86	0.40
18:R:536:GLY:O	18:R:538:ILE:HG12	2.21	0.40
20:X:73:DA:H2''	20:X:74:DA:C8	2.56	0.40
21:Y:58:DA:H2''	21:Y:59:DG:C8	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	1422/1460 (97%)	1106 (78%)	292 (20%)	24 (2%)	7	35
2	B	1112/1149 (97%)	901 (81%)	194 (17%)	17 (2%)	8	38
3	C	333/335 (99%)	282 (85%)	44 (13%)	7 (2%)	5	30
4	D	113/161 (70%)	87 (77%)	24 (21%)	2 (2%)	6	33
5	E	213/215 (99%)	182 (85%)	29 (14%)	2 (1%)	14	49
6	F	81/155 (52%)	66 (82%)	13 (16%)	2 (2%)	4	26
7	G	178/212 (84%)	145 (82%)	30 (17%)	3 (2%)	7	35
8	H	136/146 (93%)	112 (82%)	23 (17%)	1 (1%)	18	55
9	I	40/110 (36%)	30 (75%)	7 (18%)	3 (8%)	1	10
10	J	65/70 (93%)	54 (83%)	11 (17%)	0	100	100
11	K	99/142 (70%)	77 (78%)	22 (22%)	0	100	100
12	L	44/70 (63%)	33 (75%)	11 (25%)	0	100	100
13	M	160/282 (57%)	127 (79%)	31 (19%)	2 (1%)	9	41
14	N	106/422 (25%)	82 (77%)	24 (23%)	0	100	100
15	O	533/654 (82%)	401 (75%)	116 (22%)	16 (3%)	3	22
16	P	271/317 (86%)	219 (81%)	47 (17%)	5 (2%)	6	33
17	Q	33/251 (13%)	28 (85%)	5 (15%)	0	100	100
18	R	514/736 (70%)	439 (85%)	72 (14%)	3 (1%)	21	58
19	S	172/594 (29%)	157 (91%)	14 (8%)	1 (1%)	21	58
All	All	5625/7481 (75%)	4528 (80%)	1009 (18%)	88 (2%)	10	37

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	PRO
1	A	252	ARG
1	A	587	ILE
1	A	837	LYS
1	A	1033	GLU
1	A	1064	GLU
2	B	369	ARG
2	B	418	ALA
2	B	590	ILE
7	G	123	PRO
8	H	130	ARG
9	I	21	VAL

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Mol	Chain	Res	Type
13	M	84	SER
13	M	107	ILE
15	O	146	VAL
15	O	183	MET
15	O	329	PRO
15	O	473	PRO
16	P	150	LEU
16	P	315	TRP
18	R	154	VAL
1	A	251	GLY
1	A	277	SER
1	A	307	ILE
1	A	838	ASN
1	A	975	VAL
2	B	87	VAL
3	C	33	VAL
5	E	147	HIS
7	G	124	GLU
9	I	35	ILE
15	O	330	LEU
15	O	518	SER
16	P	267	SER
1	A	39	LEU
1	A	278	PRO
1	A	995	VAL
1	A	998	TYR
1	A	1035	PRO
1	A	1371	ILE
2	B	168	GLU
2	B	344	GLU
2	B	416	TYR
2	B	586	GLU
2	B	589	SER
3	C	16	THR
3	C	87	ASN
3	C	255	VAL
6	F	144	GLU
7	G	191	PRO
15	O	163	VAL
18	R	274	LYS
1	A	276	ASP
1	A	444	LEU

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Mol	Chain	Res	Type
1	A	483	LEU
1	A	1328	ILE
2	B	277	SER
2	B	713	ILE
2	B	767	ILE
3	C	88	ASN
4	D	128	PRO
9	I	23	THR
15	O	186	THR
15	O	517	VAL
16	P	202	PRO
19	S	491	ASN
2	B	624	ASP
3	C	62	SER
4	D	64	ASN
15	O	39	GLN
1	A	68	ALA
6	F	116	ASP
15	O	472	LYS
15	O	586	ALA
2	B	142	ILE
1	A	599	LYS
2	B	215	ILE
3	C	101	ILE
1	A	186	VAL
2	B	601	ILE
2	B	1137	ILE
15	O	88	VAL
15	O	352	VAL
16	P	192	PRO
5	E	125	PRO
15	O	495	VAL
15	O	620	LEU
18	R	435	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1232/1257 (98%)	1217 (99%)	15 (1%)	63	73
2	B	975/1006 (97%)	969 (99%)	6 (1%)	78	80
3	C	296/296 (100%)	294 (99%)	2 (1%)	76	79
4	D	110/145 (76%)	109 (99%)	1 (1%)	70	76
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	73/137 (53%)	72 (99%)	1 (1%)	59	71
7	G	164/190 (86%)	161 (98%)	3 (2%)	51	67
8	H	123/128 (96%)	122 (99%)	1 (1%)	73	77
9	I	38/98 (39%)	37 (97%)	1 (3%)	40	60
10	J	62/65 (95%)	62 (100%)	0	100	100
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	142/249 (57%)	142 (100%)	0	100	100
14	N	92/360 (26%)	92 (100%)	0	100	100
15	O	495/593 (84%)	491 (99%)	4 (1%)	73	77
16	P	255/285 (90%)	252 (99%)	3 (1%)	63	73
17	Q	31/195 (16%)	31 (100%)	0	100	100
18	R	450/623 (72%)	450 (100%)	0	100	100
19	S	157/494 (32%)	157 (100%)	0	100	100
All	All	5023/6505 (77%)	4986 (99%)	37 (1%)	73	79

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	THR
1	A	276	ASP
1	A	277	SER
1	A	290	THR
1	A	444	LEU
1	A	483	LEU
1	A	484	SER
1	A	485	ILE
1	A	622	VAL
1	A	705	LEU
1	A	830	ARG
1	A	837	LYS

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Mol	Chain	Res	Type
1	A	848	VAL
1	A	1063	SER
1	A	1064	GLU
2	B	298	GLN
2	B	601	ILE
2	B	603	THR
2	B	772	VAL
2	B	824	LEU
2	B	863	GLN
3	C	103	LEU
3	C	294	VAL
4	D	127	LEU
6	F	115	THR
7	G	58	GLN
7	G	59	LEU
7	G	124	GLU
8	H	130	ARG
9	I	35	ILE
15	O	181	ASP
15	O	187	ILE
15	O	516	LEU
15	O	517	VAL
16	P	203	LYS
16	P	293	ILE
16	P	313	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	92	HIS
1	A	147	GLN
1	A	151	GLN
1	A	156	HIS
1	A	161	ASN
1	A	281	ASN
1	A	386	ASN
1	A	412	ASN
1	A	437	ASN
1	A	455	ASN
1	A	477	GLN
1	A	518	ASN

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Mol	Chain	Res	Type
1	A	520	HIS
1	A	523	GLN
1	A	533	ASN
1	A	566	HIS
1	A	589	HIS
1	A	725	GLN
1	A	808	GLN
1	A	815	GLN
1	A	828	GLN
1	A	850	ASN
1	A	913	GLN
1	A	1385	GLN
2	B	116	HIS
2	B	140	ASN
2	B	175	ASN
2	B	197	GLN
2	B	217	GLN
2	B	275	ASN
2	B	286	ASN
2	B	299	GLN
2	B	396	ASN
2	B	411	ASN
2	B	423	ASN
2	B	441	ASN
2	B	456	HIS
2	B	519	HIS
2	B	558	ASN
2	B	693	HIS
2	B	699	ASN
2	B	754	ASN
2	B	800	ASN
2	B	863	GLN
2	B	883	GLN
2	B	902	GLN
2	B	928	GLN
2	B	936	GLN
2	B	1148	GLN
3	C	29	ASN
3	C	93	GLN
3	C	207	HIS
3	C	296	ASN
4	D	8	ASN

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Mol	Chain	Res	Type
4	D	56	GLN
4	D	64	ASN
4	D	69	ASN
4	D	71	ASN
4	D	126	GLN
5	E	3	GLN
5	E	54	GLN
5	E	104	ASN
5	E	114	ASN
5	E	153	HIS
5	E	174	GLN
7	G	28	HIS
7	G	58	GLN
8	H	133	ASN
8	H	134	ASN
10	J	23	ASN
13	M	86	HIS
13	M	92	ASN
13	M	178	GLN
13	M	190	ASN
13	M	254	GLN
14	N	288	GLN
14	N	377	ASN
14	N	392	GLN
15	O	43	ASN
15	O	100	GLN
15	O	147	ASN
15	O	222	HIS
15	O	244	ASN
15	O	298	ASN
15	O	310	GLN
15	O	337	GLN
15	O	346	GLN
15	O	454	ASN
15	O	544	ASN
15	O	549	GLN
15	O	584	ASN
15	O	607	ASN
15	O	626	GLN
16	P	33	GLN
16	P	34	GLN
16	P	53	GLN

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Mol	Chain	Res	Type
16	P	73	GLN
16	P	117	HIS
16	P	118	GLN
16	P	119	HIS
16	P	189	ASN
16	P	305	HIS
18	R	20	ASN
18	R	95	HIS
18	R	118	GLN
18	R	184	HIS
18	R	394	GLN
18	R	414	HIS
18	R	631	ASN
19	S	444	GLN
19	S	453	GLN
19	S	499	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
19	S	1
17	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	319:UNK	C	360:THR	N	39.73
1	Q	70:PHE	C	1070:UNK	N	13.87

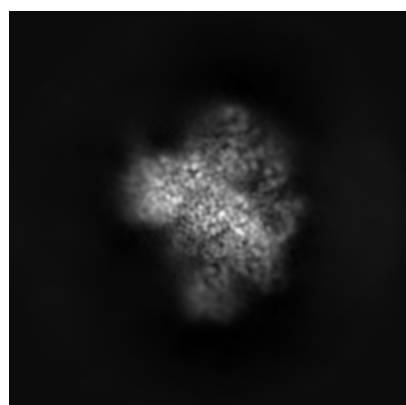
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7533. These allow visual inspection of the internal detail of the map and identification of artifacts.

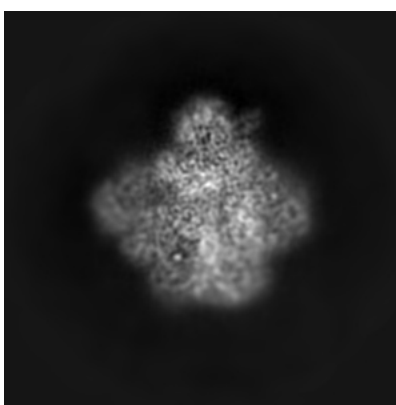
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

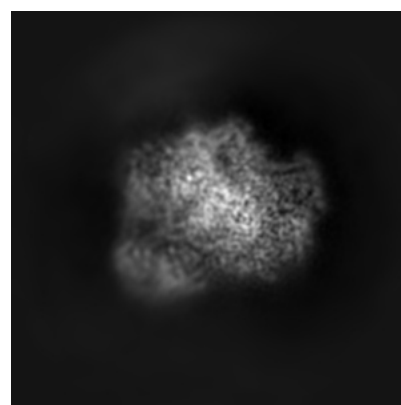
6.1.1 Primary map



X



Y

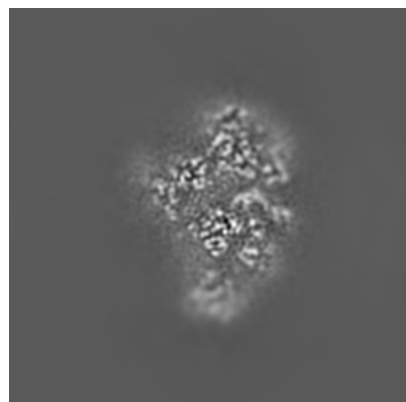


Z

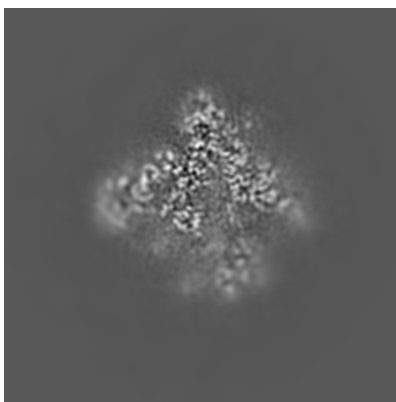
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

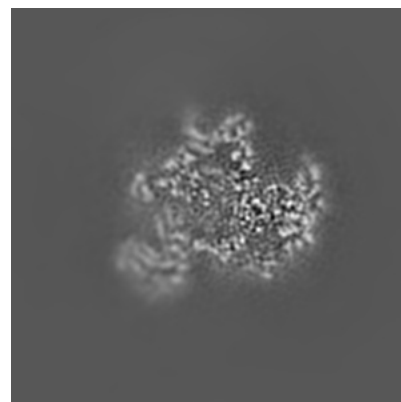
6.2.1 Primary map



X Index: 144



Y Index: 144

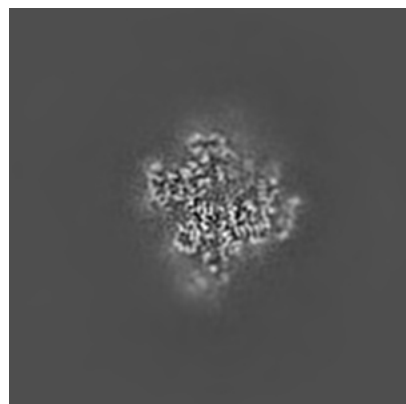


Z Index: 144

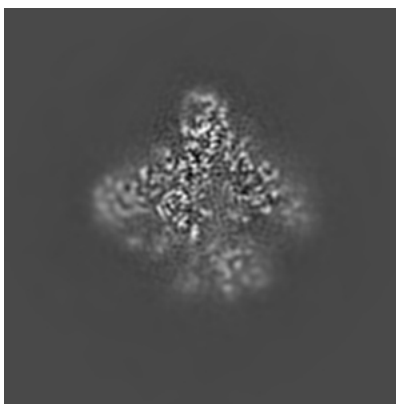
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

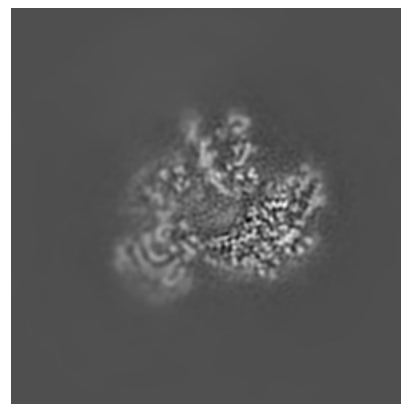
6.3.1 Primary map



X Index: 169



Y Index: 147

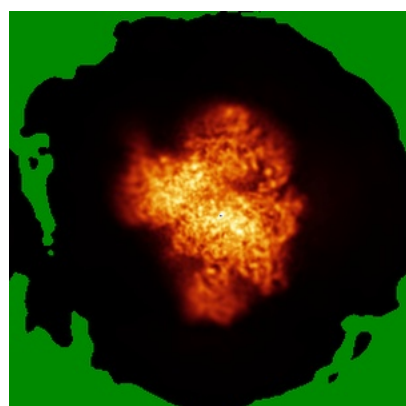


Z Index: 150

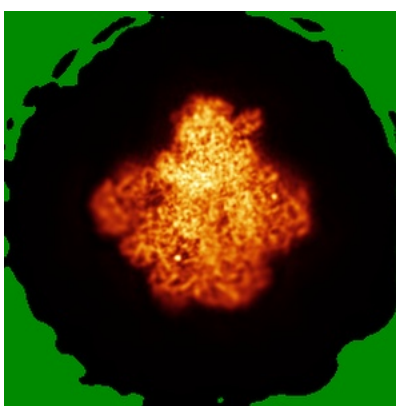
The images above show the largest variance slices of the map in three orthogonal directions.

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

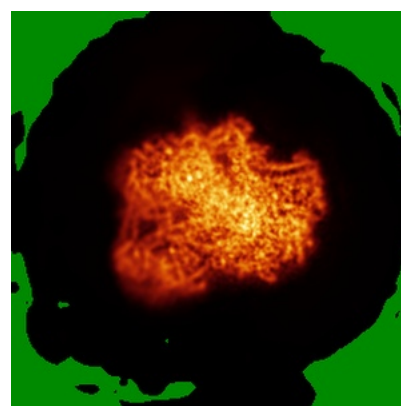
6.4.1 Primary map



X



Y

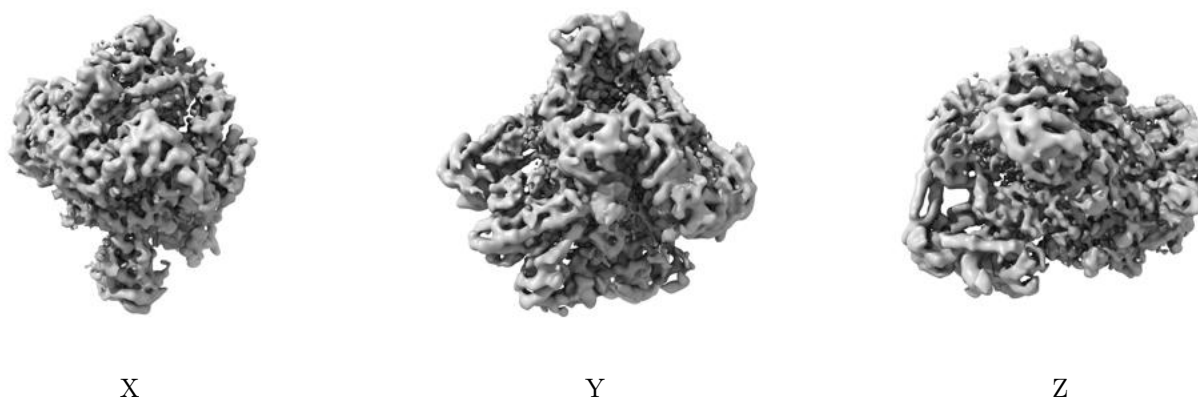


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

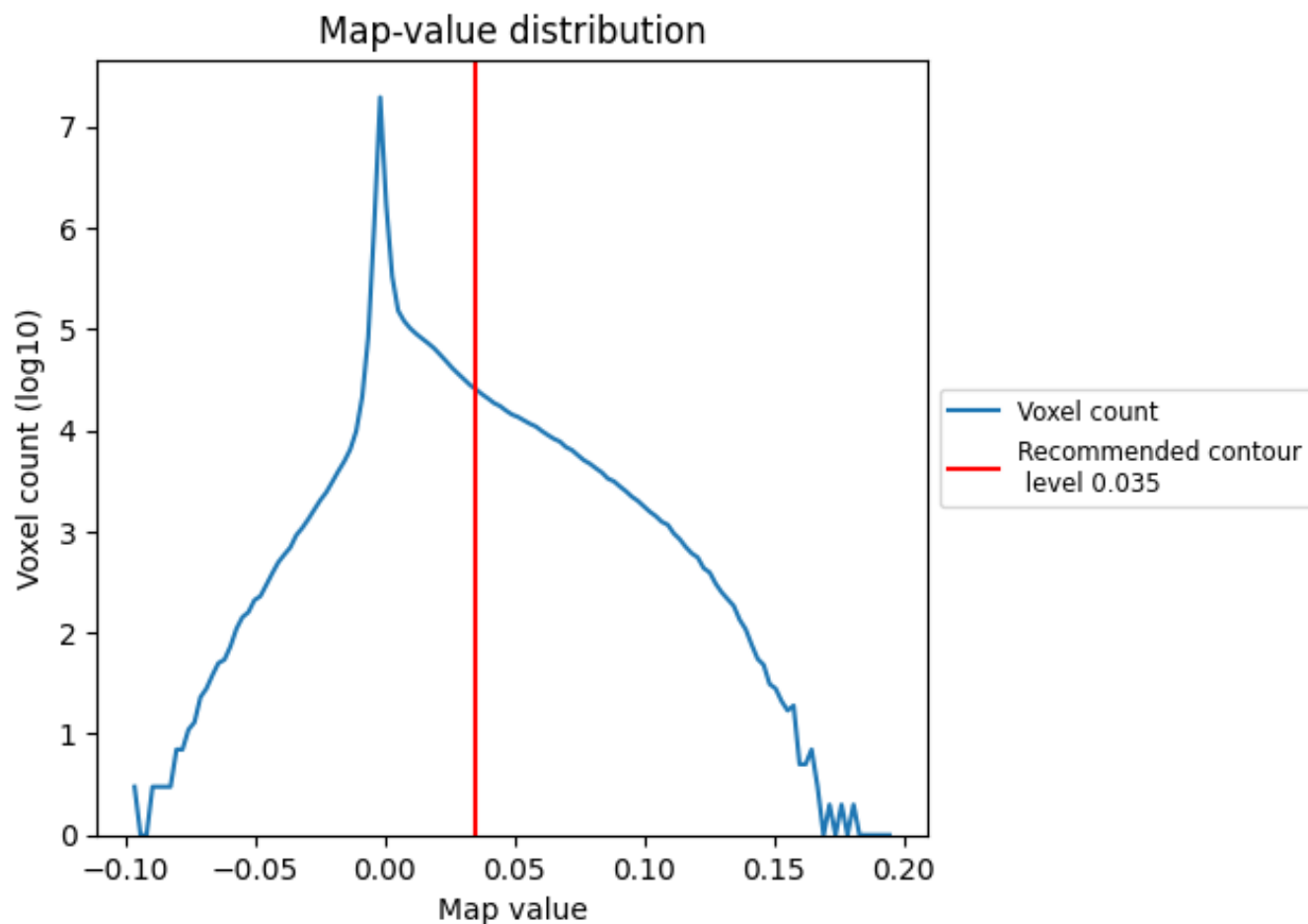
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

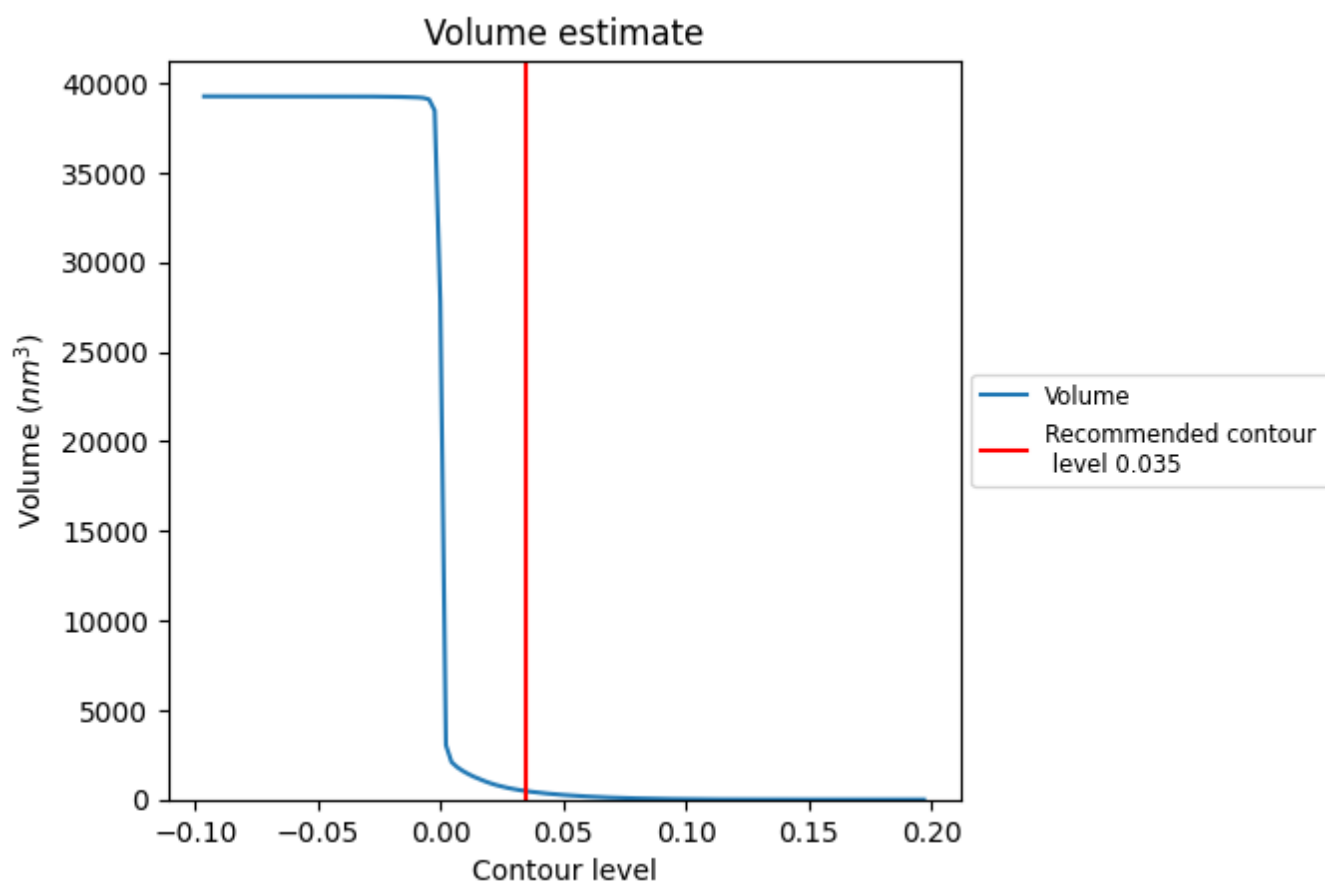
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

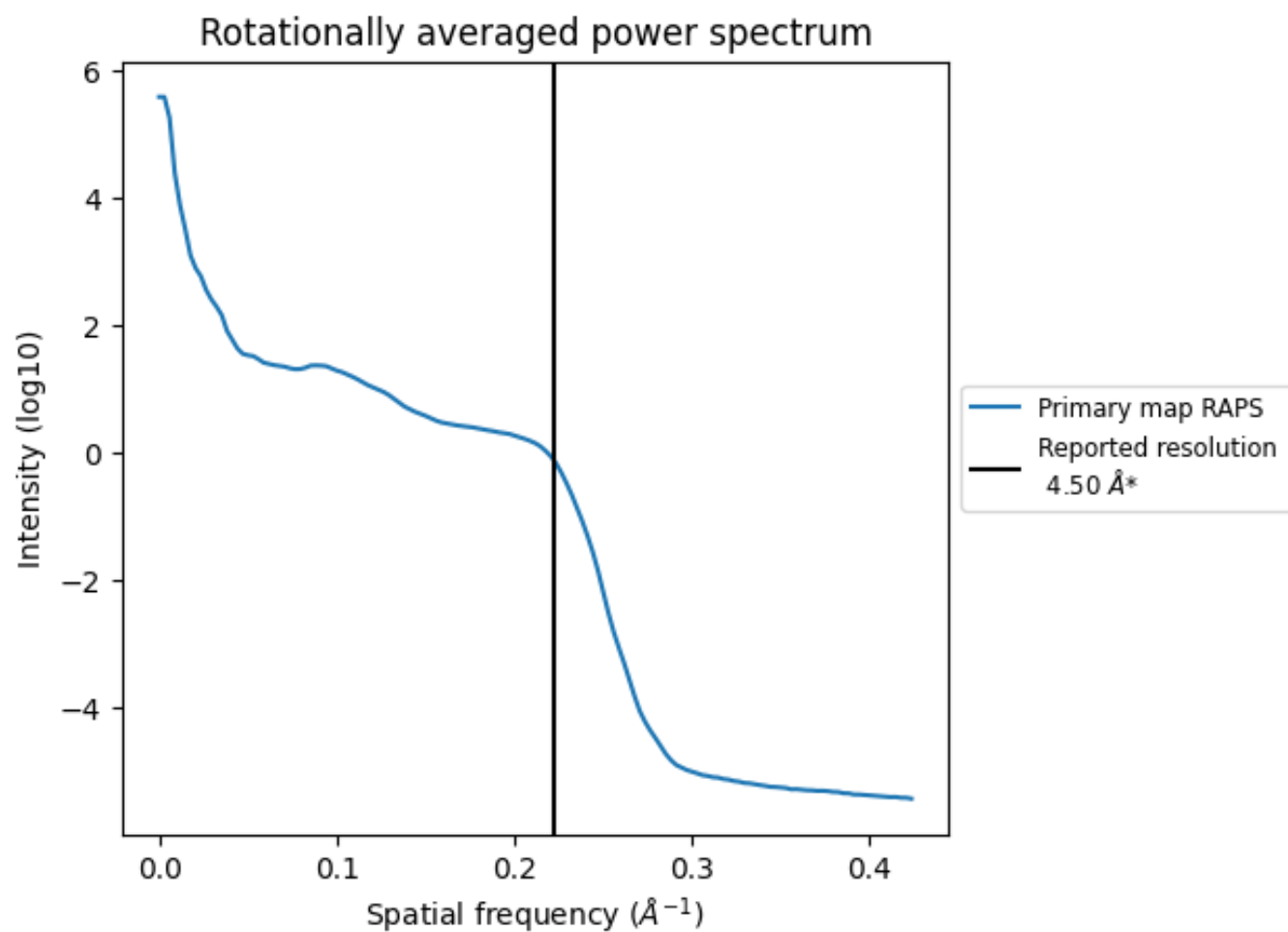
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 470 nm³; this corresponds to an approximate mass of 424 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 ⓘ

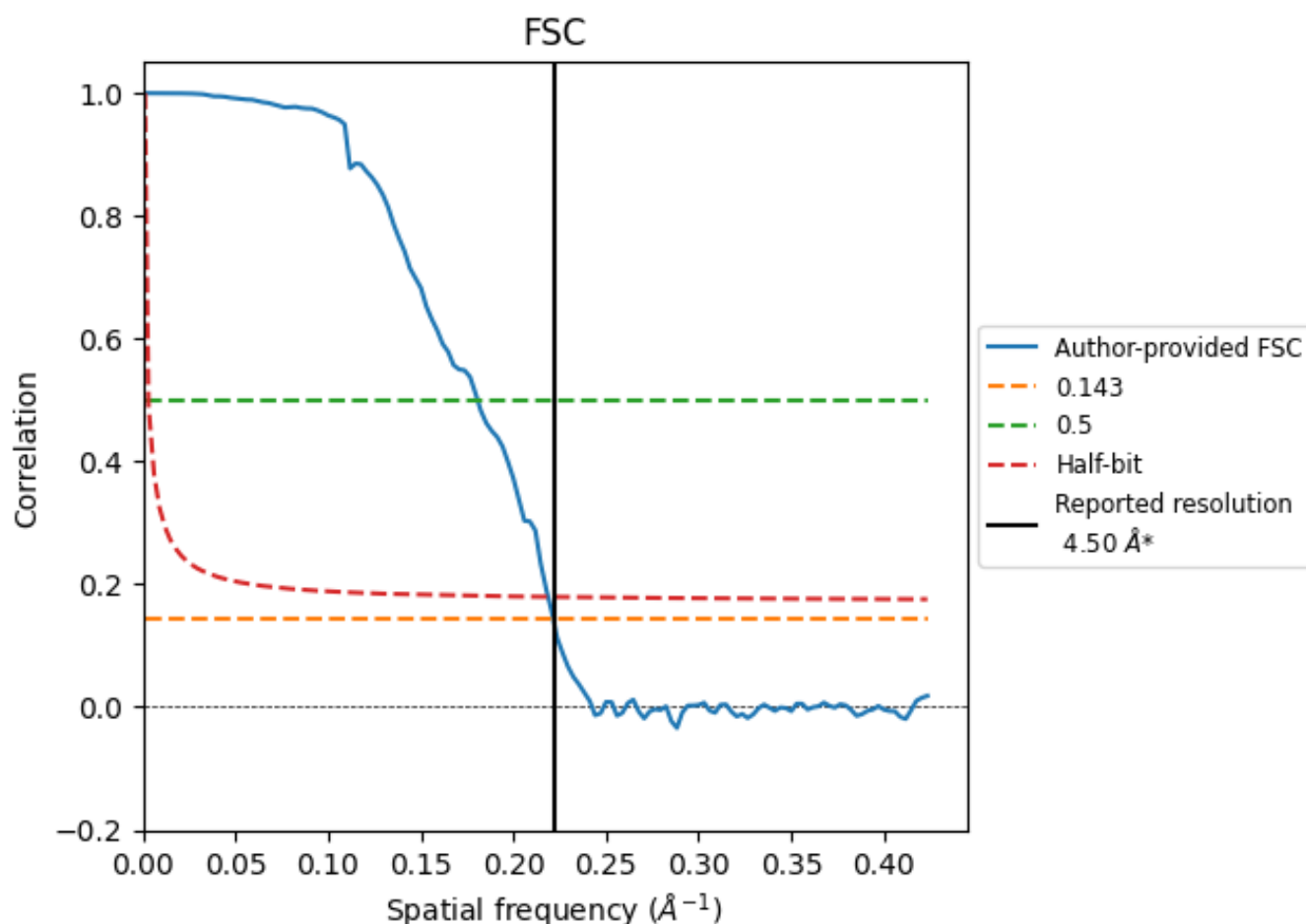


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.51	5.53	4.57
Unmasked-calculated*	-	-	-

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

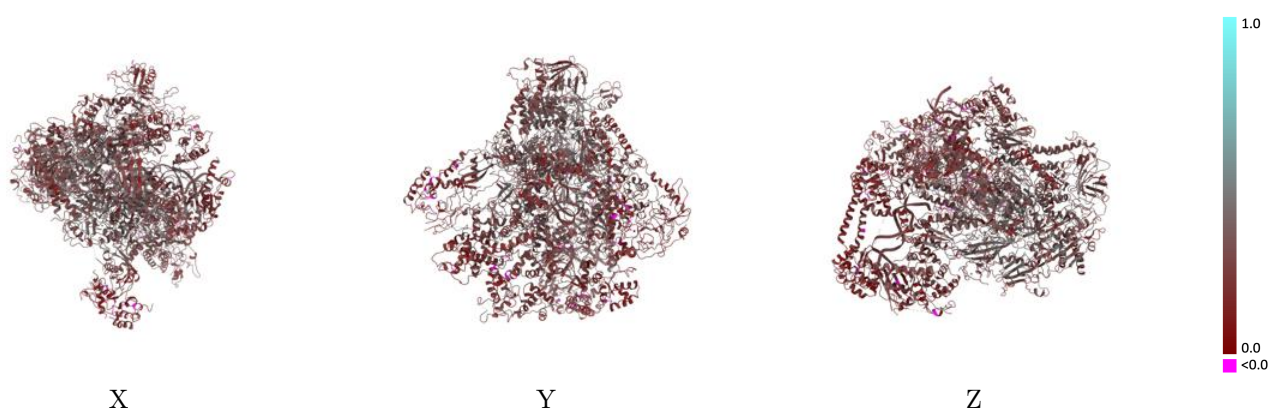
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7533 and PDB model 6CNF. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

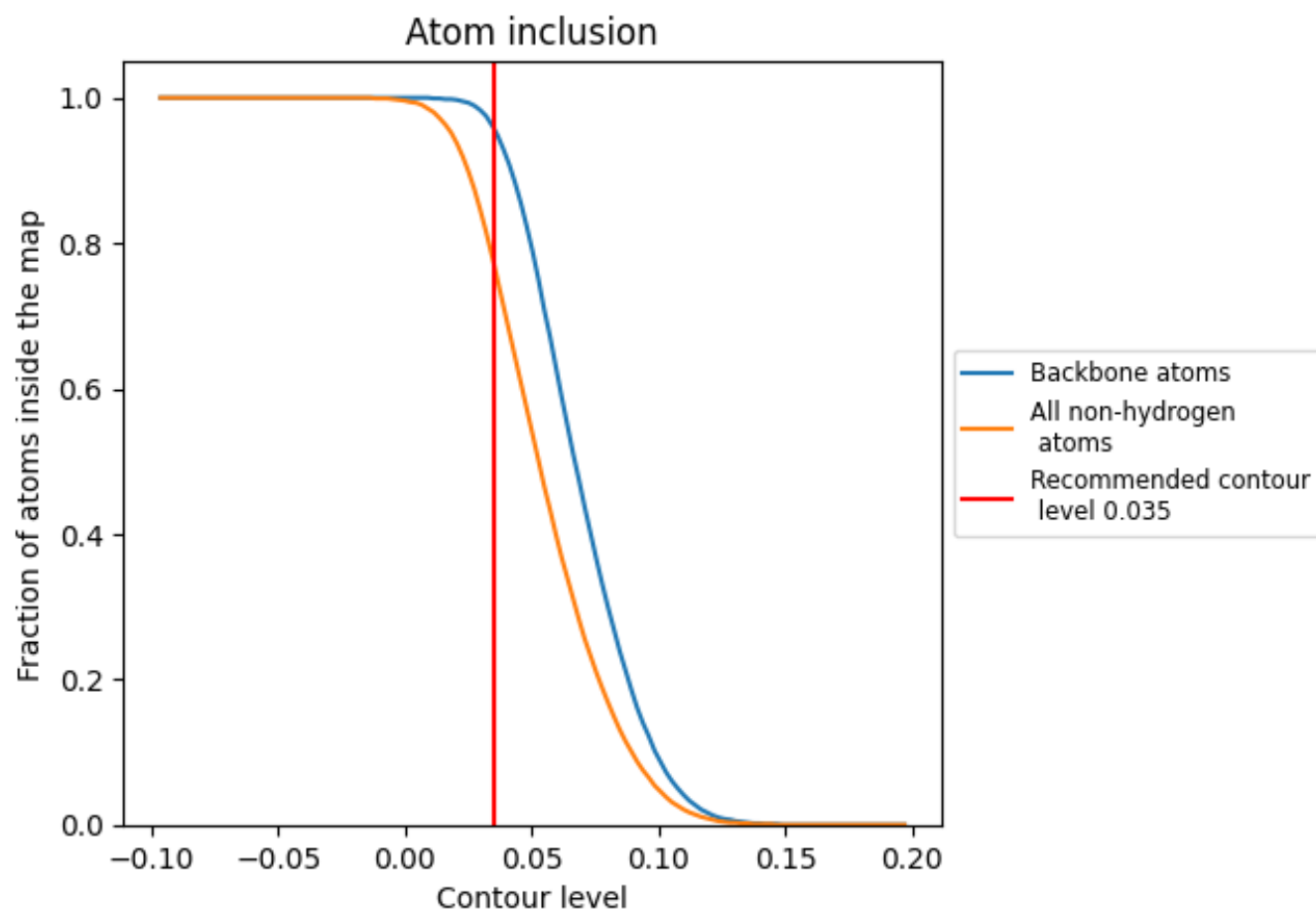


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 77% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7720	 0.2950
A	 0.7880	 0.3320
B	 0.7870	 0.3390
C	 0.8500	 0.3350
D	 0.7270	 0.1820
E	 0.7870	 0.2910
F	 0.8640	 0.3640
G	 0.7800	 0.2340
H	 0.8340	 0.3170
I	 0.7760	 0.2400
J	 0.8410	 0.3440
K	 0.8290	 0.3360
L	 0.8380	 0.3490
M	 0.7080	 0.2280
N	 0.7530	 0.2430
O	 0.7260	 0.2560
P	 0.6670	 0.2290
Q	 0.8790	 0.3320
R	 0.7000	 0.2270
S	 0.6270	 0.2160
X	 0.9200	 0.2960
Y	 0.8920	 0.3150

