



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:54 AM UTC

PDB ID : 6CNC / pdb_00006cnc
EMDB ID : EMD-7531
Title : Yeast RNA polymerase III open complex
Authors : Han, Y.; He, Y.
Deposited on : 2018-03-08
Resolution : 4.10 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

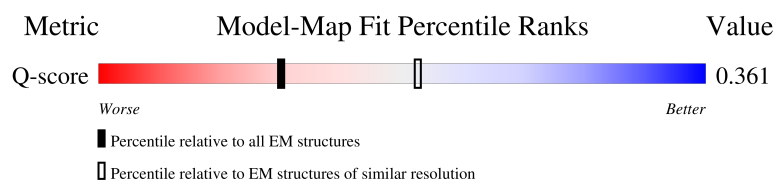
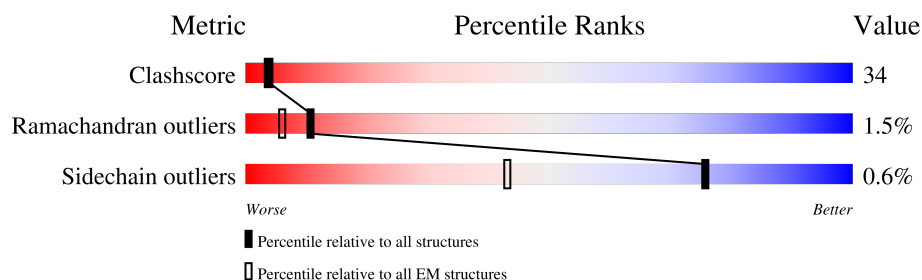
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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.



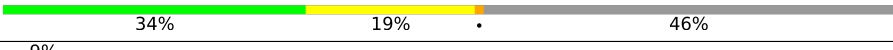
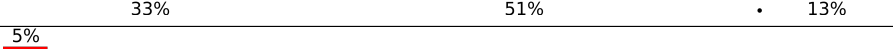
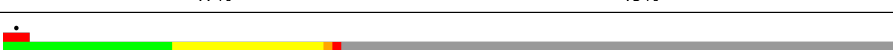
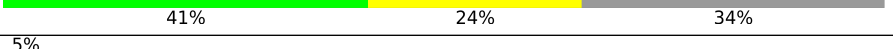
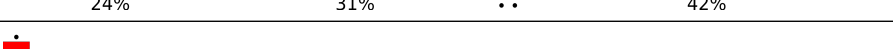
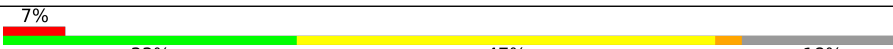
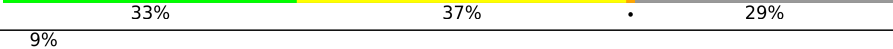
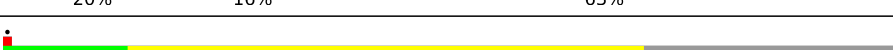
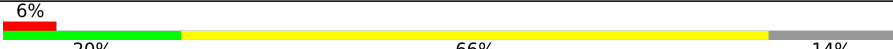
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	
2	B	1149	
3	C	335	
4	D	161	

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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	71	
21	Y	71	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 47836 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 (71-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	51	Total	C	N	O	P	0	0
			1040	503	181	306	50		

- Molecule 21 is a DNA chain called DNA (71-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	61	Total	C	N	O	P	0	0
			1249	602	223	364	60		

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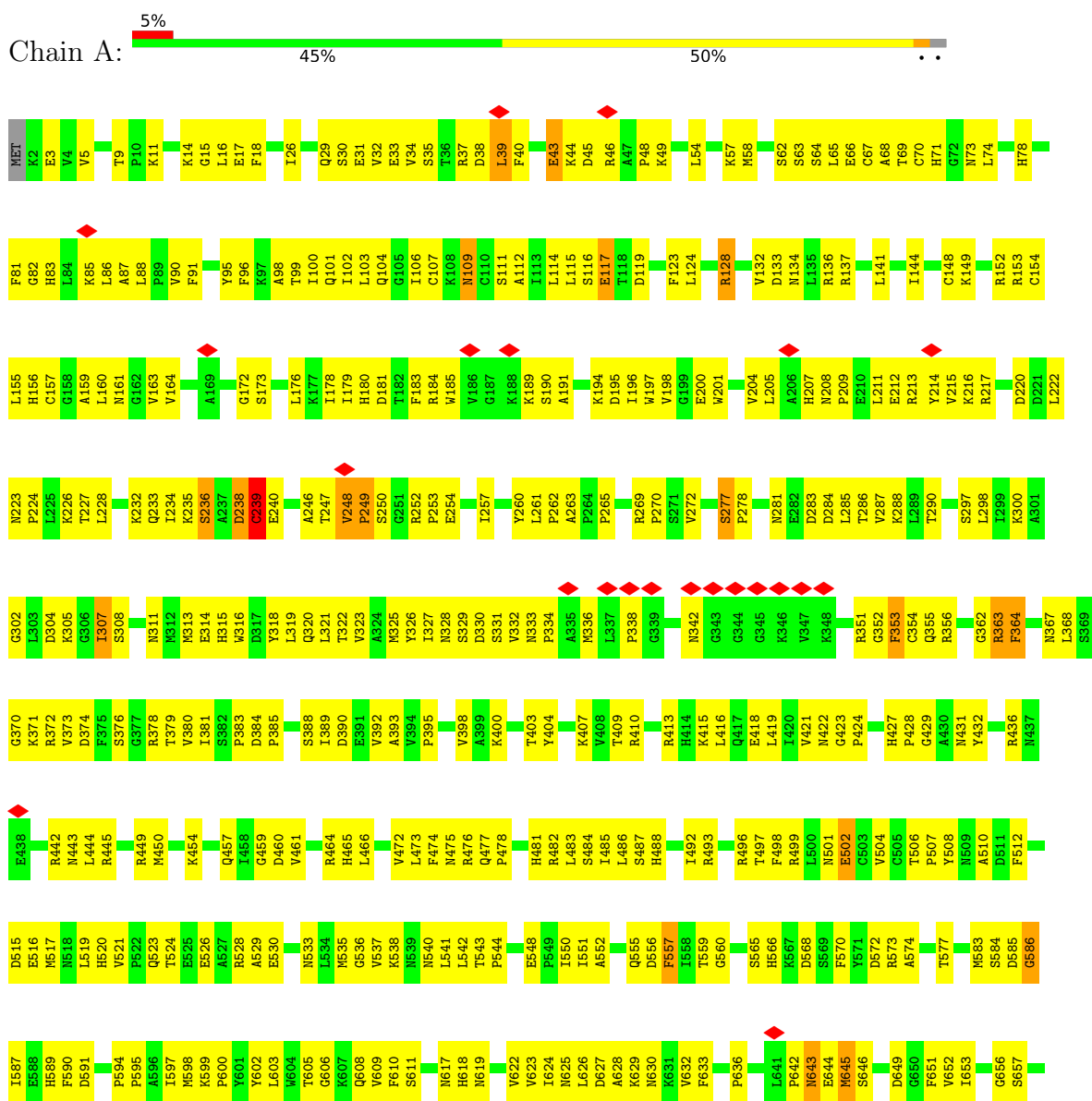
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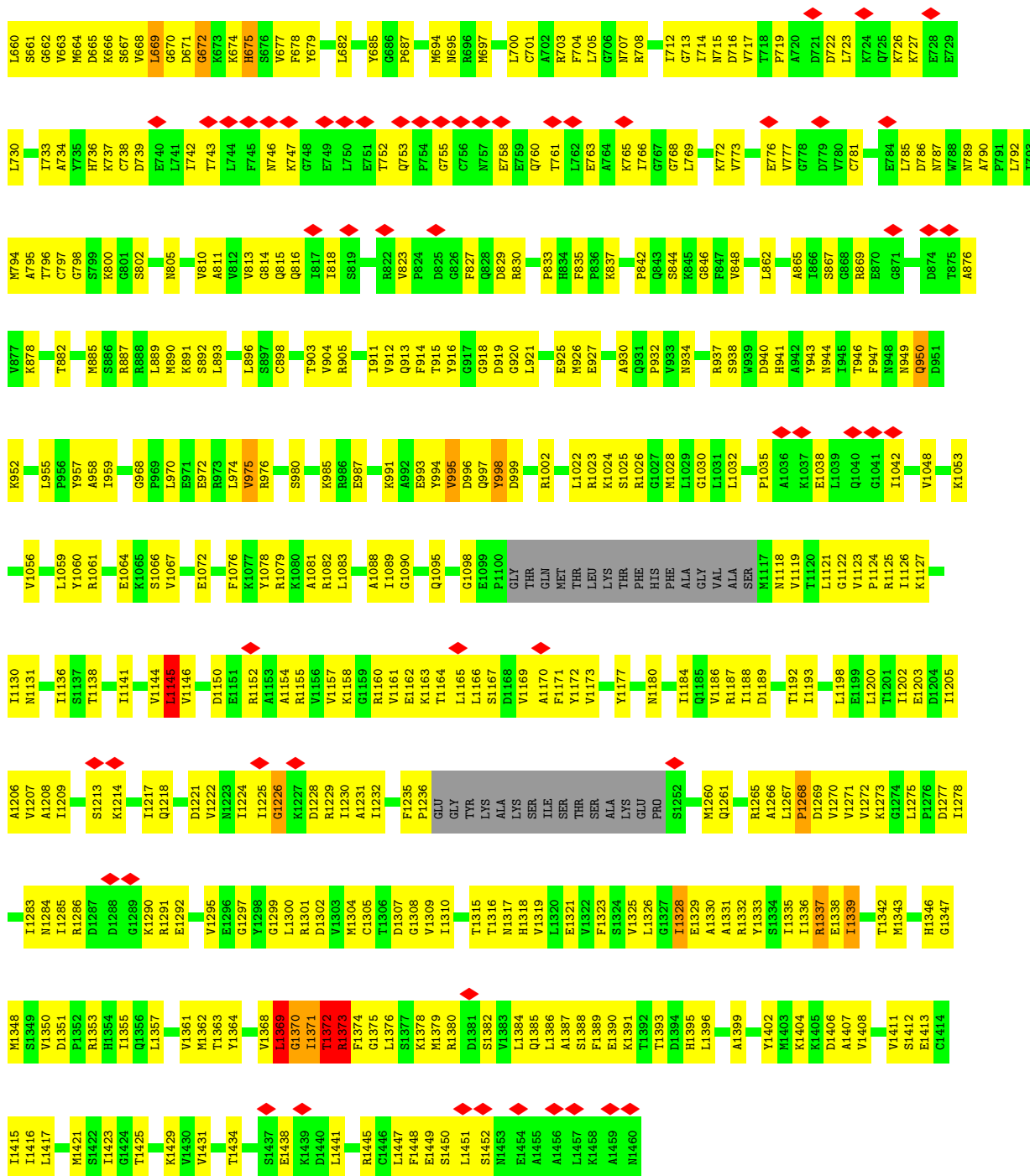
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
22	R	1	1	1	0

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.

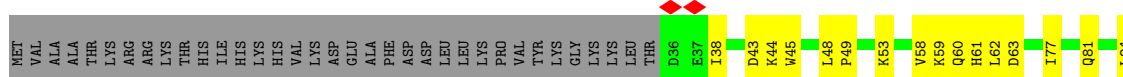
• Molecule 1: DNA-directed RNA polymerase III subunit RPC1





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

Chain B: 45% 50%

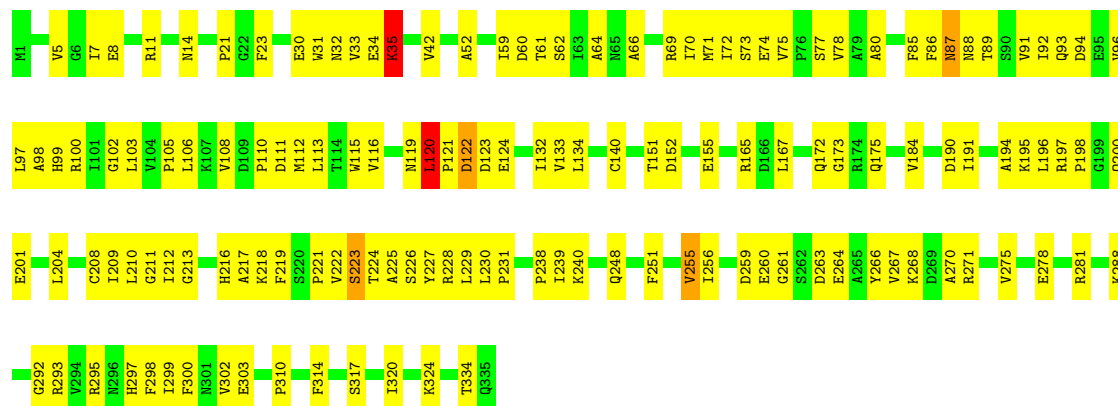


D1068	K1001	V926	S851	E768	P697	L627	L551	K479	L317	H244	D167	S85
I1071	D1002	R927	A852	D769	R698	R628	N552	S480	N396	I247	D168	D86
I1072	M1003	Q928	P855	A770	R698	K629	N553	R481	N397	A248	S169	V87
I1073	L1004	E929	L771	L771	C703	L630	G554	K482	F399	E249	K170	F91
I1074	Y1005	D930	M705	L772	A704	L635	V555	V483	K400	E250	M171	Y92
A1075	S1006	N931	M705	L773	M705	D636	N556	S484	I403	I251	A172	L93
S1076	G1007	P932	N774	L774	I710	F637	N557	S487	L407	P252	C177	K94
I1008	L1008	F933	N859	K775	I710	D638	L561	G485	D404	I253	P178	D87
Q1009	L1009	N934	V860	S776	I713	D639	L562	P486	I407	A254	I98	I98
L1078	G1010	D935	N861	S777	I713	F640	G563	R487	P410	I255	R99	R99
L1079	E1011	Q936	V862	S778	I714	F640	S564	Q490	N411	V256	V100	V100
L1080	C1012	G937	Q863	D779	A714	F640	S565	S492	R412	L257	G101	G101
E1081	L1013	I938	Q864	R780	I715	G644	S566	S493	R413	K258	K102	K102
R1082	L1083	V939	Q865	G781	F718	G644	S567	Q494	A413	C260	G189	G189
M1084	F1018	D941	Y866	F782	K719	L645	R566	F494	M414	L263	E191	S106
M1084	F1019	I942	T864	F782	K719	L645	R567	F494	A415	S264	K192	S107
D1088	I1022	I943	T864	F782	K719	L645	R568	G495	E416	S265	V193	T108
A1089	Y1023	I944	C785	C785	I722	L649	P568	M496	A418	D266	K109	K109
F1090	Y1024	I945	C785	C785	I722	D650	P571	L497	A419	L267	Q197	D110
D1093	Q1025	H947	I881	R788	L724	D651	Q674	D501	L419	I268	E198	Y111
V1094	K1026	H947	D882	R789	L724	V651	P575	D502	L420	M269	L112	L112
C1095	L1027	F949	Q883	T791	L727	E653	K583	T502	L421	C273	T113	T113
G1099	L1028	P950	M885	L795	M728	E654	V584	G505	S421		S201	S201
L1100	H1029	S951	R797	K796	P731	E655	S585	S506	I422		R204	R204
M1101	M1030	R952	Y798	R797	Q733	D656	S586	L510	N423	Y279	I205	I205
G1102	Q1031	M953	A799	Y798	Q733	S657	F587	L510	V424	Q280	I206	I206
Y1103	L1032	T954	N800	N800	M735	L659	P587	L510	H425		E208	E208
S1104	D1033	K957	Q803	Q803	V736	A660	Y591	N513	S426	V285	Y207	Y207
G1105	K1034	M958	D892	K796	L736	L661	S592	N514	N427	N286	A209	A209
M1106	H1036	P959	Q893	R797	I738	E662	S597	M517	R428	L287	D210	D210
C1107	A1037	E960	A894	I806	I738	E663	M597	H518	L429	E288	E211	E211
T1108	R1038	L961	K897	V811	E742	P666	A598	H519	T430	E289	K212	K212
T1109	A1039	I962	V898	V811	L743	P667	H600	L520	S438	S290	K213	K213
S1112	R1040		L899	I818		P668	Y601	T521	N442	S291	G214	G214
A1113	G1041	L969	L900	I818	Y746	S669	A602		S443	K292	I215	I215
N1115	V1045	G971	R901	H821	D747	M670	T603	E525	L444	Y296	V216	V216
I1116	L1046	E974	R904	Q822	K748	H672	G605	E526		T297	Q217	Q217
I1117	R1047	Y975	R905	Q822	L749	H672	G606	E527	M449	Q298	H225	H225
K1118	G1048	G976	P906	L824	P750	E676	R607	P528	E450	Q300	E226	E226
T1121	Q1049	T977	E907	E831	A751	P677	T608	I529	R451	A301	R227	R227
P1122	P1050	C978	L908	V832	G752	F678	G609	K530	V454	L302	K230	K230
Y1123	G981		G910	G833	Q753	T679	R610	K531	T455	E303	T231	T231
K1126	R1053		K911	M834	A755	L680	L612	Y534	L461	Y304	Y232	Y232
F1129	S1055	N987	S914	Q837	T756	L681	L613	V535	T464	G306	V233	V233
Q1130	D1057	S988	R915	Q840	A758	A685	V615	V536	T464	A307	I234	I234
E1131	G1058	L991	H916	Q840	V759	G886	Q619	E538	S465	K308	T235	T235
L1132	G1059	V992	Q917	Y842	S761	L687	D540	E539	N374	V309	K236	K236
Q1135	L1060	D993	Q918	Y842	V762	Y690	L541	D540	G468	K310	M237	M237
M1136	R1061	Q994	S846	S846	G763	P691	V622	T542	T471	M312	G238	G238
N1137	L1062	N997	V847	V847	G764	P691	K623	L543	S475	K239	I240	I240
A1138	G1063	Y998	P848	P848	Y765	N694	D624	L544	Q476	R313	Y241	Y241
	E1064		C922	T949	I767	Q695	T625	S546	F477	R314	L242	L242
			I924	N850		S696	H626		E478	Q315	K243	K243
			1925							K316		



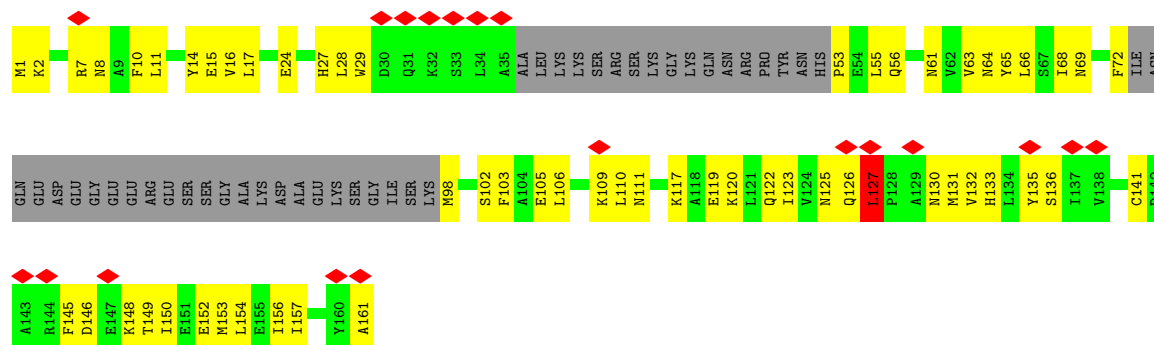
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 58% 41% ..



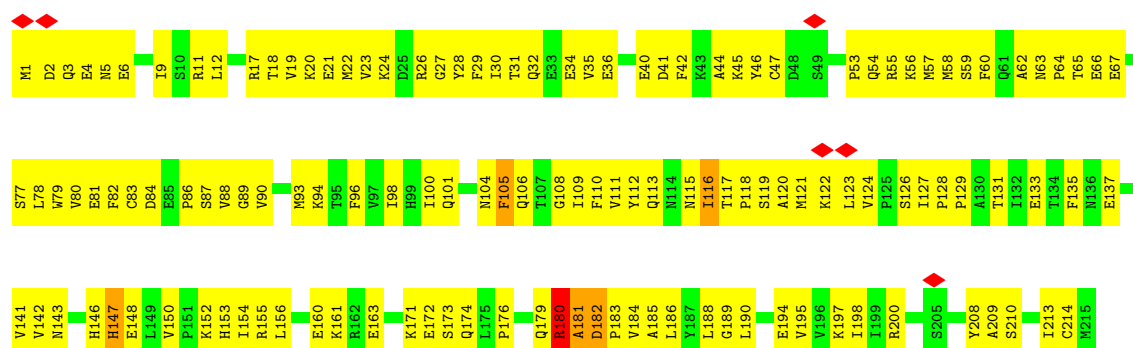
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

Chain D: 12% 37% 36% 26%



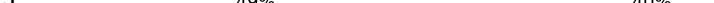
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 37% 60%



- | | | | | | | | |
|----|----|----|----|----|----|----|-----|
| M1 | F4 | C5 | P6 | S7 | C8 | N9 | M10 | M11 | L12 | T15 | D18 | S19 | G20 | V21 | Y22 | T23 | L24 | C29 | P30 | V31 | E32 | F33 | P34 | I35 | E36 | I40 | Y41 | D42 | ARG | LYS | LYS | LEU | PRO | ARG | GLU | VAL | ASP | ASP | VAL | LEU | GLY | GLY | TRP | ASP | ASN | VAL | ASP | GLN | THR | LYS | THR | THR |
|----|----|----|----|----|----|----|-----|

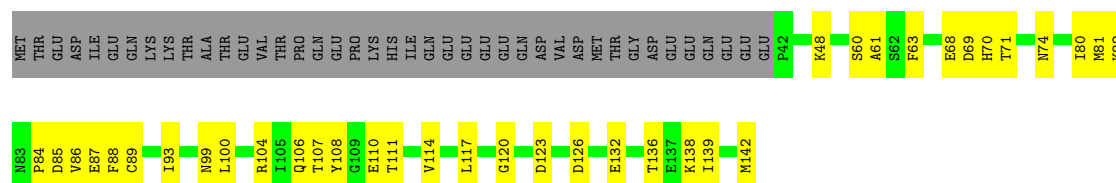
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  49% 40% 6% . .

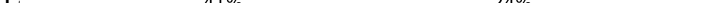


- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K: 45% 26% 29%



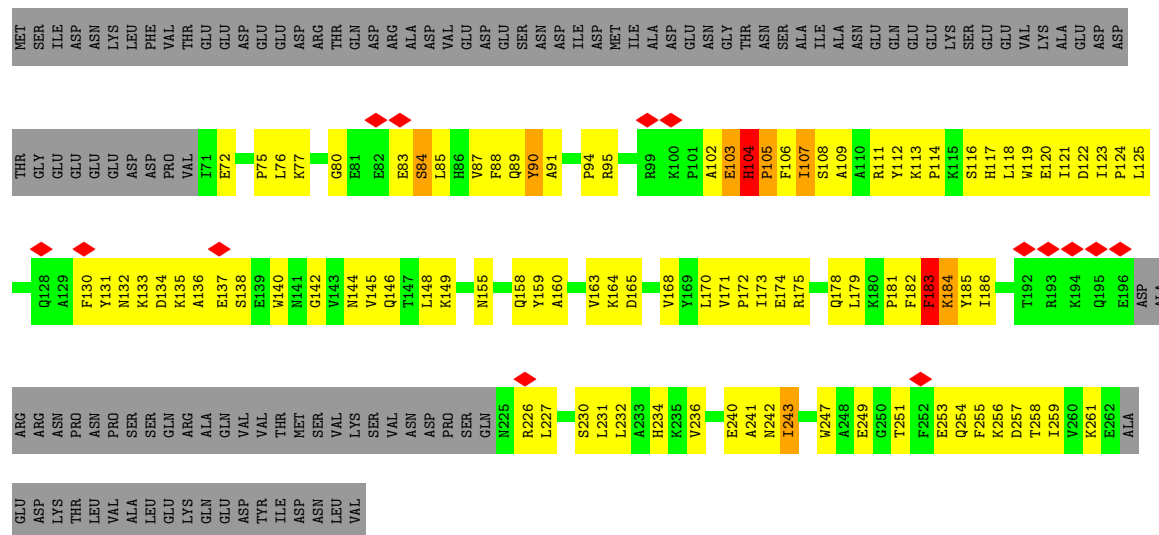
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  41% 24% 34%

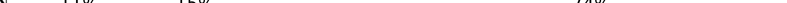


- Molecule 13: DNA-directed RNA polymerase III subunit RPC5

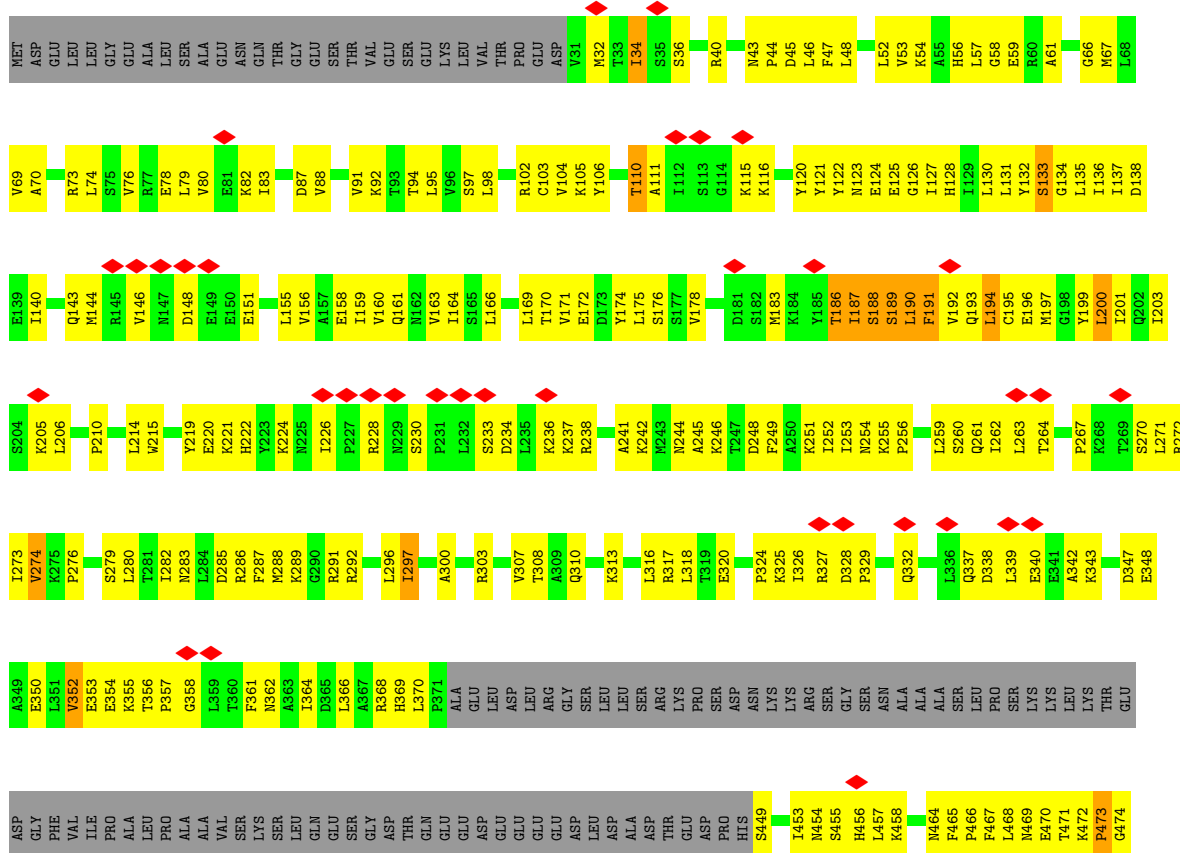
Chain M: 

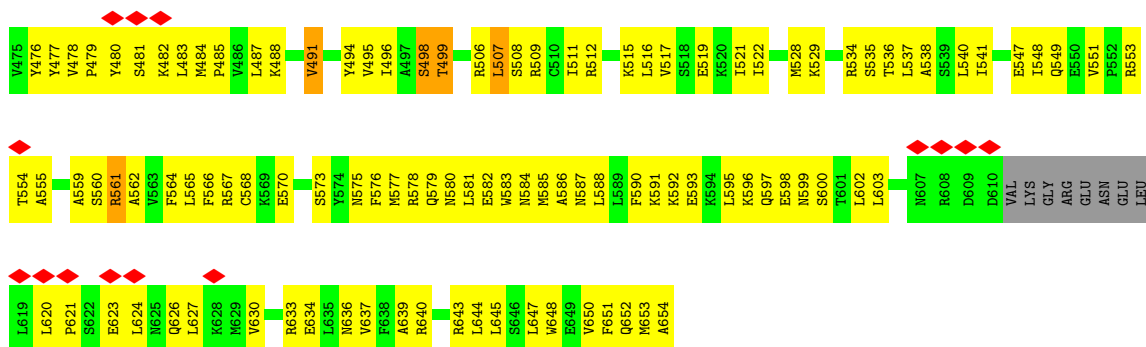


- Molecule 14: DNA-directed RNA polymerase III subunit RPC4

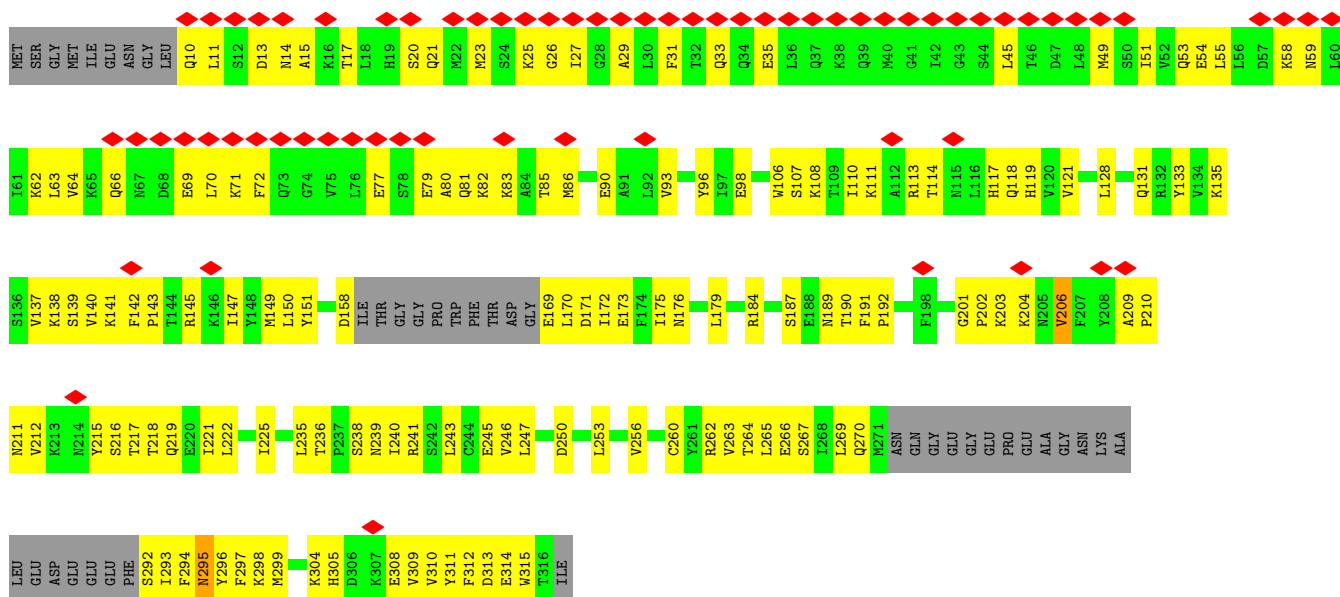
Chain N:  11% 15% 74%

- Molecule 15: DNA-directed RNA polymerase III subunit RPC3

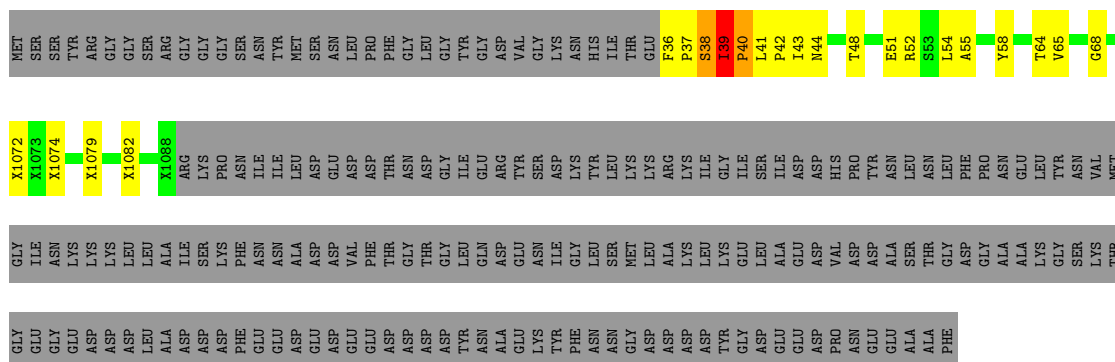


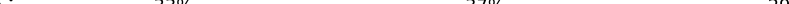


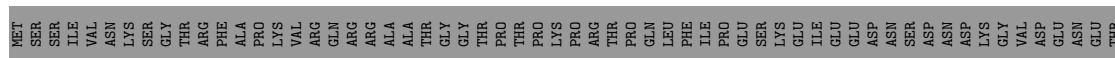
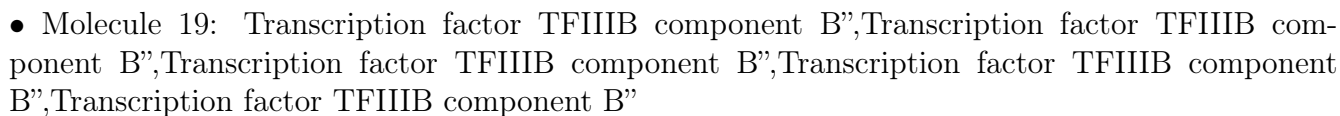
• Molecule 16: DNA-directed RNA polymerase III subunit RPC6

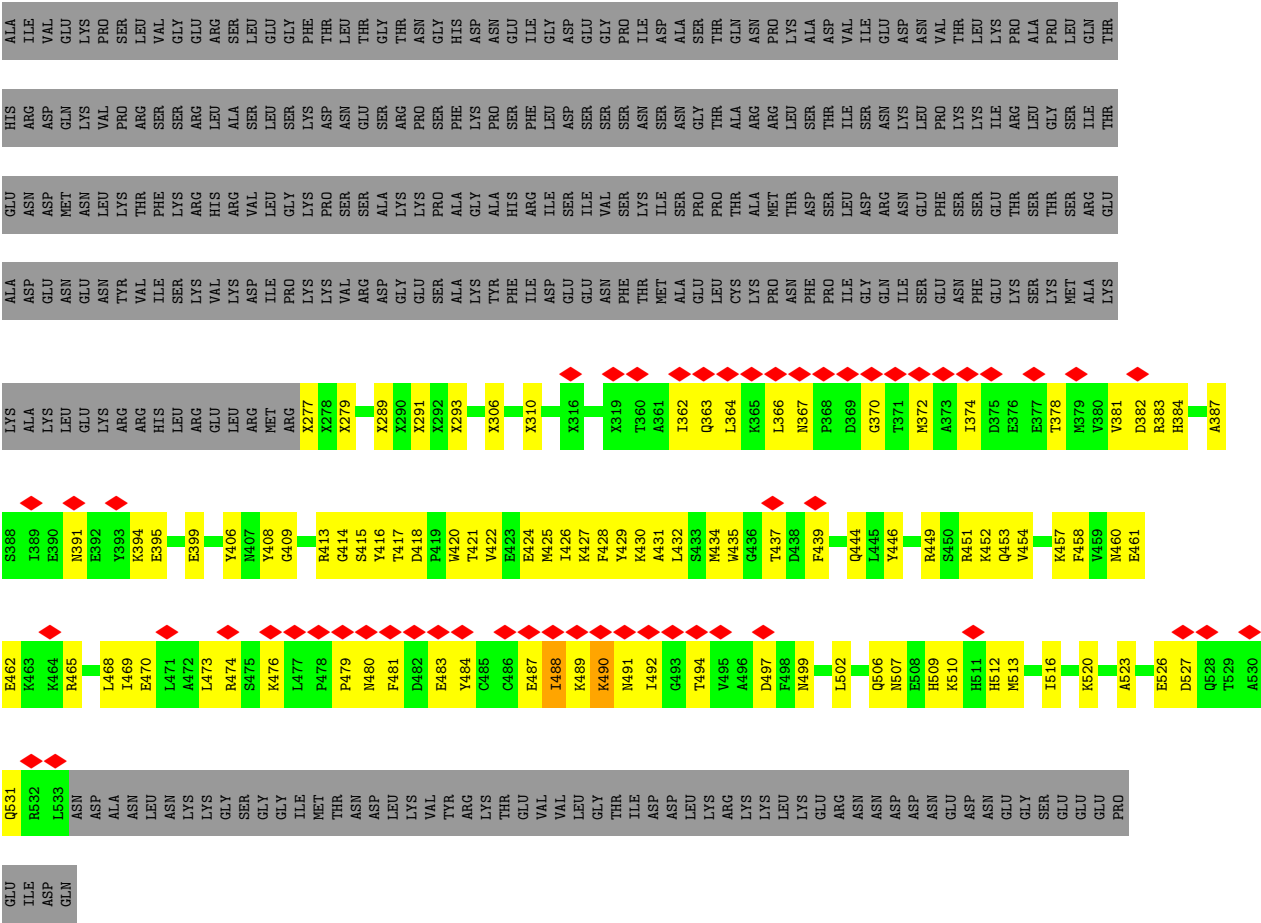


• Molecule 17: DNA-directed RNA polymerase III subunit RPC7, DNA-directed RNA polymerase III subunit RPC7, DNA-directed RNA polymerase III subunit RPC7, DNA-directed RNA polymerase III subunit RPC7, DNA-directed RNA polymerase III subunit RPC7

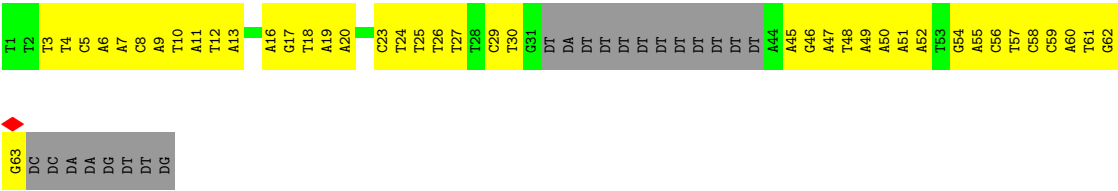
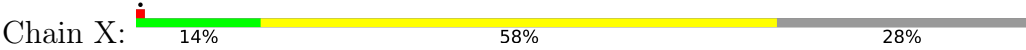


- Chain R: 

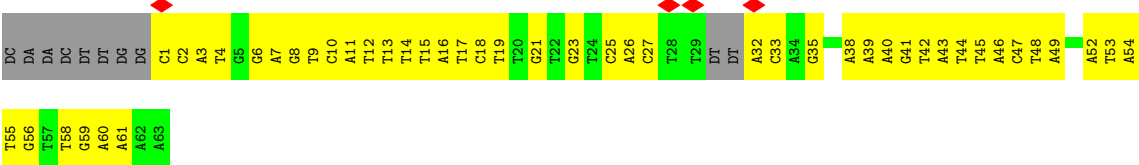




• Molecule 20: DNA (71-MER)



• Molecule 21: DNA (71-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	74281	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	0.279	Depositor
Minimum map value	-0.190	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	339.84, 339.84, 339.84	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.41	2/11358 (0.0%)	0.81	29/15345 (0.2%)
2	B	0.40	1/8943 (0.0%)	0.79	13/12068 (0.1%)
3	C	0.42	1/2711 (0.0%)	0.71	1/3676 (0.0%)
4	D	0.21	0/991	0.63	0/1328
5	E	0.30	0/1795	0.71	2/2416 (0.1%)
6	F	0.44	1/683 (0.1%)	0.74	0/923
7	G	0.27	0/1523	0.68	2/2066 (0.1%)
8	H	0.38	0/1138	0.74	2/1540 (0.1%)
9	I	0.30	0/328	0.76	0/445
10	J	0.54	1/558 (0.2%)	0.97	7/750 (0.9%)
11	K	0.44	0/803	0.77	0/1083
12	L	0.37	0/365	0.79	0/485
13	M	0.24	0/1369	0.75	7/1851 (0.4%)
14	N	0.25	0/855	0.72	1/1149 (0.1%)
15	O	0.31	0/4394	0.79	8/5928 (0.1%)
16	P	0.22	0/2282	0.64	0/3075
17	Q	0.26	0/281	0.72	1/381 (0.3%)
18	R	0.26	0/4200	0.64	7/5659 (0.1%)
19	S	0.21	0/1464	0.60	3/1971 (0.2%)
20	X	0.27	0/1164	0.51	0/1792
21	Y	0.27	0/1400	0.49	0/2157
All	All	0.35	6/48605 (0.0%)	0.74	83/66088 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	63	TYR	C-N	-6.71	1.25	1.33
1	A	502	GLU	CA-C	-5.82	1.44	1.52
3	C	151	THR	C-N	-5.57	1.25	1.33
6	F	130	ILE	C-N	-5.44	1.21	1.33
2	B	915	ARG	CA-C	5.44	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	SER	C-N	-5.06	1.25	1.33

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S	489	LYS	N-CA-C	-10.20	99.11	112.68
3	C	35	LYS	N-CA-C	-9.57	100.84	111.28
10	J	45	CYS	N-CA-C	-9.49	100.62	110.97
15	O	491	VAL	N-CA-C	-9.11	102.76	113.42
2	B	916	HIS	N-CA-C	9.03	124.36	113.16
18	R	211	LYS	N-CA-C	9.00	121.09	111.28
1	A	1270	VAL	N-CA-C	8.97	123.55	110.09
7	G	110	ILE	CA-C-N	7.58	129.32	119.84
7	G	110	ILE	C-N-CA	7.58	129.32	119.84
19	S	488	ILE	N-CA-C	7.51	118.41	106.32
18	R	213	TRP	N-CA-C	7.42	121.90	111.52
15	O	354	GLU	N-CA-C	-7.30	103.47	112.38
13	M	184	LYS	N-CA-C	-7.13	104.31	112.87
1	A	1214	LYS	N-CA-C	-7.13	104.58	113.20
19	S	490	LYS	N-CA-C	-6.97	97.85	109.07
15	O	34	ILE	N-CA-C	-6.92	104.01	113.00
18	R	215	PHE	N-CA-C	-6.92	104.97	113.41
2	B	1047	THR	N-CA-C	6.89	118.87	111.36
1	A	1337	ARG	N-CA-C	6.75	118.72	111.36
2	B	914	SER	N-CA-C	6.74	120.48	112.93
2	B	1135	MET	CA-C-N	-6.67	113.55	122.42
2	B	1135	MET	C-N-CA	-6.67	113.55	122.42
1	A	190	SER	CA-C-N	-6.61	111.52	121.83
1	A	190	SER	C-N-CA	-6.61	111.52	121.83
13	M	183	PHE	N-CA-C	6.59	118.41	107.20
18	R	259	LEU	N-CA-C	6.57	119.04	111.02
2	B	551	LEU	N-CA-C	6.55	119.73	109.96
1	A	645	MET	N-CA-C	6.50	120.21	112.93
1	A	1032	LEU	CA-C-N	6.50	129.93	120.51
1	A	1032	LEU	C-N-CA	6.50	129.93	120.51
15	O	507	LEU	N-CA-C	6.49	118.44	111.36
1	A	1370	GLY	N-CA-C	6.49	123.09	112.84
1	A	643	ASN	N-CA-C	-6.48	105.44	113.15
10	J	45	CYS	N-CA-CB	6.41	119.26	109.91
18	R	214	MET	CA-C-O	6.30	125.89	119.97
1	A	878	LYS	N-CA-C	-6.25	104.91	112.54
1	A	1339	ILE	N-CA-C	-6.21	104.46	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	876	ALA	N-CA-C	6.08	117.57	111.07
13	M	104	HIS	CA-C-N	5.99	127.33	119.84
13	M	104	HIS	C-N-CA	5.99	127.33	119.84
15	O	110	THR	N-CA-C	5.96	119.25	109.72
15	O	186	THR	N-CA-C	-5.87	105.78	113.12
15	O	111	ALA	N-CA-C	-5.84	102.29	110.35
2	B	416	TYR	CA-C-N	5.82	132.65	121.54
2	B	416	TYR	C-N-CA	5.82	132.65	121.54
18	R	23	LEU	N-CA-CB	5.81	119.97	110.90
1	A	363	ARG	N-CA-C	5.80	123.16	110.80
1	A	645	MET	N-CA-CB	-5.80	102.55	110.56
8	H	108	SER	CB-CA-C	-5.79	109.88	116.54
10	J	63	TYR	CA-C-N	-5.74	111.01	122.90
10	J	63	TYR	C-N-CA	-5.74	111.01	122.90
1	A	557	PHE	N-CA-C	5.68	118.20	111.33
15	O	200	LEU	N-CA-C	5.67	118.81	109.85
1	A	1369	LEU	N-CA-C	5.65	115.48	108.19
1	A	1268	PRO	CA-C-N	5.62	129.12	122.44
1	A	1268	PRO	C-N-CA	5.62	129.12	122.44
2	B	915	ARG	CA-C-O	5.56	128.46	120.51
1	A	353	PHE	N-CA-C	5.54	116.94	108.30
10	J	10	CYS	N-CA-C	5.53	118.07	111.71
1	A	1098	GLY	N-CA-C	5.53	119.33	112.64
8	H	83	GLN	CB-CA-C	-5.50	108.64	116.34
17	Q	38	SER	N-CA-C	5.49	115.49	108.24
1	A	1372	THR	N-CA-CB	5.45	119.70	110.49
2	B	916	HIS	N-CA-CB	-5.39	102.20	110.44
1	A	1152	ARG	CB-CA-C	-5.33	109.99	117.23
5	E	105	PHE	CB-CA-C	-5.32	108.87	115.89
1	A	1226	GLY	N-CA-C	-5.29	104.67	110.96
5	E	116	ILE	N-CA-C	-5.29	99.90	107.78
1	A	117	GLU	CB-CA-C	-5.26	109.53	115.79
18	R	153	SER	N-CA-C	5.23	119.76	113.17
14	N	406	ALA	N-CA-C	5.22	117.02	110.91
10	J	43	ARG	N-CA-C	-5.21	103.04	110.59
13	M	165	ASP	CB-CA-C	-5.20	110.60	116.63
10	J	42	LYS	N-CA-C	-5.18	107.12	113.50
1	A	1373	ARG	N-CA-C	-5.16	105.65	111.28
13	M	90	TYR	CA-C-N	-5.16	115.68	122.85
13	M	90	TYR	C-N-CA	-5.16	115.68	122.85
1	A	128	ARG	CA-C-N	-5.11	113.82	120.67
1	A	128	ARG	C-N-CA	-5.11	113.82	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	635	LEU	CA-C-N	5.05	132.70	122.04
2	B	635	LEU	C-N-CA	5.05	132.70	122.04
2	B	339	ALA	CB-CA-C	-5.04	109.28	116.34
1	A	586	GLY	N-CA-C	-5.02	103.84	111.42

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	895	0
2	B	8788	0	8902	726	0
3	C	2655	0	2628	156	0
4	D	977	0	983	61	0
5	E	1759	0	1788	130	0
6	F	671	0	692	27	0
7	G	1484	0	1485	120	0
8	H	1120	0	1089	72	0
9	I	321	0	303	28	0
10	J	549	0	560	63	0
11	K	792	0	790	46	0
12	L	363	0	386	20	0
13	M	1338	0	1307	162	0
14	N	845	0	891	108	0
15	O	4329	0	4497	359	0
16	P	2242	0	2265	146	0
17	Q	368	0	308	22	0
18	R	4131	0	4230	264	0
19	S	1649	0	1457	91	0
20	X	1040	0	584	67	0
21	Y	1249	0	696	69	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	L	1	0	0	0	0
22	R	1	0	0	0	0
All	All	47836	0	47126	3173	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 34.

All (3173) 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)
13:M:84:SER:O	13:M:85:LEU:HD12	1.26	1.31
2:B:546:SER:HB2	14:N:391:LEU:CD2	1.63	1.29
1:A:249:PRO:CD	1:A:250:SER:H	1.43	1.29
16:P:264:THR:O	16:P:265:LEU:HG	1.23	1.29
1:A:1145:LEU:HD11	1:A:1157:VAL:CG2	1.61	1.28
15:O:516:LEU:HD12	15:O:516:LEU:O	1.17	1.24
1:A:1369:LEU:CD2	1:A:1374:PHE:HE2	1.49	1.23
13:M:183:PHE:CE1	13:M:185:TYR:CD2	2.27	1.23
1:A:327:ILE:HA	1:A:353:PHE:CD2	1.74	1.20
10:J:42:LYS:HE3	10:J:43:ARG:NH1	1.55	1.20
8:H:104:PHE:O	8:H:105:GLU:HG3	1.42	1.18
13:M:104:HIS:CG	13:M:105:PRO:HD2	1.77	1.18
18:R:7:CYS:SG	18:R:28:CYS:HB3	1.82	1.18
2:B:933:PHE:CE2	3:C:226:SER:HB2	1.79	1.17
1:A:1145:LEU:CD1	1:A:1157:VAL:HG21	1.74	1.17
1:A:1169:VAL:HG23	1:A:1170:ALA:H	1.10	1.15
13:M:183:PHE:CD1	13:M:185:TYR:CD2	2.34	1.14
15:O:303:ARG:HA	16:P:265:LEU:HD21	1.22	1.14
2:B:934:ASN:HB3	2:B:1004:LEU:HD23	1.26	1.12
1:A:1369:LEU:CD2	1:A:1374:PHE:CE2	2.33	1.11
1:A:372:ARG:HD2	2:B:1050:PRO:O	1.49	1.11
15:O:353:GLU:HA	15:O:357:PRO:HD2	1.29	1.10
15:O:515:LYS:O	15:O:516:LEU:HG	1.48	1.10
16:P:311:TYR:HA	17:Q:40:PRO:HA	1.30	1.09
1:A:371:LYS:NZ	2:B:1122:PRO:HB3	1.67	1.08
2:B:780:ARG:HH12	10:J:6:ARG:CD	1.65	1.08
7:G:87:GLY:O	7:G:146:ILE:HB	1.54	1.08
12:L:31:CYS:HB2	12:L:34:CYS:SG	1.94	1.08
2:B:546:SER:CB	14:N:391:LEU:CD2	2.30	1.08
1:A:1369:LEU:HD21	1:A:1374:PHE:HE2	1.19	1.08
15:O:352:VAL:HG13	15:O:353:GLU:OE1	1.53	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:PRO:HD2	1:A:250:SER:N	1.54	1.07
13:M:183:PHE:CE1	13:M:185:TYR:HD2	1.66	1.06
2:B:546:SER:CB	14:N:391:LEU:HD23	1.84	1.06
1:A:18:PHE:HE1	2:B:1139:PRO:HB3	1.22	1.05
1:A:235:LYS:HB3	1:A:252:ARG:HE	1.16	1.05
2:B:671:THR:HG22	2:B:672:HIS:CE1	1.92	1.05
13:M:183:PHE:CD1	13:M:185:TYR:HD2	1.73	1.05
1:A:974:LEU:HD21	1:A:998:TYR:HB3	1.40	1.04
2:B:780:ARG:HH12	10:J:6:ARG:HD3	1.21	1.04
15:O:498:SER:HB2	16:P:296:TYR:HB2	1.39	1.04
2:B:780:ARG:NH2	3:C:217:ALA:HB1	1.72	1.04
2:B:1045:VAL:HG23	2:B:1046:LEU:HD12	1.40	1.04
2:B:780:ARG:NH1	10:J:6:ARG:CD	2.20	1.03
15:O:516:LEU:O	15:O:516:LEU:CD1	2.06	1.03
10:J:42:LYS:HE3	10:J:43:ARG:HH12	0.86	1.02
13:M:183:PHE:CE1	13:M:185:TYR:CE2	2.47	1.01
19:S:483:GLU:O	19:S:487:GLU:HB2	1.61	1.01
15:O:110:THR:HG22	15:O:116:LYS:HA	1.41	1.00
2:B:546:SER:HB2	14:N:391:LEU:HD23	1.38	0.99
11:K:88:PHE:HB3	11:K:106:GLN:HG2	1.41	0.99
1:A:239:CYS:SG	1:A:246:ALA:HB2	2.03	0.99
7:G:83:GLU:O	7:G:149:ARG:HA	1.63	0.99
2:B:551:LEU:HD11	14:N:388:THR:H	1.25	0.98
2:B:671:THR:CG2	2:B:672:HIS:CE1	2.47	0.98
15:O:498:SER:CB	16:P:296:TYR:HB2	1.94	0.98
13:M:104:HIS:CG	13:M:105:PRO:CD	2.47	0.98
2:B:671:THR:HG22	2:B:672:HIS:ND1	1.78	0.98
1:A:371:LYS:HZ3	2:B:1122:PRO:HB3	1.22	0.98
1:A:975:VAL:HG22	1:A:976:ARG:H	1.30	0.97
13:M:84:SER:C	13:M:85:LEU:HD12	1.89	0.97
2:B:933:PHE:CE2	3:C:226:SER:CB	2.47	0.97
15:O:498:SER:HB2	16:P:296:TYR:CB	1.94	0.97
2:B:415:GLU:HG2	2:B:416:TYR:H	1.30	0.96
1:A:285:LEU:HD21	1:A:353:PHE:HD1	1.28	0.96
3:C:119:ASN:C	3:C:120:LEU:HG	1.90	0.96
2:B:933:PHE:HE2	3:C:226:SER:CB	1.76	0.95
2:B:780:ARG:NH1	10:J:6:ARG:HD3	1.79	0.95
3:C:222:VAL:HG11	3:C:225:ALA:HB2	1.48	0.95
2:B:780:ARG:NH1	10:J:6:ARG:HD2	1.81	0.95
1:A:617:ASN:OD1	1:A:618:HIS:N	2.00	0.94
1:A:18:PHE:CE1	2:B:1139:PRO:HB3	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:94:PRO:HA	14:N:391:LEU:O	1.67	0.94
1:A:18:PHE:HD1	2:B:1139:PRO:HA	1.30	0.94
4:D:126:GLN:O	4:D:127:LEU:HG	1.68	0.93
1:A:373:VAL:O	2:B:1050:PRO:HG2	1.67	0.93
2:B:772:VAL:HG13	2:B:943:ILE:HG23	1.49	0.93
3:C:33:VAL:O	3:C:34:GLU:HB2	1.68	0.93
13:M:104:HIS:HE1	14:N:395:ILE:HD13	1.31	0.93
1:A:1266:ALA:O	1:A:1269:ASP:HB3	1.67	0.93
4:D:110:LEU:HB3	4:D:120:LYS:HE3	1.50	0.92
18:R:22:ASP:OD1	18:R:23:LEU:N	2.02	0.92
1:A:664:MET:HB3	1:A:669:LEU:CD2	2.00	0.92
1:A:15:GLY:H	1:A:1408:VAL:HG12	1.31	0.92
5:E:181:ALA:O	5:E:182:ASP:C	2.12	0.91
1:A:285:LEU:HD21	1:A:353:PHE:CD1	2.05	0.91
1:A:196:ILE:O	1:A:200:GLU:HG3	1.67	0.91
16:P:33:GLN:NE2	16:P:49:MET:SD	2.44	0.91
11:K:88:PHE:HB3	11:K:106:GLN:CG	2.02	0.90
15:O:303:ARG:HA	16:P:265:LEU:CD2	2.01	0.90
15:O:105:LYS:HB2	15:O:121:TYR:HB2	1.53	0.90
19:S:458:PHE:O	19:S:462:GLU:HB2	1.71	0.90
2:B:1139:PRO:O	2:B:1140:ARG:O	1.87	0.90
18:R:213:TRP:HH2	18:R:497:ARG:HA	1.36	0.90
1:A:444:LEU:HD11	1:A:445:ARG:HH11	1.37	0.89
1:A:393:ALA:HB3	1:A:499:ARG:HB2	1.52	0.89
1:A:1369:LEU:HD22	1:A:1374:PHE:HE2	1.38	0.89
1:A:314:GLU:HB2	15:O:559:ALA:HB1	1.54	0.89
2:B:734:PRO:HB2	2:B:915:ARG:HH12	1.37	0.89
5:E:181:ALA:O	5:E:182:ASP:O	1.91	0.89
3:C:172:GLN:H	3:C:175:GLN:HB3	1.38	0.89
1:A:154:CYS:CB	1:A:157:CYS:SG	2.60	0.88
2:B:933:PHE:HE1	2:B:1005:TYR:HD2	1.17	0.88
15:O:554:THR:HG23	15:O:561:ARG:HE	1.36	0.88
13:M:183:PHE:HE1	13:M:185:TYR:CE2	1.90	0.88
18:R:397:VAL:HA	18:R:449:VAL:O	1.74	0.88
1:A:235:LYS:HB3	1:A:252:ARG:NE	1.88	0.88
1:A:109:ASN:HD22	1:A:159:ALA:CB	1.85	0.88
1:A:1369:LEU:HD21	1:A:1374:PHE:CE2	2.03	0.88
1:A:1145:LEU:CD2	1:A:1308:GLY:O	2.21	0.88
18:R:232:CYS:HB3	18:R:237:LEU:HD11	1.54	0.88
20:X:6:DA:H4'	20:X:7:DA:OP1	1.73	0.88
1:A:100:ILE:O	1:A:104:GLN:HB2	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:CYS:HB3	1:A:157:CYS:SG	2.14	0.87
1:A:1369:LEU:HD22	1:A:1374:PHE:CE2	2.09	0.87
16:P:11:LEU:O	16:P:15:ALA:HB2	1.73	0.87
16:P:264:THR:O	16:P:265:LEU:CG	2.18	0.87
1:A:249:PRO:HD2	1:A:250:SER:H	0.71	0.87
15:O:193:GLN:O	15:O:195:CYS:N	2.08	0.87
1:A:1169:VAL:HG23	1:A:1170:ALA:N	1.88	0.87
2:B:735:MET:HB2	2:B:754:ASN:HD21	1.39	0.87
7:G:53:THR:HG21	7:G:71:THR:HG22	1.57	0.86
1:A:327:ILE:HG22	1:A:353:PHE:CE2	2.11	0.86
7:G:125:GLU:HG2	7:G:126:SER:N	1.88	0.86
13:M:94:PRO:CA	14:N:391:LEU:O	2.22	0.86
1:A:172:GLY:HA3	1:A:331:SER:HB3	1.58	0.86
1:A:238:ASP:OD1	1:A:239:CYS:N	2.09	0.86
1:A:664:MET:CB	1:A:669:LEU:HD21	2.06	0.86
3:C:119:ASN:O	3:C:120:LEU:HG	1.76	0.86
16:P:138:LYS:HD2	16:P:143:PRO:HB3	1.57	0.86
4:D:126:GLN:C	4:D:127:LEU:HG	2.01	0.86
13:M:90:TYR:O	14:N:392:GLN:HG3	1.76	0.86
15:O:156:VAL:HG12	15:O:189:SER:HB3	1.56	0.85
12:L:31:CYS:SG	12:L:48:CYS:HB3	2.16	0.85
1:A:946:THR:HG21	1:A:1066:SER:HA	1.58	0.85
4:D:145:PHE:HB2	4:D:149:THR:HG21	1.56	0.85
1:A:49:LYS:HD2	1:A:54:LEU:HB3	1.59	0.85
13:M:158:GLN:HE21	14:N:308:GLN:HE21	1.25	0.85
10:J:42:LYS:CE	10:J:43:ARG:HH12	1.82	0.85
15:O:143:GLN:HE21	15:O:196:GLU:HG2	1.41	0.85
15:O:263:LEU:HB3	15:O:272:ARG:HH21	1.41	0.85
1:A:327:ILE:HA	1:A:353:PHE:CE2	2.12	0.85
15:O:190:LEU:HD13	15:O:194:LEU:HD23	1.57	0.85
1:A:1166:LEU:HA	1:A:1169:VAL:HG22	1.56	0.84
12:L:31:CYS:SG	12:L:48:CYS:CB	2.64	0.84
1:A:356:ARG:HG3	2:B:1131:GLU:OE2	1.76	0.84
13:M:90:TYR:O	14:N:392:GLN:CG	2.26	0.84
15:O:190:LEU:HA	15:O:193:GLN:HB3	1.60	0.84
15:O:547:GLU:HG2	15:O:548:ILE:H	1.43	0.84
15:O:640:ARG:HH12	16:P:309:VAL:HA	1.43	0.84
2:B:780:ARG:CZ	3:C:217:ALA:HB1	2.07	0.84
13:M:89:GLN:HE21	13:M:178:GLN:HE22	1.20	0.84
1:A:235:LYS:HD2	1:A:252:ARG:HB2	1.58	0.84
2:B:933:PHE:CD2	2:B:937:GLY:HA2	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:302:GLU:HB3	14:N:410:GLY:HA2	1.59	0.83
15:O:597:GLN:HA	15:O:600:SER:HB2	1.61	0.83
7:G:84:ILE:HA	7:G:148:PHE:O	1.78	0.83
1:A:235:LYS:CB	1:A:252:ARG:HE	1.91	0.83
2:B:931:MET:CG	2:B:932:PRO:HD2	2.09	0.83
1:A:556:ASP:HB3	2:B:767:ILE:CD1	2.09	0.83
1:A:1305:CYS:SG	5:E:11:ARG:NH1	2.49	0.83
2:B:321:GLN:H	2:B:324:ILE:HB	1.41	0.83
9:I:8:CYS:HB3	9:I:29:CYS:SG	2.17	0.83
15:O:288:MET:SD	15:O:291:ARG:NH2	2.51	0.83
1:A:664:MET:HB3	1:A:669:LEU:HD21	1.60	0.83
15:O:292:ARG:HH12	15:O:650:VAL:HA	1.44	0.82
1:A:235:LYS:CE	1:A:254:GLU:HG3	2.09	0.82
1:A:239:CYS:SG	1:A:240:GLU:N	2.51	0.82
2:B:109:LYS:HG3	2:B:111:TYR:H	1.42	0.82
2:B:373:GLY:HA2	2:B:651:VAL:HG21	1.61	0.82
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.43	0.82
13:M:104:HIS:CD2	13:M:105:PRO:HD2	2.14	0.82
8:H:104:PHE:O	8:H:105:GLU:CG	2.27	0.82
17:Q:38:SER:O	17:Q:39:ILE:O	1.98	0.82
2:B:936:GLN:HB3	10:J:43:ARG:HD3	1.62	0.82
1:A:642:PRO:HB2	1:A:644:GLU:HG2	1.62	0.81
2:B:538:VAL:HG12	2:B:565:ILE:HB	1.62	0.81
5:E:109:ILE:HG22	5:E:133:GLU:HB3	1.59	0.81
1:A:644:GLU:OE2	1:A:651:PHE:HD2	1.63	0.81
2:B:933:PHE:CE2	2:B:937:GLY:HA2	2.15	0.81
13:M:112:TYR:HD1	13:M:119:TRP:HE1	1.28	0.81
15:O:292:ARG:HD2	15:O:488:LYS:HZ2	1.44	0.81
1:A:373:VAL:O	2:B:1050:PRO:CG	2.28	0.81
2:B:934:ASN:HB3	2:B:1004:LEU:CD2	2.07	0.81
1:A:1330:ALA:HB2	5:E:150:VAL:HG22	1.63	0.81
2:B:933:PHE:CG	2:B:934:ASN:N	2.48	0.81
5:E:179:GLN:O	5:E:180:ARG:O	1.98	0.80
15:O:124:GLU:HG3	15:O:126:GLY:H	1.44	0.80
1:A:1038:GLU:HB3	1:A:1042:ILE:HD11	1.62	0.80
2:B:933:PHE:CZ	3:C:226:SER:HB2	2.15	0.80
2:B:1047:THR:HG22	2:B:1049:GLN:H	1.45	0.80
13:M:94:PRO:HB3	14:N:391:LEU:O	1.81	0.80
15:O:183:MET:O	15:O:187:ILE:HG12	1.81	0.80
15:O:105:LYS:HG2	15:O:123:ASN:HA	1.62	0.80
13:M:112:TYR:H	13:M:243:ILE:HG21	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PHE:CD1	2:B:1139:PRO:HA	2.16	0.80
18:R:213:TRP:HD1	18:R:287:PRO:HD3	1.46	0.80
2:B:834:MET:HE1	12:L:63:ARG:HD2	1.63	0.80
15:O:48:LEU:HD22	15:O:581:LEU:HD11	1.63	0.80
15:O:324:PRO:HB2	15:O:328:ASP:HB3	1.64	0.80
2:B:364:LYS:HG3	2:B:365:MET:H	1.46	0.79
2:B:1026:LYS:NZ	2:B:1030:MET:SD	2.54	0.79
16:P:176:ASN:HA	16:P:179:LEU:HB2	1.64	0.79
5:E:88:VAL:HG23	5:E:117:THR:HG22	1.64	0.79
5:E:117:THR:HG23	5:E:120:ALA:H	1.45	0.79
1:A:400:LYS:HA	1:A:465:HIS:HD2	1.45	0.79
2:B:915:ARG:HD3	2:B:960:GLU:OE2	1.82	0.79
15:O:200:LEU:HB3	15:O:280:LEU:HB3	1.64	0.79
2:B:546:SER:CB	14:N:391:LEU:HD21	2.12	0.79
13:M:104:HIS:ND1	13:M:105:PRO:HD3	1.98	0.79
1:A:371:LYS:NZ	2:B:1122:PRO:CB	2.45	0.79
2:B:932:PRO:O	2:B:940:PRO:HD2	1.82	0.79
9:I:29:CYS:HA	13:M:183:PHE:HE2	1.47	0.79
1:A:235:LYS:NZ	1:A:254:GLU:HG3	1.96	0.79
1:A:353:PHE:O	1:A:356:ARG:HG2	1.82	0.79
2:B:1112:SER:HB2	2:B:1114:GLU:HG2	1.63	0.79
1:A:675:HIS:HA	1:A:937:ARG:HH22	1.46	0.79
13:M:94:PRO:HA	14:N:392:GLN:HA	1.63	0.79
15:O:110:THR:HG21	15:O:115:LYS:O	1.83	0.79
1:A:197:TRP:CZ3	15:O:567:ARG:NH1	2.51	0.78
15:O:80:VAL:HG11	15:O:87:ASP:HB2	1.64	0.78
12:L:31:CYS:CB	12:L:34:CYS:SG	2.63	0.78
1:A:163:VAL:C	1:A:180:HIS:HD2	1.91	0.78
1:A:124:LEU:HB3	1:A:128:ARG:HH12	1.48	0.78
16:P:235:LEU:HD21	16:P:239:ASN:HB3	1.65	0.78
19:S:494:THR:HB	19:S:497:ASP:HB2	1.65	0.78
3:C:134:LEU:HD23	3:C:167:LEU:HD23	1.65	0.78
2:B:741:ILE:HG23	2:B:746:TYR:HB3	1.66	0.78
2:B:915:ARG:HD2	2:B:1023:TYR:HB3	1.66	0.78
3:C:103:LEU:HD22	10:J:5:VAL:HG23	1.66	0.78
2:B:931:MET:HG2	2:B:932:PRO:HD2	1.66	0.78
2:B:108:THR:HG22	2:B:109:LYS:H	1.49	0.77
2:B:757:VAL:O	2:B:1019:PHE:HB2	1.83	0.77
13:M:183:PHE:HE1	13:M:185:TYR:HE2	1.30	0.77
7:G:5:SER:O	7:G:73:ARG:HA	1.83	0.77
1:A:269:ARG:NH2	1:A:286:THR:H	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:LEU:HD23	1:A:1308:GLY:O	1.84	0.77
1:A:1163:LYS:HG3	1:A:1164:THR:H	1.47	0.77
15:O:156:VAL:HG12	15:O:189:SER:CB	2.15	0.77
19:S:458:PHE:O	19:S:462:GLU:CB	2.33	0.77
19:S:470:GLU:O	19:S:474:ARG:HB3	1.84	0.77
1:A:1048:VAL:HG11	1:A:1053:LYS:HG3	1.65	0.77
16:P:69:GLU:HG3	16:P:70:LEU:H	1.50	0.77
1:A:235:LYS:CD	1:A:252:ARG:HB2	2.14	0.77
3:C:224:THR:HB	10:J:10:CYS:SG	2.25	0.77
2:B:266:LEU:HD21	9:I:4:PHE:HA	1.66	0.77
1:A:705:LEU:CD2	2:B:761:SER:HB2	2.15	0.77
3:C:152:ASP:HB2	3:C:155:GLU:HG2	1.67	0.77
15:O:172:GLU:HG3	15:O:276:PRO:HB2	1.66	0.77
2:B:1139:PRO:O	2:B:1140:ARG:C	2.27	0.77
5:E:29:PHE:HB2	5:E:65:THR:HB	1.65	0.77
18:R:632:ALA:O	18:R:636:LEU:HB2	1.85	0.77
1:A:200:GLU:HB3	15:O:516:LEU:CD2	2.15	0.76
2:B:971:GLY:HA2	10:J:51:LEU:HD11	1.66	0.76
3:C:231:PRO:HB3	3:C:275:VAL:HG22	1.67	0.76
11:K:60:SER:HA	11:K:106:GLN:HA	1.65	0.76
15:O:515:LYS:O	15:O:516:LEU:CG	2.33	0.76
16:P:264:THR:C	16:P:265:LEU:HG	2.09	0.76
13:M:105:PRO:O	13:M:106:PHE:HB2	1.85	0.76
2:B:671:THR:CG2	2:B:672:HIS:ND1	2.47	0.76
15:O:98:LEU:HB3	15:O:103:CYS:HB2	1.65	0.76
3:C:275:VAL:HG21	3:C:293:ARG:HD3	1.66	0.76
3:C:70:ILE:HG13	3:C:74:GLU:HB2	1.68	0.76
15:O:91:VAL:O	15:O:95:LEU:HB2	1.85	0.76
15:O:196:GLU:HG3	15:O:197:MET:H	1.49	0.76
1:A:1396:LEU:HD13	2:B:1132:LEU:HD21	1.68	0.76
2:B:551:LEU:CD1	14:N:388:THR:H	1.99	0.75
1:A:329:SER:O	1:A:351:ARG:NH2	2.20	0.75
1:A:1184:ILE:HB	1:A:1232:ILE:HB	1.66	0.75
1:A:373:VAL:HG12	1:A:374:ASP:H	1.51	0.75
15:O:353:GLU:CA	15:O:357:PRO:HD2	2.12	0.75
18:R:200:LYS:HG2	18:R:276:ARG:HH22	1.50	0.75
1:A:197:TRP:HZ3	15:O:567:ARG:NH1	1.85	0.75
2:B:901:ARG:NH2	3:C:94:ASP:OD1	2.20	0.75
1:A:332:VAL:HG13	1:A:333:ASN:H	1.51	0.75
1:A:541:LEU:HG	1:A:551:ILE:HD11	1.69	0.75
2:B:930:ASP:OD1	3:C:69:ARG:NH1	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:419:GLU:HB3	18:R:429:ILE:HD13	1.68	0.75
2:B:1057:ASP:CG	2:B:1058:GLY:H	1.93	0.75
15:O:353:GLU:HB2	15:O:481:SER:OG	1.85	0.75
1:A:114:LEU:HD11	1:A:148:CYS:HA	1.68	0.75
2:B:1055:SER:O	2:B:1056:ARG:C	2.27	0.75
3:C:119:ASN:O	3:C:120:LEU:O	2.05	0.75
1:A:1170:ALA:HA	1:A:1188:ILE:HG12	1.67	0.74
2:B:671:THR:HG21	2:B:672:HIS:CE1	2.22	0.74
8:H:96:VAL:HG12	8:H:143:LEU:HD13	1.69	0.74
15:O:124:GLU:HG3	15:O:126:GLY:N	2.02	0.74
1:A:1166:LEU:O	1:A:1166:LEU:HD23	1.86	0.74
16:P:172:ILE:HG22	16:P:173:GLU:H	1.52	0.74
1:A:321:LEU:O	1:A:325:MET:HB2	1.88	0.74
1:A:373:VAL:C	2:B:1050:PRO:HG2	2.12	0.74
1:A:645:MET:HE1	8:H:124:ARG:HB2	1.67	0.74
1:A:1169:VAL:CG2	1:A:1170:ALA:H	1.94	0.74
2:B:546:SER:OG	14:N:391:LEU:HD23	1.87	0.74
18:R:467:ARG:HB2	18:R:602:LEU:HD11	1.68	0.74
2:B:551:LEU:HD11	14:N:388:THR:N	2.02	0.74
15:O:54:LYS:HA	15:O:58:GLY:HA2	1.68	0.74
15:O:515:LYS:C	15:O:516:LEU:HG	2.13	0.74
7:G:96:GLY:N	7:G:112:GLN:HG2	2.02	0.74
7:G:104:ILE:HG23	7:G:105:PHE:H	1.52	0.74
1:A:1095:GLN:NE2	2:B:1068:ASP:OD2	2.20	0.74
18:R:266:LYS:HG2	18:R:283:GLY:HA3	1.69	0.74
1:A:181:ASP:HB2	1:A:220:ASP:OD1	1.88	0.74
1:A:200:GLU:HB3	15:O:516:LEU:HD23	1.68	0.74
5:E:87:SER:HA	5:E:115:ASN:HB3	1.70	0.74
20:X:56:DC:O2	21:Y:8:DG:N2	2.20	0.74
15:O:110:THR:CG2	15:O:115:LYS:O	2.35	0.74
2:B:933:PHE:O	2:B:1004:LEU:HD22	1.88	0.74
3:C:121:PRO:O	3:C:122:ASP:OD1	2.06	0.74
10:J:43:ARG:HH11	10:J:43:ARG:HG2	1.53	0.74
1:A:395:PRO:HB3	1:A:496:ARG:HA	1.69	0.73
3:C:256:ILE:HA	3:C:268:LYS:H	1.53	0.73
5:E:180:ARG:O	5:E:182:ASP:N	2.21	0.73
1:A:574:ALA:HA	11:K:81:MET:HE3	1.70	0.73
21:Y:45:DT:H72	21:Y:46:DA:H62	1.52	0.73
21:Y:55:DT:H2"	21:Y:56:DG:C8	2.22	0.73
7:G:39:ILE:HD12	7:G:40:PRO:HD2	1.69	0.73
1:A:238:ASP:CG	1:A:239:CYS:H	1.94	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:389:THR:HG23	14:N:390:PHE:H	1.50	0.73
13:M:104:HIS:ND1	13:M:105:PRO:CD	2.52	0.73
15:O:467:PHE:HD1	15:O:468:LEU:HD13	1.54	0.73
2:B:767:ILE:O	2:B:945:ASN:ND2	2.21	0.73
3:C:116:VAL:HB	3:C:209:ILE:HD11	1.71	0.73
5:E:21:GLU:HB3	5:E:35:VAL:HG21	1.71	0.73
15:O:292:ARG:NH2	15:O:653:MET:O	2.22	0.73
13:M:90:TYR:HB3	13:M:179:LEU:HB3	1.69	0.73
13:M:158:GLN:HG2	14:N:308:GLN:HG2	1.69	0.73
1:A:572:ASP:OD1	1:A:573:ARG:N	2.22	0.73
13:M:94:PRO:CB	14:N:391:LEU:O	2.35	0.73
2:B:167:ASP:O	2:B:169:SER:N	2.21	0.72
2:B:475:SER:HB3	2:B:510:LEU:O	1.89	0.72
2:B:929:GLU:HG2	3:C:72:ILE:HG23	1.69	0.72
1:A:665:ASP:OD1	1:A:798:GLY:N	2.23	0.72
14:N:290:ILE:O	14:N:294:LEU:HB2	1.89	0.72
18:R:467:ARG:HA	18:R:602:LEU:HD21	1.71	0.72
1:A:476:ARG:NH2	1:A:515:ASP:OD2	2.23	0.72
1:A:249:PRO:CD	1:A:250:SER:N	2.13	0.72
2:B:476:GLN:HG2	2:B:477:PHE:H	1.53	0.72
2:B:933:PHE:O	2:B:1004:LEU:CD2	2.37	0.72
2:B:1106:TRP:HE1	7:G:162:SER:HA	1.55	0.72
3:C:197:ARG:HB3	3:C:198:PRO:HD2	1.72	0.72
15:O:584:ASN:O	15:O:588:LEU:N	2.22	0.72
19:S:483:GLU:O	19:S:487:GLU:CB	2.37	0.72
6:F:76:LYS:HD2	6:F:79:ARG:HE	1.53	0.72
1:A:388:SER:OG	1:A:695:ASN:ND2	2.23	0.72
15:O:46:LEU:HD13	15:O:69:VAL:HB	1.71	0.72
1:A:327:ILE:HG22	1:A:353:PHE:CZ	2.24	0.72
5:E:86:PRO:HA	5:E:113:GLN:HB3	1.72	0.72
7:G:57:GLY:HA3	7:G:68:ILE:HG12	1.70	0.72
7:G:204:GLY:HA2	7:G:210:TRP:HB2	1.70	0.72
7:G:150:ILE:HG21	7:G:196:LEU:HD23	1.71	0.71
1:A:869:ARG:HH22	2:B:502:THR:HB	1.53	0.71
16:P:135:LYS:NZ	16:P:150:LEU:O	2.23	0.71
1:A:154:CYS:SG	1:A:155:LEU:N	2.62	0.71
1:A:164:VAL:HB	1:A:180:HIS:HB2	1.71	0.71
1:A:671:ASP:OD1	1:A:671:ASP:O	2.08	0.71
1:A:330:ASP:OD1	1:A:331:SER:N	2.23	0.71
1:A:597:ILE:HD11	1:A:603:LEU:HD12	1.73	0.71
2:B:197:GLN:NE2	2:B:476:GLN:OE1	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:156:VAL:CG1	15:O:189:SER:HB3	2.20	0.71
19:S:506:GLN:O	19:S:510:LYS:HB2	1.91	0.71
1:A:1121:LEU:O	1:A:1346:HIS:NE2	2.24	0.71
2:B:248:ALA:HB3	2:B:308:LYS:HG2	1.71	0.71
14:N:371:LEU:HD22	14:N:384:LYS:HD3	1.73	0.71
8:H:130:ARG:O	8:H:134:ASN:ND2	2.24	0.71
1:A:249:PRO:CG	1:A:250:SER:N	2.54	0.71
2:B:795:LEU:HB2	2:B:894:ALA:HB3	1.73	0.71
1:A:556:ASP:HB3	2:B:767:ILE:HD12	1.72	0.71
1:A:666:LYS:HA	1:A:670:GLY:HA3	1.72	0.71
15:O:499:THR:HG23	16:P:312:PHE:CB	2.21	0.70
2:B:481:ARG:HH21	21:Y:21:DG:H2'	1.54	0.70
16:P:54:GLU:O	16:P:58:LYS:N	2.22	0.70
1:A:1266:ALA:O	1:A:1269:ASP:CB	2.37	0.70
2:B:192:LYS:NZ	2:B:438:SER:O	2.22	0.70
8:H:21:ASN:OD1	8:H:22:LYS:N	2.25	0.70
18:R:152:VAL:HG22	18:R:153:SER:H	1.57	0.70
1:A:400:LYS:HA	1:A:465:HIS:CD2	2.26	0.70
1:A:827:PHE:HE2	1:A:833:PRO:HG3	1.55	0.70
5:E:179:GLN:C	5:E:180:ARG:O	2.34	0.70
7:G:45:CYS:HA	7:G:76:VAL:HA	1.74	0.70
2:B:658:TYR:CE2	2:B:670:MET:HG2	2.27	0.70
2:B:944:MET:HG2	2:B:945:ASN:H	1.57	0.70
3:C:229:LEU:HB2	3:C:293:ARG:HH11	1.57	0.70
13:M:104:HIS:HE1	14:N:395:ILE:CD1	2.05	0.70
1:A:552:ALA:CB	1:A:671:ASP:HB3	2.20	0.70
1:A:664:MET:HB3	1:A:669:LEU:HD23	1.71	0.70
15:O:144:MET:HE3	15:O:148:ASP:HA	1.73	0.70
1:A:1145:LEU:HD11	1:A:1157:VAL:HG21	0.79	0.70
19:S:444:GLN:HE22	19:S:490:LYS:NZ	1.90	0.70
4:D:7:ARG:HE	4:D:10:PHE:HZ	1.37	0.70
15:O:620:LEU:HD12	15:O:621:PRO:HD2	1.73	0.70
1:A:356:ARG:CG	2:B:1131:GLU:OE2	2.40	0.69
1:A:705:LEU:HD21	2:B:761:SER:HB2	1.74	0.69
1:A:1429:LYS:HD3	6:F:137:TYR:HE2	1.57	0.69
2:B:774:ASN:ND2	2:B:777:SER:OG	2.25	0.69
3:C:121:PRO:O	3:C:122:ASP:CG	2.35	0.69
10:J:36:LEU:HD23	10:J:47:ARG:HG3	1.72	0.69
1:A:82:GLY:O	1:A:263:ALA:N	2.20	0.69
1:A:109:ASN:HD22	1:A:159:ALA:HB2	1.55	0.69
1:A:141:LEU:HA	1:A:144:ILE:HG22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1370:GLY:O	1:A:1371:ILE:C	2.34	0.69
2:B:811:VAL:HA	2:B:817:PRO:HA	1.74	0.69
3:C:92:ILE:HD13	3:C:194:ALA:HB1	1.74	0.69
2:B:186:ILE:HA	2:B:191:GLU:HA	1.74	0.69
2:B:974:GLU:HG2	2:B:987:MET:HE1	1.74	0.69
1:A:1202:ILE:HD13	1:A:1224:ILE:HD12	1.75	0.69
2:B:612:LEU:HD13	2:B:672:HIS:HB3	1.75	0.69
1:A:325:MET:SD	1:A:351:ARG:NH2	2.66	0.69
1:A:429:GLY:C	1:A:465:HIS:HD1	1.99	0.69
18:R:144:ILE:HD12	18:R:154:VAL:HG21	1.75	0.69
4:D:24:GLU:HG3	4:D:29:TRP:HA	1.73	0.69
11:K:136:THR:HA	11:K:139:ILE:HG22	1.74	0.69
1:A:205:LEU:HG	1:A:212:GLU:HA	1.74	0.69
2:B:705:MET:SD	2:B:919:LYS:NZ	2.65	0.69
14:N:363:ILE:HG12	14:N:373:VAL:HG22	1.75	0.69
1:A:164:VAL:CB	1:A:180:HIS:HB2	2.23	0.69
2:B:77:ILE:HD13	2:B:98:ILE:HG12	1.73	0.69
2:B:325:GLU:HG3	2:B:328:ALA:HB3	1.75	0.69
3:C:42:VAL:O	11:K:138:LYS:NZ	2.26	0.69
16:P:131:GLN:HB3	16:P:133:TYR:CD2	2.28	0.69
18:R:213:TRP:CH2	18:R:497:ARG:HA	2.25	0.69
1:A:107:CYS:HA	1:A:161:ASN:HD22	1.57	0.69
1:A:643:ASN:HB2	1:A:651:PHE:CZ	2.27	0.69
2:B:933:PHE:CE1	2:B:1005:TYR:HD2	2.05	0.69
7:G:96:GLY:H	7:G:112:GLN:HG2	1.58	0.69
1:A:1164:THR:HB	1:A:1271:VAL:HA	1.74	0.69
5:E:172:GLU:HG2	5:E:173:SER:H	1.58	0.68
1:A:600:PRO:HG2	8:H:95:TYR:HD1	1.56	0.68
2:B:613:ILE:HA	2:B:646:VAL:HG12	1.75	0.68
20:X:47:DA:H2'	20:X:48:DT:H71	1.74	0.68
1:A:444:LEU:HD11	1:A:445:ARG:NH1	2.08	0.68
15:O:554:THR:HG23	15:O:561:ARG:NE	2.07	0.68
2:B:138:GLY:H	2:B:141:ILE:HG21	1.57	0.68
2:B:1101:MET:SD	2:B:1126:LYS:HG3	2.34	0.68
1:A:552:ALA:HB2	1:A:671:ASP:HB3	1.74	0.68
1:A:664:MET:CB	1:A:669:LEU:CD2	2.70	0.68
1:A:1166:LEU:HA	1:A:1169:VAL:CG2	2.22	0.68
21:Y:41:DG:H2'	21:Y:42:DT:H71	1.74	0.68
1:A:736:HIS:HA	1:A:739:ASP:HB3	1.74	0.68
11:K:89:CYS:HA	11:K:104:ARG:O	1.94	0.68
15:O:339:LEU:O	15:O:343:LYS:NZ	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:636:LEU:HD13	19:S:502:LEU:HD21	1.75	0.68
5:E:79:TRP:O	5:E:108:GLY:HA2	1.94	0.68
7:G:126:SER:HB3	7:G:139:TYR:CB	2.23	0.68
18:R:135:ARG:NH2	18:R:174:PRO:O	2.27	0.68
20:X:25:DT:H2'	20:X:26:DT:C6	2.29	0.68
2:B:914:SER:OG	2:B:957:LYS:NZ	2.23	0.68
13:M:171:VAL:HG13	13:M:172:PRO:HD2	1.76	0.68
18:R:402:LEU:HD22	18:R:476:ALA:HB1	1.76	0.68
18:R:467:ARG:HG3	18:R:610:LEU:HD22	1.75	0.68
1:A:327:ILE:CA	1:A:353:PHE:CD2	2.66	0.68
2:B:122:ASP:HA	2:B:189:GLY:HA3	1.74	0.68
2:B:938:ILE:HD13	10:J:44:TYR:CE2	2.30	0.68
13:M:104:HIS:CE1	14:N:395:ILE:HD13	2.21	0.68
20:X:6:DA:C6	20:X:7:DA:N6	2.62	0.68
3:C:71:MET:HE2	3:C:314:PHE:HA	1.76	0.67
3:C:209:ILE:HG13	3:C:210:LEU:H	1.59	0.67
15:O:46:LEU:HD22	15:O:70:ALA:HB2	1.74	0.67
2:B:129:ILE:HD11	2:B:152:MET:HB2	1.76	0.67
5:E:24:LYS:HB2	5:E:30:ILE:HD11	1.76	0.67
5:E:56:LYS:HE2	5:E:84:ASP:HB2	1.75	0.67
10:J:52:THR:HG22	10:J:53:HIS:H	1.57	0.67
2:B:102:LYS:NZ	2:B:106:SER:O	2.26	0.67
4:D:17:LEU:HD22	4:D:66:LEU:HB3	1.75	0.67
5:E:12:LEU:HD22	5:E:42:PHE:HZ	1.60	0.67
11:K:80:ILE:HG22	11:K:86:VAL:HG11	1.77	0.67
2:B:622:VAL:HG12	2:B:624:ASP:H	1.59	0.67
14:N:290:ILE:O	14:N:294:LEU:CB	2.42	0.67
15:O:43:ASN:HB3	15:O:47:PHE:HB2	1.75	0.67
1:A:1371:ILE:O	1:A:1372:THR:OG1	2.11	0.67
7:G:129:ILE:HG12	7:G:139:TYR:HB3	1.75	0.67
15:O:499:THR:HG23	16:P:312:PHE:HB2	1.76	0.67
1:A:248:VAL:N	1:A:249:PRO:HD3	2.09	0.67
1:A:976:ARG:HG3	1:A:1002:ARG:NH2	2.10	0.67
2:B:1103:TYR:HE2	7:G:163:PRO:HG2	1.59	0.67
3:C:190:ASP:O	10:J:16:ASP:HB3	1.95	0.67
13:M:91:ALA:HA	14:N:392:GLN:CD	2.19	0.67
15:O:303:ARG:CA	16:P:265:LEU:HD21	2.13	0.67
18:R:215:PHE:HD1	18:R:223:ILE:HD13	1.59	0.67
20:X:6:DA:C4	20:X:7:DA:N7	2.62	0.67
1:A:431:ASN:OD1	1:A:432:TYR:N	2.24	0.67
7:G:92:CYS:SG	7:G:98:LYS:N	2.61	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:292:ARG:NH1	15:O:650:VAL:HA	2.08	0.67
1:A:338:PRO:HG2	1:A:342:ASN:HD22	1.60	0.67
1:A:1145:LEU:HG	1:A:1308:GLY:O	1.94	0.67
2:B:717:GLN:HE21	2:B:727:LEU:HD22	1.60	0.67
2:B:1006:SER:HB2	2:B:1013:LEU:HD21	1.74	0.67
10:J:42:LYS:CE	10:J:43:ARG:NH1	2.47	0.67
13:M:122:ASP:HB3	13:M:145:VAL:HG21	1.77	0.67
14:N:395:ILE:HA	14:N:411:ARG:HA	1.76	0.67
18:R:455:GLU:OE1	18:R:546:ARG:NH2	2.27	0.67
2:B:141:ILE:HG23	2:B:142:ILE:H	1.60	0.67
1:A:390:ASP:OD2	1:A:538:LYS:NZ	2.24	0.66
1:A:1186:VAL:H	1:A:1230:ILE:HG12	1.60	0.66
6:F:96:THR:HG21	7:G:59:LEU:HD21	1.77	0.66
13:M:253:GLU:HB2	13:M:257:ASP:HB2	1.78	0.66
16:P:66:GLN:OE1	16:P:71:LYS:NZ	2.25	0.66
16:P:131:GLN:HB3	16:P:133:TYR:HD2	1.59	0.66
19:S:428:PHE:HE1	19:S:454:VAL:HG13	1.58	0.66
19:S:460:ASN:ND2	20:X:9:DA:OP2	2.28	0.66
1:A:372:ARG:O	2:B:1050:PRO:HD2	1.94	0.66
1:A:1145:LEU:O	1:A:1310:ILE:HG22	1.94	0.66
2:B:882:ASP:OD1	2:B:883:GLN:N	2.29	0.66
7:G:6:LYS:HA	7:G:72:PHE:O	1.94	0.66
15:O:599:ASN:O	15:O:603:LEU:N	2.25	0.66
18:R:517:PRO:HG3	21:Y:52:DA:H1'	1.78	0.66
1:A:239:CYS:SG	1:A:246:ALA:CB	2.81	0.66
1:A:952:LYS:O	1:A:1061:ARG:HD2	1.96	0.66
2:B:698:ARG:HH21	2:B:952:ARG:HG2	1.58	0.66
16:P:191:PHE:HB2	16:P:192:PRO:HD2	1.76	0.66
18:R:628:ILE:HG21	19:S:499:ASN:HD21	1.61	0.66
2:B:734:PRO:HB2	2:B:915:ARG:NH1	2.08	0.66
5:E:31:THR:HG22	5:E:34:GLU:HG2	1.77	0.66
18:R:123:GLN:HG2	18:R:150:LEU:HD21	1.77	0.66
15:O:353:GLU:O	15:O:358:GLY:N	2.29	0.66
1:A:363:ARG:HA	1:A:367:ASN:HB2	1.78	0.66
1:A:664:MET:HB2	1:A:669:LEU:HD21	1.76	0.66
1:A:1130:ILE:HA	1:A:1362:MET:HE1	1.78	0.66
7:G:87:GLY:HA3	7:G:148:PHE:HE2	1.59	0.66
15:O:102:ARG:NH2	15:O:282:ILE:O	2.28	0.66
16:P:313:ASP:O	16:P:314:GLU:HG2	1.96	0.66
2:B:734:PRO:CB	2:B:915:ARG:HH12	2.09	0.66
7:G:12:ARG:NH2	7:G:65:SER:OG	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:29:TYR:HB3	12:L:58:LYS:HA	1.78	0.66
15:O:495:VAL:HG21	15:O:577:MET:HG3	1.76	0.66
1:A:865:ALA:HA	2:B:696:SER:HB3	1.78	0.66
2:B:760:MET:HB3	2:B:943:ILE:HD11	1.77	0.66
16:P:11:LEU:O	16:P:15:ALA:CB	2.42	0.66
16:P:62:LYS:HD3	16:P:83:LYS:HE2	1.76	0.66
18:R:650:ALA:O	19:S:520:LYS:NZ	2.29	0.66
2:B:933:PHE:CD1	2:B:934:ASN:N	2.64	0.66
19:S:426:ILE:HA	19:S:429:TYR:HD2	1.61	0.66
1:A:766:ILE:HA	1:A:769:LEU:HB2	1.76	0.66
5:E:101:GLN:O	5:E:104:ASN:ND2	2.29	0.66
13:M:108:SER:HG	13:M:247:TRP:CD1	2.14	0.66
2:B:269:MET:O	2:B:273:CYS:HB3	1.95	0.65
2:B:613:ILE:HG13	2:B:675:ILE:HG22	1.77	0.65
2:B:1147:PHE:HD2	7:G:10:LEU:HD11	1.61	0.65
15:O:201:ILE:HD12	15:O:283:ASN:HD22	1.59	0.65
15:O:297:ILE:O	15:O:300:ALA:N	2.29	0.65
1:A:790:ALA:HB1	1:A:794:MET:HE2	1.77	0.65
1:A:1225:ILE:H	1:A:1229:ARG:HE	1.44	0.65
5:E:181:ALA:C	5:E:182:ASP:O	2.38	0.65
1:A:269:ARG:CZ	1:A:285:LEU:HB2	2.26	0.65
2:B:305:ILE:HG22	2:B:325:GLU:HG2	1.79	0.65
2:B:396:ASN:O	2:B:399:PHE:N	2.28	0.65
13:M:182:PHE:CD1	13:M:183:PHE:N	2.64	0.65
15:O:110:THR:CG2	15:O:116:LYS:HA	2.24	0.65
1:A:632:VAL:HG21	1:A:796:THR:HG23	1.76	0.65
1:A:1171:PHE:CD2	1:A:1172:TYR:HD2	2.14	0.65
1:A:1378:LYS:HG3	1:A:1379:MET:H	1.61	0.65
11:K:69:ASP:OD1	11:K:70:HIS:N	2.26	0.65
1:A:955:LEU:HD12	1:A:959:ILE:HG13	1.78	0.65
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.77	0.65
1:A:269:ARG:HH22	1:A:283:ASP:C	2.05	0.65
1:A:368:LEU:HD21	1:A:1416:ILE:HG23	1.79	0.65
5:E:32:GLN:HA	5:E:35:VAL:HG12	1.78	0.65
14:N:364:ARG:HH11	14:N:365:VAL:H	1.44	0.65
1:A:18:PHE:HE1	2:B:1139:PRO:CB	2.06	0.65
1:A:429:GLY:O	1:A:465:HIS:ND1	2.24	0.65
1:A:1059:LEU:HD11	8:H:106:GLU:HB3	1.76	0.65
18:R:239:ARG:NH1	19:S:291:UNK:O	2.30	0.65
1:A:674:LYS:HD2	1:A:927:GLU:O	1.97	0.65
1:A:716:ASP:OD2	1:A:790:ALA:N	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:CYS:HA	1:A:904:VAL:HA	1.77	0.65
8:H:38:LEU:HD21	8:H:40:LEU:HB2	1.77	0.65
16:P:189:ASN:ND2	16:P:217:THR:OG1	2.26	0.65
1:A:204:VAL:O	1:A:208:ASN:N	2.27	0.65
1:A:308:SER:HA	15:O:534:ARG:HD2	1.79	0.65
1:A:644:GLU:OE2	1:A:651:PHE:CD2	2.49	0.65
1:A:1170:ALA:CA	1:A:1188:ILE:HG12	2.27	0.65
2:B:914:SER:O	2:B:915:ARG:HG2	1.97	0.65
7:G:2:PHE:N	7:G:76:VAL:O	2.30	0.65
15:O:370:LEU:HD22	15:O:453:ILE:HD11	1.77	0.65
17:Q:40:PRO:HB2	17:Q:44:ASN:ND2	2.11	0.65
18:R:581:ASN:ND2	18:R:583:HIS:O	2.30	0.65
19:S:480:ASN:OD1	19:S:481:PHE:N	2.26	0.65
2:B:137:ARG:HG3	2:B:138:GLY:H	1.62	0.65
2:B:553:TYR:HB3	2:B:598:ALA:N	2.11	0.65
3:C:231:PRO:HA	3:C:293:ARG:HG2	1.79	0.65
1:A:911:ILE:HG23	5:E:176:PRO:HD3	1.79	0.64
1:A:1222:VAL:HG23	1:A:1231:ALA:H	1.62	0.64
18:R:619:ALA:O	18:R:623:LYS:CB	2.44	0.64
15:O:163:VAL:HG22	15:O:169:LEU:HD22	1.78	0.64
16:P:107:SER:O	16:P:110:ILE:HG22	1.97	0.64
2:B:797:ARG:HG2	2:B:803:GLN:HG2	1.78	0.64
6:F:115:THR:HG22	6:F:116:ASP:H	1.63	0.64
16:P:77:GLU:HA	16:P:80:ALA:HB3	1.79	0.64
1:A:649:ASP:OD2	1:A:663:VAL:N	2.30	0.64
2:B:764:GLY:O	2:B:767:ILE:HG12	1.97	0.64
3:C:88:ASN:HB3	12:L:60:ARG:NH1	2.11	0.64
5:E:18:THR:HG23	5:E:143:ASN:HB3	1.78	0.64
16:P:49:MET:HE2	19:S:364:LEU:HD11	1.79	0.64
18:R:93:ALA:O	18:R:149:ARG:NH2	2.31	0.64
1:A:99:THR:HA	1:A:102:ILE:HG22	1.79	0.64
2:B:417:ASP:C	2:B:419:LEU:H	2.05	0.64
18:R:469:ILE:O	18:R:473:GLY:N	2.31	0.64
1:A:577:THR:HG23	11:K:88:PHE:CD1	2.32	0.64
1:A:1145:LEU:CG	1:A:1308:GLY:O	2.46	0.64
1:A:1284:ASN:OD1	1:A:1285:ILE:N	2.30	0.64
2:B:214:GLY:HA3	2:B:234:ILE:HG21	1.79	0.64
15:O:47:PHE:HE2	15:O:586:ALA:HA	1.62	0.64
15:O:102:ARG:O	15:O:123:ASN:ND2	2.28	0.64
18:R:237:LEU:HD13	18:R:239:ARG:HG2	1.79	0.64
19:S:490:LYS:HG3	19:S:490:LYS:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:MET:HE3	1:A:891:LYS:HD3	1.78	0.64
1:A:1384:LEU:O	1:A:1388:SER:N	2.30	0.64
2:B:213:LYS:HD3	2:B:216:VAL:HG23	1.80	0.64
13:M:72:GLU:HB2	14:N:364:ARG:HE	1.62	0.64
18:R:131:TYR:OH	18:R:135:ARG:NH1	2.31	0.64
18:R:391:PRO:HA	18:R:490:CYS:HB3	1.80	0.64
1:A:58:MET:HE2	1:A:82:GLY:HA3	1.79	0.64
1:A:997:GLN:O	1:A:999:ASP:N	2.31	0.64
13:M:159:TYR:C	13:M:173:ILE:HD11	2.22	0.64
1:A:328:ASN:OD1	1:A:329:SER:N	2.24	0.63
1:A:1333:TYR:CE2	1:A:1337:ARG:HD2	2.33	0.63
2:B:404:ASP:O	2:B:407:LEU:N	2.30	0.63
2:B:1040:ARG:HD3	18:R:35:ASN:HD21	1.63	0.63
15:O:233:SER:O	15:O:236:LYS:HG2	1.97	0.63
19:S:469:ILE:O	19:S:473:LEU:HB3	1.98	0.63
1:A:226:LYS:NZ	15:O:547:GLU:OE2	2.31	0.63
15:O:599:ASN:OD1	15:O:626:GLN:NE2	2.30	0.63
18:R:463:ARG:NH1	18:R:601:ASN:O	2.30	0.63
19:S:306:UNK:O	19:S:310:UNK:CB	2.46	0.63
1:A:109:ASN:ND2	1:A:159:ALA:HB2	2.12	0.63
1:A:1333:TYR:CZ	1:A:1337:ARG:HD2	2.34	0.63
2:B:914:SER:C	2:B:916:HIS:H	2.06	0.63
4:D:125:ASN:OD1	4:D:126:GLN:N	2.27	0.63
1:A:493:ARG:HB2	1:A:499:ARG:HH21	1.63	0.63
1:A:1272:VAL:HG13	1:A:1273:LYS:H	1.64	0.63
3:C:190:ASP:O	3:C:191:ILE:HG13	1.98	0.63
1:A:869:ARG:HH12	2:B:502:THR:HB	1.64	0.63
2:B:1028:LYS:HG2	2:B:1029:HIS:H	1.64	0.63
13:M:183:PHE:C	13:M:185:TYR:H	2.07	0.63
15:O:47:PHE:HZ	15:O:590:PHE:CE2	2.15	0.63
16:P:10:GLN:HB3	16:P:13:ASP:HB3	1.80	0.63
18:R:245:VAL:HA	18:R:248:SER:HB3	1.79	0.63
19:S:418:ASP:O	19:S:449:ARG:NH1	2.31	0.63
6:F:80:ALA:O	6:F:81:THR:OG1	2.14	0.63
1:A:533:ASN:HD21	6:F:90:ARG:HG2	1.62	0.63
3:C:133:VAL:HG11	3:C:172:GLN:HE22	1.64	0.63
13:M:94:PRO:HB3	14:N:391:LEU:C	2.23	0.63
13:M:117:HIS:HB2	13:M:119:TRP:NE1	2.14	0.63
1:A:148:CYS:SG	1:A:149:LYS:N	2.72	0.63
2:B:258:LYS:HE2	2:B:265:ASP:HB2	1.81	0.63
2:B:337:VAL:HG23	2:B:345:LYS:HZ3	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:587:PHE:CZ	2:B:607:ARG:HD3	2.34	0.63
3:C:31:TRP:CZ2	11:K:123:ASP:HB3	2.34	0.63
17:Q:40:PRO:HB2	17:Q:44:ASN:HD21	1.64	0.63
18:R:392:THR:O	18:R:488:GLY:HA2	1.98	0.63
20:X:30:DT:O4	21:Y:33:DC:N4	2.32	0.63
20:X:63:DG:N2	21:Y:2:DC:O2	2.31	0.63
2:B:1042:PRO:HD2	2:B:1057:ASP:CG	2.23	0.62
3:C:71:MET:HE1	3:C:314:PHE:HD1	1.64	0.62
15:O:151:GLU:O	15:O:155:LEU:N	2.25	0.62
15:O:183:MET:HB2	15:O:186:THR:HB	1.80	0.62
15:O:233:SER:HA	20:X:59:DC:OP2	1.98	0.62
18:R:485:ASN:OD1	18:R:486:ILE:N	2.32	0.62
18:R:619:ALA:O	18:R:623:LYS:HB3	1.98	0.62
1:A:556:ASP:CB	2:B:767:ILE:CD1	2.77	0.62
1:A:573:ARG:NH2	11:K:87:GLU:OE1	2.32	0.62
15:O:193:GLN:C	15:O:195:CYS:N	2.57	0.62
1:A:1315:THR:HG22	1:A:1316:THR:H	1.65	0.62
1:A:1408:VAL:HG23	1:A:1413:GLU:HG3	1.81	0.62
9:I:32:GLU:HB2	13:M:130:PHE:HB3	1.80	0.62
13:M:160:ALA:N	13:M:173:ILE:HD11	2.14	0.62
15:O:222:HIS:CE1	15:O:244:ASN:HB3	2.35	0.62
15:O:499:THR:CG2	16:P:312:PHE:CG	2.82	0.62
15:O:644:LEU:HD11	16:P:310:VAL:HG21	1.81	0.62
2:B:351:MET:HE1	2:B:549:LEU:HD21	1.80	0.62
2:B:756:THR:O	2:B:941:ASP:N	2.27	0.62
2:B:757:VAL:HG11	2:B:1022:ILE:HD12	1.82	0.62
5:E:64:PRO:HD3	5:E:77:SER:HA	1.81	0.62
7:G:126:SER:HB3	7:G:139:TYR:HB2	1.80	0.62
13:M:111:ARG:NH1	13:M:120:GLU:OE1	2.33	0.62
1:A:566:HIS:CD2	1:A:568:ASP:HB3	2.35	0.62
2:B:726:TYR:HE2	2:B:1028:LYS:HG3	1.65	0.62
4:D:133:HIS:CE1	7:G:211:TRP:HB3	2.34	0.62
18:R:434:GLU:HA	18:R:436:LYS:H	1.64	0.62
20:X:26:DT:H2'	20:X:27:DT:C6	2.34	0.62
2:B:48:LEU:HD22	2:B:743:LEU:HD21	1.80	0.62
18:R:202:ALA:O	18:R:205:LEU:HB3	1.98	0.62
1:A:432:TYR:OH	18:R:20:ASN:ND2	2.32	0.62
1:A:628:ALA:CB	1:A:675:HIS:HD2	2.12	0.62
1:A:666:LYS:HG2	1:A:667:SER:H	1.65	0.62
1:A:1145:LEU:CD1	1:A:1157:VAL:CG2	2.54	0.62
2:B:713:ILE:HG13	2:B:725:LEU:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:997:ASN:OD1	2:B:998:TYR:N	2.33	0.62
18:R:196:ILE:O	18:R:199:VAL:HB	1.99	0.62
1:A:33:GLU:HG3	1:A:83:HIS:NE2	2.14	0.62
1:A:974:LEU:HD21	1:A:998:TYR:CB	2.23	0.62
7:G:9:ASP:OD1	7:G:10:LEU:N	2.33	0.62
7:G:207:LEU:HD22	7:G:210:TRP:CD1	2.35	0.62
18:R:121:ARG:HB2	18:R:124:ASN:HD22	1.63	0.62
2:B:140:ASN:HD22	19:S:394:LYS:HG2	1.65	0.62
2:B:546:SER:HB2	14:N:391:LEU:HD22	1.71	0.62
2:B:833:GLY:N	2:B:881:ILE:O	2.29	0.62
18:R:195:LYS:O	18:R:199:VAL:N	2.27	0.62
18:R:439:ALA:HA	18:R:450:THR:H	1.63	0.62
15:O:316:LEU:O	15:O:320:GLU:N	2.32	0.62
1:A:133:ASP:OD1	1:A:134:ASN:N	2.32	0.61
1:A:201:TRP:HB3	1:A:205:LEU:HD13	1.82	0.61
13:M:160:ALA:HA	14:N:306:VAL:HG12	1.81	0.61
15:O:455:SER:HA	15:O:458:LYS:HD3	1.81	0.61
1:A:1384:LEU:HB2	1:A:1413:GLU:OE1	1.99	0.61
1:A:1438:GLU:HA	1:A:1441:LEU:HD13	1.82	0.61
7:G:89:ILE:HG13	7:G:92:CYS:SG	2.39	0.61
15:O:356:THR:HB	15:O:357:PRO:HD3	1.81	0.61
15:O:567:ARG:HG2	15:O:568:CYS:H	1.65	0.61
18:R:516:PHE:HB2	20:X:13:DA:H5'	1.82	0.61
10:J:7:CYS:HB2	10:J:11:GLY:H	1.65	0.61
1:A:252:ARG:O	1:A:254:GLU:N	2.29	0.61
2:B:109:LYS:CG	2:B:111:TYR:O	2.49	0.61
16:P:106:TRP:HE1	16:P:145:ARG:HA	1.65	0.61
19:S:387:ALA:O	19:S:391:ASN:N	2.28	0.61
1:A:286:THR:O	1:A:290:THR:HB	1.99	0.61
1:A:642:PRO:HB3	8:H:103:LYS:NZ	2.16	0.61
13:M:80:GLY:HA3	13:M:261:LYS:HE2	1.80	0.61
1:A:395:PRO:HG2	1:A:398:VAL:HG22	1.83	0.61
1:A:502:GLU:OE1	2:B:767:ILE:HG13	2.01	0.61
2:B:521:THR:O	2:B:606:GLY:N	2.32	0.61
2:B:555:VAL:HG12	2:B:564:SER:H	1.65	0.61
10:J:16:ASP:OD1	10:J:17:LYS:N	2.33	0.61
18:R:28:CYS:SG	18:R:29:GLY:N	2.74	0.61
18:R:518:GLY:HA3	18:R:532:ILE:O	2.00	0.61
2:B:201:SER:OG	2:B:376:ARG:NH1	2.33	0.61
8:H:101:ALA:HB2	8:H:116:TYR:HE1	1.65	0.61
15:O:285:ASP:OD1	15:O:286:ARG:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1203:GLU:HA	1:A:1206:ALA:HB3	1.83	0.61
2:B:125:TYR:HB3	2:B:186:ILE:HG23	1.83	0.61
2:B:1003:MET:SD	3:C:293:ARG:NH2	2.73	0.61
2:B:1042:PRO:HD2	2:B:1057:ASP:CB	2.31	0.61
5:E:115:ASN:OD1	5:E:116:ILE:N	2.34	0.61
5:E:141:VAL:HG23	5:E:142:VAL:H	1.66	0.61
8:H:10:PHE:HE2	8:H:38:LEU:HD13	1.65	0.61
11:K:63:PHE:CD2	11:K:117:LEU:HD13	2.36	0.61
19:S:381:VAL:HG22	19:S:383:ARG:H	1.65	0.61
1:A:1378:LYS:HG3	1:A:1379:MET:N	2.15	0.61
2:B:234:ILE:HA	2:B:240:ILE:HA	1.82	0.61
2:B:612:LEU:HA	2:B:675:ILE:HG23	1.83	0.61
13:M:182:PHE:HD1	13:M:183:PHE:H	1.47	0.61
15:O:193:GLN:C	15:O:195:CYS:H	2.09	0.61
16:P:33:GLN:NE2	19:S:372:MET:SD	2.74	0.61
19:S:488:ILE:O	19:S:488:ILE:HG22	2.01	0.61
1:A:200:GLU:CB	15:O:516:LEU:CD2	2.78	0.61
1:A:373:VAL:HG21	2:B:1062:LEU:HG	1.82	0.61
1:A:1160:ARG:NH1	1:A:1307:ASP:OD2	2.31	0.61
2:B:126:SER:OG	2:B:151:ARG:HB3	2.00	0.61
2:B:1080:LEU:O	2:B:1084:MET:HB3	2.01	0.61
5:E:161:LYS:HE2	5:E:195:VAL:HG23	1.82	0.61
1:A:117:GLU:HG2	1:A:119:ASP:H	1.64	0.60
2:B:916:HIS:CD2	2:B:957:LYS:HB2	2.35	0.60
4:D:17:LEU:HD23	4:D:98:MET:HE1	1.83	0.60
5:E:112:TYR:CG	5:E:116:ILE:HG12	2.36	0.60
1:A:1171:PHE:HD2	1:A:1172:TYR:HD2	1.50	0.60
2:B:326:ALA:HB3	13:M:231:LEU:HD11	1.83	0.60
4:D:17:LEU:HD11	4:D:63:VAL:HG23	1.81	0.60
15:O:188:SER:O	15:O:190:LEU:N	2.34	0.60
18:R:87:LEU:CD2	18:R:105:PHE:HB2	2.31	0.60
20:X:6:DA:C6	20:X:7:DA:C6	2.90	0.60
1:A:716:ASP:OD1	1:A:789:ASN:HB2	2.01	0.60
1:A:842:PRO:C	1:A:844:SER:H	2.09	0.60
2:B:776:SER:HB2	2:B:928:GLN:HE21	1.66	0.60
7:G:94:ALA:O	7:G:128:TRP:NE1	2.34	0.60
18:R:464:LYS:NZ	18:R:605:VAL:O	2.29	0.60
1:A:364:PHE:HE2	1:A:1387:ALA:C	2.10	0.60
1:A:714:ILE:O	1:A:717:VAL:N	2.34	0.60
1:A:890:MET:HE3	1:A:891:LYS:CD	2.31	0.60
1:A:1224:ILE:HG13	1:A:1229:ARG:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1054:ARG:HG2	2:B:1055:SER:H	1.67	0.60
15:O:338:ASP:H	15:O:342:ALA:HB2	1.66	0.60
18:R:417:ASN:HA	19:S:437:THR:HG22	1.83	0.60
21:Y:47:DC:H2'	21:Y:48:DT:C4	2.37	0.60
1:A:1145:LEU:N	1:A:1292:GLU:OE1	2.30	0.60
1:A:1343:MET:HE1	1:A:1355:ILE:HD11	1.82	0.60
2:B:502:THR:HG22	2:B:510:LEU:HD11	1.83	0.60
5:E:185:ALA:O	5:E:189:GLY:N	2.34	0.60
16:P:20:SER:HA	16:P:23:MET:HG2	1.84	0.60
19:S:427:LYS:HB2	19:S:446:TYR:OH	2.00	0.60
1:A:1136:ILE:HG21	1:A:1318:HIS:HB3	1.84	0.60
2:B:534:TYR:HA	2:B:538:VAL:HG22	1.84	0.60
3:C:248:GLN:HB3	3:C:256:ILE:HD11	1.84	0.60
5:E:20:LYS:HB3	5:E:35:VAL:HG23	1.83	0.60
15:O:506:ARG:HH21	16:P:246:VAL:HG13	1.67	0.60
1:A:331:SER:O	1:A:351:ARG:NH2	2.35	0.60
2:B:643:LEU:HB3	2:B:645:LEU:HD13	1.84	0.60
13:M:84:SER:HB3	13:M:174:GLU:HG2	1.84	0.60
15:O:193:GLN:O	15:O:194:LEU:C	2.42	0.60
1:A:1130:ILE:CG2	1:A:1371:ILE:HG13	2.30	0.60
3:C:113:LEU:HD11	3:C:132:ILE:HD11	1.81	0.60
5:E:180:ARG:NH1	5:E:190:LEU:O	2.30	0.60
21:Y:17:DT:H2''	21:Y:18:DC:C5	2.36	0.60
1:A:18:PHE:CE1	2:B:1139:PRO:CB	2.83	0.60
1:A:373:VAL:HG12	1:A:374:ASP:N	2.16	0.60
1:A:1285:ILE:HA	1:A:1291:ARG:HG2	1.82	0.60
2:B:415:GLU:HG2	2:B:416:TYR:N	2.11	0.60
2:B:501:ASP:HB3	2:B:703:CYS:HB2	1.83	0.60
7:G:119:CYS:HB2	7:G:128:TRP:HB3	1.84	0.60
14:N:364:ARG:N	14:N:372:SER:O	2.34	0.60
16:P:31:PHE:CE2	16:P:72:PHE:HB2	2.37	0.60
16:P:190:THR:HA	16:P:215:TYR:CE1	2.37	0.60
16:P:253:LEU:HB2	16:P:262:ARG:O	2.02	0.60
16:P:308:GLU:HG2	16:P:308:GLU:O	2.01	0.60
19:S:432:LEU:O	19:S:476:LYS:NZ	2.35	0.60
1:A:1125:ARG:HH22	1:A:1317:ASN:HB3	1.66	0.59
1:A:980:SER:HA	5:E:163:GLU:HG2	1.84	0.59
2:B:354:ARG:NH1	2:B:549:LEU:HD13	2.17	0.59
2:B:728:MET:SD	2:B:753:GLN:NE2	2.74	0.59
2:B:961:LEU:HD11	2:B:1019:PHE:HA	1.84	0.59
2:B:1045:VAL:HG23	2:B:1046:LEU:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:218:LYS:HE2	12:L:70:ARG:HB3	1.85	0.59
5:E:47:CYS:HA	5:E:53:PRO:HA	1.83	0.59
13:M:251:THR:OG1	13:M:254:GLN:NE2	2.35	0.59
15:O:105:LYS:HB3	15:O:210:PRO:HG3	1.85	0.59
15:O:220:GLU:HG2	15:O:221:LYS:H	1.66	0.59
15:O:634:GLU:O	15:O:637:VAL:HG12	2.01	0.59
18:R:478:PHE:HB3	18:R:599:PRO:HA	1.84	0.59
18:R:583:HIS:NE2	18:R:585:LEU:O	2.35	0.59
2:B:253:ILE:HG22	2:B:286:ASN:ND2	2.17	0.59
3:C:238:PRO:O	3:C:239:ILE:HG13	2.01	0.59
15:O:496:ILE:O	15:O:496:ILE:HG22	2.02	0.59
18:R:166:LYS:HG2	18:R:522:ARG:HH12	1.68	0.59
1:A:248:VAL:HG23	1:A:248:VAL:O	2.02	0.59
1:A:786:ASP:OD1	1:A:787:ASN:N	2.35	0.59
2:B:831:GLU:N	2:B:831:GLU:OE1	2.31	0.59
15:O:52:LEU:HD11	15:O:131:LEU:HD12	1.82	0.59
15:O:132:TYR:C	15:O:134:GLY:H	2.10	0.59
15:O:506:ARG:HB3	16:P:250:ASP:OD1	2.03	0.59
2:B:1045:VAL:HG23	2:B:1046:LEU:CD1	2.25	0.59
15:O:215:TRP:O	15:O:219:TYR:HB2	2.03	0.59
16:P:184:ARG:O	16:P:187:SER:OG	2.20	0.59
18:R:213:TRP:CD1	18:R:287:PRO:HD3	2.32	0.59
1:A:132:VAL:HG13	1:A:136:ARG:HB2	1.84	0.59
20:X:7:DA:H4'	20:X:8:DC:OP1	2.03	0.59
1:A:830:ARG:NH1	2:B:657:SER:O	2.36	0.59
2:B:260:CYS:O	2:B:342:PHE:HB3	2.01	0.59
2:B:542:THR:O	13:M:178:GLN:NE2	2.36	0.59
3:C:255:VAL:HG22	3:C:256:ILE:H	1.68	0.59
4:D:119:GLU:HA	4:D:122:GLN:HB3	1.84	0.59
14:N:394:VAL:HB	14:N:412:VAL:HB	1.83	0.59
1:A:164:VAL:HA	1:A:180:HIS:HB2	1.84	0.59
1:A:370:GLY:O	2:B:1061:ARG:NH1	2.36	0.59
1:A:904:VAL:HG13	1:A:912:VAL:HG23	1.83	0.59
1:A:1224:ILE:HG12	1:A:1226:GLY:N	2.18	0.59
2:B:481:ARG:NH2	21:Y:21:DG:H2'	2.17	0.59
2:B:992:VAL:HG23	3:C:278:GLU:HG2	1.83	0.59
5:E:83:CYS:SG	5:E:84:ASP:N	2.75	0.59
13:M:84:SER:C	13:M:85:LEU:CD1	2.71	0.59
19:S:421:THR:HG23	19:S:424:GLU:H	1.67	0.59
1:A:813:VAL:HB	1:A:848:VAL:HG13	1.85	0.59
1:A:1022:LEU:HD22	1:A:1060:TYR:HE2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:SER:OG	3:C:221:PRO:HB3	2.03	0.59
7:G:112:GLN:HE22	7:G:115:LEU:HD22	1.68	0.59
8:H:107:VAL:N	8:H:111:LEU:O	2.32	0.59
16:P:14:ASN:HB3	16:P:51:ILE:HD13	1.85	0.59
1:A:327:ILE:CA	1:A:353:PHE:CE2	2.86	0.58
1:A:1380:ARG:HH11	1:A:1385:GLN:HE22	1.51	0.58
2:B:612:LEU:HD11	2:B:649:LEU:HD11	1.84	0.58
2:B:822:GLN:HG2	2:B:823:SER:H	1.68	0.58
8:H:5:LEU:HB2	8:H:59:ILE:O	2.03	0.58
11:K:85:ASP:OD2	11:K:111:THR:OG1	2.21	0.58
13:M:149:LYS:HB3	13:M:182:PHE:HE2	1.67	0.58
14:N:282:LEU:O	14:N:286:ASP:HB2	2.02	0.58
15:O:128:HIS:NE2	15:O:132:TYR:HE2	2.00	0.58
16:P:236:THR:HG23	16:P:239:ASN:H	1.68	0.58
19:S:418:ASP:HB3	19:S:449:ARG:HH12	1.68	0.58
1:A:235:LYS:CD	1:A:252:ARG:CB	2.81	0.58
2:B:1038:ARG:HE	2:B:1041:GLY:H	1.49	0.58
15:O:584:ASN:HD22	15:O:587:ASN:HB2	1.68	0.58
15:O:592:LYS:O	15:O:596:LYS:HG2	2.03	0.58
16:P:142:PHE:CZ	20:X:30:DT:H4'	2.38	0.58
20:X:60:DA:H2'	20:X:61:DT:C6	2.38	0.58
5:E:155:ARG:NH2	5:E:194:GLU:OE2	2.36	0.58
1:A:622:VAL:HB	1:A:624:ILE:HD11	1.85	0.58
1:A:1161:VAL:HG22	1:A:1275:LEU:HD13	1.84	0.58
5:E:55:ARG:HD2	5:E:82:PHE:CE2	2.38	0.58
14:N:306:VAL:HG23	14:N:415:LYS:HD3	1.85	0.58
15:O:195:CYS:SG	15:O:196:GLU:N	2.76	0.58
19:S:444:GLN:NE2	19:S:490:LYS:NZ	2.51	0.58
1:A:45:ASP:OD1	1:A:46:ARG:N	2.36	0.58
1:A:212:GLU:HG2	1:A:213:ARG:H	1.68	0.58
1:A:975:VAL:HG22	1:A:976:ARG:N	2.10	0.58
2:B:766:ASP:OD1	2:B:945:ASN:HB2	2.03	0.58
2:B:929:GLU:HG2	3:C:72:ILE:CG2	2.34	0.58
2:B:933:PHE:O	2:B:934:ASN:HB3	2.03	0.58
15:O:570:GLU:HA	15:O:573:SER:HB3	1.85	0.58
16:P:206:VAL:HB	16:P:210:PRO:HG3	1.85	0.58
18:R:623:LYS:HE2	19:S:435:TRP:HD1	1.67	0.58
1:A:31:GLU:HG3	1:A:69:THR:HG21	1.86	0.58
2:B:235:THR:HG22	2:B:236:LYS:HG3	1.86	0.58
3:C:227:TYR:HB3	3:C:300:PHE:CD1	2.38	0.58
3:C:255:VAL:HG13	3:C:256:ILE:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:24:CYS:SG	8:H:25:ARG:N	2.76	0.58
10:J:14:VAL:O	10:J:17:LYS:N	2.37	0.58
14:N:364:ARG:NH1	14:N:365:VAL:O	2.37	0.58
16:P:247:LEU:HB3	16:P:253:LEU:HG	1.85	0.58
18:R:431:ARG:NH1	18:R:438:THR:OG1	2.35	0.58
2:B:494:PHE:CE1	2:B:680:ILE:HD12	2.38	0.58
2:B:780:ARG:HH11	10:J:6:ARG:HD2	1.63	0.58
5:E:181:ALA:HA	5:E:186:LEU:HG	1.84	0.58
1:A:197:TRP:CH2	15:O:567:ARG:NH1	2.71	0.58
1:A:302:GLY:C	1:A:304:ASP:H	2.12	0.58
1:A:974:LEU:O	1:A:975:VAL:HG12	2.02	0.58
2:B:49:PRO:O	2:B:53:LYS:N	2.35	0.58
3:C:240:LYS:HB3	3:C:264:GLU:HB3	1.85	0.58
7:G:89:ILE:HG23	7:G:142:VAL:HG12	1.86	0.58
15:O:478:VAL:HG12	15:O:479:PRO:O	2.03	0.58
15:O:620:LEU:HD23	15:O:623:GLU:HB2	1.86	0.58
21:Y:44:DT:H2''	21:Y:45:DT:H2'	1.85	0.58
1:A:106:ILE:HD13	1:A:234:ILE:HG12	1.85	0.58
1:A:178:ILE:HD11	1:A:222:LEU:HB2	1.86	0.58
1:A:354:CYS:SG	1:A:1393:THR:OG1	2.58	0.58
1:A:1221:ASP:OD1	1:A:1222:VAL:N	2.36	0.58
2:B:265:ASP:HA	2:B:268:ILE:HD12	1.86	0.58
4:D:72:PHE:O	7:G:145:LYS:NZ	2.36	0.58
13:M:226:ARG:HG3	13:M:227:LEU:H	1.69	0.58
18:R:173:LEU:O	18:R:175:LEU:N	2.37	0.58
1:A:116:SER:HB3	1:A:155:LEU:HD22	1.85	0.58
1:A:501:ASN:O	1:A:504:VAL:HG22	2.04	0.58
1:A:795:ALA:HB1	1:A:802:SER:HA	1.86	0.58
2:B:1012:CYS:SG	3:C:293:ARG:NH2	2.75	0.58
3:C:222:VAL:HG11	3:C:225:ALA:CB	2.28	0.58
15:O:132:TYR:O	15:O:134:GLY:N	2.31	0.58
15:O:449:SER:HA	15:O:456:HIS:CD2	2.39	0.58
15:O:495:VAL:HG13	15:O:496:ILE:HG13	1.86	0.58
1:A:568:ASP:OD1	8:H:22:LYS:HG2	2.03	0.57
1:A:1126:ILE:HG22	1:A:1130:ILE:HD12	1.86	0.57
13:M:134:ASP:O	13:M:138:SER:N	2.36	0.57
16:P:53:GLN:NE2	19:S:363:GLN:HA	2.19	0.57
18:R:521:TYR:CE2	18:R:523:MET:HB2	2.39	0.57
1:A:200:GLU:CB	15:O:516:LEU:HD23	2.34	0.57
1:A:752:THR:HA	1:A:761:THR:HG21	1.87	0.57
1:A:1323:PHE:HD1	1:A:1328:ILE:H	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:46:TYR:CZ	5:E:58:MET:HA	2.39	0.57
7:G:126:SER:HG	7:G:139:TYR:CB	2.17	0.57
13:M:90:TYR:C	14:N:392:GLN:NE2	2.62	0.57
13:M:102:ALA:O	13:M:103:GLU:HB2	2.04	0.57
14:N:389:THR:C	14:N:391:LEU:H	2.13	0.57
15:O:104:VAL:N	15:O:123:ASN:HB2	2.18	0.57
18:R:25:CYS:SG	18:R:28:CYS:CB	2.92	0.57
18:R:463:ARG:HG3	18:R:602:LEU:HD13	1.86	0.57
19:S:364:LEU:HB3	19:S:374:ILE:HD12	1.87	0.57
2:B:1045:VAL:CG2	2:B:1046:LEU:HD12	2.27	0.57
15:O:110:THR:HG22	15:O:116:LYS:CA	2.26	0.57
15:O:581:LEU:O	15:O:585:MET:HB2	2.04	0.57
19:S:413:ARG:NE	20:X:12:DT:OP1	2.36	0.57
21:Y:55:DT:C4	21:Y:56:DG:O6	2.57	0.57
1:A:38:ASP:O	1:A:40:PHE:N	2.31	0.57
1:A:385:PRO:HG3	2:B:764:GLY:HA3	1.86	0.57
2:B:167:ASP:C	2:B:169:SER:H	2.12	0.57
4:D:127:LEU:HD12	4:D:127:LEU:O	2.04	0.57
9:I:8:CYS:SG	9:I:29:CYS:HB2	2.43	0.57
16:P:31:PHE:HE2	16:P:72:PHE:HB2	1.69	0.57
1:A:235:LYS:HD2	1:A:252:ARG:CB	2.33	0.57
1:A:1329:GLU:OE2	5:E:200:ARG:NH2	2.37	0.57
10:J:41:LEU:HD23	10:J:47:ARG:HA	1.87	0.57
15:O:471:THR:OG1	15:O:477:TYR:HB3	2.04	0.57
21:Y:7:DA:H2"	21:Y:8:DG:C8	2.39	0.57
1:A:485:ILE:O	1:A:486:LEU:HD12	2.05	0.57
1:A:668:VAL:O	1:A:677:VAL:N	2.35	0.57
7:G:45:CYS:SG	7:G:46:ILE:N	2.77	0.57
1:A:34:VAL:HG13	1:A:35:SER:H	1.70	0.57
1:A:67:CYS:HB3	1:A:70:CYS:O	2.04	0.57
1:A:189:LYS:HE3	1:A:191:ALA:HB2	1.86	0.57
1:A:1370:GLY:HA2	1:A:1375:GLY:CA	2.35	0.57
2:B:1022:ILE:HG22	2:B:1023:TYR:H	1.69	0.57
6:F:108:PHE:CE2	6:F:131:PRO:HG3	2.40	0.57
15:O:230:SER:O	15:O:237:LYS:NZ	2.36	0.57
15:O:352:VAL:HG13	15:O:353:GLU:CD	2.28	0.57
16:P:45:LEU:HD22	19:S:366:LEU:HB3	1.87	0.57
16:P:314:GLU:HB3	17:Q:37:PRO:HB3	1.85	0.57
18:R:7:CYS:SG	18:R:28:CYS:CB	2.76	0.57
1:A:327:ILE:CG2	1:A:353:PHE:CE2	2.87	0.57
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:90:TYR:O	14:N:392:GLN:CB	2.53	0.57
1:A:30:SER:OG	1:A:82:GLY:HA2	2.04	0.57
1:A:649:ASP:OD2	1:A:663:VAL:HG13	2.04	0.57
2:B:651:VAL:HG23	2:B:652:ASN:H	1.70	0.57
3:C:30:GLU:HG3	11:K:84:PRO:HG3	1.87	0.57
5:E:28:TYR:CZ	5:E:78:LEU:HD23	2.40	0.57
7:G:13:ILE:HG13	7:G:66:SER:HB3	1.87	0.57
15:O:292:ARG:HD2	15:O:488:LYS:NZ	2.16	0.57
15:O:467:PHE:CD1	15:O:468:LEU:HD13	2.39	0.57
15:O:494:TYR:HB2	16:P:294:PHE:HZ	1.69	0.57
18:R:617:GLU:HG2	18:R:621:LYS:HE2	1.87	0.57
1:A:980:SER:OG	5:E:160:GLU:HA	2.05	0.57
6:F:108:PHE:HE2	6:F:131:PRO:HG3	1.70	0.57
15:O:158:GLU:OE1	15:O:161:GLN:NE2	2.37	0.57
15:O:159:ILE:O	15:O:163:VAL:HG23	2.05	0.57
15:O:166:LEU:HB3	15:O:169:LEU:HD11	1.87	0.57
1:A:91:PHE:HE1	1:A:227:THR:HG21	1.70	0.56
1:A:584:SER:O	1:A:586:GLY:N	2.38	0.56
1:A:940:ASP:O	1:A:943:TYR:N	2.38	0.56
2:B:554:GLY:O	2:B:599:VAL:HG12	2.05	0.56
2:B:615:VAL:HA	2:B:620:SER:HA	1.87	0.56
2:B:818:ILE:O	2:B:822:GLN:N	2.37	0.56
7:G:104:ILE:HG12	7:G:105:PHE:CD1	2.39	0.56
15:O:498:SER:HB2	16:P:296:TYR:HB3	1.85	0.56
15:O:554:THR:CG2	15:O:561:ARG:HE	2.14	0.56
18:R:521:TYR:HE2	18:R:523:MET:HB2	1.69	0.56
1:A:1144:VAL:HG12	1:A:1292:GLU:HG3	1.88	0.56
2:B:496:MET:HE2	2:B:608:ILE:HG22	1.87	0.56
2:B:546:SER:HB3	14:N:391:LEU:HD21	1.86	0.56
13:M:183:PHE:C	13:M:185:TYR:N	2.57	0.56
1:A:478:PRO:HG3	21:Y:23:DG:N3	2.19	0.56
1:A:595:PRO:HG2	1:A:598:MET:HG2	1.87	0.56
1:A:943:TYR:O	1:A:947:PHE:N	2.38	0.56
2:B:59:LYS:HE2	2:B:519:HIS:CD2	2.41	0.56
2:B:62:LEU:HA	2:B:155:MET:HE1	1.86	0.56
2:B:539:GLU:HA	14:N:308:GLN:HE22	1.70	0.56
2:B:932:PRO:HB2	2:B:1004:LEU:HD13	1.85	0.56
3:C:132:ILE:O	3:C:208:CYS:HB3	2.04	0.56
4:D:65:TYR:HA	4:D:68:ILE:HG22	1.87	0.56
8:H:106:GLU:OE1	8:H:106:GLU:N	2.38	0.56
11:K:99:ASN:O	11:K:100:LEU:HD12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:123:ILE:O	13:M:146:GLN:N	2.35	0.56
18:R:401:THR:O	18:R:479:THR:OG1	2.20	0.56
18:R:510:SER:N	18:R:520:ILE:O	2.34	0.56
1:A:1319:VAL:HG21	1:A:1335:ILE:HB	1.87	0.56
2:B:855:PRO:O	18:R:106:GLN:NE2	2.38	0.56
2:B:905:ARG:O	2:B:907:GLU:N	2.38	0.56
3:C:69:ARG:HE	11:K:71:THR:HG22	1.71	0.56
15:O:251:LYS:HA	15:O:254:ASN:HB2	1.88	0.56
16:P:216:SER:OG	16:P:260:CYS:HA	2.05	0.56
18:R:397:VAL:O	18:R:484:GLN:N	2.37	0.56
1:A:106:ILE:HD11	1:A:111:SER:C	2.29	0.56
1:A:176:LEU:HB3	1:A:320:GLN:NE2	2.19	0.56
1:A:925:GLU:CD	1:A:1081:ALA:HA	2.30	0.56
2:B:332:ILE:HG13	2:B:333:ALA:H	1.68	0.56
8:H:93:TYR:HD2	8:H:143:LEU:HG	1.71	0.56
15:O:91:VAL:O	15:O:95:LEU:CB	2.52	0.56
15:O:583:TRP:CZ3	16:P:315:TRP:HB3	2.40	0.56
17:Q:38:SER:O	17:Q:39:ILE:C	2.49	0.56
1:A:496:ARG:HB2	2:B:1035:MET:SD	2.45	0.56
1:A:502:GLU:CD	2:B:767:ILE:HG13	2.30	0.56
2:B:297:THR:OG1	2:B:302:LEU:HG	2.06	0.56
2:B:961:LEU:HD13	2:B:1018:PHE:CE2	2.41	0.56
7:G:126:SER:HB3	7:G:139:TYR:HB3	1.87	0.56
15:O:498:SER:OG	16:P:296:TYR:HB2	2.04	0.56
1:A:11:LYS:HD2	2:B:1145:ASP:HA	1.88	0.56
1:A:17:GLU:O	2:B:1139:PRO:C	2.49	0.56
1:A:830:ARG:NH2	1:A:833:PRO:O	2.37	0.56
1:A:835:PHE:CE2	1:A:844:SER:HA	2.40	0.56
2:B:915:ARG:CD	2:B:1023:TYR:HB3	2.35	0.56
3:C:66:ALA:O	3:C:70:ILE:HG22	2.06	0.56
3:C:86:PHE:O	3:C:87:ASN:O	2.23	0.56
3:C:89:THR:CG2	3:C:201:GLU:H	2.18	0.56
1:A:777:VAL:HG12	1:A:811:ALA:HB1	1.86	0.56
1:A:816:GLN:HB3	1:A:867:SER:HB2	1.87	0.56
2:B:461:LEU:HD21	2:B:1028:LYS:HD3	1.87	0.56
2:B:695:GLN:HG3	2:B:697:PRO:HD2	1.88	0.56
4:D:110:LEU:HD21	4:D:123:ILE:HD11	1.88	0.56
5:E:17:ARG:HG3	5:E:35:VAL:HG22	1.87	0.56
5:E:63:ASN:HA	5:E:77:SER:HA	1.88	0.56
7:G:96:GLY:HA2	7:G:112:GLN:OE1	2.05	0.56
11:K:63:PHE:HD2	11:K:117:LEU:HD13	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:107:ILE:HD12	13:M:124:PRO:HG3	1.87	0.56
13:M:159:TYR:HD1	13:M:172:PRO:HA	1.69	0.56
15:O:46:LEU:HD11	15:O:66:GLY:HA2	1.88	0.56
15:O:234:ASP:O	15:O:238:ARG:N	2.39	0.56
18:R:6:ASN:HD22	18:R:30:VAL:HG21	1.70	0.56
2:B:177:CYS:SG	2:B:714:ALA:HB1	2.46	0.56
2:B:541:ILE:HA	2:B:544:ILE:HD12	1.88	0.56
2:B:944:MET:HE1	2:B:957:LYS:HE2	1.88	0.56
4:D:135:TYR:HA	4:D:141:CYS:SG	2.46	0.56
9:I:15:THR:HG22	9:I:24:LEU:HA	1.87	0.56
15:O:555:ALA:HB2	15:O:561:ARG:HG3	1.88	0.56
15:O:595:LEU:HD12	15:O:598:GLU:CG	2.35	0.56
1:A:329:SER:HA	1:A:351:ARG:NE	2.21	0.56
1:A:486:LEU:HD23	1:A:537:VAL:HG22	1.87	0.56
1:A:628:ALA:CB	1:A:675:HIS:CD2	2.89	0.56
1:A:955:LEU:HB2	1:A:958:ALA:HB3	1.87	0.56
2:B:109:LYS:HG2	2:B:111:TYR:O	2.05	0.56
2:B:734:PRO:CB	2:B:915:ARG:NH1	2.69	0.56
2:B:1038:ARG:NE	2:B:1041:GLY:H	2.03	0.56
18:R:639:GLU:HG3	18:R:642:ARG:HE	1.69	0.56
20:X:56:DC:N3	21:Y:8:DG:N1	2.53	0.56
1:A:330:ASP:CG	1:A:331:SER:H	2.12	0.55
1:A:890:MET:SD	2:B:1068:ASP:HB2	2.46	0.55
1:A:893:LEU:HD13	1:A:1361:VAL:HG21	1.86	0.55
1:A:1189:ASP:OD2	1:A:1192:THR:N	2.39	0.55
1:A:1202:ILE:O	1:A:1205:ILE:HG13	2.06	0.55
1:A:1385:GLN:HA	1:A:1388:SER:HB3	1.87	0.55
1:A:321:LEU:O	1:A:325:MET:CB	2.54	0.55
1:A:598:MET:HB2	8:H:96:VAL:HG21	1.87	0.55
1:A:1429:LYS:HD3	6:F:137:TYR:CE2	2.40	0.55
2:B:658:TYR:CD2	2:B:670:MET:HG2	2.41	0.55
2:B:754:ASN:O	10:J:48:ARG:NH1	2.40	0.55
2:B:932:PRO:HG2	2:B:940:PRO:CG	2.36	0.55
2:B:933:PHE:HE1	2:B:1005:TYR:CD2	2.09	0.55
2:B:936:GLN:HB2	2:B:938:ILE:HD12	1.86	0.55
3:C:96:VAL:O	3:C:99:HIS:HB3	2.06	0.55
5:E:179:GLN:O	5:E:180:ARG:C	2.49	0.55
8:H:8:ASP:OD1	8:H:9:ILE:N	2.38	0.55
18:R:219:ARG:N	21:Y:54:DA:OP1	2.26	0.55
21:Y:39:DA:H1'	21:Y:40:DA:H5'	1.88	0.55
2:B:471:THR:HG23	2:B:514:LEU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:90:TYR:CB	13:M:179:LEU:HB3	2.35	0.55
15:O:307:VAL:HG13	15:O:308:THR:H	1.70	0.55
16:P:14:ASN:HA	16:P:17:THR:HG22	1.88	0.55
1:A:207:HIS:CE1	15:O:521:ILE:HG21	2.42	0.55
3:C:240:LYS:HB2	3:C:261:GLY:O	2.06	0.55
15:O:338:ASP:OD1	15:O:339:LEU:N	2.40	0.55
21:Y:10:DC:N3	21:Y:11:DA:N6	2.54	0.55
1:A:552:ALA:HB3	1:A:671:ASP:H	1.72	0.55
1:A:633:PHE:HZ	1:A:643:ASN:HB3	1.72	0.55
2:B:81:GLN:O	2:B:94:LYS:HA	2.07	0.55
2:B:1036:HIS:NE2	2:B:1058:GLY:HA2	2.20	0.55
15:O:135:LEU:HD12	15:O:138:ASP:HB3	1.87	0.55
15:O:190:LEU:CA	15:O:193:GLN:HB3	2.36	0.55
18:R:219:ARG:NH1	18:R:514:GLU:O	2.39	0.55
19:S:417:THR:HG22	19:S:453:GLN:HE21	1.72	0.55
19:S:439:PHE:HD1	19:S:454:VAL:HG12	1.72	0.55
19:S:507:ASN:HA	19:S:510:LYS:HB3	1.87	0.55
1:A:418:GLU:O	1:A:421:VAL:HG12	2.07	0.55
1:A:523:GLN:HB2	2:B:1081:GLU:OE2	2.06	0.55
1:A:974:LEU:HD11	1:A:998:TYR:CD2	2.41	0.55
2:B:521:THR:HG22	2:B:605:GLY:HA2	1.89	0.55
2:B:931:MET:HG3	2:B:932:PRO:HD2	1.89	0.55
13:M:164:LYS:HE3	13:M:259:ILE:HG13	1.88	0.55
15:O:296:LEU:HD22	15:O:487:LEU:HD21	1.87	0.55
16:P:221:ILE:O	16:P:225:ILE:HG12	2.07	0.55
18:R:96:ILE:HG22	18:R:141:HIS:NE2	2.21	0.55
18:R:100:ILE:O	18:R:103:ALA:HB3	2.07	0.55
19:S:414:GLY:HA3	20:X:11:DA:P	2.47	0.55
1:A:134:ASN:OD1	1:A:1404:LYS:NZ	2.39	0.55
1:A:484:SER:O	1:A:508:TYR:HE1	1.90	0.55
1:A:1411:VAL:HG13	1:A:1412:SER:H	1.72	0.55
2:B:733:GLN:HG3	10:J:54:VAL:HG13	1.89	0.55
2:B:957:LYS:HZ2	2:B:1022:ILE:HD13	1.72	0.55
15:O:647:LEU:O	15:O:650:VAL:HG12	2.07	0.55
1:A:11:LYS:HG3	2:B:1117:ILE:HD13	1.87	0.55
1:A:520:HIS:HE1	2:B:1062:LEU:HD21	1.72	0.55
2:B:383:LEU:HB3	2:B:442:TRP:CH2	2.41	0.55
2:B:611:PRO:HG3	2:B:648:TYR:CE1	2.41	0.55
2:B:976:GLY:HA2	2:B:981:GLY:HA3	1.88	0.55
6:F:89:GLU:OE1	6:F:90:ARG:N	2.40	0.55
7:G:88:TRP:CD1	7:G:143:ASN:H	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:126:SER:CB	7:G:139:TYR:CB	2.85	0.55
1:A:372:ARG:HG2	2:B:1050:PRO:HB2	1.89	0.55
1:A:715:ASN:HD21	2:B:1001:LYS:HD3	1.70	0.55
5:E:77:SER:O	5:E:105:PHE:HB3	2.06	0.55
13:M:112:TYR:HD1	13:M:119:TRP:NE1	2.00	0.55
14:N:287:HIS:NE2	14:N:384:LYS:HG3	2.22	0.55
15:O:171:VAL:HB	15:O:276:PRO:HB3	1.87	0.55
1:A:164:VAL:HB	1:A:180:HIS:CB	2.37	0.55
1:A:308:SER:HA	15:O:534:ARG:CD	2.37	0.55
1:A:371:LYS:HZ1	2:B:1122:PRO:CB	2.19	0.55
1:A:404:TYR:CZ	1:A:528:ARG:HD2	2.42	0.55
1:A:636:PRO:HG2	1:A:643:ASN:HA	1.89	0.55
1:A:1125:ARG:NH2	1:A:1317:ASN:HB3	2.22	0.55
2:B:906:PRO:HB3	2:B:1026:LYS:HE3	1.89	0.55
18:R:11:GLU:N	18:R:11:GLU:OE1	2.40	0.55
18:R:270:LEU:O	18:R:273:GLN:NE2	2.36	0.55
2:B:817:PRO:HB2	2:B:822:GLN:HA	1.89	0.54
5:E:182:ASP:OD1	5:E:183:PRO:HD2	2.07	0.54
7:G:82:GLY:HA2	7:G:150:ILE:O	2.08	0.54
8:H:93:TYR:CD2	8:H:143:LEU:HG	2.42	0.54
18:R:436:LYS:NZ	19:S:462:GLU:OE2	2.25	0.54
18:R:483:ILE:HG21	18:R:486:ILE:HG13	1.89	0.54
18:R:627:TRP:O	18:R:631:ASN:ND2	2.32	0.54
1:A:371:LYS:HZ3	2:B:1122:PRO:CB	2.08	0.54
1:A:628:ALA:HB2	1:A:675:HIS:HD2	1.69	0.54
2:B:400:LYS:O	2:B:403:ILE:HG22	2.07	0.54
2:B:566:ARG:NH2	14:N:282:LEU:HD23	2.22	0.54
2:B:583:LYS:HG2	2:B:584:VAL:HG13	1.88	0.54
2:B:778:ILE:HG13	2:B:906:PRO:HG2	1.88	0.54
2:B:904:ARG:NH2	2:B:1033:ASP:OD1	2.40	0.54
7:G:114:MET:HB3	7:G:201:GLN:HB3	1.89	0.54
15:O:128:HIS:CE1	15:O:652:GLN:HE22	2.25	0.54
18:R:165:VAL:HA	18:R:170:ILE:HD13	1.90	0.54
1:A:625:ASN:HD21	1:A:941:HIS:HA	1.72	0.54
1:A:661:SER:HB2	8:H:122:LEU:HD11	1.89	0.54
2:B:260:CYS:O	2:B:346:ALA:HB2	2.07	0.54
8:H:43:ASN:ND2	8:H:46:LEU:HD13	2.22	0.54
16:P:137:VAL:HG21	16:P:149:MET:HE3	1.88	0.54
19:S:429:TYR:HA	19:S:432:LEU:HD12	1.88	0.54
1:A:238:ASP:CG	1:A:239:CYS:N	2.64	0.54
2:B:334:HIS:O	2:B:337:VAL:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:126:SER:OG	7:G:139:TYR:CG	2.58	0.54
8:H:114:VAL:HG21	8:H:130:ARG:NH1	2.22	0.54
13:M:163:VAL:HG22	13:M:168:VAL:HG22	1.89	0.54
1:A:164:VAL:CA	1:A:180:HIS:HB2	2.38	0.54
1:A:675:HIS:CA	1:A:937:ARG:HH22	2.20	0.54
2:B:932:PRO:HG2	2:B:940:PRO:HG3	1.89	0.54
4:D:61:ASN:ND2	7:G:103:GLY:O	2.41	0.54
15:O:59:GLU:HG3	15:O:61:ALA:H	1.73	0.54
18:R:213:TRP:NE1	18:R:287:PRO:HG3	2.22	0.54
1:A:66:GLU:HB3	1:A:71:HIS:HB2	1.90	0.54
1:A:921:LEU:CD2	1:A:932:PRO:HG3	2.38	0.54
1:A:1193:ILE:HG12	1:A:1200:LEU:HD11	1.90	0.54
3:C:119:ASN:O	3:C:120:LEU:CG	2.51	0.54
3:C:123:ASP:OD1	3:C:124:GLU:N	2.40	0.54
5:E:153:HIS:CE1	5:E:184:VAL:HG11	2.43	0.54
15:O:623:GLU:O	15:O:627:LEU:HG	2.07	0.54
16:P:269:LEU:HD11	16:P:296:TYR:OH	2.07	0.54
1:A:1370:GLY:C	1:A:1375:GLY:HA3	2.33	0.54
2:B:163:LEU:HD22	2:B:171:MET:HE1	1.88	0.54
2:B:1031:VAL:O	2:B:1034:LYS:N	2.41	0.54
3:C:33:VAL:C	3:C:35:LYS:H	2.16	0.54
3:C:230:LEU:HD13	3:C:297:HIS:CE1	2.42	0.54
15:O:78:GLU:HG2	15:O:82:LYS:HZ1	1.73	0.54
1:A:997:GLN:C	1:A:999:ASP:H	2.15	0.54
2:B:239:LYS:HG2	2:B:241:TYR:CE2	2.41	0.54
5:E:2:ASP:O	5:E:6:GLU:N	2.41	0.54
7:G:203:ASP:HB3	7:G:211:TRP:HE1	1.73	0.54
8:H:93:TYR:HD1	8:H:145:ARG:HD3	1.72	0.54
13:M:122:ASP:HB3	13:M:145:VAL:CG2	2.37	0.54
13:M:182:PHE:HD1	13:M:183:PHE:N	2.04	0.54
15:O:366:LEU:HD22	15:O:368:ARG:HH11	1.72	0.54
18:R:610:LEU:HA	18:R:613:HIS:CD2	2.41	0.54
20:X:16:DA:H2'	20:X:17:DG:C8	2.43	0.54
1:A:200:GLU:CB	15:O:516:LEU:HD21	2.38	0.54
1:A:211:LEU:HD22	1:A:215:VAL:HG21	1.90	0.54
1:A:830:ARG:HD2	1:A:837:LYS:HG2	1.90	0.54
1:A:869:ARG:NH2	2:B:502:THR:HB	2.22	0.54
1:A:1278:ILE:HG12	1:A:1297:GLY:HA3	1.88	0.54
2:B:254:ALA:O	2:B:258:LYS:HG2	2.08	0.54
2:B:647:GLU:OE1	2:B:647:GLU:N	2.41	0.54
5:E:112:TYR:CZ	5:E:116:ILE:HG23	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:290:ILE:HG21	14:N:384:LYS:HZ1	1.73	0.54
16:P:295:ASN:HB2	16:P:297:PHE:CE1	2.43	0.54
18:R:632:ALA:O	18:R:636:LEU:CB	2.55	0.54
1:A:516:GLU:OE2	2:B:1034:LYS:HD3	2.07	0.54
1:A:617:ASN:CG	1:A:618:HIS:N	2.66	0.54
2:B:135:TYR:O	2:B:142:ILE:HA	2.07	0.54
2:B:138:GLY:N	2:B:141:ILE:HG21	2.21	0.54
2:B:330:THR:HA	2:B:345:LYS:HE3	1.90	0.54
2:B:936:GLN:NE2	10:J:43:ARG:NH1	2.56	0.54
3:C:223:SER:HB2	3:C:303:GLU:HB2	1.89	0.54
6:F:79:ARG:NH1	6:F:145:ASP:H	2.06	0.54
11:K:123:ASP:O	11:K:126:ASP:N	2.40	0.54
13:M:106:PHE:O	13:M:107:ILE:HG22	2.07	0.54
13:M:242:ASN:O	13:M:243:ILE:HB	2.08	0.54
18:R:399:THR:HB	18:R:484:GLN:NE2	2.23	0.54
20:X:25:DT:O4	21:Y:38:DA:N6	2.41	0.54
1:A:379:THR:HG21	1:A:497:THR:HA	1.90	0.53
1:A:891:LYS:HG3	1:A:1389:PHE:HD1	1.73	0.53
2:B:723:THR:HG23	2:B:724:LEU:H	1.74	0.53
15:O:187:ILE:O	15:O:189:SER:N	2.41	0.53
15:O:190:LEU:CB	15:O:194:LEU:HG	2.38	0.53
15:O:190:LEU:CD1	15:O:194:LEU:HD23	2.32	0.53
18:R:437:THR:O	18:R:465:TYR:OH	2.26	0.53
1:A:378:ARG:O	1:A:379:THR:OG1	2.24	0.53
1:A:1024:LYS:HE2	1:A:1030:GLY:HA3	1.89	0.53
1:A:1028:MET:SD	1:A:1048:VAL:HG22	2.49	0.53
2:B:347:LEU:HB3	2:B:541:ILE:HD11	1.90	0.53
4:D:14:TYR:CE2	4:D:103:PHE:HB2	2.44	0.53
18:R:398:ALA:HB3	18:R:449:VAL:HB	1.89	0.53
20:X:3:DT:O4	21:Y:60:DA:N6	2.41	0.53
1:A:252:ARG:HB3	1:A:253:PRO:HD2	1.89	0.53
2:B:244:HIS:HB3	2:B:247:ILE:HG22	1.90	0.53
2:B:552:ASN:OD1	2:B:553:TYR:CD2	2.61	0.53
3:C:31:TRP:CG	3:C:32:ASN:N	2.74	0.53
5:E:32:GLN:O	5:E:36:GLU:N	2.41	0.53
14:N:282:LEU:O	14:N:286:ASP:CB	2.57	0.53
16:P:209:ALA:O	16:P:212:VAL:HG12	2.08	0.53
16:P:311:TYR:HA	17:Q:40:PRO:CA	2.21	0.53
18:R:395:ASN:H	18:R:487:VAL:HB	1.72	0.53
21:Y:7:DA:H2''	21:Y:8:DG:H8	1.73	0.53
21:Y:46:DA:H2''	21:Y:47:DC:O4'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:VAL:O	1:A:290:THR:HG22	2.07	0.53
1:A:389:ILE:N	1:A:695:ASN:OD1	2.37	0.53
1:A:542:LEU:HD21	1:A:679:TYR:HE1	1.73	0.53
1:A:624:ILE:HG22	1:A:625:ASN:N	2.24	0.53
3:C:105:PRO:HG3	10:J:6:ARG:NH2	2.24	0.53
7:G:2:PHE:N	7:G:77:PHE:HA	2.22	0.53
13:M:255:PHE:O	13:M:258:THR:OG1	2.25	0.53
18:R:97:PRO:HD2	18:R:100:ILE:HD12	1.89	0.53
20:X:6:DA:C4	20:X:7:DA:C5	2.96	0.53
20:X:11:DA:H2''	20:X:12:DT:C6	2.44	0.53
1:A:197:TRP:HZ3	15:O:567:ARG:HH11	1.51	0.53
1:A:308:SER:N	1:A:311:ASN:OD1	2.41	0.53
1:A:373:VAL:N	2:B:1050:PRO:HG2	2.22	0.53
1:A:628:ALA:O	1:A:651:PHE:HA	2.07	0.53
2:B:1022:ILE:HG22	2:B:1023:TYR:N	2.23	0.53
10:J:56:LEU:O	10:J:59:LYS:N	2.41	0.53
15:O:267:PRO:HD3	15:O:273:ILE:HG22	1.91	0.53
1:A:214:TYR:HD2	1:A:215:VAL:HG13	1.73	0.53
1:A:269:ARG:HH21	1:A:286:THR:H	1.55	0.53
2:B:626:HIS:HA	2:B:629:LYS:HB3	1.89	0.53
3:C:211:GLY:HA3	3:C:219:PHE:CE2	2.44	0.53
6:F:85:MET:SD	6:F:153:VAL:HA	2.49	0.53
15:O:44:PRO:HA	15:O:582:GLU:HG3	1.91	0.53
15:O:189:SER:O	15:O:190:LEU:C	2.51	0.53
15:O:496:ILE:HD11	15:O:576:PHE:CZ	2.44	0.53
15:O:584:ASN:OD1	16:P:310:VAL:HA	2.09	0.53
16:P:128:LEU:HA	16:P:131:GLN:HB2	1.91	0.53
18:R:397:VAL:HG12	18:R:484:GLN:HB2	1.90	0.53
1:A:224:PRO:O	1:A:227:THR:HG22	2.07	0.53
1:A:269:ARG:NH1	1:A:285:LEU:HB2	2.22	0.53
1:A:482:ARG:HB3	1:A:544:PRO:HG3	1.91	0.53
1:A:993:GLU:O	5:E:197:LYS:NZ	2.42	0.53
1:A:1305:CYS:SG	5:E:141:VAL:HG11	2.49	0.53
9:I:22:TYR:O	9:I:23:THR:HG22	2.07	0.53
9:I:29:CYS:HA	13:M:183:PHE:CE2	2.35	0.53
10:J:43:ARG:NH1	10:J:43:ARG:HG2	2.24	0.53
15:O:538:ALA:O	15:O:541:ILE:HG22	2.08	0.53
16:P:241:ARG:O	16:P:245:GLU:HG2	2.08	0.53
18:R:128:SER:OG	18:R:164:MET:SD	2.62	0.53
18:R:521:TYR:HB3	18:R:530:LEU:HB2	1.89	0.53
1:A:44:LYS:HG3	1:A:45:ASP:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ARG:HG3	1:A:477:GLN:HB3	1.91	0.53
1:A:678:PHE:CE2	1:A:694:MET:HG2	2.43	0.53
1:A:968:GLY:O	1:A:972:GLU:HG2	2.09	0.53
5:E:94:LYS:O	5:E:98:ILE:HG12	2.09	0.53
5:E:182:ASP:CG	5:E:183:PRO:HD2	2.34	0.53
7:G:141:ASP:OD1	7:G:142:VAL:N	2.42	0.53
8:H:97:MET:HB2	8:H:142:LEU:HB3	1.90	0.53
13:M:125:LEU:HD11	13:M:146:GLN:HB2	1.90	0.53
16:P:106:TRP:CZ3	16:P:108:LYS:HB3	2.44	0.53
16:P:256:VAL:O	16:P:260:CYS:HB3	2.08	0.53
18:R:516:PHE:CD1	18:R:517:PRO:HD2	2.43	0.53
1:A:472:VAL:HG11	1:A:519:LEU:HG	1.90	0.53
1:A:896:LEU:HB3	1:A:1090:GLY:HA3	1.91	0.53
1:A:912:VAL:HG23	1:A:913:GLN:H	1.74	0.53
1:A:995:VAL:HG23	1:A:996:ASP:H	1.74	0.53
2:B:247:ILE:HG13	2:B:248:ALA:H	1.74	0.53
2:B:464:ILE:HD11	2:B:746:TYR:CE1	2.44	0.53
2:B:529:ILE:HD11	2:B:575:PHE:CE1	2.42	0.53
2:B:551:LEU:CD1	14:N:388:THR:N	2.68	0.53
3:C:115:TRP:HH2	3:C:212:ILE:HB	1.73	0.53
8:H:13:SER:HB3	8:H:27:GLU:O	2.08	0.53
9:I:30:PRO:CD	13:M:183:PHE:HZ	2.21	0.53
14:N:287:HIS:CD2	14:N:384:LYS:HG3	2.43	0.53
15:O:507:LEU:O	15:O:511:ILE:HG12	2.08	0.53
16:P:98:GLU:HB3	16:P:150:LEU:HD21	1.89	0.53
18:R:287:PRO:HD2	18:R:290:PHE:CE1	2.44	0.53
18:R:463:ARG:NH1	18:R:598:ASP:O	2.39	0.53
1:A:45:ASP:O	1:A:48:PRO:HD3	2.10	0.53
1:A:364:PHE:CE2	1:A:1387:ALA:C	2.87	0.53
2:B:758:ALA:O	2:B:943:ILE:HD12	2.09	0.53
2:B:934:ASN:ND2	2:B:1019:PHE:HZ	2.07	0.53
3:C:7:ILE:HG12	3:C:292:GLY:HA2	1.90	0.53
3:C:108:VAL:HB	3:C:184:VAL:HG12	1.91	0.53
6:F:101:ILE:HG21	6:F:120:ILE:HD11	1.91	0.53
13:M:109:ALA:HB3	13:M:122:ASP:HB2	1.90	0.53
18:R:405:ARG:HG3	18:R:443:ALA:O	2.09	0.53
1:A:1171:PHE:HD2	1:A:1172:TYR:CD2	2.26	0.52
1:A:1299:GLY:C	1:A:1301:ARG:H	2.18	0.52
2:B:337:VAL:HG23	2:B:338:GLU:H	1.73	0.52
5:E:66:GLU:HG3	5:E:67:GLU:H	1.74	0.52
5:E:82:PHE:HZ	5:E:113:GLN:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:35:ILE:HD12	9:I:36:GLU:HG2	1.91	0.52
13:M:122:ASP:HA	13:M:146:GLN:O	2.09	0.52
15:O:332:GLN:HE22	15:O:337:GLN:NE2	2.07	0.52
1:A:32:VAL:HG11	1:A:57:LYS:HD2	1.90	0.52
1:A:109:ASN:ND2	1:A:159:ALA:CB	2.64	0.52
1:A:624:ILE:H	1:A:657:SER:HG	1.54	0.52
1:A:1391:LYS:HB2	1:A:1395:HIS:CE1	2.45	0.52
2:B:289:GLU:O	2:B:292:LYS:HG2	2.09	0.52
2:B:317:LEU:O	2:B:320:LEU:HG	2.09	0.52
3:C:172:GLN:N	3:C:175:GLN:HB3	2.16	0.52
3:C:255:VAL:O	3:C:268:LYS:HB2	2.09	0.52
5:E:153:HIS:ND1	5:E:184:VAL:HG11	2.24	0.52
7:G:115:LEU:H	7:G:199:SER:HB3	1.75	0.52
13:M:171:VAL:CG1	13:M:172:PRO:HD2	2.39	0.52
18:R:140:HIS:ND1	18:R:140:HIS:O	2.42	0.52
19:S:409:GLY:HA3	21:Y:55:DT:H4'	1.91	0.52
20:X:59:DC:C2	20:X:60:DA:N7	2.76	0.52
1:A:381:ILE:HD11	1:A:517:MET:HG2	1.90	0.52
1:A:703:ARG:NH2	11:K:93:ILE:O	2.42	0.52
1:A:1316:THR:OG1	1:A:1317:ASN:N	2.42	0.52
2:B:155:MET:HB2	2:B:185:PHE:CE1	2.44	0.52
2:B:667:VAL:HG23	2:B:670:MET:HE3	1.91	0.52
2:B:714:ALA:O	2:B:717:GLN:HB2	2.10	0.52
3:C:100:ARG:HH12	10:J:2:ILE:HB	1.73	0.52
14:N:395:ILE:HD12	14:N:411:ARG:HA	1.92	0.52
15:O:132:TYR:OH	15:O:291:ARG:NH1	2.43	0.52
16:P:106:TRP:HB2	16:P:147:ILE:HG22	1.90	0.52
18:R:195:LYS:HA	18:R:198:VAL:HB	1.92	0.52
1:A:5:VAL:HG22	7:G:37:LYS:HB3	1.90	0.52
1:A:161:ASN:HB2	1:A:180:HIS:CE1	2.43	0.52
1:A:606:GLY:HA2	1:A:609:VAL:HG12	1.90	0.52
2:B:553:TYR:HA	2:B:597:MET:HB3	1.89	0.52
2:B:726:TYR:CE2	2:B:1028:LYS:HG3	2.44	0.52
2:B:926:VAL:CG1	2:B:930:ASP:HB2	2.40	0.52
2:B:933:PHE:CE2	3:C:226:SER:HB3	2.39	0.52
2:B:1038:ARG:NH1	2:B:1058:GLY:O	2.36	0.52
3:C:211:GLY:HA3	3:C:219:PHE:CD2	2.44	0.52
15:O:110:THR:HG22	15:O:115:LYS:O	2.09	0.52
15:O:163:VAL:HG12	15:O:282:ILE:HD11	1.91	0.52
16:P:135:LYS:HB3	16:P:151:TYR:HD1	1.74	0.52
18:R:4:CYS:HB3	18:R:9:GLY:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:12:PHE:CD1	18:R:25:CYS:HB3	2.44	0.52
1:A:598:MET:HA	1:A:602:TYR:HD1	1.75	0.52
1:A:1173:VAL:HA	1:A:1186:VAL:HG12	1.91	0.52
1:A:1267:LEU:C	1:A:1269:ASP:H	2.17	0.52
2:B:774:ASN:O	2:B:777:SER:HB2	2.10	0.52
2:B:914:SER:HB3	2:B:918:GLN:HB2	1.92	0.52
2:B:933:PHE:O	2:B:1004:LEU:HD23	2.09	0.52
15:O:36:SER:O	15:O:40:ARG:HB2	2.10	0.52
18:R:392:THR:OG1	18:R:489:SER:O	2.28	0.52
21:Y:15:DT:H2'	21:Y:16:DA:C8	2.44	0.52
1:A:1431:VAL:HG13	7:G:57:GLY:O	2.10	0.52
2:B:244:HIS:CE1	2:B:332:ILE:HD12	2.45	0.52
2:B:556:TYR:HE1	2:B:561:LEU:HD12	1.74	0.52
2:B:911:LYS:HD3	2:B:1029:HIS:HB2	1.92	0.52
5:E:200:ARG:HD2	5:E:208:TYR:CZ	2.44	0.52
7:G:98:LYS:HA	7:G:109:PHE:HA	1.92	0.52
14:N:389:THR:O	14:N:391:LEU:N	2.42	0.52
16:P:27:ILE:HB	16:P:31:PHE:HB2	1.91	0.52
18:R:467:ARG:O	18:R:471:LYS:CB	2.58	0.52
18:R:502:ALA:HB2	18:R:519:LEU:HD11	1.90	0.52
19:S:431:ALA:HA	19:S:434:MET:HB2	1.91	0.52
1:A:473:LEU:HD13	1:A:485:ILE:HG23	1.92	0.52
2:B:296:TYR:HD2	13:M:186:ILE:HG13	1.73	0.52
2:B:727:LEU:HD21	2:B:788:ARG:HE	1.73	0.52
2:B:884:VAL:HG12	2:B:898:VAL:HB	1.91	0.52
2:B:958:MET:HG3	2:B:1018:PHE:CE2	2.44	0.52
4:D:1:MET:HG3	4:D:2:LYS:H	1.73	0.52
11:K:68:GLU:HG3	11:K:69:ASP:H	1.74	0.52
18:R:91:SER:HB3	18:R:101:THR:HG21	1.91	0.52
18:R:418:ALA:HA	18:R:429:ILE:O	2.09	0.52
18:R:422:PRO:HB2	18:R:634:PHE:CZ	2.45	0.52
1:A:224:PRO:HA	1:A:227:THR:HG22	1.91	0.52
5:E:26:ARG:HH22	5:E:189:GLY:N	2.08	0.52
6:F:85:MET:HA	6:F:151:LEU:HD21	1.91	0.52
8:H:101:ALA:HB2	8:H:116:TYR:CE1	2.44	0.52
15:O:499:THR:HG21	16:P:312:PHE:CG	2.45	0.52
16:P:310:VAL:HB	17:Q:43:ILE:HD11	1.91	0.52
21:Y:18:DC:H2''	21:Y:19:DT:C5	2.45	0.52
1:A:628:ALA:HB1	1:A:675:HIS:CD2	2.45	0.52
1:A:643:ASN:HB2	1:A:651:PHE:CE2	2.45	0.52
1:A:1318:HIS:CD2	1:A:1321:GLU:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:490:GLN:H	2:B:490:GLN:CD	2.18	0.52
2:B:736:VAL:HG21	2:B:960:GLU:HG3	1.91	0.52
2:B:779:ASP:OD2	3:C:216:HIS:HB3	2.10	0.52
2:B:1084:MET:HE1	2:B:1121:ILE:N	2.25	0.52
3:C:173:GLY:C	3:C:175:GLN:H	2.16	0.52
10:J:7:CYS:SG	10:J:46:CYS:HA	2.49	0.52
13:M:91:ALA:CA	14:N:392:GLN:CD	2.83	0.52
18:R:273:GLN:HB2	19:S:277:UNK:N	2.25	0.52
1:A:235:LYS:HZ3	1:A:254:GLU:HG3	1.74	0.52
1:A:372:ARG:C	2:B:1050:PRO:HD2	2.35	0.52
1:A:975:VAL:CG2	1:A:976:ARG:H	2.08	0.52
2:B:285:VAL:O	2:B:288:GLU:HB3	2.10	0.52
2:B:621:ARG:HG3	2:B:645:LEU:HG	1.92	0.52
15:O:519:GLU:OE1	15:O:519:GLU:N	2.40	0.52
16:P:63:LEU:HA	16:P:71:LYS:O	2.08	0.52
18:R:289:SER:HB2	18:R:535:SER:HB3	1.92	0.52
18:R:506:GLY:HA2	18:R:509:SER:HB2	1.92	0.52
1:A:457:GLN:N	1:A:460:ASP:OD2	2.43	0.51
2:B:197:GLN:HE22	2:B:451:ARG:HD2	1.75	0.51
2:B:337:VAL:HG23	2:B:345:LYS:NZ	2.24	0.51
2:B:464:ILE:HG12	2:B:687:LEU:HD11	1.93	0.51
5:E:190:LEU:HD23	5:E:214:CYS:HB2	1.92	0.51
13:M:95:ARG:NH2	14:N:413:ASP:O	2.43	0.51
18:R:467:ARG:HD3	18:R:602:LEU:HG	1.92	0.51
18:R:509:SER:HB3	18:R:519:LEU:HD21	1.92	0.51
1:A:277:SER:HB3	1:A:278:PRO:HD2	1.91	0.51
1:A:656:GLY:H	1:A:944:ASN:HD22	1.58	0.51
1:A:1157:VAL:HG11	1:A:1308:GLY:HA3	1.92	0.51
2:B:529:ILE:HD11	2:B:575:PHE:HE1	1.74	0.51
5:E:100:ILE:HG21	5:E:127:ILE:HG13	1.92	0.51
15:O:53:VAL:O	15:O:58:GLY:N	2.43	0.51
1:A:413:ARG:O	1:A:416:LEU:N	2.43	0.51
1:A:610:PHE:CE1	1:A:664:MET:HE1	2.46	0.51
1:A:1347:GLY:O	1:A:1348:MET:HG2	2.10	0.51
2:B:666:ILE:HA	2:B:670:MET:SD	2.50	0.51
2:B:800:ASN:HA	2:B:855:PRO:HG3	1.92	0.51
2:B:971:GLY:HA2	10:J:51:LEU:CD1	2.39	0.51
4:D:102:SER:O	4:D:106:LEU:N	2.43	0.51
5:E:118:PRO:O	5:E:122:LYS:N	2.44	0.51
15:O:190:LEU:HB3	15:O:194:LEU:HG	1.91	0.51
15:O:255:LYS:HB3	15:O:256:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:106:TRP:NE1	16:P:145:ARG:HA	2.24	0.51
18:R:401:THR:HG22	18:R:403:GLY:H	1.76	0.51
18:R:468:ILE:HG13	18:R:610:LEU:HD11	1.92	0.51
18:R:510:SER:OG	18:R:512:GLU:OE2	2.28	0.51
19:S:425:MET:HG2	19:S:429:TYR:CE2	2.45	0.51
19:S:444:GLN:HE22	19:S:490:LYS:HZ2	1.58	0.51
1:A:926:MET:HE3	1:A:930:ALA:HA	1.91	0.51
1:A:1145:LEU:HA	1:A:1309:VAL:HA	1.93	0.51
1:A:1166:LEU:HD23	1:A:1166:LEU:C	2.35	0.51
2:B:735:MET:HE2	2:B:754:ASN:ND2	2.26	0.51
3:C:85:PHE:CZ	3:C:98:ALA:HB2	2.45	0.51
3:C:251:PHE:CD2	3:C:255:VAL:HG21	2.45	0.51
8:H:95:TYR:HE2	8:H:97:MET:HE2	1.76	0.51
16:P:59:ASN:CG	16:P:80:ALA:HB1	2.35	0.51
18:R:478:PHE:O	18:R:599:PRO:HB3	2.10	0.51
19:S:506:GLN:O	19:S:510:LYS:CB	2.57	0.51
1:A:11:LYS:HG3	2:B:1117:ILE:HG21	1.93	0.51
1:A:48:PRO:C	1:A:49:LYS:HG2	2.35	0.51
1:A:329:SER:HA	1:A:351:ARG:CZ	2.39	0.51
2:B:383:LEU:HB3	2:B:442:TRP:HH2	1.75	0.51
2:B:536:LEU:HD22	2:B:571:PHE:CD1	2.45	0.51
12:L:53:HIS:CD2	12:L:54:ARG:H	2.28	0.51
13:M:135:LYS:O	13:M:138:SER:OG	2.20	0.51
13:M:159:TYR:CD1	13:M:172:PRO:HA	2.45	0.51
15:O:188:SER:HG	15:O:191:PHE:HD1	1.55	0.51
18:R:138:LYS:HZ1	18:R:173:LEU:C	2.19	0.51
1:A:528:ARG:HH12	6:F:118:LEU:HB2	1.76	0.51
1:A:589:HIS:HA	11:K:104:ARG:HH21	1.74	0.51
1:A:594:PRO:HB3	8:H:79:TRP:CD1	2.45	0.51
1:A:734:ALA:HB2	1:A:773:VAL:HG21	1.92	0.51
2:B:832:VAL:HB	12:L:60:ARG:HA	1.93	0.51
3:C:33:VAL:HG21	11:K:126:ASP:OD2	2.11	0.51
3:C:270:ALA:O	3:C:271:ARG:HG2	2.10	0.51
4:D:126:GLN:O	4:D:127:LEU:CG	2.49	0.51
7:G:88:TRP:HA	7:G:146:ILE:HD12	1.93	0.51
10:J:53:HIS:ND1	10:J:53:HIS:O	2.44	0.51
21:Y:55:DT:H2"	21:Y:56:DG:H8	1.70	0.51
1:A:974:LEU:C	1:A:975:VAL:HG12	2.36	0.51
2:B:279:TYR:OH	2:B:358:MET:HG2	2.11	0.51
2:B:755:ALA:HA	10:J:48:ARG:HH12	1.75	0.51
2:B:758:ALA:HA	2:B:1019:PHE:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:41:ASP:HA	5:E:44:ALA:HB3	1.92	0.51
10:J:1:MET:O	10:J:53:HIS:NE2	2.43	0.51
13:M:88:PHE:HB2	14:N:395:ILE:HG23	1.92	0.51
15:O:590:PHE:O	15:O:593:GLU:N	2.44	0.51
16:P:82:LYS:O	16:P:86:MET:HG2	2.10	0.51
18:R:554:GLU:HG2	18:R:582:LEU:HD22	1.92	0.51
1:A:38:ASP:OD1	1:A:38:ASP:N	2.38	0.51
1:A:38:ASP:HB3	1:A:290:THR:OG1	2.10	0.51
1:A:327:ILE:CB	1:A:353:PHE:CE2	2.94	0.51
1:A:1164:THR:OG1	1:A:1272:VAL:HG12	2.09	0.51
1:A:1382:SER:HA	1:A:1406:ASP:OD1	2.11	0.51
2:B:45:TRP:HA	2:B:676:GLU:OE2	2.11	0.51
2:B:214:GLY:HA3	2:B:234:ILE:CG2	2.41	0.51
2:B:230:LYS:HD3	2:B:334:HIS:HE1	1.76	0.51
2:B:767:ILE:HG22	2:B:768:GLU:N	2.26	0.51
5:E:153:HIS:CD2	5:E:198:ILE:HG12	2.46	0.51
7:G:95:GLU:HG3	7:G:96:GLY:H	1.75	0.51
15:O:480:TYR:HA	15:O:483:LEU:HB3	1.92	0.51
15:O:507:LEU:HD21	15:O:536:THR:HG23	1.91	0.51
15:O:602:LEU:HD11	15:O:623:GLU:HG2	1.91	0.51
16:P:266:GLU:O	16:P:269:LEU:HB3	2.10	0.51
18:R:104:ALA:HA	18:R:107:TRP:HD1	1.76	0.51
18:R:186:ALA:HA	18:R:189:LEU:HD12	1.93	0.51
1:A:504:VAL:O	1:A:507:PRO:HD2	2.11	0.51
2:B:204:ARG:HH22	2:B:602:ALA:HB1	1.76	0.51
2:B:558:ASN:HD21	2:B:603:THR:HG22	1.76	0.51
3:C:32:ASN:O	3:C:33:VAL:HG23	2.10	0.51
4:D:11:LEU:HB3	7:G:2:PHE:O	2.11	0.51
13:M:230:SER:C	13:M:234:HIS:HD1	2.18	0.51
15:O:267:PRO:HD3	15:O:273:ILE:CG2	2.40	0.51
15:O:519:GLU:HA	15:O:522:ILE:HB	1.93	0.51
18:R:498:LEU:HD13	18:R:519:LEU:HB2	1.92	0.51
1:A:753:GLN:O	1:A:755:GLY:N	2.43	0.51
1:A:1411:VAL:HG21	2:B:1071:ILE:HD12	1.92	0.51
2:B:780:ARG:CZ	3:C:217:ALA:CB	2.85	0.51
2:B:908:LEU:HA	2:B:922:CYS:SG	2.51	0.51
2:B:1019:PHE:HE1	10:J:44:TYR:OH	1.94	0.51
7:G:147:ARG:NH2	7:G:204:GLY:O	2.44	0.51
15:O:190:LEU:HD21	15:O:199:TYR:CE1	2.46	0.51
15:O:353:GLU:HA	15:O:357:PRO:CD	2.21	0.51
16:P:81:GLN:O	16:P:85:THR:OG1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:191:LEU:HB2	18:R:195:LYS:HD3	1.92	0.51
20:X:47:DA:C2'	20:X:48:DT:H71	2.40	0.51
1:A:714:ILE:HG13	2:B:962:ILE:HD12	1.93	0.50
1:A:714:ILE:HD13	2:B:958:MET:HE3	1.92	0.50
1:A:723:LEU:O	1:A:727:LYS:HB2	2.11	0.50
1:A:934:ASN:ND2	1:A:937:ARG:HE	2.09	0.50
1:A:1146:VAL:HG23	1:A:1308:GLY:O	2.11	0.50
2:B:109:LYS:HG3	2:B:111:TYR:O	2.11	0.50
2:B:771:LEU:O	2:B:923:GLY:N	2.35	0.50
8:H:115:TYR:HE1	8:H:124:ARG:HG3	1.76	0.50
15:O:578:ARG:HA	15:O:648:TRP:HZ3	1.77	0.50
18:R:213:TRP:CD1	18:R:287:PRO:HG3	2.46	0.50
1:A:98:ALA:O	1:A:101:GLN:N	2.45	0.50
1:A:270:PRO:HG3	2:B:1046:LEU:CD1	2.41	0.50
1:A:407:LYS:HG2	1:A:461:VAL:HG22	1.92	0.50
1:A:552:ALA:HB3	1:A:671:ASP:CB	2.41	0.50
1:A:773:VAL:O	1:A:777:VAL:HG23	2.11	0.50
1:A:1180:ASN:HB3	9:I:21:VAL:H	1.75	0.50
1:A:1386:LEU:HB3	1:A:1395:HIS:CD2	2.47	0.50
2:B:97:ASP:OD2	2:B:99:ARG:NH1	2.45	0.50
2:B:371:TYR:HB2	2:B:492:SER:OG	2.10	0.50
2:B:454:VAL:HG13	2:B:455:THR:HG23	1.93	0.50
2:B:629:LYS:O	2:B:635:LEU:HB2	2.11	0.50
2:B:849:THR:HG22	2:B:865:GLN:O	2.11	0.50
5:E:152:LYS:HE2	5:E:154:ILE:HD11	1.94	0.50
15:O:595:LEU:HD12	15:O:598:GLU:HG3	1.93	0.50
16:P:64:VAL:HB	16:P:71:LYS:HB2	1.92	0.50
1:A:37:ARG:HG2	1:A:38:ASP:OD1	2.11	0.50
1:A:235:LYS:HE3	1:A:254:GLU:HG3	1.91	0.50
1:A:548:GLU:OE2	1:A:672:GLY:O	2.28	0.50
1:A:1445:ARG:HG3	1:A:1447:LEU:HD12	1.93	0.50
2:B:263:LEU:HD11	2:B:296:TYR:HA	1.93	0.50
2:B:279:TYR:HE1	2:B:358:MET:HA	1.75	0.50
2:B:415:GLU:OE1	2:B:415:GLU:N	2.45	0.50
2:B:662:TYR:HE1	2:B:677:PRO:HG3	1.75	0.50
2:B:731:PRO:HB2	2:B:750:PRO:HG2	1.92	0.50
2:B:1036:HIS:CE1	2:B:1054:ARG:HA	2.46	0.50
4:D:126:GLN:O	4:D:127:LEU:O	2.30	0.50
7:G:53:THR:CG2	7:G:71:THR:HG22	2.37	0.50
7:G:112:GLN:NE2	7:G:115:LEU:HD22	2.26	0.50
15:O:69:VAL:HG22	15:O:122:TYR:CG	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:251:LYS:O	15:O:255:LYS:N	2.38	0.50
18:R:168:LEU:HB2	18:R:170:ILE:HD11	1.94	0.50
18:R:281:GLU:OE1	18:R:281:GLU:N	2.40	0.50
1:A:200:GLU:HG2	15:O:515:LYS:HD3	1.93	0.50
1:A:476:ARG:NH1	1:A:477:GLN:HB3	2.26	0.50
1:A:949:ASN:OD1	1:A:950:GLN:N	2.45	0.50
1:A:1022:LEU:HA	1:A:1025:SER:HB3	1.93	0.50
2:B:1004:LEU:HD21	2:B:1019:PHE:HE2	1.76	0.50
2:B:1107:CYS:SG	2:B:1109:THR:HG22	2.52	0.50
8:H:81:PRO:HD2	11:K:108:TYR:OH	2.12	0.50
14:N:395:ILE:HD11	14:N:408:LEU:HD21	1.92	0.50
15:O:78:GLU:O	15:O:82:LYS:NZ	2.45	0.50
15:O:483:LEU:O	15:O:487:LEU:N	2.44	0.50
15:O:643:ARG:NH2	17:Q:51:GLU:OE1	2.45	0.50
18:R:523:MET:O	18:R:527:LYS:HA	2.12	0.50
1:A:153:ARG:HG3	1:A:160:LEU:HB3	1.94	0.50
1:A:224:PRO:HD2	1:A:316:TRP:HH2	1.76	0.50
1:A:427:HIS:NE2	1:A:492:ILE:HG21	2.26	0.50
1:A:642:PRO:HB2	1:A:644:GLU:H	1.77	0.50
1:A:705:LEU:HD22	2:B:761:SER:HB2	1.91	0.50
1:A:733:ILE:HD12	1:A:736:HIS:CE1	2.47	0.50
1:A:1452:SER:HA	4:D:120:LYS:NZ	2.27	0.50
2:B:58:VAL:HA	2:B:60:GLN:OE1	2.12	0.50
2:B:109:LYS:HG3	2:B:111:TYR:N	2.21	0.50
2:B:884:VAL:HG23	12:L:58:LYS:HB3	1.94	0.50
4:D:65:TYR:OH	4:D:69:ASN:ND2	2.36	0.50
5:E:59:SER:HA	5:E:81:GLU:HA	1.94	0.50
14:N:380:MET:SD	14:N:421:GLN:NE2	2.84	0.50
15:O:73:ARG:HD3	15:O:121:TYR:OH	2.11	0.50
16:P:106:TRP:CG	16:P:107:SER:N	2.79	0.50
18:R:287:PRO:HD2	18:R:290:PHE:HE1	1.76	0.50
1:A:38:ASP:C	1:A:40:PHE:H	2.18	0.50
1:A:236:SER:H	1:A:252:ARG:HD2	1.76	0.50
1:A:272:VAL:HB	1:A:281:ASN:HB3	1.92	0.50
2:B:152:MET:HE1	2:B:384:ILE:HG21	1.93	0.50
2:B:354:ARG:CZ	2:B:549:LEU:HD13	2.40	0.50
2:B:778:ILE:CD1	2:B:906:PRO:HG2	2.41	0.50
3:C:14:ASN:ND2	3:C:295:ARG:HH12	2.08	0.50
4:D:146:ASP:O	4:D:150:ILE:HG12	2.12	0.50
5:E:2:ASP:HA	5:E:5:ASN:HB2	1.94	0.50
7:G:203:ASP:O	7:G:205:MET:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:256:GLN:HA	18:R:259:LEU:HB3	1.93	0.50
1:A:746:ASN:OD1	1:A:747:LYS:N	2.45	0.50
2:B:143:MET:CG	19:S:399:GLU:HB2	2.42	0.50
2:B:775:LYS:HG3	2:B:925:ILE:HG22	1.93	0.50
7:G:54:VAL:HA	7:G:70:VAL:HG12	1.93	0.50
7:G:88:TRP:O	7:G:99:VAL:HA	2.12	0.50
13:M:121:ILE:N	13:M:148:LEU:O	2.29	0.50
13:M:255:PHE:O	13:M:259:ILE:HG12	2.11	0.50
15:O:282:ILE:H	15:O:282:ILE:HD12	1.77	0.50
16:P:218:THR:HG23	16:P:219:GLN:H	1.77	0.50
1:A:100:ILE:HD11	1:A:178:ILE:HG21	1.94	0.50
1:A:520:HIS:CE1	2:B:1062:LEU:HD21	2.47	0.50
1:A:610:PHE:CD1	1:A:664:MET:HE1	2.46	0.50
1:A:1286:ARG:N	1:A:1290:LYS:O	2.44	0.50
2:B:362:ASN:ND2	2:B:365:MET:SD	2.76	0.50
2:B:553:TYR:HD1	2:B:597:MET:HA	1.77	0.50
2:B:933:PHE:CZ	2:B:934:ASN:O	2.64	0.50
3:C:112:MET:C	3:C:113:LEU:HD12	2.37	0.50
10:J:12:LYS:O	10:J:14:VAL:HG23	2.12	0.50
11:K:138:LYS:O	11:K:142:MET:N	2.41	0.50
18:R:194:LYS:O	18:R:197:LYS:HB3	2.11	0.50
18:R:468:ILE:O	18:R:472:ILE:N	2.43	0.50
18:R:502:ALA:O	18:R:506:GLY:N	2.36	0.50
20:X:6:DA:N1	20:X:7:DA:C6	2.80	0.50
1:A:552:ALA:HB3	1:A:671:ASP:HB3	1.92	0.50
1:A:1078:TYR:O	1:A:1081:ALA:N	2.45	0.50
1:A:1224:ILE:HG12	1:A:1226:GLY:H	1.77	0.50
2:B:424:VAL:O	18:R:92:TYR:OH	2.25	0.50
3:C:61:THR:HA	3:C:298:PHE:HZ	1.77	0.50
3:C:209:ILE:HG13	3:C:210:LEU:N	2.26	0.50
7:G:203:ASP:OD1	7:G:204:GLY:N	2.41	0.50
15:O:125:GLU:HB3	15:O:128:HIS:HB2	1.94	0.50
17:Q:36:PHE:N	17:Q:37:PRO:HD2	2.26	0.50
18:R:172:GLU:HG3	18:R:506:GLY:HA3	1.94	0.50
18:R:424:ARG:HG2	21:Y:46:DA:OP1	2.12	0.50
21:Y:59:DG:H1'	21:Y:60:DA:C8	2.46	0.50
1:A:278:PRO:HD3	2:B:852:ALA:HB1	1.94	0.49
1:A:376:SER:HB2	2:B:1060:LEU:HD12	1.93	0.49
1:A:424:PRO:HG2	1:A:444:LEU:CD2	2.41	0.49
2:B:100:VAL:HG12	2:B:129:ILE:HD13	1.94	0.49
2:B:543:LEU:HD22	13:M:158:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:ILE:HG23	3:C:317:SER:OG	2.12	0.49
3:C:197:ARG:HB3	3:C:198:PRO:CD	2.41	0.49
13:M:117:HIS:HB2	13:M:119:TRP:HE1	1.76	0.49
13:M:247:TRP:CH2	13:M:249:GLU:HB2	2.47	0.49
15:O:273:ILE:HG23	15:O:274:VAL:O	2.11	0.49
16:P:298:LYS:HG2	16:P:298:LYS:O	2.11	0.49
1:A:37:ARG:HG2	1:A:38:ASP:H	1.76	0.49
1:A:73:ASN:OD1	1:A:74:LEU:N	2.45	0.49
1:A:903:THR:HA	1:A:914:PHE:O	2.12	0.49
5:E:31:THR:HG23	5:E:34:GLU:H	1.76	0.49
13:M:159:TYR:CD2	13:M:170:LEU:HD21	2.47	0.49
15:O:95:LEU:HD21	15:O:120:TYR:CZ	2.47	0.49
18:R:398:ALA:HA	18:R:484:GLN:H	1.77	0.49
1:A:351:ARG:HD2	1:A:355:GLN:HE22	1.78	0.49
1:A:733:ILE:O	1:A:737:LYS:HG3	2.11	0.49
1:A:1163:LYS:HG3	1:A:1164:THR:N	2.21	0.49
1:A:1165:LEU:HD22	1:A:1198:LEU:HD21	1.93	0.49
2:B:141:ILE:HG23	2:B:142:ILE:N	2.26	0.49
2:B:417:ASP:C	2:B:419:LEU:N	2.70	0.49
2:B:538:VAL:HB	2:B:563:GLY:HA3	1.94	0.49
2:B:724:LEU:HD21	2:B:726:TYR:CZ	2.48	0.49
5:E:96:PHE:O	5:E:100:ILE:HG12	2.12	0.49
5:E:112:TYR:CD2	5:E:116:ILE:HG12	2.48	0.49
6:F:97:ARG:O	6:F:101:ILE:HG12	2.12	0.49
7:G:21:ASP:OD1	7:G:22:THR:N	2.42	0.49
14:N:276:ALA:HB1	14:N:280:LEU:HD23	1.94	0.49
19:S:430:LYS:O	19:S:434:MET:HG2	2.13	0.49
19:S:470:GLU:O	19:S:474:ARG:CB	2.58	0.49
21:Y:52:DA:H2'	21:Y:53:DT:O5'	2.11	0.49
1:A:937:ARG:HG3	1:A:938:SER:N	2.27	0.49
2:B:490:GLN:OE1	2:B:490:GLN:N	2.45	0.49
8:H:123:MET:HE2	8:H:125:LEU:HD23	1.94	0.49
9:I:34:PRO:O	9:I:35:ILE:HG13	2.13	0.49
14:N:384:LYS:HA	14:N:416:ILE:HD11	1.93	0.49
15:O:140:ILE:O	15:O:144:MET:N	2.42	0.49
15:O:590:PHE:O	15:O:591:LYS:C	2.54	0.49
16:P:15:ALA:HA	16:P:55:LEU:HD11	1.93	0.49
16:P:211:ASN:OD1	16:P:212:VAL:N	2.46	0.49
18:R:440:LEU:O	18:R:447:MET:HB2	2.12	0.49
1:A:298:LEU:HD21	1:A:315:HIS:CE1	2.48	0.49
1:A:373:VAL:N	2:B:1060:LEU:O	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:ASP:CG	1:A:789:ASN:HB2	2.38	0.49
1:A:1434:THR:HG23	7:G:56:GLU:HA	1.95	0.49
2:B:454:VAL:HG13	2:B:455:THR:H	1.77	0.49
2:B:529:ILE:HD13	2:B:584:VAL:HG11	1.94	0.49
2:B:540:ASP:OD1	2:B:541:ILE:N	2.45	0.49
2:B:1004:LEU:HD21	2:B:1019:PHE:CE2	2.47	0.49
2:B:1126:LYS:O	2:B:1129:PHE:N	2.45	0.49
8:H:10:PHE:CE2	8:H:38:LEU:HD13	2.45	0.49
15:O:288:MET:O	15:O:291:ARG:HG2	2.13	0.49
15:O:554:THR:CG2	15:O:561:ARG:NE	2.74	0.49
16:P:292:SER:OG	16:P:293:ILE:N	2.43	0.49
18:R:268:ALA:O	18:R:272:VAL:HB	2.12	0.49
18:R:290:PHE:CE1	18:R:495:PRO:HG3	2.47	0.49
1:A:1217:ILE:HG22	1:A:1218:GLN:N	2.27	0.49
2:B:59:LYS:O	2:B:63:ASP:N	2.42	0.49
2:B:615:VAL:HG12	2:B:620:SER:HA	1.94	0.49
2:B:961:LEU:HD22	2:B:1018:PHE:CZ	2.47	0.49
3:C:75:VAL:HG12	3:C:320:ILE:HD12	1.95	0.49
3:C:224:THR:CB	10:J:10:CYS:SG	2.98	0.49
14:N:364:ARG:HB3	14:N:372:SER:HB3	1.93	0.49
15:O:260:SER:HB3	15:O:264:THR:OG1	2.12	0.49
1:A:403:THR:HG21	1:A:431:ASN:HD21	1.78	0.49
1:A:498:PHE:CE2	1:A:519:LEU:HD13	2.47	0.49
1:A:1123:VAL:N	1:A:1124:PRO:HD2	2.28	0.49
2:B:251:ILE:HG21	2:B:256:VAL:HG23	1.94	0.49
3:C:32:ASN:CG	3:C:33:VAL:H	2.21	0.49
3:C:80:ALA:HA	3:C:208:CYS:HA	1.94	0.49
5:E:22:MET:HE1	5:E:135:PHE:CZ	2.48	0.49
5:E:188:LEU:HD23	5:E:190:LEU:HD11	1.94	0.49
14:N:402:ASP:O	14:N:405:SER:HB2	2.13	0.49
15:O:516:LEU:HA	15:O:566:PHE:O	2.13	0.49
17:Q:1072:UNK:O	17:Q:1074:UNK:N	2.46	0.49
19:S:451:ARG:HG3	19:S:452:LYS:H	1.78	0.49
21:Y:13:DT:H2'	21:Y:14:DT:C6	2.47	0.49
1:A:214:TYR:CD2	1:A:215:VAL:HG13	2.48	0.49
1:A:285:LEU:O	1:A:288:LYS:N	2.46	0.49
1:A:487:SER:OG	1:A:536:GLY:HA2	2.13	0.49
4:D:14:TYR:HD2	4:D:15:GLU:HG2	1.77	0.49
13:M:149:LYS:CB	13:M:182:PHE:HE2	2.25	0.49
13:M:159:TYR:C	13:M:173:ILE:CD1	2.86	0.49
15:O:595:LEU:HD21	15:O:630:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:6:ASN:ND2	18:R:30:VAL:HG21	2.27	0.49
18:R:394:GLN:HB3	21:Y:49:DA:H4'	1.94	0.49
1:A:213:ARG:HA	1:A:216:LYS:HB2	1.95	0.49
1:A:481:HIS:HA	1:A:1095:GLN:OE1	2.13	0.49
1:A:497:THR:HG23	1:A:499:ARG:HG3	1.95	0.49
1:A:557:PHE:HA	1:A:701:CYS:SG	2.53	0.49
1:A:633:PHE:CZ	1:A:643:ASN:HB3	2.48	0.49
2:B:539:GLU:O	2:B:563:GLY:HA2	2.13	0.49
2:B:652:ASN:O	2:B:655:ASN:HB3	2.12	0.49
2:B:936:GLN:HB2	2:B:938:ILE:CD1	2.42	0.49
2:B:1106:TRP:HE1	7:G:162:SER:CA	2.26	0.49
5:E:64:PRO:HD3	5:E:77:SER:CA	2.42	0.49
7:G:124:GLU:O	7:G:126:SER:N	2.44	0.49
16:P:106:TRP:CG	16:P:107:SER:H	2.31	0.49
18:R:158:GLY:HA3	18:R:515:LEU:HD11	1.95	0.49
1:A:618:HIS:CE1	1:A:619:ASN:OD1	2.66	0.49
2:B:546:SER:HB2	14:N:391:LEU:HD21	1.68	0.49
2:B:671:THR:HG21	2:B:672:HIS:HE1	1.76	0.49
2:B:1004:LEU:HD12	2:B:1017:ILE:HB	1.95	0.49
3:C:228:ARG:HH21	3:C:299:ILE:HG21	1.78	0.49
11:K:85:ASP:OD1	11:K:108:TYR:HB2	2.12	0.49
13:M:142:GLY:HA2	13:M:185:TYR:CZ	2.48	0.49
18:R:216:GLU:OE2	18:R:498:LEU:HB2	2.13	0.49
18:R:218:ARG:CZ	21:Y:53:DT:H5'	2.43	0.49
20:X:48:DT:C4	20:X:49:DA:N6	2.81	0.49
2:B:417:ASP:OD1	2:B:418:ALA:N	2.46	0.48
2:B:721:ILE:HG12	2:B:899:LEU:HD22	1.95	0.48
2:B:821:HIS:CE1	2:B:824:LEU:HD22	2.48	0.48
3:C:227:TYR:HB3	3:C:300:PHE:HD1	1.78	0.48
8:H:12:VAL:HG22	8:H:26:ILE:HD11	1.94	0.48
15:O:285:ASP:O	15:O:288:MET:HB2	2.13	0.48
16:P:173:GLU:HA	16:P:175:ILE:HD12	1.95	0.48
16:P:267:SER:O	16:P:270:GLN:HB3	2.13	0.48
18:R:191:LEU:HD21	18:R:239:ARG:HE	1.77	0.48
1:A:1154:ALA:HB1	1:A:1283:ILE:HD12	1.95	0.48
2:B:61:HIS:O	2:B:155:MET:HE1	2.13	0.48
2:B:97:ASP:OD1	2:B:98:ILE:N	2.46	0.48
2:B:377:LEU:HD11	2:B:520:ILE:HD13	1.94	0.48
2:B:501:ASP:OD2	2:B:513:ASN:ND2	2.46	0.48
2:B:822:GLN:O	2:B:824:LEU:N	2.46	0.48
3:C:229:LEU:HB2	3:C:293:ARG:NH1	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:132:VAL:HA	4:D:135:TYR:HB3	1.95	0.48
5:E:180:ARG:C	5:E:182:ASP:H	2.19	0.48
6:F:79:ARG:HH22	6:F:145:ASP:HB2	1.78	0.48
6:F:125:LEU:HD12	6:F:130:ILE:HD12	1.94	0.48
7:G:115:LEU:HD21	7:G:130:TRP:CZ2	2.49	0.48
7:G:157:ASP:OD1	7:G:158:VAL:N	2.40	0.48
15:O:172:GLU:O	15:O:176:SER:HB2	2.12	0.48
15:O:214:LEU:HD11	15:O:249:PHE:HE1	1.79	0.48
15:O:579:GLN:O	15:O:583:TRP:N	2.46	0.48
16:P:240:ILE:HD13	16:P:243:LEU:HD22	1.95	0.48
18:R:274:LYS:O	18:R:275:PHE:CG	2.65	0.48
19:S:381:VAL:HG22	19:S:383:ARG:N	2.27	0.48
19:S:434:MET:HE3	19:S:479:PRO:HB3	1.95	0.48
20:X:62:DG:N1	21:Y:2:DC:N3	2.61	0.48
21:Y:9:DT:H2"	21:Y:10:DC:C6	2.47	0.48
1:A:892:SER:O	1:A:1380:ARG:NH2	2.46	0.48
1:A:1384:LEU:HD12	1:A:1413:GLU:OE2	2.13	0.48
2:B:204:ARG:NH2	2:B:558:ASN:HA	2.28	0.48
7:G:55:GLU:N	7:G:55:GLU:OE1	2.47	0.48
8:H:96:VAL:HG12	8:H:143:LEU:CD1	2.40	0.48
14:N:400:ALA:HB3	14:N:405:SER:HA	1.94	0.48
16:P:201:GLY:N	16:P:202:PRO:CD	2.76	0.48
18:R:191:LEU:HD23	18:R:239:ARG:HH21	1.78	0.48
18:R:195:LYS:O	18:R:198:VAL:HB	2.13	0.48
1:A:96:PHE:O	1:A:99:THR:N	2.46	0.48
1:A:354:CYS:HG	1:A:1393:THR:HG1	1.58	0.48
1:A:362:GLY:O	1:A:367:ASN:ND2	2.47	0.48
1:A:626:LEU:HD23	1:A:627:ASP:N	2.29	0.48
2:B:252:PRO:HD2	2:B:255:ILE:HD12	1.95	0.48
2:B:554:GLY:HA2	2:B:564:SER:HA	1.94	0.48
2:B:555:VAL:HG12	2:B:564:SER:N	2.27	0.48
2:B:762:TYR:HE2	2:B:926:VAL:HG21	1.78	0.48
3:C:260:GLU:HB2	3:C:263:ASP:HB2	1.95	0.48
5:E:41:ASP:O	5:E:45:LYS:N	2.46	0.48
7:G:110:ILE:O	7:G:110:ILE:HG13	2.13	0.48
10:J:57:ILE:O	10:J:61:LEU:HG	2.13	0.48
13:M:72:GLU:HB2	14:N:364:ARG:NE	2.27	0.48
13:M:113:LYS:HE2	13:M:118:LEU:HB2	1.95	0.48
14:N:308:GLN:HB2	14:N:417:VAL:HG12	1.96	0.48
15:O:318:LEU:HD11	15:O:368:ARG:HD3	1.95	0.48
18:R:214:MET:SD	18:R:265:THR:HG22	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:O	1:A:371:LYS:HG3	2.13	0.48
1:A:373:VAL:CG1	1:A:374:ASP:H	2.23	0.48
1:A:415:LYS:O	1:A:419:LEU:N	2.45	0.48
1:A:543:THR:HB	1:A:550:ILE:HB	1.96	0.48
1:A:608:GLN:O	1:A:611:SER:N	2.47	0.48
1:A:704:PHE:CZ	1:A:708:ARG:HD2	2.49	0.48
1:A:1064:GLU:O	1:A:1067:VAL:N	2.44	0.48
2:B:525:GLU:HG3	2:B:526:GLU:H	1.78	0.48
2:B:848:PRO:HB2	2:B:851:SER:HB3	1.94	0.48
3:C:218:LYS:HE2	12:L:69:ALA:O	2.14	0.48
4:D:103:PHE:O	4:D:106:LEU:HB3	2.13	0.48
7:G:30:LEU:HB3	7:G:48:ILE:HG13	1.96	0.48
13:M:90:TYR:O	14:N:392:GLN:HB2	2.13	0.48
13:M:117:HIS:HD1	13:M:119:TRP:CD1	2.32	0.48
15:O:32:MET:C	15:O:34:ILE:H	2.21	0.48
18:R:213:TRP:HB3	18:R:285:ALA:HB1	1.95	0.48
18:R:392:THR:O	18:R:488:GLY:CA	2.61	0.48
1:A:636:PRO:HG3	1:A:646:SER:N	2.27	0.48
1:A:714:ILE:HG12	2:B:958:MET:HG2	1.95	0.48
2:B:415:GLU:CG	2:B:416:TYR:H	2.13	0.48
2:B:591:TYR:HB2	2:B:656:ASP:HB2	1.95	0.48
2:B:611:PRO:HG3	2:B:648:TYR:HE1	1.78	0.48
2:B:914:SER:O	2:B:915:ARG:CG	2.61	0.48
3:C:35:LYS:HD2	3:C:35:LYS:HA	1.45	0.48
13:M:113:LYS:HG2	13:M:117:HIS:O	2.14	0.48
13:M:253:GLU:O	13:M:257:ASP:N	2.40	0.48
14:N:288:GLN:HE21	14:N:292:ARG:HG3	1.79	0.48
15:O:352:VAL:O	15:O:355:LYS:HB3	2.14	0.48
15:O:495:VAL:O	15:O:495:VAL:HG22	2.13	0.48
21:Y:43:DA:C4	21:Y:44:DT:N3	2.81	0.48
21:Y:59:DG:H4'	21:Y:60:DA:H5'	1.96	0.48
1:A:18:PHE:CD1	2:B:1139:PRO:CA	2.94	0.48
1:A:493:ARG:HB2	1:A:499:ARG:NH2	2.28	0.48
2:B:788:ARG:HH22	3:C:93:GLN:NE2	2.10	0.48
2:B:1053:GLY:O	2:B:1057:ASP:O	2.31	0.48
5:E:82:PHE:HD1	5:E:111:VAL:HB	1.77	0.48
7:G:138:LEU:HD12	7:G:139:TYR:O	2.13	0.48
9:I:33:PHE:CD1	9:I:34:PRO:HD2	2.48	0.48
13:M:83:GLU:O	13:M:84:SER:O	2.32	0.48
13:M:148:LEU:HA	13:M:181:PRO:HA	1.96	0.48
15:O:599:ASN:O	15:O:602:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:12:PHE:HD1	18:R:25:CYS:HB3	1.79	0.48
18:R:434:GLU:HA	18:R:436:LYS:N	2.28	0.48
18:R:619:ALA:O	18:R:623:LYS:HB2	2.13	0.48
20:X:6:DA:C2	20:X:7:DA:C5	3.02	0.48
1:A:69:THR:O	7:G:163:PRO:HB2	2.13	0.48
1:A:236:SER:H	1:A:252:ARG:CD	2.27	0.48
1:A:284:ASP:OD2	1:A:352:GLY:HA3	2.14	0.48
1:A:1261:GLN:HG3	1:A:1265:ARG:HH12	1.79	0.48
1:A:1391:LYS:O	1:A:1395:HIS:ND1	2.46	0.48
2:B:112:LEU:HD23	2:B:113:THR:H	1.79	0.48
2:B:517:MET:SD	2:B:675:ILE:HD11	2.54	0.48
2:B:885:MET:HE2	2:B:897:LYS:HB3	1.95	0.48
2:B:933:PHE:CD1	2:B:933:PHE:C	2.91	0.48
3:C:224:THR:HG23	3:C:224:THR:O	2.14	0.48
5:E:1:MET:HG3	5:E:4:GLU:H	1.79	0.48
5:E:19:VAL:O	5:E:22:MET:HB3	2.14	0.48
15:O:650:VAL:HG13	15:O:651:PHE:N	2.29	0.48
16:P:90:GLU:HA	16:P:93:VAL:HB	1.96	0.48
18:R:198:VAL:O	18:R:202:ALA:N	2.39	0.48
1:A:1187:ARG:HA	1:A:1228:ASP:O	2.14	0.48
2:B:236:LYS:O	2:B:239:LYS:HB3	2.13	0.48
2:B:244:HIS:HE1	2:B:332:ILE:HB	1.78	0.48
2:B:849:THR:HG23	2:B:850:ASN:H	1.78	0.48
2:B:874:ARG:HG2	18:R:16:LEU:HD13	1.95	0.48
5:E:40:GLU:HG3	5:E:41:ASP:H	1.79	0.48
5:E:82:PHE:HE1	5:E:112:TYR:O	1.96	0.48
13:M:88:PHE:HB2	14:N:395:ILE:CG2	2.44	0.48
14:N:286:ASP:OD2	14:N:385:GLY:N	2.47	0.48
16:P:308:GLU:OE1	16:P:308:GLU:N	2.46	0.48
18:R:607:ASP:C	18:R:609:GLU:H	2.22	0.48
20:X:6:DA:C4	20:X:7:DA:C8	3.02	0.48
1:A:101:GLN:OE1	1:A:1402:TYR:OH	2.30	0.48
1:A:422:ASN:ND2	1:A:428:PRO:O	2.44	0.48
2:B:264:SER:O	9:I:10:ASN:HA	2.14	0.48
9:I:7:SER:OG	9:I:8:CYS:N	2.45	0.48
13:M:123:ILE:N	13:M:145:VAL:HG22	2.28	0.48
15:O:191:PHE:HD2	15:O:192:VAL:HG13	1.79	0.48
18:R:492:VAL:HG11	18:R:560:LEU:HD13	1.94	0.48
19:S:513:MET:HA	19:S:516:ILE:HD12	1.96	0.48
1:A:307:ILE:HB	1:A:311:ASN:OD1	2.14	0.47
1:A:559:THR:HG21	2:B:947:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:ASP:O	1:A:726:LYS:N	2.27	0.47
2:B:552:ASN:HD21	2:B:568:PRO:N	2.12	0.47
2:B:635:LEU:HD21	2:B:640:PHE:HE1	1.79	0.47
2:B:678:PHE:HB3	2:B:978:CYS:O	2.14	0.47
3:C:5:VAL:HG22	3:C:293:ARG:O	2.14	0.47
5:E:89:GLY:HA2	5:E:117:THR:HG21	1.95	0.47
5:E:185:ALA:HA	5:E:190:LEU:HD13	1.95	0.47
8:H:137:GLN:HB3	8:H:139:ASN:OD1	2.13	0.47
12:L:29:TYR:CB	12:L:58:LYS:HA	2.44	0.47
13:M:87:VAL:HA	14:N:396:ALA:HA	1.95	0.47
15:O:478:VAL:HB	15:O:480:TYR:CZ	2.49	0.47
18:R:439:ALA:HA	18:R:450:THR:N	2.28	0.47
20:X:24:DT:H2''	20:X:25:DT:O4'	2.14	0.47
1:A:235:LYS:HD2	1:A:252:ARG:NE	2.29	0.47
1:A:444:LEU:HD21	1:A:445:ARG:NH1	2.29	0.47
1:A:830:ARG:NH2	1:A:835:PHE:O	2.47	0.47
1:A:1088:ALA:HB2	1:A:1423:ILE:HD13	1.96	0.47
1:A:1202:ILE:O	1:A:1205:ILE:N	2.48	0.47
2:B:1147:PHE:CD2	7:G:10:LEU:HD11	2.45	0.47
4:D:148:LYS:O	4:D:152:GLU:HB2	2.13	0.47
7:G:126:SER:CB	7:G:139:TYR:HB2	2.42	0.47
13:M:113:LYS:HG3	13:M:116:SER:O	2.14	0.47
17:Q:41:LEU:HB3	17:Q:42:PRO:HD2	1.97	0.47
18:R:22:ASP:CG	18:R:23:LEU:N	2.71	0.47
18:R:24:VAL:HG23	18:R:30:VAL:O	2.13	0.47
19:S:453:GLN:O	19:S:457:LYS:CB	2.62	0.47
1:A:106:ILE:CD1	1:A:234:ILE:HG12	2.44	0.47
1:A:1425:THR:HG23	6:F:92:ARG:HB2	1.97	0.47
2:B:137:ARG:C	2:B:415:GLU:HB2	2.39	0.47
2:B:301:ALA:O	2:B:305:ILE:HG12	2.14	0.47
2:B:659:ILE:HG12	2:B:672:HIS:HB2	1.95	0.47
2:B:776:SER:HB3	3:C:217:ALA:HB2	1.95	0.47
3:C:32:ASN:OD1	3:C:33:VAL:N	2.48	0.47
7:G:88:TRP:CG	7:G:143:ASN:H	2.32	0.47
14:N:287:HIS:CD2	14:N:384:LYS:HE2	2.49	0.47
14:N:297:MET:HE3	14:N:305:MET:HG3	1.95	0.47
15:O:499:THR:HG23	16:P:312:PHE:CG	2.49	0.47
18:R:511:TYR:CE2	18:R:513:PRO:HG3	2.49	0.47
21:Y:42:DT:H2''	21:Y:43:DA:C8	2.50	0.47
1:A:226:LYS:HD3	15:O:547:GLU:HG3	1.96	0.47
1:A:974:LEU:O	1:A:975:VAL:CG1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1166:LEU:HD21	1:A:1268:PRO:HA	1.96	0.47
2:B:120:LEU:HD23	2:B:885:MET:SD	2.53	0.47
2:B:201:SER:HB2	2:B:374:ASN:O	2.14	0.47
2:B:306:GLY:HA3	2:B:324:ILE:HG23	1.96	0.47
3:C:122:ASP:OD1	3:C:123:ASP:N	2.47	0.47
3:C:152:ASP:HB2	3:C:155:GLU:CG	2.42	0.47
5:E:1:MET:HB3	5:E:4:GLU:HG2	1.96	0.47
15:O:121:TYR:CE1	15:O:210:PRO:HG2	2.49	0.47
18:R:387:SER:HA	18:R:579:PRO:HA	1.97	0.47
18:R:496:ILE:HD12	18:R:536:GLY:HA2	1.97	0.47
1:A:15:GLY:HA2	1:A:1407:ALA:HA	1.96	0.47
1:A:106:ILE:HG13	1:A:112:ALA:O	2.15	0.47
1:A:327:ILE:O	1:A:354:CYS:HB2	2.14	0.47
1:A:483:LEU:HD13	1:A:550:ILE:HG21	1.95	0.47
1:A:649:ASP:HB3	1:A:662:GLY:HA2	1.96	0.47
1:A:919:ASP:OD1	1:A:921:LEU:HD13	2.14	0.47
2:B:140:ASN:ND2	19:S:394:LYS:HG2	2.28	0.47
2:B:192:LYS:O	2:B:193:VAL:HG23	2.15	0.47
2:B:424:VAL:HA	18:R:93:ALA:HB2	1.95	0.47
2:B:465:SER:C	2:B:468:GLY:H	2.23	0.47
2:B:543:LEU:HD22	13:M:158:GLN:HE22	1.79	0.47
2:B:776:SER:CB	2:B:928:GLN:HE21	2.27	0.47
13:M:160:ALA:H	13:M:173:ILE:HG13	1.79	0.47
15:O:125:GLU:HB3	15:O:128:HIS:CB	2.45	0.47
15:O:362:ASN:O	15:O:477:TYR:HD1	1.97	0.47
16:P:33:GLN:HB2	16:P:72:PHE:HE2	1.78	0.47
16:P:142:PHE:HZ	20:X:30:DT:H4'	1.80	0.47
18:R:498:LEU:HD22	18:R:519:LEU:HD13	1.96	0.47
19:S:418:ASP:HB3	19:S:449:ARG:NH1	2.29	0.47
21:Y:2:DC:H2''	21:Y:3:DA:N7	2.30	0.47
1:A:1155:ARG:HA	1:A:1158:LYS:HB3	1.96	0.47
2:B:77:ILE:CD1	2:B:98:ILE:HG12	2.44	0.47
2:B:217:GLN:HE21	2:B:232:TYR:HB3	1.79	0.47
2:B:694:ASN:HD21	2:B:916:HIS:CE1	2.31	0.47
4:D:130:ASN:OD1	4:D:133:HIS:ND1	2.47	0.47
5:E:81:GLU:O	5:E:110:PHE:HA	2.14	0.47
15:O:171:VAL:O	15:O:175:LEU:HB3	2.14	0.47
16:P:27:ILE:HG21	16:P:35:GLU:HG3	1.97	0.47
17:Q:64:THR:O	17:Q:68:GLY:N	2.47	0.47
18:R:25:CYS:SG	18:R:28:CYS:HB3	2.55	0.47
18:R:91:SER:O	18:R:96:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:247:VAL:O	18:R:249:HIS:ND1	2.42	0.47
18:R:555:ALA:O	18:R:558:PRO:HD2	2.15	0.47
1:A:9:THR:OG1	4:D:1:MET:HE1	2.14	0.47
1:A:29:GLN:HE21	2:B:1100:LEU:HD13	1.80	0.47
1:A:114:LEU:HD12	1:A:115:LEU:N	2.29	0.47
1:A:476:ARG:HD3	1:A:510:ALA:HB2	1.95	0.47
1:A:591:ASP:OD1	1:A:591:ASP:N	2.47	0.47
1:A:1026:ARG:HH12	8:H:110:ASP:HB3	1.79	0.47
1:A:1150:ASP:OD1	1:A:1291:ARG:HD2	2.14	0.47
2:B:263:LEU:HD21	2:B:296:TYR:CD1	2.49	0.47
3:C:94:ASP:OD1	3:C:94:ASP:N	2.46	0.47
5:E:96:PHE:CZ	5:E:100:ILE:HD11	2.50	0.47
9:I:5:CYS:SG	9:I:9:ASN:N	2.88	0.47
13:M:112:TYR:HA	13:M:119:TRP:CD1	2.49	0.47
13:M:136:ALA:HA	13:M:140:TRP:O	2.15	0.47
15:O:92:LYS:NZ	17:Q:1082:UNK:HA	2.29	0.47
15:O:484:MET:HB2	15:O:485:PRO:HD3	1.95	0.47
16:P:219:GLN:NE2	16:P:222:LEU:HD12	2.29	0.47
18:R:122:SER:N	20:X:25:DT:OP1	2.47	0.47
18:R:155:TYR:CE1	20:X:12:DT:H3'	2.50	0.47
18:R:200:LYS:HG2	18:R:276:ARG:NH2	2.25	0.47
18:R:501:LEU:HA	18:R:563:PHE:CE2	2.49	0.47
19:S:444:GLN:HE22	19:S:490:LYS:HZ1	1.61	0.47
1:A:33:GLU:HB3	1:A:35:SER:OG	2.15	0.47
1:A:197:TRP:HH2	15:O:549:GLN:NE2	2.13	0.47
2:B:698:ARG:NH2	2:B:952:ARG:HG2	2.28	0.47
2:B:926:VAL:HB	2:B:931:MET:HE3	1.96	0.47
3:C:225:ALA:HB2	3:C:302:VAL:HG23	1.96	0.47
15:O:132:TYR:CD1	15:O:645:LEU:HD11	2.50	0.47
15:O:338:ASP:HB3	15:O:342:ALA:H	1.79	0.47
16:P:304:LYS:HG3	16:P:305:HIS:CD2	2.50	0.47
20:X:26:DT:H2'	20:X:27:DT:H71	1.97	0.47
21:Y:25:DC:H2''	21:Y:26:DA:C8	2.49	0.47
1:A:201:TRP:CD1	1:A:216:LYS:HZ3	2.33	0.47
1:A:566:HIS:HD2	1:A:568:ASP:HB3	1.80	0.47
1:A:919:ASP:OD2	1:A:1353:ARG:NH2	2.48	0.47
1:A:1202:ILE:CD1	1:A:1224:ILE:HD12	2.43	0.47
1:A:1369:LEU:CD2	1:A:1374:PHE:CD2	2.92	0.47
2:B:1105:GLY:O	2:B:1116:ILE:HD12	2.14	0.47
5:E:46:TYR:HA	5:E:57:MET:HE3	1.96	0.47
9:I:30:PRO:HD2	13:M:183:PHE:HZ	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:480:TYR:O	15:O:483:LEU:HB3	2.15	0.47
16:P:118:GLN:HA	16:P:121:VAL:HG22	1.96	0.47
18:R:587:THR:O	18:R:590:THR:OG1	2.28	0.47
1:A:842:PRO:C	1:A:844:SER:N	2.73	0.47
1:A:1275:LEU:O	1:A:1277:ASP:N	2.39	0.47
2:B:232:TYR:CE1	2:B:253:ILE:HD13	2.50	0.47
2:B:454:VAL:HG13	2:B:455:THR:N	2.30	0.47
2:B:531:LYS:O	2:B:535:VAL:HG23	2.15	0.47
2:B:675:ILE:HG13	2:B:676:GLU:N	2.29	0.47
2:B:929:GLU:HB3	3:C:69:ARG:HG2	1.97	0.47
3:C:78:VAL:HG23	3:C:209:ILE:O	2.15	0.47
4:D:126:GLN:HE21	7:G:85:VAL:HA	1.81	0.47
4:D:133:HIS:O	4:D:136:SER:OG	2.29	0.47
13:M:134:ASP:HA	13:M:137:GLU:HB2	1.97	0.47
15:O:80:VAL:HG21	15:O:87:ASP:OD1	2.14	0.47
19:S:425:MET:O	19:S:428:PHE:HB3	2.14	0.47
1:A:62:SER:OG	1:A:63:SER:N	2.48	0.46
1:A:424:PRO:HG3	1:A:431:ASN:HA	1.97	0.46
1:A:560:GLY:HA2	1:A:705:LEU:HD12	1.95	0.46
1:A:653:ILE:O	1:A:660:LEU:HB2	2.16	0.46
1:A:667:SER:OG	1:A:668:VAL:N	2.41	0.46
1:A:976:ARG:CG	1:A:1002:ARG:NH2	2.76	0.46
2:B:296:TYR:CE2	13:M:183:PHE:HD2	2.33	0.46
2:B:936:GLN:NE2	10:J:43:ARG:HH11	2.12	0.46
5:E:82:PHE:CD1	5:E:111:VAL:HB	2.50	0.46
8:H:100:THR:OG1	8:H:138:GLU:HA	2.15	0.46
15:O:468:LEU:HG	15:O:478:VAL:CG1	2.44	0.46
15:O:553:ARG:NH1	15:O:554:THR:HB	2.30	0.46
18:R:147:SER:O	18:R:150:LEU:N	2.33	0.46
18:R:610:LEU:HA	18:R:613:HIS:HB2	1.97	0.46
1:A:1317:ASN:O	1:A:1318:HIS:ND1	2.48	0.46
2:B:399:PHE:CE1	2:B:422:ILE:HG22	2.49	0.46
5:E:106:GLN:O	5:E:131:THR:N	2.43	0.46
7:G:58:GLN:N	7:G:67:TYR:O	2.48	0.46
8:H:130:ARG:NH2	8:H:134:ASN:OD1	2.48	0.46
13:M:227:LEU:HG	13:M:232:LEU:HA	1.98	0.46
15:O:126:GLY:C	15:O:128:HIS:N	2.72	0.46
15:O:190:LEU:HB3	15:O:194:LEU:N	2.31	0.46
15:O:350:GLU:OE1	15:O:482:LYS:HG3	2.14	0.46
20:X:7:DA:H2"	20:X:8:DC:C6	2.50	0.46
1:A:239:CYS:SG	1:A:240:GLU:OE1	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:LYS:C	1:A:667:SER:HG	2.23	0.46
1:A:704:PHE:HZ	1:A:708:ARG:HD2	1.80	0.46
1:A:800:LYS:HB3	2:B:951:SER:OG	2.15	0.46
1:A:1130:ILE:HG22	1:A:1371:ILE:HG21	1.96	0.46
1:A:1165:LEU:C	1:A:1167:SER:N	2.73	0.46
2:B:140:ASN:HD22	19:S:394:LYS:HA	1.81	0.46
2:B:191:GLU:OE1	2:B:191:GLU:N	2.48	0.46
2:B:757:VAL:HA	2:B:942:ILE:O	2.16	0.46
2:B:775:LYS:HA	2:B:778:ILE:HG22	1.97	0.46
5:E:181:ALA:HA	5:E:186:LEU:CG	2.45	0.46
7:G:114:MET:HG3	7:G:149:ARG:NH2	2.30	0.46
7:G:156:VAL:O	7:G:193:ALA:HA	2.16	0.46
9:I:6:PRO:C	9:I:7:SER:HG	2.21	0.46
13:M:125:LEU:HD23	13:M:131:TYR:HE1	1.79	0.46
15:O:45:ASP:N	15:O:582:GLU:OE2	2.48	0.46
16:P:297:PHE:C	16:P:299:MET:H	2.23	0.46
18:R:122:SER:OG	20:X:25:DT:H5'	2.15	0.46
18:R:623:LYS:HE2	19:S:435:TRP:CD1	2.50	0.46
1:A:356:ARG:HE	1:A:363:ARG:HH12	1.62	0.46
1:A:598:MET:HB2	8:H:96:VAL:CG2	2.46	0.46
1:A:974:LEU:HD11	1:A:998:TYR:CG	2.50	0.46
1:A:1217:ILE:HG22	1:A:1218:GLN:H	1.80	0.46
2:B:778:ILE:HA	2:B:782:PHE:HB3	1.97	0.46
2:B:944:MET:HG2	2:B:945:ASN:N	2.27	0.46
3:C:33:VAL:HG12	3:C:34:GLU:N	2.29	0.46
3:C:334:THR:HG23	11:K:48:LYS:HG3	1.97	0.46
5:E:20:LYS:O	5:E:23:VAL:HG12	2.15	0.46
8:H:1:MET:HG3	8:H:3:ASN:H	1.81	0.46
8:H:104:PHE:C	8:H:105:GLU:HG3	2.31	0.46
13:M:77:LYS:HA	14:N:360:VAL:HG22	1.96	0.46
16:P:79:GLU:HA	16:P:82:LYS:HE3	1.97	0.46
18:R:198:VAL:HA	18:R:201:ASP:HB2	1.98	0.46
18:R:249:HIS:HD2	19:S:406:TYR:CE2	2.33	0.46
19:S:465:ARG:HB3	19:S:468:LEU:HD13	1.97	0.46
1:A:577:THR:HG21	11:K:89:CYS:H	1.80	0.46
1:A:642:PRO:HB3	8:H:103:LYS:HZ2	1.80	0.46
1:A:652:VAL:HB	1:A:668:VAL:HG11	1.97	0.46
1:A:818:ILE:HG22	1:A:867:SER:HA	1.96	0.46
1:A:892:SER:HB2	1:A:1376:LEU:HD11	1.97	0.46
1:A:985:LYS:O	1:A:987:GLU:HG3	2.15	0.46
2:B:800:ASN:HD22	2:B:851:SER:HA	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:85:LEU:HG	14:N:398:SER:HB2	1.98	0.46
15:O:576:PHE:O	15:O:579:GLN:HG2	2.16	0.46
16:P:202:PRO:C	16:P:203:LYS:HG2	2.41	0.46
18:R:467:ARG:O	18:R:471:LYS:HB2	2.16	0.46
18:R:500:GLY:HA2	18:R:503:PHE:HB3	1.96	0.46
19:S:451:ARG:HG3	19:S:452:LYS:N	2.31	0.46
21:Y:43:DA:C8	21:Y:43:DA:H5'	2.50	0.46
1:A:705:LEU:HD23	1:A:705:LEU:C	2.40	0.46
1:A:1325:VAL:HG23	1:A:1326:LEU:H	1.81	0.46
2:B:122:ASP:HA	2:B:189:GLY:CA	2.44	0.46
2:B:325:GLU:O	2:B:328:ALA:N	2.49	0.46
2:B:1093:ASP:HB2	2:B:1102:GLY:O	2.16	0.46
3:C:85:PHE:CE2	3:C:94:ASP:HB2	2.50	0.46
5:E:2:ASP:O	5:E:6:GLU:HG2	2.16	0.46
13:M:125:LEU:HD13	13:M:144:ASN:O	2.16	0.46
19:S:461:GLU:OE1	19:S:465:ARG:NH2	2.46	0.46
21:Y:55:DT:C2'	21:Y:56:DG:C8	2.98	0.46
1:A:481:HIS:CD2	1:A:483:LEU:H	2.34	0.46
1:A:642:PRO:HB3	8:H:103:LYS:HZ3	1.80	0.46
1:A:827:PHE:HB3	2:B:655:ASN:OD1	2.16	0.46
1:A:827:PHE:CE2	1:A:833:PRO:HG3	2.44	0.46
1:A:1131:ASN:OD1	1:A:1372:THR:OG1	2.30	0.46
2:B:232:TYR:HD1	2:B:242:LEU:HD23	1.79	0.46
2:B:327:ILE:HG12	13:M:231:LEU:HD22	1.98	0.46
2:B:421:SER:O	2:B:424:VAL:HB	2.15	0.46
2:B:501:ASP:HB3	2:B:703:CYS:CB	2.46	0.46
2:B:721:ILE:HG12	2:B:899:LEU:CD2	2.45	0.46
2:B:1013:LEU:HD13	2:B:1017:ILE:HD11	1.98	0.46
5:E:26:ARG:HH12	5:E:189:GLY:HA3	1.81	0.46
8:H:3:ASN:O	8:H:5:LEU:HD12	2.16	0.46
12:L:32:ALA:HB3	12:L:53:HIS:CE1	2.51	0.46
12:L:38:LEU:HD22	12:L:48:CYS:HA	1.98	0.46
15:O:134:GLY:O	15:O:137:ILE:HB	2.15	0.46
15:O:136:ILE:HG21	15:O:164:ILE:HD11	1.97	0.46
18:R:288:PRO:HA	18:R:291:VAL:HB	1.98	0.46
18:R:467:ARG:HB3	18:R:610:LEU:HD13	1.98	0.46
19:S:422:VAL:O	19:S:426:ILE:N	2.48	0.46
1:A:233:GLN:HG2	15:O:575:ASN:HD21	1.80	0.46
1:A:392:VAL:HG23	1:A:488:HIS:CG	2.51	0.46
1:A:476:ARG:HG3	1:A:477:GLN:OE1	2.16	0.46
1:A:550:ILE:HG23	1:A:551:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:PRO:HB2	8:H:46:LEU:HD23	1.97	0.46
1:A:921:LEU:HA	1:A:1082:ARG:HA	1.98	0.46
1:A:1177:TYR:OH	1:A:1260:MET:HG2	2.16	0.46
2:B:112:LEU:HD22	2:B:162:ILE:HG12	1.97	0.46
2:B:636:ASP:OD1	2:B:637:PHE:N	2.49	0.46
2:B:785:CYS:SG	2:B:1026:LYS:NZ	2.64	0.46
2:B:849:THR:HG23	2:B:850:ASN:N	2.31	0.46
3:C:33:VAL:C	3:C:35:LYS:N	2.72	0.46
5:E:200:ARG:HD2	5:E:208:TYR:OH	2.16	0.46
16:P:53:GLN:NE2	19:S:362:ILE:O	2.38	0.46
16:P:82:LYS:HE2	16:P:133:TYR:CE1	2.50	0.46
18:R:155:TYR:HE1	20:X:13:DA:P	2.38	0.46
1:A:423:GLY:HA3	1:A:449:ARG:NH1	2.30	0.46
1:A:506:THR:OG1	1:A:507:PRO:HD3	2.16	0.46
2:B:177:CYS:SG	2:B:179:LEU:N	2.84	0.46
2:B:338:GLU:H	2:B:345:LYS:HZ3	1.64	0.46
2:B:493:GLN:HG3	2:B:497:LEU:HB2	1.98	0.46
2:B:691:PRO:HD2	2:B:978:CYS:HA	1.98	0.46
2:B:840:GLN:O	2:B:872:ILE:HG23	2.15	0.46
2:B:1019:PHE:HE1	10:J:44:TYR:HH	1.63	0.46
7:G:111:PRO:HD2	7:G:198:GLY:H	1.81	0.46
8:H:110:ASP:O	8:H:128:ASN:HA	2.16	0.46
13:M:159:TYR:O	14:N:307:PHE:N	2.35	0.46
15:O:47:PHE:HZ	15:O:590:PHE:HE2	1.62	0.46
16:P:108:LYS:HA	16:P:111:LYS:HD3	1.98	0.46
1:A:646:SER:OG	1:A:649:ASP:O	2.26	0.46
1:A:1119:VAL:HA	1:A:1138:THR:HG21	1.98	0.46
1:A:1186:VAL:HG22	1:A:1230:ILE:HD13	1.98	0.46
1:A:1202:ILE:HD12	1:A:1228:ASP:HA	1.97	0.46
1:A:1363:THR:OG1	1:A:1368:VAL:HG22	2.16	0.46
2:B:140:ASN:HA	19:S:394:LYS:HB3	1.98	0.46
2:B:210:ASP:OD1	2:B:211:GLU:N	2.49	0.46
2:B:574:GLN:HE22	14:N:422:ILE:HG12	1.81	0.46
3:C:85:PHE:HE1	3:C:204:LEU:HD22	1.80	0.46
5:E:200:ARG:NH2	5:E:210:SER:OG	2.49	0.46
7:G:4:LEU:HD21	7:G:73:ARG:HE	1.80	0.46
11:K:110:GLU:CD	11:K:111:THR:HG23	2.40	0.46
15:O:132:TYR:C	15:O:134:GLY:N	2.73	0.46
16:P:137:VAL:HG11	16:P:149:MET:HE3	1.98	0.46
21:Y:11:DA:H2'	21:Y:12:DT:H71	1.98	0.46
1:A:622:VAL:HA	1:A:685:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:813:VAL:HG12	1:A:814:GLY:N	2.31	0.45
2:B:1112:SER:OG	2:B:1113:ALA:N	2.49	0.45
3:C:80:ALA:HB3	3:C:102:GLY:HA2	1.97	0.45
3:C:278:GLU:N	3:C:278:GLU:OE1	2.50	0.45
15:O:516:LEU:HD13	15:O:565:LEU:HD23	1.97	0.45
15:O:580:ASN:HA	15:O:583:TRP:HB2	1.97	0.45
16:P:96:TYR:OH	16:P:113:ARG:HG3	2.16	0.45
16:P:216:SER:OG	16:P:217:THR:N	2.49	0.45
16:P:309:VAL:HG21	16:P:311:TYR:CZ	2.51	0.45
1:A:26:ILE:HD13	1:A:262:PRO:HD3	1.99	0.45
1:A:123:PHE:CG	1:A:144:ILE:HD13	2.51	0.45
1:A:216:LYS:HG3	1:A:217:ARG:H	1.81	0.45
1:A:805:ASN:HD21	2:B:951:SER:HA	1.81	0.45
1:A:1127:LYS:O	1:A:1131:ASN:CB	2.65	0.45
1:A:1225:ILE:N	1:A:1229:ARG:HE	2.11	0.45
2:B:92:TYR:N	2:B:136:THR:OG1	2.40	0.45
2:B:230:LYS:HD3	2:B:334:HIS:CE1	2.50	0.45
2:B:254:ALA:HB3	2:B:290:SER:HB2	1.98	0.45
2:B:1039:ALA:HB3	18:R:20:ASN:OD1	2.14	0.45
15:O:470:GLU:HB2	15:O:479:PRO:HD3	1.98	0.45
16:P:263:VAL:HG12	16:P:265:LEU:H	1.81	0.45
18:R:121:ARG:NH2	20:X:23:DC:O3'	2.49	0.45
19:S:413:ARG:NH1	20:X:11:DA:H3'	2.31	0.45
20:X:6:DA:N6	20:X:7:DA:N6	2.64	0.45
20:X:47:DA:H2''	20:X:48:DT:H5'	1.98	0.45
1:A:232:LYS:HD3	16:P:315:TRP:CH2	2.51	0.45
1:A:328:ASN:O	1:A:351:ARG:NE	2.49	0.45
1:A:623:VAL:O	1:A:685:TYR:OH	2.30	0.45
1:A:1203:GLU:O	1:A:1207:VAL:HG12	2.16	0.45
1:A:1272:VAL:HG13	1:A:1273:LYS:N	2.28	0.45
2:B:109:LYS:HD2	2:B:110:ASP:H	1.82	0.45
2:B:134:GLU:HA	2:B:144:HIS:HB3	1.98	0.45
2:B:412:ARG:HH22	18:R:151:GLN:HB2	1.81	0.45
2:B:958:MET:HG3	2:B:1018:PHE:CZ	2.51	0.45
3:C:255:VAL:HG13	3:C:256:ILE:H	1.80	0.45
4:D:17:LEU:HB2	4:D:66:LEU:HD23	1.97	0.45
4:D:149:THR:O	4:D:153:MET:HG3	2.16	0.45
5:E:171:LYS:H	5:E:174:GLN:NE2	2.13	0.45
6:F:84:TYR:HD1	6:F:152:ILE:HG23	1.82	0.45
7:G:112:GLN:OE1	7:G:115:LEU:HD13	2.15	0.45
10:J:1:MET:HB3	10:J:2:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:254:GLN:OE1	14:N:409:LEU:HG	2.15	0.45
15:O:551:VAL:O	15:O:562:ALA:HB1	2.15	0.45
15:O:634:GLU:O	15:O:637:VAL:N	2.50	0.45
16:P:190:THR:HA	16:P:215:TYR:HE1	1.81	0.45
1:A:49:LYS:HD2	1:A:54:LEU:CB	2.40	0.45
1:A:195:ASP:O	1:A:198:VAL:HG12	2.17	0.45
1:A:777:VAL:O	1:A:781:CYS:HB2	2.16	0.45
2:B:649:LEU:HD22	2:B:653:GLU:OE1	2.17	0.45
2:B:723:THR:HG23	2:B:724:LEU:N	2.31	0.45
2:B:755:ALA:HB2	2:B:782:PHE:HE1	1.82	0.45
2:B:791:THR:HG22	2:B:842:TYR:HE2	1.81	0.45
3:C:278:GLU:O	3:C:281:ARG:HG2	2.16	0.45
8:H:128:ASN:CG	8:H:129:TYR:H	2.24	0.45
14:N:373:VAL:HB	14:N:381:ASP:O	2.16	0.45
15:O:205:LYS:HG3	15:O:206:LEU:N	2.32	0.45
15:O:353:GLU:HB2	15:O:481:SER:HG	1.80	0.45
15:O:369:HIS:CG	15:O:370:LEU:H	2.35	0.45
15:O:454:ASN:O	15:O:457:LEU:HB3	2.15	0.45
16:P:118:GLN:OE1	21:Y:35:DG:H5"	2.16	0.45
18:R:213:TRP:CD1	18:R:287:PRO:CD	2.99	0.45
18:R:434:GLU:CA	18:R:436:LYS:H	2.30	0.45
1:A:3:GLU:O	7:G:37:LYS:HG3	2.15	0.45
1:A:34:VAL:HG13	1:A:35:SER:N	2.31	0.45
1:A:90:VAL:HG21	1:A:320:GLN:HA	1.97	0.45
1:A:114:LEU:HD21	1:A:148:CYS:HB2	1.97	0.45
1:A:781:CYS:O	1:A:785:LEU:HB2	2.16	0.45
1:A:903:THR:O	1:A:905:ARG:HG3	2.16	0.45
1:A:1170:ALA:HA	1:A:1188:ILE:CG1	2.42	0.45
1:A:1329:GLU:CD	5:E:200:ARG:HH21	2.25	0.45
1:A:1411:VAL:HG13	1:A:1412:SER:N	2.30	0.45
2:B:112:LEU:HD23	2:B:113:THR:N	2.30	0.45
2:B:178:PRO:HD3	10:J:63:TYR:OH	2.16	0.45
2:B:239:LYS:HZ2	2:B:241:TYR:HE2	1.64	0.45
2:B:242:LEU:HD12	2:B:256:VAL:HG21	1.99	0.45
2:B:298:GLN:HA	2:B:302:LEU:HD12	1.98	0.45
2:B:552:ASN:OD1	2:B:553:TYR:N	2.50	0.45
2:B:698:ARG:HE	2:B:952:ARG:HB3	1.82	0.45
3:C:229:LEU:HD23	3:C:295:ARG:HA	1.98	0.45
4:D:157:ILE:O	4:D:161:ALA:N	2.49	0.45
9:I:5:CYS:HB3	9:I:10:ASN:H	1.82	0.45
15:O:623:GLU:OE1	15:O:624:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:151:TYR:OH	18:R:647:ALA:HB1	2.17	0.45
18:R:431:ARG:HH12	21:Y:48:DT:P	2.40	0.45
1:A:134:ASN:HD21	1:A:1404:LYS:HD3	1.82	0.45
1:A:179:ILE:HG23	1:A:220:ASP:O	2.17	0.45
1:A:200:GLU:HG2	15:O:515:LYS:CD	2.47	0.45
1:A:436:ARG:N	1:A:460:ASP:OD1	2.49	0.45
2:B:44:LYS:NZ	2:B:663:GLU:HB2	2.32	0.45
2:B:273:CYS:O	2:B:354:ARG:NH1	2.50	0.45
2:B:832:VAL:HG13	2:B:882:ASP:O	2.17	0.45
2:B:932:PRO:O	2:B:940:PRO:CD	2.60	0.45
2:B:944:MET:CG	2:B:945:ASN:H	2.26	0.45
2:B:991:LEU:O	2:B:994:GLN:N	2.47	0.45
3:C:231:PRO:HB3	3:C:275:VAL:CG2	2.41	0.45
8:H:95:TYR:CE2	8:H:97:MET:HE2	2.51	0.45
15:O:310:GLN:NE2	15:O:313:LYS:HD3	2.31	0.45
15:O:317:ARG:HA	15:O:320:GLU:CD	2.42	0.45
15:O:482:LYS:C	15:O:485:PRO:HD2	2.42	0.45
18:R:267:ALA:O	18:R:271:SER:OG	2.24	0.45
1:A:152:ARG:HH12	21:Y:9:DT:P	2.39	0.45
1:A:269:ARG:CZ	1:A:286:THR:H	2.30	0.45
1:A:315:HIS:O	1:A:318:TYR:N	2.49	0.45
1:A:1122:GLY:C	1:A:1124:PRO:HD2	2.42	0.45
1:A:1373:ARG:HB2	1:A:1390:GLU:HG2	1.97	0.45
2:B:798:TYR:C	18:R:99:TYR:HE1	2.25	0.45
2:B:884:VAL:CG2	12:L:58:LYS:HB3	2.47	0.45
2:B:914:SER:OG	2:B:914:SER:O	2.19	0.45
2:B:1004:LEU:HD12	2:B:1017:ILE:HD12	1.99	0.45
3:C:31:TRP:HE3	11:K:82:LYS:HD2	1.81	0.45
5:E:112:TYR:O	5:E:137:GLU:HB2	2.17	0.45
7:G:15:PRO:HA	7:G:18:PHE:CZ	2.51	0.45
14:N:284:ASN:O	14:N:287:HIS:N	2.49	0.45
15:O:259:LEU:HD23	15:O:261:GLN:H	1.81	0.45
15:O:366:LEU:HD22	15:O:368:ARG:NH1	2.31	0.45
20:X:50:DA:H2	21:Y:15:DT:O2	2.00	0.45
21:Y:42:DT:N3	21:Y:43:DA:N6	2.64	0.45
1:A:283:ASP:OD1	1:A:284:ASP:N	2.43	0.45
1:A:760:GLN:HA	1:A:763:GLU:HB3	1.99	0.45
1:A:1364:TYR:HE2	1:A:1379:MET:SD	2.40	0.45
5:E:112:TYR:CD1	5:E:116:ILE:HG12	2.51	0.45
5:E:123:LEU:HD21	5:E:126:SER:HB2	1.99	0.45
11:K:132:GLU:O	11:K:136:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:29:TYR:HB3	12:L:59:ALA:H	1.82	0.45
18:R:425:PHE:HB2	21:Y:46:DA:OP1	2.17	0.45
18:R:492:VAL:HB	18:R:494:PHE:CE2	2.52	0.45
18:R:602:LEU:O	18:R:606:ASP:N	2.50	0.45
21:Y:1:DC:H1'	21:Y:2:DC:C2	2.51	0.45
1:A:891:LYS:HG3	1:A:1389:PHE:CD1	2.52	0.45
1:A:1286:ARG:H	1:A:1291:ARG:HA	1.81	0.45
1:A:1315:THR:HG22	1:A:1316:THR:N	2.29	0.45
1:A:1339:ILE:HD13	1:A:1339:ILE:HA	1.84	0.45
2:B:536:LEU:HD23	2:B:536:LEU:O	2.17	0.45
2:B:766:ASP:O	2:B:770:ALA:HB3	2.16	0.45
2:B:775:LYS:C	2:B:777:SER:N	2.74	0.45
4:D:109:LYS:HB2	4:D:156:ILE:HD11	1.99	0.45
5:E:9:ILE:HG22	5:E:53:PRO:CG	2.47	0.45
7:G:126:SER:OG	7:G:139:TYR:CB	2.65	0.45
12:L:25:ALA:N	12:L:37:LYS:HE2	2.32	0.45
15:O:69:VAL:HG22	15:O:122:TYR:CD1	2.51	0.45
15:O:197:MET:HG3	15:O:286:ARG:HB3	1.97	0.45
15:O:221:LYS:N	15:O:224:LYS:HB3	2.32	0.45
21:Y:58:DT:H4'	21:Y:59:DG:H5'	1.99	0.45
2:B:130:TYR:CE1	2:B:148:GLU:HG3	2.52	0.45
3:C:31:TRP:HB2	11:K:82:LYS:HG3	1.99	0.45
5:E:46:TYR:O	5:E:54:GLN:N	2.49	0.45
9:I:29:CYS:CA	13:M:183:PHE:HE2	2.25	0.45
14:N:304:PHE:HB2	14:N:411:ARG:O	2.17	0.45
14:N:365:VAL:HG13	14:N:370:LYS:O	2.16	0.45
15:O:67:MET:HE3	15:O:82:LYS:HB3	1.99	0.45
15:O:484:MET:O	15:O:488:LYS:N	2.39	0.45
18:R:408:LEU:HD13	18:R:427:ALA:HA	1.99	0.45
18:R:425:PHE:HE2	18:R:427:ALA:HB3	1.82	0.45
20:X:25:DT:H2'	20:X:26:DT:H6	1.78	0.45
1:A:103:LEU:HD21	1:A:222:LEU:HD22	1.99	0.44
1:A:442:ARG:HA	18:R:29:GLY:O	2.17	0.44
1:A:645:MET:CE	8:H:124:ARG:HB2	2.42	0.44
1:A:1206:ALA:O	1:A:1209:ILE:HB	2.17	0.44
1:A:1332:ARG:HA	1:A:1335:ILE:HG22	1.99	0.44
1:A:1447:LEU:HB3	1:A:1450:SER:HB3	1.98	0.44
2:B:660:ALA:HB2	2:B:670:MET:SD	2.57	0.44
3:C:195:LYS:HD2	10:J:57:ILE:HG21	1.98	0.44
3:C:255:VAL:HG22	3:C:256:ILE:N	2.32	0.44
6:F:143:PHE:O	6:F:144:GLU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:94:PRO:HA	14:N:392:GLN:CA	2.42	0.44
13:M:123:ILE:HB	13:M:146:GLN:HB3	2.00	0.44
15:O:364:ILE:HA	15:O:476:TYR:OH	2.17	0.44
16:P:311:TYR:CD1	17:Q:40:PRO:HB3	2.52	0.44
19:S:523:ALA:HA	19:S:526:GLU:HB3	1.99	0.44
21:Y:15:DT:O4	21:Y:16:DA:N6	2.50	0.44
1:A:173:SER:HB2	1:A:334:PRO:HB2	1.99	0.44
1:A:326:TYR:CD2	1:A:327:ILE:HG23	2.53	0.44
1:A:378:ARG:NE	1:A:516:GLU:OE1	2.49	0.44
1:A:919:ASP:OD2	1:A:921:LEU:HB2	2.17	0.44
1:A:1329:GLU:OE2	5:E:200:ARG:NE	2.46	0.44
2:B:84:LEU:HG	2:B:85:SER:O	2.18	0.44
2:B:259:ALA:HB1	2:B:302:LEU:HD23	1.99	0.44
2:B:971:GLY:CA	10:J:51:LEU:HD11	2.43	0.44
4:D:102:SER:HA	4:D:105:GLU:HB2	1.99	0.44
7:G:4:LEU:HD12	7:G:74:ALA:O	2.17	0.44
13:M:104:HIS:CB	13:M:105:PRO:HD2	2.43	0.44
15:O:267:PRO:HG2	15:O:270:SER:HB2	1.99	0.44
18:R:414:HIS:HD2	18:R:615:LEU:O	2.01	0.44
1:A:16:LEU:HD11	1:A:1417:LEU:HD11	2.00	0.44
1:A:372:ARG:HD2	2:B:1050:PRO:C	2.34	0.44
1:A:373:VAL:CA	2:B:1050:PRO:HG2	2.48	0.44
1:A:726:LYS:O	1:A:730:LEU:HG	2.17	0.44
1:A:1023:ARG:O	1:A:1028:MET:HB2	2.17	0.44
2:B:93:LEU:HD12	2:B:135:TYR:HB3	1.99	0.44
2:B:493:GLN:CG	2:B:497:LEU:HB2	2.48	0.44
2:B:842:TYR:CE1	2:B:873:TYR:HB2	2.52	0.44
3:C:59:ILE:HD11	3:C:64:ALA:HB2	1.99	0.44
3:C:239:ILE:HG22	3:C:288:LYS:HD2	2.00	0.44
4:D:14:TYR:CD2	4:D:15:GLU:HG2	2.53	0.44
4:D:126:GLN:NE2	7:G:85:VAL:HA	2.32	0.44
5:E:9:ILE:HG22	5:E:53:PRO:HG3	1.99	0.44
7:G:189:GLU:HG3	7:G:191:PRO:HD3	2.00	0.44
8:H:9:ILE:O	8:H:31:THR:HG22	2.18	0.44
11:K:63:PHE:CZ	11:K:114:VAL:HG12	2.52	0.44
13:M:253:GLU:HA	13:M:256:LYS:HB2	1.99	0.44
14:N:371:LEU:HD22	14:N:384:LYS:CD	2.46	0.44
20:X:58:DC:C4	20:X:59:DC:C4	3.05	0.44
1:A:483:LEU:HD21	1:A:540:ASN:HB3	1.99	0.44
1:A:1188:ILE:HB	1:A:1228:ASP:HB3	1.99	0.44
1:A:1302:ASP:N	1:A:1302:ASP:OD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:PRO:HA	2:B:151:ARG:HG2	1.99	0.44
2:B:263:LEU:HD21	2:B:296:TYR:CE1	2.52	0.44
2:B:427:ASN:HA	2:B:430:THR:H	1.82	0.44
2:B:591:TYR:CZ	2:B:600:HIS:HB2	2.51	0.44
2:B:696:SER:OG	2:B:697:PRO:HD3	2.17	0.44
2:B:747:ASP:O	10:J:54:VAL:HG11	2.18	0.44
2:B:791:THR:O	2:B:791:THR:HG23	2.17	0.44
5:E:22:MET:CE	5:E:26:ARG:HH21	2.23	0.44
8:H:104:PHE:HE1	8:H:114:VAL:HG13	1.81	0.44
13:M:257:ASP:O	13:M:261:LYS:HG3	2.17	0.44
14:N:388:THR:HG23	14:N:390:PHE:CD2	2.53	0.44
15:O:288:MET:SD	15:O:326:ILE:HG21	2.57	0.44
16:P:202:PRO:O	16:P:203:LYS:HG2	2.17	0.44
18:R:229:LEU:HB2	18:R:244:ILE:HD13	1.98	0.44
21:Y:14:DT:H2'	21:Y:14:DT:OP2	2.17	0.44
21:Y:53:DT:H2''	21:Y:54:DA:H5''	2.00	0.44
1:A:235:LYS:HZ3	1:A:254:GLU:CG	2.30	0.44
1:A:372:ARG:O	2:B:1050:PRO:CD	2.64	0.44
1:A:379:THR:HG22	1:A:380:VAL:N	2.32	0.44
1:A:474:PHE:CZ	1:A:517:MET:HG3	2.52	0.44
1:A:524:THR:N	2:B:1081:GLU:OE2	2.40	0.44
1:A:598:MET:O	1:A:600:PRO:HD2	2.18	0.44
1:A:704:PHE:O	1:A:707:ASN:N	2.51	0.44
1:A:733:ILE:HA	1:A:736:HIS:NE2	2.32	0.44
1:A:815:GLN:HA	1:A:846:GLY:O	2.18	0.44
1:A:869:ARG:NH1	2:B:502:THR:HB	2.29	0.44
2:B:240:ILE:CG1	2:B:286:ASN:HD22	2.31	0.44
2:B:969:LEU:HB3	2:B:994:GLN:OE1	2.17	0.44
2:B:1088:ASP:OD1	2:B:1088:ASP:N	2.49	0.44
3:C:21:PRO:HD3	3:C:30:GLU:HA	1.98	0.44
3:C:260:GLU:O	3:C:264:GLU:N	2.50	0.44
4:D:27:HIS:NE2	4:D:53:PRO:HG3	2.32	0.44
13:M:159:TYR:CG	13:M:170:LEU:HD21	2.53	0.44
15:O:307:VAL:HG13	15:O:308:THR:N	2.32	0.44
16:P:297:PHE:C	16:P:299:MET:N	2.75	0.44
18:R:120:ARG:HE	21:Y:42:DT:H4'	1.81	0.44
18:R:192:ALA:O	18:R:195:LYS:NZ	2.50	0.44
18:R:633:ASP:O	18:R:636:LEU:HB3	2.18	0.44
1:A:785:LEU:HD21	1:A:789:ASN:HD21	1.82	0.44
2:B:77:ILE:HG21	2:B:98:ILE:HD11	2.00	0.44
2:B:320:LEU:HA	2:B:324:ILE:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:592:SER:N	2:B:656:ASP:OD2	2.29	0.44
2:B:658:TYR:HE2	2:B:670:MET:HG2	1.81	0.44
9:I:32:GLU:HG3	13:M:132:ASN:HB2	2.00	0.44
13:M:125:LEU:HD22	13:M:142:GLY:O	2.18	0.44
15:O:241:ALA:O	15:O:245:ALA:N	2.34	0.44
18:R:116:PHE:CE2	18:R:164:MET:HB3	2.52	0.44
18:R:399:THR:O	18:R:481:PHE:HA	2.18	0.44
18:R:522:ARG:HD3	18:R:529:VAL:HG22	2.00	0.44
20:X:61:DT:H3	21:Y:4:DT:H3	1.64	0.44
1:A:477:GLN:HG2	1:A:478:PRO:N	2.32	0.44
1:A:1157:VAL:HG12	1:A:1160:ARG:HD2	1.98	0.44
3:C:89:THR:HG23	3:C:200:GLN:HA	1.98	0.44
7:G:116:PHE:HZ	7:G:203:ASP:HA	1.83	0.44
8:H:80:ARG:HG3	11:K:108:TYR:CZ	2.52	0.44
14:N:299:ASN:CG	14:N:301:PRO:HD3	2.43	0.44
14:N:384:LYS:HD2	14:N:416:ILE:HD11	1.99	0.44
15:O:164:ILE:HG12	15:O:282:ILE:HD13	1.99	0.44
15:O:203:ILE:HG13	15:O:203:ILE:O	2.18	0.44
15:O:248:ASP:O	15:O:252:ILE:HG12	2.18	0.44
15:O:471:THR:HA	15:O:477:TYR:HD2	1.81	0.44
18:R:96:ILE:HD11	18:R:101:THR:HG22	2.00	0.44
18:R:630:LEU:HD11	19:S:444:GLN:HG3	1.99	0.44
20:X:51:DA:H2''	20:X:52:DA:C8	2.52	0.44
21:Y:55:DT:C2	21:Y:56:DG:C5	3.05	0.44
1:A:183:PHE:C	1:A:184:ARG:HG2	2.43	0.44
1:A:476:ARG:HA	1:A:517:MET:SD	2.58	0.44
1:A:890:MET:O	1:A:893:LEU:N	2.50	0.44
1:A:1399:ALA:HA	1:A:1404:LYS:HD2	1.99	0.44
2:B:208:GLU:O	2:B:215:ILE:HA	2.17	0.44
2:B:552:ASN:HD21	2:B:568:PRO:CA	2.31	0.44
8:H:112:ILE:O	8:H:126:GLU:HA	2.18	0.44
10:J:2:ILE:HD12	10:J:2:ILE:H	1.82	0.44
15:O:56:HIS:CG	15:O:130:LEU:HD23	2.53	0.44
15:O:488:LYS:HD3	15:O:488:LYS:HA	1.64	0.44
17:Q:54:LEU:O	17:Q:58:TYR:N	2.51	0.44
19:S:453:GLN:O	19:S:457:LYS:HB3	2.17	0.44
20:X:10:DT:C4	20:X:11:DA:N6	2.86	0.44
1:A:57:LYS:HA	1:A:68:ALA:HB3	2.00	0.44
1:A:323:VAL:O	1:A:326:TYR:HB3	2.18	0.44
1:A:427:HIS:HB3	1:A:428:PRO:HD3	2.00	0.44
1:A:727:LYS:HA	1:A:730:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1213:SER:OG	1:A:1217:ILE:HB	2.18	0.44
2:B:760:MET:HE3	2:B:762:TYR:HB2	1.99	0.44
2:B:775:LYS:C	2:B:777:SER:H	2.26	0.44
2:B:778:ILE:CG1	2:B:906:PRO:HG2	2.47	0.44
3:C:75:VAL:HG23	3:C:221:PRO:HG3	2.00	0.44
4:D:106:LEU:HG	4:D:110:LEU:HD22	2.00	0.44
8:H:98:TYR:HD1	8:H:141:TYR:CE2	2.34	0.44
14:N:386:ALA:HB2	14:N:416:ILE:HA	1.99	0.44
15:O:199:TYR:C	15:O:200:LEU:HD12	2.43	0.44
15:O:221:LYS:H	15:O:224:LYS:HB3	1.83	0.44
19:S:509:HIS:HA	19:S:512:HIS:HB3	2.00	0.44
20:X:3:DT:H2''	20:X:4:DT:H71	1.99	0.44
21:Y:55:DT:C4	21:Y:56:DG:C6	3.06	0.44
1:A:445:ARG:NH2	18:R:17:SER:OG	2.51	0.43
1:A:501:ASN:OD1	1:A:502:GLU:N	2.52	0.43
1:A:976:ARG:HH21	1:A:994:TYR:HB2	1.83	0.43
2:B:191:GLU:HG2	2:B:192:LYS:N	2.32	0.43
2:B:410:PRO:HA	2:B:414:MET:HE2	2.00	0.43
2:B:626:HIS:CD2	2:B:645:LEU:HD21	2.53	0.43
3:C:100:ARG:NH1	10:J:2:ILE:HB	2.33	0.43
7:G:87:GLY:HA3	7:G:148:PHE:CE2	2.45	0.43
10:J:43:ARG:HH11	10:J:43:ARG:CG	2.25	0.43
13:M:72:GLU:OE1	14:N:364:ARG:NH2	2.50	0.43
13:M:174:GLU:HB3	13:M:175:ARG:H	1.65	0.43
15:O:132:TYR:CE1	15:O:645:LEU:HD21	2.53	0.43
15:O:327:ARG:C	15:O:329:PRO:HD2	2.43	0.43
15:O:352:VAL:HG13	15:O:353:GLU:H	1.83	0.43
15:O:464:ASN:HA	15:O:469:ASN:CG	2.43	0.43
18:R:195:LYS:O	18:R:199:VAL:HG23	2.18	0.43
18:R:213:TRP:CD1	18:R:213:TRP:O	2.70	0.43
18:R:420:TYR:HB2	18:R:428:VAL:HG22	2.00	0.43
20:X:45:DA:H2''	20:X:46:DG:C8	2.53	0.43
20:X:60:DA:N6	21:Y:4:DT:C4	2.86	0.43
21:Y:8:DG:H2'	21:Y:9:DT:H71	1.99	0.43
1:A:78:HIS:ND1	2:B:1090:PHE:HZ	2.16	0.43
1:A:232:LYS:HG2	1:A:254:GLU:OE2	2.19	0.43
1:A:332:VAL:HG13	1:A:333:ASN:N	2.27	0.43
1:A:432:TYR:CD1	1:A:443:ASN:HB3	2.53	0.43
1:A:436:ARG:HH11	1:A:459:GLY:HA3	1.83	0.43
1:A:666:LYS:HA	1:A:670:GLY:CA	2.46	0.43
1:A:715:ASN:OD1	1:A:716:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:LEU:O	1:A:796:THR:N	2.50	0.43
1:A:818:ILE:HD11	1:A:823:VAL:HA	2.00	0.43
1:A:916:TYR:O	1:A:920:GLY:N	2.48	0.43
1:A:921:LEU:HD23	1:A:932:PRO:HG3	1.99	0.43
1:A:1079:ARG:HG2	6:F:84:TYR:HE2	1.83	0.43
1:A:1083:LEU:HA	1:A:1083:LEU:HD23	1.60	0.43
1:A:1222:VAL:HA	1:A:1231:ALA:O	2.17	0.43
1:A:1370:GLY:O	1:A:1371:ILE:O	2.36	0.43
2:B:719:LYS:NZ	10:J:65:PRO:HG3	2.33	0.43
2:B:759:VAL:HG12	2:B:946:PRO:HG3	2.00	0.43
2:B:911:LYS:HA	2:B:920:GLY:O	2.18	0.43
5:E:147:HIS:ND1	5:E:148:GLU:N	2.66	0.43
13:M:94:PRO:CA	14:N:392:GLN:HA	2.40	0.43
16:P:253:LEU:HA	16:P:263:VAL:HA	2.00	0.43
1:A:161:ASN:HB2	1:A:180:HIS:HE1	1.82	0.43
1:A:733:ILE:HD12	1:A:736:HIS:NE2	2.33	0.43
1:A:1415:ILE:HG22	2:B:1079:LEU:HD21	2.00	0.43
1:A:1421:MET:HE3	1:A:1421:MET:HB2	1.87	0.43
2:B:619:GLN:OE1	2:B:619:GLN:N	2.52	0.43
2:B:855:PRO:N	18:R:106:GLN:HE22	2.17	0.43
4:D:68:ILE:O	4:D:72:PHE:N	2.41	0.43
4:D:127:LEU:HB2	4:D:133:HIS:HB3	1.99	0.43
7:G:49:TYR:HB2	7:G:75:VAL:HG23	2.00	0.43
8:H:116:TYR:HB2	8:H:123:MET:HB3	2.00	0.43
14:N:361:GLY:HA3	14:N:374:LYS:O	2.19	0.43
15:O:53:VAL:O	15:O:57:LEU:N	2.50	0.43
15:O:347:ASP:HA	15:O:350:GLU:CG	2.48	0.43
18:R:519:LEU:HB3	18:R:532:ILE:HB	2.00	0.43
18:R:528:ILE:HG12	18:R:543:ALA:HB2	2.00	0.43
1:A:216:LYS:HG3	1:A:217:ARG:N	2.33	0.43
1:A:538:LYS:HB3	1:A:687:PRO:HB2	2.01	0.43
1:A:590:PHE:O	11:K:106:GLN:NE2	2.51	0.43
1:A:694:MET:O	1:A:697:MET:HB3	2.18	0.43
1:A:1165:LEU:C	1:A:1167:SER:H	2.26	0.43
1:A:1235:PHE:HB2	1:A:1236:PRO:HD2	1.99	0.43
1:A:1265:ARG:NH2	2:B:285:VAL:HG22	2.34	0.43
1:A:1378:LYS:CG	1:A:1379:MET:N	2.82	0.43
2:B:108:THR:HG22	2:B:109:LYS:N	2.26	0.43
2:B:525:GLU:HG3	2:B:528:PRO:HD2	2.01	0.43
2:B:726:TYR:O	2:B:727:LEU:HB3	2.18	0.43
5:E:156:LEU:HD11	5:E:195:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:15:PRO:HA	7:G:18:PHE:CE2	2.53	0.43
7:G:142:VAL:C	7:G:144:GLU:H	2.26	0.43
11:K:110:GLU:OE2	11:K:111:THR:HG23	2.18	0.43
11:K:120:GLY:O	11:K:123:ASP:HB2	2.19	0.43
13:M:144:ASN:CG	13:M:145:VAL:H	2.27	0.43
14:N:366:HIS:H	14:N:370:LYS:HB2	1.84	0.43
14:N:366:HIS:CG	14:N:367:LYS:H	2.36	0.43
15:O:170:THR:HG22	15:O:279:SER:HA	2.00	0.43
15:O:364:ILE:HA	15:O:476:TYR:CZ	2.54	0.43
18:R:99:TYR:HD2	18:R:100:ILE:HG13	1.82	0.43
18:R:413:LEU:HB3	18:R:620:SER:OG	2.19	0.43
1:A:172:GLY:HA3	1:A:331:SER:CB	2.38	0.43
1:A:313:MET:SD	15:O:548:ILE:HD13	2.59	0.43
1:A:388:SER:C	1:A:501:ASN:HD22	2.27	0.43
1:A:713:GLY:HA2	2:B:1018:PHE:CG	2.54	0.43
1:A:753:GLN:HE22	1:A:765:LYS:HE2	1.83	0.43
1:A:943:TYR:HA	1:A:946:THR:HG22	2.01	0.43
2:B:136:THR:HG22	2:B:142:ILE:HG22	2.01	0.43
2:B:269:MET:CE	2:B:280:GLN:HG2	2.49	0.43
2:B:556:TYR:HD1	2:B:561:LEU:HA	1.84	0.43
2:B:938:ILE:HG23	10:J:45:CYS:HB3	2.00	0.43
7:G:41:ASN:HA	7:G:155:PHE:CD2	2.54	0.43
7:G:114:MET:HB2	7:G:199:SER:HB2	1.98	0.43
8:H:99:GLY:HA3	8:H:118:PHE:HD1	1.83	0.43
10:J:48:ARG:O	10:J:52:THR:N	2.22	0.43
13:M:75:PRO:HA	14:N:362:SER:OG	2.19	0.43
18:R:143:LEU:HD11	18:R:157:ILE:HG22	1.99	0.43
1:A:14:LYS:O	2:B:1142:ARG:HB2	2.19	0.43
1:A:116:SER:OG	1:A:117:GLU:OE1	2.16	0.43
1:A:153:ARG:NH2	15:O:338:ASP:HA	2.33	0.43
1:A:270:PRO:HG3	2:B:1046:LEU:HD12	1.99	0.43
1:A:388:SER:OG	1:A:389:ILE:N	2.51	0.43
1:A:629:LYS:HE3	1:A:633:PHE:CD2	2.53	0.43
1:A:642:PRO:HB2	1:A:644:GLU:CG	2.42	0.43
1:A:777:VAL:CG1	1:A:811:ALA:HB1	2.49	0.43
1:A:813:VAL:HG12	1:A:814:GLY:H	1.84	0.43
1:A:1166:LEU:CA	1:A:1169:VAL:HG22	2.37	0.43
1:A:1335:ILE:HG23	1:A:1336:ILE:H	1.84	0.43
2:B:630:LEU:HD12	2:B:635:LEU:HB3	2.00	0.43
2:B:888:VAL:CG1	12:L:54:ARG:HD3	2.48	0.43
2:B:954:THR:HG23	2:B:954:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:121:MET:HA	5:E:124:VAL:HB	2.00	0.43
16:P:235:LEU:HD23	16:P:236:THR:O	2.19	0.43
18:R:75:SER:OG	20:X:27:DT:H2'	2.18	0.43
18:R:604:ASP:OD1	18:R:605:VAL:N	2.50	0.43
21:Y:6:DG:C6	21:Y:7:DA:C6	3.07	0.43
21:Y:26:DA:H2''	21:Y:27:DC:H5''	2.00	0.43
1:A:302:GLY:O	1:A:304:ASP:N	2.50	0.43
1:A:541:LEU:HD22	1:A:682:LEU:HD22	1.99	0.43
1:A:573:ARG:O	1:A:577:THR:CB	2.67	0.43
1:A:738:CYS:SG	1:A:842:PRO:HD3	2.59	0.43
1:A:975:VAL:O	1:A:976:ARG:HG3	2.19	0.43
1:A:1335:ILE:HG23	1:A:1336:ILE:N	2.34	0.43
2:B:137:ARG:HB3	2:B:417:ASP:HA	2.01	0.43
2:B:300:GLN:HE22	13:M:186:ILE:HG22	1.83	0.43
3:C:97:LEU:HD12	3:C:194:ALA:HB2	2.00	0.43
3:C:324:LYS:HD3	11:K:68:GLU:OE2	2.19	0.43
8:H:5:LEU:HG	8:H:133:ASN:HB3	2.01	0.43
8:H:93:TYR:HB2	8:H:143:LEU:HD11	2.00	0.43
8:H:107:VAL:O	8:H:111:LEU:HB2	2.18	0.43
10:J:37:SER:OG	10:J:47:ARG:NH2	2.52	0.43
15:O:183:MET:CB	15:O:186:THR:HB	2.48	0.43
15:O:499:THR:O	17:Q:39:ILE:HD13	2.18	0.43
15:O:555:ALA:HB2	15:O:561:ARG:CG	2.48	0.43
18:R:238:ARG:HB3	19:S:289:UNK:O	2.18	0.43
1:A:11:LYS:HZ2	2:B:1145:ASP:N	2.17	0.43
1:A:209:PRO:O	1:A:212:GLU:HB2	2.18	0.43
1:A:450:MET:O	1:A:454:LYS:HG2	2.18	0.43
1:A:1378:LYS:CG	1:A:1379:MET:H	2.29	0.43
1:A:1380:ARG:NH1	1:A:1385:GLN:HE22	2.14	0.43
2:B:169:SER:O	2:B:172:ALA:N	2.51	0.43
2:B:586:GLU:HG2	2:B:587:PHE:N	2.34	0.43
4:D:126:GLN:O	4:D:127:LEU:C	2.61	0.43
5:E:23:VAL:HG22	5:E:28:TYR:HB2	2.00	0.43
5:E:146:HIS:O	5:E:146:HIS:ND1	2.51	0.43
5:E:194:GLU:O	5:E:213:ILE:HG13	2.19	0.43
7:G:95:GLU:HG3	7:G:96:GLY:N	2.33	0.43
11:K:106:GLN:HG3	11:K:106:GLN:O	2.18	0.43
13:M:112:TYR:OH	13:M:114:PRO:HA	2.18	0.43
15:O:187:ILE:C	15:O:189:SER:H	2.27	0.43
17:Q:55:ALA:O	17:Q:58:TYR:HB3	2.19	0.43
18:R:99:TYR:CD2	18:R:100:ILE:HG13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:273:GLN:H	18:R:273:GLN:CD	2.25	0.43
20:X:59:DC:N3	20:X:60:DA:N6	2.67	0.43
1:A:869:ARG:HH12	2:B:502:THR:CB	2.29	0.43
1:A:1408:VAL:HG23	1:A:1413:GLU:CG	2.48	0.43
1:A:1452:SER:C	4:D:117:LYS:HZ2	2.27	0.43
2:B:296:TYR:CD2	13:M:186:ILE:HG13	2.52	0.43
2:B:909:GLY:HA2	2:B:921:VAL:HG13	2.01	0.43
7:G:105:PHE:HD2	7:G:107:ASP:H	1.66	0.43
15:O:125:GLU:HB3	15:O:128:HIS:CG	2.54	0.43
15:O:547:GLU:O	15:O:548:ILE:HG13	2.18	0.43
16:P:238:SER:HA	16:P:241:ARG:CZ	2.49	0.43
18:R:274:LYS:HB3	18:R:275:PHE:H	1.74	0.43
18:R:430:MET:HE3	18:R:441:ILE:HG21	2.01	0.43
19:S:277:UNK:O	19:S:279:UNK:N	2.52	0.43
19:S:367:ASN:HB3	19:S:370:GLY:O	2.19	0.43
20:X:29:DC:C6	20:X:30:DT:H72	2.53	0.43
1:A:373:VAL:HG11	2:B:1082:ARG:HD2	2.01	0.43
1:A:585:ASP:N	1:A:585:ASP:OD1	2.51	0.43
1:A:1304:MET:HE1	1:A:1326:LEU:HD11	2.01	0.43
2:B:217:GLN:HB3	2:B:356:VAL:CG1	2.49	0.43
2:B:1008:ILE:HD11	11:K:70:HIS:NE2	2.34	0.43
3:C:73:SER:HA	3:C:213:GLY:HA3	2.01	0.43
4:D:10:PHE:HA	7:G:3:ILE:HG22	2.01	0.43
9:I:5:CYS:O	9:I:9:ASN:HA	2.19	0.43
11:K:88:PHE:HB3	11:K:106:GLN:HG3	1.95	0.43
13:M:104:HIS:CB	13:M:105:PRO:CD	2.89	0.43
18:R:286:ARG:HA	18:R:290:PHE:CZ	2.54	0.43
18:R:610:LEU:HA	18:R:613:HIS:HD2	1.81	0.43
1:A:16:LEU:HD23	2:B:1139:PRO:HB2	2.01	0.42
2:B:732:GLN:O	2:B:750:PRO:HB2	2.19	0.42
5:E:26:ARG:HH22	5:E:189:GLY:CA	2.32	0.42
13:M:76:LEU:HB3	13:M:168:VAL:HB	2.01	0.42
13:M:155:ASN:OD1	13:M:155:ASN:N	2.51	0.42
16:P:141:LYS:HG2	16:P:142:PHE:H	1.84	0.42
16:P:216:SER:CB	16:P:260:CYS:HA	2.49	0.42
18:R:73:LEU:HD22	21:Y:32:DA:N7	2.34	0.42
19:S:527:ASP:O	19:S:531:GLN:HG3	2.19	0.42
20:X:55:DA:H1'	20:X:56:DC:H5'	2.01	0.42
21:Y:60:DA:H2''	21:Y:61:DA:H8	1.84	0.42
1:A:9:THR:O	1:A:11:LYS:HG2	2.19	0.42
1:A:185:TRP:O	1:A:189:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LEU:HD22	1:A:336:MET:HG2	2.02	0.42
1:A:383:PRO:HG3	1:A:512:PHE:CE2	2.54	0.42
1:A:583:MET:HG3	1:A:700:LEU:HB2	2.01	0.42
1:A:705:LEU:HD22	2:B:761:SER:CB	2.48	0.42
1:A:869:ARG:NH2	2:B:502:THR:O	2.52	0.42
2:B:417:ASP:O	2:B:419:LEU:N	2.52	0.42
2:B:552:ASN:ND2	2:B:565:ILE:O	2.50	0.42
2:B:556:TYR:HD2	2:B:600:HIS:CE1	2.37	0.42
2:B:778:ILE:HD11	2:B:906:PRO:HG2	2.00	0.42
7:G:97:ILE:HG21	7:G:140:PHE:HZ	1.85	0.42
9:I:34:PRO:C	9:I:35:ILE:HG13	2.43	0.42
11:K:107:THR:HG23	11:K:108:TYR:O	2.20	0.42
13:M:72:GLU:OE1	14:N:364:ARG:NE	2.50	0.42
13:M:113:LYS:O	13:M:117:HIS:HA	2.19	0.42
13:M:160:ALA:N	13:M:173:ILE:CD1	2.81	0.42
15:O:205:LYS:HG3	15:O:206:LEU:H	1.84	0.42
15:O:325:LYS:HE3	15:O:484:MET:SD	2.59	0.42
15:O:499:THR:HG21	16:P:312:PHE:CD1	2.54	0.42
1:A:67:CYS:H	1:A:71:HIS:HA	1.84	0.42
1:A:152:ARG:HE	1:A:184:ARG:NE	2.17	0.42
1:A:916:TYR:HB3	1:A:920:GLY:HA2	2.02	0.42
2:B:140:ASN:HB3	19:S:395:GLU:H	1.82	0.42
2:B:199:GLN:HG3	2:B:477:PHE:CE2	2.54	0.42
2:B:364:LYS:HG3	2:B:365:MET:N	2.25	0.42
2:B:398:ASP:C	2:B:425:HIS:HE1	2.27	0.42
2:B:475:SER:CB	2:B:510:LEU:O	2.64	0.42
3:C:8:GLU:HG3	3:C:11:ARG:CZ	2.48	0.42
3:C:52:ALA:HB2	3:C:310:PRO:HG2	2.01	0.42
3:C:60:ASP:CG	3:C:62:SER:H	2.27	0.42
3:C:256:ILE:HG22	3:C:267:VAL:HA	2.01	0.42
5:E:79:TRP:HE1	5:E:81:GLU:CD	2.27	0.42
5:E:180:ARG:C	5:E:182:ASP:N	2.76	0.42
7:G:207:LEU:HD23	7:G:209:SER:H	1.84	0.42
15:O:262:ILE:O	15:O:274:VAL:HA	2.19	0.42
15:O:484:MET:HA	15:O:487:LEU:HB3	2.01	0.42
15:O:517:VAL:HG11	15:O:522:ILE:HD11	2.01	0.42
15:O:573:SER:O	15:O:576:PHE:CD2	2.72	0.42
17:Q:65:VAL:C	17:Q:68:GLY:H	2.27	0.42
18:R:142:MET:HG3	18:R:144:ILE:HG22	2.01	0.42
18:R:144:ILE:HB	19:S:408:TYR:CE1	2.54	0.42
1:A:155:LEU:HD11	1:A:156:HIS:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:SER:HB2	1:A:664:MET:HE2	2.00	0.42
1:A:1373:ARG:CG	1:A:1374:PHE:N	2.83	0.42
1:A:1449:GLU:OE2	4:D:10:PHE:N	2.52	0.42
2:B:149:ILE:HD12	2:B:429:ILE:HG21	2.01	0.42
2:B:338:GLU:OE1	2:B:339:ALA:N	2.50	0.42
2:B:350:ALA:O	2:B:353:THR:N	2.52	0.42
2:B:837:GLN:OE1	2:B:837:GLN:N	2.52	0.42
2:B:1057:ASP:CG	2:B:1058:GLY:N	2.62	0.42
2:B:1088:ASP:OD2	2:B:1123:TYR:N	2.53	0.42
6:F:99:LEU:O	6:F:102:SER:OG	2.26	0.42
9:I:35:ILE:HB	9:I:36:GLU:H	1.59	0.42
13:M:91:ALA:HA	14:N:392:GLN:OE1	2.19	0.42
15:O:106:TYR:OH	17:Q:1079:UNK:N	2.52	0.42
15:O:242:LYS:O	15:O:246:LYS:N	2.40	0.42
15:O:528:MET:HE3	15:O:529:LYS:HG2	2.00	0.42
16:P:202:PRO:O	16:P:204:LYS:N	2.48	0.42
18:R:491:ASP:HB2	18:R:537:LYS:HG2	2.02	0.42
20:X:19:DA:H4'	20:X:20:DA:OP1	2.19	0.42
20:X:62:DG:O6	21:Y:2:DC:N4	2.53	0.42
1:A:269:ARG:HH22	1:A:284:ASP:N	2.17	0.42
1:A:444:LEU:HD12	1:A:444:LEU:C	2.45	0.42
1:A:552:ALA:HB3	1:A:671:ASP:CG	2.43	0.42
1:A:768:GLY:O	1:A:772:LYS:HB2	2.20	0.42
1:A:862:LEU:HD22	2:B:494:PHE:HB2	2.01	0.42
2:B:539:GLU:OE1	2:B:539:GLU:N	2.53	0.42
5:E:62:ALA:O	5:E:78:LEU:N	2.49	0.42
7:G:52:LEU:O	7:G:53:THR:HG22	2.20	0.42
15:O:507:LEU:HD12	15:O:508:SER:N	2.35	0.42
18:R:2:PRO:HG2	18:R:12:PHE:HE2	1.83	0.42
18:R:188:LYS:HB2	18:R:247:VAL:HG11	2.01	0.42
18:R:199:VAL:O	18:R:203:VAL:HG23	2.19	0.42
18:R:213:TRP:O	18:R:213:TRP:CG	2.72	0.42
19:S:382:ASP:C	19:S:384:HIS:H	2.27	0.42
21:Y:38:DA:C6	21:Y:39:DA:C6	3.07	0.42
1:A:223:ASN:O	1:A:226:LYS:HB3	2.20	0.42
1:A:541:LEU:HD13	1:A:682:LEU:HD22	2.02	0.42
1:A:916:TYR:CZ	1:A:1089:ILE:HG21	2.55	0.42
1:A:1141:ILE:HB	1:A:1295:VAL:HB	1.99	0.42
1:A:1338:GLU:O	1:A:1342:THR:HG22	2.19	0.42
1:A:1370:GLY:HA2	1:A:1375:GLY:HA2	2.01	0.42
1:A:1395:HIS:O	1:A:1399:ALA:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:ILE:HG13	2:B:43:ASP:HB3	2.00	0.42
2:B:230:LYS:HD2	2:B:242:LEU:HD22	2.01	0.42
2:B:354:ARG:O	2:B:358:MET:HG3	2.20	0.42
2:B:846:SER:OG	2:B:866:TYR:HB3	2.19	0.42
2:B:1025:GLN:O	2:B:1027:LEU:HD12	2.19	0.42
4:D:53:PRO:C	4:D:55:LEU:H	2.28	0.42
8:H:104:PHE:CE1	8:H:114:VAL:HG13	2.55	0.42
9:I:33:PHE:CE2	9:I:35:ILE:HA	2.55	0.42
13:M:131:TYR:HE2	13:M:133:LYS:HA	1.84	0.42
15:O:132:TYR:CZ	15:O:291:ARG:NH1	2.88	0.42
15:O:189:SER:O	15:O:190:LEU:O	2.38	0.42
16:P:135:LYS:HB3	16:P:151:TYR:CD1	2.52	0.42
16:P:218:THR:HG23	16:P:219:GLN:N	2.34	0.42
1:A:957:TYR:CD2	1:A:1035:PRO:HD3	2.54	0.42
1:A:1382:SER:HB2	1:A:1385:GLN:HG2	2.01	0.42
2:B:732:GLN:HB3	10:J:52:THR:CG2	2.50	0.42
2:B:790:LYS:HA	2:B:898:VAL:O	2.19	0.42
2:B:988:SER:HB2	2:B:998:TYR:HB2	2.00	0.42
3:C:100:ARG:HH21	10:J:5:VAL:HG13	1.84	0.42
4:D:1:MET:HG3	4:D:2:LYS:N	2.33	0.42
8:H:47:PHE:CZ	8:H:146:ARG:HG3	2.55	0.42
13:M:140:TRP:CD1	13:M:185:TYR:HB3	2.55	0.42
15:O:190:LEU:HB2	15:O:194:LEU:HG	2.01	0.42
15:O:471:THR:OG1	15:O:472:LYS:N	2.53	0.42
15:O:561:ARG:HD2	15:O:561:ARG:HA	1.41	0.42
15:O:599:ASN:ND2	15:O:630:VAL:HG11	2.34	0.42
16:P:21:GLN:O	16:P:26:GLY:N	2.50	0.42
18:R:81:ASN:CG	18:R:84:ARG:HH21	2.27	0.42
18:R:241:HIS:HD2	18:R:255:LEU:HD23	1.85	0.42
18:R:509:SER:OG	18:R:521:TYR:HD1	2.03	0.42
19:S:291:UNK:O	19:S:293:UNK:N	2.53	0.42
1:A:81:PHE:CD1	1:A:265:PRO:HD3	2.55	0.42
1:A:297:SER:HA	1:A:300:LYS:HB3	2.02	0.42
1:A:475:ASN:OD1	1:A:476:ARG:N	2.48	0.42
1:A:730:LEU:O	1:A:733:ILE:HG22	2.19	0.42
1:A:739:ASP:O	1:A:743:THR:HG22	2.19	0.42
1:A:758:GLU:C	1:A:760:GLN:H	2.27	0.42
1:A:991:LYS:HG3	1:A:993:GLU:HG2	2.01	0.42
1:A:1118:ASN:O	1:A:1138:THR:OG1	2.28	0.42
2:B:306:GLY:HA2	2:B:325:GLU:HB2	2.01	0.42
2:B:334:HIS:C	2:B:336:THR:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:615:VAL:HG22	2:B:671:THR:C	2.44	0.42
2:B:681:LEU:HD23	2:B:685:ALA:HB1	2.00	0.42
2:B:1036:HIS:CE1	2:B:1057:ASP:O	2.73	0.42
3:C:260:GLU:HB2	3:C:263:ASP:H	1.84	0.42
8:H:16:ASP:O	8:H:18:GLY:N	2.51	0.42
9:I:4:PHE:O	9:I:12:LEU:HD11	2.20	0.42
15:O:135:LEU:HB3	15:O:287:PHE:HZ	1.85	0.42
15:O:156:VAL:CG1	15:O:189:SER:CB	2.87	0.42
15:O:160:VAL:O	15:O:163:VAL:N	2.53	0.42
15:O:271:LEU:HD23	15:O:272:ARG:N	2.34	0.42
19:S:363:GLN:HB2	19:S:378:THR:HG21	2.02	0.42
21:Y:40:DA:H1'	21:Y:41:DG:O4'	2.19	0.42
1:A:95:TYR:O	1:A:98:ALA:HB3	2.20	0.42
1:A:134:ASN:O	1:A:137:ARG:HB2	2.19	0.42
1:A:235:LYS:HB3	1:A:252:ARG:CZ	2.49	0.42
1:A:269:ARG:NH2	1:A:283:ASP:C	2.74	0.42
1:A:912:VAL:HG23	1:A:913:GLN:N	2.35	0.42
2:B:322:GLU:C	2:B:324:ILE:H	2.27	0.42
2:B:1095:CYS:O	2:B:1099:GLY:HA2	2.20	0.42
4:D:11:LEU:H	7:G:3:ILE:HA	1.85	0.42
4:D:64:ASN:HD22	7:G:102:LEU:HD22	1.85	0.42
14:N:389:THR:C	14:N:391:LEU:N	2.76	0.42
15:O:76:VAL:HG23	15:O:120:TYR:HE1	1.85	0.42
15:O:190:LEU:HD13	15:O:194:LEU:CD2	2.40	0.42
15:O:347:ASP:OD1	15:O:348:GLU:N	2.53	0.42
16:P:170:LEU:HD23	16:P:171:ASP:N	2.34	0.42
18:R:470:GLN:HG2	18:R:475:ALA:O	2.20	0.42
18:R:486:ILE:N	18:R:543:ALA:O	2.52	0.42
19:S:458:PHE:O	19:S:462:GLU:HB3	2.17	0.42
19:S:484:TYR:CE1	19:S:488:ILE:HD13	2.55	0.42
1:A:163:VAL:C	1:A:180:HIS:CD2	2.83	0.42
1:A:176:LEU:HB3	1:A:320:GLN:HE21	1.85	0.42
1:A:235:LYS:HD3	1:A:252:ARG:HB3	2.02	0.42
1:A:625:ASN:N	1:A:625:ASN:OD1	2.51	0.42
2:B:300:GLN:O	2:B:304:TYR:N	2.37	0.42
2:B:552:ASN:OD1	2:B:553:TYR:HD2	2.02	0.42
2:B:690:TYR:N	2:B:691:PRO:HD3	2.35	0.42
2:B:713:ILE:O	2:B:749:LEU:HD13	2.19	0.42
2:B:842:TYR:HB2	2:B:881:ILE:HD11	2.02	0.42
2:B:909:GLY:HA2	2:B:921:VAL:CG1	2.49	0.42
3:C:78:VAL:HG11	3:C:108:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:LYS:HD2	10:J:57:ILE:CG2	2.50	0.42
10:J:48:ARG:HG3	10:J:49:MET:N	2.35	0.42
13:M:90:TYR:O	14:N:392:GLN:CD	2.62	0.42
13:M:164:LYS:HG3	14:N:300:LYS:HD3	2.01	0.42
15:O:125:GLU:OE1	15:O:288:MET:HE1	2.20	0.42
15:O:488:LYS:HD2	15:O:654:ALA:HB1	2.02	0.42
1:A:15:GLY:N	1:A:1408:VAL:HG12	2.14	0.41
1:A:235:LYS:O	1:A:236:SER:C	2.63	0.41
1:A:555:GLN:O	1:A:556:ASP:C	2.62	0.41
1:A:805:ASN:ND2	2:B:951:SER:HA	2.35	0.41
1:A:882:THR:O	1:A:885:MET:HB3	2.20	0.41
2:B:206:ILE:HD13	2:B:374:ASN:ND2	2.35	0.41
2:B:495:GLY:HA3	2:B:610:ARG:NH1	2.35	0.41
2:B:949:PHE:O	2:B:953:MET:N	2.52	0.41
2:B:1038:ARG:HD2	2:B:1057:ASP:OD2	2.20	0.41
3:C:110:PRO:O	3:C:111:ASP:HB2	2.19	0.41
3:C:256:ILE:HG22	3:C:267:VAL:HG22	2.01	0.41
13:M:84:SER:O	13:M:85:LEU:CD1	2.23	0.41
13:M:113:LYS:HD3	13:M:241:ALA:HA	2.01	0.41
15:O:74:LEU:HG	15:O:79:LEU:HD12	2.02	0.41
15:O:488:LYS:HA	15:O:491:VAL:HG23	2.02	0.41
15:O:597:GLN:OE1	15:O:597:GLN:N	2.53	0.41
16:P:169:GLU:CD	16:P:239:ASN:HD21	2.27	0.41
18:R:467:ARG:CG	18:R:610:LEU:HD22	2.49	0.41
1:A:38:ASP:CG	1:A:39:LEU:H	2.27	0.41
1:A:86:LEU:HD21	1:A:319:LEU:HD21	2.01	0.41
1:A:533:ASN:ND2	6:F:94:LEU:HD22	2.35	0.41
2:B:93:LEU:CD1	2:B:133:ILE:HG21	2.49	0.41
2:B:217:GLN:CG	2:B:232:TYR:HB3	2.50	0.41
2:B:767:ILE:HD12	2:B:767:ILE:HG23	1.80	0.41
2:B:1009:THR:O	11:K:74:ASN:ND2	2.53	0.41
14:N:385:GLY:O	14:N:416:ILE:HA	2.21	0.41
15:O:47:PHE:HB3	15:O:582:GLU:OE1	2.21	0.41
15:O:67:MET:HG2	15:O:83:ILE:HD11	2.01	0.41
15:O:472:LYS:CG	15:O:473:PRO:HD2	2.50	0.41
15:O:560:SER:O	15:O:560:SER:OG	2.31	0.41
16:P:69:GLU:HG3	16:P:70:LEU:N	2.28	0.41
18:R:455:GLU:HB3	18:R:592:LEU:HD23	2.02	0.41
20:X:57:DT:H2"	20:X:58:DC:C5	2.55	0.41
1:A:43:GLU:OE1	1:A:44:LYS:HG2	2.19	0.41
1:A:194:LYS:O	1:A:197:TRP:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:HD12	1:A:262:PRO:HD2	2.02	0.41
1:A:521:VAL:C	2:B:1082:ARG:HH22	2.26	0.41
1:A:602:TYR:N	3:C:23:PHE:O	2.54	0.41
1:A:712:ILE:HG13	2:B:946:PRO:HB3	2.02	0.41
1:A:896:LEU:HD11	1:A:912:VAL:HG21	2.02	0.41
1:A:1328:ILE:O	1:A:1331:ALA:N	2.53	0.41
2:B:1006:SER:O	2:B:1010:GLY:N	2.53	0.41
3:C:91:VAL:HG21	10:J:61:LEU:HD23	2.01	0.41
9:I:6:PRO:O	9:I:8:CYS:N	2.53	0.41
19:S:420:TRP:CD1	19:S:457:LYS:HD2	2.55	0.41
1:A:68:ALA:O	1:A:69:THR:C	2.64	0.41
1:A:200:GLU:HB3	15:O:516:LEU:HD21	1.96	0.41
1:A:235:LYS:HD3	1:A:252:ARG:CB	2.50	0.41
1:A:918:GLY:HA3	5:E:208:TYR:CD1	2.56	0.41
1:A:968:GLY:C	1:A:970:LEU:H	2.28	0.41
1:A:1053:LYS:O	1:A:1056:VAL:N	2.52	0.41
1:A:1162:GLU:O	1:A:1163:LYS:C	2.63	0.41
2:B:390:ASP:OD2	2:B:444:LEU:HG	2.20	0.41
2:B:751:ALA:C	2:B:1023:TYR:HH	2.28	0.41
2:B:883:GLN:HB3	2:B:899:LEU:HD21	2.03	0.41
2:B:961:LEU:HD22	2:B:1018:PHE:CE1	2.55	0.41
2:B:969:LEU:HB3	2:B:994:GLN:CD	2.46	0.41
2:B:1054:ARG:C	2:B:1055:SER:HG	2.19	0.41
5:E:128:PRO:N	5:E:129:PRO:HD2	2.35	0.41
5:E:143:ASN:OD1	5:E:143:ASN:N	2.52	0.41
7:G:129:ILE:HG23	7:G:138:LEU:HA	2.03	0.41
13:M:104:HIS:CE1	14:N:395:ILE:CD1	2.91	0.41
15:O:581:LEU:HB2	15:O:648:TRP:CH2	2.55	0.41
15:O:630:VAL:O	15:O:633:ARG:HB3	2.21	0.41
18:R:425:PHE:CE2	18:R:427:ALA:HB3	2.55	0.41
18:R:622:LEU:HD21	19:S:487:GLU:CD	2.46	0.41
1:A:152:ARG:HH21	1:A:184:ARG:HE	1.69	0.41
1:A:200:GLU:C	15:O:516:LEU:HD21	2.45	0.41
1:A:308:SER:HB3	1:A:311:ASN:ND2	2.36	0.41
1:A:833:PRO:CB	2:B:659:ILE:HD12	2.50	0.41
1:A:925:GLU:OE2	1:A:1081:ALA:HA	2.20	0.41
1:A:1026:ARG:NH2	8:H:129:TYR:OH	2.53	0.41
1:A:1451:LEU:O	4:D:111:ASN:ND2	2.52	0.41
2:B:232:TYR:CD1	2:B:242:LEU:HD23	2.55	0.41
2:B:306:GLY:CA	2:B:325:GLU:HB2	2.50	0.41
2:B:806:ILE:H	2:B:806:ILE:HG13	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1028:LYS:HG2	2:B:1029:HIS:N	2.33	0.41
4:D:28:LEU:HD13	4:D:56:GLN:HG3	2.02	0.41
4:D:131:MET:H	4:D:154:LEU:HD11	1.85	0.41
5:E:55:ARG:HB3	5:E:82:PHE:HD2	1.85	0.41
5:E:93:MET:HE1	5:E:124:VAL:HA	2.02	0.41
7:G:105:PHE:HD2	7:G:107:ASP:N	2.19	0.41
11:K:110:GLU:CD	11:K:111:THR:H	2.28	0.41
13:M:131:TYR:CE2	13:M:133:LYS:HA	2.55	0.41
13:M:251:THR:HG21	13:M:255:PHE:CD2	2.56	0.41
15:O:472:LYS:O	15:O:474:GLY:N	2.53	0.41
16:P:29:ALA:O	16:P:71:LYS:HD3	2.21	0.41
18:R:190:ASP:O	18:R:195:LYS:NZ	2.43	0.41
18:R:537:LYS:HD3	21:Y:52:DA:P	2.61	0.41
20:X:6:DA:H2"	20:X:7:DA:H8	1.84	0.41
1:A:191:ALA:HB3	1:A:194:LYS:HB3	2.02	0.41
1:A:385:PRO:HG3	2:B:764:GLY:CA	2.51	0.41
1:A:624:ILE:N	1:A:657:SER:OG	2.42	0.41
1:A:738:CYS:O	1:A:742:ILE:HG22	2.21	0.41
1:A:1169:VAL:O	1:A:1170:ALA:C	2.64	0.41
2:B:84:LEU:HD22	2:B:91:PHE:O	2.20	0.41
2:B:587:PHE:CE1	2:B:607:ARG:HD3	2.56	0.41
2:B:623:LYS:O	2:B:625:ILE:N	2.53	0.41
2:B:667:VAL:HG12	2:B:669:SER:H	1.85	0.41
2:B:710:ILE:HG12	2:B:1026:LYS:O	2.19	0.41
2:B:916:HIS:NE2	2:B:957:LYS:N	2.68	0.41
2:B:933:PHE:CE2	2:B:937:GLY:CA	2.94	0.41
2:B:936:GLN:CB	2:B:938:ILE:HD12	2.51	0.41
4:D:8:ASN:HB3	7:G:4:LEU:O	2.20	0.41
5:E:60:PHE:CZ	5:E:80:VAL:HG11	2.56	0.41
7:G:203:ASP:HB3	7:G:211:TRP:NE1	2.36	0.41
15:O:573:SER:HA	15:O:576:PHE:CD2	2.56	0.41
18:R:213:TRP:HD1	18:R:287:PRO:CD	2.22	0.41
18:R:387:SER:HB3	18:R:578:SER:C	2.45	0.41
1:A:64:SER:OG	1:A:65:LEU:N	2.53	0.41
1:A:305:LYS:HA	15:O:535:SER:OG	2.20	0.41
1:A:466:LEU:HD12	1:A:466:LEU:HA	1.91	0.41
1:A:1205:ILE:HA	1:A:1208:ALA:HB3	2.02	0.41
1:A:1299:GLY:O	1:A:1301:ARG:N	2.52	0.41
2:B:217:GLN:NE2	2:B:352:MET:HE3	2.35	0.41
2:B:531:LYS:HA	2:B:534:TYR:HD2	1.86	0.41
2:B:756:THR:H	10:J:48:ARG:HH12	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:106:LEU:HD12	3:C:208:CYS:SG	2.60	0.41
3:C:140:CYS:HB2	3:C:196:LEU:HD13	2.01	0.41
5:E:90:VAL:HG23	5:E:119:SER:OG	2.21	0.41
6:F:144:GLU:HG3	6:F:145:ASP:N	2.36	0.41
14:N:290:ILE:O	14:N:294:LEU:HB3	2.19	0.41
16:P:139:SER:OG	16:P:140:VAL:N	2.53	0.41
18:R:467:ARG:O	18:R:471:LYS:HB3	2.21	0.41
1:A:543:THR:OG1	1:A:544:PRO:HD2	2.21	0.41
1:A:719:PRO:HD3	1:A:810:VAL:HG13	2.02	0.41
1:A:896:LEU:HD23	1:A:1357:LEU:HD21	2.02	0.41
1:A:975:VAL:O	1:A:1002:ARG:NH2	2.47	0.41
2:B:464:ILE:HD11	2:B:746:TYR:HE1	1.84	0.41
2:B:797:ARG:NH1	18:R:137:GLU:OE1	2.54	0.41
2:B:957:LYS:HZ2	2:B:1022:ILE:HG21	1.86	0.41
2:B:1045:VAL:CG2	2:B:1046:LEU:N	2.83	0.41
5:E:27:GLY:O	5:E:65:THR:HG22	2.20	0.41
5:E:82:PHE:CG	5:E:83:CYS:N	2.89	0.41
8:H:15:VAL:HG13	8:H:24:CYS:SG	2.61	0.41
13:M:77:LYS:HG2	14:N:360:VAL:N	2.36	0.41
13:M:227:LEU:O	13:M:232:LEU:HB2	2.20	0.41
15:O:94:THR:HA	15:O:97:SER:HB2	2.02	0.41
15:O:570:GLU:OE1	15:O:570:GLU:N	2.40	0.41
1:A:33:GLU:HG3	1:A:83:HIS:HE2	1.84	0.41
1:A:228:LEU:HD12	1:A:257:ILE:HD11	2.03	0.41
1:A:322:THR:O	1:A:326:TYR:N	2.47	0.41
1:A:404:TYR:HD2	1:A:464:ARG:HH21	1.68	0.41
1:A:541:LEU:HG	1:A:551:ILE:CD1	2.47	0.41
1:A:665:ASP:OD2	1:A:797:CYS:HA	2.21	0.41
1:A:792:LEU:O	1:A:796:THR:HB	2.20	0.41
1:A:887:ARG:HE	2:B:1064:GLU:CD	2.28	0.41
1:A:975:VAL:HG13	1:A:976:ARG:N	2.35	0.41
1:A:1448:PHE:CZ	4:D:16:VAL:HG23	2.56	0.41
2:B:98:ILE:CD1	2:B:131:VAL:HG12	2.51	0.41
2:B:112:LEU:HD22	2:B:162:ILE:CG1	2.51	0.41
2:B:239:LYS:NZ	2:B:241:TYR:HE2	2.19	0.41
2:B:368:ASP:C	2:B:370:ASP:H	2.28	0.41
2:B:622:VAL:O	2:B:626:HIS:HD2	2.04	0.41
2:B:625:ILE:HD11	2:B:628:ARG:HH21	1.86	0.41
2:B:738:THR:H	2:B:741:ILE:HD13	1.86	0.41
2:B:738:THR:HA	2:B:976:GLY:O	2.21	0.41
2:B:800:ASN:OD1	2:B:855:PRO:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:889:SER:OG	2:B:891:ASN:OD1	2.36	0.41
2:B:1077:GLN:O	2:B:1081:GLU:HB2	2.20	0.41
4:D:157:ILE:HG13	4:D:161:ALA:HB3	2.03	0.41
5:E:181:ALA:O	5:E:186:LEU:HG	2.21	0.41
7:G:44:LEU:HD21	7:G:105:PHE:CE1	2.56	0.41
7:G:46:ILE:N	7:G:75:VAL:O	2.51	0.41
7:G:126:SER:CB	7:G:139:TYR:HB3	2.49	0.41
7:G:152:ARG:HB3	7:G:197:LEU:HD11	2.03	0.41
13:M:236:VAL:O	13:M:240:GLU:N	2.51	0.41
15:O:172:GLU:O	15:O:176:SER:CB	2.69	0.41
15:O:547:GLU:HG2	15:O:548:ILE:N	2.22	0.41
15:O:595:LEU:HD22	15:O:633:ARG:CZ	2.51	0.41
15:O:639:ALA:O	15:O:643:ARG:HG3	2.21	0.41
16:P:25:LYS:HG3	16:P:26:GLY:N	2.36	0.41
16:P:96:TYR:OH	16:P:113:ARG:NH1	2.54	0.41
17:Q:48:THR:HG23	17:Q:51:GLU:H	1.86	0.41
18:R:172:GLU:HG2	18:R:502:ALA:O	2.21	0.41
18:R:249:HIS:CD2	19:S:406:TYR:CE2	3.09	0.41
18:R:471:LYS:HD3	18:R:614:LEU:HD23	2.02	0.41
18:R:508:PHE:O	18:R:522:ARG:N	2.28	0.41
19:S:491:ASN:OD1	19:S:492:ILE:N	2.53	0.41
20:X:60:DA:C6	21:Y:4:DT:C4	3.09	0.41
1:A:87:ALA:O	1:A:88:LEU:HB2	2.21	0.41
1:A:565:SER:OG	1:A:663:VAL:HA	2.21	0.41
1:A:570:PHE:CE1	1:A:605:THR:HG22	2.56	0.41
1:A:660:LEU:HG	8:H:117:SER:OG	2.21	0.41
1:A:773:VAL:O	1:A:776:GLU:HB3	2.21	0.41
1:A:792:LEU:HG	1:A:796:THR:OG1	2.21	0.41
1:A:1072:GLU:O	1:A:1076:PHE:HB2	2.21	0.41
2:B:225:HIS:CD2	2:B:226:GLU:HG2	2.56	0.41
2:B:521:THR:HG21	2:B:587:PHE:CD2	2.56	0.41
2:B:930:ASP:O	2:B:931:MET:HB3	2.20	0.41
2:B:938:ILE:CG1	10:J:45:CYS:SG	3.09	0.41
2:B:961:LEU:HD21	2:B:1019:PHE:C	2.46	0.41
2:B:1093:ASP:OD1	2:B:1118:LYS:HG2	2.21	0.41
4:D:133:HIS:HE1	7:G:212:GLU:H	1.68	0.41
5:E:3:GLN:O	5:E:6:GLU:HB2	2.21	0.41
6:F:81:THR:HG22	6:F:82:THR:N	2.35	0.41
13:M:184:LYS:HD2	13:M:184:LYS:HA	1.70	0.41
15:O:174:TYR:O	15:O:178:VAL:HG23	2.21	0.41
15:O:197:MET:HE1	15:O:320:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:340:GLU:O	15:O:343:LYS:N	2.51	0.41
17:Q:52:ARG:O	17:Q:55:ALA:N	2.54	0.41
18:R:231:ALA:HA	18:R:234:MET:HB3	2.03	0.41
18:R:420:TYR:CZ	18:R:422:PRO:HG3	2.56	0.41
18:R:528:ILE:HG23	18:R:541:THR:O	2.21	0.41
1:A:201:TRP:CD1	1:A:216:LYS:NZ	2.90	0.40
1:A:409:THR:O	1:A:410:ARG:C	2.64	0.40
1:A:424:PRO:HG2	1:A:444:LEU:HD23	2.03	0.40
1:A:535:MET:HG3	2:B:1073:TYR:CD1	2.57	0.40
1:A:630:ASN:ND2	1:A:663:VAL:O	2.55	0.40
1:A:717:VAL:O	1:A:810:VAL:HG22	2.20	0.40
1:A:794:MET:SD	2:B:947:HIS:ND1	2.93	0.40
1:A:913:GLN:HG2	1:A:915:THR:O	2.21	0.40
1:A:921:LEU:HG	1:A:1081:ALA:O	2.21	0.40
2:B:251:ILE:CG2	2:B:256:VAL:HG23	2.51	0.40
2:B:526:GLU:O	2:B:529:ILE:HG22	2.21	0.40
5:E:54:GLN:HB2	5:E:57:MET:HE2	2.02	0.40
6:F:76:LYS:HD3	6:F:79:ARG:HH21	1.86	0.40
10:J:52:THR:HG22	10:J:53:HIS:N	2.32	0.40
13:M:91:ALA:N	14:N:392:GLN:NE2	2.69	0.40
15:O:103:CYS:C	15:O:123:ASN:HB2	2.46	0.40
15:O:516:LEU:O	15:O:516:LEU:CG	2.66	0.40
16:P:110:ILE:O	16:P:114:THR:HG22	2.22	0.40
18:R:505:HIS:O	18:R:508:PHE:N	2.50	0.40
20:X:7:DA:H2"	20:X:8:DC:C5	2.56	0.40
20:X:52:DA:H8	20:X:52:DA:OP2	2.03	0.40
1:A:526:GLU:O	1:A:529:ALA:N	2.54	0.40
1:A:530:GLU:OE2	2:B:1075:ALA:HA	2.21	0.40
1:A:1350:VAL:O	1:A:1351:ASP:HB2	2.22	0.40
2:B:249:GLU:HB3	2:B:250:GLU:HG2	2.03	0.40
2:B:637:PHE:C	2:B:639:ASP:H	2.29	0.40
2:B:789:ARG:O	2:B:899:LEU:HA	2.21	0.40
2:B:929:GLU:OE2	3:C:73:SER:OG	2.28	0.40
2:B:1005:TYR:OH	3:C:293:ARG:NH1	2.54	0.40
2:B:1042:PRO:HB3	18:R:38:VAL:HG22	2.04	0.40
8:H:18:GLY:C	8:H:20:TYR:H	2.28	0.40
9:I:19:SER:O	9:I:21:VAL:HG23	2.21	0.40
12:L:29:TYR:HB2	12:L:30:ILE:H	1.75	0.40
13:M:158:GLN:NE2	14:N:308:GLN:HE21	2.05	0.40
14:N:279:GLU:O	14:N:282:LEU:HB2	2.22	0.40
14:N:287:HIS:ND1	14:N:369:GLY:O	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:127:ILE:O	15:O:130:LEU:HB2	2.21	0.40
15:O:133:SER:O	15:O:137:ILE:HG13	2.22	0.40
15:O:190:LEU:CD1	15:O:194:LEU:CD2	2.97	0.40
15:O:509:ARG:O	15:O:512:ARG:HB3	2.20	0.40
15:O:636:ASN:O	15:O:640:ARG:HG2	2.20	0.40
16:P:140:VAL:CG2	16:P:158:ASP:HB3	2.51	0.40
18:R:509:SER:HA	18:R:521:TYR:HA	2.02	0.40
19:S:415:SER:OG	19:S:416:TYR:N	2.53	0.40
20:X:11:DA:C5	20:X:12:DT:C4	3.09	0.40
20:X:18:DT:H73	20:X:19:DA:N7	2.36	0.40
1:A:496:ARG:O	1:A:497:THR:HB	2.21	0.40
1:A:498:PHE:CZ	1:A:519:LEU:HD13	2.57	0.40
1:A:552:ALA:CB	1:A:671:ASP:H	2.33	0.40
1:A:792:LEU:HD11	8:H:19:ARG:NH2	2.37	0.40
1:A:1127:LYS:O	1:A:1131:ASN:HB3	2.21	0.40
1:A:1145:LEU:HB3	1:A:1146:VAL:H	1.48	0.40
1:A:1217:ILE:H	1:A:1217:ILE:HD12	1.87	0.40
1:A:1318:HIS:NE2	1:A:1321:GLU:HB3	2.36	0.40
2:B:517:MET:HE2	2:B:611:PRO:HD2	2.03	0.40
3:C:259:ASP:HB2	3:C:266:TYR:CE1	2.57	0.40
7:G:2:PHE:CD2	7:G:79:PRO:HB3	2.56	0.40
7:G:52:LEU:HD12	7:G:53:THR:HG22	2.04	0.40
11:K:61:ALA:O	11:K:104:ARG:HD2	2.21	0.40
15:O:226:ILE:O	15:O:228:ARG:N	2.46	0.40
15:O:253:ILE:O	15:O:256:PRO:HD2	2.21	0.40
15:O:465:PHE:HA	15:O:466:PRO:HA	1.86	0.40
15:O:498:SER:HG	16:P:296:TYR:HB2	1.85	0.40
15:O:519:GLU:HG3	15:O:534:ARG:NH2	2.36	0.40
15:O:564:PHE:C	15:O:565:LEU:HD12	2.45	0.40
16:P:117:HIS:HB3	16:P:119:HIS:ND1	2.36	0.40
18:R:237:LEU:C	18:R:237:LEU:HD12	2.46	0.40
18:R:609:GLU:HG2	18:R:613:HIS:NE2	2.36	0.40
20:X:5:DC:H2"	20:X:6:DA:H8	1.85	0.40
1:A:395:PRO:CB	1:A:496:ARG:HA	2.43	0.40
1:A:400:LYS:CA	1:A:465:HIS:HD2	2.26	0.40
1:A:1164:THR:CB	1:A:1271:VAL:HA	2.49	0.40
2:B:227:ARG:NH1	2:B:449:MET:HE3	2.36	0.40
2:B:721:ILE:HG22	2:B:790:LYS:HD3	2.04	0.40
2:B:1041:GLY:HA3	2:B:1057:ASP:OD2	2.22	0.40
3:C:31:TRP:CE3	11:K:82:LYS:HD2	2.56	0.40
7:G:195:ALA:C	7:G:196:LEU:HD12	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:110:ASP:O	8:H:111:LEU:HD12	2.21	0.40
13:M:140:TRP:CG	13:M:185:TYR:HB3	2.57	0.40
14:N:286:ASP:O	14:N:290:ILE:HG22	2.22	0.40
15:O:358:GLY:HA2	15:O:361:PHE:CD2	2.56	0.40
16:P:218:THR:OG1	16:P:219:GLN:N	2.54	0.40
18:R:269:LYS:O	18:R:272:VAL:HG12	2.21	0.40
20:X:54:DG:H2"	20:X:55:DA:C8	2.57	0.40
1:A:85:LYS:HD2	1:A:260:TYR:HE1	1.87	0.40
1:A:228:LEU:HD21	1:A:232:LYS:HE3	2.03	0.40
1:A:384:ASP:HA	2:B:765:TYR:CE2	2.57	0.40
1:A:666:LYS:O	1:A:667:SER:C	2.64	0.40
1:A:889:LEU:HD12	1:A:889:LEU:HA	1.88	0.40
1:A:995:VAL:HG21	5:E:209:ALA:HB2	2.02	0.40
2:B:244:HIS:ND1	2:B:332:ILE:HD12	2.37	0.40
2:B:309:VAL:HG22	2:B:310:LYS:N	2.35	0.40
2:B:756:THR:N	10:J:48:ARG:HH12	2.19	0.40
2:B:888:VAL:HG23	2:B:893:GLN:O	2.21	0.40
7:G:157:ASP:CG	7:G:158:VAL:H	2.29	0.40
7:G:207:LEU:HB3	7:G:210:TRP:CE2	2.56	0.40
8:H:94:ASP:HB3	8:H:145:ARG:HA	2.04	0.40
8:H:123:MET:HE1	8:H:142:LEU:HD13	2.04	0.40
14:N:364:ARG:HG3	14:N:365:VAL:N	2.36	0.40
15:O:289:LYS:HZ3	15:O:325:LYS:HD3	1.87	0.40
15:O:528:MET:HG3	15:O:529:LYS:N	2.37	0.40
15:O:537:LEU:O	15:O:540:LEU:HB3	2.21	0.40
16:P:203:LYS:HD2	16:P:206:VAL:CG2	2.52	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%)	1135 (80%)	265 (19%)	22 (2%)	8	39
2	B	1112/1149 (97%)	912 (82%)	183 (16%)	17 (2%)	8	39
3	C	333/335 (99%)	278 (84%)	50 (15%)	5 (2%)	8	39
4	D	113/161 (70%)	85 (75%)	27 (24%)	1 (1%)	14	49
5	E	213/215 (99%)	177 (83%)	32 (15%)	4 (2%)	6	34
6	F	81/155 (52%)	69 (85%)	11 (14%)	1 (1%)	10	42
7	G	178/212 (84%)	147 (83%)	27 (15%)	4 (2%)	5	31
8	H	136/146 (93%)	111 (82%)	25 (18%)	0	100	100
9	I	40/110 (36%)	30 (75%)	8 (20%)	2 (5%)	1	18
10	J	65/70 (93%)	54 (83%)	11 (17%)	0	100	100
11	K	99/142 (70%)	82 (83%)	17 (17%)	0	100	100
12	L	44/70 (63%)	37 (84%)	7 (16%)	0	100	100
13	M	160/282 (57%)	126 (79%)	29 (18%)	5 (3%)	3	25
14	N	106/422 (25%)	84 (79%)	21 (20%)	1 (1%)	14	49
15	O	533/654 (82%)	411 (77%)	108 (20%)	14 (3%)	4	28
16	P	271/317 (86%)	225 (83%)	44 (16%)	2 (1%)	18	55
17	Q	33/251 (13%)	26 (79%)	5 (15%)	2 (6%)	1	15
18	R	514/736 (70%)	453 (88%)	59 (12%)	2 (0%)	30	65
19	S	172/594 (29%)	156 (91%)	16 (9%)	0	100	100
All	All	5625/7481 (75%)	4598 (82%)	945 (17%)	82 (2%)	11	39

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	PRO
1	A	587	ILE
1	A	599	LYS
1	A	1371	ILE
2	B	1046	LEU
2	B	1140	ARG
3	C	87	ASN
5	E	180	ARG
5	E	181	ALA
9	I	21	VAL
13	M	84	SER
13	M	103	GLU

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Mol	Chain	Res	Type
13	M	107	ILE
14	N	391	LEU
15	O	146	VAL
15	O	188	SER
15	O	189	SER
15	O	194	LEU
17	Q	39	ILE
1	A	975	VAL
1	A	995	VAL
1	A	1372	THR
2	B	87	VAL
2	B	168	GLU
3	C	120	LEU
7	G	125	GLU
9	I	35	ILE
13	M	105	PRO
15	O	352	VAL
16	P	295	ASN
1	A	39	LEU
1	A	236	SER
1	A	238	ASP
1	A	239	CYS
1	A	307	ILE
1	A	675	HIS
1	A	998	TYR
2	B	335	LEU
2	B	418	ALA
2	B	1056	ARG
3	C	122	ASP
3	C	255	VAL
13	M	243	ILE
15	O	133	SER
15	O	190	LEU
18	R	274	LYS
1	A	109	ASN
1	A	1328	ILE
2	B	713	ILE
2	B	766	ASP
2	B	767	ILE
2	B	823	SER
2	B	934	ASN
2	B	1057	ASP

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Mol	Chain	Res	Type
5	E	147	HIS
5	E	182	ASP
6	F	144	GLU
7	G	111	PRO
15	O	191	PHE
1	A	43	GLU
1	A	829	ASP
1	A	1145	LEU
3	C	223	SER
7	G	191	PRO
15	O	499	THR
1	A	277	SER
1	A	1300	LEU
2	B	822	GLN
2	B	215	ILE
15	O	274	VAL
1	A	672	GLY
4	D	127	LEU
15	O	187	ILE
15	O	297	ILE
2	B	811	VAL
2	B	1137	ILE
15	O	88	VAL
15	O	473	PRO
16	P	206	VAL
17	Q	40	PRO
18	R	516	PHE
7	G	158	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1232/1257 (98%)	1223 (99%)	9 (1%)	76	79
2	B	975/1006 (97%)	968 (99%)	7 (1%)	76	79
3	C	296/296 (100%)	294 (99%)	2 (1%)	76	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	110/145 (76%)	109 (99%)	1 (1%)	70	76
5	E	197/197 (100%)	196 (100%)	1 (0%)	81	82
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	164/190 (86%)	163 (99%)	1 (1%)	78	80
8	H	123/128 (96%)	123 (100%)	0	100	100
9	I	38/98 (39%)	37 (97%)	1 (3%)	40	61
10	J	62/65 (95%)	61 (98%)	1 (2%)	55	69
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%)	140 (99%)	2 (1%)	59	71
14	N	92/360 (26%)	90 (98%)	2 (2%)	45	64
15	O	495/593 (84%)	493 (100%)	2 (0%)	84	83
16	P	255/285 (90%)	255 (100%)	0	100	100
17	Q	31/195 (16%)	30 (97%)	1 (3%)	34	56
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%)	4993 (99%)	30 (1%)	76	80

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	CYS
1	A	247	THR
1	A	248	VAL
1	A	364	PHE
1	A	669	LEU
1	A	950	GLN
1	A	1145	LEU
1	A	1369	LEU
1	A	1373	ARG
2	B	110	ASP
2	B	112	LEU
2	B	551	LEU
2	B	741	ILE
2	B	772	VAL
2	B	933	PHE

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Mol	Chain	Res	Type
2	B	1047	THR
3	C	35	LYS
3	C	120	LEU
4	D	127	LEU
5	E	180	ARG
7	G	125	GLU
9	I	35	ILE
10	J	43	ARG
13	M	104	HIS
13	M	183	PHE
14	N	391	LEU
14	N	392	GLN
15	O	498	SER
15	O	561	ARG
17	Q	39	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	161	ASN
1	A	207	HIS
1	A	315	HIS
1	A	386	ASN
1	A	437	ASN
1	A	520	HIS
1	A	523	GLN
1	A	533	ASN
1	A	566	HIS
1	A	589	HIS
1	A	618	HIS
1	A	619	ASN
1	A	675	HIS
1	A	707	ASN
1	A	725	GLN
1	A	828	GLN
1	A	899	GLN
1	A	913	GLN
1	A	1385	GLN
1	A	1419	GLN
2	B	140	ASN
2	B	217	GLN

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Mol	Chain	Res	Type
2	B	225	HIS
2	B	270	GLN
2	B	286	ASN
2	B	299	GLN
2	B	374	ASN
2	B	411	ASN
2	B	425	HIS
2	B	519	HIS
2	B	574	GLN
2	B	600	HIS
2	B	626	HIS
2	B	693	HIS
2	B	717	GLN
2	B	754	ASN
2	B	774	ASN
2	B	800	ASN
2	B	865	GLN
2	B	880	HIS
2	B	902	GLN
2	B	928	GLN
2	B	936	GLN
2	B	1029	HIS
3	C	65	ASN
3	C	93	GLN
3	C	99	HIS
3	C	130	ASN
3	C	175	GLN
3	C	207	HIS
3	C	330	ASN
4	D	31	GLN
5	E	54	GLN
5	E	104	ASN
5	E	114	ASN
5	E	153	HIS
5	E	174	GLN
8	H	133	ASN
11	K	74	ASN
11	K	118	GLN
13	M	86	HIS
13	M	178	GLN
13	M	190	ASN
13	M	254	GLN

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Mol	Chain	Res	Type
14	N	288	GLN
14	N	308	GLN
14	N	377	ASN
15	O	43	ASN
15	O	56	HIS
15	O	100	GLN
15	O	147	ASN
15	O	222	HIS
15	O	298	ASN
15	O	332	GLN
15	O	337	GLN
15	O	346	GLN
15	O	549	GLN
15	O	587	ASN
15	O	626	GLN
15	O	652	GLN
16	P	33	GLN
16	P	34	GLN
16	P	117	HIS
16	P	189	ASN
16	P	219	GLN
16	P	305	HIS
18	R	6	ASN
18	R	8	HIS
18	R	20	ASN
18	R	35	ASN
18	R	82	ASN
18	R	169	HIS
18	R	183	GLN
18	R	184	HIS
18	R	278	ASN
18	R	414	HIS
19	S	444	GLN
19	S	499	ASN
19	S	506	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	37.73
1	Q	70:PHE	C	1070:UNK	N	12.87

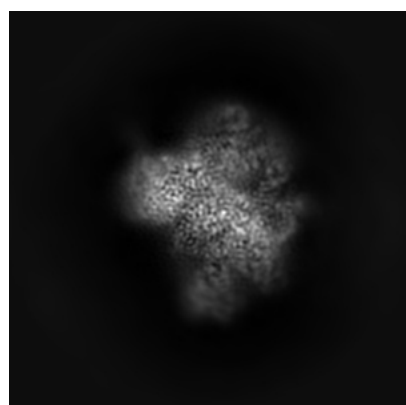
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7531. These allow visual inspection of the internal detail of the map and identification of artifacts.

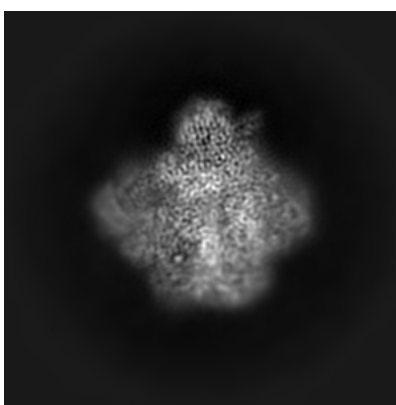
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

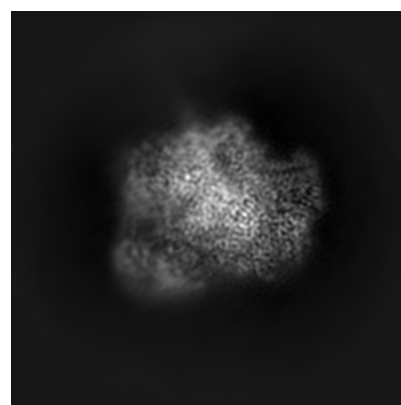
6.1.1 Primary map



X



Y

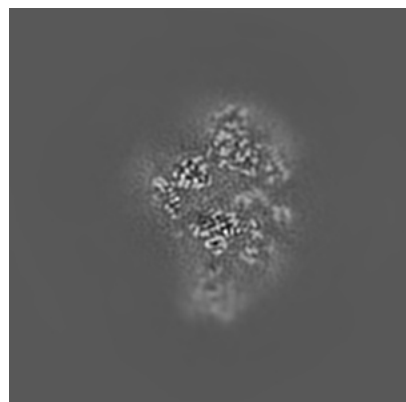


Z

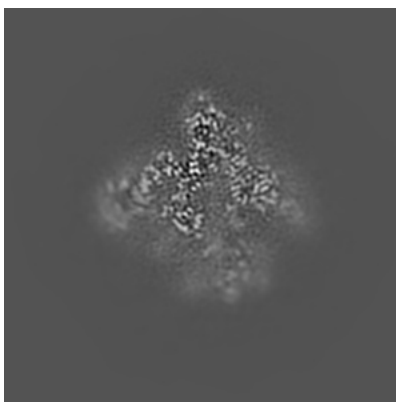
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

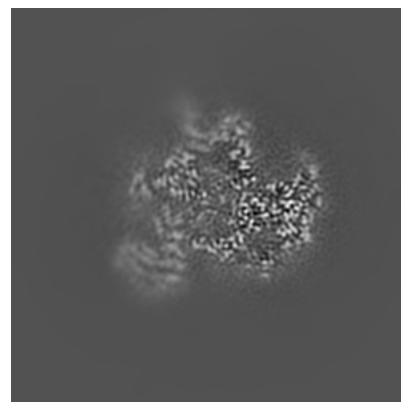
6.2.1 Primary map



X Index: 144



Y Index: 144

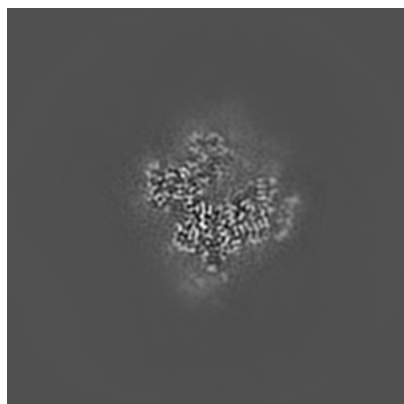


Z Index: 144

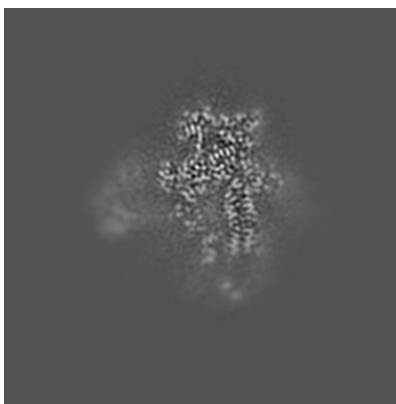
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

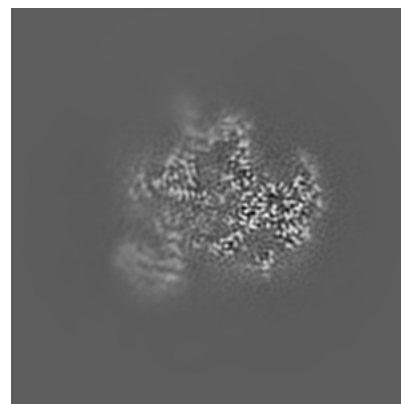
6.3.1 Primary map



X Index: 168



Y Index: 133

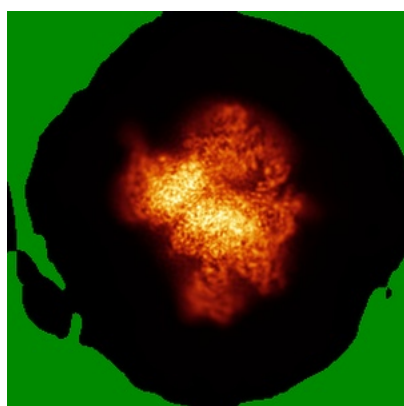


Z Index: 143

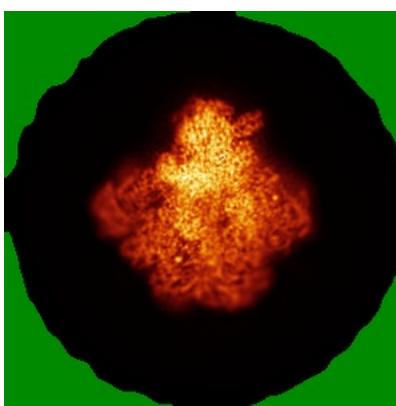
The images above show the largest variance slices of the map in three orthogonal directions.

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

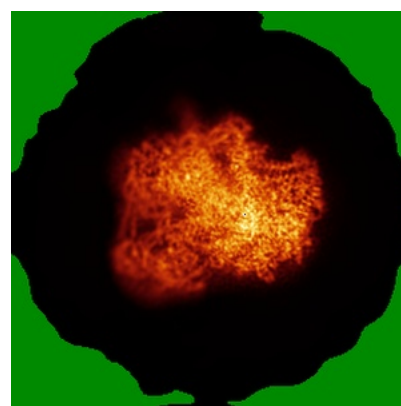
6.4.1 Primary map



X



Y

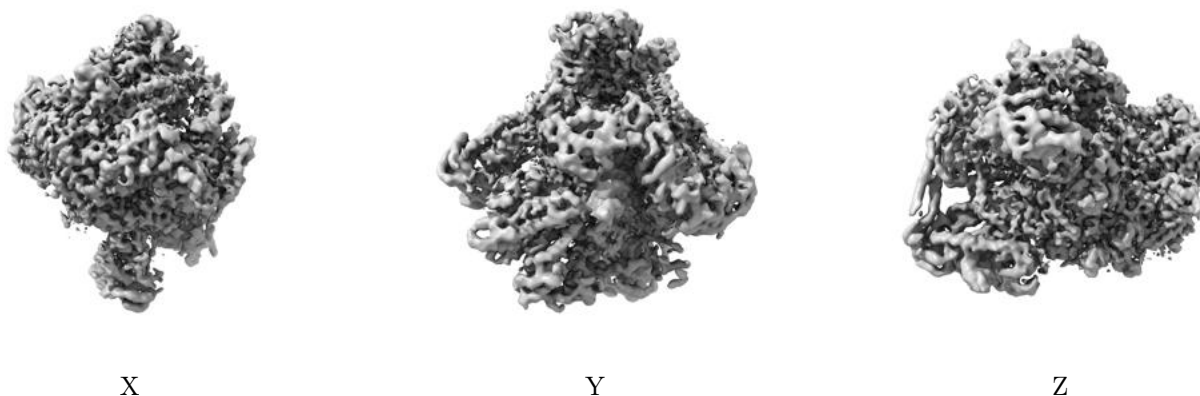


Z

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

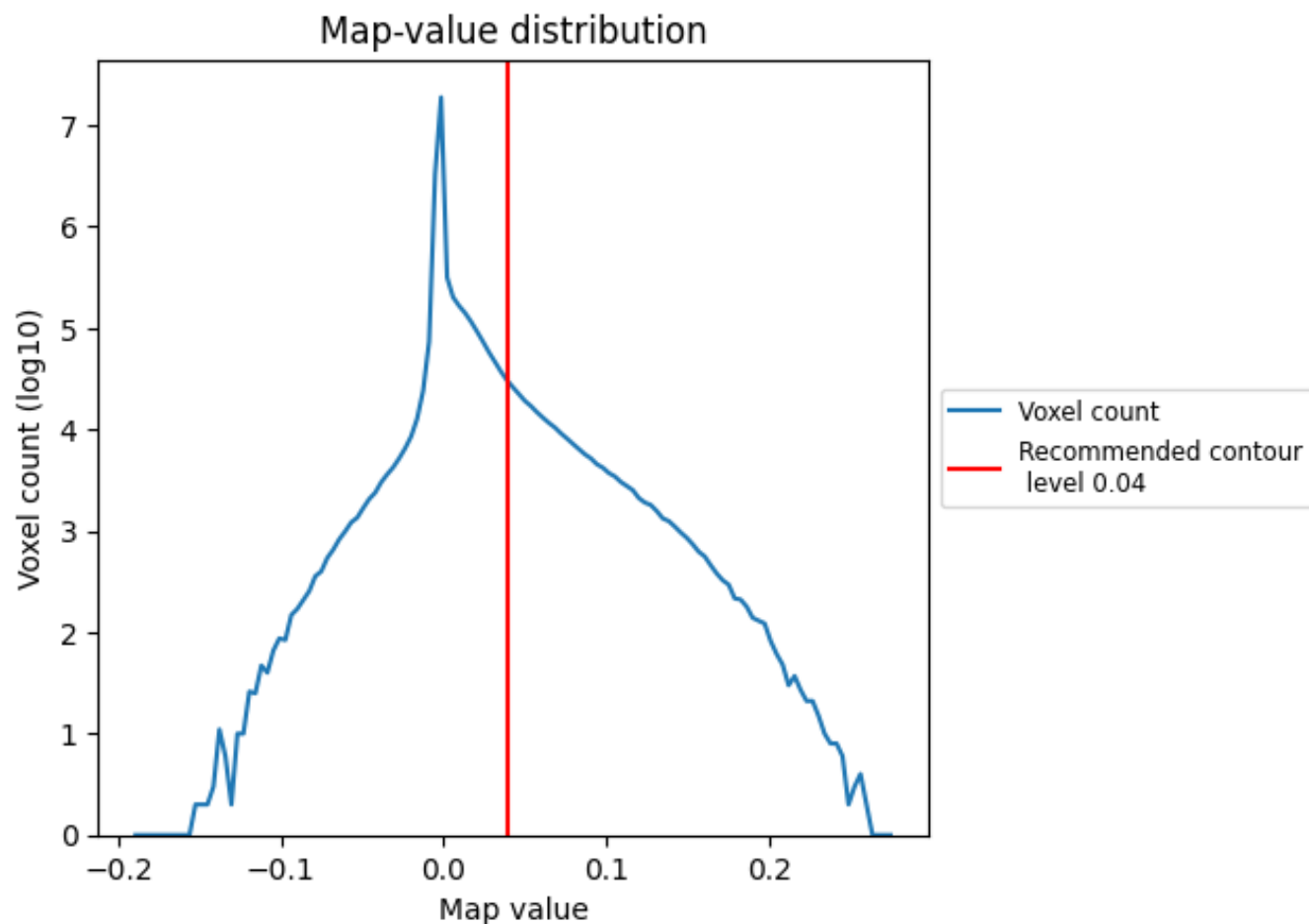
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

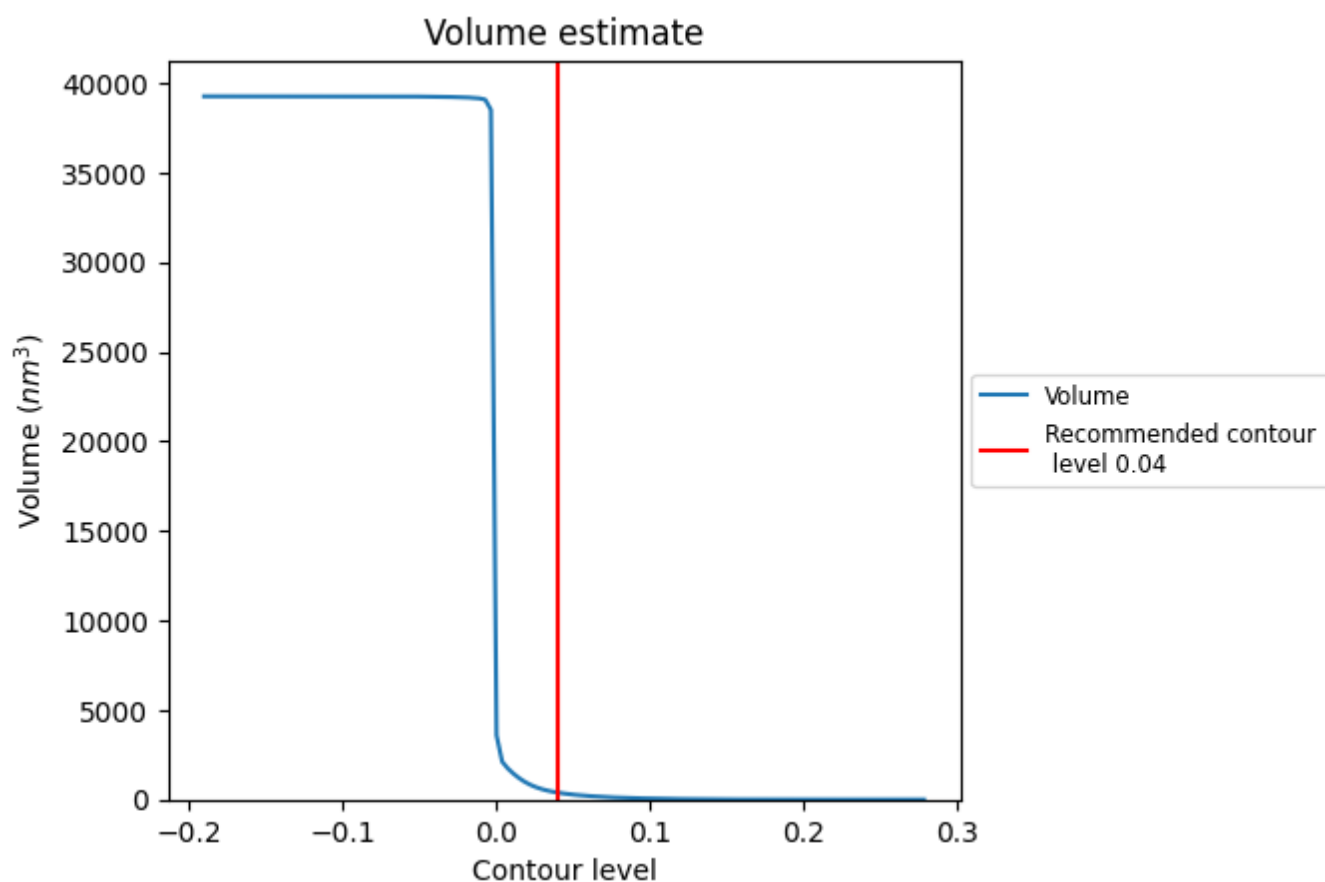
This section contains the results of statistical analysis of the map.

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.

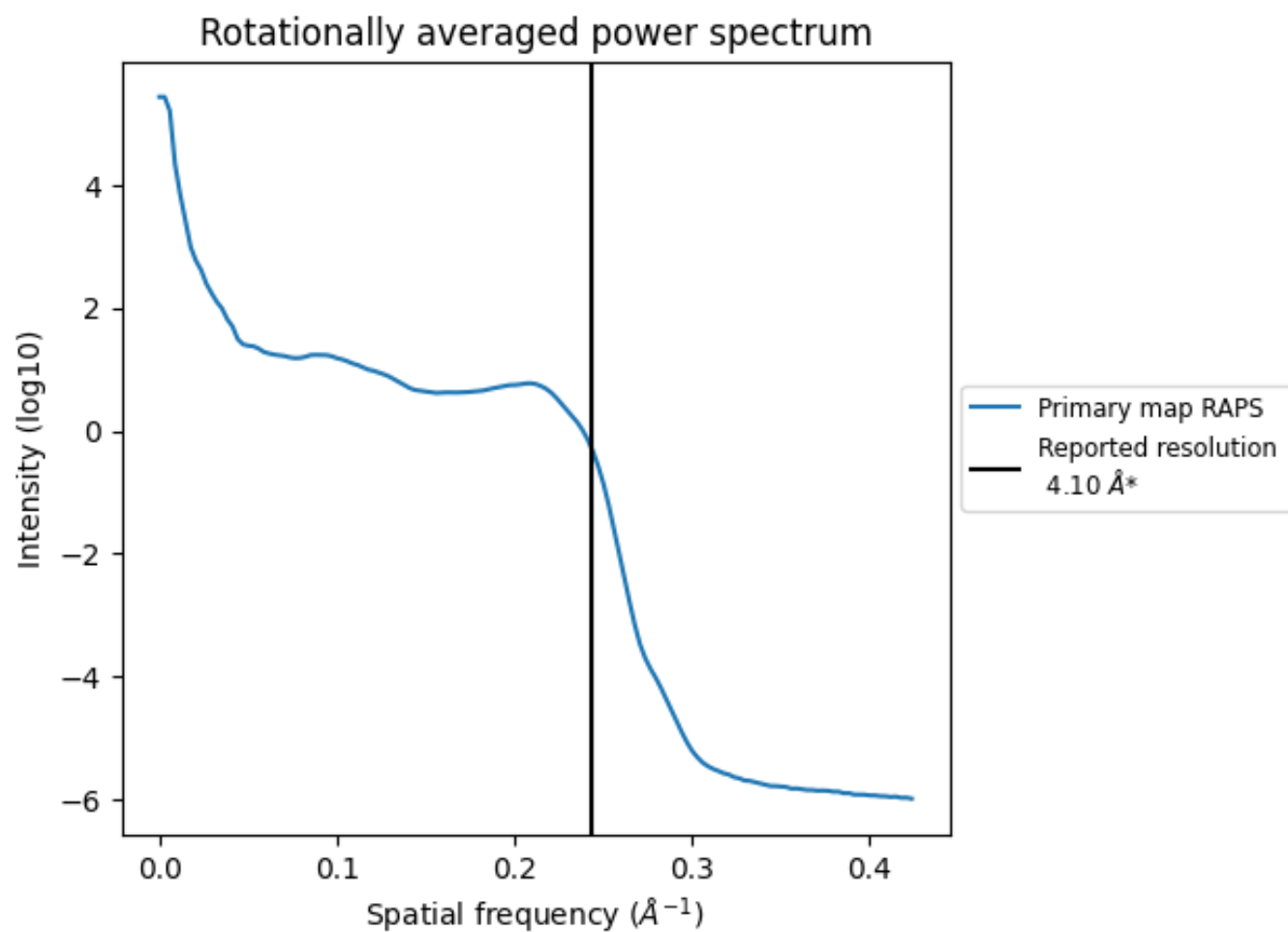
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 395 nm³; this corresponds to an approximate mass of 357 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 ⓘ

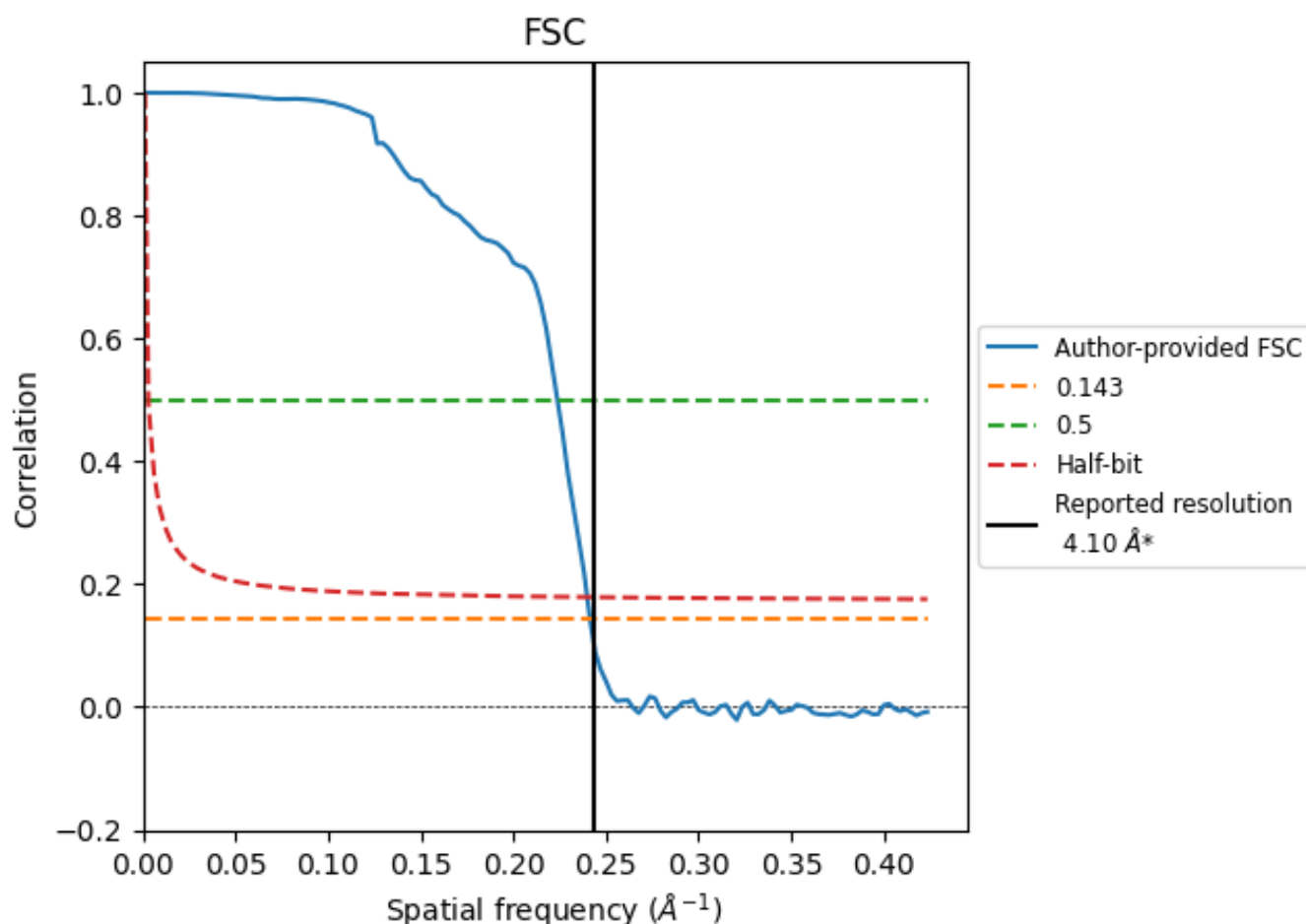


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.14	4.47	4.17
Unmasked-calculated*	-	-	-

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

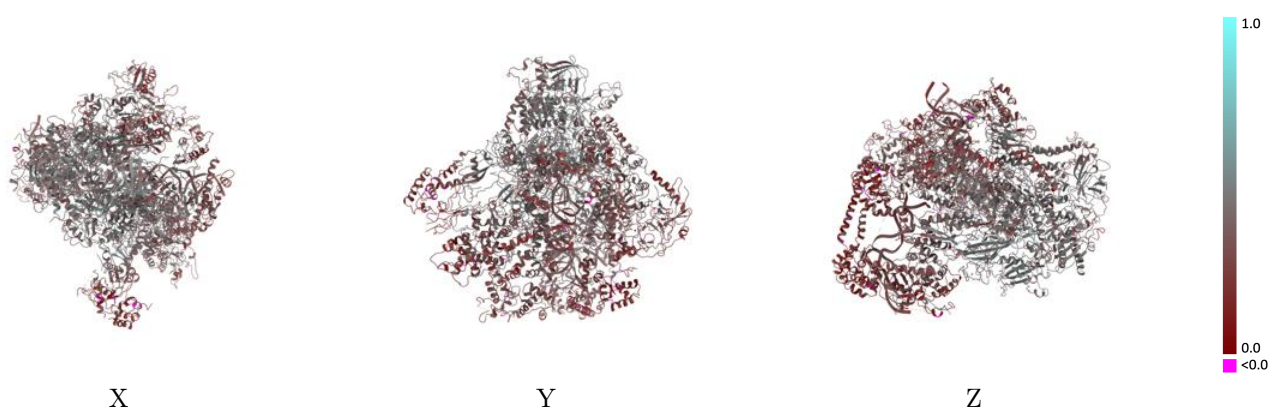
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7531 and PDB model 6CNC. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

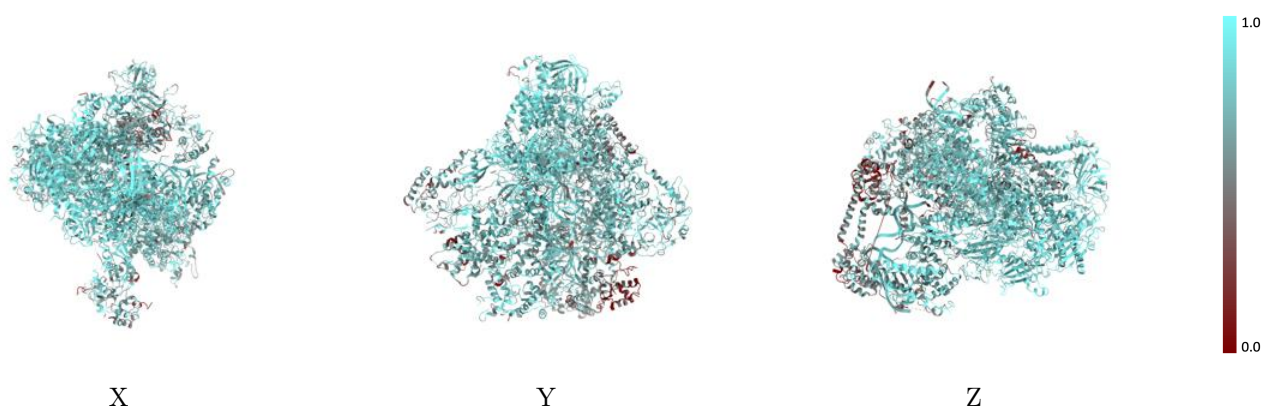
This section was not generated.

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



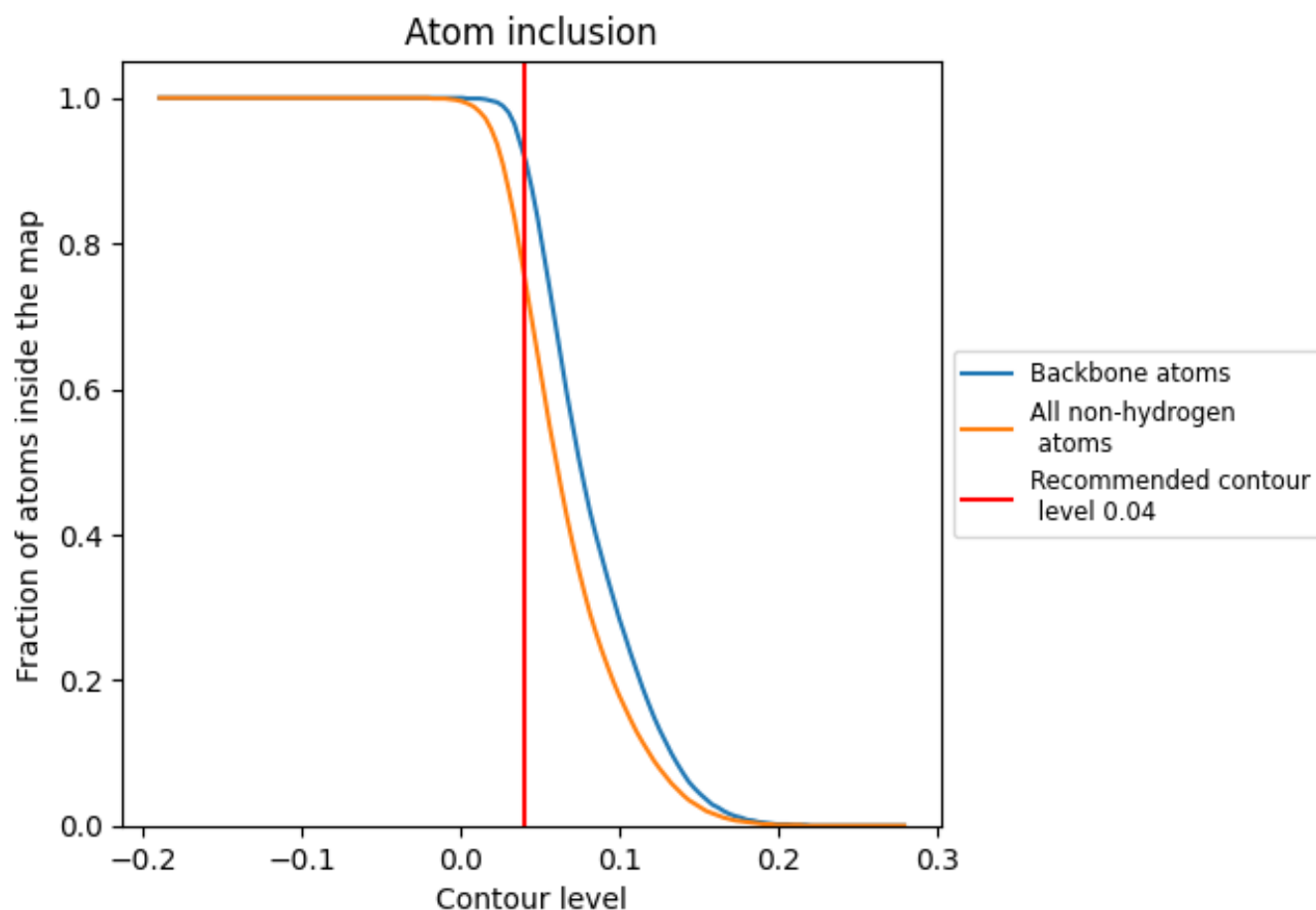
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 75% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7530	 0.3610
A	 0.7810	 0.3990
B	 0.8030	 0.4160
C	 0.8750	 0.4350
D	 0.6050	 0.2130
E	 0.7830	 0.3590
F	 0.8820	 0.4480
G	 0.7220	 0.3000
H	 0.8320	 0.4340
I	 0.7450	 0.3340
J	 0.8800	 0.4440
K	 0.8630	 0.4420
L	 0.8260	 0.4250
M	 0.6800	 0.2940
N	 0.6980	 0.3070
O	 0.6900	 0.3110
P	 0.5810	 0.2640
Q	 0.8600	 0.3920
R	 0.6510	 0.2820
S	 0.5480	 0.2580
X	 0.8850	 0.3190
Y	 0.8430	 0.3360

