Full wwPDB EM Validation Report ⓘ

Jul 31, 2024 – 11:08 AM JST

PDB ID	:	8I0V
EMDB ID	:	EMD-35111
Title	:	The cryo-EM structure of human post-Bact complex
Authors	:	Zhan, X.; Lu, Y.; Shi, Y.
Deposited on	:	2023-01-11
Resolution	:	3.00 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:

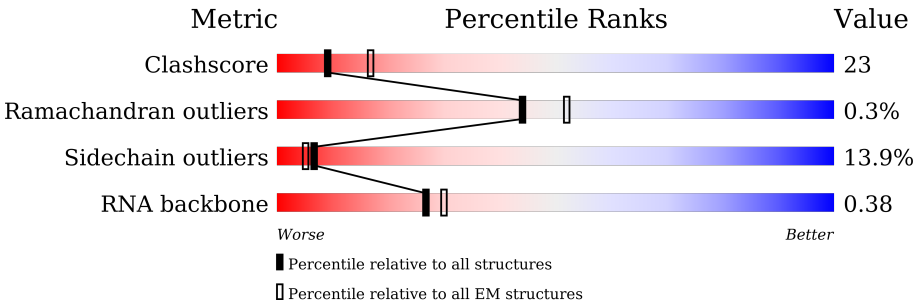
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	2335	53% 27% 5% 16%
2	B	117	29% 38% 14% 16%
3	C	972	45% 38% 5% 12%
4	E	357	33% 44% 6% 16%
5	F	107	23% 37% 25% 5% 9%
6	G	220	5% 18% 10% 64%
7	H	188	55% 20% 46% 13% 20%

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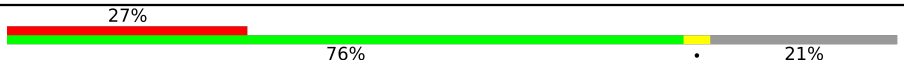
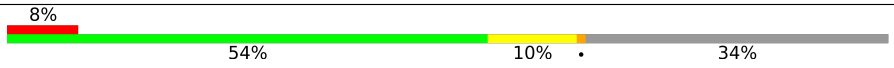
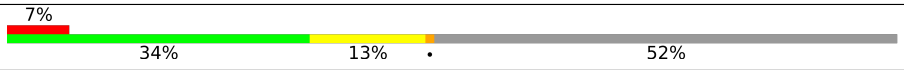
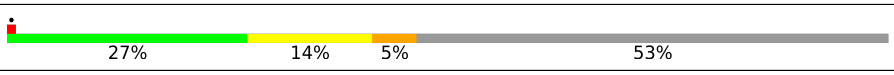
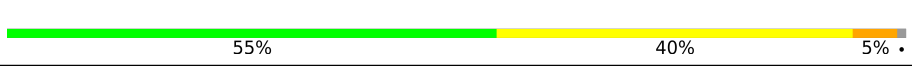
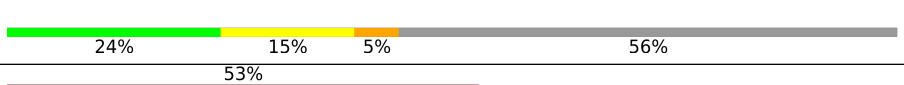
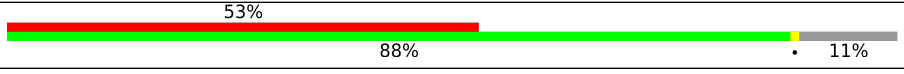
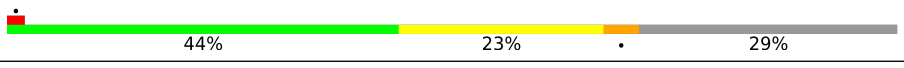
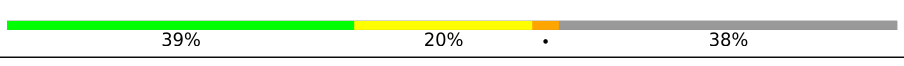
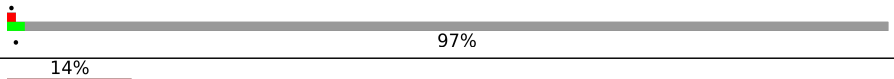
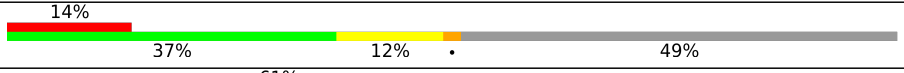
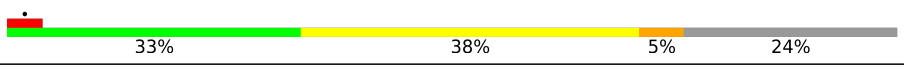
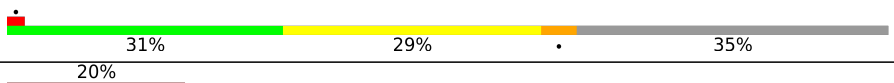
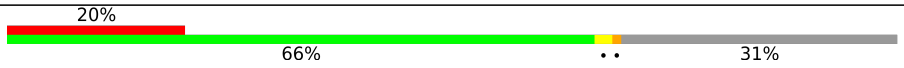
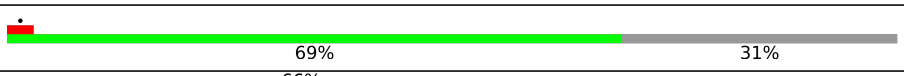
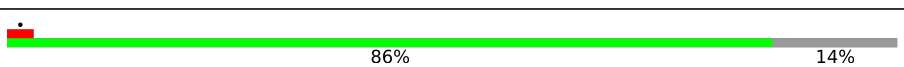
Mol	Chain	Length	Quality of chain
8	I	855	
9	J	848	
10	L	802	
11	M	243	
12	N	144	
13	O	420	
14	P	229	
15	Q	1485	
16	R	536	
17	S	166	
18	T	514	
19	U	2752	
20	V	908	
21	W	579	
22	X	1041	
23	Y	492	
24	Z	225	
25	a	240	
25	m	240	
26	b	119	
26	n	119	
27	c	118	
27	h	118	
28	d	86	
28	i	86	

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Mol	Chain	Length	Quality of chain
29	e	92	86% 14%
29	j	92	88% 88% 12%
30	f	76	14% 97%
30	k	76	95% 96%
31	g	126	64% 36%
31	l	126	60% 66% 34%
32	q	504	17% 26% 74%
32	r	504	12% 26% 74%
32	s	504	15% 25% 74%
32	t	504	17% 26% 74%
33	y	301	16% 26% 74%
34	1	1304	49% 24% 33% 6% 37%
35	3	1217	81% 35% 51% 11%
36	2	895	23% 18% 7% 72%
37	4	424	28% 34% 62%
38	7	110	50% 25% 34% 15% 26%
39	5	86	57% 28% 50% 12% 10%
40	p	225	40% 40% 60%
41	o	255	63% 64% 36%

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 104205 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 Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1969	16331	10528	2863	2872	68	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	98	2066	925	347	696	98	0	0

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	860	6724	4298	1122	1272	32	0	0

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	299	2338	1470	410	445	13	0	0

- Molecule 5 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	F	97	2075	928	381	669	97	0	0

- Molecule 6 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	G	79	1587	708	248	552	79	0	0

- Molecule 7 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	151	Total	C	N	O	P	0	0
			3203	1431	551	1070	151		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	672	Total	C	N	O	0	0
			3387	2043	672	672		

- Molecule 9 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	563	Total	C	N	O	S	0	0
			3789	2361	712	710	6		

- Molecule 10 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	387	Total	C	N	O	S	0	0
			2584	1596	494	489	5		

- Molecule 11 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	114	Total	C	N	O	S	0	0
			971	605	181	183	2		

- Molecule 12 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	143	Total	C	N	O	S	0	0
			1184	746	217	209	12		

- Molecule 13 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	O	290	Total	C	N	O	0	0
			1447	862	292	293		

- Molecule 14 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	101	Total	C	N	O	S	0	0
			876	537	175	162	2		

- Molecule 15 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	Q	1322	Total	C	N	O	0	0
			5288	2644	1322	1322		

- Molecule 16 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	R	380	Total	C	N	O	P	S	0	0
			2915	1791	552	558	2	12		

- Molecule 17 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	S	158	Total	C	N	O	0	0
			770	454	158	158		

- Molecule 18 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	320	Total	C	N	O	S	0	0
			2507	1582	456	462	7		

- Molecule 19 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	72	Total	C	N	O	S	0	0
			422	257	82	82	1		

- Molecule 20 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	462	Total	C	N	O	S	0	0
			2959	1842	537	567	13		

- Molecule 21 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	W	501	Total	C	N	O	0	0
			2473	1471	501	501		

- Molecule 22 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	786	Total	C	N	O	S	0	0
			6357	4010	1133	1184	30		

- Molecule 23 is a protein called Peptidyl-prolyl cis-trans isomerase-like 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	320	Total	C	N	O	S	0	0
			2556	1616	420	508	12		

- Molecule 24 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Z	155	Total	C	N	O	0	0
			772	462	155	155		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	a	86	Total	C	N	O	0	0
			344	172	86	86		
25	m	82	Total	C	N	O	0	0
			413	249	82	82		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	b	82	Total	C	N	O	0	0
			328	164	82	82		
26	n	80	Total	C	N	O	0	0
			402	242	80	80		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	c	97	Total 388	C 194	N 97	O 97	0	0
27	h	95	Total 482	C 292	N 95	O 95	0	0

- Molecule 28 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	d	74	Total 296	C 148	N 74	O 74	0	0
28	i	72	Total 359	C 215	N 72	O 72	0	0

- Molecule 29 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	e	79	Total 316	C 158	N 79	O 79	0	0
29	j	81	Total 403	C 241	N 81	O 81	0	0

- Molecule 30 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	f	74	Total 296	C 148	N 74	O 74	0	0
30	k	73	Total 364	C 218	N 73	O 73	0	0

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	g	81	Total 324	C 162	N 81	O 81	0	0
31	l	83	Total 415	C 249	N 83	O 83	0	0

- Molecule 32 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	q	132	Total 659	C 395	N 132	O 132	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
32	r	131	Total 654	C 392	N 131	O 131	0	0
32	s	132	Total 659	C 395	N 132	O 132	0	0
32	t	131	Total 654	C 392	N 131	O 131	0	0

- Molecule 33 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	y	79	Total 316	C 158	N 79	O 79	0	0

- Molecule 34 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1	816	Total 6378	C 4084	N 1106	O 1151	S 37	0	0

- Molecule 35 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	3	1177	Total 9210	C 5848	N 1562	O 1755	S 45	0	0

- Molecule 36 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2	250	Total 1576	C 973	N 307	O 294	S 2	0	0

- Molecule 37 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	4	161	Total 792	C 470	N 161	O 161	0	0

- Molecule 38 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	7	81	Total	C	N	O	S	0	0
			613	376	109	115	13		

- Molecule 39 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5	77	Total	C	N	O	S	0	0
			635	403	110	117	5		

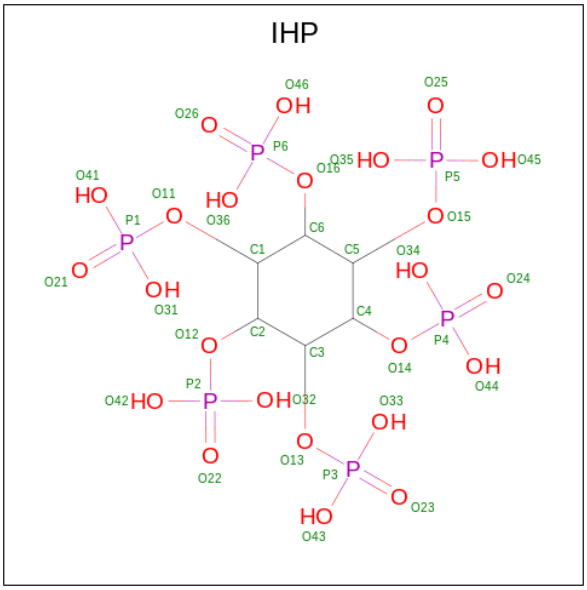
- Molecule 40 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
40	p	90	Total	C	N	O	0	0
			451	271	90	90		

- Molecule 41 is a protein called U2 small nuclear ribonucleoprotein A'.

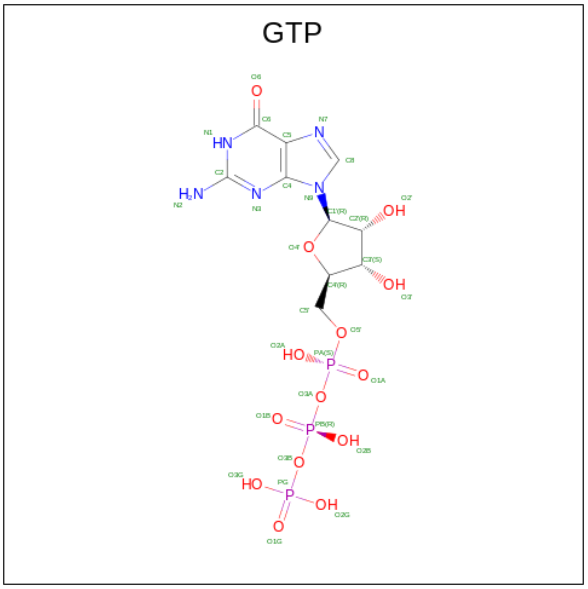
Mol	Chain	Residues	Atoms				AltConf	Trace
41	o	162	Total	C	N	O	0	0
			816	492	162	162		

- Molecule 42 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
42	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 43 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
43	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 44 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
44	C	1	Total	Mg	0
			1	1	
44	F	5	Total	Mg	0
			5	5	
44	L	1	Total	Mg	0
			1	1	

- Molecule 45 is ZINC ION (three-letter code: ZN) (formula: Zn).

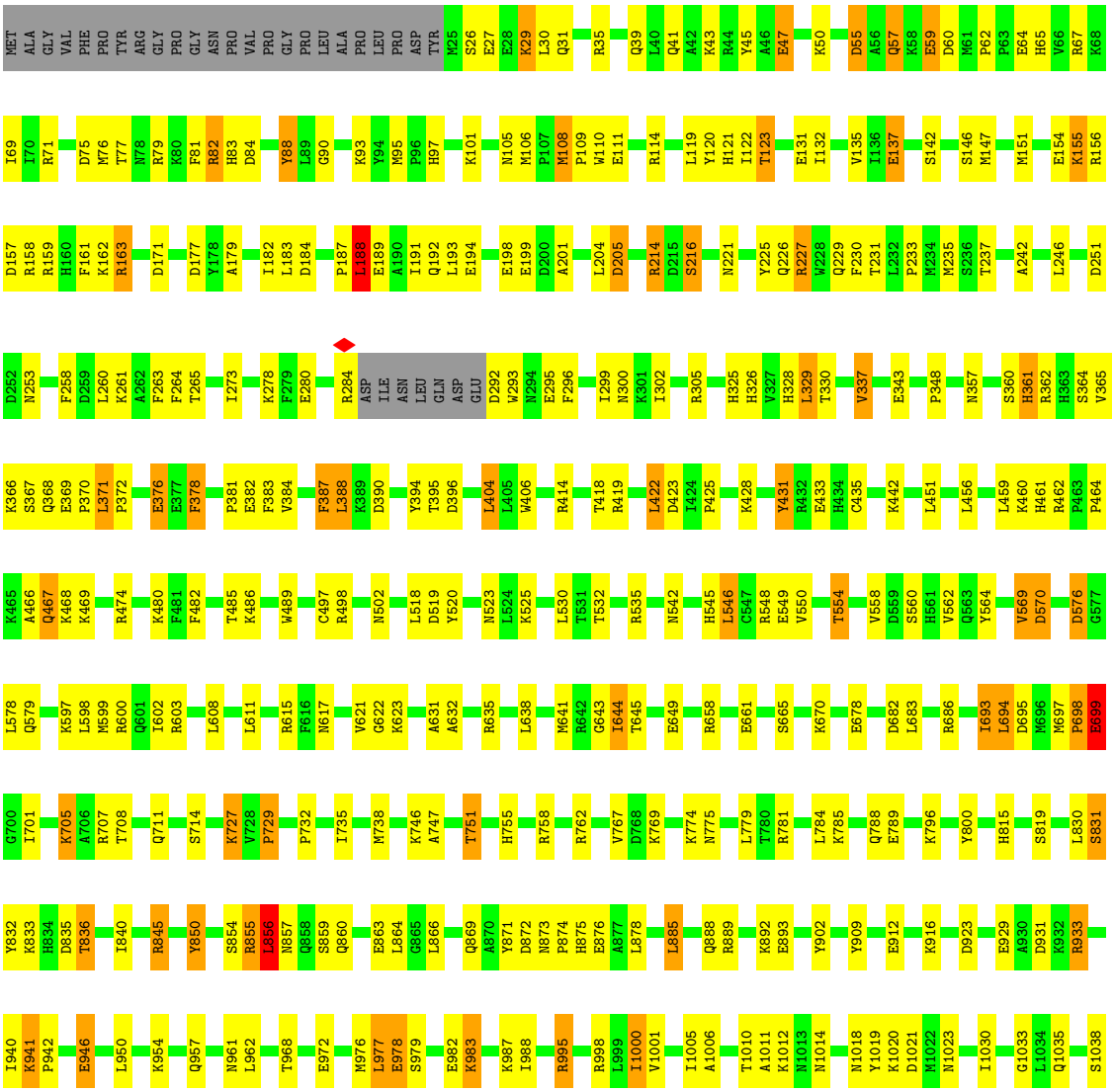
Mol	Chain	Residues	Atoms		AltConf
45	N	3	Total	Zn	0
			3	3	
45	7	3	Total	Zn	0
			3	3	

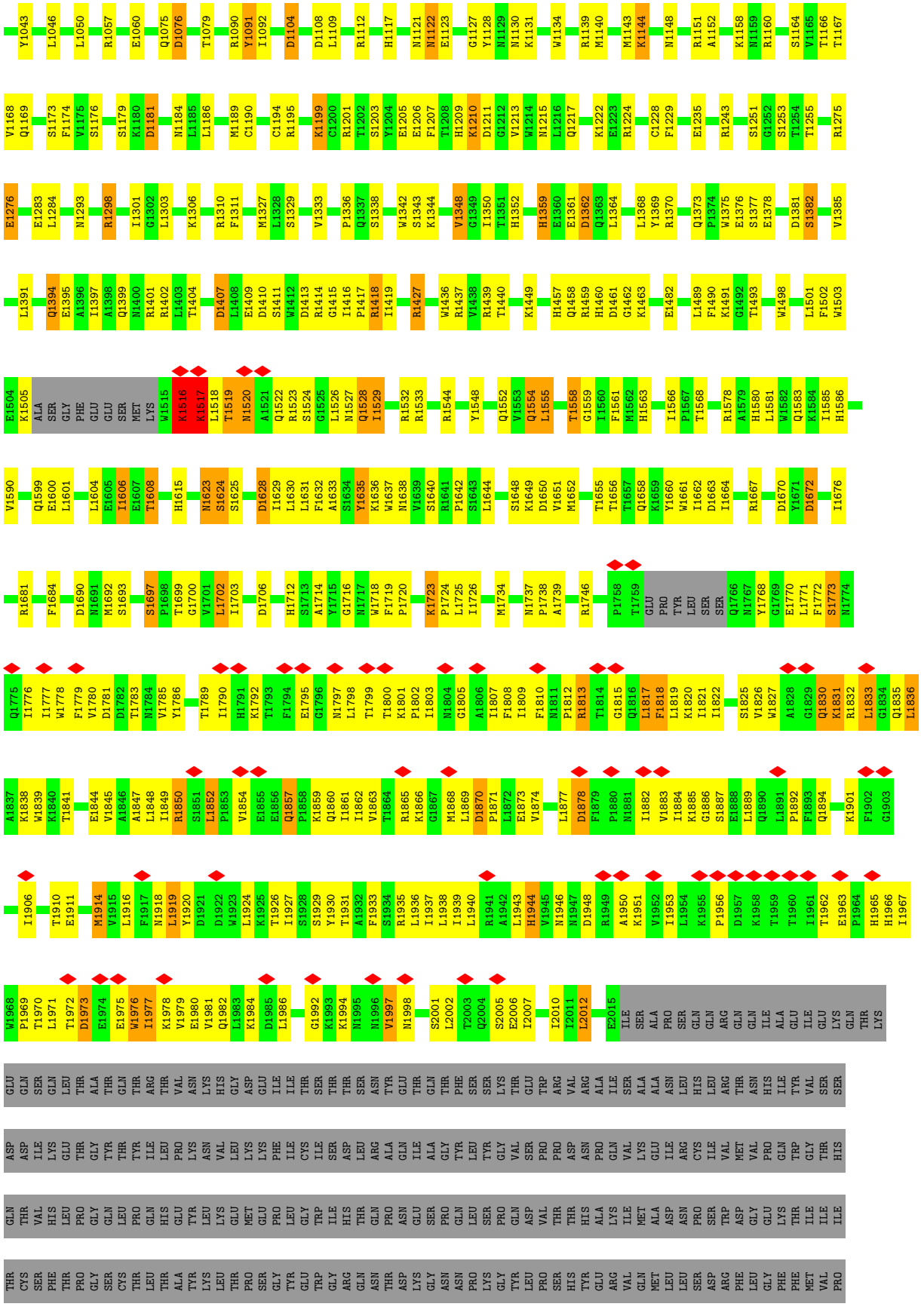
3 Residue-property plots (i)

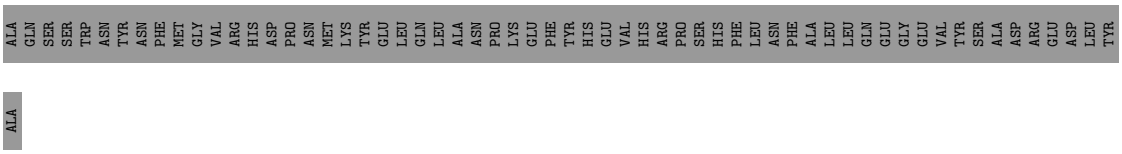
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Pre-mRNA-processing-splicing factor 8

Chain A:

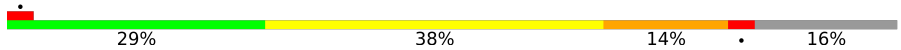


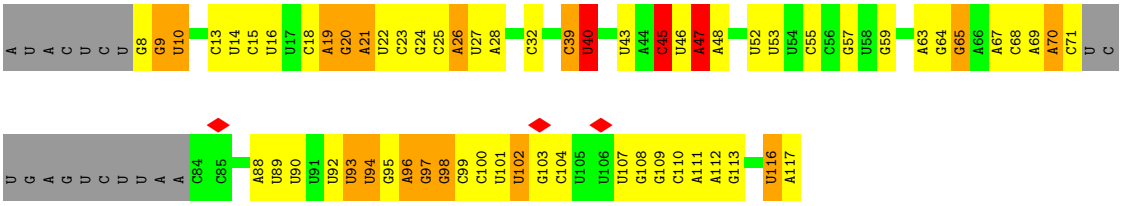




• Molecule 2: U5 snRNA

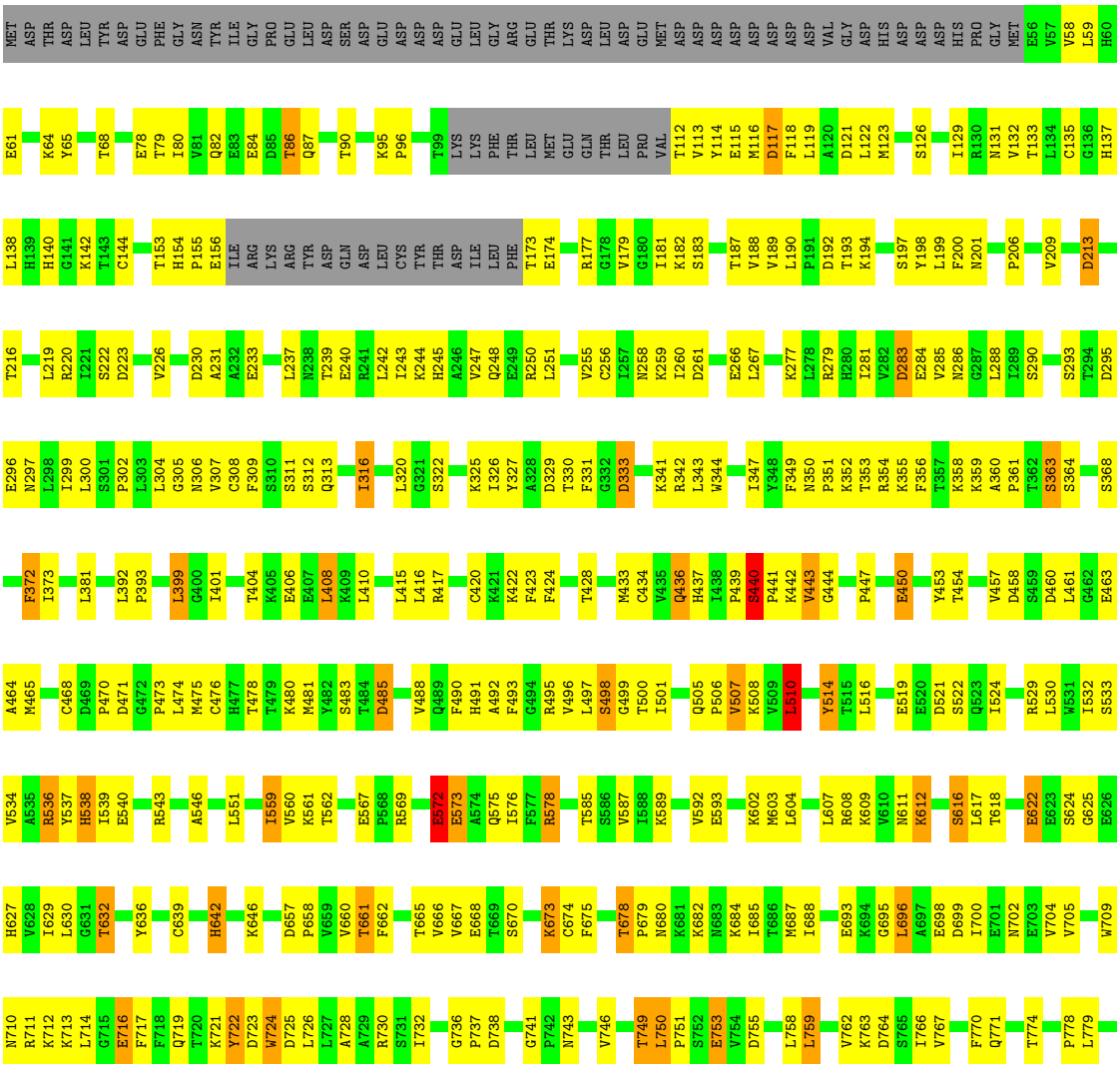
Chain B:





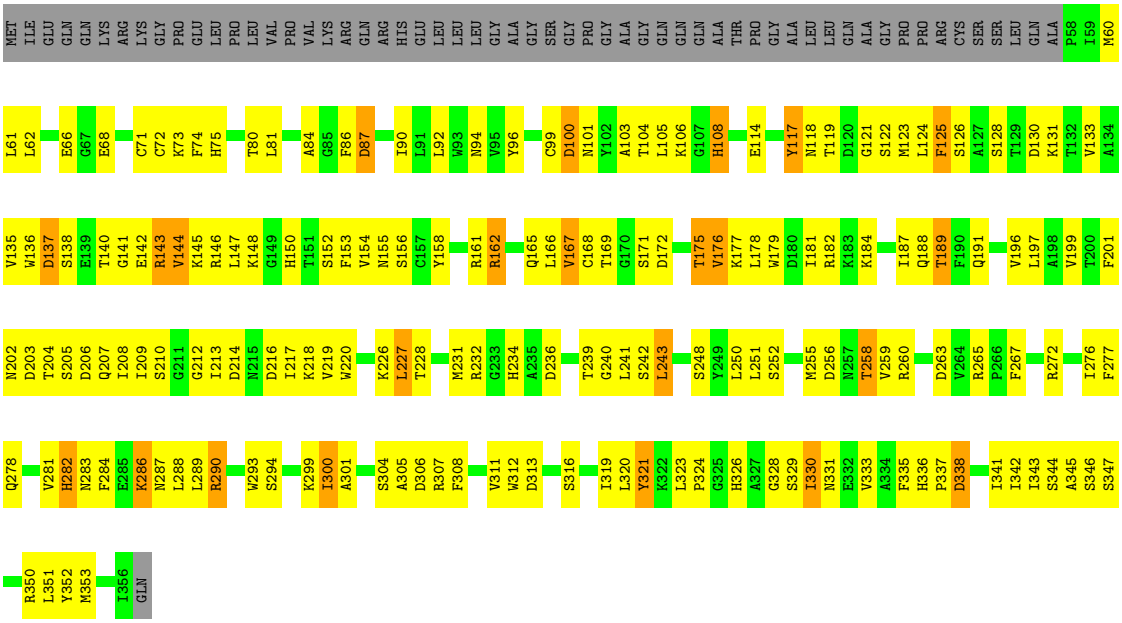
• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

Chain C:



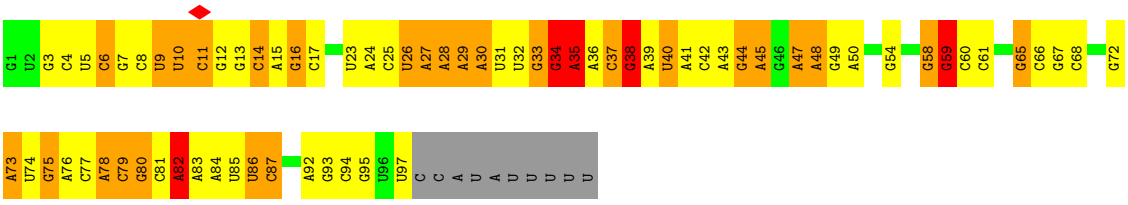
• Molecule 4: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E:



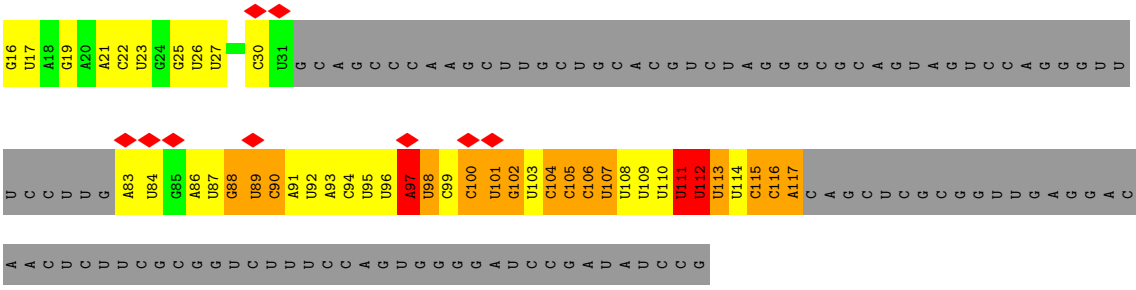
• Molecule 5: U6 snRNA

Chain F:



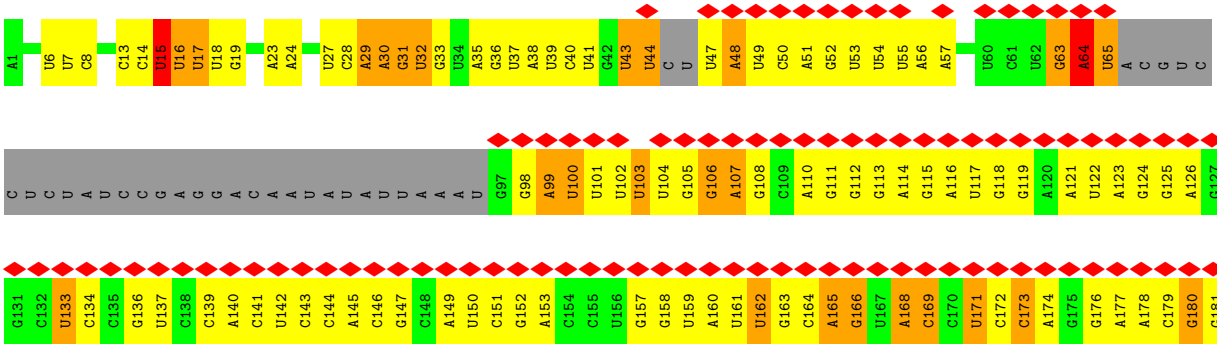
• Molecule 6: Pre-mRNA

Chain G:



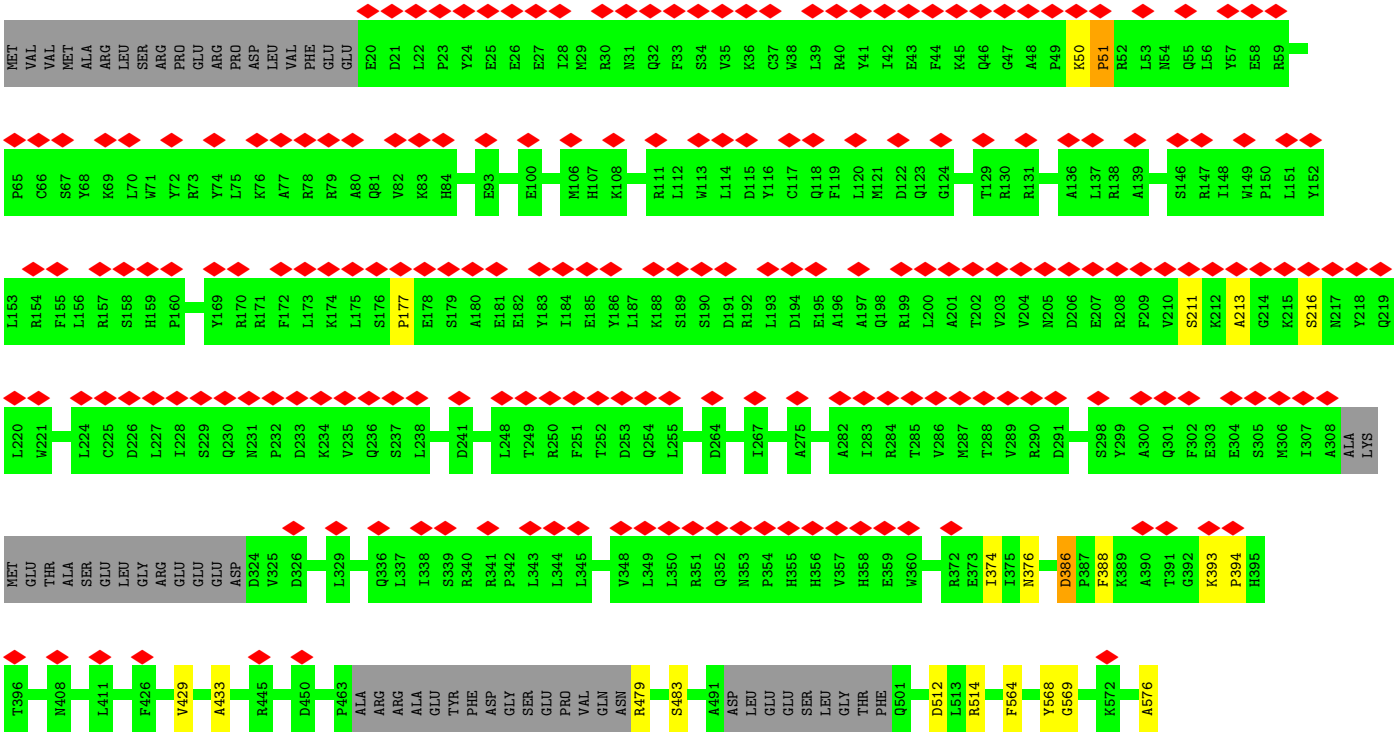
• Molecule 7: U2 snRNA

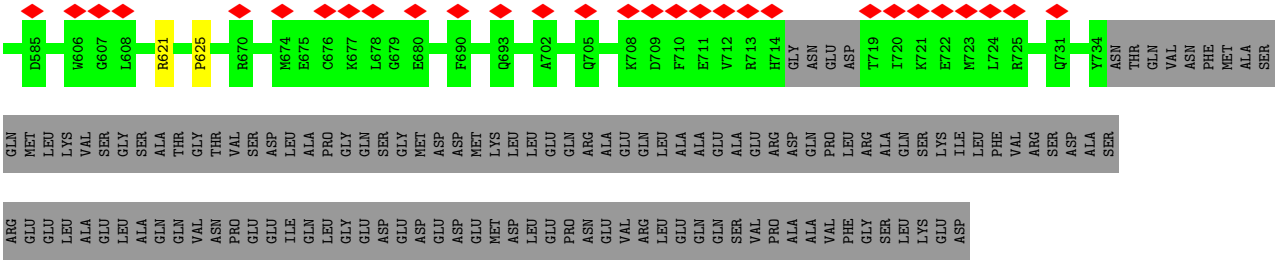
Chain H:



• Molecule 8: Pre-mRNA-splicing factor SYF1

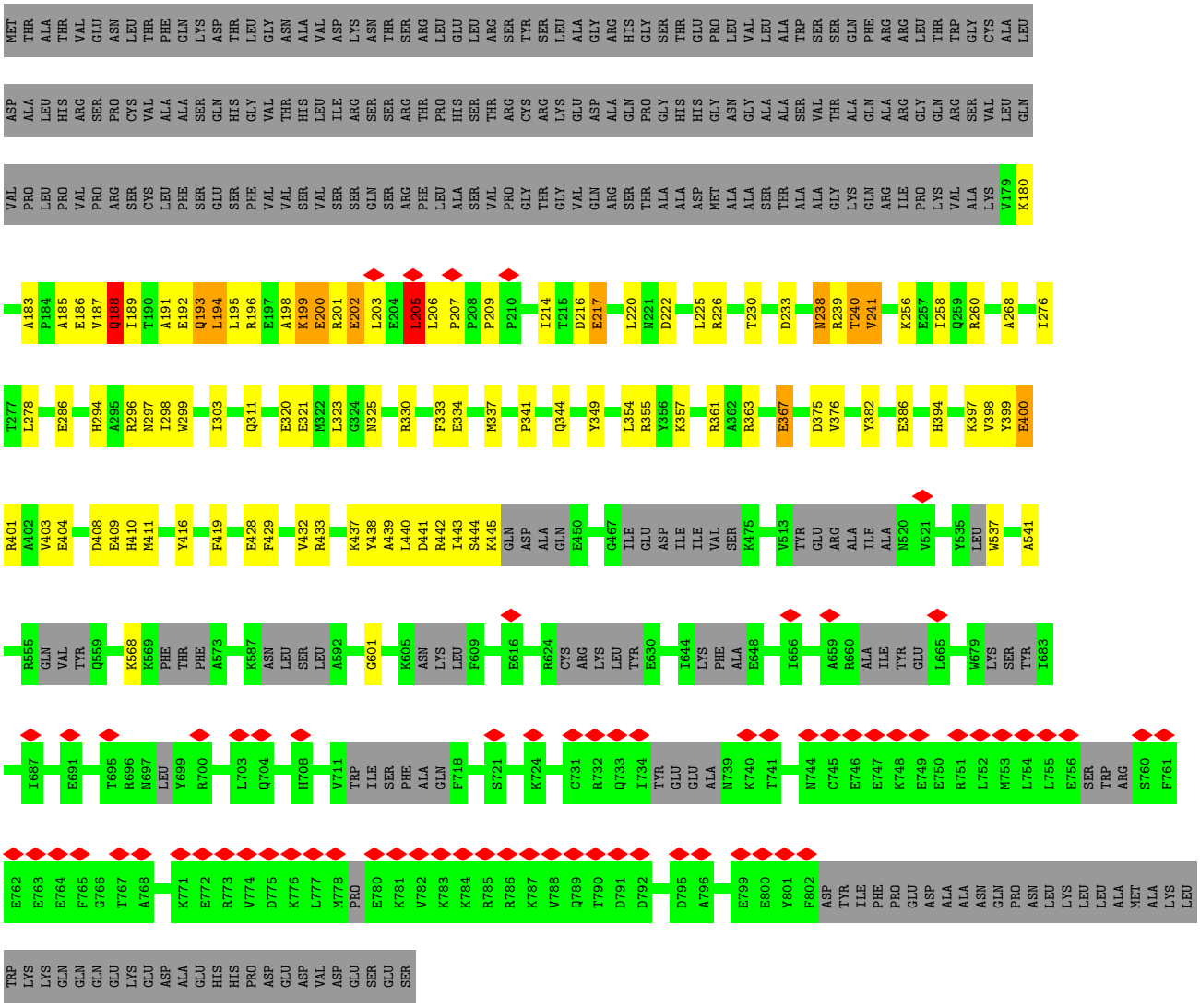
Chain I:





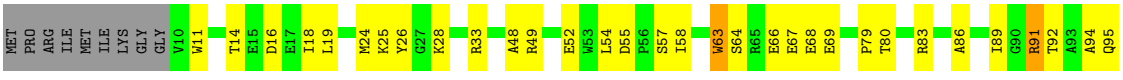
• Molecule 9: Crooked neck-like protein 1

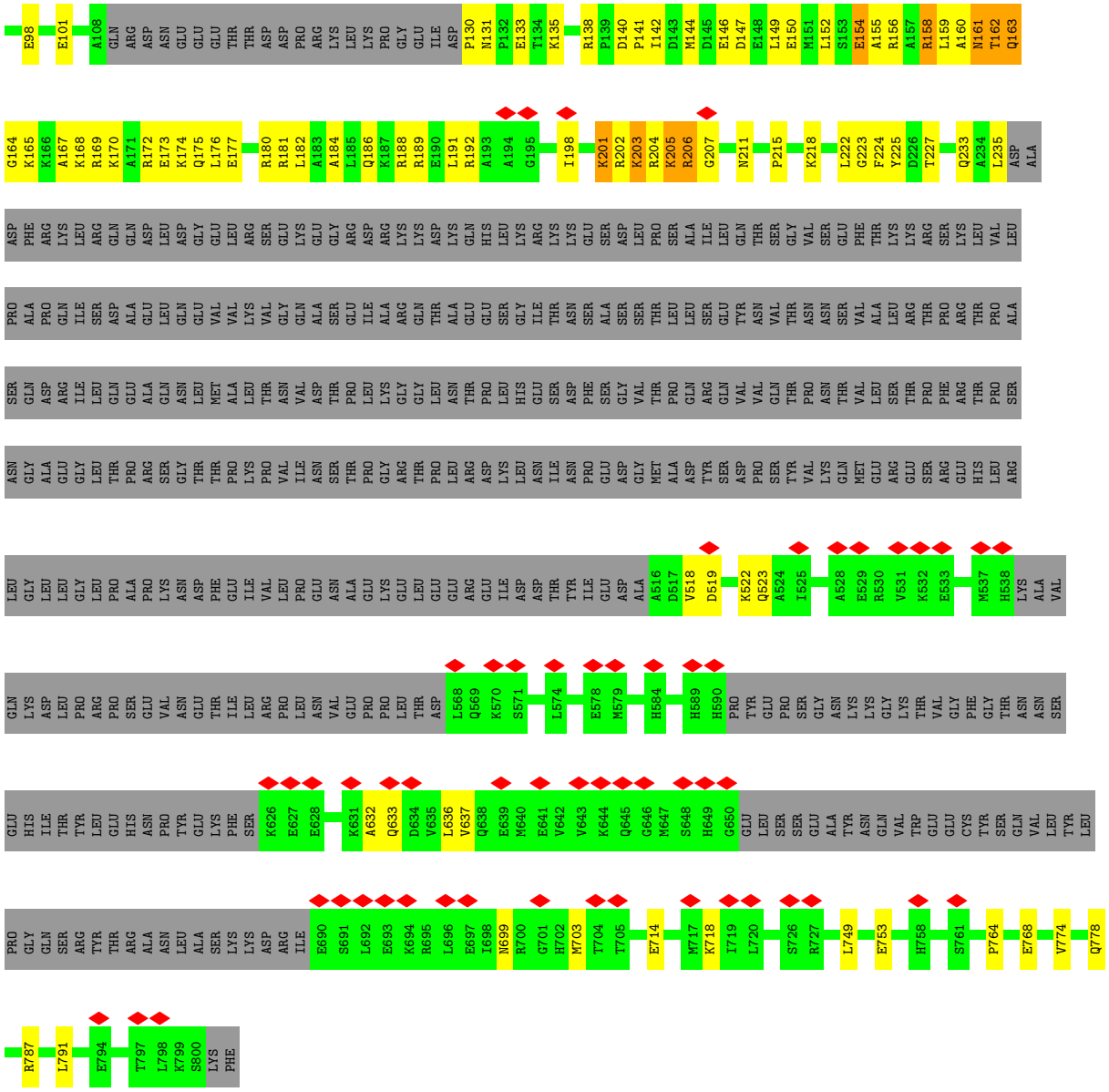
Chain J:



• Molecule 10: Cell division cycle 5-like protein

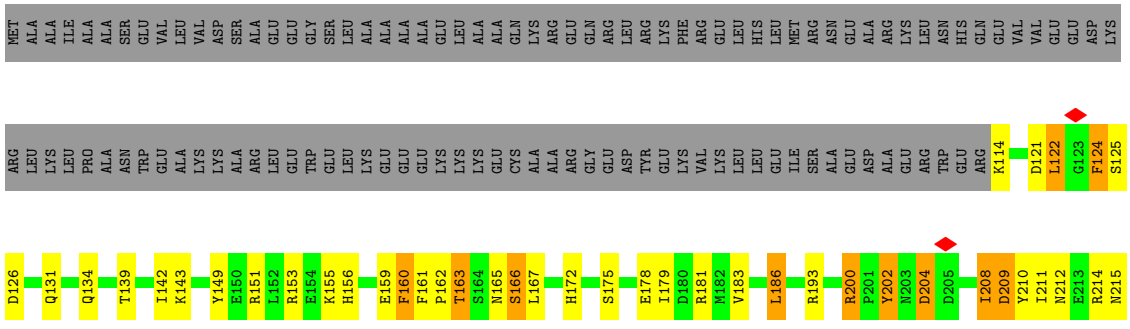
Chain L:

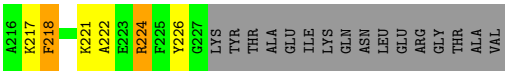




• Molecule 11: Pre-mRNA-splicing factor SYF2

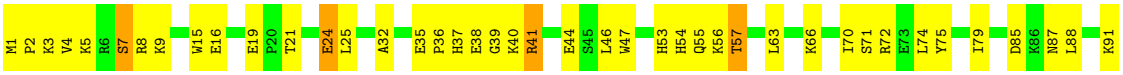
Chain M:

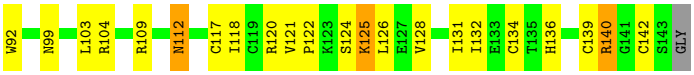




• Molecule 12: Protein BUD31 homolog

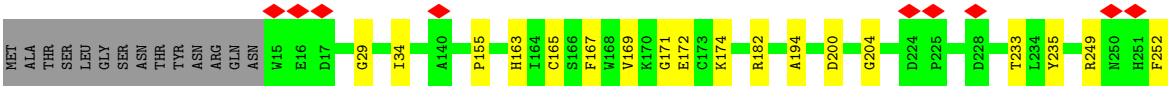
Chain N:

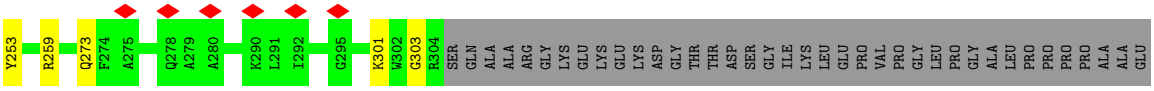




• Molecule 13: Pre-mRNA-splicing factor RBM22

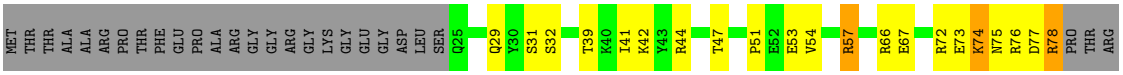
Chain O:

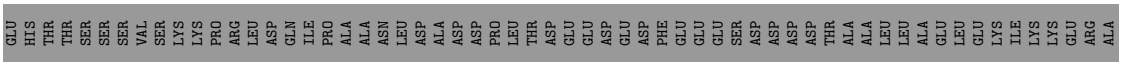




• Molecule 14: Spliceosome-associated protein CWC15 homolog

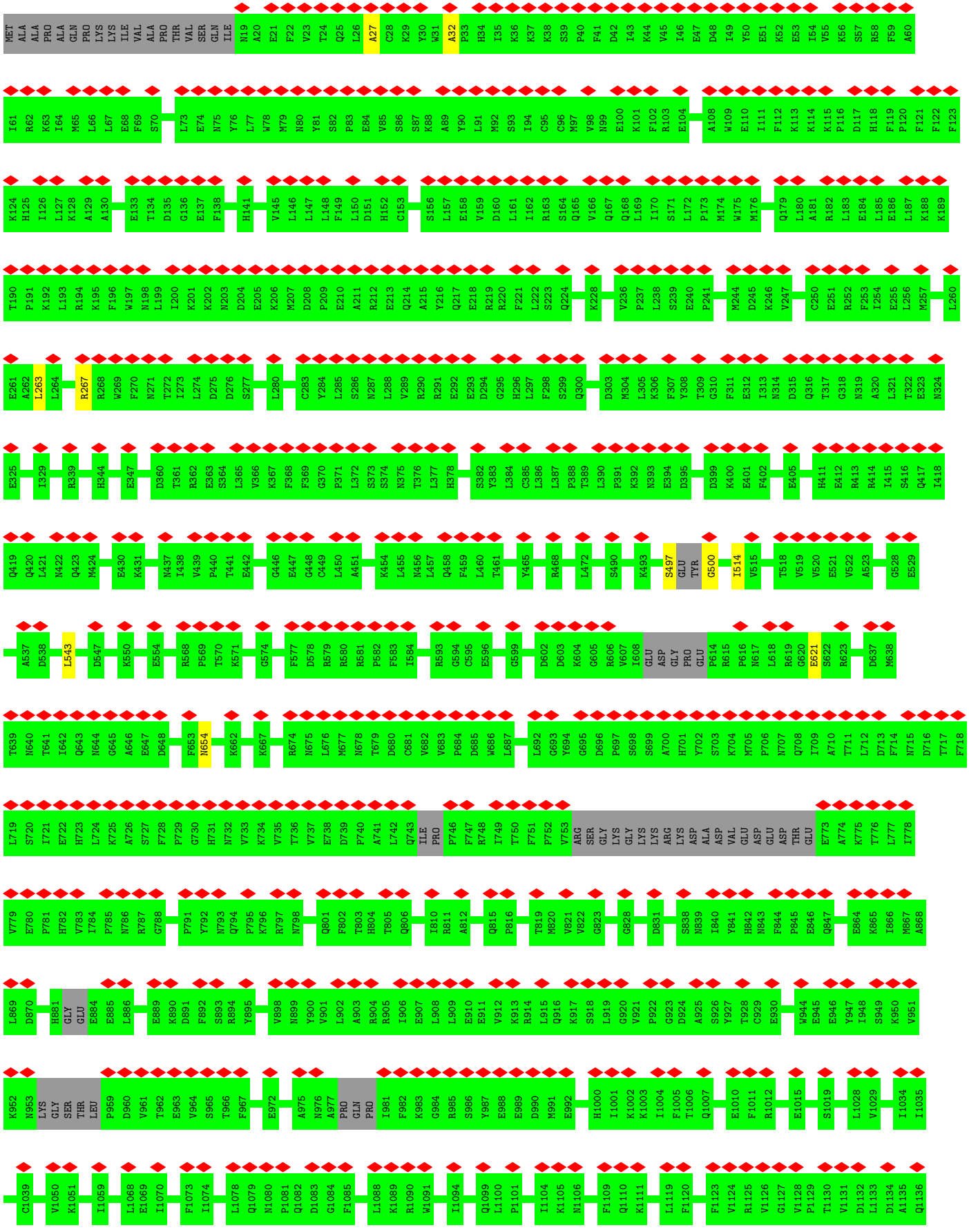
Chain P:

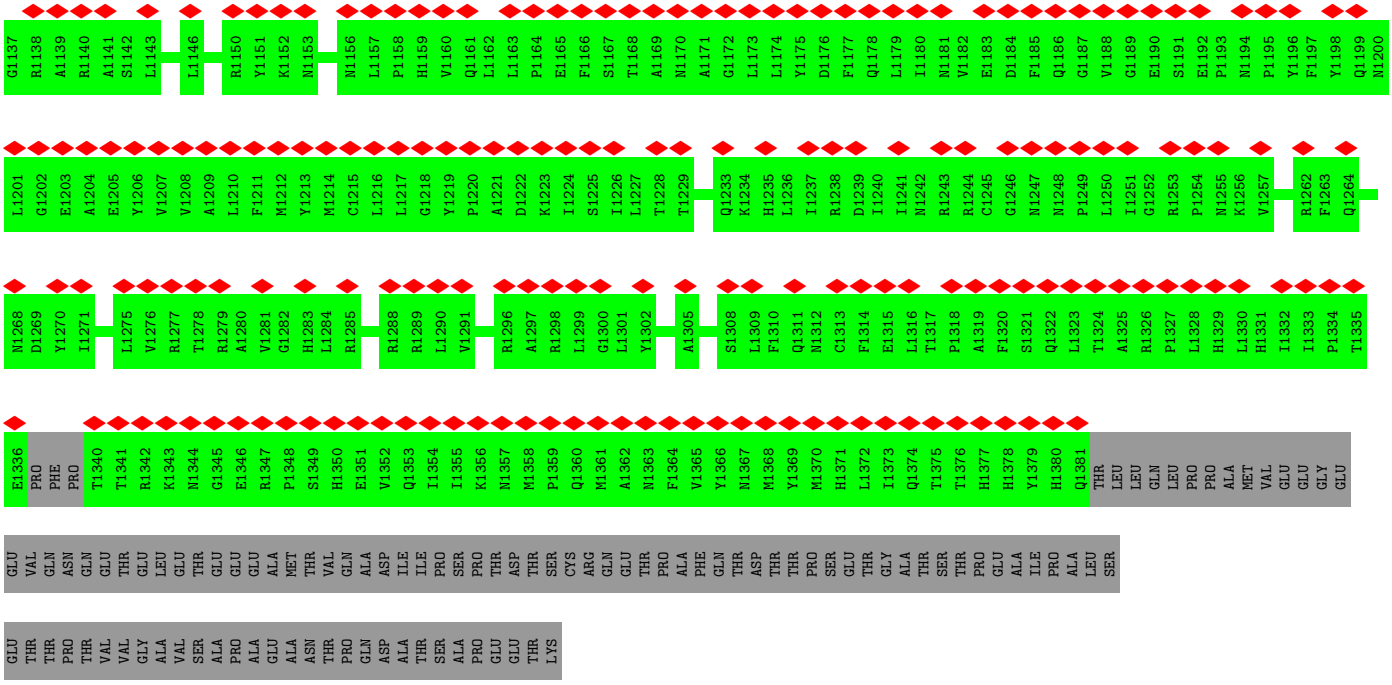




• Molecule 15: RNA helicase aquarius

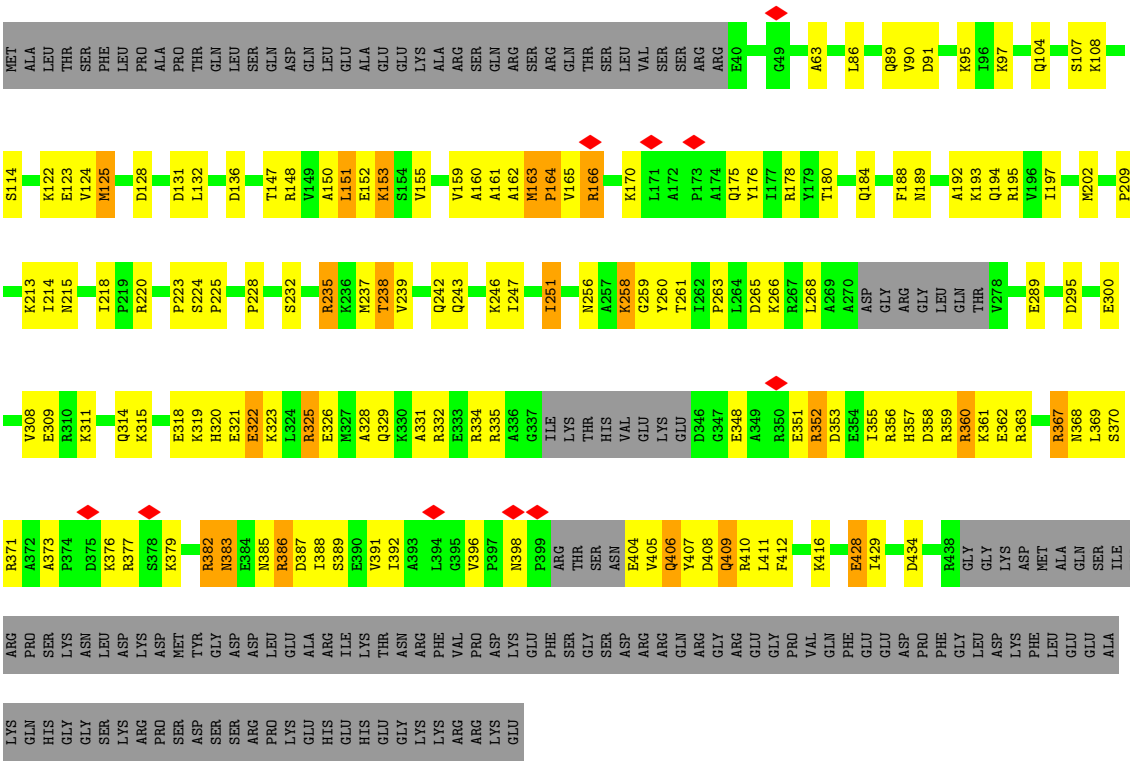
Chain Q:


MET ALA ALA PRO ALA GLN PRO LYS LYS ILE VAL ALA PRO THR VAL SER GLN ILE N19 A20 E21 F22 Y23 T24 Q25 L26 A27 C28 K29 Y30 W31 A32 P33 H34 I35 K36 K37 K38 S39 P40 F41 D42 I43 K44 V45 I46 E47 D48 I49 Y50 E51 K52 E53 I54 V55 K56 S57 R58 F59 A60
I61 R62 K63 I64 M65 L66 L67 E68 F69 S70 L73 E74 N75 Y76 L77 W78 M79 N80 Y81 S82 P83 E84 V85 S86 S87 K88 A89 Y90 L91 M92 S93 I94 C95 C96 M97 V98 N99 E100 K101 F102 R103 E104 A108 W109 E110 I111 F112 K113 K114 K115 P116 D117 H118 F119 P120 F121 F122 F123
K124 H125 I126 L127 K128 A129 A130 E133 T134 D135 G136 E137 F138 H141 V145 L146 L147 L148 F149 L150 D151 H152 C153 S156 L157 E158 V159 D160 L161 I162 R163 S164 Q165 V166 Q167 Q168 L169 I170 S171 L172 P173 M174 W175 M176 Q179 L180 A181 R182 L183 E184 L185 E186 L187 K188 K189
T190 P191 K192 L193 R194 K195 F196 W197 N198 L199 I200 K201 K202 N203 D204 E205 K206 M207 D208 P209 E210 A211 R212 E213 Q214 A215 Y216 Q217 E218 R219 R220 F221 L222 S223 Q224 K228 V236 P237 L238 S239 E240 P241 M244 D245 K246 V247 C250 E251 R252 F253 I254 E255 L256 M257 L260
E261 A262 L263 L264 R267 R268 W269 F270 N271 T272 I273 L274 D275 D276 S277 L280 C283 Y284 L285 S286 N287 L288 V289 R290 R291 E292 E293 D294 G295 H296 L297 F298 S299 Q300 D303 M304 L305 K306 F307 Y308 T309 G310 F311 E312 I313 N314 D315 Q316 T317 G318 N319 A320 L321 T322 E323 N324
E325 I329 R339 H344 E347 D360 T361 R362 E363 S364 L365 V366 K367 F368 F369 G370 P371 L372 S373 S374 N375 T376 L377 H378 S382 Y383 L384 C385 L386 L387 P388 T389 L390 P391 K392 N393 E394 D395 D399 K400 E401 F402 E405 H411 E412 R413 R414 I415 S416 Q417 I418
Q419 Q420 L421 N422 Q423 M424 E430 K431 N437 I438 V439 P440 T441 E442 G446 E447 G448 C449 L450 A451 K454 L455 N456 L457 Q458 F459 L460 T461 Y465 R468 L472 S490 K493 S497 GLU TYR G500 I514 V515 T518 V519 V520 E521 V522 A523 G528 E529
A537 D538 L543 D547 K550 E554 R568 P569 T570 K571 G574 F577 D578 R579 R580 R581 P582 F583 I584 R593 G594 C595 E596 G599 D602 D603 K604 G605 R606 V607 I608 GLU ASP GLY PRO GLU P614 R615 P616 N617 L618 R619 G620 E621 S622 R623 D637 M638
T639 N640 T641 I642 Q643 N644 G645 A646 E647 D648 F653 N654 K662 K667 R674 N675 L676 M677 N678 T679 D680 C681 V682 V683 P684 D685 W686 L687 L692 G693 Y694 G695 D696 P697 S698 S699 A700 H701 Y702 S703 K704 M705 P706 N707 Q708 I709 A710 T711 L712 D713 F714 W715 D716 T717 F718
L719 S720 I721 E722 H723 L724 K725 A726 S727 F728 P729 G730 H731 N732 V733 K734 V735 T736 V737 E738 D739 P740 A741 L742 Q743 ILE PRO P746 F747 R748 I749 T750 F751 P752 V753 ARG SER GLY LYS GLY LYS LYS ARG LYS ASP ALA ASP VAL GLU ASP GLU ASP THR GLU E773 A774 K775 T776 L777 I778
V779 E780 P781 H782 V783 I784 P785 N786 R787 G788 P791 Y792 N793 Q794 P795 K796 R797 N798 Q801 F802 T803 H804 T805 Q806 I810 R811 A812 Q815 P816 T819 M820 V821 V822 G823 G828 D831 S838 N839 I840 Y841 H842 N843 F844 P845 E846 Q847 E864 K865 I866 M867 A868
L869 D870 H881 GLY GLU E884 E885 L886 E889 K890 D891 F892 S893 R894 Y895 V898 N899 Y900 V901 L902 A903 R904 R905 I906 E907 L908 L909 E910 E911 V912 K913 R914 L915 Q916 K917 S918 L919 G920 V921 P922 G923 D924 A925 S926 Y927 T928 C929 E930 W944 E945 E946 Y947 I948 S949 K950 V951
K952 N953 LYS GLY SER THR LEU P959 D960 V961 T962 E963 V964 S965 T966 F967 E972 A975 N976 A977 PRO GLN PRO I981 F982 K983 G984 R985 S986 Y987 E988 E989 D990 M991 E992 H1000 I1001 K1002 K1003 I1004 F1005 T1006 Q1007 E1010 F1011 R1012 E1015 S1019 L1028 V1029 I1034 I1035
C1039 V1050 K1051 I1059 L1068 E1069 I1070 F1073 I1074 L1078 Q1079 N1080 P1081 Q1082 D1083 G1084 F1085 L1088 K1089 R1090 W1091 I1094 Q1099 L1100 P1101 I1104 K1105 N1106 F1109 Q1110 K1111 L1119 F1120 F1123 V1124 R1125 V1126 G1127 V1128 P1129 T1130 V1131 D1132 L1133 D1134 A1135 Q1136



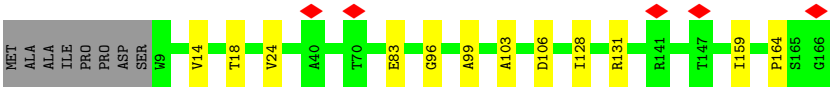
• Molecule 16: SNW domain-containing protein 1

Chain R:



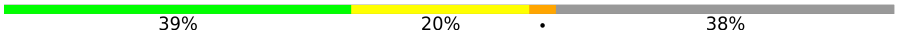
• Molecule 17: Peptidyl-prolyl cis-trans isomerase-like 1

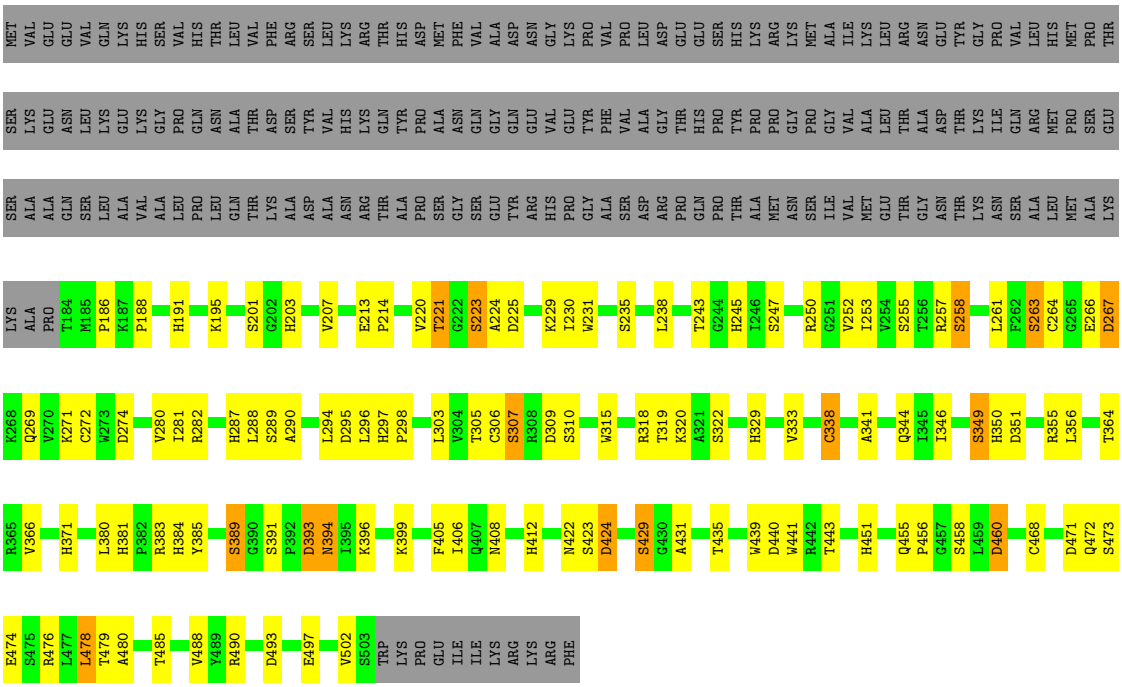
Chain S:



• Molecule 18: Pleiotropic regulator 1

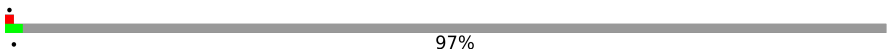
Chain T:

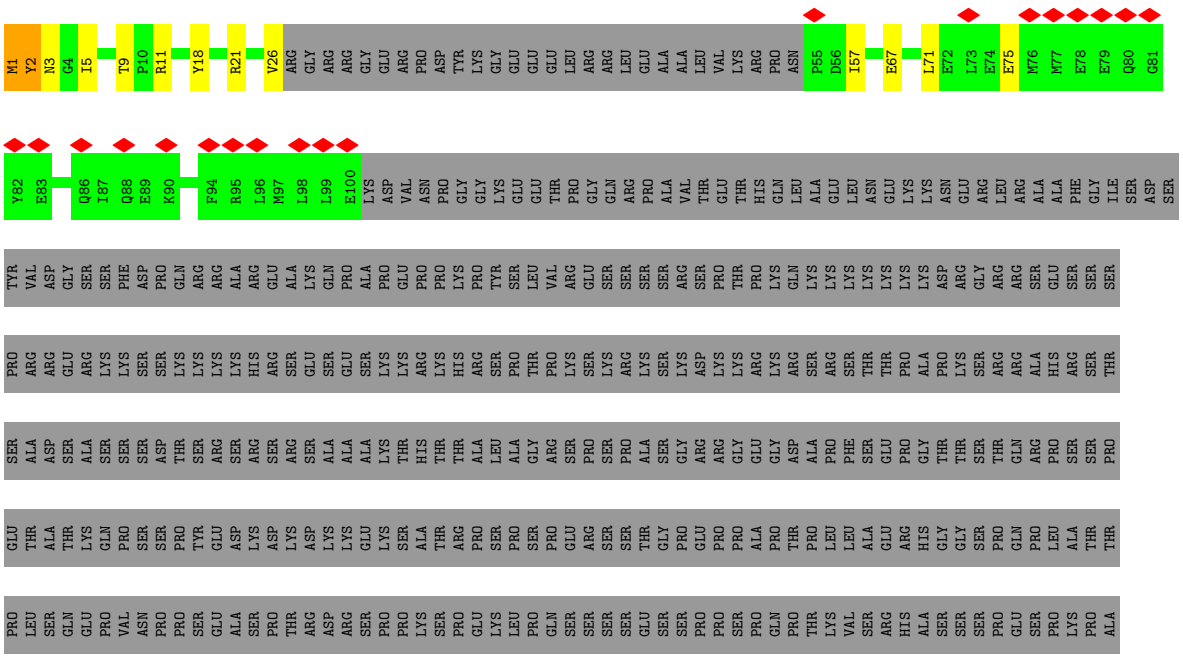


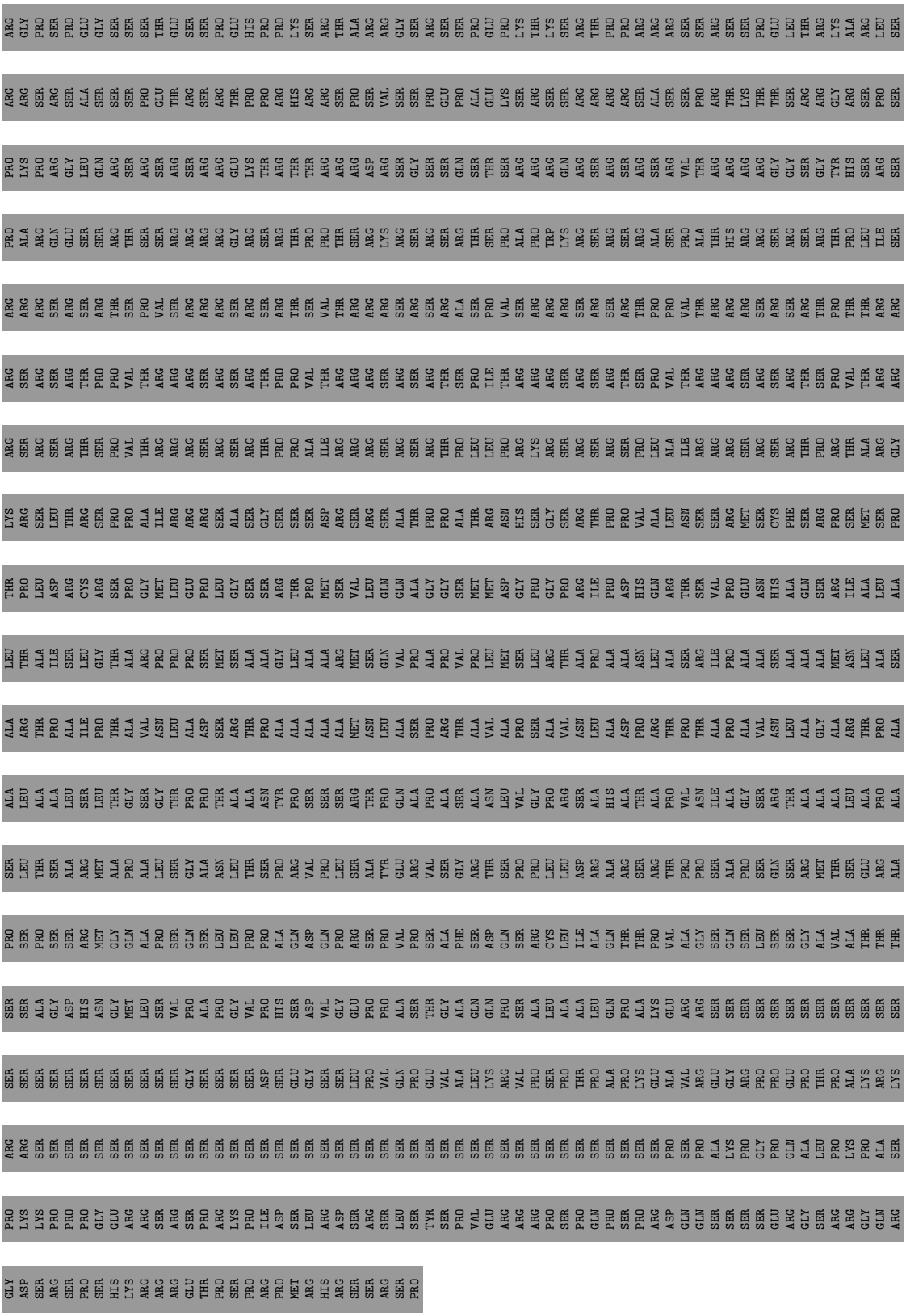


• Molecule 19: Serine/arginine repetitive matrix protein 2

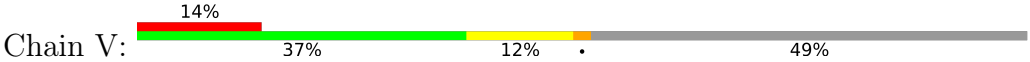
Chain U:

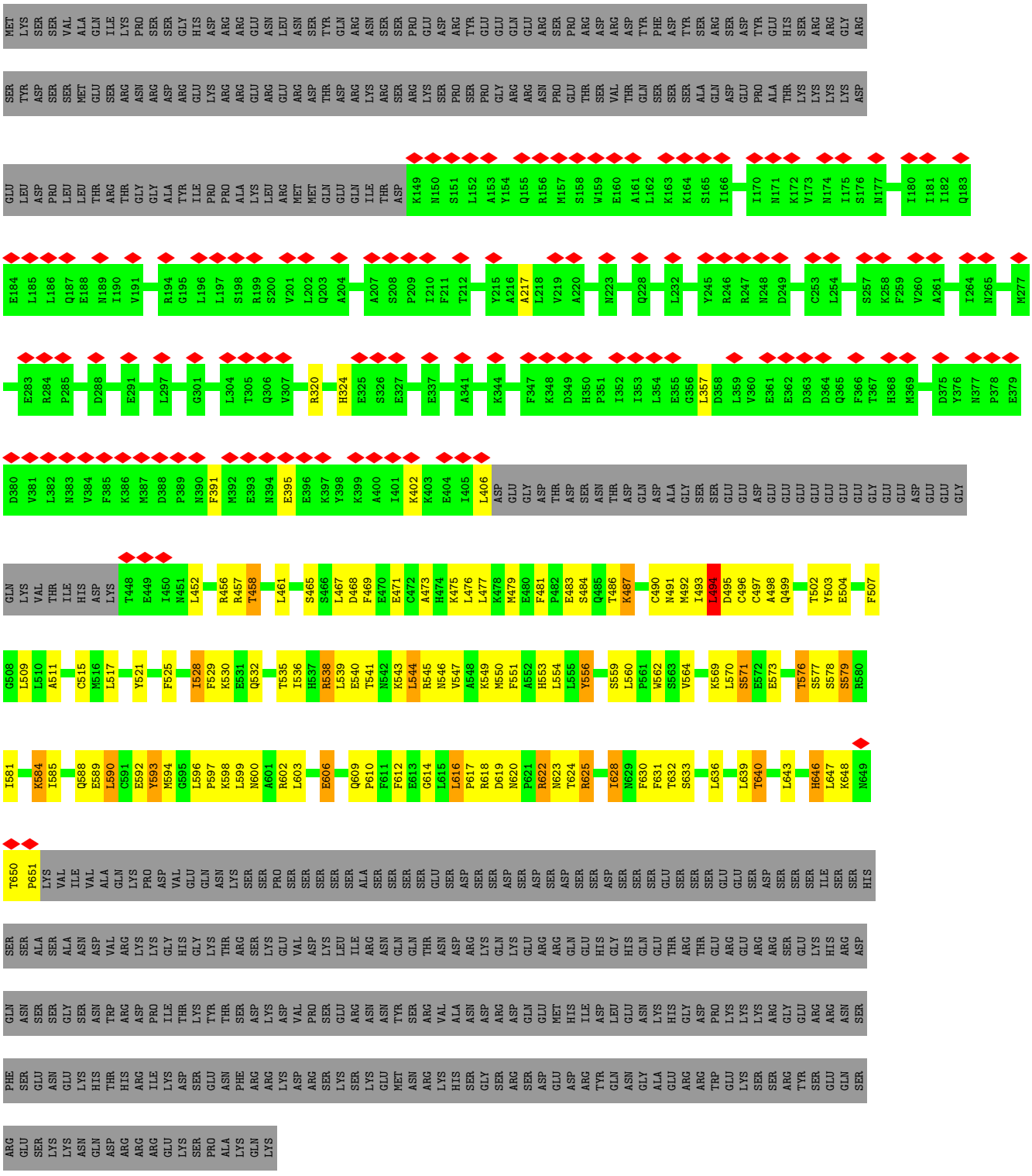






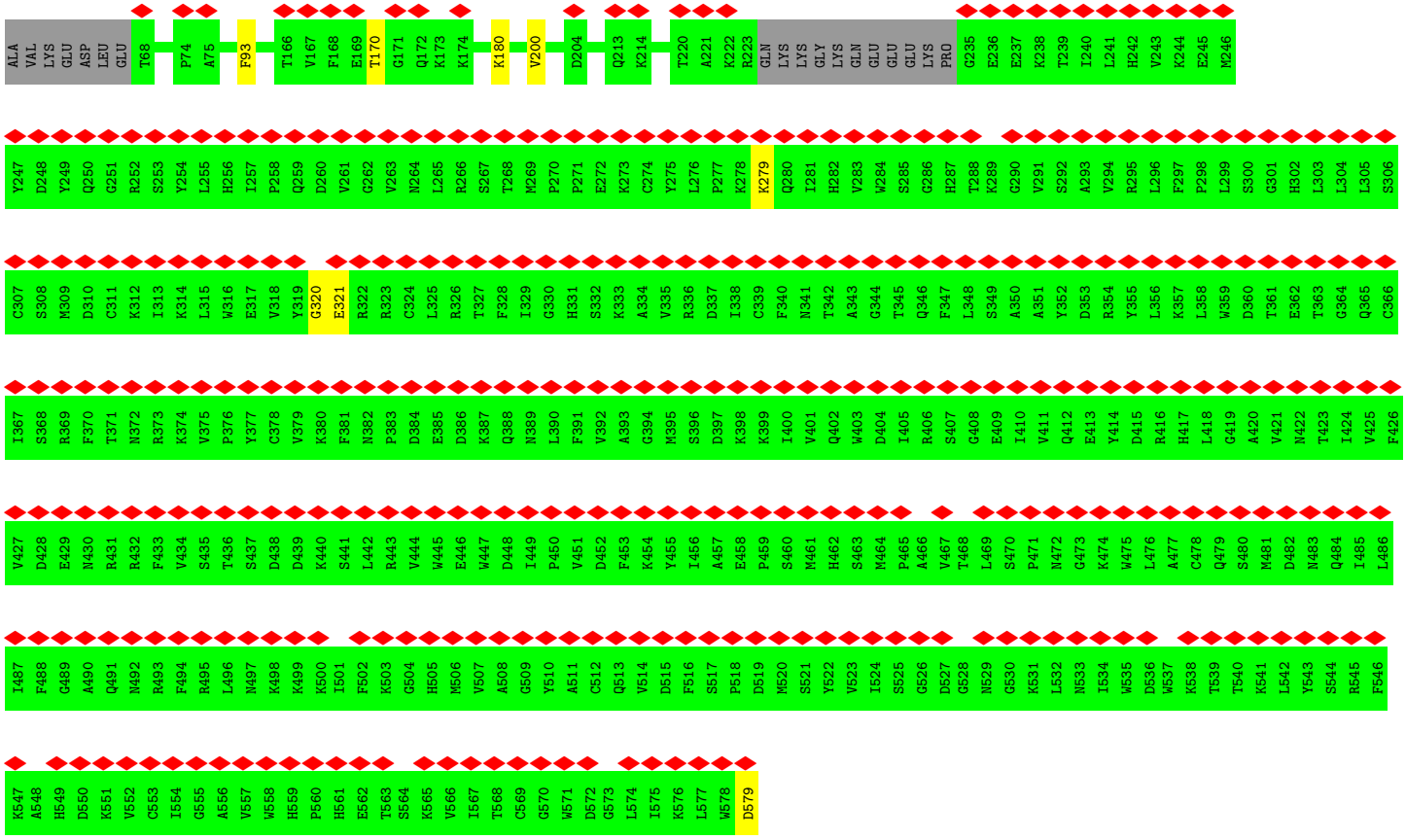
• Molecule 20: Pre-mRNA-splicing factor CWC22 homolog





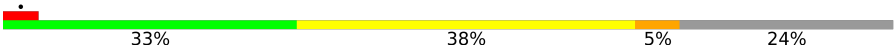
• Molecule 21: Pre-mRNA-processing factor 17

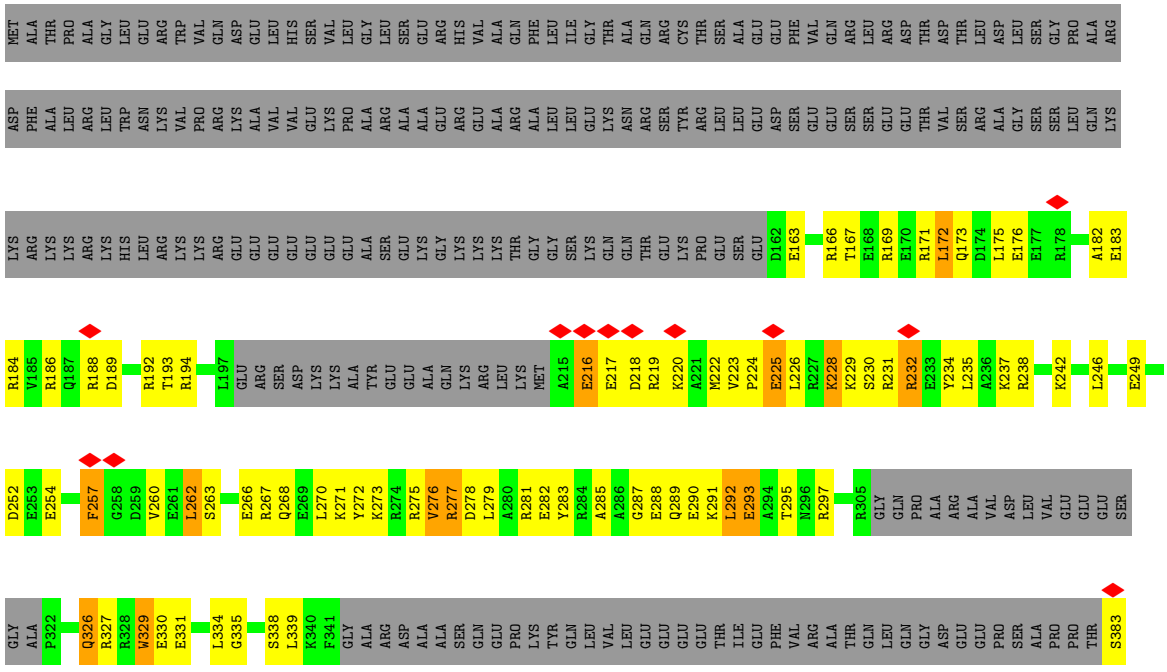
Chain W:

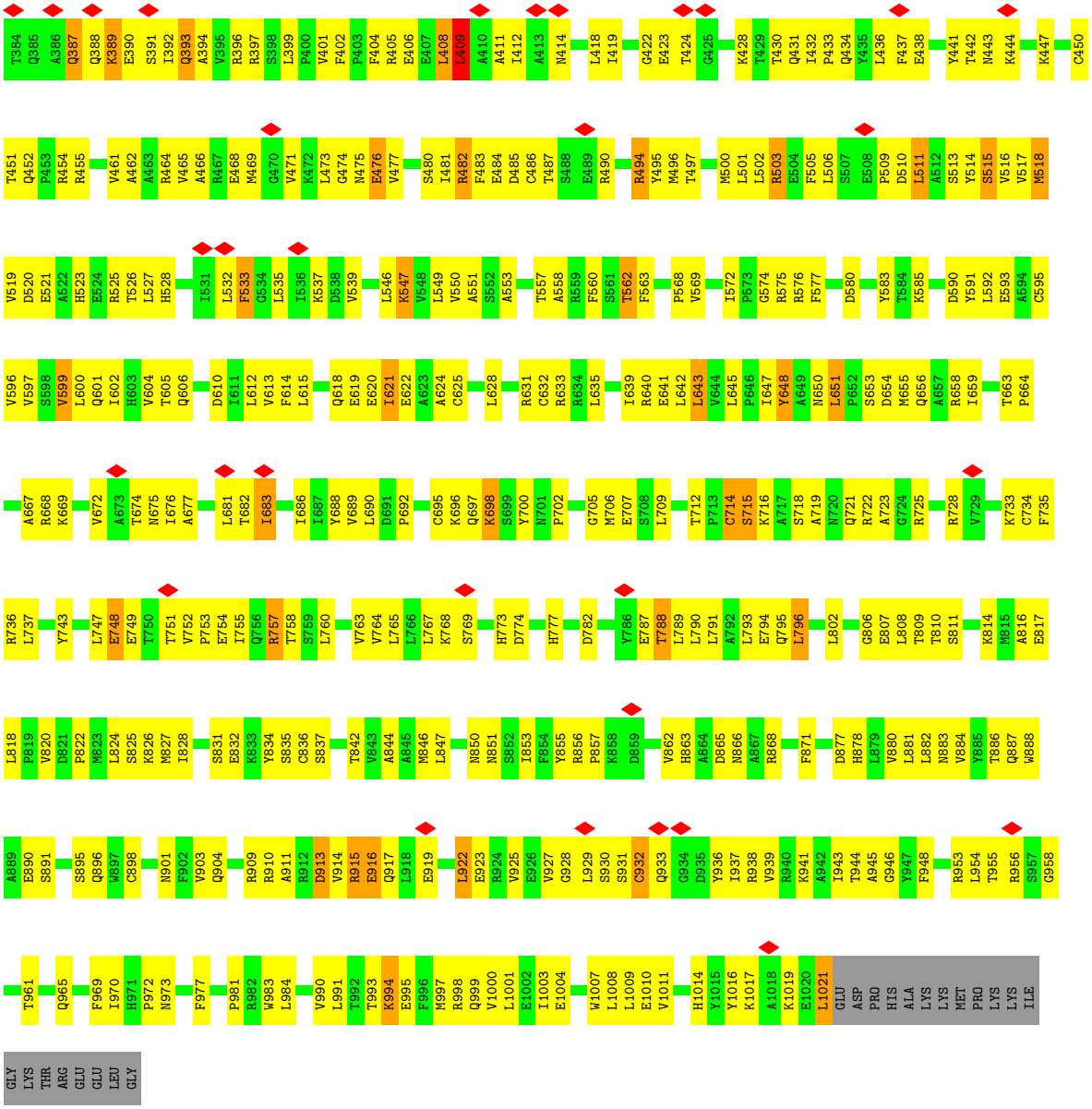


• Molecule 22: Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16

Chain X:

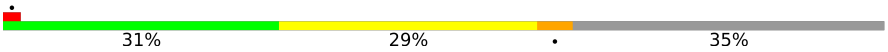


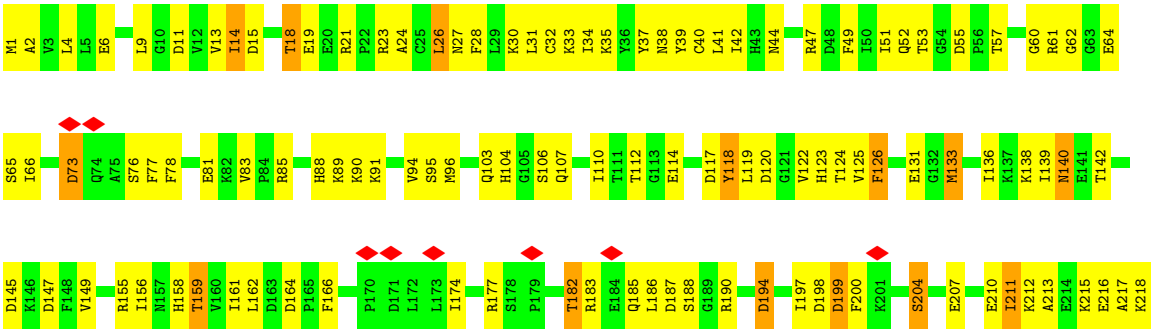


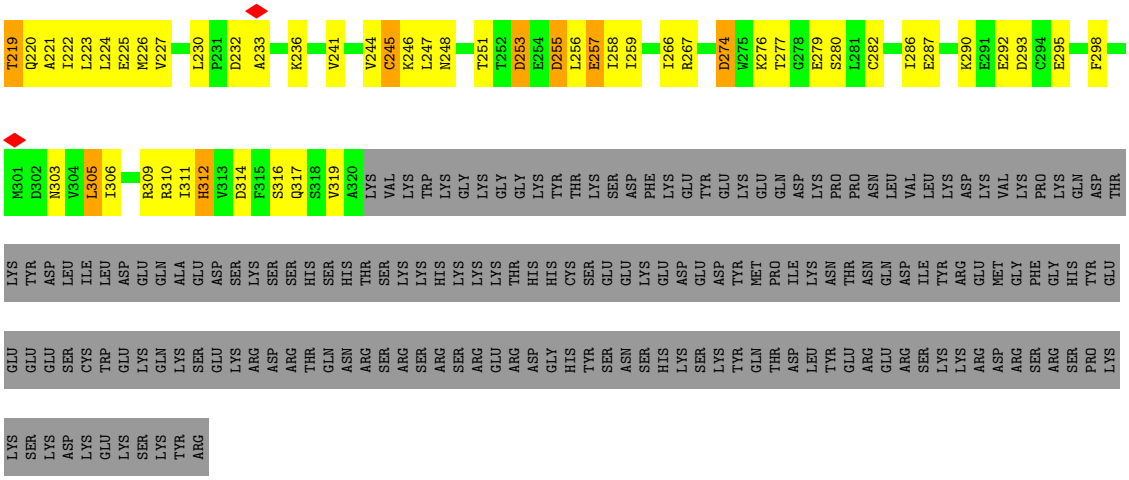


• Molecule 23: Peptidyl-prolyl cis-trans isomerase-like 4

Chain Y:

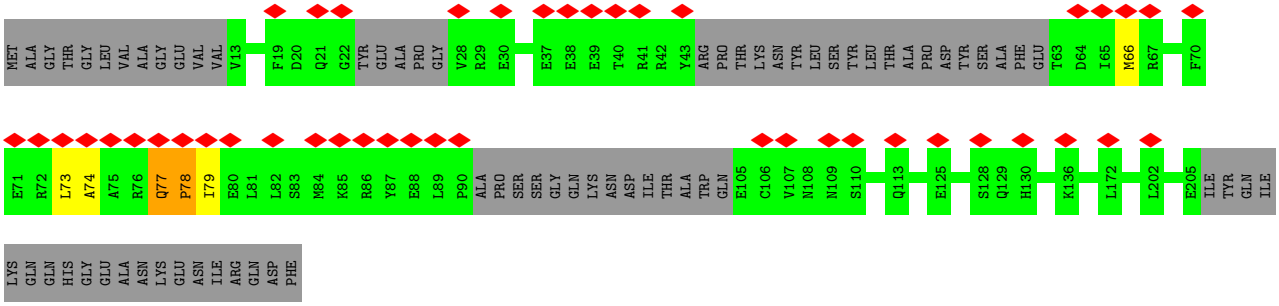






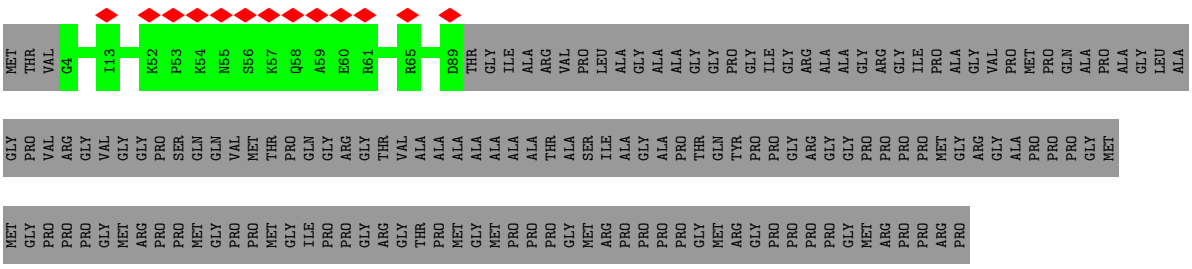
• Molecule 24: Pre-mRNA-splicing factor SPF27

Chain Z:



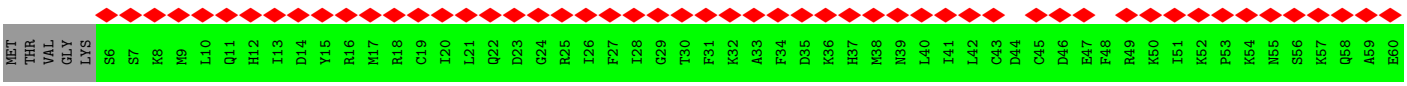
• Molecule 25: Small nuclear ribonucleoprotein-associated proteins B and B'

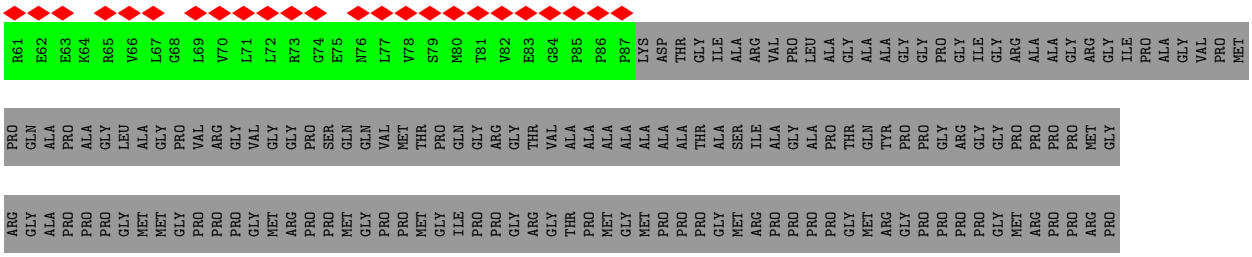
Chain a:



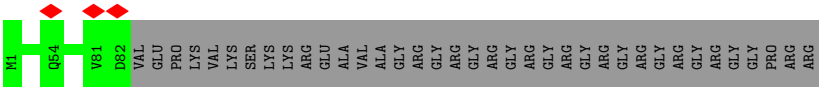
• Molecule 25: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain m:

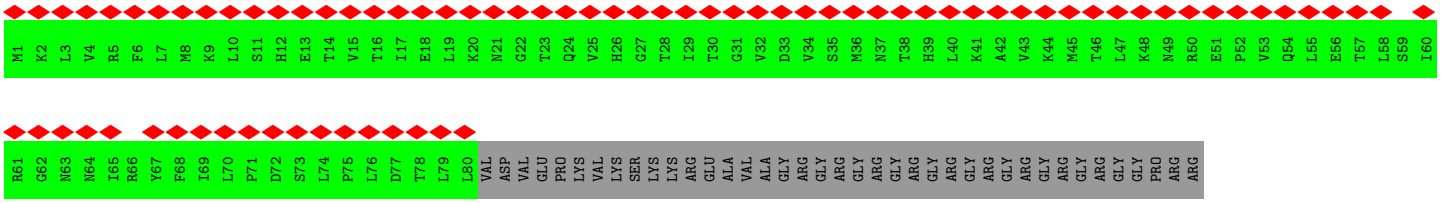




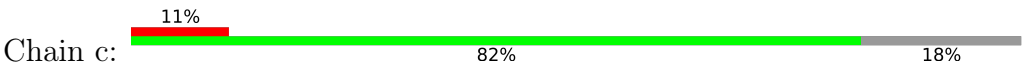
• Molecule 26: Small nuclear ribonucleoprotein Sm D1

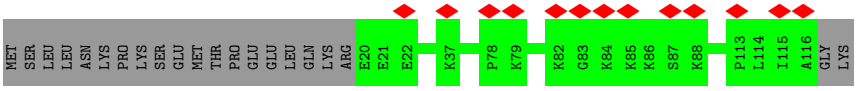


• Molecule 26: Small nuclear ribonucleoprotein Sm D1

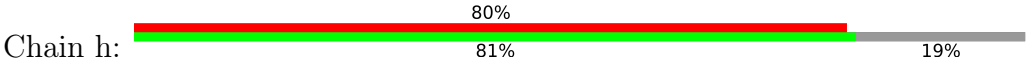


• Molecule 27: Small nuclear ribonucleoprotein Sm D2

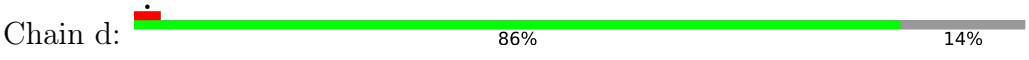


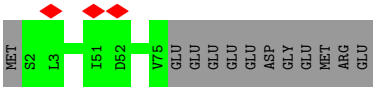


• Molecule 27: Small nuclear ribonucleoprotein Sm D2

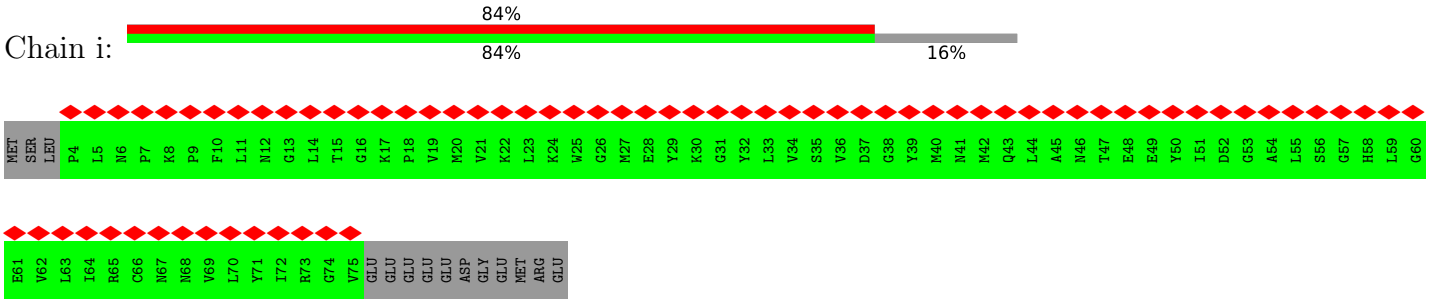


• Molecule 28: Small nuclear ribonucleoprotein F

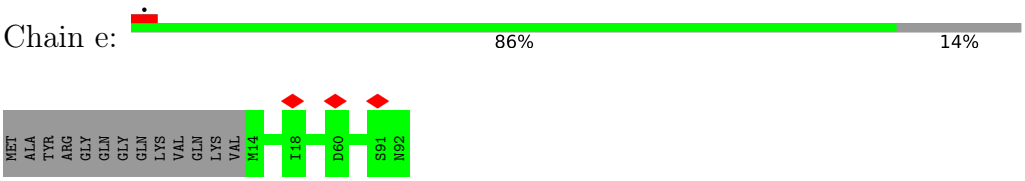




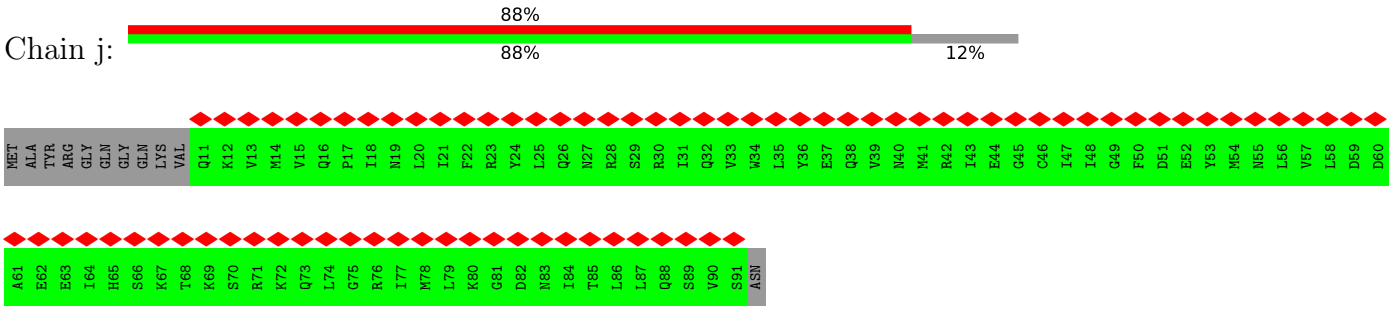
• Molecule 28: Small nuclear ribonucleoprotein F



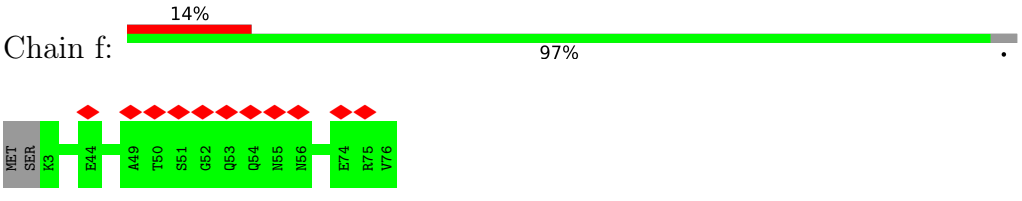
• Molecule 29: Small nuclear ribonucleoprotein E



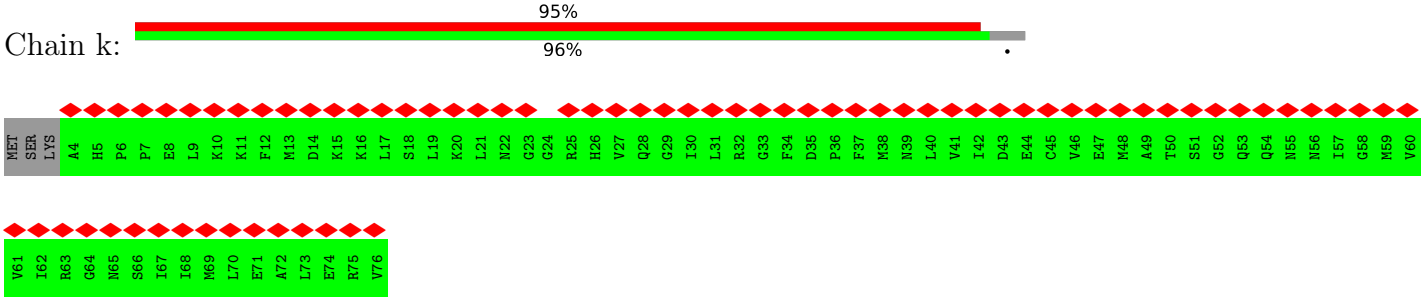
• Molecule 29: Small nuclear ribonucleoprotein E



• Molecule 30: Small nuclear ribonucleoprotein G

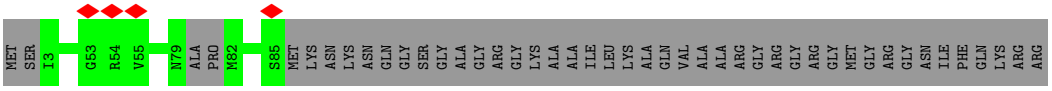


• Molecule 30: Small nuclear ribonucleoprotein G



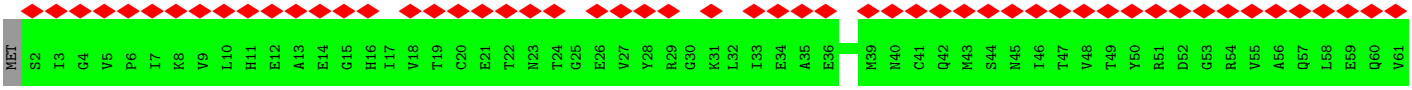
• Molecule 31: Small nuclear ribonucleoprotein Sm D3

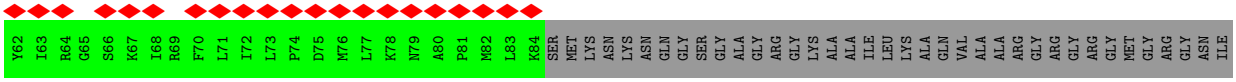
Chain g:



• Molecule 31: Small nuclear ribonucleoprotein Sm D3

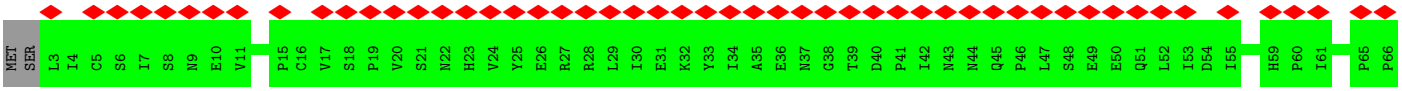
Chain l:

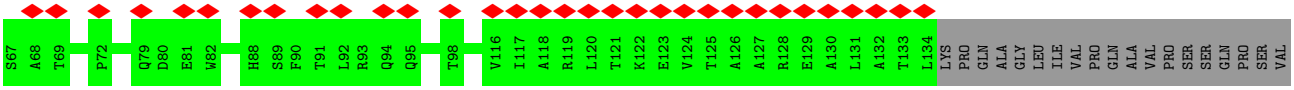




• Molecule 32: Pre-mRNA-processing factor 19

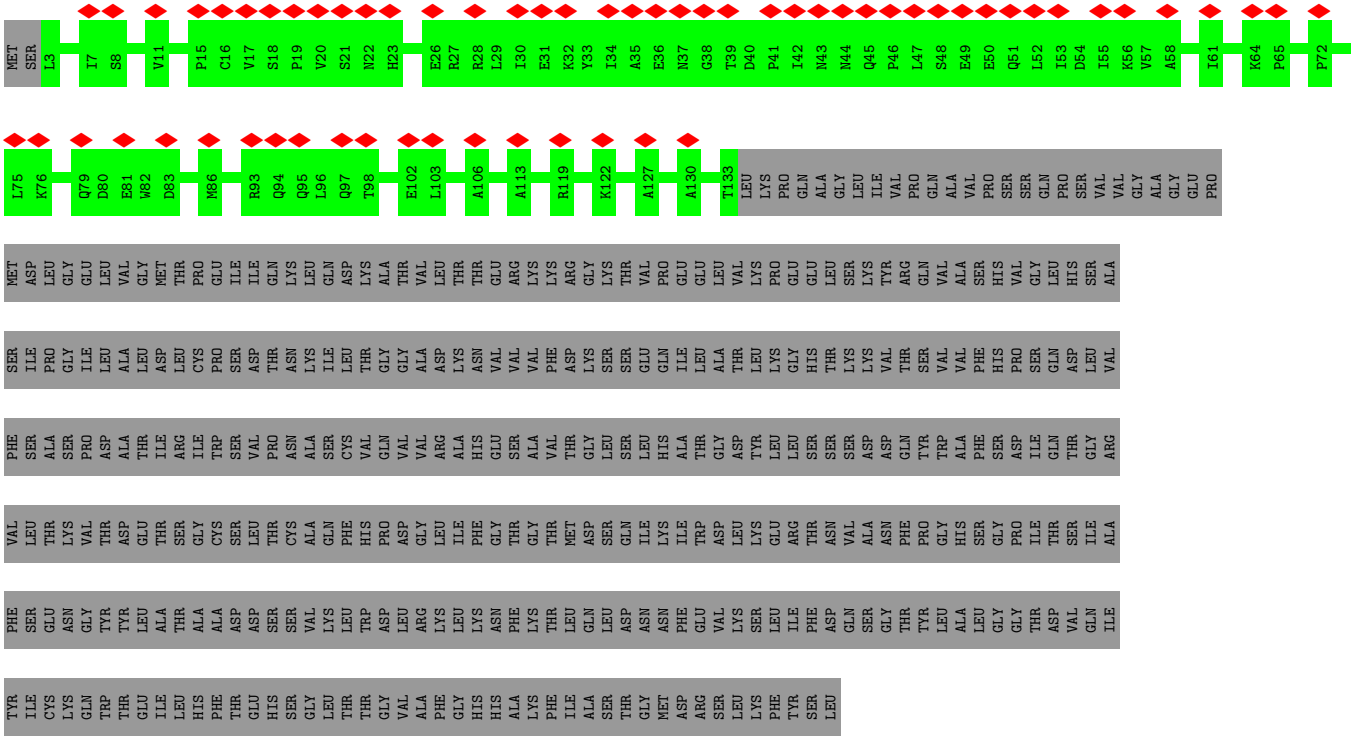
Chain q:





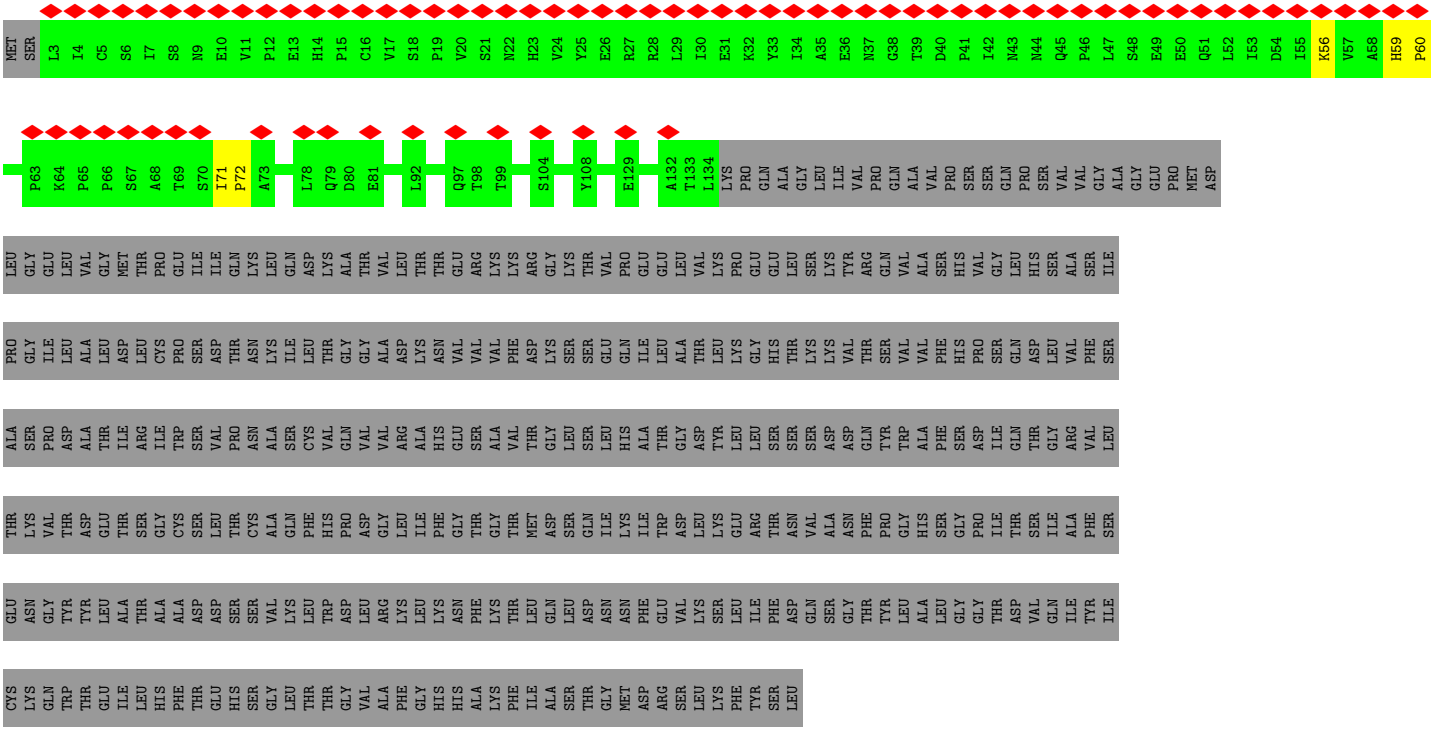
• Molecule 32: Pre-mRNA-processing factor 19

Chain r:



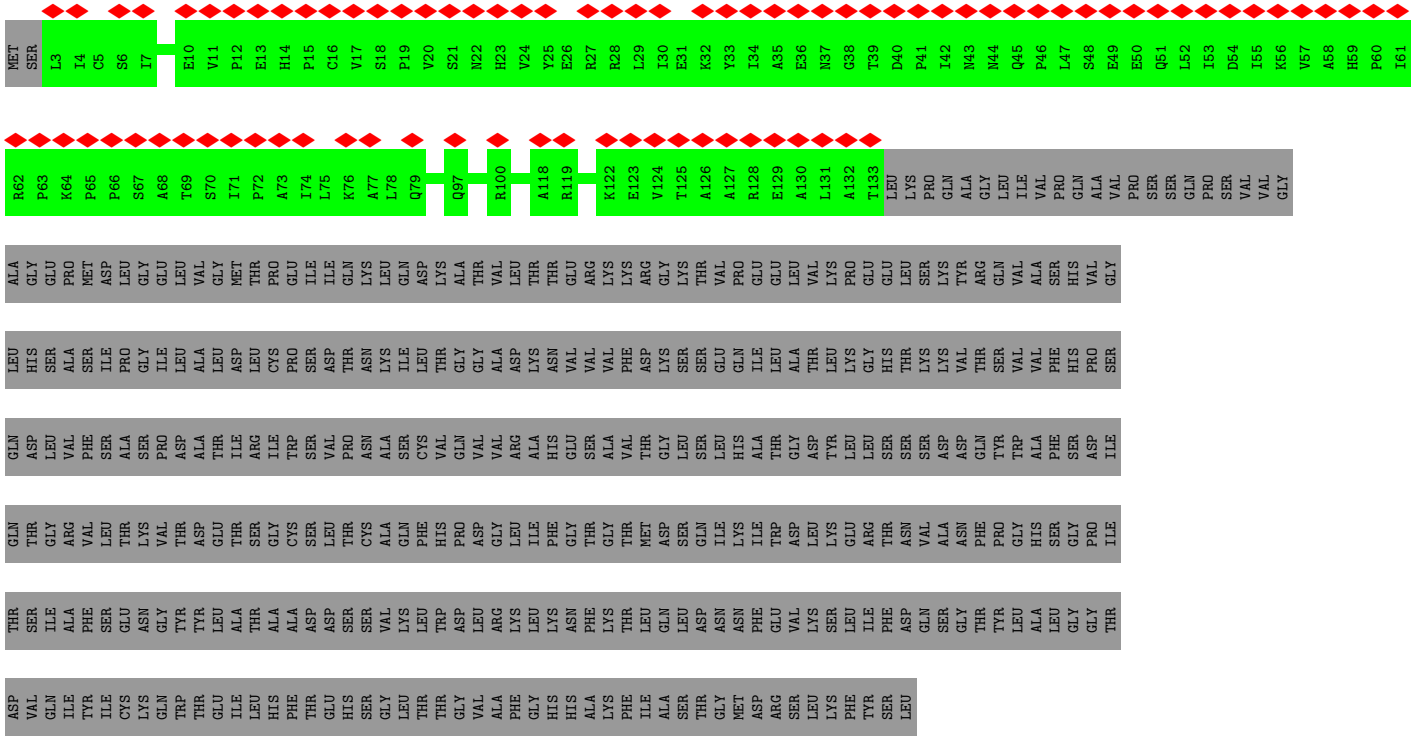
• Molecule 32: Pre-mRNA-processing factor 19

Chain s:



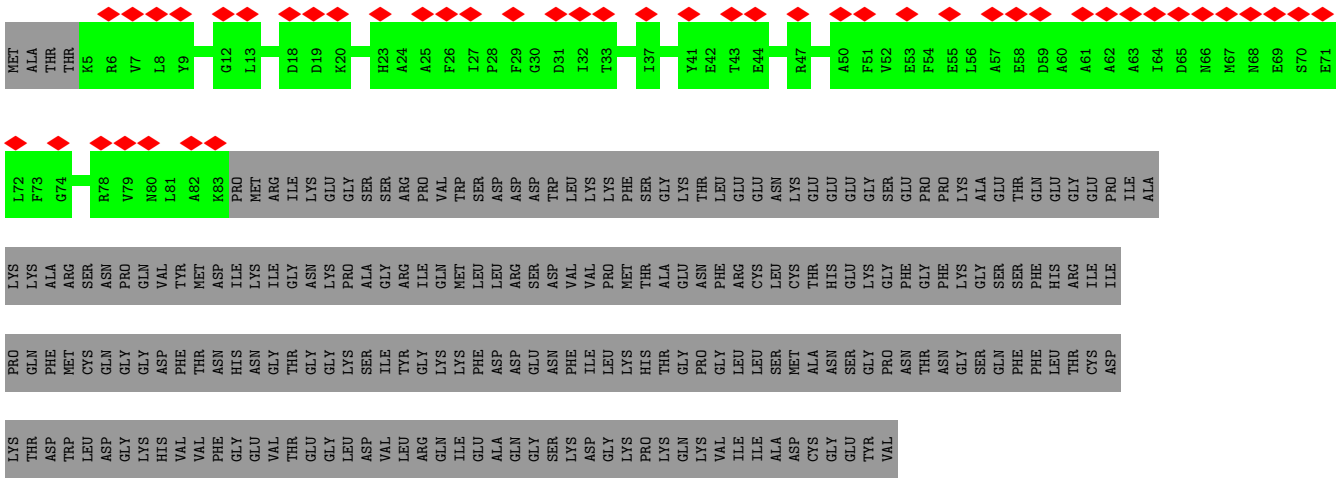
• Molecule 32: Pre-mRNA-processing factor 19

Chain t:



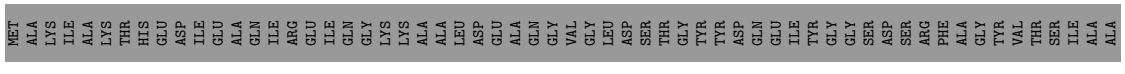
• Molecule 33: Peptidyl-prolyl cis-trans isomerase E

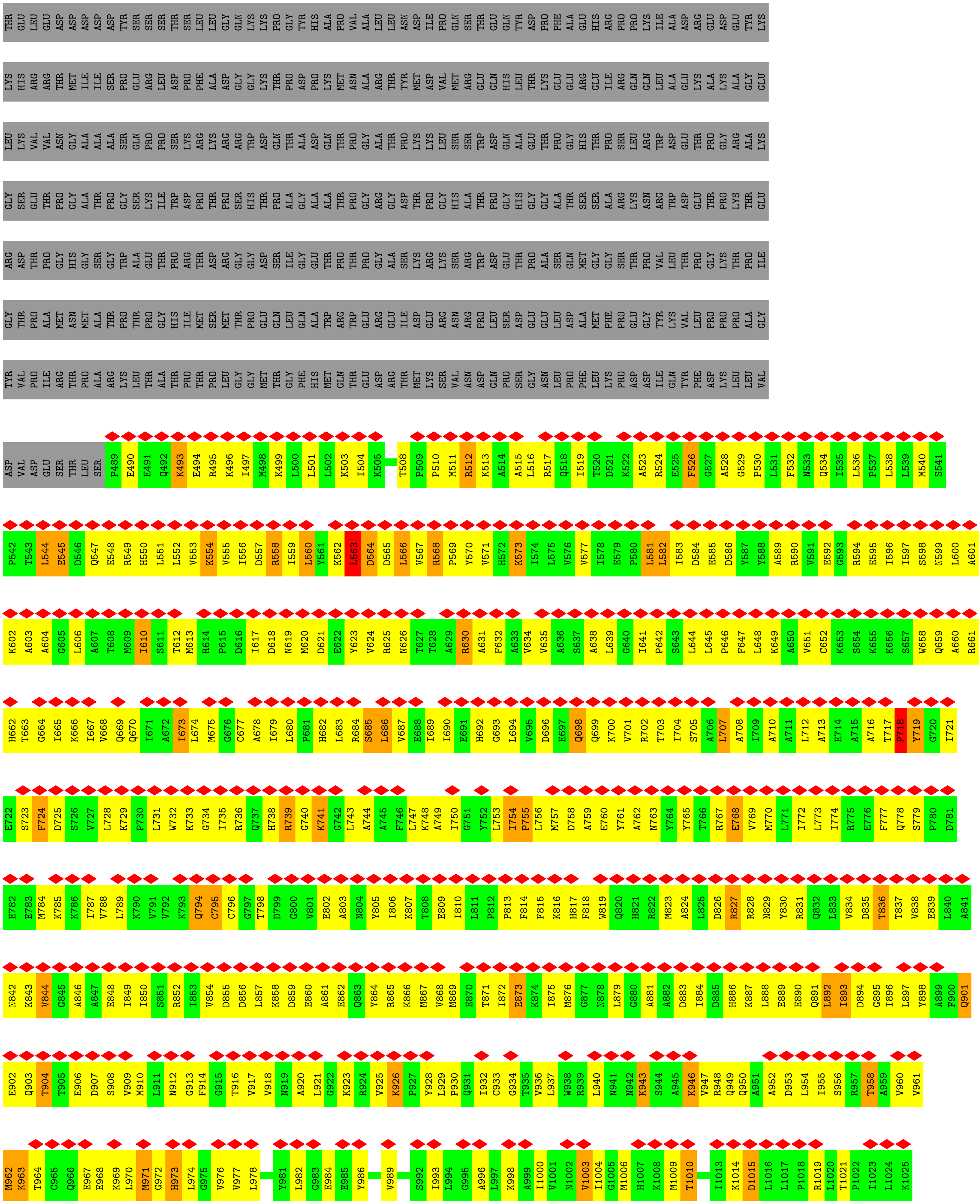
Chain y:



• Molecule 34: Splicing factor 3B subunit 1

Chain 1:

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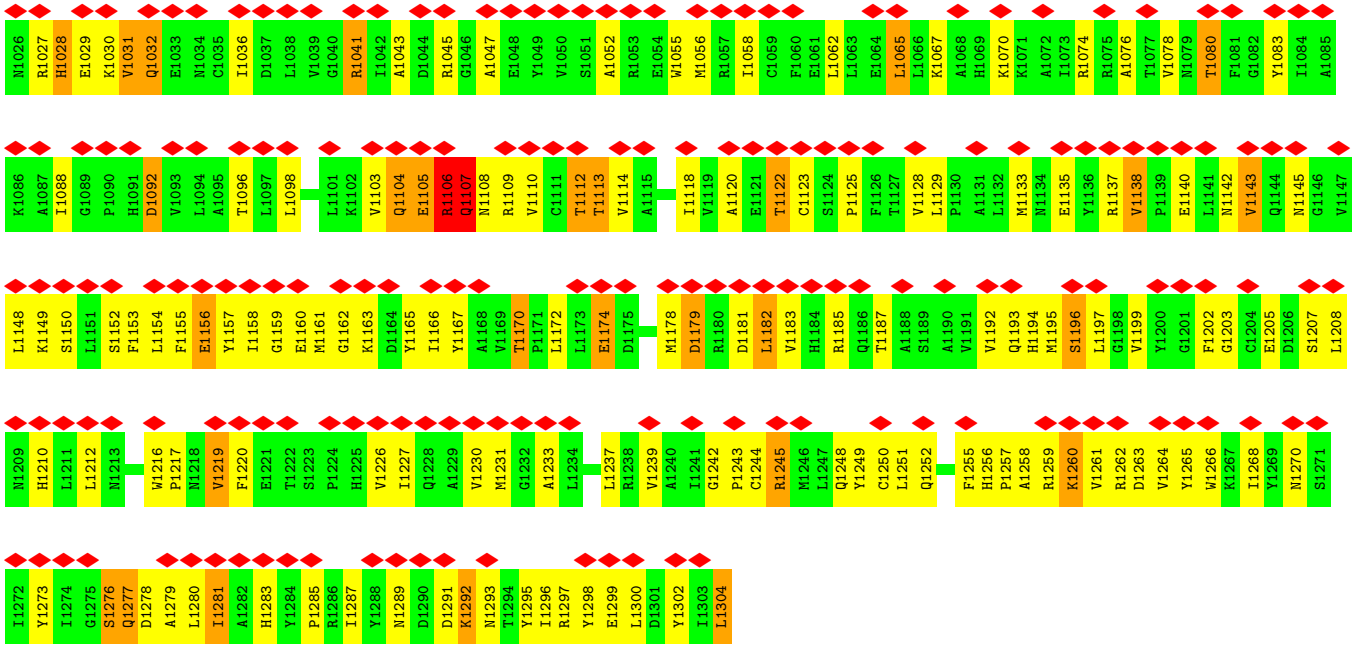
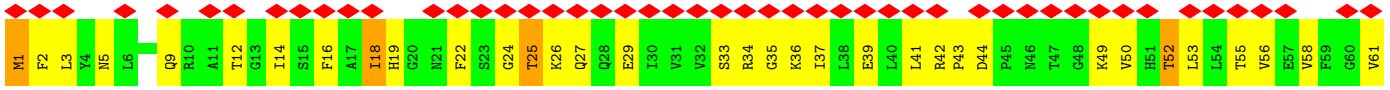
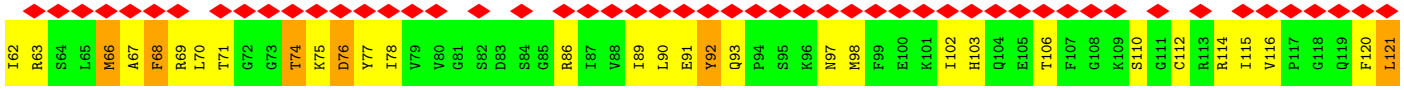
LYS HIS ARG ARG THR MET ILE ILE SER PRO GLU ARG LEU ASP PRO PHE ALA ASP GLY GLY LYS THR PRO ASP PRO LYS MET ASN ALA ARG THR TYR MET ASP VAL MET ARG GLU GLN HIS LEU THR LYS GLU GLU ARG GLU ILE ARG GLN GLN LEU ALA GLU LYS ALA LYS ALA GLY GLU
LEU LYS VAL VAL ASN GLY ALA ALA ALA SER GLN PRO PRO SER LYS ARG LYS ARG ARG TRP ASP GLN THR ALA ASP GLN THR PRO GLY ALA THR PRO LYS LYS LEU SER SER TRP ASP GLN ALA GLU THR PRO GLY HIS THR PRO SER LEU ARG TRP ASP GLU THR PRO GLY ARG ALA LYS
GLY SER GLU THR PRO GLY ALA THR PRO GLY SER LYS ILE TRP ASP PRO THR PRO SER HIS THR PRO ALA GLY ALA ALA THR PRO GLY ARG GLY ASP THR PRO GLY HIS ALA THR PRO GLY HIS GLY GLY ALA THR SER SER ALA ARG LYS ASN ARG TRP ASP GLU THR PRO LYS THR GLU
ARG ASP THR PRO GLY HIS GLY SER GLY TRP ALA GLU THR PRO ARG THR ASP ARG GLY GLY ASP SER ILE GLY GLU THR PRO THR PRO GLY ALA SER LYS ARG LYS SER ARG TRP ASP GLU THR PRO ALA SER GLN MET GLY GLY SER THR PRO VAL LEU THR PRO GLY LYS THR PRO ILE
GLY THR PRO ALA MET ASN MET ALA THR PRO THR PRO GLY HIS ILE MET SER MET THR PRO GLU GLN LEU GLN ALA TRP ARG TRP GLU ARG GLU ILE ASP GLU ARG ASN ARG PRO LEU SER ASP GLU GLU LEU ASP ALA MET PHE PRO GLU GLY TYR LYS VAL LEU PRO PRO PRO ALA GLY
TYR VAL PRO ILE ARG THR PRO ALA ARG LYS LEU THR ALA THR PRO THR PRO LEU GLY GLY MET THR GLY PHE HIS MET GLN THR GLU ASP ARG THR MET LYS SER VAL ASN ASP GLN PRO SER GLY ASN LEU PRO PHE LEU LYS PRO ASP ASP ILE GLN TYR PHE ASP LYS LEU LEU VAL
ASP VAL ASP GLU SER THR LEU SER P489 E490 E491 Q492 K493 E494 R495 K496 I497 M498 K499 L500 L501 L502 K503 I504 K505 T508 P509 P510 M511 R512 K513 A514 A515 L516 R517 Q518 I519 T520 D521 K522 A523 R524 E525 F526 G527 A528 G529 P530 L531 F532 N533 Q534 I535 L536 P537 L538 L539 M540 S541
P542 T543 L544 E545 D546 Q547 E548 R549 H550 L551 L552 V553 K554 V555 I556 D557 R558 I559 L560 Y561 K562 L563 D564 D565 L566 V567 R568 P569 Y570 V571 H572 K573 I574 L575 V576 V577 I578 E579 P580 L581 L582 I583 D584 E585 D586 Y587 Y588 A589 R590 V591 E592 G593 R594 E595 I596 I597 S598 N599 L600 A601
K602 A603 A604 G605 L606 A607 T608 M609 I610 S611 T612 M613 R614 P615 D616 I617 D618 N619 M620 D621 E622 Y623 V624 R625 N626 T627 T628 A629 R630 A631 F632 A633 V634 V635 A636 S637 A638 L639 G640 I641 P642 S643 L644 L645 P646 F647 L648 K649 A650 V651 C652 K653 S654 K655 K656 S657 W658 Q659 A660 R661
H662 T663 G664 I665 K666 I667 V668 Q669 Q670 I671 A672 I673 L674 M675 G676 C677 A678 I679 L680 P681 H682 L683 R684 S685 L686 V687 E688 I689 I690 E691 H692 G693 L694 V695 D696 E697 Q698 Q699 K700 V701 R702 T703 I704 S705 A706 L707 A708 I709 A710 A711 L712 A713 E714 A715 A716 T717 P718 Y719 G720 I721
E722 S723 F724 D725 S726 V727 L728 K729 P730 L731 W732 K733 G734 I735 R736 Q737 H738 R739 G740 K741 G742 L743 A744 A745 F746 L747 K748 A749 I750 G751 Y752 L753 I754 P755 L756 M757 D758 A759 E760 Y761 A762 N763 Y764 Y765 T766 R767 E768 V769 M770 L771 I772 L773 I774 R775 E776 F777 Q778 S779 P780 D781
E782 E783 M784 K785 K786 I787 V788 L789 K790 V791 V792 K793 Q794 C795 C796 G797 T798 D799 G800 V801 E802 A803 N804 Y805 I806 K807 T808 E809 I810 L811 P812 P813 F814 F815 K816 H817 F818 W819 Q820 H821 R822 M823 A824 L825 D826 R827 R828 N829 Y830 R831 Q832 L833 V834 D835 T836 T837 V838 E839 L840 A841
N842 K843 V844 G845 A846 A847 E848 I849 I850 S851 R852 I853 V854 D855 D856 L857 K858 D859 E860 A861 E862 Q863 Y864 R865 K866 M867 V868 M869 E870 T871 I872 E873 K874 I875 M876 G877 N878 L879 G880 A881 A882 D883 I884 D885 H886 K887 L888 E889 E890 Q891 L892 I893 D894 G895 I896 L897 Y898 A899 F900 Q901
E902 Q903 T904 T905 E906 D907 S908 V909 M910 L911 N912 G913 F914 G915 T916 V917 V918 N919 A920 L921 G922 K923 R924 V925 K926 P927 Y928 L929 P930 Q931 I932 C933 G934 T935 V936 L937 W938 R939 L940 N941 N942 K943 S944 A945 K946 V947 R948 Q949 Q950 A951 A952 D953 L954 I955 S956 R957 T958 A959 V960 V961
M962 K963 T964 C965 Q966 E967 E968 K969 L970 M971 G972 H973 L974 G975 V976 V977 L978 Y981 L982 G983 E984 E985 Y986 V989 S992 I993 L994 G995 A996 L997 K998 A999 I1000 V1001 N1002 V1003 I1004 G1005 M1006 H1007 K1008 M1009 T1010 I1013 K1014 D1015 L1016 L1017 P1018 R1019 L1020 T1021 P1022 I1023 L1024 K1025

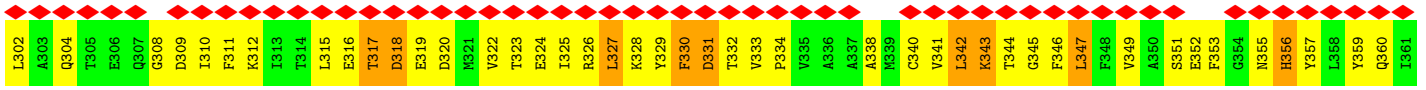


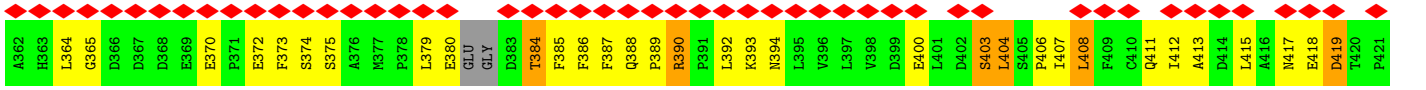
• Molecule 35: Splicing factor 3B subunit 3

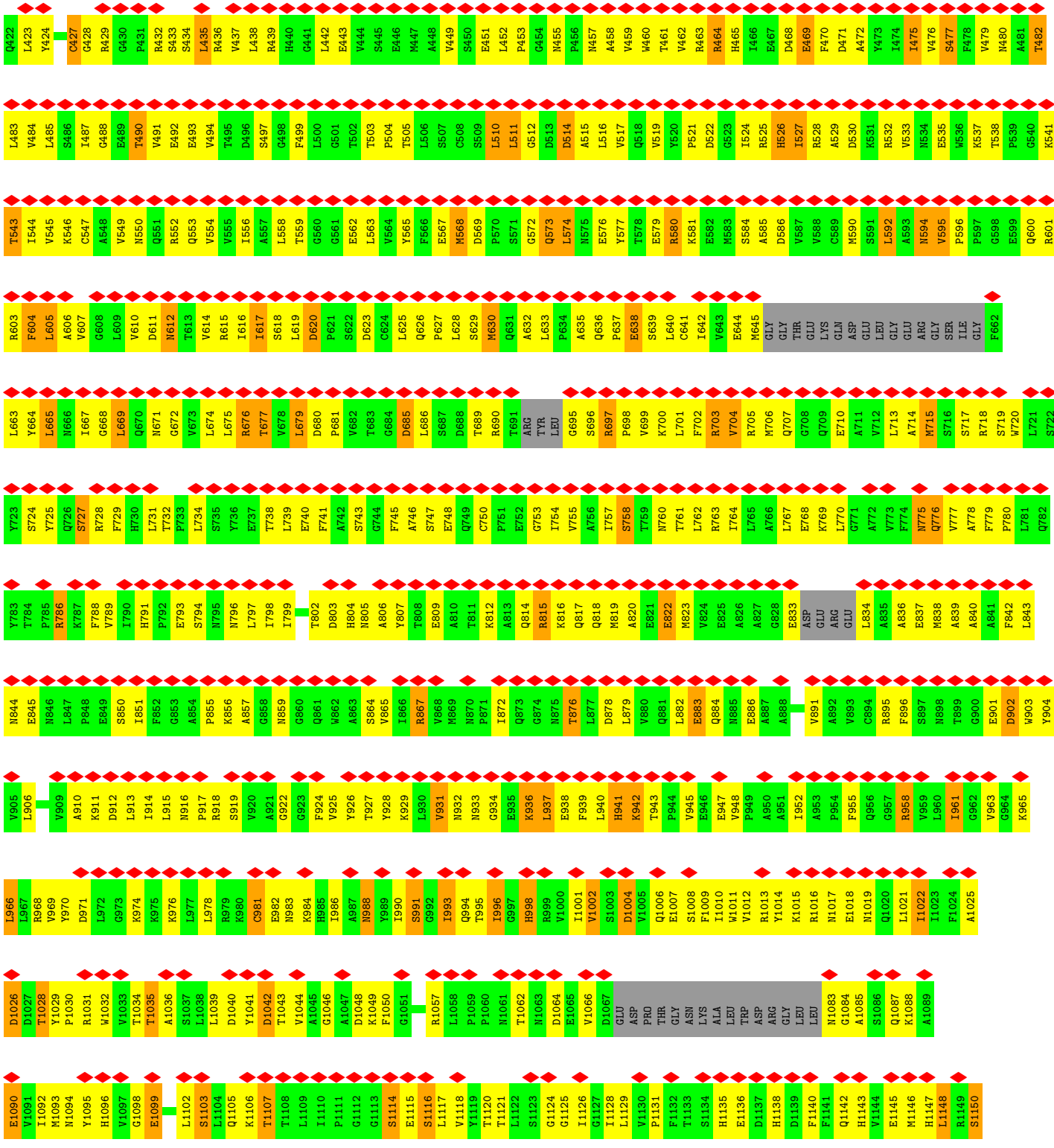
Chain 3:







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L483 V484 L485 S486 I487 G488 E489 T490 V491 E492 E493 V494 T495 D496 S497 G498 F499 L500 G501 T502 T503 P504 T505 L506 S507 C508 S509 L510 L511 G512 D513 D514 A515 L516 V517 Q518 V519 Y520 P521 D522 G523 I524 R525 H526 I527 R528 A529 D530 K531 R532 V533 N534 E535 W536 K537 T538 P539 G540 K541 K542
T543 I544 V545 K546 C547 A548 V549 N550 Q551 R552 Q553 V554 V555 I556 A557 L558 T559 G560 G561 E562 L563 V564 Y565 F566 E567 M568 D569 P570 S571 G572 Q573 L574 N575 E576 Y577 T578 E579 R580 K581 E582 M583 S584 A585 D586 V587 V588 C589 M590 S591 L592 A593 N594 V595 P596 P597 G598 E599 Q600 R601 S602
R603 F604 L605 A606 V607 G608 L609 V610 D611 N612 T613 V614 R615 I616 I617 S618 L619 D620 P621 S622 D623 C624 L625 Q626 P627 L628 S629 M630 Q631 A632 L633 P634 A635 Q636 P637 E638 S639 L640 C641 I642 V643 E644 M645 GLY GLY THR GLU LYS GLN ASP GLU LEU GLY GLU ARG GLY SER ILE GLY F662
L663 Y664 L665 N666 I667 G668 L669 Q670 N671 G672 V673 L674 L675 R676 T677 V678 L679 D680 P681 V682 T683 G684 D685 L686 S687 D688 T689 R690 T691 ARG TYR LEU G695 S696 R697 P698 V699 K700 L701 F702 R703 V704 R705 M706 Q707 G708 Q709 E710 A711 V712 L713 A714 M715 S716 S717 R718 S719 W720 L721 S722
Y723 S724 Y725 Q726 S727 R728 F729 H730 L731 T732 P733 L734 S735 Y736 E737 T738 L739 E740 F741 A742 S743 G744 F745 A746 S747 E748 Q749 C750 P751 E752 G753 I754 V755 A756 I757 S758 T759 N760 T761 L762 R763 I764 L765 A766 L767 E768 K769 L770 G771 A772 V773 F774 N775 Q776 V777 A778 F779 P780 L781 Q782
Y783 T784 P785 R786 K787 F788 V789 I790 H791 P792 E793 S794 N795 N796 L797 T798 I799 T802 D803 H804 N805 A806 Y807 T808 E809 A810 T811 K812 A813 Q814 R815 K816 Q817 Q818 M819 A820 E821 E822 M823 V824 E825 A826 A827 G828 E833 ASP GLU ARG GLU L834 A835 A836 E837 M838 A839 A840 A841 F842 L843
N844 E845 N846 L847 P848 E849 S850 I851 F852 G853 A854 P855 K856 A857 G858 N859 G860 Q861 W862 A863 S864 V865 I866 R867 V868 M869 N870 P871 I872 Q873 G874 N875 T876 L877 D878 L879 V880 Q881 L882 E883 Q884 N885 E886 A887 A888 V891 A892 V893 C894 R895 F896 S897 N898 T899 G900 E901 D902 W903 Y904
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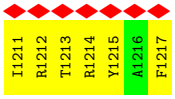
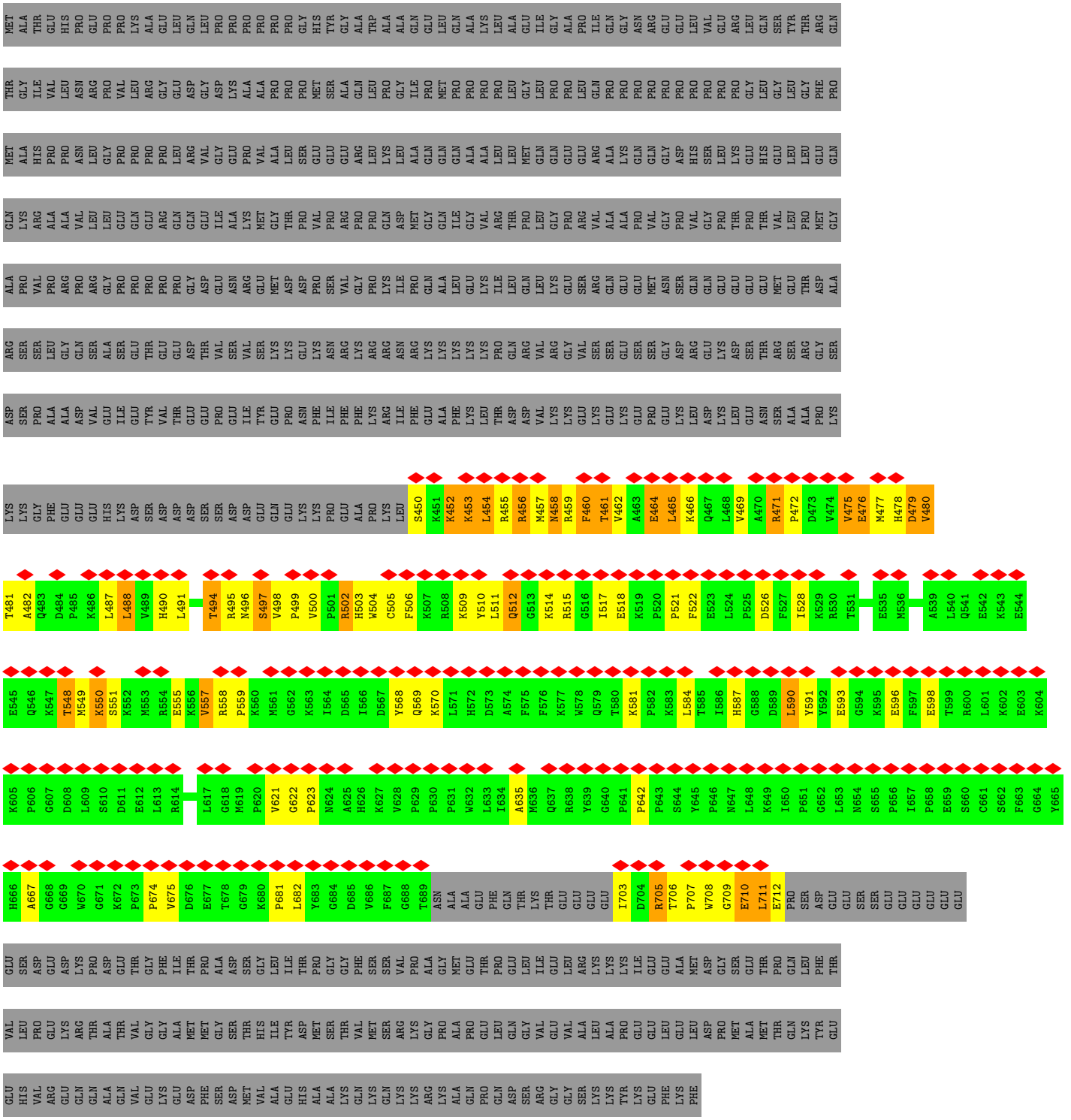
L966 L967 R968 V969 Y970 D971 L972 G973 K974 K975 K976 L977 L978 R979 K980 C981 E982 N983 K984 H985 I986 A987 N988 Y989 I990 S991 Q992 I993 Q994 T995 I996 G997 H998 R999 V1000 I1001 V1002 S1003 D1004 V1005 Q1006 E1007 S1008 F1009 I1010 W1011 V1012 R1013 Y1014 K1015 R1016 N1017 E1018 N1019 Q1020 L1021 I1022 I1023 F1024 A1025
D1026 D1027 T1028 Y1029 P1030 R1031 W1032 V1033 T1034 T1035 A1036 S1037 L1038 L1039 D1040 Y1041 D1042 T1043 V1044 A1045 G1046 A1047 D1048 K1049 F1050 G1051 R1057 L1058 P1059 P1060 N1061 T1062 N1063 D1064 E1065 V1066 D1067 GLU ASP PRO THR GLY ASN LYS ALA LEU TRP ASP ARG GLY LEU LEU N1083 G1084 A1085 S1086 Q1087 K1088 A1089
E1090 Y1091 I1092 M1093 N1094 Y1095 H1096 V1097 G1098 E1099 L1102 S1103 L1104 Q1105 K1106 T1107 T1108 L1109 I1110 P1111 G1112 G1113 S1114 E1115 S1116 L1117 V1118 Y1119 T1120 T1121 L1122 S1123 G1124 G1125 I1126 G1127 I1128 L1129 V1130 P1131 F1132 T1133 S1134 H1135 E1136 D1137 H1138 D1139 F1140 F1141 Q1142 H1143 V1144 E1145 M1146 H1147 L1148 R1149 S1150
E1151 H1152 P1153 P1154 L1155 C1156 G1157 R1158 D1159 H1160 L1161 S1162 F1163 R1164 S1165 Y1166 Y1167 F1168 P1169 V1170 K1171 N1172 V1173 I1174 D1175 G1176 D1177 L1178 C1179 E1180 Q1181 F1182 N1183 S1184 M1185 E1186 P1187 N1188 K1189 Q1190 K1191 N1192 V1193 S1194 E1195 E1196 L1197 D1198 R1199 T1200 P1201 P1202 E1203 V1204 S1205 K1206 K1207 L1208 E1209 D1210



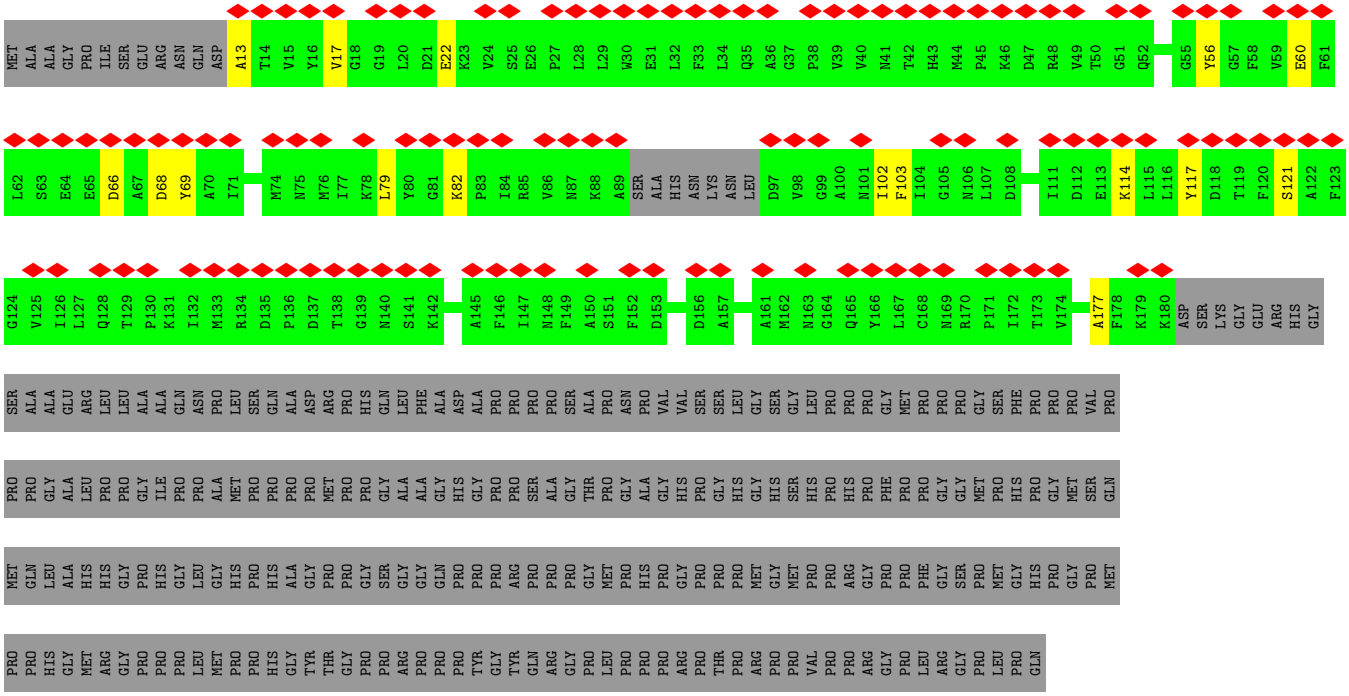
• Molecule 36: Splicing factor 3B subunit 2

Chain 2:



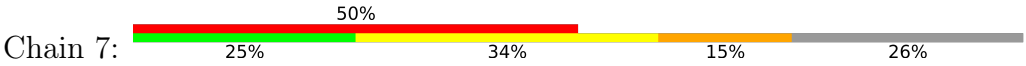
• Molecule 37: Splicing factor 3B subunit 4

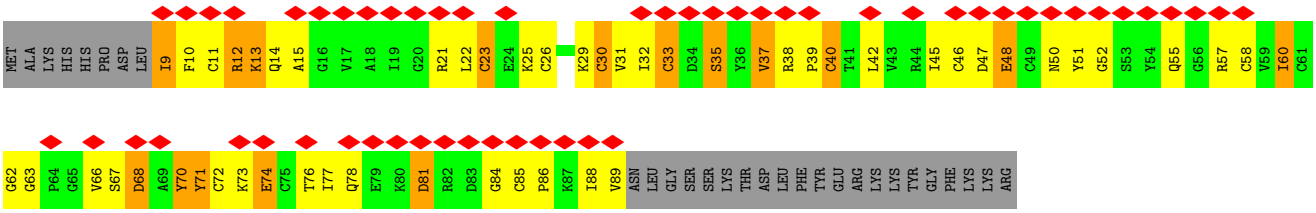
Chain 4:



• Molecule 38: PHD finger-like domain-containing protein 5A

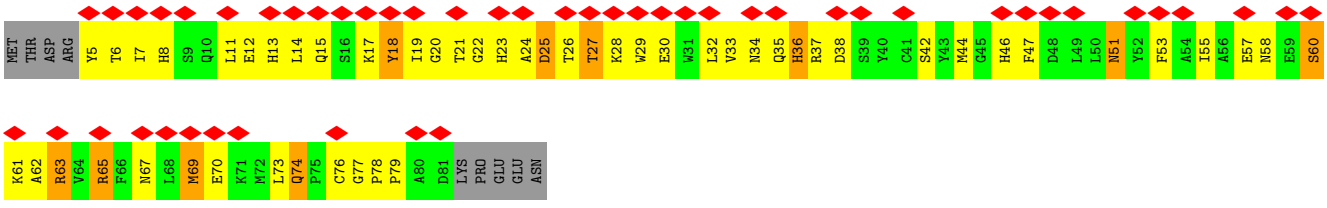
Chain 7:





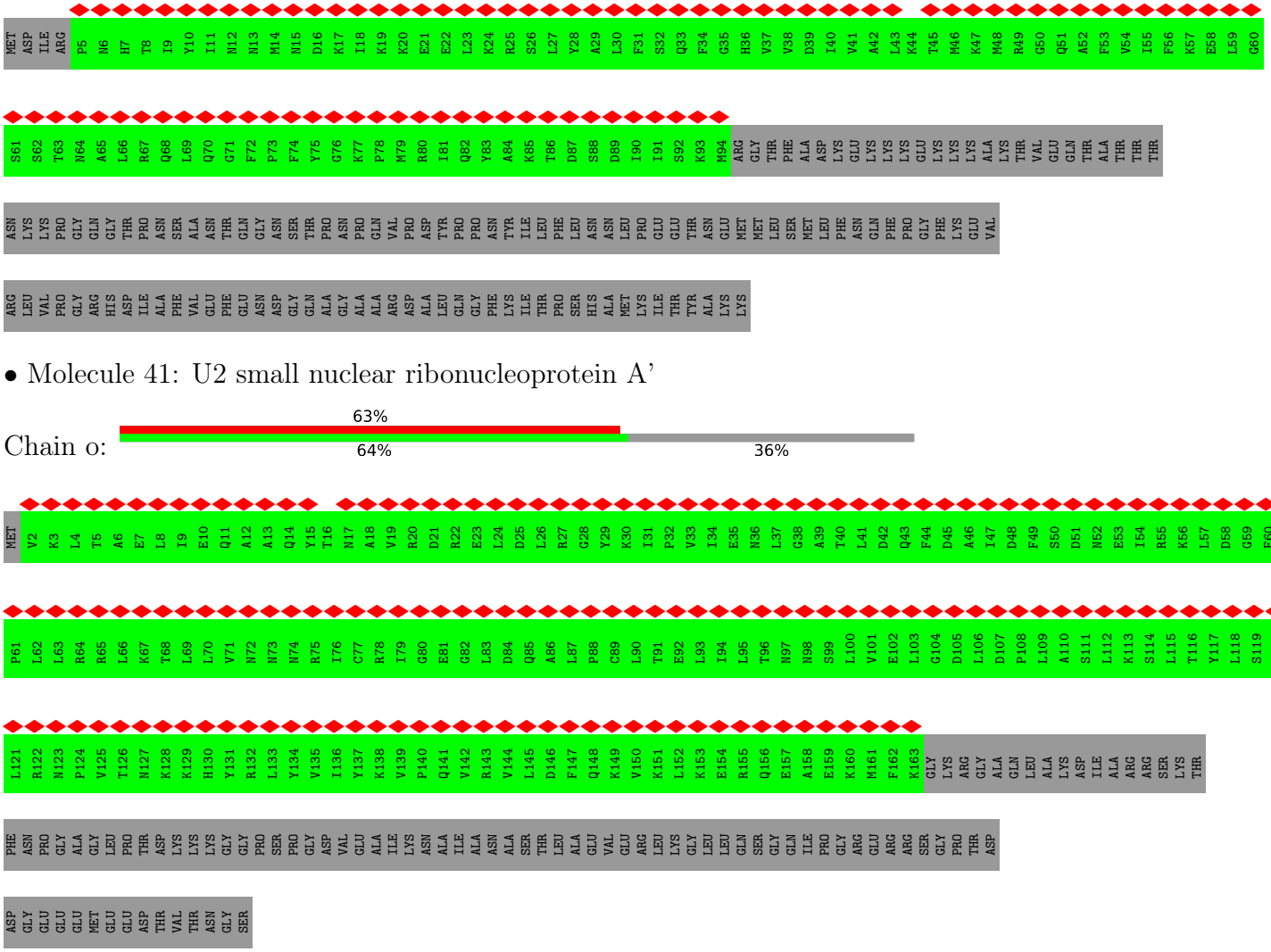
• Molecule 39: Splicing factor 3B subunit 5

Chain 5:



• Molecule 40: U2 small nuclear ribonucleoprotein B”

Chain p:



• Molecule 41: U2 small nuclear ribonucleoprotein A'

Chain o:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92596	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.253	Depositor
Minimum map value	-1.475	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	516.96, 516.96, 516.96	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.077, 1.077, 1.077	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, IHP, GTP, SEP, MG

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	0.78	1/16774 (0.0%)	0.66	5/22749 (0.0%)
2	B	1.08	2/2303 (0.1%)	1.04	6/3579 (0.2%)
3	C	0.55	0/6873	0.63	2/9346 (0.0%)
4	E	0.42	0/2392	0.63	1/3242 (0.0%)
5	F	1.21	3/2323 (0.1%)	1.17	11/3619 (0.3%)
6	G	0.70	3/1764 (0.2%)	1.30	19/2737 (0.7%)
7	H	0.66	2/3574 (0.1%)	1.07	10/5560 (0.2%)
8	I	0.25	0/3406	0.42	0/4767
9	J	0.58	0/3833	0.55	0/5205
10	L	0.46	0/2612	0.53	0/3548
11	M	0.48	0/991	0.73	0/1325
12	N	0.64	0/1210	0.60	0/1622
13	O	0.33	0/1447	0.48	0/2013
14	P	0.74	0/888	0.80	1/1177 (0.1%)
15	Q	0.24	0/5279	0.45	0/6583
16	R	0.52	0/2937	0.58	0/3945
17	S	0.27	0/769	0.50	0/1063
18	T	1.02	0/2574	0.73	3/3511 (0.1%)
19	U	0.43	0/424	0.48	0/582
20	V	0.32	0/2993	0.50	1/4088 (0.0%)
21	W	0.34	0/2471	0.71	0/3437
22	X	0.34	0/6479	0.59	4/8747 (0.0%)
23	Y	0.33	0/2605	0.58	0/3522
24	Z	0.25	0/768	0.39	0/1067
25	a	0.26	0/343	0.55	0/427
25	m	0.25	0/416	0.54	0/581
26	b	0.25	0/327	0.52	0/407
26	n	0.24	0/404	0.50	0/564
27	c	0.24	0/387	0.52	0/482
27	h	0.24	0/485	0.48	0/677
28	d	0.24	0/295	0.54	0/367
28	i	0.27	0/362	0.53	0/502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	e	0.23	0/315	0.51	0/392
29	j	0.25	0/403	0.46	0/561
30	f	0.24	0/295	0.53	0/367
30	k	0.26	0/366	0.53	0/509
31	g	0.24	0/322	0.51	0/399
31	l	0.26	0/417	0.51	0/581
32	q	0.25	0/658	0.41	0/919
32	r	0.27	0/653	0.41	0/912
32	s	0.27	0/658	0.45	0/919
32	t	0.26	0/653	0.38	0/912
33	y	0.26	0/315	0.51	0/392
34	1	0.63	0/6494	0.70	7/8801 (0.1%)
35	3	0.52	0/9398	0.66	1/12756 (0.0%)
36	2	0.56	0/1593	0.75	1/2170 (0.0%)
37	4	0.27	0/790	0.48	0/1095
38	7	0.56	0/621	0.61	0/833
39	5	0.72	0/654	0.64	0/885
40	p	0.25	0/453	0.46	0/631
41	o	0.24	0/821	0.48	0/1149
All	All	0.59	11/106587 (0.0%)	0.68	72/146224 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
3	C	0	4
4	E	0	1
8	I	0	1
9	J	0	3
11	M	0	1
12	N	0	1
14	P	0	1
16	R	0	1
22	X	0	1
23	Y	0	1
24	Z	0	1
34	1	0	4
35	3	0	5
36	2	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
38	7	0	1
39	5	0	1
All	All	0	40

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	97	A	N7-C5	7.07	1.43	1.39
6	G	97	A	N9-C4	-6.39	1.34	1.37
1	A	705	LYS	CD-CE	5.89	1.66	1.51
7	H	15	U	C4-O4	-5.71	1.19	1.23
2	B	32	C	N3-C4	-5.67	1.29	1.33
7	H	15	U	C2-O2	-5.47	1.17	1.22
5	F	65	G	N9-C8	-5.42	1.34	1.37
2	B	55	C	N1-C6	-5.33	1.33	1.37
5	F	72	G	C5-C4	-5.09	1.34	1.38
5	F	65	G	C5-C4	-5.02	1.34	1.38
6	G	-3	A	N3-C4	-5.01	1.31	1.34

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	97	A	C8-N9-C4	20.50	114.00	105.80
34	1	755	PRO	CA-N-CD	-15.48	89.83	111.50
6	G	97	A	N9-C4-C5	-13.31	100.47	105.80
7	H	15	U	N3-C4-O4	-12.76	110.47	119.40
7	H	15	U	N3-C2-O2	-11.44	114.19	122.20
6	G	97	A	C4-C5-C6	-10.90	111.55	117.00
6	G	97	A	N1-C2-N3	-10.17	124.22	129.30
6	G	97	A	N7-C8-N9	-9.90	108.85	113.80
6	G	97	A	N3-C4-C5	9.47	133.43	126.80
7	H	15	U	N3-C4-C5	9.06	120.03	114.60
18	T	186	PRO	C-N-CA	-9.00	99.21	121.70
7	H	15	U	C2-N3-C4	-8.29	122.03	127.00
5	F	38	G	O5'-P-OP2	-7.63	98.83	105.70
5	F	78	A	C8-N9-C4	7.40	108.76	105.80
36	2	550	LYS	N-CA-CB	-7.06	97.89	110.60
2	B	40	U	C2-N1-C1'	6.99	126.09	117.70
5	F	82	A	C2-N3-C4	-6.96	107.12	110.60
6	G	9	C	N3-C2-O2	-6.90	117.07	121.90
2	B	19	A	N9-C4-C5	-6.84	103.07	105.80
7	H	15	U	N1-C2-N3	6.51	118.81	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	97	A	N9-C1'-C2'	-6.35	105.01	112.00
20	V	494	LEU	CA-CB-CG	6.34	129.88	115.30
34	1	1107	GLN	C-N-CA	-6.33	105.88	121.70
6	G	112	U	N1-C2-O2	6.31	127.22	122.80
6	G	-5	C	C2-N1-C1'	6.14	125.56	118.80
7	H	173	C	N1-C2-O2	5.96	122.48	118.90
5	F	59	G	C4-C5-N7	5.93	113.17	110.80
34	1	718	PRO	CA-N-CD	-5.90	103.24	111.50
5	F	34	G	C4-N9-C1'	5.89	134.16	126.50
6	G	112	U	C2-N1-C1'	5.88	124.75	117.70
5	F	82	A	C5-C6-N1	-5.84	114.78	117.70
7	H	64	A	C5-C6-N6	-5.84	119.03	123.70
4	E	227	LEU	CA-CB-CG	5.78	128.60	115.30
6	G	112	U	O5'-P-OP2	-5.77	100.51	105.70
1	A	1518	LEU	CB-CG-CD2	5.77	120.81	111.00
6	G	111	U	OP2-P-O3'	5.60	117.52	105.20
5	F	59	G	C5-N7-C8	-5.58	101.51	104.30
6	G	97	A	C6-N1-C2	5.57	121.94	118.60
7	H	15	U	OP2-P-O3'	5.55	117.41	105.20
34	1	963	LYS	CB-CA-C	-5.49	99.42	110.40
5	F	38	G	C8-N9-C4	-5.48	104.21	106.40
6	G	9	C	N1-C2-O2	5.47	122.18	118.90
2	B	40	U	C6-N1-C1'	-5.46	113.56	121.20
14	P	216	ARG	NE-CZ-NH1	-5.43	117.58	120.30
5	F	38	G	N7-C8-N9	5.42	115.81	113.10
1	A	598	LEU	CB-CG-CD2	-5.41	101.80	111.00
35	3	235	LEU	CA-CB-CG	5.40	127.72	115.30
22	X	651	LEU	CA-CB-CG	5.40	127.72	115.30
7	H	15	U	N1-C2-O2	5.39	126.58	122.80
1	A	1517	LYS	CA-CB-CG	5.39	125.25	113.40
34	1	718	PRO	N-CA-CB	-5.36	96.70	102.60
22	X	262	LEU	CA-CB-CG	5.35	127.61	115.30
5	F	34	G	C8-N9-C1'	-5.34	120.06	127.00
7	H	15	U	C5-C4-O4	5.29	129.07	125.90
6	G	2	U	C6-N1-C2	-5.25	117.85	121.00
2	B	19	A	N3-C4-N9	5.25	131.60	127.40
18	T	303	LEU	CA-CB-CG	5.24	127.35	115.30
3	C	510	LEU	CA-CB-CG	5.23	127.33	115.30
3	C	251	LEU	CA-CB-CG	5.23	127.33	115.30
34	1	563	LEU	CA-CB-CG	5.20	127.26	115.30
6	G	113	U	P-O3'-C3'	5.18	125.91	119.70
2	B	45	C	N3-C2-O2	-5.15	118.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	X	172	LEU	CA-CB-CG	5.15	127.14	115.30
5	F	35	A	N1-C2-N3	5.10	131.85	129.30
34	1	1280	LEU	CB-CG-CD2	-5.10	102.33	111.00
6	G	112	U	N3-C2-O2	-5.09	118.63	122.20
1	A	1516	LYS	C-N-CA	5.09	134.43	121.70
6	G	115	C	N1-C2-O2	5.07	121.94	118.90
2	B	47	A	O4'-C1'-N9	5.07	112.26	108.20
1	A	1817	LEU	CA-CB-CG	5.07	126.95	115.30
18	T	351	ASP	C-N-CA	5.02	134.25	121.70
22	X	409	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	1	1105	GLU	Peptide
34	1	1107	GLN	Peptide
34	1	1179	ASP	Peptide
34	1	962	MET	Mainchain
36	2	502	ARG	Peptide
36	2	548	THR	Mainchain
35	3	268	ARG	Peptide
35	3	342	LEU	Peptide
35	3	490	THR	Peptide
35	3	916	ASN	Peptide
35	3	971	ASP	Peptide
39	5	79	PRO	Peptide
38	7	13	LYS	Peptide
1	A	1338	SER	Peptide
1	A	1416	ILE	Peptide
1	A	1516	LYS	Peptide
1	A	187	PRO	Peptide
1	A	365	VAL	Peptide
1	A	433	GLU	Peptide
1	A	699	GLU	Peptide
1	A	855	ARG	Peptide
1	A	940	ILE	Peptide
1	A	941	LYS	Peptide
1	A	982	GLU	Peptide
3	C	443	VAL	Peptide
3	C	533	SER	Peptide
3	C	572	GLU	Peptide

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Mol	Chain	Res	Type	Group
3	C	823	ALA	Peptide
4	E	321	TYR	Peptide
8	I	386	ASP	Peptide
9	J	202	GLU	Peptide
9	J	205	LEU	Peptide
9	J	240	THR	Peptide
11	M	124	PHE	Peptide
12	N	36	PRO	Peptide
14	P	29	GLN	Peptide
16	R	163	MET	Peptide
22	X	326	GLN	Peptide
23	Y	204	SER	Peptide
24	Z	77	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16331	0	16276	594	0
2	B	2066	0	1047	50	0
3	C	6724	0	6696	316	0
4	E	2338	0	2275	144	0
5	F	2075	0	1048	86	0
6	G	1587	0	808	77	0
7	H	3203	0	1618	100	0
8	I	3387	0	1651	13	0
9	J	3789	0	2891	95	0
10	L	2584	0	2096	97	0
11	M	971	0	950	69	0
12	N	1184	0	1190	44	0
13	O	1447	0	638	15	0
14	P	876	0	875	51	0
15	Q	5288	0	1361	5	0
16	R	2915	0	2794	134	0
17	S	770	0	356	8	0
18	T	2507	0	2451	79	0
19	U	422	0	291	14	0
20	V	2959	0	2237	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	W	2473	0	1096	19	0
22	X	6357	0	6349	345	0
23	Y	2556	0	2492	135	0
24	Z	772	0	342	2	0
25	a	344	0	93	0	0
25	m	413	0	194	0	0
26	b	328	0	89	0	0
26	n	402	0	184	0	0
27	c	388	0	102	0	0
27	h	482	0	220	0	0
28	d	296	0	87	0	0
28	i	359	0	179	0	0
29	e	316	0	85	0	0
29	j	403	0	173	0	0
30	f	296	0	84	0	0
30	k	364	0	176	0	0
31	g	324	0	89	0	0
31	l	415	0	198	0	0
32	q	659	0	296	0	0
32	r	654	0	294	0	0
32	s	659	0	296	0	0
32	t	654	0	294	0	0
33	y	316	0	86	0	0
34	1	6378	0	6511	959	0
35	3	9210	0	9117	813	0
36	2	1576	0	1191	294	0
37	4	792	0	367	11	0
38	7	613	0	596	56	0
39	5	635	0	595	137	0
40	p	451	0	215	0	0
41	o	816	0	386	0	0
42	A	36	0	6	5	0
43	C	32	0	12	0	0
44	C	1	0	0	0	0
44	F	5	0	0	0	0
44	L	1	0	0	0	0
45	7	3	0	0	0	0
45	N	3	0	0	0	0
All	All	104205	0	82043	4180	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 23.

All (4180) 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)
34:1:1279:ALA:HA	35:3:1167:TYR:CD1	1.35	1.61
1:A:1798:LEU:HD21	34:1:973:HIS:CD2	1.35	1.58
34:1:495:ARG:CG	34:1:530:PRO:HB3	1.36	1.54
21:W:279:LYS:CB	36:2:622:GLY:HA3	1.10	1.51
34:1:495:ARG:HG2	34:1:530:PRO:CB	1.44	1.45
34:1:933:CYS:CB	34:1:970:LEU:HD11	1.45	1.44
34:1:1300:LEU:HB3	35:3:1032:TRP:CZ3	1.51	1.44
34:1:598:SER:HA	34:1:638:ALA:CB	1.46	1.43
34:1:594:ARG:NH1	34:1:674:LEU:HD22	1.16	1.43
35:3:353:PHE:CE1	39:5:55:ILE:HD11	1.51	1.42
34:1:598:SER:HA	34:1:638:ALA:CA	1.50	1.41
34:1:1257:PRO:CB	36:2:481:THR:HG23	1.49	1.40
36:2:487:LEU:CD2	39:5:28:LYS:HB2	1.48	1.40
34:1:594:ARG:HA	34:1:634:VAL:CG1	1.53	1.38
34:1:1281:ILE:HG22	35:3:1050:PHE:CE1	1.59	1.37
21:W:279:LYS:CB	36:2:622:GLY:CA	2.02	1.36
34:1:778:GLN:HG3	34:1:817:HIS:CG	1.64	1.32
34:1:594:ARG:HH11	34:1:674:LEU:CD2	1.42	1.32
34:1:1256:HIS:CD2	34:1:1257:PRO:HD2	1.65	1.31
35:3:1116:SER:CA	36:2:708:TRP:HZ2	1.44	1.29
34:1:933:CYS:SG	34:1:970:LEU:HD11	1.73	1.29
34:1:1154:LEU:O	34:1:1158:ILE:HG12	1.34	1.28
34:1:1148:LEU:CD1	34:1:1187:THR:HB	1.61	1.28
34:1:582:LEU:HG	34:1:634:VAL:CG2	1.63	1.27
1:A:1798:LEU:CD2	34:1:973:HIS:CD2	2.18	1.26
34:1:1148:LEU:HD13	34:1:1187:THR:CB	1.62	1.26
38:7:9:ILE:CG1	39:5:6:THR:HG21	1.66	1.26
34:1:1153:PHE:O	34:1:1157:TYR:HD2	1.19	1.26
3:C:213:ASP:OD1	3:C:616:SER:HB2	1.32	1.23
36:2:487:LEU:HD22	39:5:28:LYS:CB	1.69	1.22
34:1:933:CYS:SG	34:1:974:LEU:HD21	1.80	1.22
34:1:1125:PRO:HD2	34:1:1165:TYR:OH	1.35	1.21
34:1:601:ALA:O	34:1:639:LEU:HD21	1.39	1.21
1:A:1792:LYS:HE2	34:1:973:HIS:NE2	1.57	1.19
34:1:1148:LEU:HB3	34:1:1187:THR:HG22	1.23	1.19
35:3:353:PHE:CZ	39:5:55:ILE:HD11	1.75	1.19
34:1:1160:GLU:HG3	35:3:1146:MET:HE1	1.22	1.18
34:1:1281:ILE:CG2	35:3:1050:PHE:HE1	1.55	1.18
7:H:56:A:N7	36:2:505:CYS:HB3	1.57	1.18
34:1:594:ARG:HD3	34:1:674:LEU:CD1	1.72	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:1256:HIS:CD2	34:1:1257:PRO:CD	2.27	1.18
34:1:854:VAL:HG11	34:1:891:GLN:HE21	1.01	1.17
34:1:1257:PRO:CB	36:2:481:THR:CG2	2.23	1.17
34:1:1263:ASP:CA	39:5:24:ALA:HB2	1.75	1.17
34:1:933:CYS:HB2	34:1:970:LEU:CD1	1.73	1.16
34:1:777:PHE:CE2	34:1:814:PHE:HB2	1.79	1.16
34:1:1279:ALA:CA	35:3:1167:TYR:CD1	2.26	1.16
34:1:606:LEU:HG	34:1:639:LEU:CD1	1.75	1.16
1:A:1994:LYS:HD3	34:1:986:TYR:OH	1.41	1.16
34:1:598:SER:CA	34:1:638:ALA:CB	2.23	1.15
35:3:1041:TYR:CD2	36:2:705:ARG:NE	2.15	1.15
34:1:1279:ALA:HA	35:3:1167:TYR:CE1	1.82	1.14
34:1:1257:PRO:HB3	36:2:481:THR:CG2	1.77	1.14
34:1:1217:PRO:HB2	36:2:510:TYR:CZ	1.82	1.14
34:1:702:ARG:HD2	34:1:738:HIS:CD2	1.82	1.13
34:1:754:ILE:HG21	34:1:795:CYS:HA	1.21	1.13
34:1:495:ARG:HD3	34:1:530:PRO:HA	1.29	1.13
34:1:1256:HIS:CG	34:1:1257:PRO:HD2	1.84	1.13
34:1:598:SER:CA	34:1:638:ALA:HB2	1.77	1.13
34:1:707:LEU:HD12	34:1:741:LYS:HD3	1.30	1.12
34:1:778:GLN:HG3	34:1:817:HIS:ND1	1.63	1.12
34:1:1160:GLU:CG	35:3:1146:MET:HE1	1.80	1.12
34:1:1300:LEU:CB	35:3:1032:TRP:CZ3	2.33	1.12
35:3:1116:SER:C	36:2:708:TRP:CZ2	2.22	1.12
34:1:582:LEU:HD23	34:1:631:ALA:HA	1.28	1.12
35:3:1041:TYR:CE2	36:2:705:ARG:NH2	2.18	1.12
34:1:582:LEU:CG	34:1:634:VAL:HG21	1.80	1.11
34:1:1300:LEU:HD13	35:3:1032:TRP:CH2	1.85	1.11
35:3:1116:SER:CA	36:2:708:TRP:CZ2	2.32	1.11
35:3:1041:TYR:CD2	36:2:705:ARG:CZ	2.33	1.11
34:1:1248:GLN:NE2	36:2:496:ASN:HB3	1.63	1.10
34:1:1302:TYR:CE1	35:3:915:LEU:HB3	1.86	1.10
35:3:35:GLY:HA2	39:5:47:PHE:CZ	1.87	1.10
34:1:1257:PRO:HB2	36:2:481:THR:HG23	1.34	1.10
34:1:869:MET:SD	34:1:896:ILE:HD13	1.92	1.10
36:2:482:ALA:HB2	36:2:488:LEU:HD12	1.13	1.09
38:7:9:ILE:HG13	39:5:6:THR:HG21	1.27	1.09
34:1:1302:TYR:HE1	35:3:915:LEU:HB3	1.14	1.09
35:3:189:TYR:HA	39:5:73:LEU:CD1	1.81	1.09
34:1:719:TYR:CE1	35:3:146:ARG:NH1	2.21	1.08
34:1:850:ILE:HG22	34:1:888:LEU:HD11	1.30	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:1279:ALA:HB2	35:3:1167:TYR:HA	1.27	1.08
1:A:1798:LEU:HD11	34:1:973:HIS:CD2	1.88	1.08
34:1:523:ALA:C	34:1:563:LEU:HD11	1.71	1.08
34:1:1179:ASP:HB2	36:2:511:LEU:CB	1.84	1.08
34:1:1153:PHE:O	34:1:1157:TYR:CD2	2.06	1.07
34:1:1217:PRO:HD3	36:2:590:LEU:HD13	1.34	1.07
34:1:1263:ASP:HA	39:5:24:ALA:HB2	1.31	1.07
36:2:482:ALA:CB	36:2:488:LEU:HD12	1.85	1.07
34:1:594:ARG:CA	34:1:634:VAL:HG13	1.83	1.07
34:1:598:SER:HA	34:1:638:ALA:HA	1.34	1.07
34:1:1281:ILE:CG2	35:3:1050:PHE:CE1	2.33	1.07
34:1:598:SER:HA	34:1:638:ALA:HB2	1.19	1.06
34:1:933:CYS:HB2	34:1:970:LEU:HD11	1.13	1.06
35:3:1041:TYR:CB	36:2:705:ARG:HG3	1.84	1.06
34:1:606:LEU:HG	34:1:639:LEU:HD13	1.11	1.06
34:1:774:ILE:HG23	34:1:813:PRO:HG3	1.16	1.06
35:3:805:ASN:HB3	39:5:58:ASN:HB2	1.35	1.06
34:1:598:SER:CA	34:1:638:ALA:HA	1.84	1.06
34:1:1179:ASP:HB2	36:2:511:LEU:HB2	1.08	1.06
34:1:1279:ALA:CB	35:3:1167:TYR:HA	1.83	1.06
34:1:1257:PRO:HB3	36:2:481:THR:HG23	1.07	1.06
36:2:459:ARG:HD2	36:2:480:VAL:O	1.53	1.06
34:1:1125:PRO:HB2	34:1:1165:TYR:CZ	1.91	1.05
34:1:582:LEU:HG	34:1:634:VAL:HG21	1.11	1.05
34:1:1155:PHE:HA	34:1:1158:ILE:CG1	1.86	1.05
35:3:353:PHE:CE1	39:5:55:ILE:CD1	2.39	1.05
35:3:616:ILE:HB	35:3:629:SER:O	1.54	1.05
34:1:1125:PRO:HB2	34:1:1165:TYR:CE2	1.91	1.05
34:1:1242:GLY:HA2	35:3:1169:PRO:HD3	1.35	1.05
34:1:1251:LEU:HD12	36:2:497:SER:CB	1.86	1.05
34:1:778:GLN:CG	34:1:817:HIS:CG	2.38	1.04
34:1:1153:PHE:HB3	34:1:1157:TYR:HE2	1.21	1.04
34:1:1300:LEU:HD13	35:3:1032:TRP:CZ2	1.92	1.04
34:1:933:CYS:CB	34:1:970:LEU:CD1	2.29	1.04
34:1:949:GLN:HB2	34:1:989:VAL:HG22	1.38	1.04
34:1:598:SER:CA	34:1:638:ALA:CA	2.35	1.04
35:3:805:ASN:CB	39:5:58:ASN:HB2	1.87	1.04
34:1:854:VAL:HG11	34:1:891:GLN:NE2	1.73	1.03
34:1:857:LEU:HD13	34:1:895:GLY:HA3	1.36	1.03
34:1:1167:TYR:CE2	36:2:581:LYS:HA	1.94	1.03
34:1:1249:TYR:HA	36:2:498:VAL:HB	1.41	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:1041:TYR:CE2	36:2:705:ARG:CZ	2.42	1.03
7:H:56:A:C5	36:2:505:CYS:HB3	1.93	1.02
34:1:774:ILE:HG23	34:1:813:PRO:CG	1.89	1.02
34:1:594:ARG:NH1	34:1:674:LEU:CD2	2.08	1.02
34:1:869:MET:CE	34:1:896:ILE:HA	1.89	1.02
35:3:35:GLY:HA2	39:5:47:PHE:CE1	1.94	1.02
34:1:1179:ASP:CB	36:2:511:LEU:HB2	1.88	1.02
35:3:114:ARG:NH1	39:5:37:ARG:HB2	1.74	1.02
1:A:1798:LEU:CD2	34:1:973:HIS:HD2	1.60	1.02
21:W:279:LYS:CB	36:2:621:VAL:O	2.08	1.01
34:1:789:LEU:HB3	34:1:836:THR:HG21	1.38	1.01
1:A:1798:LEU:HD21	34:1:973:HIS:NE2	1.75	1.01
10:L:162:THR:HG22	16:R:259:GLY:O	1.60	1.01
34:1:495:ARG:HD3	34:1:530:PRO:CA	1.89	1.00
34:1:594:ARG:HA	34:1:634:VAL:HG13	1.04	1.00
6:G:83:A:H62	37:4:22:GLU:CB	1.73	1.00
9:J:199:LYS:HE2	9:J:199:LYS:HA	1.43	1.00
34:1:1251:LEU:HD12	36:2:497:SER:HB3	1.43	1.00
34:1:594:ARG:CD	34:1:674:LEU:HD13	1.92	0.99
36:2:514:LYS:CE	36:2:591:TYR:OH	2.10	0.99
34:1:869:MET:CE	34:1:896:ILE:HD13	1.93	0.99
10:L:164:GLY:O	10:L:167:ALA:N	1.95	0.99
34:1:789:LEU:CD2	34:1:836:THR:HG21	1.93	0.99
34:1:1160:GLU:CD	35:3:1146:MET:CE	2.31	0.99
34:1:1285:PRO:HB3	36:2:494:THR:HG21	1.44	0.99
34:1:1160:GLU:CB	34:1:1202:PHE:CE2	2.46	0.99
35:3:1041:TYR:HB3	36:2:705:ARG:HG3	1.02	0.99
34:1:1278:ASP:OD2	35:3:1166:TYR:CE2	2.14	0.98
36:2:498:VAL:HG21	36:2:587:HIS:CE1	1.97	0.98
34:1:1160:GLU:HG3	35:3:1146:MET:CE	1.93	0.98
35:3:115:ILE:HD13	39:5:19:ILE:H	1.26	0.98
35:3:115:ILE:HG21	39:5:19:ILE:HB	1.43	0.98
36:2:487:LEU:HD13	39:5:28:LYS:HD2	0.99	0.98
36:2:487:LEU:CD1	39:5:28:LYS:HD2	1.94	0.98
10:L:161:ASN:OD1	10:L:168:LYS:HD2	1.64	0.97
36:2:482:ALA:HB2	36:2:488:LEU:CD1	1.93	0.97
1:A:1792:LYS:HE3	34:1:973:HIS:CE1	1.99	0.97
5:F:38:G:H2'	5:F:39:A:H8	1.25	0.97
34:1:1148:LEU:HD13	34:1:1187:THR:HB	0.99	0.97
34:1:1148:LEU:CB	34:1:1187:THR:HG22	1.95	0.97
35:3:353:PHE:CZ	39:5:55:ILE:CD1	2.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2:511:LEU:HD11	36:2:591:TYR:HE1	1.25	0.97
1:A:855:ARG:HG3	1:A:1520:ASN:HB3	1.43	0.97
34:1:606:LEU:CG	34:1:639:LEU:HD13	1.95	0.97
34:1:850:ILE:HG22	34:1:888:LEU:CD1	1.95	0.97
34:1:869:MET:HE1	34:1:896:ILE:HA	1.47	0.97
34:1:1292:LYS:NZ	39:5:78:PRO:HG2	1.81	0.96
36:2:487:LEU:HD13	39:5:28:LYS:CD	1.93	0.96
35:3:1041:TYR:HB3	36:2:705:ARG:CG	1.96	0.96
35:3:477:SER:HB2	35:3:505:THR:H	1.28	0.96
34:1:558:ARG:NH1	35:3:217:LEU:HD22	1.81	0.96
35:3:1040:ASP:HB3	36:2:706:THR:O	1.65	0.96
34:1:949:GLN:HB2	34:1:989:VAL:CG2	1.97	0.95
34:1:949:GLN:HA	34:1:989:VAL:HG13	1.47	0.95
3:C:618:THR:OG1	3:C:630:LEU:HB3	1.64	0.95
34:1:1043:ALA:HB2	34:1:1055:TRP:CH2	2.01	0.95
34:1:1125:PRO:CD	34:1:1165:TYR:OH	2.14	0.95
11:M:215:ASN:ND2	16:R:260:TYR:HA	1.82	0.95
17:S:83:GLU:HA	17:S:106:ASP:HA	1.46	0.95
1:A:1792:LYS:CE	34:1:973:HIS:NE2	2.30	0.95
34:1:1148:LEU:CB	34:1:1187:THR:CG2	2.43	0.95
34:1:707:LEU:CD1	34:1:741:LYS:HD3	1.96	0.95
34:1:1148:LEU:HD13	34:1:1187:THR:CG2	1.96	0.95
38:7:9:ILE:CG1	39:5:6:THR:CG2	2.45	0.94
10:L:16:ASP:HB2	10:L:54:LEU:HD21	1.47	0.94
34:1:1300:LEU:HB3	35:3:1032:TRP:CE3	2.03	0.94
34:1:1279:ALA:HA	35:3:1167:TYR:HD1	1.19	0.94
34:1:582:LEU:HD23	34:1:631:ALA:CA	1.97	0.94
34:1:1153:PHE:HB3	34:1:1157:TYR:CE2	2.02	0.94
34:1:937:LEU:HD23	34:1:977:VAL:HG21	1.47	0.94
34:1:1178:MET:SD	36:2:514:LYS:NZ	2.41	0.94
36:2:487:LEU:HD21	39:5:28:LYS:HB2	1.50	0.94
34:1:1178:MET:HG2	36:2:591:TYR:CZ	2.03	0.93
34:1:778:GLN:CG	34:1:817:HIS:ND1	2.30	0.93
34:1:866:LYS:HG2	34:1:909:VAL:HG11	1.48	0.93
34:1:1125:PRO:HG2	34:1:1165:TYR:CE2	2.02	0.93
34:1:594:ARG:CD	34:1:674:LEU:CD1	2.45	0.93
2:B:40:U:O4	6:G:0:G:N2	2.01	0.93
34:1:933:CYS:SG	34:1:970:LEU:CD1	2.57	0.93
34:1:774:ILE:CG2	34:1:813:PRO:HG3	1.98	0.93
34:1:1179:ASP:CB	36:2:511:LEU:CB	2.46	0.93
2:B:46:U:O2	19:U:11:ARG:NH2	2.00	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:59:G:H1	5:F:76:A:H61	1.09	0.93
39:5:36:HIS:HD1	39:5:76:CYS:HG	1.08	0.93
35:3:805:ASN:HB3	39:5:58:ASN:CB	1.98	0.92
34:1:937:LEU:CD2	34:1:977:VAL:HG21	1.98	0.92
34:1:1262:ARG:CB	39:5:24:ALA:HB1	1.99	0.92
34:1:1263:ASP:N	39:5:24:ALA:HB2	1.84	0.92
36:2:487:LEU:HD22	39:5:28:LYS:HB2	0.93	0.92
2:B:20:G:O6	2:B:57:G:N1	2.02	0.92
34:1:850:ILE:CG2	34:1:888:LEU:HD11	1.99	0.92
35:3:1116:SER:HA	36:2:708:TRP:CZ2	2.03	0.92
34:1:594:ARG:HA	34:1:634:VAL:HG11	1.49	0.92
34:1:1148:LEU:HB2	34:1:1187:THR:HG21	1.52	0.92
1:A:467:GLN:OE1	2:B:20:G:N2	2.03	0.91
34:1:1257:PRO:HB2	36:2:481:THR:CG2	1.94	0.91
34:1:857:LEU:HD13	34:1:895:GLY:CA	1.99	0.91
21:W:320:GLY:O	36:2:667:ALA:O	1.87	0.91
35:3:516:LEU:O	35:3:527:ILE:HB	1.70	0.91
14:P:207:ASP:HB2	14:P:218:GLU:HB2	1.50	0.91
34:1:1125:PRO:HG2	34:1:1165:TYR:HE2	1.35	0.91
35:3:35:GLY:CA	39:5:47:PHE:CZ	2.53	0.91
34:1:1257:PRO:HG3	36:2:478:HIS:CA	2.01	0.91
34:1:884:ILE:HD13	34:1:889:GLU:HB3	1.50	0.91
34:1:1148:LEU:CD1	34:1:1187:THR:CG2	2.48	0.91
9:J:199:LYS:HG3	11:M:208:ILE:HD13	1.53	0.91
4:E:150:HIS:HE2	4:E:169:THR:HG1	1.13	0.90
34:1:884:ILE:HB	34:1:888:LEU:HD23	1.52	0.90
34:1:778:GLN:HG2	34:1:817:HIS:CE1	2.04	0.90
35:3:459:VAL:HG21	35:3:757:ILE:HG21	1.51	0.90
3:C:350:ASN:HD22	3:C:353:THR:HG22	1.36	0.90
34:1:1160:GLU:CD	35:3:1146:MET:HE2	1.89	0.90
8:I:394:PRO:HG2	8:I:429:VAL:HA	1.53	0.90
34:1:967:GLU:CB	34:1:970:LEU:HB3	2.00	0.90
35:3:463:ARG:H	35:3:510:LEU:HD22	1.36	0.90
34:1:1155:PHE:HA	34:1:1158:ILE:HD11	1.52	0.90
34:1:1155:PHE:HA	34:1:1158:ILE:CD1	2.00	0.90
34:1:1160:GLU:HB2	34:1:1202:PHE:CE2	2.07	0.90
34:1:789:LEU:HD22	34:1:836:THR:HG21	1.52	0.90
34:1:778:GLN:CG	34:1:817:HIS:CE1	2.55	0.89
1:A:705:LYS:NZ	16:R:247:ILE:O	2.04	0.89
38:7:9:ILE:HG12	39:5:6:THR:CG2	2.02	0.89
34:1:962:MET:HG2	34:1:974:LEU:HD12	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:1292:LYS:HZ2	39:5:78:PRO:HG2	1.37	0.89
34:1:789:LEU:HD22	34:1:836:THR:CG2	2.01	0.89
34:1:582:LEU:CD2	34:1:631:ALA:HA	2.03	0.89
34:1:719:TYR:CD1	35:3:146:ARG:NH1	2.41	0.89
34:1:960:VAL:O	34:1:963:LYS:HB3	1.72	0.89
34:1:1278:ASP:HB3	35:3:1166:TYR:HE2	1.38	0.89
34:1:1281:ILE:HG22	35:3:1050:PHE:CZ	2.06	0.89
1:A:1798:LEU:CD1	34:1:973:HIS:CD2	2.55	0.88
11:M:215:ASN:HD21	16:R:261:THR:N	1.70	0.88
34:1:1245:ARG:HH22	35:3:1028:THR:HB	1.37	0.88
1:A:39:GLN:HE22	21:W:170:THR:H	1.18	0.88
34:1:962:MET:SD	34:1:974:LEU:HD11	2.13	0.88
34:1:1160:GLU:HB3	34:1:1202:PHE:CE2	2.08	0.88
1:A:1792:LYS:CE	34:1:973:HIS:CE1	2.56	0.88
34:1:1217:PRO:CB	36:2:510:TYR:CZ	2.55	0.88
34:1:594:ARG:HD3	34:1:674:LEU:CD2	2.03	0.88
34:1:1256:HIS:CD2	34:1:1257:PRO:HD3	2.09	0.88
35:3:189:TYR:CB	39:5:73:LEU:HD12	2.04	0.88
34:1:1125:PRO:CB	34:1:1165:TYR:CE2	2.57	0.88
34:1:1266:TRP:CE3	39:5:22:GLY:HA3	2.08	0.88
9:J:195:LEU:HD23	11:M:209:ASP:HA	1.56	0.88
34:1:497:ILE:HG12	34:1:526:PHE:HZ	1.37	0.88
34:1:601:ALA:O	34:1:639:LEU:CD2	2.21	0.88
34:1:1160:GLU:HB2	34:1:1202:PHE:CZ	2.08	0.88
34:1:1178:MET:HA	36:2:511:LEU:HD13	1.55	0.88
34:1:1300:LEU:HB3	35:3:1032:TRP:HZ3	1.33	0.88
34:1:1148:LEU:HB3	34:1:1187:THR:CG2	2.00	0.88
34:1:1160:GLU:CG	35:3:1146:MET:CE	2.50	0.87
34:1:1293:ASN:OD1	39:5:77:GLY:HA3	1.73	0.87
35:3:353:PHE:CE1	39:5:51:ASN:HB3	2.09	0.87
34:1:594:ARG:HD3	34:1:674:LEU:HD11	1.54	0.87
36:2:514:LYS:HE3	36:2:591:TYR:OH	1.72	0.87
36:2:642:PRO:CB	37:4:66:ASP:CB	2.51	0.87
3:C:213:ASP:OD1	3:C:616:SER:CB	2.20	0.87
18:T:307:SER:OG	18:T:309:ASP:OD1	1.92	0.87
34:1:564:ASP:O	34:1:568:ARG:NH2	2.06	0.87
34:1:1255:PHE:O	36:2:488:LEU:HG	1.75	0.87
1:A:372:PRO:O	3:C:342:ARG:NH2	2.07	0.87
1:A:1526:LEU:HD13	1:A:1528:GLN:H	1.40	0.87
22:X:690:LEU:HD22	22:X:735:PHE:HB2	1.57	0.87
23:Y:246:LYS:HE3	23:Y:312:HIS:HB2	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ARG:HH12	7:H:18:U:H5'	1.37	0.87
34:1:710:ALA:HA	34:1:749:ALA:HB2	1.57	0.87
35:3:1129:LEU:O	36:2:708:TRP:HH2	1.58	0.87
34:1:1242:GLY:HA2	35:3:1169:PRO:CD	2.05	0.86
36:2:478:HIS:O	36:2:481:THR:HG22	1.73	0.86
34:1:952:ALA:HB2	34:1:993:ILE:HD11	1.56	0.86
35:3:1007:GLU:HB3	36:2:495:ARG:NH2	1.89	0.86
5:F:36:A:H3'	5:F:37:C:H5"	1.55	0.86
3:C:478:THR:HG21	3:C:492:ALA:HB1	1.56	0.86
34:1:582:LEU:CD1	34:1:634:VAL:HG21	2.04	0.86
34:1:1302:TYR:CE1	35:3:915:LEU:HD13	2.09	0.86
34:1:949:GLN:HA	34:1:989:VAL:CG1	2.05	0.86
35:3:1116:SER:C	36:2:708:TRP:HZ2	1.64	0.86
35:3:1008:SER:OG	35:3:1009:PHE:N	2.07	0.86
1:A:414:ARG:NH1	3:C:410:LEU:O	2.09	0.85
10:L:161:ASN:O	10:L:161:ASN:ND2	2.07	0.85
1:A:1994:LYS:CD	34:1:986:TYR:OH	2.24	0.85
34:1:594:ARG:CZ	34:1:674:LEU:HD22	2.06	0.85
35:3:668:GLY:HA3	35:3:699:VAL:HG11	1.57	0.85
34:1:1125:PRO:CG	34:1:1165:TYR:CE2	2.58	0.85
5:F:38:G:H2'	5:F:39:A:C8	2.10	0.85
34:1:712:LEU:O	34:1:716:ALA:HB3	1.76	0.85
34:1:594:ARG:CA	34:1:634:VAL:CG1	2.46	0.85
34:1:1248:GLN:NE2	36:2:496:ASN:CB	2.40	0.85
1:A:1018:ASN:ND2	1:A:1023:ASN:OD1	2.09	0.85
34:1:1257:PRO:HB3	36:2:478:HIS:O	1.77	0.85
36:2:452:LYS:HD2	36:2:452:LYS:O	1.75	0.85
35:3:139:LYS:HG3	35:3:160:ALA:HB3	1.57	0.85
35:3:353:PHE:CD1	39:5:55:ILE:HD11	2.11	0.85
34:1:497:ILE:HG23	34:1:526:PHE:HE1	1.42	0.84
9:J:187:VAL:HG13	9:J:188:GLN:H	1.43	0.84
34:1:582:LEU:HG	34:1:634:VAL:HG23	1.59	0.84
34:1:949:GLN:OE1	34:1:989:VAL:HG22	1.76	0.84
35:3:115:ILE:HD11	39:5:18:TYR:HA	1.57	0.84
35:3:568:MET:HB3	35:3:574:LEU:HD12	1.60	0.84
35:3:253:GLU:OE1	39:5:63:ARG:NH1	2.10	0.84
38:7:40:CYS:SG	38:7:73:LYS:NZ	2.51	0.84
34:1:1242:GLY:CA	35:3:1169:PRO:CD	2.55	0.84
3:C:117:ASP:N	3:C:117:ASP:OD1	2.11	0.84
9:J:193:GLN:HA	9:J:193:GLN:HE21	1.42	0.84
34:1:744:ALA:HB1	34:1:784:MET:HA	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:991:LEU:HA	22:X:995:GLU:HA	1.60	0.84
34:1:1257:PRO:HG3	36:2:478:HIS:C	1.97	0.84
3:C:488:VAL:HG13	3:C:609:LYS:HD3	1.59	0.84
34:1:962:MET:SD	34:1:974:LEU:CD1	2.65	0.84
35:3:280:ASP:HB3	35:3:283:ARG:HG3	1.60	0.83
35:3:806:ALA:HA	35:3:856:LYS:HB3	1.58	0.83
35:3:1116:SER:N	36:2:708:TRP:HZ2	1.76	0.83
34:1:926:LYS:HE2	34:1:964:THR:O	1.78	0.83
34:1:1251:LEU:HD12	36:2:497:SER:HB2	1.57	0.83
35:3:585:ALA:HB1	35:3:610:VAL:HG12	1.59	0.83
35:3:114:ARG:HD3	39:5:38:ASP:OD1	1.78	0.83
34:1:754:ILE:HG21	34:1:795:CYS:CA	2.08	0.83
34:1:1263:ASP:N	39:5:24:ALA:CB	2.41	0.83
35:3:429:ARG:HD3	39:5:55:ILE:HG23	1.60	0.83
34:1:777:PHE:CD1	34:1:818:PHE:HE2	1.96	0.83
34:1:1300:LEU:CD1	35:3:1032:TRP:CH2	2.61	0.83
34:1:598:SER:O	34:1:638:ALA:HB1	1.79	0.83
1:A:1636:LYS:HD3	1:A:1658:GLN:HE21	1.44	0.83
7:H:56:A:C5	36:2:505:CYS:CB	2.62	0.83
34:1:1125:PRO:HD2	34:1:1165:TYR:HH	1.40	0.83
4:E:92:LEU:HD12	4:E:103:ALA:HB3	1.61	0.83
34:1:734:GLY:O	34:1:738:HIS:HB2	1.77	0.83
39:5:36:HIS:ND1	39:5:76:CYS:SG	2.49	0.83
3:C:618:THR:HG1	3:C:630:LEU:HB3	1.44	0.83
34:1:1281:ILE:HG21	35:3:1050:PHE:HE1	1.42	0.83
35:3:352:GLU:OE2	35:3:429:ARG:NH1	2.12	0.83
11:M:215:ASN:ND2	16:R:260:TYR:CA	2.40	0.82
1:A:325:HIS:HD2	1:A:326:HIS:HD2	1.25	0.82
34:1:558:ARG:NH1	35:3:217:LEU:CD2	2.42	0.82
7:H:56:A:N7	36:2:505:CYS:CB	2.42	0.82
34:1:857:LEU:CD1	34:1:895:GLY:HA3	2.09	0.82
11:M:215:ASN:HD21	16:R:261:THR:H	1.24	0.82
3:C:670:SER:HA	3:C:823:ALA:HB3	1.61	0.82
36:2:511:LEU:HD23	36:2:593:GLU:HB3	1.61	0.82
34:1:1285:PRO:CB	36:2:494:THR:HG21	2.09	0.82
1:A:1838:LYS:HB3	1:A:1868:MET:HG3	1.60	0.81
5:F:59:G:H1	5:F:76:A:N6	1.76	0.81
34:1:665:ILE:HD13	34:1:705:SER:HB2	1.61	0.81
34:1:1148:LEU:CD1	34:1:1187:THR:CB	2.34	0.81
34:1:1205:GLU:OE1	35:3:1171:LYS:HD3	1.79	0.81
35:3:162:LYS:HE3	35:3:165:THR:HG21	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2:517:ILE:HD12	36:2:517:ILE:O	1.80	0.81
34:1:702:ARG:HD2	34:1:738:HIS:CG	2.15	0.81
34:1:929:LEU:CB	34:1:970:LEU:HD22	2.10	0.81
34:1:725:ASP:HA	34:1:728:LEU:HG	1.61	0.81
11:M:215:ASN:HD22	16:R:260:TYR:HA	1.45	0.81
1:A:1835:GLN:HA	1:A:1838:LYS:HG3	1.63	0.81
36:2:454:LEU:HD12	36:2:454:LEU:O	1.80	0.81
22:X:242:LYS:NZ	23:Y:220:GLN:O	2.14	0.81
34:1:1242:GLY:CA	35:3:1169:PRO:HD3	2.11	0.81
36:2:511:LEU:CD2	36:2:593:GLU:HB3	2.10	0.81
4:E:92:LEU:O	4:E:101:ASN:ND2	2.14	0.80
4:E:197:LEU:HG	4:E:212:GLY:HA2	1.62	0.80
36:2:487:LEU:CD2	39:5:28:LYS:CB	2.42	0.80
38:7:33:CYS:SG	38:7:35:SER:OG	2.31	0.80
1:A:1807:ILE:HB	1:A:1820:LYS:HB3	1.63	0.80
35:3:412:ILE:HG12	35:3:423:LEU:HD22	1.63	0.80
34:1:1259:ARG:NH2	39:5:25:ASP:OD1	2.15	0.80
4:E:87:ASP:N	4:E:87:ASP:OD1	2.13	0.80
34:1:929:LEU:CB	34:1:970:LEU:CD2	2.59	0.80
1:A:701:ILE:HD11	16:R:237:MET:HG3	1.64	0.80
35:3:170:VAL:HG23	35:3:184:CYS:HB3	1.64	0.80
36:2:511:LEU:CD1	36:2:591:TYR:HE1	1.94	0.80
34:1:652:CYS:HB2	34:1:692:HIS:HE1	1.46	0.80
34:1:778:GLN:HG2	34:1:817:HIS:NE2	1.97	0.80
22:X:604:VAL:HG13	22:X:605:THR:HG23	1.64	0.80
3:C:534:VAL:HG22	3:C:537:TYR:HB2	1.65	0.79
35:3:115:ILE:CD1	39:5:19:ILE:H	1.95	0.79
34:1:497:ILE:HG12	34:1:526:PHE:CZ	2.17	0.79
34:1:558:ARG:HH12	35:3:217:LEU:HD22	1.47	0.79
34:1:1178:MET:HB3	36:2:514:LYS:NZ	1.98	0.79
3:C:343:LEU:HD13	3:C:373:ILE:HD11	1.63	0.79
34:1:929:LEU:C	34:1:970:LEU:HD22	2.02	0.79
34:1:1160:GLU:CD	35:3:1146:MET:HE1	1.96	0.79
35:3:29:GLU:HG3	35:3:42:ARG:HG3	1.63	0.79
34:1:1257:PRO:HG3	36:2:478:HIS:O	1.83	0.79
16:R:376:LYS:HA	16:R:379:LYS:HB2	1.65	0.79
34:1:598:SER:O	34:1:602:LYS:HB2	1.83	0.79
34:1:598:SER:N	34:1:638:ALA:HB2	1.98	0.79
35:3:136:GLU:OE2	35:3:189:TYR:OH	2.00	0.79
35:3:228:LEU:HD21	35:3:250:ILE:HG21	1.65	0.79
2:B:97:G:H1	2:B:116:U:H3	1.29	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:367:ARG:NH1	23:Y:282:CYS:SG	2.55	0.78
34:1:854:VAL:CG1	34:1:891:GLN:HE21	1.91	0.78
34:1:952:ALA:CB	34:1:993:ILE:HD11	2.12	0.78
35:3:412:ILE:HD12	35:3:1107:THR:HG21	1.64	0.78
35:3:929:LYS:HE3	35:3:938:GLU:HB2	1.65	0.78
34:1:834:VAL:HG22	34:1:871:THR:HG23	1.65	0.78
14:P:67:GLU:OE2	18:T:476:ARG:NH2	2.15	0.78
34:1:805:TYR:O	34:1:809:GLU:HB2	1.82	0.78
34:1:1217:PRO:HG2	36:2:510:TYR:OH	1.83	0.78
18:T:191:HIS:NE2	18:T:440:ASP:OD1	2.16	0.78
34:1:523:ALA:O	34:1:563:LEU:HD11	1.83	0.78
34:1:1279:ALA:CA	35:3:1167:TYR:HD1	1.80	0.78
16:R:163:MET:O	16:R:165:VAL:N	2.15	0.78
34:1:757:MET:HB3	34:1:762:ALA:HB2	1.64	0.78
36:2:479:ASP:HA	36:2:488:LEU:HD13	1.64	0.78
1:A:221:ASN:HB2	1:A:227:ARG:HB2	1.64	0.78
34:1:778:GLN:CG	34:1:817:HIS:CD2	2.67	0.78
1:A:1826:VAL:O	1:A:1830:GLN:NE2	2.17	0.77
34:1:544:LEU:HD21	34:1:549:ARG:HG3	1.64	0.77
34:1:972:GLY:HA2	34:1:1010:THR:HG21	1.64	0.77
34:1:1283:HIS:HE1	35:3:1168:PHE:CZ	2.01	0.77
21:W:180:LYS:HA	21:W:200:VAL:H	1.49	0.77
34:1:1125:PRO:CB	34:1:1165:TYR:CZ	2.67	0.77
34:1:554:LYS:HA	34:1:558:ARG:HH21	1.50	0.77
35:3:1041:TYR:CZ	36:2:705:ARG:NH2	2.53	0.77
34:1:1244:CYS:SG	35:3:1030:PRO:HD2	2.25	0.77
23:Y:245:CYS:SG	23:Y:246:LYS:N	2.58	0.77
34:1:866:LYS:CG	34:1:909:VAL:HG11	2.14	0.77
34:1:1160:GLU:HB3	34:1:1202:PHE:HE2	1.49	0.77
16:R:348:GLU:O	16:R:352:ARG:HB2	1.84	0.77
34:1:952:ALA:HB1	34:1:993:ILE:CD1	2.15	0.77
34:1:1251:LEU:CB	36:2:497:SER:HB2	2.14	0.77
35:3:89:ILE:HD12	35:3:103:HIS:HB2	1.67	0.77
35:3:189:TYR:CA	39:5:73:LEU:CD1	2.61	0.77
1:A:923:ASP:OD2	1:A:1439:ARG:NH1	2.18	0.77
16:R:308:VAL:HA	23:Y:197:ILE:HG21	1.66	0.77
34:1:1302:TYR:HE1	35:3:915:LEU:CB	1.96	0.77
35:3:878:ASP:OD1	35:3:879:LEU:N	2.18	0.77
35:3:996:ILE:HD13	36:2:703:ILE:N	2.00	0.77
3:C:144:CYS:SG	3:C:313:GLN:NE2	2.58	0.77
34:1:1257:PRO:CG	36:2:478:HIS:O	2.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:464:ARG:HG2	35:3:516:LEU:HD11	1.67	0.77
21:W:321:GLU:HA	36:2:667:ALA:HB3	1.65	0.76
36:2:568:TYR:O	36:2:570:LYS:N	2.18	0.76
14:P:183:LYS:HA	23:Y:52:GLN:HE22	1.50	0.76
22:X:480:SER:OG	22:X:485:ASP:OD1	2.04	0.76
34:1:712:LEU:O	34:1:716:ALA:CB	2.33	0.76
34:1:884:ILE:CD1	34:1:889:GLU:HB3	2.15	0.76
36:2:498:VAL:CG2	36:2:587:HIS:CE1	2.67	0.76
3:C:684:LYS:HB3	3:C:795:VAL:HB	1.67	0.76
34:1:495:ARG:CD	34:1:530:PRO:HB3	2.15	0.76
35:3:351:SER:H	35:3:356:HIS:HB3	1.50	0.76
35:3:1013:ARG:NH2	35:3:1064:ASP:OD1	2.18	0.76
22:X:242:LYS:O	22:X:246:LEU:HB2	1.86	0.76
34:1:1178:MET:HA	36:2:511:LEU:CD1	2.14	0.76
36:2:711:LEU:O	36:2:711:LEU:HD13	1.85	0.76
34:1:739:ARG:HA	34:1:743:LEU:CD2	2.16	0.76
34:1:1148:LEU:CB	34:1:1187:THR:HG21	2.12	0.76
35:3:592:LEU:HD22	35:3:605:LEU:HD13	1.65	0.76
36:2:498:VAL:HG21	36:2:587:HIS:HE1	1.45	0.76
1:A:1830:GLN:HB3	1:A:1836:LEU:HD22	1.68	0.76
4:E:216:ASP:OD2	4:E:218:LYS:NZ	2.18	0.76
22:X:961:THR:O	22:X:965:GLN:NE2	2.19	0.76
34:1:838:VAL:HG13	34:1:875:ILE:HG12	1.67	0.76
38:7:22:LEU:N	38:7:67:SER:O	2.18	0.76
1:A:1798:LEU:CG	34:1:973:HIS:CD2	2.68	0.76
34:1:747:LEU:HD12	34:1:750:ILE:HD11	1.68	0.76
10:L:159:LEU:O	11:M:211:ILE:HD13	1.86	0.76
35:3:459:VAL:HG22	35:3:476:VAL:HA	1.68	0.76
4:E:135:VAL:HG13	4:E:144:VAL:HG23	1.68	0.76
6:G:88:G:H1	7:H:41:U:H3	1.28	0.76
20:V:576:THR:HB	20:V:579:SER:H	1.49	0.76
34:1:565:ASP:HA	34:1:568:ARG:HE	1.51	0.76
34:1:1160:GLU:OE2	35:3:1146:MET:CE	2.33	0.76
34:1:1193:GLN:NE2	38:7:78:GLN:NE2	2.34	0.76
35:3:525:ARG:HG3	35:3:533:VAL:HG13	1.67	0.76
1:A:57:GLN:N	1:A:57:GLN:HE21	1.84	0.75
34:1:744:ALA:O	34:1:787:ILE:CB	2.34	0.75
34:1:702:ARG:CD	34:1:738:HIS:CD2	2.65	0.75
35:3:412:ILE:H	35:3:1105:GLN:HE22	1.34	0.75
1:A:729:PRO:HG2	11:M:226:TYR:CE1	2.22	0.75
8:I:621:ARG:O	8:I:625:PRO:HD2	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:1262:ARG:C	39:5:24:ALA:CB	2.55	0.75
34:1:1178:MET:HG2	36:2:591:TYR:CE2	2.21	0.75
35:3:1026:ASP:OD1	35:3:1026:ASP:N	2.18	0.75
2:B:18:C:O2	2:B:59:G:N2	2.19	0.75
7:H:28:C:O2'	7:H:29:A:N3	2.18	0.75
9:J:193:GLN:HE21	9:J:193:GLN:CA	2.00	0.75
35:3:463:ARG:HB2	35:3:510:LEU:HD13	1.66	0.75
16:R:359:ARG:HB3	16:R:363:ARG:HH21	1.52	0.75
34:1:1243:PRO:CD	35:3:1167:TYR:O	2.34	0.75
1:A:1104:ASP:OD1	1:A:1104:ASP:N	2.19	0.75
4:E:312:TRP:HE1	4:E:319:ILE:HG12	1.50	0.75
35:3:115:ILE:HD13	39:5:19:ILE:N	2.01	0.75
17:S:18:THR:HA	17:S:159:ILE:HA	1.69	0.75
34:1:754:ILE:CG2	34:1:795:CYS:HA	2.11	0.75
34:1:778:GLN:HG2	34:1:817:HIS:CD2	2.21	0.75
34:1:789:LEU:HB3	34:1:836:THR:CG2	2.15	0.75
34:1:861:ALA:O	34:1:864:TYR:N	2.17	0.75
34:1:869:MET:HE2	34:1:896:ILE:HD13	1.68	0.75
34:1:1262:ARG:CB	39:5:24:ALA:O	2.34	0.75
35:3:969:VAL:HB	35:3:981:CYS:HB2	1.69	0.75
23:Y:246:LYS:HB2	23:Y:311:ILE:HA	1.67	0.75
6:G:98:U:O4	7:H:33:G:N1	2.19	0.74
20:V:539:LEU:HD13	20:V:543:LYS:HB3	1.68	0.74
35:3:1040:ASP:OD2	35:3:1043:THR:N	2.20	0.74
1:A:658:ARG:NH1	5:F:67:G:OP2	2.19	0.74
14:P:206:LYS:HB3	14:P:218:GLU:HG2	1.69	0.74
18:T:267:ASP:OD1	18:T:267:ASP:N	2.21	0.74
34:1:1285:PRO:HB3	36:2:494:THR:CG2	2.17	0.74
1:A:1870:ASP:N	1:A:1870:ASP:OD1	2.20	0.74
16:R:325:ARG:HE	23:Y:222:ILE:HG23	1.51	0.74
34:1:789:LEU:CB	34:1:836:THR:HG21	2.15	0.74
12:N:53:HIS:NE2	12:N:85:ASP:OD2	2.19	0.74
35:3:902:ASP:OD1	35:3:902:ASP:N	2.20	0.74
1:A:850:TYR:OH	1:A:863:GLU:OE1	2.05	0.74
4:E:166:LEU:HD11	4:E:178:LEU:HG	1.70	0.74
22:X:919:GLU:HA	22:X:922:LEU:HB2	1.69	0.74
34:1:884:ILE:HD13	34:1:889:GLU:CB	2.17	0.74
35:3:206:GLN:HG3	35:3:231:HIS:HD2	1.52	0.74
35:3:325:ILE:N	35:3:375:SER:OG	2.20	0.74
35:3:511:LEU:HD23	35:3:512:GLY:H	1.52	0.74
1:A:184:ASP:HB2	12:N:1:MET:HA	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:22:PHE:O	35:3:75:LYS:NZ	2.19	0.74
35:3:487:ILE:HA	35:3:491:VAL:HG13	1.69	0.74
9:J:199:LYS:HE2	9:J:199:LYS:CA	2.18	0.74
34:1:717:THR:CB	34:1:718:PRO:HD2	2.16	0.74
34:1:1043:ALA:HB2	34:1:1055:TRP:HH2	1.53	0.74
9:J:438:TYR:O	9:J:442:ARG:HB2	1.88	0.74
36:2:491:LEU:O	36:2:494:THR:OG1	2.06	0.74
16:R:125:MET:N	16:R:125:MET:SD	2.61	0.73
34:1:869:MET:HE2	34:1:896:ILE:HA	1.70	0.73
34:1:1203:GLY:HA2	35:3:1171:LYS:CG	2.18	0.73
6:G:108:U:H5"	22:X:676:ILE:HB	1.70	0.73
22:X:428:LYS:HD2	22:X:551:ALA:HB1	1.70	0.73
34:1:850:ILE:HG21	34:1:888:LEU:HD21	1.68	0.73
1:A:1382:SER:HB2	1:A:1415:GLY:HA2	1.69	0.73
11:M:165:ASN:HB2	16:R:95:LYS:HB3	1.69	0.73
1:A:55:ASP:OD1	1:A:55:ASP:N	2.17	0.73
20:V:581:ILE:HA	20:V:584:LYS:HG2	1.71	0.73
35:3:228:LEU:HD12	35:3:229:GLU:H	1.52	0.73
4:E:189:THR:OG1	4:E:191:GLN:OE1	2.06	0.73
4:E:255:MET:HB2	4:E:282:HIS:HB3	1.71	0.73
34:1:1251:LEU:HB2	36:2:497:SER:HB2	1.68	0.73
18:T:223:SER:OG	18:T:225:ASP:OD2	2.02	0.73
34:1:1205:GLU:OE1	35:3:1171:LYS:CD	2.36	0.73
34:1:1257:PRO:CB	36:2:478:HIS:O	2.37	0.73
1:A:1838:LYS:O	1:A:1841:THR:OG1	2.07	0.73
34:1:597:ILE:O	34:1:638:ALA:CB	2.36	0.73
22:X:752:VAL:O	22:X:757:ARG:NH2	2.21	0.73
34:1:1249:TYR:HE2	36:2:587:HIS:HD1	1.36	0.73
35:3:932:ASN:HB2	35:3:936:LYS:HE3	1.69	0.73
14:P:186:ARG:CB	14:P:186:ARG:HH11	2.02	0.72
34:1:702:ARG:HD2	34:1:738:HIS:NE2	2.03	0.72
34:1:962:MET:HG2	34:1:974:LEU:CD1	2.18	0.72
1:A:1652:MET:HG2	1:A:1719:PHE:HA	1.72	0.72
34:1:952:ALA:HB1	34:1:993:ILE:HD13	1.71	0.72
36:2:457:MET:HA	36:2:457:MET:CE	2.19	0.72
6:G:105:C:H4'	6:G:106:C:OP2	1.88	0.72
34:1:1145:ASN:HD21	34:1:1183:VAL:HG11	1.52	0.72
4:E:128:SER:OG	4:E:130:ASP:OD1	2.03	0.72
4:E:137:ASP:O	4:E:141:GLY:N	2.19	0.72
34:1:1160:GLU:CB	34:1:1202:PHE:CZ	2.69	0.72
34:1:1248:GLN:HE22	36:2:496:ASN:HB3	1.49	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ARG:NH1	2:B:15:C:OP2	2.23	0.72
1:A:1878:ASP:OD1	1:A:1878:ASP:N	2.13	0.72
3:C:778:PRO:HB2	3:C:821:LEU:HD21	1.71	0.72
18:T:188:PRO:HG2	18:T:502:VAL:HG11	1.70	0.72
22:X:689:VAL:O	22:X:734:CYS:HA	1.89	0.72
38:7:73:LYS:O	38:7:77:ILE:HG13	1.88	0.72
34:1:758:ASP:O	34:1:762:ALA:N	2.15	0.72
34:1:796:CYS:HB3	34:1:806:ILE:HG12	1.71	0.72
35:3:581:LYS:HD2	35:3:625:LEU:HD22	1.71	0.72
1:A:888:GLN:O	1:A:889:ARG:NH1	2.22	0.72
2:B:18:C:N3	2:B:59:G:N1	2.34	0.72
4:E:126:SER:HG	4:E:136:TRP:HE1	1.34	0.72
23:Y:51:ILE:HD11	23:Y:112:THR:HG23	1.72	0.72
34:1:962:MET:CG	34:1:974:LEU:HD12	2.19	0.72
1:A:159:ARG:NH1	1:A:159:ARG:HA	2.05	0.72
22:X:945:ALA:HA	22:X:1011:VAL:HG11	1.71	0.72
34:1:594:ARG:HG3	34:1:634:VAL:HG22	1.72	0.72
34:1:597:ILE:C	34:1:638:ALA:HB2	2.10	0.72
34:1:963:LYS:HB2	34:1:1003:VAL:HG21	1.71	0.72
1:A:27:GLU:OE1	1:A:31:GLN:NE2	2.22	0.71
1:A:419:ARG:NH2	1:A:423:ASP:O	2.23	0.71
15:Q:497:SER:O	15:Q:500:GLY:N	2.23	0.71
23:Y:62:GLY:O	23:Y:107:GLN:NE2	2.23	0.71
23:Y:122:VAL:HB	23:Y:123:HIS:HD2	1.53	0.71
1:A:1637:TRP:O	1:A:1656:THR:HA	1.89	0.71
34:1:1287:ILE:HA	36:2:490:HIS:NE2	2.05	0.71
34:1:1299:GLU:HA	34:1:1302:TYR:HE2	1.55	0.71
35:3:208:LEU:HD13	35:3:250:ILE:HD11	1.71	0.71
38:7:71:TYR:CE2	38:7:81:ASP:HB2	2.25	0.71
9:J:363:ARG:NH1	9:J:386:GLU:OE2	2.23	0.71
13:O:163:HIS:O	13:O:182:ARG:N	2.23	0.71
35:3:353:PHE:HE1	39:5:51:ASN:HB3	1.54	0.71
11:M:215:ASN:ND2	16:R:261:THR:H	1.88	0.71
22:X:405:ARG:NH2	22:X:438:GLU:OE1	2.24	0.71
35:3:805:ASN:CB	39:5:58:ASN:CB	2.64	0.71
36:2:462:VAL:HG22	36:2:480:VAL:HG11	1.73	0.71
36:2:479:ASP:N	36:2:479:ASP:OD1	2.23	0.71
6:G:111:U:H4'	6:G:112:U:OP2	1.90	0.71
35:3:565:TYR:HB3	35:3:577:TYR:HB3	1.72	0.71
35:3:565:TYR:HE1	35:3:619:LEU:HB2	1.54	0.71
3:C:258:ASN:OD1	3:C:259:LYS:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:5:U:H5'	5:F:6:C:H4'	1.73	0.71
1:A:1992:GLY:HA2	1:A:1997:VAL:HG23	1.73	0.71
34:1:777:PHE:CD1	34:1:818:PHE:CE2	2.79	0.71
34:1:933:CYS:SG	34:1:974:LEU:CD2	2.71	0.71
34:1:952:ALA:CB	34:1:993:ILE:CD1	2.68	0.71
1:A:325:HIS:CD2	1:A:326:HIS:HD2	2.09	0.71
18:T:195:LYS:HZ3	18:T:490:ARG:HD2	1.56	0.71
22:X:219:ARG:NH2	23:Y:292:GLU:OE2	2.24	0.71
34:1:503:LYS:HE2	34:1:511:MET:HG2	1.72	0.71
34:1:857:LEU:HD13	34:1:895:GLY:C	2.11	0.71
34:1:1256:HIS:HD2	34:1:1257:PRO:HD3	1.54	0.71
34:1:1298:TYR:CD1	35:3:918:ARG:HB2	2.25	0.71
35:3:1129:LEU:O	36:2:708:TRP:CH2	2.43	0.71
1:A:1935:ARG:NE	1:A:1980:GLU:OE2	2.24	0.71
4:E:277:PHE:HE2	4:E:300:ILE:HG21	1.56	0.71
34:1:884:ILE:HD12	34:1:884:ILE:O	1.91	0.71
34:1:1178:MET:HB3	36:2:514:LYS:HD2	1.72	0.71
38:7:21:ARG:NH1	38:7:68:ASP:OD1	2.21	0.71
1:A:1399:GLN:OE1	1:A:1401:ARG:NH1	2.24	0.70
7:H:18:U:OP2	11:M:221:LYS:NZ	2.23	0.70
7:H:56:A:OP1	36:2:504:TRP:HZ3	1.73	0.70
34:1:1108:ASN:O	34:1:1112:THR:HG22	1.91	0.70
35:3:1048:ASP:OD1	35:3:1049:LYS:N	2.24	0.70
34:1:598:SER:CB	34:1:638:ALA:HA	2.21	0.70
35:3:384:THR:OG1	35:3:385:PHE:O	2.08	0.70
35:3:812:LYS:HD2	35:3:856:LYS:HE3	1.74	0.70
11:M:209:ASP:OD1	11:M:209:ASP:N	2.23	0.70
34:1:777:PHE:HA	34:1:818:PHE:CE2	2.26	0.70
36:2:514:LYS:CD	36:2:591:TYR:OH	2.38	0.70
1:A:39:GLN:HE22	21:W:170:THR:N	1.89	0.70
1:A:857:ASN:ND2	1:A:860:GLN:OE1	2.23	0.70
35:3:286:ILE:CD1	39:5:63:ARG:HA	2.20	0.70
39:5:62:ALA:HA	39:5:65:ARG:HH12	1.55	0.70
1:A:41:GLN:HE22	1:A:45:TYR:HD2	1.38	0.70
34:1:707:LEU:HD12	34:1:741:LYS:CD	2.17	0.70
34:1:1276:SER:O	34:1:1276:SER:OG	2.07	0.70
35:3:1160:HIS:NE2	35:3:1175:ASP:OD2	2.20	0.70
35:3:189:TYR:HA	39:5:73:LEU:HD11	1.74	0.70
36:2:675:VAL:HA	36:2:681:PRO:HA	1.73	0.70
9:J:225:LEU:HG	10:L:211:ASN:HB2	1.74	0.70
22:X:231:ARG:O	22:X:235:LEU:HG	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:597:ILE:O	34:1:638:ALA:HB2	1.92	0.70
35:3:1057:ARG:NH2	36:2:707:PRO:HB3	2.06	0.70
34:1:1242:GLY:HA3	35:3:1169:PRO:HD2	1.74	0.70
35:3:1182:PHE:O	35:3:1190:GLN:NE2	2.24	0.70
1:A:382:GLU:HG3	3:C:354:ARG:HG3	1.72	0.70
6:G:92:U:H2'	6:G:93:A:H8	1.57	0.70
34:1:594:ARG:NE	34:1:674:LEU:HD13	2.06	0.70
34:1:739:ARG:HA	34:1:743:LEU:HD22	1.74	0.70
35:3:286:ILE:HD11	39:5:63:ARG:HA	1.74	0.70
35:3:642:ILE:O	35:3:703:ARG:NE	2.24	0.70
1:A:1057:ARG:NH1	1:A:1060:GLU:OE1	2.25	0.69
22:X:501:LEU:HB3	22:X:532:LEU:HD21	1.73	0.69
34:1:1056:MET:HE2	34:1:1096:THR:HG21	1.73	0.69
34:1:734:GLY:O	34:1:738:HIS:CB	2.40	0.69
34:1:789:LEU:CD2	34:1:836:THR:CG2	2.65	0.69
34:1:1181:ASP:OD1	34:1:1182:LEU:N	2.24	0.69
1:A:155:LYS:NZ	1:A:622:GLY:O	2.25	0.69
10:L:55:ASP:HB3	10:L:58:ILE:HD12	1.74	0.69
22:X:592:LEU:HD23	22:X:593:GLU:H	1.57	0.69
34:1:553:VAL:HA	34:1:556:ILE:HG22	1.72	0.69
34:1:929:LEU:O	34:1:970:LEU:HD22	1.91	0.69
35:3:1:MET:CG	36:2:709:GLY:O	2.40	0.69
35:3:487:ILE:HG13	35:3:491:VAL:HG22	1.73	0.69
35:3:983:ASN:ND2	35:3:1021:LEU:O	2.25	0.69
4:E:277:PHE:CE2	4:E:300:ILE:HG21	2.28	0.69
12:N:120:ARG:NH1	12:N:142:CYS:SG	2.66	0.69
18:T:245:HIS:HE2	18:T:263:SER:HG	1.41	0.69
35:3:189:TYR:CA	39:5:73:LEU:HD12	2.21	0.69
35:3:499:PHE:HZ	35:3:516:LEU:HD22	1.57	0.69
36:2:477:MET:HA	36:2:480:VAL:HG13	1.74	0.69
7:H:56:A:C5	36:2:505:CYS:SG	2.85	0.69
34:1:872:ILE:CD1	34:1:892:LEU:HD11	2.22	0.69
38:7:46:CYS:H	38:7:85:CYS:HB2	1.58	0.69
3:C:137:HIS:CD2	3:C:138:LEU:H	2.11	0.69
10:L:519:ASP:O	10:L:523:GLN:N	2.23	0.69
34:1:680:LEU:HA	34:1:683:LEU:HB2	1.75	0.69
34:1:1302:TYR:CD1	35:3:915:LEU:HD13	2.27	0.69
1:A:1889:LEU:HD11	1:A:2012:LEU:HD21	1.73	0.69
3:C:682:LYS:HB3	3:C:797:ALA:HB2	1.74	0.69
22:X:835:SER:OG	22:X:938:ARG:NH1	2.26	0.69
34:1:586:ASP:OD1	34:1:589:ALA:N	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:1052:ALA:HA	34:1:1088:ILE:HD11	1.75	0.69
34:1:1153:PHE:CB	34:1:1157:TYR:HE2	2.04	0.69
35:3:981:CYS:SG	35:3:1019:ASN:ND2	2.66	0.69
39:5:62:ALA:HA	39:5:65:ARG:NH1	2.07	0.69
5:F:86:U:OP2	11:M:193:ARG:NH1	2.25	0.69
34:1:630:ARG:HE	34:1:670:GLN:CD	1.95	0.69
35:3:114:ARG:NH2	39:5:37:ARG:HD2	2.07	0.69
36:2:452:LYS:HD2	36:2:452:LYS:C	2.11	0.69
3:C:131:ASN:HA	3:C:201:ASN:HB2	1.75	0.69
14:P:41:ILE:HG13	18:T:318:ARG:HG3	1.75	0.69
1:A:1179:SER:O	1:A:1201:ARG:NH1	2.23	0.68
5:F:82:A:H4'	5:F:82:A:OP2	1.92	0.68
11:M:217:LYS:HD2	11:M:217:LYS:O	1.93	0.68
1:A:1134:TRP:O	1:A:1139:ARG:NH1	2.25	0.68
3:C:759:LEU:HA	3:C:762:VAL:HG12	1.74	0.68
34:1:774:ILE:HD11	34:1:810:ILE:HA	1.75	0.68
35:3:353:PHE:CZ	39:5:51:ASN:HB3	2.28	0.68
35:3:968:ARG:HB2	35:3:970:TYR:HE2	1.57	0.68
35:3:1041:TYR:CG	36:2:705:ARG:NE	2.60	0.68
1:A:705:LYS:HD3	16:R:247:ILE:HB	1.76	0.68
4:E:68:GLU:HG2	4:E:347:SER:HB2	1.75	0.68
34:1:854:VAL:CG1	34:1:891:GLN:HG3	2.23	0.68
34:1:1249:TYR:CE2	36:2:587:HIS:CE1	2.80	0.68
35:3:775:ASN:HD22	35:3:775:ASN:H	1.40	0.68
34:1:1217:PRO:CB	36:2:510:TYR:OH	2.41	0.68
35:3:1194:SER:OG	35:3:1199:ARG:O	2.10	0.68
1:A:682:ASP:OD1	1:A:746:LYS:NZ	2.25	0.68
9:J:330:ARG:NH2	11:M:149:TYR:OH	2.24	0.68
10:L:67:GLU:OE1	10:L:91:ARG:NH2	2.26	0.68
34:1:850:ILE:HG21	34:1:888:LEU:CD2	2.24	0.68
34:1:1174:GLU:OE2	34:1:1210:HIS:NE2	2.26	0.68
34:1:1217:PRO:HD3	36:2:590:LEU:CD1	2.19	0.68
34:1:1242:GLY:CA	35:3:1169:PRO:HD2	2.23	0.68
34:1:770:MET:SD	34:1:810:ILE:HD11	2.34	0.68
35:3:39:GLU:OE2	35:3:55:THR:OG1	2.12	0.68
35:3:1057:ARG:HH22	36:2:707:PRO:HB3	1.57	0.68
4:E:146:ARG:HD2	4:E:148:LYS:HE2	1.75	0.68
7:H:173:C:H2'	7:H:174:A:C8	2.28	0.68
11:M:215:ASN:HD21	16:R:260:TYR:CA	2.07	0.68
18:T:471:ASP:OD1	18:T:473:SER:OG	2.07	0.68
22:X:281:ARG:NH1	22:X:281:ARG:HA	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:955:ILE:HG21	34:1:978:LEU:HD11	1.74	0.68
34:1:1006:MET:HE2	34:1:1045:ARG:HD3	1.74	0.68
1:A:1831:LYS:HG3	1:A:1832:ARG:N	2.07	0.68
6:G:92:U:H2'	6:G:93:A:C8	2.29	0.68
12:N:25:LEU:HD13	12:N:56:LYS:HG2	1.76	0.68
34:1:1043:ALA:CB	34:1:1055:TRP:CH2	2.77	0.68
1:A:1011:ALA:HB2	10:L:80:THR:HB	1.76	0.68
1:A:1544:ARG:NE	1:A:1672:ASP:OD2	2.26	0.68
35:3:705:ARG:HA	35:3:710:GLU:HA	1.76	0.68
36:2:511:LEU:HD11	36:2:591:TYR:CE1	2.18	0.68
2:B:8:G:H22	2:B:70:A:H1'	1.57	0.68
34:1:732:TRP:NE1	34:1:768:GLU:OE2	2.27	0.68
1:A:1578:ARG:HE	1:A:1746:ARG:NH2	1.91	0.67
4:E:294:SER:OG	4:E:299:LYS:O	2.10	0.67
20:V:543:LYS:HA	20:V:546:ASN:ND2	2.08	0.67
35:3:288:VAL:HG23	35:3:289:CYS:H	1.59	0.67
35:3:328:LYS:NZ	35:3:370:GLU:OE2	2.26	0.67
35:3:876:THR:O	35:3:876:THR:OG1	2.12	0.67
34:1:601:ALA:C	34:1:639:LEU:HD21	2.13	0.67
35:3:603:ARG:HG3	35:3:604:PHE:CE1	2.29	0.67
1:A:1807:ILE:HD11	1:A:1841:THR:HG22	1.75	0.67
3:C:193:THR:HG23	3:C:194:LYS:HD2	1.75	0.67
16:R:367:ARG:O	16:R:371:ARG:HG3	1.93	0.67
35:3:185:LEU:HG	35:3:235:LEU:HD11	1.76	0.67
35:3:449:VAL:HG13	35:3:763:ARG:HG2	1.76	0.67
1:A:1723:LYS:HB3	1:A:1724:PRO:HD3	1.75	0.67
9:J:311:GLN:OE1	9:J:311:GLN:N	2.24	0.67
16:R:389:SER:HA	16:R:392:ILE:HD12	1.75	0.67
34:1:933:CYS:SG	34:1:974:LEU:HD11	2.35	0.67
35:3:215:LEU:H	35:3:215:LEU:HD12	1.59	0.67
35:3:697:ARG:NH2	35:3:717:SER:OG	2.28	0.67
38:7:37:VAL:HB	38:7:38:ARG:HG3	1.76	0.67
1:A:873:ASN:ND2	1:A:876:GLU:OE1	2.28	0.67
4:E:217:ILE:HB	4:E:231:MET:HG3	1.74	0.67
9:J:196:ARG:NH1	9:J:196:ARG:HB2	2.09	0.67
35:3:427:CYS:SG	35:3:428:GLY:N	2.66	0.67
35:3:620:ASP:N	35:3:620:ASP:OD1	2.27	0.67
1:A:946:GLU:HB3	1:A:950:LEU:HD23	1.75	0.67
5:F:43:A:H1'	6:G:5:G:N2	2.10	0.67
20:V:484:SER:O	20:V:487:LYS:NZ	2.20	0.67
36:2:455:ARG:HA	36:2:458:ASN:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:HIS:CE1	22:X:866:ASN:HB3	2.30	0.67
3:C:137:HIS:HB2	3:C:239:THR:HG23	1.77	0.67
4:E:251:LEU:HD21	4:E:300:ILE:HG13	1.76	0.67
14:P:212:ASN:ND2	18:T:458:SER:OG	2.27	0.67
34:1:1156:GLU:HB3	38:7:38:ARG:HH12	1.58	0.67
36:2:568:TYR:C	36:2:570:LYS:H	1.96	0.67
1:A:1792:LYS:HE3	34:1:973:HIS:HE1	1.56	0.67
1:A:1936:LEU:O	1:A:1940:LEU:HG	1.93	0.67
22:X:430:THR:HG23	22:X:465:VAL:HG22	1.77	0.67
34:1:1207:SER:HA	36:2:584:LEU:HD22	1.77	0.67
34:1:1220:PHE:CE2	36:2:504:TRP:HB3	2.30	0.67
1:A:747:ALA:O	1:A:751:THR:HG22	1.94	0.67
34:1:1299:GLU:HA	34:1:1302:TYR:CE2	2.30	0.67
35:3:288:VAL:HA	39:5:62:ALA:HB2	1.77	0.67
3:C:64:LYS:HA	14:P:206:LYS:NZ	2.10	0.66
3:C:508:LYS:HG3	3:C:524:ILE:HG13	1.77	0.66
6:G:19:G:N2	13:O:194:ALA:O	2.28	0.66
22:X:583:TYR:O	22:X:585:LYS:NZ	2.22	0.66
35:3:169:HIS:ND1	35:3:234:PHE:HB2	2.10	0.66
35:3:191:GLU:HA	35:3:194:ASN:HD22	1.59	0.66
35:3:745:PHE:HB2	35:3:755:VAL:HG23	1.76	0.66
35:3:1136:GLU:OE1	35:3:1136:GLU:N	2.27	0.66
9:J:411:MET:SD	9:J:416:TYR:HE2	2.18	0.66
10:L:201:LYS:HD2	10:L:202:ARG:H	1.58	0.66
34:1:767:ARG:HE	34:1:805:TYR:HE1	1.44	0.66
34:1:1193:GLN:NE2	38:7:78:GLN:HE22	1.93	0.66
1:A:1664:ILE:HG22	1:A:1703:ILE:HB	1.77	0.66
3:C:758:LEU:HB3	3:C:796:VAL:HG11	1.78	0.66
20:V:547:VAL:O	20:V:550:MET:HB2	1.95	0.66
20:V:628:ILE:O	20:V:632:THR:OG1	2.12	0.66
22:X:234:TYR:O	22:X:238:ARG:HB2	1.96	0.66
34:1:621:ASP:HB3	34:1:624:VAL:HG22	1.75	0.66
35:3:168:TYR:CE1	39:5:69:MET:HB3	2.30	0.66
35:3:485:LEU:HD23	35:3:491:VAL:HG12	1.76	0.66
20:V:456:ARG:NE	20:V:492:MET:SD	2.68	0.66
1:A:372:PRO:HG3	3:C:341:LYS:HB3	1.76	0.66
1:A:1962:THR:HG23	1:A:1966:HIS:HB2	1.75	0.66
5:F:41:A:N1	6:G:6:A:N6	2.41	0.66
34:1:694:LEU:HD12	34:1:694:LEU:H	1.59	0.66
34:1:859:ASP:O	34:1:865:ARG:NE	2.27	0.66
35:3:147:ASP:OD1	35:3:151:ARG:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:511:LEU:HD21	35:3:517:VAL:HG23	1.78	0.66
35:3:700:LYS:HB3	35:3:702:PHE:CZ	2.30	0.66
35:3:833:GLU:O	35:3:836:ALA:N	2.23	0.66
35:3:926:TYR:HB3	35:3:928:TYR:HE2	1.60	0.66
36:2:514:LYS:HE3	36:2:591:TYR:HH	1.59	0.66
1:A:532:THR:OG1	6:G:3:A:OP1	2.13	0.66
7:H:43:U:O2'	7:H:44:U:O5'	2.13	0.66
9:J:194:LEU:HD13	10:L:156:ARG:HG3	1.77	0.66
34:1:929:LEU:CA	34:1:970:LEU:HD22	2.25	0.66
35:3:777:VAL:HG22	35:3:779:PHE:HE1	1.61	0.66
1:A:1457:HIS:ND1	1:A:1460:HIS:HD2	1.94	0.66
3:C:64:LYS:HD3	14:P:209:ARG:HH12	1.60	0.66
34:1:1217:PRO:HB2	36:2:510:TYR:OH	1.95	0.66
34:1:1217:PRO:CG	36:2:510:TYR:OH	2.43	0.66
34:1:1251:LEU:CD1	36:2:497:SER:HB2	2.25	0.66
3:C:255:VAL:HB	3:C:307:VAL:HG12	1.77	0.66
6:G:95:U:H2'	6:G:96:U:C6	2.31	0.66
9:J:409:GLU:HG2	9:J:410:HIS:CD2	2.31	0.66
22:X:827:MET:HB3	22:X:946:GLY:HA3	1.78	0.66
34:1:850:ILE:CG2	34:1:888:LEU:CG	2.73	0.66
34:1:1179:ASP:CB	36:2:511:LEU:HB3	2.25	0.66
34:1:1216:TRP:HD1	36:2:590:LEU:HD11	1.61	0.66
35:3:1188:ASN:OD1	35:3:1189:LYS:N	2.28	0.66
1:A:75:ASP:O	1:A:77:THR:N	2.29	0.66
1:A:1629:ILE:HB	1:A:1662:ILE:HB	1.77	0.66
1:A:1631:LEU:HB2	1:A:1660:TYR:HB3	1.76	0.66
1:A:1860:GLN:HG2	1:A:1883:VAL:HB	1.78	0.66
5:F:80:G:OP2	10:L:174:LYS:NZ	2.27	0.66
14:P:186:ARG:HD3	14:P:190:ASP:HB2	1.76	0.66
34:1:1278:ASP:O	35:3:1167:TYR:CE1	2.49	0.66
35:3:121:LEU:HB2	35:3:132:ILE:HD12	1.78	0.66
35:3:840:ALA:O	35:3:844:ASN:ND2	2.28	0.66
35:3:911:LYS:HB3	35:3:922:GLY:O	1.96	0.66
16:R:315:LYS:O	16:R:318:GLU:HG3	1.96	0.66
34:1:755:PRO:HD2	34:1:794:GLN:HB3	1.78	0.66
34:1:937:LEU:HD21	34:1:977:VAL:HG21	1.78	0.66
36:2:454:LEU:HD12	36:2:454:LEU:C	2.16	0.66
22:X:698:LYS:HD3	22:X:707:GLU:HG3	1.78	0.65
22:X:769:SER:OG	22:X:816:ALA:HB1	1.96	0.65
34:1:523:ALA:C	34:1:563:LEU:CD1	2.58	0.65
34:1:1217:PRO:O	36:2:503:HIS:CE1	2.48	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:1279:ALA:HB1	35:3:1167:TYR:HA	1.74	0.65
35:3:169:HIS:HD2	35:3:170:VAL:H	1.44	0.65
35:3:635:ALA:HB3	35:3:669:LEU:HD13	1.78	0.65
1:A:678:GLU:OE1	1:A:774:LYS:NZ	2.27	0.65
1:A:1255:THR:HG22	1:A:1526:LEU:HD21	1.78	0.65
7:H:125:G:H2'	7:H:126:A:C8	2.30	0.65
34:1:696:ASP:O	34:1:702:ARG:NH1	2.29	0.65
34:1:1249:TYR:HE2	36:2:587:HIS:ND1	1.92	0.65
36:2:674:PRO:O	36:2:682:LEU:N	2.24	0.65
3:C:618:THR:OG1	3:C:618:THR:O	2.13	0.65
34:1:495:ARG:HH21	34:1:530:PRO:HA	1.61	0.65
1:A:59:GLU:OE1	12:N:87:ASN:HB2	1.95	0.65
3:C:925:PRO:HG2	3:C:928:HIS:CE1	2.31	0.65
23:Y:94:VAL:HG13	23:Y:110:ILE:HG13	1.77	0.65
34:1:962:MET:CG	34:1:974:LEU:CD1	2.75	0.65
34:1:1257:PRO:HG3	36:2:478:HIS:CB	2.26	0.65
35:3:568:MET:HA	35:3:574:LEU:HA	1.79	0.65
35:3:586:ASP:HB3	35:3:610:VAL:HB	1.77	0.65
7:H:56:A:H4'	36:2:478:HIS:HA	1.77	0.65
13:O:29:GLY:O	16:R:195:ARG:NH2	2.23	0.65
21:W:320:GLY:C	36:2:667:ALA:O	2.35	0.65
34:1:1278:ASP:O	35:3:1167:TYR:HE1	1.80	0.65
35:3:1:MET:SD	36:2:709:GLY:O	2.53	0.65
35:3:1117:LEU:O	35:3:1128:ILE:HA	1.96	0.65
38:7:10:PHE:HB3	38:7:12:ARG:HG2	1.79	0.65
34:1:594:ARG:HD3	34:1:674:LEU:CG	2.27	0.65
34:1:1155:PHE:HA	34:1:1158:ILE:HG12	1.76	0.65
35:3:434:SER:HG	35:3:436:ARG:HE	1.43	0.65
36:2:469:VAL:HG12	36:2:471:ARG:H	1.62	0.65
7:H:32:U:O2'	7:H:33:G:N7	2.26	0.65
22:X:527:LEU:HD22	22:X:763:VAL:HG11	1.77	0.65
36:2:476:GLU:O	36:2:480:VAL:HG13	1.97	0.65
1:A:1703:ILE:HD13	1:A:1714:ALA:HB2	1.77	0.65
2:B:99:C:H2'	2:B:100:C:C6	2.32	0.65
22:X:910:ARG:O	22:X:914:VAL:HG13	1.96	0.65
23:Y:267:ARG:N	23:Y:287:GLU:O	2.29	0.65
34:1:789:LEU:HD22	34:1:836:THR:HG23	1.79	0.65
34:1:955:ILE:HG22	34:1:996:ALA:HB1	1.79	0.65
35:3:206:GLN:HG3	35:3:231:HIS:CD2	2.30	0.65
22:X:824:LEU:HD21	22:X:844:ALA:HB1	1.77	0.65
23:Y:39:TYR:N	23:Y:156:ILE:O	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:253:ASP:OD1	23:Y:253:ASP:N	2.29	0.65
34:1:1302:TYR:HE1	35:3:915:LEU:HD13	1.58	0.65
35:3:260:ASN:OD1	35:3:261:PHE:N	2.30	0.65
38:7:9:ILE:HG12	39:5:6:THR:HG22	1.78	0.65
1:A:154:GLU:OE2	1:A:158:ARG:NE	2.29	0.65
4:E:118:ASN:HD21	4:E:122:SER:H	1.45	0.65
4:E:236:ASP:HB2	4:E:256:ASP:HB3	1.78	0.65
5:F:43:A:H2	6:G:4:A:H61	1.44	0.65
7:H:119:G:H8	7:H:119:G:O5'	1.80	0.65
34:1:495:ARG:CD	34:1:530:PRO:HA	2.19	0.65
34:1:940:LEU:HD23	34:1:977:VAL:CG1	2.27	0.65
35:3:545:VAL:HG12	35:3:546:LYS:HG2	1.79	0.65
20:V:622:ARG:HA	20:V:625:ARG:HE	1.61	0.64
22:X:618:GLN:HG2	22:X:648:TYR:CD2	2.32	0.64
34:1:850:ILE:HG21	34:1:888:LEU:CG	2.27	0.64
1:A:1014:ASN:HD21	10:L:83:ARG:HB2	1.62	0.64
3:C:926:ALA:HA	3:C:929:LEU:HG	1.80	0.64
10:L:149:LEU:HA	10:L:152:LEU:HD12	1.79	0.64
1:A:357:ASN:HD22	3:C:862:PRO:HB3	1.62	0.64
1:A:707:ARG:HH22	7:H:17:U:H4'	1.62	0.64
20:V:525:PHE:HB3	20:V:560:LEU:HD21	1.80	0.64
35:3:1004:ASP:OD1	35:3:1006:GLN:N	2.28	0.64
1:A:1201:ARG:O	1:A:1203:SER:N	2.30	0.64
1:A:1778:TRP:O	1:A:1862:ILE:HG13	1.98	0.64
7:H:56:A:C6	36:2:505:CYS:HB3	2.33	0.64
34:1:850:ILE:CG2	34:1:888:LEU:CD1	2.68	0.64
35:3:233:ASN:ND2	35:3:233:ASN:H	1.95	0.64
1:A:1994:LYS:HD3	34:1:986:TYR:CZ	2.32	0.64
10:L:188:ARG:O	10:L:192:ARG:HG2	1.97	0.64
14:P:206:LYS:CB	14:P:218:GLU:HG2	2.27	0.64
22:X:272:TYR:OH	23:Y:227:VAL:O	2.10	0.64
24:Z:74:ALA:O	24:Z:78:PRO:HA	1.97	0.64
34:1:582:LEU:CG	34:1:634:VAL:CG2	2.54	0.64
34:1:933:CYS:HB2	34:1:970:LEU:HD13	1.72	0.64
1:A:1768:TYR:HA	1:A:1771:LEU:HB2	1.79	0.64
1:A:1798:LEU:CD1	34:1:973:HIS:HD2	2.06	0.64
1:A:1809:ILE:HB	1:A:1818:PHE:HD2	1.62	0.64
34:1:662:HIS:CD2	34:1:704:ILE:HG21	2.33	0.64
1:A:57:GLN:HE21	1:A:57:GLN:H	1.45	0.64
1:A:201:ALA:HA	1:A:204:LEU:HD23	1.78	0.64
4:E:153:PHE:HB2	4:E:172:ASP:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:175:THR:HG22	4:E:191:GLN:HG3	1.80	0.64
5:F:82:A:H2'	7:H:17:U:OP1	1.97	0.64
23:Y:32:CYS:SG	23:Y:159:THR:OG1	2.50	0.64
35:3:452:LEU:HD12	35:3:453:PRO:HD2	1.80	0.64
35:3:734:LEU:HD12	35:3:767:LEU:HD22	1.79	0.64
35:3:1009:PHE:HE1	35:3:1036:ALA:HB2	1.61	0.64
22:X:232:ARG:HA	22:X:235:LEU:HD12	1.80	0.64
34:1:744:ALA:CB	34:1:784:MET:HA	2.26	0.64
34:1:869:MET:SD	34:1:896:ILE:CD1	2.80	0.64
35:3:434:SER:OG	35:3:436:ARG:NE	2.25	0.64
35:3:665:LEU:HD11	35:3:667:ILE:HG13	1.78	0.64
35:3:805:ASN:HB2	39:5:58:ASN:HB2	1.77	0.64
35:3:1201:PRO:HA	35:3:1204:VAL:HG22	1.80	0.64
38:7:33:CYS:HG	38:7:35:SER:HG	1.09	0.64
1:A:1778:TRP:HB2	1:A:1861:ILE:HD12	1.79	0.64
1:A:1789:THR:HG22	1:A:1803:ILE:HD11	1.78	0.64
5:F:37:C:H4'	5:F:38:G:OP2	1.97	0.64
22:X:937:ILE:HG22	22:X:941:LYS:HD2	1.78	0.64
34:1:662:HIS:CE1	34:1:700:LYS:HB3	2.32	0.64
34:1:923:LYS:HG2	34:1:926:LYS:HE3	1.78	0.64
34:1:1155:PHE:HA	34:1:1158:ILE:HG13	1.74	0.64
34:1:1217:PRO:HB3	36:2:510:TYR:CE2	2.33	0.64
34:1:1248:GLN:HE21	36:2:496:ASN:CB	2.11	0.64
35:3:189:TYR:CD1	39:5:37:ARG:NH2	2.66	0.64
35:3:512:GLY:HA3	35:3:515:ALA:HB3	1.79	0.64
38:7:9:ILE:CD1	39:5:6:THR:HG21	2.28	0.64
1:A:535:ARG:NH1	6:G:2:U:OP2	2.31	0.64
1:A:1528:GLN:O	1:A:1532:ARG:HB2	1.99	0.64
3:C:381:LEU:HD22	3:C:416:LEU:HD21	1.78	0.64
3:C:737:PRO:HD2	3:C:741:GLY:HA3	1.78	0.64
9:J:185:ALA:HA	10:L:142:ILE:HD13	1.79	0.64
22:X:619:GLU:HA	22:X:622:GLU:OE1	1.97	0.64
34:1:499:LYS:HD2	34:1:534:GLN:NE2	2.12	0.64
34:1:1262:ARG:C	39:5:24:ALA:HB1	2.19	0.63
35:3:794:SER:O	35:3:796:ASN:ND2	2.31	0.63
36:2:596:GLU:H	36:2:596:GLU:CD	2.02	0.63
3:C:493:PHE:HD2	3:C:551:LEU:HG	1.62	0.63
12:N:112:ASN:N	12:N:112:ASN:OD1	2.28	0.63
20:V:609:GLN:HE22	20:V:616:LEU:HD21	1.63	0.63
23:Y:303:ASN:O	23:Y:310:ARG:NH1	2.30	0.63
34:1:826:ASP:OD1	34:1:827:ARG:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:958:ARG:NH2	35:3:1014:TYR:OH	2.31	0.63
7:H:29:A:H4'	7:H:29:A:OP1	1.96	0.63
9:J:296:ARG:NH1	9:J:320:GLU:OE2	2.29	0.63
16:R:357:HIS:CD2	16:R:361:LYS:HE2	2.33	0.63
34:1:1217:PRO:CB	36:2:510:TYR:CE2	2.81	0.63
34:1:490:GLU:O	34:1:494:GLU:HG2	1.98	0.63
35:3:1017:ASN:OD1	35:3:1018:GLU:N	2.31	0.63
36:2:517:ILE:HD12	36:2:517:ILE:C	2.19	0.63
34:1:617:ILE:HD12	34:1:660:ALA:HB1	1.81	0.63
34:1:1160:GLU:OE1	34:1:1160:GLU:N	2.19	0.63
35:3:1031:ARG:HG2	35:3:1031:ARG:HH11	1.63	0.63
3:C:709:TRP:HB3	3:C:713:LYS:HB2	1.81	0.63
5:F:79:C:H1'	5:F:82:A:H2	1.62	0.63
22:X:621:ILE:HG12	22:X:672:VAL:HG12	1.81	0.63
34:1:719:TYR:CZ	35:3:146:ARG:NH1	2.66	0.63
34:1:843:LYS:HB3	34:1:844:VAL:HG22	1.80	0.63
34:1:1160:GLU:CD	34:1:1160:GLU:H	2.01	0.63
35:3:330:PHE:O	35:3:390:ARG:NH2	2.32	0.63
38:7:30:CYS:SG	38:7:31:VAL:N	2.72	0.63
1:A:762:ARG:HH12	14:P:226:LYS:HZ1	1.47	0.63
1:A:1948:ASP:HA	1:A:1951:LYS:HD3	1.80	0.63
10:L:79:PRO:O	10:L:80:THR:OG1	2.16	0.63
14:P:77:ASP:O	14:P:78:ARG:NE	2.32	0.63
23:Y:14:ILE:HD12	23:Y:94:VAL:HG21	1.80	0.63
35:3:207:THR:O	35:3:207:THR:OG1	2.15	0.63
35:3:387:PHE:HE1	35:3:389:PRO:HG3	1.64	0.63
1:A:1014:ASN:ND2	1:A:1014:ASN:O	2.32	0.63
5:F:79:C:H1'	5:F:82:A:C2	2.33	0.63
10:L:188:ARG:HE	10:L:191:LEU:HD12	1.64	0.63
34:1:1155:PHE:CA	34:1:1158:ILE:CG1	2.72	0.63
3:C:464:ALA:HB1	3:C:473:PRO:HG3	1.80	0.63
4:E:312:TRP:HD1	4:E:319:ILE:HA	1.63	0.63
9:J:311:GLN:HG3	11:M:131:GLN:HG2	1.79	0.63
16:R:348:GLU:HB2	22:X:263:SER:H	1.64	0.63
34:1:625:ARG:NH1	34:1:659:GLN:OE1	2.31	0.63
34:1:1249:TYR:HA	36:2:498:VAL:CB	2.25	0.63
35:3:565:TYR:CE1	35:3:619:LEU:HB2	2.33	0.63
1:A:485:THR:HG22	1:A:486:LYS:H	1.63	0.62
9:J:198:ALA:HB1	10:L:160:ALA:HB2	1.80	0.62
16:R:325:ARG:NH1	23:Y:222:ILE:O	2.32	0.62
20:V:620:ASN:ND2	20:V:623:ASN:OD1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:521:PRO:O	35:3:543:THR:OG1	2.13	0.62
1:A:90:GLY:HA3	16:R:209:PRO:HD3	1.80	0.62
5:F:49:G:H2'	5:F:50:A:H8	1.64	0.62
23:Y:27:ASN:O	23:Y:31:LEU:HD12	1.99	0.62
23:Y:39:TYR:O	23:Y:185:GLN:NE2	2.32	0.62
35:3:70:LEU:HD11	35:3:152:LEU:HD13	1.80	0.62
38:7:52:GLY:H	38:7:55:GLN:HE21	1.47	0.62
6:G:105:C:OP1	22:X:993:THR:OG1	2.16	0.62
13:O:235:TYR:N	13:O:301:LYS:O	2.32	0.62
34:1:550:HIS:HD2	34:1:551:LEU:HD22	1.64	0.62
34:1:872:ILE:HD13	34:1:892:LEU:HD11	1.79	0.62
34:1:1278:ASP:OD2	35:3:1166:TYR:CZ	2.52	0.62
35:3:966:LEU:HB2	35:3:968:ARG:HD2	1.81	0.62
3:C:560:VAL:HG22	3:C:561:LYS:H	1.64	0.62
3:C:750:LEU:HD23	3:C:751:PRO:HD3	1.82	0.62
34:1:1120:ALA:HB2	34:1:1128:VAL:HG21	1.80	0.62
35:3:1:MET:CB	36:2:709:GLY:O	2.47	0.62
3:C:561:LYS:NZ	3:C:611:ASN:O	2.32	0.62
20:V:609:GLN:HA	20:V:612:PHE:HB2	1.80	0.62
34:1:598:SER:C	34:1:638:ALA:CB	2.67	0.62
34:1:1155:PHE:CG	34:1:1158:ILE:HD11	2.35	0.62
35:3:884:GLN:NE2	35:3:884:GLN:O	2.32	0.62
1:A:758:ARG:HH21	1:A:775:ASN:HD22	1.45	0.62
1:A:957:GLN:O	1:A:961:ASN:ND2	2.26	0.62
9:J:330:ARG:HD3	9:J:361:ARG:HH22	1.64	0.62
34:1:1278:ASP:CB	35:3:1166:TYR:HE2	2.11	0.62
35:3:207:THR:O	35:3:209:THR:HG22	1.99	0.62
35:3:747:SER:N	35:3:750:CYS:O	2.31	0.62
35:3:947:GLU:HB3	35:3:963:VAL:HG13	1.82	0.62
37:4:68:ASP:CB	37:4:114:LYS:CB	2.78	0.62
38:7:39:PRO:HB2	38:7:70:TYR:HD1	1.63	0.62
1:A:1251:SER:O	1:A:1251:SER:OG	2.17	0.62
22:X:580:ASP:OD2	22:X:733:LYS:NZ	2.31	0.62
34:1:495:ARG:CD	34:1:530:PRO:CB	2.75	0.62
34:1:929:LEU:CB	34:1:970:LEU:HD23	2.30	0.62
34:1:1137:ARG:NH1	36:2:522:PHE:H	1.97	0.62
35:3:1193:VAL:HA	35:3:1196:GLU:HG2	1.81	0.62
36:2:514:LYS:HD2	36:2:591:TYR:OH	1.98	0.62
2:B:53:U:OP1	14:P:39:THR:OG1	2.17	0.62
14:P:184:VAL:HB	23:Y:123:HIS:HE1	1.65	0.62
22:X:632:CYS:SG	22:X:642:LEU:HD13	2.39	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:1249:TYR:CA	36:2:498:VAL:HB	2.24	0.62
35:3:384:THR:OG1	35:3:385:PHE:N	2.31	0.62
20:V:540:GLU:HG3	20:V:541:THR:H	1.65	0.62
22:X:396:ARG:NH1	22:X:468:GLU:OE1	2.32	0.62
2:B:63:A:H2'	2:B:64:G:H8	1.65	0.62
2:B:64:G:H2'	2:B:65:G:C8	2.35	0.62
9:J:206:LEU:HD22	9:J:207:PRO:HD2	1.81	0.62
20:V:532:GLN:HE21	20:V:547:VAL:HG11	1.64	0.62
22:X:249:GLU:HB3	22:X:273:LYS:HE2	1.82	0.62
23:Y:147:ASP:HB2	23:Y:149:VAL:HG12	1.80	0.62
23:Y:219:THR:O	23:Y:223:LEU:HB2	2.00	0.62
35:3:680:ASP:CG	35:3:681:PRO:HD2	2.21	0.62
35:3:807:TYR:H	35:3:856:LYS:HD2	1.65	0.62
35:3:996:ILE:CD1	36:2:703:ILE:N	2.63	0.62
35:3:1009:PHE:HZ	35:3:1046:GLY:HA3	1.65	0.62
3:C:64:LYS:HA	14:P:206:LYS:HZ3	1.65	0.61
22:X:824:LEU:HD11	22:X:844:ALA:HA	1.82	0.61
34:1:528:ALA:HB2	34:1:567:VAL:HG12	1.82	0.61
34:1:600:LEU:O	34:1:604:ALA:CB	2.48	0.61
35:3:293:HIS:NE2	35:3:295:THR:HB	2.15	0.61
36:2:478:HIS:O	36:2:481:THR:CG2	2.47	0.61
1:A:1780:VAL:HB	1:A:1863:VAL:HG23	1.81	0.61
16:R:320:HIS:O	16:R:323:LYS:HG2	1.99	0.61
1:A:231:THR:HG22	1:A:233:PRO:HD2	1.83	0.61
1:A:987:LYS:NZ	3:C:61:GLU:OE1	2.27	0.61
1:A:1181:ASP:OD1	1:A:1181:ASP:N	2.32	0.61
9:J:344:GLN:N	9:J:344:GLN:OE1	2.33	0.61
22:X:558:ALA:O	22:X:562:THR:OG1	2.17	0.61
34:1:738:HIS:ND1	34:1:743:LEU:HD11	2.15	0.61
35:3:325:ILE:O	35:3:374:SER:HA	2.00	0.61
35:3:429:ARG:NE	39:5:55:ILE:HG12	2.15	0.61
1:A:784:LEU:O	1:A:788:GLN:HG3	2.00	0.61
1:A:1608:THR:HB	1:A:1632:PHE:HB2	1.83	0.61
4:E:126:SER:OG	4:E:136:TRP:NE1	2.26	0.61
34:1:606:LEU:HD12	34:1:606:LEU:N	2.15	0.61
35:3:114:ARG:CZ	39:5:37:ARG:HB2	2.29	0.61
35:3:191:GLU:O	35:3:194:ASN:N	2.26	0.61
1:A:1336:PRO:HB2	1:A:1350:ILE:HG12	1.83	0.61
20:V:511:ALA:HB1	20:V:525:PHE:HZ	1.64	0.61
34:1:703:THR:OG1	34:1:738:HIS:HE1	1.84	0.61
34:1:1129:LEU:CD1	34:1:1165:TYR:HB3	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:12:THR:O	35:3:34:ARG:NH1	2.34	0.61
35:3:61:VAL:HG21	39:5:46:HIS:CE1	2.35	0.61
1:A:81:PHE:O	1:A:83:HIS:N	2.34	0.61
1:A:732:PRO:HG2	1:A:735:ILE:HD13	1.83	0.61
1:A:1276:GLU:OE1	1:A:1375:TRP:N	2.31	0.61
3:C:209:VAL:HG21	3:C:237:LEU:HD23	1.82	0.61
4:E:108:HIS:CD2	4:E:128:SER:HB2	2.36	0.61
9:J:195:LEU:HD23	11:M:209:ASP:CA	2.29	0.61
9:J:441:ASP:OD1	9:J:445:LYS:NZ	2.33	0.61
22:X:651:LEU:HG	22:X:656:GLN:NE2	2.15	0.61
23:Y:40:CYS:O	23:Y:156:ILE:N	2.28	0.61
34:1:595:GLU:O	34:1:599:ASN:ND2	2.33	0.61
34:1:1028:HIS:O	34:1:1032:GLN:HB2	2.01	0.61
34:1:1302:TYR:HE1	35:3:915:LEU:CD1	2.13	0.61
35:3:928:TYR:HB3	35:3:937:LEU:HB3	1.81	0.61
35:3:1010:ILE:HG12	35:3:1026:ASP:HB3	1.80	0.61
35:3:1040:ASP:CB	36:2:706:THR:O	2.45	0.61
1:A:988:ILE:HD12	1:A:1030:ILE:HG13	1.81	0.61
1:A:1869:LEU:HD22	1:A:1884:ILE:HG22	1.83	0.61
10:L:699:ASN:O	10:L:703:MET:N	2.32	0.61
34:1:1133:MET:HG2	34:1:1172:LEU:HD13	1.82	0.61
34:1:1179:ASP:HB3	36:2:511:LEU:HB3	1.81	0.61
10:L:63:TRP:CD1	10:L:67:GLU:HB3	2.36	0.61
11:M:163:THR:HG23	11:M:166:SER:HB2	1.82	0.61
13:O:172:GLU:O	13:O:174:LYS:N	2.32	0.61
34:1:1166:ILE:O	34:1:1170:THR:HG22	2.01	0.61
34:1:1212:LEU:HD13	34:1:1237:LEU:HD13	1.81	0.61
35:3:318:ASP:OD1	35:3:319:GLU:N	2.33	0.61
38:7:13:LYS:NZ	38:7:48:GLU:OE1	2.26	0.61
3:C:724:TRP:HH2	3:C:788:LYS:HZ2	1.48	0.61
4:E:135:VAL:HG12	4:E:145:LYS:HB2	1.82	0.61
5:F:15:A:H2'	5:F:16:G:C8	2.35	0.61
38:7:46:CYS:O	38:7:50:ASN:HB2	1.99	0.61
1:A:1870:ASP:O	1:A:1874:VAL:HG23	2.01	0.61
1:A:1919:LEU:HD12	1:A:1936:LEU:HD11	1.83	0.61
2:B:63:A:H2'	2:B:64:G:C8	2.36	0.61
7:H:56:A:C6	36:2:505:CYS:CB	2.84	0.61
16:R:122:LYS:HG2	16:R:124:VAL:HG23	1.83	0.61
35:3:25:THR:OG1	35:3:27:GLN:N	2.31	0.61
36:2:596:GLU:OE2	36:2:596:GLU:N	2.21	0.61
2:B:102:U:H2'	2:B:103:G:C8	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:209:ILE:HG13	4:E:219:VAL:HG13	1.83	0.60
5:F:35:A:C8	6:G:12:G:C6	2.89	0.60
34:1:834:VAL:O	34:1:838:VAL:HG23	2.01	0.60
34:1:850:ILE:CG2	34:1:888:LEU:HD21	2.30	0.60
34:1:949:GLN:CB	34:1:989:VAL:HG22	2.24	0.60
1:A:641:MET:O	1:A:645:THR:HG23	1.99	0.60
1:A:1969:PRO:HB2	1:A:1971:LEU:HD23	1.83	0.60
22:X:257:PHE:CZ	22:X:270:LEU:HB2	2.36	0.60
22:X:677:ALA:O	22:X:725:ARG:NE	2.34	0.60
34:1:617:ILE:HD13	34:1:651:VAL:HB	1.83	0.60
37:4:17:VAL:O	37:4:56:TYR:HA	2.01	0.60
5:F:36:A:H2'	5:F:38:G:OP2	2.02	0.60
34:1:630:ARG:HG3	34:1:670:GLN:HG3	1.83	0.60
35:3:139:LYS:NZ	35:3:160:ALA:O	2.34	0.60
35:3:706:MET:HG3	35:3:707:GLN:HG2	1.83	0.60
1:A:384:VAL:HG12	3:C:331:PHE:HB3	1.82	0.60
1:A:1578:ARG:HE	1:A:1746:ARG:HH21	1.48	0.60
9:J:361:ARG:HD3	11:M:161:PHE:CE2	2.36	0.60
34:1:549:ARG:NH2	34:1:592:GLU:OE1	2.30	0.60
34:1:777:PHE:CD2	34:1:814:PHE:HB2	2.35	0.60
34:1:953:ASP:O	34:1:956:SER:OG	2.18	0.60
34:1:1178:MET:CG	36:2:591:TYR:CZ	2.82	0.60
35:3:418:GLU:OE1	35:3:419:ASP:N	2.28	0.60
34:1:677:CYS:O	34:1:680:LEU:HD12	2.01	0.60
34:1:949:GLN:CA	34:1:989:VAL:HG13	2.27	0.60
34:1:1258:ALA:HB3	34:1:1261:VAL:HG13	1.83	0.60
35:3:214:ASP:O	35:3:218:ASN:N	2.33	0.60
1:A:729:PRO:HG2	11:M:226:TYR:HE1	1.64	0.60
1:A:892:LYS:HD2	1:A:912:GLU:OE1	2.00	0.60
1:A:1490:PHE:O	1:A:1493:THR:OG1	2.19	0.60
7:H:99:A:O2'	7:H:100:U:OP2	2.18	0.60
11:M:215:ASN:ND2	16:R:260:TYR:CB	2.65	0.60
34:1:664:GLY:HA2	34:1:667:ILE:HD12	1.82	0.60
35:3:71:THR:O	35:3:146:ARG:NH2	2.33	0.60
35:3:910:ALA:HB1	35:3:913:LEU:HD11	1.83	0.60
1:A:47:GLU:H	1:A:47:GLU:CD	2.03	0.60
1:A:857:ASN:OD1	1:A:860:GLN:N	2.26	0.60
1:A:1892:PRO:HB3	1:A:1944:HIS:CD2	2.36	0.60
22:X:802:LEU:HB3	22:X:806:GLY:HA2	1.83	0.60
34:1:508:THR:HB	34:1:510:PRO:HD2	1.83	0.60
34:1:1155:PHE:CA	34:1:1158:ILE:HD11	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:1292:LYS:CD	39:5:78:PRO:HG2	2.32	0.60
35:3:112:CYS:HG	39:5:46:HIS:CD2	2.18	0.60
36:2:514:LYS:NZ	36:2:591:TYR:OH	2.34	0.60
14:P:72:ARG:HA	14:P:75:ASN:ND2	2.17	0.60
22:X:765:LEU:HD22	22:X:822:PRO:HG3	1.82	0.60
23:Y:96:MET:HB2	23:Y:124:THR:HB	1.84	0.60
34:1:1192:VAL:O	34:1:1196:SER:OG	2.20	0.60
35:3:329:TYR:CE2	35:3:389:PRO:HA	2.37	0.60
35:3:477:SER:CB	35:3:505:THR:H	2.11	0.60
35:3:615:ARG:NH2	35:3:630:MET:HB3	2.17	0.60
3:C:192:ASP:CG	3:C:193:THR:H	2.04	0.60
3:C:811:THR:O	3:C:815:VAL:HG23	2.00	0.60
4:E:105:LEU:HD11	4:E:136:TRP:CD2	2.37	0.60
7:H:48:A:C2	7:H:65:U:H2'	2.37	0.60
18:T:271:LYS:HG2	18:T:280:VAL:HG11	1.84	0.60
22:X:406:GLU:HA	22:X:409:LEU:HD23	1.84	0.60
34:1:675:MET:HB3	34:1:678:ALA:HB3	1.84	0.60
34:1:803:ALA:HB1	34:1:844:VAL:CG1	2.32	0.60
34:1:1178:MET:HB3	36:2:514:LYS:CD	2.30	0.60
35:3:883:GLU:OE2	35:3:884:GLN:N	2.33	0.60
1:A:39:GLN:NE2	21:W:170:THR:H	1.96	0.60
1:A:875:HIS:HE1	22:X:866:ASN:HB3	1.65	0.60
1:A:972:GLU:OE1	1:A:972:GLU:N	2.30	0.60
1:A:1160:ARG:HD3	14:P:192:VAL:HG11	1.84	0.60
4:E:203:ASP:N	4:E:203:ASP:OD1	2.32	0.60
34:1:528:ALA:CB	34:1:567:VAL:HG12	2.32	0.60
34:1:777:PHE:CZ	34:1:810:ILE:HG23	2.37	0.60
34:1:1178:MET:HB3	36:2:514:LYS:HZ3	1.67	0.60
35:3:680:ASP:OD2	35:3:681:PRO:HD2	2.02	0.60
39:5:65:ARG:HB3	39:5:65:ARG:CZ	2.32	0.60
5:F:79:C:H4'	5:F:80:G:OP1	2.02	0.59
6:G:117:A:H2'	23:Y:246:LYS:HE2	1.84	0.59
34:1:590:ARG:O	34:1:594:ARG:HB2	2.02	0.59
34:1:1148:LEU:CD1	34:1:1187:THR:HG21	2.31	0.59
1:A:390:ASP:OD1	1:A:390:ASP:N	2.35	0.59
1:A:693:ILE:HG22	1:A:694:LEU:HD23	1.82	0.59
1:A:1527:ASN:O	1:A:1529:ILE:N	2.36	0.59
3:C:724:TRP:HE1	3:C:732:ILE:HD11	1.67	0.59
4:E:114:GLU:OE2	4:E:290:ARG:NH2	2.36	0.59
23:Y:42:ILE:HA	23:Y:53:THR:HG22	1.83	0.59
23:Y:77:PHE:HB3	23:Y:103:GLN:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:497:ILE:CG1	34:1:526:PHE:HZ	2.11	0.59
34:1:698:GLN:HB3	34:1:701:VAL:HG12	1.84	0.59
35:3:1140:PHE:HE1	35:3:1197:LEU:HD13	1.67	0.59
1:A:1663:ASP:O	1:A:1703:ILE:N	2.34	0.59
4:E:202:ASN:ND2	4:E:204:THR:OG1	2.36	0.59
4:E:300:ILE:HG23	4:E:312:TRP:HB2	1.83	0.59
22:X:272:TYR:O	22:X:276:VAL:HB	2.02	0.59
22:X:802:LEU:HA	22:X:807:GLU:O	2.02	0.59
34:1:495:ARG:CD	34:1:530:PRO:CA	2.74	0.59
34:1:815:PHE:HZ	34:1:849:ILE:HG23	1.67	0.59
35:3:462:VAL:O	35:3:472:ALA:N	2.30	0.59
1:A:1558:THR:OG1	1:A:1559:GLY:N	2.33	0.59
1:A:1841:THR:O	1:A:1845:VAL:HG23	2.02	0.59
4:E:312:TRP:CD1	4:E:319:ILE:HA	2.37	0.59
9:J:439:ALA:HA	9:J:442:ARG:HB3	1.84	0.59
12:N:70:ILE:HB	12:N:74:LEU:HD23	1.83	0.59
12:N:121:VAL:HG11	12:N:126:LEU:HD21	1.83	0.59
22:X:225:GLU:O	22:X:229:LYS:HD3	2.03	0.59
23:Y:91:LYS:HG3	23:Y:114:GLU:HG3	1.84	0.59
35:3:982:GLU:HG2	35:3:984:LYS:HE3	1.84	0.59
42:A:3000:IHP:H1	42:A:3000:IHP:O46	2.01	0.59
5:F:28:A:O2'	12:N:39:GLY:O	2.19	0.59
7:H:50:C:H2'	7:H:51:A:C8	2.38	0.59
9:J:196:ARG:HB2	9:J:196:ARG:HH11	1.68	0.59
17:S:99:ALA:HB2	17:S:128:ILE:HA	1.83	0.59
23:Y:161:ILE:HG21	23:Y:164:ASP:HB2	1.84	0.59
34:1:1295:TYR:HH	39:5:29:TRP:HD1	1.50	0.59
35:3:138:GLN:HG2	35:3:161:HIS:CE1	2.36	0.59
35:3:1039:LEU:HD13	36:2:708:TRP:HB3	1.85	0.59
34:1:597:ILE:HB	34:1:634:VAL:HG12	1.83	0.59
34:1:598:SER:O	34:1:638:ALA:CB	2.48	0.59
34:1:669:GLN:HB2	34:1:708:ALA:HA	1.83	0.59
34:1:759:ALA:O	34:1:763:ASN:N	2.35	0.59
35:3:112:CYS:SG	39:5:46:HIS:NE2	2.65	0.59
35:3:1116:SER:N	36:2:708:TRP:CZ2	2.60	0.59
3:C:137:HIS:O	3:C:142:LYS:NZ	2.26	0.59
5:F:59:G:N2	5:F:76:A:N1	2.42	0.59
21:W:279:LYS:CB	36:2:621:VAL:C	2.71	0.59
22:X:612:LEU:O	22:X:689:VAL:HA	2.03	0.59
22:X:698:LYS:NZ	22:X:758:THR:HA	2.17	0.59
34:1:1203:GLY:HA2	35:3:1171:LYS:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:1116:SER:HA	36:2:708:TRP:CH2	2.38	0.59
1:A:729:PRO:HG2	11:M:226:TYR:CD1	2.38	0.59
9:J:199:LYS:O	9:J:199:LYS:HD3	2.03	0.59
22:X:557:THR:HA	22:X:560:PHE:HB2	1.85	0.59
34:1:777:PHE:CE2	34:1:814:PHE:CB	2.72	0.59
1:A:83:HIS:NE2	6:G:16:G:O6	2.36	0.59
1:A:1946:ASN:O	34:1:943:LYS:HE2	2.03	0.59
3:C:453:TYR:CZ	3:C:575:GLN:HB2	2.38	0.59
4:E:251:LEU:HB2	4:E:293:TRP:CE2	2.38	0.59
18:T:455:GLN:HG2	18:T:456:PRO:HD2	1.85	0.59
20:V:545:ARG:HG3	20:V:585:ILE:HG21	1.85	0.59
22:X:219:ARG:NE	23:Y:295:GLU:OE1	2.34	0.59
34:1:850:ILE:HG21	34:1:888:LEU:HG	1.85	0.59
34:1:881:ALA:HB3	34:1:920:ALA:O	2.02	0.59
34:1:1255:PHE:O	36:2:488:LEU:CG	2.51	0.59
35:3:114:ARG:HH12	39:5:34:ASN:HA	1.68	0.59
35:3:1039:LEU:HB3	36:2:708:TRP:HB2	1.84	0.59
1:A:47:GLU:HA	1:A:50:LYS:HG3	1.83	0.59
1:A:425:PRO:HB2	1:A:428:LYS:HG3	1.85	0.59
1:A:498:ARG:O	1:A:502:ASN:ND2	2.35	0.59
1:A:1776:ILE:HG22	1:A:1859:LYS:HZ3	1.67	0.59
35:3:435:LEU:HD13	35:3:799:ILE:HD11	1.84	0.59
35:3:525:ARG:HD3	35:3:533:VAL:HG22	1.85	0.59
35:3:700:LYS:HE2	35:3:715:MET:HB3	1.84	0.59
1:A:1298:ARG:HH11	1:A:1298:ARG:HB2	1.68	0.58
16:R:334:ARG:O	22:X:268:GLN:NE2	2.35	0.58
20:V:606:GLU:HA	20:V:609:GLN:CG	2.33	0.58
34:1:739:ARG:HD2	34:1:739:ARG:C	2.23	0.58
34:1:940:LEU:HD23	34:1:977:VAL:HG12	1.85	0.58
34:1:1110:VAL:O	34:1:1113:THR:HG22	2.02	0.58
35:3:35:GLY:CA	39:5:47:PHE:CE1	2.77	0.58
35:3:212:GLU:HB2	35:3:223:LYS:HG3	1.84	0.58
35:3:528:ARG:HG2	35:3:532:ARG:HH21	1.67	0.58
7:H:180:G:H2'	7:H:181:G:C8	2.38	0.58
9:J:443:ILE:HG13	9:J:444:SER:N	2.18	0.58
10:L:163:GLN:HA	10:L:163:GLN:HE21	1.68	0.58
20:V:497:CYS:HB3	20:V:507:PHE:CG	2.38	0.58
22:X:526:THR:HG22	22:X:528:HIS:H	1.68	0.58
34:1:597:ILE:HB	34:1:634:VAL:CG1	2.33	0.58
34:1:739:ARG:HA	34:1:743:LEU:HD21	1.84	0.58
34:1:778:GLN:HA	34:1:817:HIS:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:1078:VAL:HG12	34:1:1118:ILE:HD12	1.85	0.58
35:3:189:TYR:HB2	39:5:73:LEU:HD12	1.84	0.58
35:3:387:PHE:CE1	35:3:389:PRO:HG3	2.38	0.58
35:3:758:SER:N	35:3:761:THR:O	2.25	0.58
35:3:1041:TYR:H	36:2:705:ARG:HA	1.68	0.58
1:A:163:ARG:NH2	1:A:576:ASP:OD1	2.36	0.58
1:A:263:PHE:HE1	1:A:273:ILE:HD11	1.68	0.58
1:A:758:ARG:HD3	1:A:779:LEU:HD11	1.85	0.58
1:A:1222:LYS:O	20:V:592:GLU:HG3	2.02	0.58
1:A:1519:THR:OG1	1:A:1522:GLN:HB2	2.04	0.58
4:E:218:LYS:HD2	4:E:220:TRP:CZ2	2.38	0.58
9:J:433:ARG:O	9:J:437:LYS:HG2	2.03	0.58
34:1:777:PHE:CA	34:1:818:PHE:CE2	2.87	0.58
35:3:607:VAL:N	35:3:615:ARG:O	2.29	0.58
35:3:1117:LEU:N	36:2:708:TRP:CH2	2.72	0.58
1:A:1407:ASP:OD1	1:A:1407:ASP:N	2.32	0.58
22:X:546:LEU:HD22	22:X:547:LYS:H	1.68	0.58
23:Y:13:VAL:HB	23:Y:131:GLU:HB3	1.85	0.58
34:1:558:ARG:HH11	35:3:217:LEU:CD2	2.15	0.58
34:1:1110:VAL:O	34:1:1114:VAL:HG23	2.03	0.58
34:1:1193:GLN:HE21	38:7:78:GLN:NE2	2.01	0.58
35:3:195:ASP:OD2	35:3:198:GLY:N	2.36	0.58
36:2:458:ASN:O	36:2:458:ASN:ND2	2.35	0.58
1:A:1815:GLY:O	1:A:1918:ASN:HA	2.04	0.58
1:A:1862:ILE:HA	1:A:1885:LYS:O	2.01	0.58
2:B:14:U:H2'	2:B:15:C:H6	1.69	0.58
4:E:140:THR:HB	4:E:142:GLU:HG2	1.85	0.58
34:1:755:PRO:CD	34:1:794:GLN:HB3	2.33	0.58
34:1:884:ILE:HD12	34:1:884:ILE:C	2.22	0.58
34:1:1148:LEU:HB2	34:1:1187:THR:CG2	2.16	0.58
1:A:909:TYR:HB2	1:A:1033:GLY:HA3	1.85	0.58
3:C:879:ASP:OD1	3:C:879:ASP:N	2.36	0.58
12:N:32:ALA:HA	12:N:35:GLU:HG2	1.85	0.58
16:R:328:ALA:HB2	23:Y:226:MET:SD	2.43	0.58
16:R:373:ALA:HB3	16:R:376:LYS:HB3	1.84	0.58
34:1:850:ILE:O	34:1:854:VAL:HG13	2.04	0.58
35:3:695:GLY:O	35:3:697:ARG:NE	2.30	0.58
6:G:101:U:O3'	6:G:102:G:H2'	2.04	0.58
9:J:193:GLN:HA	9:J:193:GLN:NE2	2.13	0.58
10:L:49:ARG:NH1	10:L:133:GLU:O	2.37	0.58
22:X:192:ARG:HG2	22:X:192:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:141:VAL:HB	35:3:158:LEU:HD12	1.86	0.58
4:E:313:ASP:OD1	4:E:316:SER:N	2.28	0.58
6:G:106:C:OP2	22:X:998:ARG:NH2	2.36	0.58
17:S:14:VAL:O	17:S:24:VAL:HA	2.03	0.58
1:A:707:ARG:NH1	7:H:18:U:H5'	2.13	0.58
1:A:711:GLN:HE22	7:H:18:U:H5"	1.69	0.58
3:C:250:ARG:NH1	3:C:447:PRO:O	2.36	0.58
7:H:125:G:H2'	7:H:126:A:H8	1.67	0.58
14:P:184:VAL:HB	23:Y:123:HIS:CE1	2.38	0.58
20:V:543:LYS:HA	20:V:546:ASN:HD21	1.69	0.58
21:W:321:GLU:CA	36:2:667:ALA:HB3	2.34	0.58
22:X:653:SER:HA	22:X:656:GLN:HG3	1.85	0.58
34:1:1074:ARG:O	34:1:1078:VAL:HG23	2.03	0.58
35:3:69:ARG:NH1	35:3:74:THR:HA	2.18	0.58
35:3:310:ILE:O	35:3:311:PHE:HD2	1.87	0.58
35:3:642:ILE:H	35:3:703:ARG:HE	1.52	0.58
39:5:14:LEU:HA	39:5:17:LYS:HB2	1.86	0.58
1:A:1519:THR:HB	6:G:97:A:N6	2.19	0.58
5:F:35:A:C2	5:F:36:A:C6	2.91	0.58
20:V:491:ASN:HA	20:V:528:ILE:HD11	1.85	0.58
22:X:664:PRO:HG2	22:X:667:ALA:HB3	1.85	0.58
1:A:755:HIS:CD2	14:P:219:PHE:HE2	2.22	0.57
1:A:1436:TRP:O	1:A:1440:THR:HG23	2.04	0.57
1:A:1779:PHE:HB2	1:A:1810:PHE:HB3	1.85	0.57
3:C:444:GLY:O	3:C:447:PRO:HD2	2.04	0.57
4:E:150:HIS:NE2	4:E:169:THR:OG1	2.19	0.57
11:M:179:ILE:O	11:M:183:VAL:HG23	2.04	0.57
12:N:57:THR:HG21	12:N:88:LEU:HD23	1.86	0.57
16:R:161:ALA:HA	16:R:166:ARG:HH12	1.69	0.57
22:X:850:ASN:O	22:X:853:ILE:HG12	2.03	0.57
34:1:524:ARG:HD2	34:1:563:LEU:HD12	1.85	0.57
34:1:854:VAL:HG23	34:1:855:ASP:H	1.68	0.57
34:1:876:MET:HE3	34:1:920:ALA:HB3	1.85	0.57
34:1:1256:HIS:HD2	36:2:488:LEU:HD11	1.68	0.57
35:3:791:HIS:HD2	35:3:794:SER:OG	1.87	0.57
22:X:650:ASN:O	22:X:904:GLN:NE2	2.37	0.57
22:X:714:CYS:SG	22:X:718:SER:OG	2.61	0.57
34:1:512:ARG:O	34:1:516:LEU:HB2	2.04	0.57
34:1:1104:GLN:O	34:1:1105:GLU:HB3	2.03	0.57
35:3:449:VAL:HG22	35:3:763:ARG:HB3	1.85	0.57
35:3:607:VAL:HB	35:3:615:ARG:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:7:33:CYS:HB2	38:7:74:GLU:OE1	2.04	0.57
1:A:194:GLU:HA	1:A:194:GLU:OE2	2.03	0.57
3:C:711:ARG:NH2	3:C:732:ILE:O	2.38	0.57
11:M:165:ASN:HD22	16:R:95:LYS:HE2	1.70	0.57
35:3:345:GLY:O	35:3:360:GLN:HG3	2.04	0.57
39:5:7:ILE:HG13	39:5:8:HIS:N	2.18	0.57
1:A:1604:LEU:HD21	1:A:1725:LEU:HD22	1.85	0.57
1:A:1676:ILE:HD12	1:A:1706:ASP:HB2	1.85	0.57
1:A:1927:ILE:HD12	1:A:1931:THR:HG22	1.87	0.57
3:C:779:LEU:O	3:C:938:ARG:HD2	2.04	0.57
10:L:11:TRP:CE2	10:L:49:ARG:HD3	2.39	0.57
18:T:195:LYS:NZ	18:T:490:ARG:HD2	2.19	0.57
34:1:499:LYS:HG2	34:1:534:GLN:OE1	2.04	0.57
34:1:826:ASP:HB3	34:1:829:ASN:HB2	1.87	0.57
34:1:1178:MET:CG	36:2:514:LYS:HZ2	2.17	0.57
34:1:1244:CYS:HB3	35:3:1029:TYR:CE1	2.39	0.57
39:5:8:HIS:NE2	39:5:12:GLU:OE2	2.37	0.57
1:A:665:SER:O	1:A:665:SER:OG	2.18	0.57
1:A:1275:ARG:NH1	1:A:1373:GLN:O	2.36	0.57
1:A:1333:VAL:HG11	20:V:467:LEU:HD13	1.87	0.57
1:A:1978:LYS:O	1:A:1981:VAL:HG12	2.05	0.57
1:A:1994:LYS:HD3	34:1:986:TYR:HH	1.62	0.57
3:C:113:VAL:HG23	3:C:114:TYR:H	1.68	0.57
3:C:461:LEU:HB3	3:C:465:MET:HE1	1.85	0.57
22:X:394:ALA:HA	22:X:397:ARG:HD2	1.86	0.57
22:X:707:GLU:O	22:X:990:VAL:HA	2.03	0.57
23:Y:2:ALA:HA	23:Y:15:ASP:HA	1.87	0.57
23:Y:24:ALA:HA	23:Y:78:PHE:HZ	1.69	0.57
34:1:1098:LEU:HD12	34:1:1135:GLU:HG2	1.87	0.57
34:1:1178:MET:CB	36:2:514:LYS:NZ	2.67	0.57
35:3:479:VAL:HG23	35:3:480:ASN:ND2	2.20	0.57
35:3:538:THR:OG1	35:3:542:LYS:O	2.22	0.57
1:A:406:TRP:CZ2	3:C:266:GLU:HG3	2.39	0.57
2:B:96:A:H4'	2:B:97:G:H5"	1.85	0.57
4:E:158:TYR:HB3	4:E:168:CYS:SG	2.44	0.57
4:E:260:ARG:HD3	4:E:276:ILE:HG12	1.87	0.57
22:X:593:GLU:O	22:X:597:VAL:HG22	2.04	0.57
22:X:1009:LEU:HD21	22:X:1021:LEU:HD11	1.85	0.57
23:Y:55:ASP:OD2	23:Y:60:GLY:N	2.37	0.57
23:Y:139:ILE:HA	23:Y:142:THR:HG23	1.86	0.57
34:1:557:ASP:HB2	34:1:558:ARG:NH2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1397:ILE:HD11	16:R:405:VAL:HA	1.87	0.57
3:C:261:ASP:OD2	3:C:261:ASP:N	2.35	0.57
11:M:163:THR:OG1	11:M:165:ASN:OD1	2.21	0.57
22:X:462:ALA:HB1	22:X:473:LEU:HD11	1.86	0.57
22:X:760:LEU:O	22:X:764:VAL:HG23	2.05	0.57
34:1:777:PHE:CE2	34:1:810:ILE:HG23	2.39	0.57
35:3:365:GLY:HA2	35:3:394:ASN:ND2	2.19	0.57
3:C:126:SER:O	3:C:126:SER:OG	2.22	0.57
9:J:334:GLU:OE2	9:J:349:TYR:OH	2.10	0.57
20:V:491:ASN:O	20:V:494:LEU:HB3	2.05	0.57
22:X:640:ARG:HH22	22:X:668:ARG:HB2	1.70	0.57
34:1:495:ARG:HD3	34:1:530:PRO:CB	2.35	0.57
34:1:777:PHE:CD2	34:1:814:PHE:CA	2.87	0.57
34:1:898:TYR:OH	34:1:902:GLU:HG2	2.04	0.57
35:3:616:ILE:HG22	35:3:628:LEU:HB3	1.86	0.57
35:3:638:GLU:OE2	35:3:698:PRO:HB3	2.04	0.57
35:3:1147:HIS:O	35:3:1151:GLU:HG3	2.03	0.57
35:3:1200:THR:O	35:3:1203:GLU:N	2.37	0.57
1:A:1635:TYR:CZ	1:A:1636:LYS:HB2	2.40	0.57
9:J:199:LYS:HD3	9:J:199:LYS:C	2.25	0.57
16:R:175:GLN:OE1	16:R:176:TYR:N	2.33	0.57
20:V:551:PHE:HD1	20:V:554:LEU:HD12	1.69	0.57
23:Y:23:ARG:O	23:Y:26:LEU:HD23	2.05	0.57
34:1:739:ARG:HH11	34:1:740:GLY:HA2	1.70	0.57
34:1:747:LEU:HD21	34:1:773:LEU:HD22	1.86	0.57
35:3:552:ARG:HH21	35:3:567:GLU:HB3	1.70	0.57
3:C:461:LEU:HB3	3:C:465:MET:CE	2.35	0.57
14:P:42:LYS:O	18:T:258:SER:HB3	2.04	0.57
14:P:44:ARG:NH2	18:T:255:SER:O	2.36	0.57
17:S:14:VAL:HA	17:S:164:PRO:HA	1.87	0.57
20:V:636:LEU:O	20:V:640:THR:OG1	2.18	0.57
23:Y:33:LYS:HG3	23:Y:174:ILE:HD13	1.85	0.57
34:1:719:TYR:CD1	34:1:719:TYR:N	2.73	0.57
34:1:1160:GLU:OE2	35:3:1146:MET:HE1	2.02	0.57
34:1:1239:VAL:O	35:3:1169:PRO:HB3	2.05	0.57
1:A:1167:THR:OG1	1:A:1168:VAL:N	2.38	0.56
11:M:208:ILE:O	11:M:208:ILE:HG22	2.04	0.56
22:X:511:LEU:HG	22:X:514:TYR:HB2	1.86	0.56
35:3:86:ARG:NH1	35:3:1157:GLY:O	2.38	0.56
1:A:1839:TRP:CZ3	1:A:1871:PRO:HA	2.40	0.56
14:P:209:ARG:O	14:P:209:ARG:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:543:LEU:N	15:Q:621:GLU:O	2.35	0.56
34:1:1178:MET:HB3	36:2:591:TYR:OH	2.05	0.56
1:A:1768:TYR:HA	1:A:1771:LEU:CB	2.34	0.56
1:A:1980:GLU:O	1:A:1984:LYS:HG2	2.06	0.56
3:C:463:GLU:H	3:C:463:GLU:CD	2.08	0.56
3:C:829:GLU:HG2	3:C:907:VAL:HB	1.86	0.56
21:W:579:ASP:O	36:2:623:PRO:CB	2.53	0.56
22:X:217:GLU:HA	22:X:220:LYS:HB2	1.87	0.56
22:X:519:VAL:HB	22:X:550:VAL:HG13	1.87	0.56
34:1:619:ASN:OD1	34:1:620:MET:N	2.32	0.56
34:1:652:CYS:HB2	34:1:692:HIS:CE1	2.35	0.56
34:1:1006:MET:CE	34:1:1045:ARG:HD3	2.36	0.56
34:1:1155:PHE:O	34:1:1159:GLY:N	2.35	0.56
35:3:246:SER:OG	35:3:247:GLY:N	2.35	0.56
35:3:373:PHE:HE1	35:3:385:PHE:HB3	1.70	0.56
35:3:1057:ARG:HH22	36:2:707:PRO:CB	2.17	0.56
35:3:1145:GLU:HA	35:3:1148:LEU:HB2	1.88	0.56
3:C:490:PHE:O	3:C:491:HIS:ND1	2.33	0.56
12:N:16:GLU:OE1	12:N:16:GLU:N	2.33	0.56
23:Y:224:LEU:HD11	23:Y:230:LEU:HD23	1.86	0.56
35:3:286:ILE:HD11	39:5:63:ARG:CA	2.35	0.56
35:3:429:ARG:HE	39:5:55:ILE:HG12	1.70	0.56
35:3:1180:GLU:CD	35:3:1212:ARG:HH21	2.08	0.56
1:A:431:TYR:HB3	1:A:611:LEU:HD21	1.88	0.56
2:B:99:C:H2'	2:B:100:C:H6	1.69	0.56
16:R:162:ALA:C	16:R:164:PRO:HD3	2.26	0.56
22:X:716:LYS:HG3	22:X:747:LEU:HB3	1.87	0.56
34:1:1249:TYR:CE2	36:2:587:HIS:ND1	2.73	0.56
35:3:353:PHE:CZ	39:5:55:ILE:CG1	2.89	0.56
35:3:592:LEU:HD11	35:3:619:LEU:HD21	1.88	0.56
35:3:1148:LEU:HA	35:3:1151:GLU:OE2	2.05	0.56
1:A:1006:ALA:O	1:A:1010:THR:HG22	2.05	0.56
1:A:1410:ASP:OD2	1:A:1411:SER:N	2.38	0.56
1:A:1817:LEU:HD23	1:A:1919:LEU:HD21	1.87	0.56
10:L:28:LYS:HE2	16:R:268:LEU:HD23	1.88	0.56
22:X:246:LEU:HG	22:X:277:ARG:NE	2.21	0.56
23:Y:216:GLU:HA	23:Y:219:THR:HG23	1.86	0.56
23:Y:247:LEU:HD11	23:Y:256:LEU:HD11	1.86	0.56
34:1:631:ALA:O	34:1:635:VAL:HG13	2.05	0.56
35:3:342:LEU:HB3	35:3:343:LYS:O	2.06	0.56
35:3:527:ILE:HG12	35:3:532:ARG:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:PRO:O	1:A:383:PHE:N	2.32	0.56
3:C:833:PHE:HB3	3:C:900:VAL:HG23	1.88	0.56
4:E:197:LEU:HD11	4:E:213:ILE:HD13	1.88	0.56
4:E:243:LEU:HG	4:E:250:LEU:HB2	1.87	0.56
16:R:321:GLU:HB2	22:X:283:TYR:CE2	2.41	0.56
22:X:430:THR:O	22:X:434:GLN:HG3	2.06	0.56
23:Y:246:LYS:HD2	23:Y:310:ARG:O	2.06	0.56
34:1:523:ALA:CB	34:1:563:LEU:HD11	2.35	0.56
34:1:954:LEU:O	34:1:958:THR:HG22	2.05	0.56
35:3:25:THR:OG1	35:3:26:LYS:N	2.35	0.56
35:3:206:GLN:NE2	35:3:231:HIS:HA	2.21	0.56
35:3:717:SER:HB2	35:3:718:ARG:NH1	2.21	0.56
1:A:854:SER:OG	1:A:855:ARG:N	2.37	0.56
1:A:1790:ILE:HD12	34:1:977:VAL:HG22	1.86	0.56
1:A:1798:LEU:CD2	34:1:973:HIS:NE2	2.54	0.56
2:B:15:C:H2'	2:B:16:U:H6	1.71	0.56
3:C:401:ILE:HD11	3:C:423:PHE:HB2	1.88	0.56
6:G:104:C:O2'	6:G:105:C:O2	2.14	0.56
9:J:321:GLU:OE1	9:J:355:ARG:NH1	2.39	0.56
10:L:147:ASP:HA	10:L:150:GLU:HG3	1.88	0.56
22:X:476:GLU:HG3	22:X:477:VAL:H	1.70	0.56
34:1:970:LEU:O	34:1:973:HIS:HB2	2.06	0.56
35:3:329:TYR:HE2	35:3:389:PRO:HA	1.69	0.56
35:3:1143:HIS:O	35:3:1147:HIS:ND1	2.39	0.56
1:A:378:PHE:O	3:C:355:LYS:HG3	2.05	0.56
3:C:529:ARG:NH2	3:C:540:GLU:HB2	2.20	0.56
3:C:617:LEU:HD11	3:C:629:ILE:HG23	1.88	0.56
7:H:50:C:H2'	7:H:51:A:H8	1.71	0.56
22:X:242:LYS:NZ	23:Y:224:LEU:HB2	2.21	0.56
22:X:331:GLU:O	22:X:335:GLY:N	2.39	0.56
22:X:430:THR:HG22	22:X:434:GLN:NE2	2.20	0.56
34:1:789:LEU:HD23	34:1:836:THR:HG21	1.87	0.56
34:1:819:TRP:HZ2	34:1:837:THR:HG21	1.71	0.56
34:1:1270:ASN:OD1	39:5:21:THR:HB	2.06	0.56
35:3:1:MET:HA	36:2:709:GLY:O	2.05	0.56
35:3:1083:ASN:OD1	35:3:1084:GLY:N	2.39	0.56
1:A:35:ARG:O	1:A:39:GLN:HG3	2.06	0.56
22:X:518:MET:HA	22:X:549:LEU:O	2.06	0.56
22:X:580:ASP:HB2	22:X:733:LYS:HG3	1.88	0.56
22:X:698:LYS:O	22:X:757:ARG:HD3	2.05	0.56
34:1:1278:ASP:HB3	35:3:1166:TYR:CE2	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:ARG:HH22	14:P:226:LYS:HZ3	1.54	0.55
3:C:678:THR:HG22	3:C:679:PRO:HD2	1.88	0.55
7:H:27:U:O2'	7:H:28:C:H5'	2.06	0.55
10:L:223:GLY:HA2	16:R:86:LEU:CD2	2.36	0.55
16:R:357:HIS:O	16:R:361:LYS:HD2	2.06	0.55
35:3:510:LEU:HD23	35:3:510:LEU:H	1.70	0.55
36:2:511:LEU:CD1	36:2:591:TYR:CE1	2.83	0.55
1:A:1636:LYS:HD3	1:A:1658:GLN:NE2	2.18	0.55
10:L:66:GLU:O	10:L:69:GLU:HG3	2.05	0.55
14:P:198:ALA:O	14:P:201:VAL:HG23	2.06	0.55
22:X:700:TYR:HA	22:X:706:MET:O	2.07	0.55
38:7:30:CYS:SG	38:7:33:CYS:N	2.79	0.55
1:A:758:ARG:HH21	1:A:775:ASN:ND2	2.03	0.55
1:A:1382:SER:CB	1:A:1415:GLY:HA2	2.36	0.55
10:L:714:GLU:O	10:L:718:LYS:N	2.32	0.55
16:R:160:ALA:O	16:R:166:ARG:NH1	2.40	0.55
22:X:602:ILE:O	22:X:606:GLN:HB2	2.06	0.55
22:X:811:SER:HA	22:X:814:LYS:NZ	2.21	0.55
23:Y:257:GLU:OE2	23:Y:266:ILE:HG21	2.06	0.55
34:1:784:MET:O	34:1:788:VAL:HG12	2.05	0.55
34:1:807:LYS:HG3	34:1:844:VAL:HG11	1.88	0.55
35:3:68:PHE:CE2	35:3:77:TYR:HB2	2.41	0.55
35:3:169:HIS:CD2	35:3:170:VAL:H	2.22	0.55
35:3:477:SER:HB2	35:3:505:THR:N	2.11	0.55
35:3:703:ARG:HH11	35:3:703:ARG:HB2	1.70	0.55
35:3:926:TYR:HB3	35:3:928:TYR:CE2	2.41	0.55
1:A:1303:LEU:HD12	1:A:1311:PHE:CE1	2.41	0.55
5:F:35:A:H8	6:G:12:G:C6	2.23	0.55
7:H:165:A:O2'	7:H:166:G:O5'	2.24	0.55
22:X:443:ASN:O	22:X:444:LYS:HB2	2.05	0.55
35:3:92:TYR:OH	35:3:97:ASN:OD1	2.18	0.55
35:3:226:GLU:OE1	35:3:259:LYS:HD3	2.07	0.55
36:2:456:ARG:HD2	36:2:456:ARG:C	2.27	0.55
3:C:86:THR:OG1	3:C:87:GLN:N	2.38	0.55
4:E:165:GLN:HG3	4:E:181:ILE:HD13	1.89	0.55
7:H:6:U:H2'	7:H:7:U:H6	1.70	0.55
15:Q:27:ALA:O	15:Q:32:ALA:N	2.32	0.55
22:X:275:ARG:O	22:X:279:LEU:HD23	2.07	0.55
22:X:647:ILE:HA	22:X:651:LEU:HD21	1.88	0.55
34:1:598:SER:HA	34:1:638:ALA:N	2.18	0.55
34:1:1062:LEU:HA	34:1:1065:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:542:LYS:HB2	35:3:558:LEU:HD11	1.88	0.55
35:3:943:THR:HG23	35:3:976:LYS:HB3	1.89	0.55
35:3:1041:TYR:HD2	36:2:705:ARG:CG	2.18	0.55
37:4:13:ALA:O	37:4:60:GLU:HA	2.06	0.55
1:A:227:ARG:HH22	1:A:229:GLN:HE21	1.54	0.55
3:C:441:PRO:HB3	3:C:495:ARG:HH21	1.72	0.55
3:C:529:ARG:HH22	3:C:540:GLU:HB2	1.71	0.55
5:F:42:C:H2'	5:F:43:A:O4'	2.06	0.55
6:G:111:U:O2'	22:X:482:ARG:HD2	2.07	0.55
7:H:107:A:H2'	7:H:108:G:C8	2.42	0.55
19:U:71:LEU:O	19:U:75:GLU:N	2.38	0.55
23:Y:122:VAL:HB	23:Y:123:HIS:CD2	2.39	0.55
24:Z:73:LEU:O	24:Z:77:GLN:CB	2.55	0.55
34:1:524:ARG:HE	34:1:566:LEU:HD22	1.72	0.55
36:2:510:TYR:OH	36:2:591:TYR:O	2.23	0.55
1:A:214:ARG:HH12	1:A:225:TYR:HB2	1.72	0.55
1:A:1502:PHE:HZ	1:A:1505:LYS:HG3	1.72	0.55
3:C:711:ARG:HB3	3:C:730:ARG:HH22	1.72	0.55
12:N:38:GLU:C	12:N:40:LYS:H	2.10	0.55
22:X:640:ARG:HG3	22:X:640:ARG:HH11	1.70	0.55
34:1:1257:PRO:HG3	36:2:478:HIS:HA	1.85	0.55
35:3:233:ASN:HD21	35:3:286:ILE:CG2	2.19	0.55
35:3:312:LYS:HB2	35:3:330:PHE:HD1	1.72	0.55
35:3:406:PRO:HG2	35:3:408:LEU:HD11	1.89	0.55
35:3:747:SER:OG	35:3:748:GLU:N	2.40	0.55
39:5:14:LEU:HD23	39:5:17:LYS:HD2	1.88	0.55
1:A:548:ARG:HG2	1:A:548:ARG:HH21	1.72	0.55
3:C:632:THR:H	3:C:636:TYR:HD2	1.55	0.55
4:E:105:LEU:HD11	4:E:136:TRP:CG	2.42	0.55
14:P:67:GLU:CD	18:T:476:ARG:HH21	2.07	0.55
18:T:349:SER:OG	18:T:350:HIS:N	2.39	0.55
22:X:537:LYS:HD2	22:X:563:PHE:CZ	2.41	0.55
35:3:69:ARG:HH12	35:3:74:THR:HA	1.71	0.55
35:3:567:GLU:OE2	35:3:601:ARG:NH2	2.40	0.55
39:5:27:THR:HG23	39:5:30:GLU:HG3	1.88	0.55
1:A:121:HIS:ND1	1:A:123:THR:HG23	2.21	0.55
1:A:831:SER:O	1:A:831:SER:OG	2.18	0.55
3:C:360:ALA:H	3:C:361:PRO:HD3	1.72	0.55
3:C:506:PRO:HB2	3:C:569:ARG:NH2	2.22	0.55
4:E:188:GLN:NE2	4:E:189:THR:H	2.05	0.55
12:N:131:ILE:H	12:N:131:ILE:HD12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:606:GLU:OE2	20:V:609:GLN:HG3	2.06	0.55
22:X:1008:LEU:HB3	22:X:1016:TYR:HD2	1.71	0.55
23:Y:104:HIS:CD2	23:Y:124:THR:HG1	2.24	0.55
34:1:850:ILE:CG2	34:1:888:LEU:HG	2.37	0.55
34:1:1148:LEU:HD12	34:1:1187:THR:HG21	1.89	0.55
35:3:530:ASP:O	35:3:532:ARG:N	2.40	0.55
35:3:718:ARG:HB2	35:3:720:TRP:NE1	2.21	0.55
1:A:348:PRO:HB3	1:A:394:TYR:CZ	2.42	0.55
1:A:1108:ASP:O	1:A:1112:ARG:HG3	2.06	0.55
9:J:438:TYR:O	9:J:442:ARG:CB	2.55	0.55
18:T:371:HIS:CE1	18:T:396:LYS:HG3	2.42	0.55
34:1:803:ALA:HB1	34:1:844:VAL:HG12	1.88	0.55
35:3:35:GLY:HA3	39:5:47:PHE:CZ	2.40	0.55
5:F:38:G:P	5:F:38:G:H8	2.29	0.54
16:R:408:ASP:OD1	16:R:410:ARG:N	2.28	0.54
18:T:429:SER:HB3	18:T:439:TRP:HE1	1.72	0.54
22:X:515:SER:O	22:X:547:LYS:HB2	2.07	0.54
22:X:631:ARG:HG3	22:X:635:LEU:HD23	1.88	0.54
34:1:1263:ASP:N	39:5:24:ALA:HB1	2.20	0.54
1:A:1861:ILE:HG22	1:A:1882:ILE:HG12	1.89	0.54
1:A:1920:TYR:HE1	1:A:1936:LEU:HD22	1.72	0.54
3:C:216:THR:HG22	3:C:245:HIS:CE1	2.41	0.54
10:L:164:GLY:O	10:L:167:ALA:CA	2.55	0.54
10:L:518:VAL:O	10:L:522:LYS:N	2.37	0.54
11:M:204:ASP:OD2	11:M:204:ASP:N	2.40	0.54
20:V:584:LYS:HG3	20:V:585:ILE:N	2.21	0.54
22:X:412:ILE:HB	22:X:418:LEU:HD22	1.88	0.54
34:1:747:LEU:HD23	34:1:788:VAL:HB	1.90	0.54
34:1:1279:ALA:CA	35:3:1167:TYR:CE1	2.72	0.54
1:A:1519:THR:HG23	1:A:1519:THR:O	2.08	0.54
1:A:1979:VAL:HA	1:A:1982:GLN:HB2	1.88	0.54
3:C:112:THR:OG1	3:C:116:MET:N	2.41	0.54
3:C:514:TYR:HE2	3:C:522:SER:HB3	1.73	0.54
3:C:713:LYS:HA	3:C:716:GLU:OE2	2.07	0.54
4:E:201:PHE:CD1	4:E:208:ILE:HD13	2.42	0.54
5:F:41:A:H2'	5:F:42:C:C6	2.43	0.54
22:X:695:CYS:HB3	22:X:722:ARG:HH22	1.73	0.54
34:1:869:MET:HE2	34:1:896:ILE:CD1	2.37	0.54
35:3:115:ILE:CD1	39:5:18:TYR:HA	2.33	0.54
35:3:526:HIS:CG	35:3:573:GLN:HE21	2.25	0.54
35:3:791:HIS:NE2	35:3:934:GLY:HA3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:911:LYS:CB	35:3:922:GLY:O	2.55	0.54
35:3:1191:LYS:O	35:3:1195:GLU:HG3	2.07	0.54
1:A:1206:GLU:HG2	1:A:1207:PHE:N	2.21	0.54
1:A:1975:GLU:O	1:A:1979:VAL:HG22	2.07	0.54
3:C:297:ASN:N	3:C:297:ASN:OD1	2.37	0.54
3:C:465:MET:HE3	3:C:475:MET:HG3	1.90	0.54
4:E:62:LEU:O	4:E:350:ARG:HB2	2.07	0.54
4:E:90:ILE:HD12	4:E:105:LEU:HD22	1.90	0.54
4:E:166:LEU:HD12	4:E:167:VAL:H	1.73	0.54
7:H:7:U:H2'	7:H:8:C:C6	2.42	0.54
10:L:224:PHE:H	16:R:86:LEU:HD23	1.72	0.54
18:T:371:HIS:NE2	18:T:389:SER:OG	2.37	0.54
34:1:778:GLN:N	34:1:778:GLN:OE1	2.41	0.54
34:1:1300:LEU:HD22	35:3:1032:TRP:CE3	2.42	0.54
35:3:18:ILE:HG21	35:3:67:ALA:H	1.72	0.54
35:3:289:CYS:SG	35:3:338:ALA:HA	2.48	0.54
35:3:1015:LYS:O	35:3:1019:ASN:N	2.40	0.54
37:4:79:LEU:N	37:4:82:LYS:O	2.41	0.54
1:A:41:GLN:NE2	1:A:41:GLN:O	2.41	0.54
1:A:135:VAL:O	1:A:418:THR:OG1	2.22	0.54
1:A:1352:HIS:CD2	19:U:5:ILE:HG21	2.42	0.54
1:A:1642:PRO:HA	1:A:1716:GLY:O	2.08	0.54
2:B:8:G:H1	2:B:70:A:H1'	1.71	0.54
5:F:16:G:H2'	5:F:17:C:C6	2.42	0.54
10:L:205:LYS:H	10:L:205:LYS:HD3	1.71	0.54
22:X:937:ILE:HD12	22:X:937:ILE:H	1.72	0.54
23:Y:4:LEU:HD11	23:Y:11:ASP:HB3	1.89	0.54
34:1:785:LYS:O	34:1:789:LEU:HD12	2.07	0.54
34:1:1154:LEU:C	34:1:1158:ILE:HG12	2.23	0.54
34:1:1155:PHE:CA	34:1:1158:ILE:HG12	2.37	0.54
35:3:1:MET:SD	36:2:709:GLY:N	2.79	0.54
35:3:189:TYR:HA	39:5:73:LEU:HD13	1.78	0.54
1:A:1946:ASN:O	34:1:943:LYS:CE	2.55	0.54
5:F:15:A:H2'	5:F:16:G:H8	1.73	0.54
9:J:216:ASP:HB3	9:J:217:GLU:OE1	2.08	0.54
22:X:837:SER:HB2	22:X:930:SER:O	2.08	0.54
23:Y:255:ASP:HA	23:Y:258:ILE:HD12	1.89	0.54
35:3:1041:TYR:HB2	36:2:703:ILE:O	2.07	0.54
1:A:122:ILE:HD12	1:A:123:THR:HG22	1.90	0.54
1:A:371:LEU:HD21	3:C:347:ILE:HD11	1.87	0.54
1:A:701:ILE:H	1:A:701:ILE:HD12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:ASN:OD1	1:A:1139:ARG:HB3	2.07	0.54
1:A:1681:ARG:NH1	1:A:1681:ARG:HB3	2.23	0.54
3:C:674:CYS:HB3	3:C:818:SER:HB2	1.90	0.54
9:J:200:GLU:OE1	9:J:200:GLU:HA	2.06	0.54
23:Y:88:HIS:ND1	23:Y:120:ASP:OD1	2.35	0.54
34:1:565:ASP:OD1	34:1:566:LEU:N	2.41	0.54
38:7:68:ASP:OD1	38:7:68:ASP:N	2.38	0.54
1:A:1795:GLU:HG2	1:A:1797:ASN:H	1.71	0.54
1:A:1894:GLN:HE21	1:A:1944:HIS:CE1	2.26	0.54
3:C:213:ASP:CG	3:C:616:SER:HB2	2.20	0.54
7:H:56:A:O4'	36:2:504:TRP:HH2	1.91	0.54
9:J:568:LYS:HA	9:J:601:GLY:HA3	1.89	0.54
11:M:178:GLU:HA	11:M:181:ARG:HD3	1.90	0.54
14:P:208:LYS:O	14:P:208:LYS:NZ	2.29	0.54
20:V:589:GLU:O	20:V:593:TYR:HB2	2.07	0.54
22:X:648:TYR:O	22:X:656:GLN:NE2	2.40	0.54
3:C:119:LEU:O	3:C:123:MET:HG3	2.08	0.54
3:C:349:PHE:HB2	3:C:356:PHE:CD1	2.43	0.54
3:C:699:ASP:OD1	3:C:722:TYR:OH	2.24	0.54
3:C:928:HIS:ND1	3:C:928:HIS:N	2.55	0.54
4:E:283:ASN:N	4:E:283:ASN:OD1	2.41	0.54
10:L:184:ALA:O	10:L:188:ARG:N	2.31	0.54
18:T:346:ILE:HD13	18:T:380:LEU:HD21	1.89	0.54
22:X:635:LEU:HB2	22:X:639:ILE:HD11	1.89	0.54
22:X:639:ILE:HG22	22:X:640:ARG:H	1.73	0.54
34:1:815:PHE:HA	34:1:819:TRP:CD1	2.43	0.54
34:1:1092:ASP:O	34:1:1096:THR:HG23	2.08	0.54
3:C:129:ILE:HG22	3:C:199:LEU:HB3	1.90	0.54
3:C:216:THR:HG22	3:C:245:HIS:HE1	1.73	0.54
6:G:99:C:O2'	6:G:102:G:O6	2.25	0.54
22:X:696:LYS:HB3	22:X:709:LEU:HD11	1.90	0.54
22:X:793:LEU:HA	22:X:796:LEU:HD12	1.90	0.54
34:1:598:SER:C	34:1:638:ALA:HB1	2.28	0.54
34:1:731:LEU:O	34:1:735:ILE:HG12	2.08	0.54
35:3:286:ILE:HD11	39:5:63:ARG:HD3	1.90	0.54
35:3:429:ARG:HD3	39:5:55:ILE:HG12	1.89	0.54
35:3:803:ASP:OD1	35:3:804:HIS:N	2.41	0.54
35:3:883:GLU:HB3	35:3:886:GLU:HG3	1.89	0.54
38:7:46:CYS:N	38:7:85:CYS:HB2	2.22	0.54
3:C:220:ARG:NH1	3:C:578:ARG:O	2.38	0.53
4:E:202:ASN:ND2	4:E:207:GLN:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:239:THR:OG1	4:E:289:LEU:O	2.22	0.53
7:H:151:C:H2'	7:H:152:G:C8	2.43	0.53
22:X:455:ARG:NE	22:X:481:ILE:HD13	2.23	0.53
23:Y:104:HIS:NE2	23:Y:124:THR:OG1	2.38	0.53
34:1:693:GLY:HA2	34:1:696:ASP:HB2	1.90	0.53
34:1:881:ALA:CB	34:1:920:ALA:O	2.56	0.53
34:1:1279:ALA:CB	35:3:1167:TYR:CA	2.74	0.53
35:3:234:PHE:CE1	35:3:236:ILE:HG12	2.42	0.53
35:3:356:HIS:CD2	35:3:403:SER:HG	2.25	0.53
1:A:57:GLN:HE21	1:A:57:GLN:CA	2.20	0.53
1:A:1189:MET:HG2	1:A:1190:CYS:H	1.72	0.53
1:A:1771:LEU:HD21	1:A:1779:PHE:HE2	1.73	0.53
3:C:187:THR:HA	3:C:200:PHE:O	2.08	0.53
3:C:818:SER:O	3:C:822:MET:HB2	2.09	0.53
4:E:260:ARG:CD	4:E:276:ILE:HG12	2.39	0.53
20:V:628:ILE:HD11	20:V:643:LEU:HB2	1.90	0.53
22:X:527:LEU:HD23	22:X:755:ILE:HD13	1.89	0.53
23:Y:118:TYR:N	23:Y:118:TYR:CD1	2.77	0.53
34:1:933:CYS:O	34:1:936:VAL:N	2.41	0.53
34:1:1058:ILE:O	34:1:1062:LEU:HG	2.08	0.53
34:1:1255:PHE:HD2	36:2:491:LEU:HD12	1.73	0.53
35:3:266:ASP:OD1	35:3:266:ASP:N	2.40	0.53
35:3:994:GLN:HE22	35:3:1036:ALA:C	2.10	0.53
36:2:568:TYR:C	36:2:570:LYS:N	2.58	0.53
1:A:214:ARG:NH1	1:A:225:TYR:HB2	2.24	0.53
1:A:263:PHE:CE1	1:A:273:ILE:HD11	2.43	0.53
1:A:395:THR:HG22	1:A:396:ASP:H	1.73	0.53
1:A:836:THR:O	1:A:840:ILE:HG12	2.07	0.53
9:J:443:ILE:HG13	9:J:444:SER:H	1.73	0.53
16:R:351:GLU:O	16:R:355:ILE:HG13	2.08	0.53
18:T:250:ARG:HD2	18:T:266:GLU:HG3	1.90	0.53
20:V:609:GLN:NE2	20:V:616:LEU:HD21	2.23	0.53
22:X:643:LEU:HG	22:X:669:LYS:HA	1.89	0.53
35:3:164:ASN:HA	35:3:189:TYR:CZ	2.43	0.53
35:3:229:GLU:HB2	35:3:230:GLU:OE1	2.09	0.53
35:3:286:ILE:CD1	39:5:63:ARG:CA	2.87	0.53
35:3:642:ILE:N	35:3:703:ARG:HE	2.06	0.53
1:A:661:GLU:HB3	16:R:214:ILE:HG12	1.91	0.53
3:C:825:PRO:O	3:C:826:ARG:HG2	2.08	0.53
6:G:116:C:O4'	16:R:371:ARG:HA	2.07	0.53
16:R:386:ARG:NH1	16:R:391:VAL:HG21	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:700:TYR:HE2	22:X:705:GLY:HA2	1.73	0.53
23:Y:21:ARG:HH12	23:Y:83:VAL:N	2.07	0.53
34:1:594:ARG:HD3	34:1:674:LEU:HD21	1.86	0.53
34:1:652:CYS:SG	34:1:689:ILE:HG23	2.48	0.53
34:1:728:LEU:HB3	34:1:765:TYR:OH	2.08	0.53
34:1:777:PHE:O	34:1:818:PHE:CE2	2.62	0.53
35:3:1131:PRO:CG	36:2:709:GLY:HA2	2.38	0.53
1:A:1817:LEU:CD2	1:A:1919:LEU:HD21	2.39	0.53
3:C:725:ASP:HB3	3:C:728:ALA:H	1.74	0.53
4:E:311:VAL:HB	4:E:321:TYR:HB2	1.90	0.53
11:M:125:SER:O	16:R:242:GLN:NE2	2.42	0.53
16:R:150:ALA:O	16:R:153:LYS:HG3	2.09	0.53
16:R:328:ALA:HB1	23:Y:226:MET:HA	1.89	0.53
22:X:842:THR:HB	22:X:882:LEU:HD23	1.91	0.53
34:1:594:ARG:CD	34:1:674:LEU:CD2	2.81	0.53
34:1:1163:LYS:HE3	35:3:1142:GLN:HE22	1.73	0.53
36:2:495:ARG:O	36:2:497:SER:N	2.41	0.53
1:A:142:SER:HA	1:A:242:ALA:HB2	1.91	0.53
6:G:83:A:N6	37:4:22:GLU:CB	2.58	0.53
9:J:397:LYS:O	9:J:400:GLU:HG3	2.09	0.53
10:L:201:LYS:NZ	10:L:203:LYS:HG2	2.23	0.53
22:X:640:ARG:HH12	22:X:668:ARG:HB2	1.74	0.53
38:7:21:ARG:NH1	38:7:66:VAL:O	2.27	0.53
39:5:63:ARG:O	39:5:67:ASN:ND2	2.42	0.53
1:A:1143:MET:SD	1:A:1143:MET:N	2.81	0.53
3:C:441:PRO:O	3:C:444:GLY:HA3	2.09	0.53
3:C:460:ASP:OD2	3:C:461:LEU:N	2.41	0.53
3:C:481:MET:SD	3:C:612:LYS:HG3	2.48	0.53
4:E:240:GLY:O	4:E:252:SER:HA	2.09	0.53
6:G:12:G:H3'	6:G:13:C:C6	2.44	0.53
11:M:215:ASN:HD21	16:R:260:TYR:C	2.11	0.53
12:N:63:LEU:O	12:N:70:ILE:HG12	2.09	0.53
23:Y:306:ILE:HG12	23:Y:311:ILE:HD13	1.89	0.53
34:1:896:ILE:HD12	34:1:917:VAL:HG11	1.90	0.53
36:2:457:MET:CE	36:2:457:MET:CA	2.85	0.53
1:A:1831:LYS:NZ	1:A:1832:ARG:HB2	2.24	0.53
3:C:439:PRO:O	3:C:443:VAL:HB	2.09	0.53
4:E:208:ILE:HG23	4:E:220:TRP:HD1	1.74	0.53
18:T:287:HIS:NE2	18:T:305:THR:OG1	2.33	0.53
22:X:725:ARG:HD3	22:X:728:ARG:NH1	2.23	0.53
34:1:702:ARG:HD2	34:1:738:HIS:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:769:VAL:HA	34:1:772:ILE:HD13	1.89	0.53
34:1:806:ILE:HG23	34:1:810:ILE:HB	1.90	0.53
34:1:850:ILE:CB	34:1:888:LEU:HD11	2.38	0.53
34:1:1216:TRP:CD1	36:2:590:LEU:HD11	2.43	0.53
35:3:269:CYS:SG	35:3:327:LEU:HD11	2.48	0.53
35:3:605:LEU:O	35:3:617:ILE:N	2.42	0.53
35:3:642:ILE:HB	35:3:703:ARG:HH21	1.73	0.53
35:3:769:LYS:HD3	35:3:769:LYS:N	2.24	0.53
35:3:939:PHE:CZ	35:3:942:LYS:HG2	2.44	0.53
35:3:1025:ALA:HA	35:3:1087:GLN:O	2.09	0.53
1:A:41:GLN:HE22	1:A:45:TYR:HB2	1.74	0.53
3:C:938:ARG:HG2	3:C:942:GLY:HA3	1.91	0.53
18:T:203:HIS:CE1	18:T:229:LYS:HG3	2.44	0.53
34:1:713:ALA:CB	34:1:749:ALA:HA	2.37	0.53
34:1:1103:VAL:O	34:1:1109:ARG:HD3	2.08	0.53
35:3:34:ARG:HB2	35:3:37:ILE:HB	1.91	0.53
35:3:698:PRO:O	35:3:700:LYS:NZ	2.34	0.53
35:3:777:VAL:HG22	35:3:779:PHE:CE1	2.43	0.53
3:C:514:TYR:CE2	3:C:522:SER:HB3	2.44	0.53
4:E:108:HIS:NE2	4:E:128:SER:HB2	2.24	0.53
34:1:743:LEU:HD12	34:1:743:LEU:N	2.23	0.53
34:1:1036:ILE:HD11	34:1:1080:THR:HG21	1.90	0.53
1:A:65:HIS:O	1:A:69:ILE:HG13	2.10	0.52
1:A:1381:ASP:OD1	1:A:1414:ARG:HG2	2.09	0.52
6:G:8:C:H2'	6:G:9:C:C2	2.44	0.52
18:T:468:CYS:HB3	18:T:479:THR:HG22	1.89	0.52
22:X:167:THR:O	22:X:171:ARG:HG3	2.09	0.52
22:X:936:TYR:HA	22:X:939:VAL:HG22	1.91	0.52
23:Y:6:GLU:HG3	23:Y:158:HIS:HB3	1.91	0.52
34:1:523:ALA:CA	34:1:563:LEU:HD11	2.39	0.52
34:1:1266:TRP:CD1	39:5:24:ALA:HA	2.44	0.52
35:3:519:VAL:HB	35:3:524:ILE:HG23	1.92	0.52
35:3:623:ASP:OD2	35:3:626:GLN:NE2	2.41	0.52
1:A:325:HIS:HD2	1:A:326:HIS:CD2	2.16	0.52
1:A:384:VAL:HA	3:C:331:PHE:HD2	1.73	0.52
3:C:750:LEU:HA	3:C:753:GLU:HB2	1.91	0.52
4:E:145:LYS:NZ	4:E:184:LYS:HG3	2.24	0.52
4:E:258:THR:HG23	4:E:278:GLN:HE22	1.73	0.52
9:J:375:ASP:OD1	9:J:376:VAL:N	2.42	0.52
20:V:490:CYS:SG	20:V:521:TYR:HB3	2.50	0.52
34:1:499:LYS:HD2	34:1:534:GLN:HE22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:515:ALA:O	34:1:519:ILE:HG22	2.09	0.52
34:1:774:ILE:CD1	34:1:810:ILE:HA	2.39	0.52
34:1:1122:THR:OG1	34:1:1123:CYS:N	2.41	0.52
34:1:1260:LYS:O	34:1:1264:VAL:HG22	2.10	0.52
35:3:1117:LEU:N	36:2:708:TRP:CZ2	2.75	0.52
1:A:233:PRO:O	1:A:237:THR:HG23	2.10	0.52
1:A:885:LEU:HD23	1:A:1005:ILE:HG12	1.90	0.52
1:A:1972:THR:O	1:A:1976:TRP:HB2	2.09	0.52
6:G:112:U:OP1	22:X:503:ARG:HG2	2.09	0.52
9:J:443:ILE:HG23	9:J:444:SER:O	2.10	0.52
11:M:208:ILE:HG12	11:M:210:TYR:CE1	2.44	0.52
13:O:249:ARG:O	13:O:252:PHE:N	2.42	0.52
22:X:390:GLU:O	22:X:393:GLN:HG3	2.09	0.52
34:1:1148:LEU:HD12	34:1:1187:THR:CB	2.32	0.52
35:3:991:SER:O	35:3:991:SER:OG	2.28	0.52
1:A:845:ARG:HH11	1:A:1440:THR:HG22	1.74	0.52
1:A:1283:GLU:OE1	1:A:1283:GLU:N	2.42	0.52
3:C:559:ILE:HD12	3:C:560:VAL:O	2.09	0.52
4:E:281:VAL:HG21	4:E:306:ASP:HB2	1.91	0.52
34:1:545:GLU:HG2	34:1:548:GLU:HG3	1.91	0.52
34:1:842:ASN:OD1	34:1:879:LEU:HD11	2.10	0.52
34:1:846:ALA:HB1	34:1:850:ILE:HG12	1.91	0.52
34:1:886:HIS:HD2	34:1:887:LYS:HD3	1.74	0.52
34:1:1152:SER:HG	34:1:1194:HIS:CE1	2.27	0.52
34:1:1283:HIS:CE1	35:3:1168:PHE:CE1	2.97	0.52
35:3:632:ALA:O	35:3:633:LEU:HD23	2.09	0.52
35:3:940:LEU:HB3	35:3:941:HIS:CE1	2.43	0.52
2:B:64:G:H2'	2:B:65:G:H8	1.74	0.52
6:G:91:A:H2'	6:G:92:U:C6	2.45	0.52
16:R:91:ASP:OD1	16:R:95:LYS:N	2.27	0.52
34:1:600:LEU:O	34:1:604:ALA:HB3	2.10	0.52
34:1:854:VAL:HG12	34:1:891:GLN:HG3	1.90	0.52
1:A:597:LYS:N	2:B:45:C:OP1	2.42	0.52
1:A:832:TYR:OH	1:A:929:GLU:OE2	2.25	0.52
4:E:100:ASP:N	4:E:100:ASP:OD1	2.42	0.52
7:H:118:G:H2'	7:H:119:G:C8	2.43	0.52
16:R:189:ASN:ND2	16:R:192:ALA:O	2.42	0.52
35:3:91:GLU:HG2	35:3:92:TYR:N	2.25	0.52
35:3:147:ASP:OD1	35:3:150:ALA:N	2.43	0.52
35:3:1041:TYR:CD2	36:2:705:ARG:HG3	2.43	0.52
36:2:457:MET:HA	36:2:457:MET:HE3	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1785:VAL:O	1:A:1805:GLY:HA3	2.10	0.52
1:A:1844:GLU:O	1:A:1848:LEU:HD23	2.10	0.52
2:B:112:A:H2'	2:B:113:G:C8	2.44	0.52
3:C:497:LEU:O	3:C:546:ALA:HB1	2.10	0.52
4:E:208:ILE:O	4:E:219:VAL:HA	2.10	0.52
22:X:223:VAL:HA	22:X:226:LEU:HG	1.92	0.52
34:1:962:MET:CE	34:1:974:LEU:HD13	2.39	0.52
34:1:1248:GLN:O	36:2:498:VAL:HB	2.10	0.52
34:1:1249:TYR:CD2	36:2:587:HIS:HE1	2.28	0.52
34:1:1255:PHE:HD2	36:2:491:LEU:CD1	2.23	0.52
35:3:206:GLN:NE2	35:3:232:GLY:H	2.07	0.52
35:3:233:ASN:HD21	35:3:286:ILE:HG22	1.75	0.52
35:3:429:ARG:CD	39:5:55:ILE:HG12	2.40	0.52
1:A:1737:ASN:OD1	1:A:1739:ALA:N	2.39	0.52
4:E:145:LYS:HE2	4:E:184:LYS:HE2	1.92	0.52
10:L:63:TRP:HB3	10:L:68:GLU:HG3	1.91	0.52
22:X:432:ILE:HB	22:X:433:PRO:HD3	1.90	0.52
23:Y:27:ASN:HD21	23:Y:65:SER:HA	1.75	0.52
35:3:1115:GLU:CG	36:2:708:TRP:HE1	2.23	0.52
37:4:117:TYR:O	37:4:121:SER:CB	2.58	0.52
38:7:58:CYS:HB3	38:7:62:GLY:N	2.25	0.52
1:A:75:ASP:O	1:A:77:THR:HG22	2.10	0.52
1:A:357:ASN:ND2	3:C:862:PRO:HB3	2.25	0.52
1:A:872:ASP:O	1:A:874:PRO:HD3	2.10	0.52
1:A:1650:ASP:OD1	1:A:1718:TRP:HB2	2.10	0.52
3:C:478:THR:CG2	3:C:492:ALA:HB1	2.37	0.52
5:F:48:A:H2'	10:L:165:LYS:NZ	2.24	0.52
7:H:172:C:N4	7:H:173:C:H41	2.07	0.52
11:M:217:LYS:NZ	11:M:224:ARG:HH12	2.08	0.52
34:1:601:ALA:C	34:1:639:LEU:CD2	2.77	0.52
34:1:648:LEU:HA	34:1:651:VAL:HG22	1.92	0.52
34:1:750:ILE:HG22	34:1:753:LEU:HD12	1.92	0.52
34:1:777:PHE:HA	34:1:818:PHE:CZ	2.44	0.52
34:1:1125:PRO:CG	34:1:1165:TYR:CZ	2.92	0.52
34:1:1289:ASN:HB3	34:1:1295:TYR:H	1.75	0.52
34:1:1291:ASP:OD1	34:1:1292:LYS:N	2.43	0.52
35:3:390:ARG:HD3	35:3:393:LYS:HE3	1.91	0.52
35:3:515:ALA:HB2	35:3:528:ARG:CZ	2.40	0.52
35:3:606:ALA:HA	35:3:616:ILE:HA	1.92	0.52
35:3:695:GLY:HA3	35:3:717:SER:OG	2.10	0.52
3:C:209:VAL:HG23	3:C:898:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:320:LEU:HD13	3:C:343:LEU:HB2	1.92	0.52
3:C:333:ASP:OD1	3:C:333:ASP:N	2.43	0.52
4:E:135:VAL:CG1	4:E:145:LYS:HB2	2.40	0.52
16:R:319:LYS:O	16:R:322:GLU:HG3	2.10	0.52
20:V:511:ALA:HB1	20:V:525:PHE:CZ	2.43	0.52
22:X:287:GLY:O	22:X:291:LYS:HG2	2.10	0.52
34:1:523:ALA:HB1	34:1:563:LEU:HD11	1.91	0.52
34:1:606:LEU:N	34:1:606:LEU:CD1	2.73	0.52
34:1:1257:PRO:HB3	36:2:481:THR:HG22	1.83	0.52
34:1:1302:TYR:CE1	35:3:915:LEU:CB	2.77	0.52
35:3:442:LEU:HD13	35:3:770:LEU:HD23	1.91	0.52
35:3:872:ILE:HD12	35:3:872:ILE:H	1.75	0.52
35:3:1008:SER:HG	35:3:1009:PHE:N	2.06	0.52
36:2:460:PHE:HB3	36:2:464:GLU:HG2	1.91	0.52
1:A:1831:LYS:HG3	1:A:1832:ARG:H	1.75	0.51
2:B:69:A:H3'	2:B:70:A:C8	2.45	0.51
3:C:131:ASN:OD1	3:C:201:ASN:ND2	2.43	0.51
6:G:116:C:H2'	6:G:117:A:H5'	1.91	0.51
14:P:39:THR:O	18:T:318:ARG:HD3	2.10	0.51
22:X:401:VAL:HG12	22:X:572:ILE:HD12	1.91	0.51
22:X:700:TYR:HB3	22:X:757:ARG:O	2.09	0.51
35:3:189:TYR:CB	39:5:73:LEU:CD1	2.83	0.51
35:3:451:GLU:HA	35:3:761:THR:HG22	1.92	0.51
36:2:711:LEU:C	36:2:711:LEU:HD22	2.30	0.51
38:7:57:ARG:NH1	38:7:62:GLY:O	2.39	0.51
1:A:1014:ASN:ND2	10:L:83:ARG:HB2	2.25	0.51
1:A:1786:TYR:CD1	1:A:1833:LEU:HB2	2.45	0.51
3:C:713:LYS:HA	3:C:716:GLU:CD	2.30	0.51
5:F:41:A:C2	6:G:7:G:N1	2.78	0.51
14:P:213:ASP:OD2	14:P:216:ARG:HB2	2.10	0.51
22:X:424:THR:HG21	22:X:728:ARG:NH2	2.25	0.51
22:X:441:TYR:OH	22:X:547:LYS:NZ	2.39	0.51
22:X:683:ILE:HD13	22:X:686:ILE:HG13	1.91	0.51
34:1:873:GLU:HG3	34:1:916:THR:HG21	1.92	0.51
35:3:181:MET:HB3	35:3:212:GLU:HA	1.92	0.51
35:3:275:ARG:HB3	35:3:275:ARG:HH21	1.75	0.51
35:3:1168:PHE:N	35:3:1168:PHE:CD2	2.77	0.51
7:H:103:U:H4'	7:H:104:U:H5'	1.92	0.51
22:X:289:GLN:HG2	22:X:293:GLU:OE1	2.11	0.51
22:X:877:ASP:O	22:X:881:LEU:HG	2.10	0.51
34:1:560:LEU:HD23	34:1:603:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:831:ARG:O	34:1:834:VAL:HB	2.11	0.51
1:A:280:GLU:HG3	19:U:9:THR:HG21	1.93	0.51
1:A:1770:GLU:O	1:A:1773:SER:OG	2.29	0.51
1:A:1819:LEU:HD21	1:A:1906:ILE:HD11	1.91	0.51
11:M:210:TYR:C	11:M:210:TYR:CD2	2.84	0.51
16:R:367:ARG:HH11	16:R:371:ARG:NH1	2.08	0.51
22:X:882:LEU:O	22:X:886:THR:OG1	2.20	0.51
34:1:687:VAL:O	34:1:690:ILE:HG13	2.11	0.51
34:1:743:LEU:N	34:1:743:LEU:CD1	2.73	0.51
35:3:120:PHE:HB2	35:3:133:SER:OG	2.09	0.51
35:3:614:VAL:HG23	35:3:633:LEU:HD11	1.93	0.51
35:3:1041:TYR:CD2	36:2:705:ARG:CG	2.94	0.51
35:3:1041:TYR:CD2	36:2:705:ARG:NH2	2.62	0.51
1:A:71:ARG:NH1	1:A:177:ASP:OD1	2.43	0.51
1:A:1718:TRP:CZ3	1:A:1726:ILE:HD11	2.45	0.51
1:A:1738:PRO:HB2	36:2:550:LYS:CB	2.41	0.51
2:B:98:G:H2'	2:B:99:C:C6	2.45	0.51
3:C:213:ASP:OD2	3:C:213:ASP:N	2.42	0.51
4:E:84:ALA:HB2	4:E:90:ILE:HG12	1.93	0.51
5:F:40:U:H2'	5:F:41:A:C8	2.45	0.51
6:G:88:G:O6	7:H:41:U:O4	2.28	0.51
14:P:186:ARG:CB	14:P:186:ARG:NH1	2.73	0.51
14:P:188:TRP:O	14:P:188:TRP:CG	2.62	0.51
16:R:148:ARG:O	16:R:152:GLU:HG3	2.11	0.51
18:T:381:HIS:HD2	18:T:441:TRP:CE2	2.29	0.51
22:X:412:ILE:HD13	22:X:418:LEU:HB2	1.91	0.51
23:Y:95:SER:OG	23:Y:125:VAL:HA	2.11	0.51
23:Y:213:ALA:HA	23:Y:216:GLU:HG3	1.91	0.51
34:1:747:LEU:HD11	34:1:773:LEU:HD21	1.92	0.51
34:1:960:VAL:O	34:1:963:LYS:CB	2.52	0.51
35:3:413:ALA:HB1	35:3:415:LEU:HD13	1.92	0.51
35:3:550:ASN:HD22	35:3:553:GLN:HB2	1.75	0.51
35:3:700:LYS:O	35:3:714:ALA:HA	2.11	0.51
1:A:26:SER:HB3	1:A:29:LYS:HB2	1.93	0.51
1:A:874:PRO:HG2	22:X:866:ASN:HD21	1.75	0.51
1:A:1502:PHE:CZ	1:A:1505:LYS:HG3	2.46	0.51
3:C:112:THR:OG1	3:C:112:THR:O	2.25	0.51
4:E:72:CYS:SG	4:E:81:LEU:HD11	2.51	0.51
7:H:181:G:H2'	7:H:182:U:C6	2.46	0.51
14:P:74:LYS:O	14:P:77:ASP:HB3	2.11	0.51
18:T:272:CYS:HB3	18:T:282:ARG:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:244:VAL:HG13	23:Y:312:HIS:O	2.11	0.51
34:1:573:LYS:H	34:1:573:LYS:HD2	1.75	0.51
34:1:641:ILE:N	34:1:642:PRO:HD2	2.26	0.51
34:1:661:ARG:HG2	34:1:692:HIS:NE2	2.25	0.51
35:3:424:TYR:CD1	35:3:437:VAL:HG22	2.46	0.51
35:3:720:TRP:CE3	35:3:731:LEU:HG	2.45	0.51
35:3:1114:SER:HB2	35:3:1215:TYR:CE1	2.46	0.51
36:2:458:ASN:HD22	36:2:458:ASN:C	2.13	0.51
1:A:693:ILE:O	1:A:695:ASP:N	2.43	0.51
1:A:1935:ARG:O	1:A:1938:LEU:HG	2.11	0.51
5:F:40:U:H3	6:G:7:G:H1	1.59	0.51
11:M:165:ASN:HB2	16:R:95:LYS:CB	2.37	0.51
19:U:1:MET:O	19:U:3:ASN:N	2.44	0.51
22:X:418:LEU:HD12	22:X:568:PRO:HG2	1.92	0.51
23:Y:215:LYS:O	23:Y:218:LYS:N	2.44	0.51
34:1:1179:ASP:H	36:2:511:LEU:CD1	2.22	0.51
35:3:458:ALA:HB1	35:3:460:TRP:HZ3	1.76	0.51
35:3:628:LEU:HD21	35:3:681:PRO:HA	1.92	0.51
1:A:1121:ASN:HB2	1:A:1123:GLU:OE2	2.11	0.51
1:A:1554:GLN:HG3	1:A:1561:PHE:CE1	2.46	0.51
1:A:1785:VAL:O	1:A:1822:ILE:HD11	2.11	0.51
3:C:782:GLU:OE2	3:C:941:LYS:NZ	2.44	0.51
9:J:193:GLN:CA	9:J:193:GLN:NE2	2.72	0.51
34:1:830:TYR:O	34:1:834:VAL:HG23	2.11	0.51
34:1:1080:THR:HA	34:1:1083:TYR:HD2	1.74	0.51
34:1:1179:ASP:H	36:2:511:LEU:HD13	1.74	0.51
38:7:71:TYR:CD2	38:7:81:ASP:HB2	2.46	0.51
1:A:422:LEU:HD22	1:A:638:LEU:HD13	1.93	0.51
1:A:467:GLN:HG3	2:B:19:A:N7	2.26	0.51
1:A:1375:TRP:O	1:A:1378:GLU:N	2.44	0.51
1:A:1516:LYS:O	1:A:1517:LYS:HD2	2.10	0.51
2:B:101:U:H2'	2:B:102:U:C6	2.45	0.51
4:E:152:SER:OG	4:E:153:PHE:N	2.43	0.51
4:E:308:PHE:HE1	4:E:324:PRO:HB3	1.76	0.51
8:I:393:LYS:N	8:I:394:PRO:HD3	2.26	0.51
10:L:172:ARG:HA	10:L:175:GLN:HE21	1.75	0.51
12:N:54:HIS:CE1	12:N:92:TRP:HZ2	2.28	0.51
12:N:104:ARG:HD3	12:N:136:HIS:HB3	1.92	0.51
18:T:274:ASP:HB2	18:T:281:ILE:HD13	1.92	0.51
22:X:235:LEU:HD22	23:Y:217:ALA:HA	1.91	0.51
22:X:330:GLU:O	22:X:334:LEU:HD12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:596:VAL:O	22:X:600:LEU:HG	2.11	0.51
34:1:738:HIS:C	34:1:743:LEU:HD21	2.32	0.51
35:3:932:ASN:O	35:3:933:ASN:ND2	2.44	0.51
36:2:555:GLU:O	36:2:559:PRO:HA	2.11	0.51
38:7:39:PRO:HB2	38:7:70:TYR:CD1	2.44	0.51
1:A:59:GLU:HB3	12:N:103:LEU:HD21	1.92	0.51
1:A:1590:VAL:HG21	1:A:1628:ASP:OD1	2.11	0.51
1:A:1599:GLN:HB2	1:A:1600:GLU:OE1	2.10	0.51
1:A:1973:ASP:OD1	1:A:1973:ASP:N	2.42	0.51
22:X:257:PHE:CE1	22:X:270:LEU:HB2	2.46	0.51
22:X:451:THR:HA	22:X:496:MET:O	2.10	0.51
22:X:483:PHE:HE1	22:X:917:GLN:HB2	1.76	0.51
34:1:972:GLY:O	34:1:976:VAL:HG12	2.10	0.51
34:1:1251:LEU:CG	36:2:497:SER:HB2	2.41	0.51
35:3:317:THR:HB	35:3:322:VAL:HA	1.92	0.51
35:3:819:MET:HA	35:3:822:GLU:OE1	2.10	0.51
35:3:940:LEU:HB3	35:3:941:HIS:ND1	2.26	0.51
35:3:1011:TRP:HB2	35:3:1025:ALA:O	2.11	0.51
1:A:767:VAL:HG21	2:B:39:C:O2'	2.11	0.50
4:E:60:MET:CB	4:E:353:MET:HB3	2.41	0.50
5:F:30:A:H61	6:G:16:G:H1'	1.76	0.50
5:F:45:A:C6	6:G:3:A:C5	2.99	0.50
10:L:192:ARG:NH1	10:L:198:ILE:HB	2.26	0.50
11:M:159:GLU:OE2	11:M:167:LEU:HB3	2.12	0.50
22:X:721:GLN:O	22:X:725:ARG:N	2.43	0.50
22:X:880:VAL:O	22:X:884:VAL:HG23	2.11	0.50
34:1:594:ARG:CA	34:1:634:VAL:HG11	2.30	0.50
34:1:594:ARG:C	34:1:634:VAL:HG13	2.32	0.50
34:1:702:ARG:CD	34:1:738:HIS:NE2	2.74	0.50
34:1:777:PHE:HD1	34:1:818:PHE:CE2	2.29	0.50
34:1:1266:TRP:HD1	39:5:24:ALA:HA	1.76	0.50
35:3:42:ARG:HB2	35:3:53:LEU:HD11	1.93	0.50
35:3:146:ARG:HB3	35:3:150:ALA:HA	1.93	0.50
36:2:452:LYS:HE3	36:2:456:ARG:HB2	1.93	0.50
1:A:1845:VAL:O	1:A:1849:ILE:HG12	2.11	0.50
3:C:343:LEU:HA	3:C:368:SER:OG	2.11	0.50
3:C:534:VAL:CG2	3:C:537:TYR:HB2	2.38	0.50
10:L:26:TYR:OH	10:L:158:ARG:NH1	2.36	0.50
12:N:139:CYS:SG	12:N:140:ARG:N	2.84	0.50
20:V:536:ILE:HG21	20:V:579:SER:OG	2.11	0.50
20:V:550:MET:O	20:V:554:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:601:GLN:HA	22:X:604:VAL:HG12	1.93	0.50
22:X:697:GLN:NE2	22:X:751:THR:OG1	2.42	0.50
22:X:810:THR:O	22:X:814:LYS:HG3	2.11	0.50
22:X:944:THR:HG23	22:X:1003:ILE:HD11	1.93	0.50
34:1:598:SER:C	34:1:638:ALA:HA	2.31	0.50
34:1:1125:PRO:HD2	34:1:1165:TYR:CZ	2.39	0.50
34:1:1205:GLU:OE1	35:3:1171:LYS:HD2	2.10	0.50
35:3:379:LEU:HD12	35:3:380:GLU:H	1.76	0.50
7:H:133:U:H2'	7:H:134:C:C6	2.46	0.50
22:X:430:THR:HG22	22:X:434:GLN:HE21	1.77	0.50
23:Y:217:ALA:O	23:Y:220:GLN:HG3	2.12	0.50
34:1:594:ARG:CD	34:1:674:LEU:HD22	2.40	0.50
34:1:872:ILE:HD12	34:1:892:LEU:HD11	1.93	0.50
35:3:706:MET:HG2	35:3:770:LEU:HD12	1.94	0.50
35:3:823:MET:SD	35:3:838:MET:HG3	2.52	0.50
1:A:1785:VAL:HG23	1:A:1786:TYR:CD2	2.47	0.50
7:H:151:C:H2'	7:H:152:G:H8	1.76	0.50
9:J:429:PHE:O	9:J:432:VAL:HG22	2.11	0.50
18:T:309:ASP:OD1	18:T:309:ASP:N	2.43	0.50
22:X:856:ARG:NH2	22:X:865:ASP:OD1	2.44	0.50
34:1:547:GLN:HA	34:1:550:HIS:HB3	1.92	0.50
34:1:597:ILE:O	34:1:638:ALA:HB1	2.12	0.50
34:1:602:LYS:HA	34:1:639:LEU:HD23	1.92	0.50
34:1:618:ASP:HA	34:1:660:ALA:HB2	1.92	0.50
34:1:906:GLU:N	34:1:906:GLU:OE1	2.44	0.50
35:3:2:PHE:C	35:3:3:LEU:HD23	2.32	0.50
35:3:326:ARG:NE	35:3:372:GLU:OE2	2.19	0.50
35:3:1031:ARG:HG2	35:3:1031:ARG:NH1	2.26	0.50
1:A:79:ARG:HB3	1:A:79:ARG:NH1	2.26	0.50
1:A:225:TYR:O	1:A:418:THR:HG21	2.11	0.50
1:A:916:LYS:HD2	1:A:1035:GLN:NE2	2.26	0.50
3:C:300:LEU:HD23	3:C:306:ASN:HB3	1.92	0.50
3:C:406:GLU:OE1	3:C:406:GLU:N	2.39	0.50
3:C:687:MET:HE2	3:C:791:ILE:HG12	1.93	0.50
11:M:218:PHE:CD1	11:M:218:PHE:C	2.85	0.50
18:T:497:GLU:OE1	18:T:497:GLU:N	2.33	0.50
34:1:583:ILE:CB	34:1:626:ASN:OD1	2.60	0.50
34:1:777:PHE:CD2	34:1:814:PHE:HA	2.47	0.50
34:1:1265:TYR:OH	36:2:500:VAL:HG13	2.12	0.50
35:3:238:VAL:HB	35:3:247:GLY:O	2.12	0.50
35:3:463:ARG:HD3	35:3:468:ASP:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:663:LEU:HD23	35:3:679:LEU:HB3	1.92	0.50
35:3:819:MET:HA	35:3:822:GLU:CD	2.31	0.50
1:A:216:SER:O	1:A:216:SER:OG	2.27	0.50
1:A:1712:HIS:ND1	1:A:1734:MET:HG3	2.26	0.50
7:H:152:G:H2'	7:H:153:A:C8	2.47	0.50
9:J:222:ASP:OD1	9:J:226:ARG:NH1	2.44	0.50
18:T:422:ASN:OD1	18:T:474:GLU:HB3	2.11	0.50
22:X:171:ARG:HH22	22:X:509:PRO:HD3	1.77	0.50
22:X:230:SER:O	22:X:234:TYR:HB2	2.11	0.50
23:Y:274:ASP:HB3	23:Y:277:THR:OG1	2.12	0.50
34:1:523:ALA:O	34:1:563:LEU:CD1	2.58	0.50
34:1:1266:TRP:CZ3	39:5:22:GLY:HA3	2.46	0.50
35:3:677:THR:HA	35:3:685:ASP:O	2.12	0.50
35:3:929:LYS:HG3	35:3:931:VAL:HG22	1.93	0.50
1:A:1207:PHE:HB2	1:A:1209:HIS:CD2	2.47	0.50
2:B:107:U:H2'	2:B:108:G:O4'	2.12	0.50
3:C:115:GLU:OE1	3:C:115:GLU:N	2.45	0.50
3:C:710:ASN:OD1	3:C:712:LYS:HB3	2.12	0.50
6:G:94:C:H2'	6:G:95:U:C6	2.47	0.50
8:I:386:ASP:O	8:I:388:PHE:N	2.44	0.50
10:L:63:TRP:HD1	10:L:67:GLU:HB3	1.77	0.50
10:L:632:ALA:O	10:L:636:LEU:N	2.40	0.50
16:R:235:ARG:NE	16:R:235:ARG:H	2.10	0.50
18:T:231:TRP:CZ3	18:T:238:LEU:HB2	2.46	0.50
22:X:834:TYR:CZ	22:X:941:LYS:HB3	2.47	0.50
34:1:581:LEU:O	34:1:584:ASP:HB3	2.12	0.50
34:1:1179:ASP:HB3	36:2:511:LEU:CB	2.35	0.50
34:1:1248:GLN:HE21	36:2:496:ASN:HB2	1.77	0.50
35:3:776:GLN:HG2	35:3:777:VAL:N	2.27	0.50
35:3:945:VAL:HG21	35:3:963:VAL:HG21	1.93	0.50
35:3:1207:LYS:O	35:3:1211:ILE:HG12	2.12	0.50
1:A:550:VAL:O	1:A:554:THR:HG23	2.12	0.50
3:C:300:LEU:HA	3:C:306:ASN:ND2	2.27	0.50
3:C:726:LEU:O	3:C:730:ARG:HG2	2.11	0.50
5:F:35:A:H8	6:G:12:G:O6	1.93	0.50
7:H:165:A:O2'	7:H:166:G:O4'	2.29	0.50
10:L:19:LEU:HD23	10:L:54:LEU:HD22	1.92	0.50
18:T:243:THR:O	18:T:243:THR:OG1	2.23	0.50
20:V:540:GLU:O	20:V:544:LEU:HB2	2.12	0.50
20:V:553:HIS:CD2	20:V:556:TYR:HE1	2.30	0.50
23:Y:37:TYR:O	23:Y:40:CYS:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:777:PHE:CG	34:1:818:PHE:HE2	2.29	0.50
34:1:1003:VAL:HG22	34:1:1004:ILE:N	2.27	0.50
34:1:1292:LYS:NZ	39:5:78:PRO:CG	2.66	0.50
35:3:642:ILE:H	35:3:703:ARG:NE	2.09	0.50
35:3:644:GLU:HG2	35:3:645:MET:N	2.25	0.50
35:3:1040:ASP:OD2	35:3:1042:ASP:N	2.45	0.50
35:3:1131:PRO:HB3	36:2:709:GLY:HA2	1.93	0.50
35:3:1187:PRO:O	35:3:1191:LYS:HG3	2.12	0.50
3:C:687:MET:HA	3:C:790:LYS:O	2.12	0.50
4:E:248:SER:HB2	4:E:263:ASP:OD2	2.12	0.50
18:T:213:GLU:HG2	18:T:214:PRO:N	2.26	0.50
22:X:612:LEU:HB2	22:X:686:ILE:HD12	1.93	0.50
23:Y:183:ARG:HA	23:Y:183:ARG:NE	2.26	0.50
34:1:1283:HIS:HE1	35:3:1168:PHE:CE1	2.30	0.50
35:3:616:ILE:O	35:3:628:LEU:N	2.45	0.50
38:7:52:GLY:N	38:7:55:GLN:HE21	2.10	0.50
1:A:93:LYS:O	1:A:649:GLU:HG2	2.11	0.49
1:A:1418:ARG:HB2	1:A:1462:GLY:HA3	1.94	0.49
1:A:1866:LYS:HG3	1:A:1886:GLY:HA3	1.94	0.49
4:E:105:LEU:HD21	4:E:136:TRP:CE2	2.47	0.49
4:E:243:LEU:HA	4:E:250:LEU:HA	1.93	0.49
20:V:217:ALA:HB2	20:V:357:LEU:HA	1.94	0.49
22:X:184:ARG:O	22:X:188:ARG:HG3	2.12	0.49
22:X:480:SER:HB3	22:X:500:MET:CE	2.42	0.49
22:X:715:SER:O	22:X:718:SER:OG	2.29	0.49
23:Y:298:PHE:HE2	23:Y:314:ASP:HA	1.76	0.49
23:Y:305:LEU:HD23	23:Y:305:LEU:H	1.77	0.49
35:3:115:ILE:CG2	39:5:19:ILE:HB	2.28	0.49
35:3:185:LEU:HD13	35:3:206:GLN:OE1	2.11	0.49
35:3:234:PHE:C	35:3:235:LEU:HD12	2.33	0.49
35:3:581:LYS:HB2	35:3:625:LEU:HD22	1.94	0.49
2:B:39:C:H4'	2:B:40:U:OP1	2.12	0.49
7:H:54:U:H2'	7:H:55:U:C6	2.47	0.49
8:I:433:ALA:HA	8:I:479:ARG:HA	1.94	0.49
9:J:238:ASN:C	9:J:240:THR:H	2.15	0.49
20:V:503:TYR:CD1	20:V:549:LYS:HD2	2.47	0.49
22:X:471:VAL:HG21	22:X:476:GLU:CD	2.33	0.49
34:1:803:ALA:HB1	34:1:807:LYS:HE3	1.93	0.49
35:3:757:ILE:HG22	35:3:762:LEU:HG	1.94	0.49
38:7:15:ALA:HB2	38:7:84:GLY:HA2	1.94	0.49
3:C:404:THR:O	3:C:408:LEU:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:536:ARG:O	3:C:536:ARG:HD3	2.12	0.49
3:C:832:TYR:CD2	3:C:899:SER:HB2	2.47	0.49
4:E:66:GLU:N	4:E:87:ASP:OD2	2.45	0.49
5:F:86:U:H5"	11:M:134:GLN:HE22	1.77	0.49
10:L:86:ALA:HB1	10:L:91:ARG:O	2.12	0.49
18:T:201:SER:HB3	18:T:485:THR:HG22	1.94	0.49
18:T:297:HIS:HA	18:T:338:CYS:SG	2.53	0.49
20:V:571:SER:OG	20:V:573:GLU:OE2	2.29	0.49
22:X:856:ARG:HD2	22:X:868:ARG:HH12	1.77	0.49
22:X:1007:TRP:HA	22:X:1010:GLU:HB2	1.94	0.49
34:1:777:PHE:HA	34:1:818:PHE:HE2	1.76	0.49
34:1:1279:ALA:CB	35:3:1167:TYR:CD1	2.92	0.49
1:A:1517:LYS:HG3	6:G:97:A:N7	2.27	0.49
1:A:1661:TRP:NE1	1:A:1697:SER:O	2.41	0.49
1:A:1874:VAL:O	1:A:1877:LEU:HG	2.13	0.49
5:F:49:G:N2	7:H:29:A:N7	2.61	0.49
9:J:320:GLU:OE1	9:J:325:ASN:HB3	2.13	0.49
10:L:162:THR:CG2	16:R:259:GLY:O	2.48	0.49
14:P:186:ARG:HH11	14:P:186:ARG:HB3	1.76	0.49
16:R:263:PRO:HB2	16:R:265:ASP:OD1	2.12	0.49
20:V:391:PHE:O	20:V:395:GLU:CB	2.61	0.49
20:V:596:LEU:N	20:V:597:PRO:HD2	2.27	0.49
22:X:171:ARG:CZ	22:X:509:PRO:HB3	2.43	0.49
22:X:419:ILE:HD11	22:X:560:PHE:HB3	1.95	0.49
23:Y:182:THR:OG1	23:Y:183:ARG:N	2.45	0.49
23:Y:211:ILE:O	23:Y:215:LYS:HG2	2.13	0.49
23:Y:290:LYS:HB3	23:Y:293:ASP:H	1.78	0.49
34:1:1125:PRO:CD	34:1:1165:TYR:CZ	2.95	0.49
1:A:1352:HIS:HD2	19:U:5:ILE:HG21	1.77	0.49
2:B:13:C:H2'	2:B:14:U:C6	2.48	0.49
3:C:132:VAL:HG11	3:C:226:VAL:HG23	1.93	0.49
3:C:474:LEU:HA	3:C:498:SER:O	2.11	0.49
3:C:750:LEU:HD22	19:U:67:GLU:HA	1.95	0.49
3:C:770:PHE:HE1	3:C:789:PHE:CD1	2.30	0.49
4:E:182:ARG:NE	4:E:182:ARG:HA	2.28	0.49
5:F:80:G:H22	9:J:209:PRO:HD3	1.78	0.49
9:J:189:ILE:HG22	9:J:189:ILE:O	2.12	0.49
9:J:330:ARG:CZ	9:J:361:ARG:HH12	2.26	0.49
11:M:155:LYS:HD2	11:M:156:HIS:NE2	2.27	0.49
34:1:663:THR:HA	34:1:666:LYS:CE	2.43	0.49
34:1:663:THR:HA	34:1:666:LYS:HE3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:884:ILE:CB	34:1:888:LEU:HD23	2.33	0.49
34:1:1076:ALA:O	34:1:1080:THR:HG23	2.12	0.49
34:1:1256:HIS:HA	36:2:488:LEU:HD11	1.94	0.49
35:3:469:GLU:HG2	35:3:470:PHE:CD1	2.47	0.49
35:3:757:ILE:HA	35:3:762:LEU:HA	1.94	0.49
35:3:1095:TYR:CE1	35:3:1164:ARG:HD2	2.48	0.49
36:2:462:VAL:O	36:2:466:LYS:HG3	2.12	0.49
38:7:42:LEU:HG	38:7:70:TYR:CE2	2.47	0.49
1:A:162:LYS:HE2	1:A:163:ARG:O	2.13	0.49
1:A:485:THR:HG22	1:A:486:LYS:N	2.27	0.49
3:C:480:LYS:HB2	3:C:493:PHE:HB3	1.93	0.49
3:C:514:TYR:OH	3:C:519:GLU:HG2	2.13	0.49
4:E:75:HIS:HB2	4:E:80:THR:H	1.78	0.49
6:G:109:U:H5”	22:X:454:ARG:HD3	1.93	0.49
9:J:185:ALA:HB2	10:L:141:PRO:O	2.13	0.49
13:O:259:ARG:N	13:O:273:GLN:O	2.39	0.49
16:R:104:GLN:HE21	16:R:225:PRO:HB3	1.77	0.49
18:T:460:ASP:OD2	18:T:460:ASP:N	2.45	0.49
22:X:743:TYR:O	22:X:747:LEU:HB2	2.12	0.49
22:X:828:ILE:O	22:X:831:SER:OG	2.29	0.49
22:X:972:PRO:HA	22:X:977:PHE:CD2	2.47	0.49
23:Y:104:HIS:CE1	23:Y:124:THR:HG1	2.29	0.49
34:1:754:ILE:HD13	34:1:754:ILE:N	2.27	0.49
34:1:862:GLU:HA	34:1:865:ARG:NH1	2.27	0.49
35:3:22:PHE:N	35:3:29:GLU:OE1	2.45	0.49
35:3:43:PRO:HB3	35:3:50:VAL:HG22	1.93	0.49
35:3:259:LYS:HE2	35:3:266:ASP:HB3	1.94	0.49
35:3:968:ARG:HG2	35:3:982:GLU:OE1	2.12	0.49
35:3:1165:SER:HB2	35:3:1169:PRO:HA	1.94	0.49
2:B:14:U:H2’	2:B:15:C:C6	2.46	0.49
3:C:447:PRO:HA	3:C:450:GLU:OE1	2.13	0.49
3:C:767:VAL:O	3:C:771:GLN:HG3	2.12	0.49
10:L:164:GLY:O	10:L:167:ALA:HB3	2.12	0.49
22:X:496:MET:HB2	22:X:500:MET:HB3	1.95	0.49
22:X:855:TYR:CE2	22:X:857:PRO:HG3	2.46	0.49
23:Y:89:LYS:HB3	23:Y:90:LYS:HD3	1.95	0.49
34:1:767:ARG:HA	34:1:805:TYR:OH	2.13	0.49
34:1:862:GLU:OE1	34:1:904:THR:OG1	2.30	0.49
34:1:963:LYS:O	34:1:963:LYS:HD2	2.12	0.49
35:3:18:ILE:HD12	35:3:67:ALA:HB2	1.95	0.49
35:3:168:TYR:OH	39:5:70:GLU:OE2	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:713:LEU:HD13	35:3:714:ALA:N	2.27	0.49
36:2:705:ARG:N	36:2:705:ARG:HD2	2.28	0.49
3:C:114:TYR:N	3:C:115:GLU:OE1	2.46	0.49
3:C:538:HIS:CE1	3:C:551:LEU:HD13	2.47	0.49
5:F:31:U:H3'	5:F:32:U:H6	1.76	0.49
6:G:107:U:OP2	22:X:618:GLN:NE2	2.46	0.49
9:J:286:GLU:HG3	9:J:298:ILE:HD12	1.94	0.49
11:M:142:ILE:HD12	11:M:143:LYS:H	1.78	0.49
14:P:184:VAL:HG21	23:Y:119:LEU:HD22	1.95	0.49
16:R:89:GLN:OE1	16:R:90:VAL:N	2.39	0.49
18:T:396:LYS:HD3	18:T:405:PHE:HE1	1.78	0.49
23:Y:77:PHE:O	23:Y:103:GLN:NE2	2.46	0.49
23:Y:246:LYS:CE	23:Y:312:HIS:HB2	2.38	0.49
34:1:523:ALA:HB1	34:1:563:LEU:CD1	2.43	0.49
34:1:898:TYR:CZ	34:1:902:GLU:HG2	2.47	0.49
34:1:970:LEU:O	34:1:974:LEU:HG	2.13	0.49
34:1:1148:LEU:HD13	34:1:1187:THR:HG22	1.87	0.49
35:3:346:PHE:HA	35:3:360:GLN:HA	1.95	0.49
35:3:603:ARG:HD2	35:3:603:ARG:O	2.13	0.49
1:A:226:GLN:HA	1:A:418:THR:HG22	1.94	0.49
1:A:643:GLY:HA3	2:B:28:A:O2'	2.13	0.49
1:A:1771:LEU:HD21	1:A:1779:PHE:CE2	2.47	0.49
1:A:1862:ILE:HG22	1:A:1885:LYS:HB3	1.95	0.49
4:E:145:LYS:HZ3	4:E:184:LYS:HG3	1.78	0.49
4:E:181:ILE:H	4:E:181:ILE:HD12	1.77	0.49
7:H:16:U:H6	7:H:16:U:OP1	1.96	0.49
10:L:48:ALA:O	10:L:52:GLU:HG2	2.12	0.49
16:R:369:LEU:HG	16:R:376:LYS:HG3	1.94	0.49
34:1:998:LYS:HZ1	34:1:1041:ARG:NH1	2.11	0.49
34:1:1217:PRO:HB2	36:2:510:TYR:CE1	2.43	0.49
35:3:253:GLU:CD	39:5:63:ARG:HH12	2.16	0.49
35:3:804:HIS:NE2	35:3:859:ASN:O	2.46	0.49
1:A:156:ARG:NH2	1:A:157:ASP:OD2	2.46	0.49
1:A:983:LYS:HE3	1:A:983:LYS:HB3	1.52	0.49
3:C:302:PRO:HB2	3:C:320:LEU:HG	1.94	0.49
4:E:75:HIS:CE1	4:E:121:GLY:HA3	2.47	0.49
6:G:11:A:H2'	6:G:12:G:O4'	2.12	0.49
9:J:286:GLU:HG3	9:J:298:ILE:CD1	2.43	0.49
9:J:399:TYR:O	9:J:403:VAL:HG23	2.13	0.49
16:R:123:GLU:HB3	16:R:125:MET:CE	2.43	0.49
18:T:220:VAL:HG13	18:T:252:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:424:ASP:OD1	18:T:424:ASP:N	2.46	0.49
20:V:473:ALA:O	20:V:477:LEU:HG	2.12	0.49
22:X:447:LYS:HB2	22:X:514:TYR:CD1	2.47	0.49
22:X:533:PHE:CE1	22:X:550:VAL:HG11	2.48	0.49
34:1:517:ARG:HB3	34:1:517:ARG:CZ	2.43	0.49
34:1:582:LEU:HD12	34:1:634:VAL:HG21	1.90	0.49
34:1:600:LEU:O	34:1:604:ALA:HB2	2.13	0.49
34:1:770:MET:HA	34:1:773:LEU:HG	1.95	0.49
35:3:316:GLU:O	35:3:323:THR:OG1	2.29	0.49
35:3:740:GLU:HB2	35:3:758:SER:HA	1.95	0.49
35:3:952:ILE:HG12	35:3:961:ILE:HG12	1.95	0.49
3:C:133:THR:OG1	3:C:222:SER:OG	2.30	0.48
3:C:476:CYS:SG	3:C:496:VAL:HG12	2.53	0.48
3:C:843:VAL:O	3:C:846:VAL:HG13	2.13	0.48
4:E:94:ASN:O	4:E:99:CYS:HA	2.13	0.48
4:E:337:PRO:HG2	4:E:338:ASP:OD2	2.12	0.48
16:R:189:ASN:HA	16:R:195:ARG:HH21	1.78	0.48
21:W:321:GLU:CB	36:2:667:ALA:HB3	2.43	0.48
22:X:281:ARG:HA	22:X:281:ARG:CZ	2.42	0.48
22:X:618:GLN:HG2	22:X:648:TYR:CG	2.48	0.48
22:X:648:TYR:CE2	22:X:651:LEU:HB3	2.48	0.48
23:Y:241:VAL:HG22	23:Y:287:GLU:HA	1.95	0.48
34:1:815:PHE:O	34:1:819:TRP:HB2	2.13	0.48
34:1:824:ALA:HB3	34:1:864:TYR:HD1	1.76	0.48
34:1:1283:HIS:CE1	35:3:1168:PHE:CZ	2.91	0.48
35:3:249:LEU:HA	35:3:257:THR:O	2.12	0.48
35:3:914:ILE:HD12	35:3:919:SER:HB3	1.95	0.48
35:3:1102:LEU:HD12	35:3:1102:LEU:HA	1.66	0.48
39:5:60:SER:O	39:5:63:ARG:N	2.46	0.48
1:A:1301:ILE:HD11	1:A:1306:LYS:HD3	1.96	0.48
3:C:325:LYS:HG2	3:C:329:ASP:OD2	2.14	0.48
3:C:471:ASP:H	3:C:499:GLY:HA2	1.78	0.48
3:C:618:THR:OG1	3:C:630:LEU:CB	2.51	0.48
3:C:724:TRP:HA	3:C:724:TRP:CE3	2.48	0.48
4:E:156:SER:HB2	4:E:199:VAL:HG12	1.95	0.48
5:F:77:C:H2'	5:F:78:A:O4'	2.13	0.48
7:H:56:A:O4'	36:2:504:TRP:CH2	2.65	0.48
7:H:64:A:H2'	7:H:65:U:C6	2.48	0.48
11:M:165:ASN:HB2	16:R:95:LYS:HA	1.95	0.48
16:R:408:ASP:OD1	16:R:409:GLN:N	2.46	0.48
22:X:768:LYS:HE3	22:X:802:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:495:ARG:CG	34:1:530:PRO:CB	2.31	0.48
34:1:497:ILE:HG23	34:1:526:PHE:CE1	2.33	0.48
34:1:569:PRO:HD2	34:1:570:TYR:CE2	2.48	0.48
34:1:632:PHE:O	34:1:635:VAL:HG22	2.13	0.48
35:3:70:LEU:HD13	35:3:146:ARG:HG2	1.95	0.48
35:3:503:THR:HG22	35:3:504:PRO:HD2	1.95	0.48
35:3:665:LEU:HD21	35:3:667:ILE:HD11	1.94	0.48
1:A:147:MET:O	1:A:151:MET:HG2	2.13	0.48
1:A:1786:TYR:HD1	1:A:1833:LEU:HB2	1.78	0.48
3:C:363:SER:O	3:C:364:SER:OG	2.28	0.48
3:C:764:ASP:OD2	3:C:764:ASP:N	2.45	0.48
4:E:162:ARG:HE	4:E:162:ARG:HB2	1.52	0.48
4:E:255:MET:HB2	4:E:282:HIS:CB	2.43	0.48
7:H:106:G:N3	7:H:107:A:C6	2.81	0.48
16:R:256:ASN:ND2	16:R:259:GLY:HA2	2.28	0.48
18:T:220:VAL:HG23	18:T:230:ILE:HG12	1.94	0.48
22:X:820:VAL:HG21	22:X:824:LEU:HD22	1.94	0.48
34:1:606:LEU:CD1	34:1:606:LEU:H	2.25	0.48
35:3:75:LYS:HE3	35:3:76:ASP:H	1.79	0.48
35:3:436:ARG:HD3	35:3:776:GLN:OE1	2.14	0.48
1:A:251:ASP:N	1:A:251:ASP:OD2	2.45	0.48
4:E:242:SER:O	4:E:293:TRP:NE1	2.45	0.48
8:I:479:ARG:O	8:I:483:SER:N	2.36	0.48
18:T:355:ARG:HH11	18:T:364:THR:HG21	1.78	0.48
22:X:527:LEU:HG	22:X:754:GLU:OE1	2.13	0.48
34:1:850:ILE:HG22	34:1:888:LEU:CG	2.38	0.48
35:3:388:GLN:NE2	35:3:845:GLU:OE1	2.46	0.48
35:3:484:VAL:O	35:3:485:LEU:HD12	2.13	0.48
1:A:111:GLU:OE2	1:A:114:ARG:NH2	2.41	0.48
1:A:205:ASP:OD2	1:A:205:ASP:N	2.43	0.48
1:A:525:LYS:HB2	1:A:525:LYS:HZ3	1.77	0.48
3:C:589:LYS:HD2	3:C:661:THR:HG22	1.96	0.48
3:C:746:VAL:O	3:C:791:ILE:HG13	2.13	0.48
4:E:105:LEU:HD21	4:E:136:TRP:CZ2	2.49	0.48
7:H:182:U:H2'	7:H:183:G:C8	2.48	0.48
9:J:230:THR:HA	9:J:233:ASP:OD2	2.13	0.48
12:N:21:THR:O	12:N:24:GLU:HG3	2.13	0.48
16:R:124:VAL:O	16:R:124:VAL:HG12	2.13	0.48
19:U:26:VAL:HG22	20:V:517:LEU:HD12	1.95	0.48
34:1:795:CYS:O	34:1:798:THR:HG23	2.14	0.48
34:1:1244:CYS:SG	35:3:1029:TYR:HD1	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:1299:GLU:O	34:1:1302:TYR:HD2	1.97	0.48
1:A:1792:LYS:HE2	1:A:1798:LEU:HG	1.95	0.48
3:C:230:ASP:OD2	3:C:259:LYS:HD2	2.13	0.48
3:C:719:GLN:NE2	3:C:726:LEU:HA	2.28	0.48
7:H:31:G:H2'	7:H:31:G:N3	2.28	0.48
7:H:139:C:H2'	7:H:140:A:H8	1.78	0.48
16:R:358:ASP:O	16:R:362:GLU:HB2	2.13	0.48
20:V:535:THR:HB	20:V:538:ARG:HG3	1.95	0.48
22:X:818:LEU:HD21	22:X:925:VAL:HG21	1.95	0.48
23:Y:133:MET:HA	23:Y:136:ILE:HB	1.96	0.48
35:3:181:MET:HB2	35:3:211:TYR:O	2.13	0.48
35:3:189:TYR:HB3	39:5:73:LEU:HD12	1.92	0.48
35:3:209:THR:OG1	35:3:210:PHE:N	2.45	0.48
35:3:407:ILE:HD11	35:3:1124:GLY:CA	2.44	0.48
39:5:51:ASN:OD1	39:5:51:ASN:N	2.46	0.48
1:A:105:ASN:O	1:A:489:TRP:NE1	2.46	0.48
1:A:835:ASP:HB3	1:A:878:LEU:HD13	1.95	0.48
1:A:1635:TYR:CE1	1:A:1636:LYS:HB2	2.49	0.48
1:A:1866:LYS:HE2	1:A:1886:GLY:H	1.79	0.48
3:C:820:PHE:HD1	3:C:821:LEU:HD23	1.77	0.48
4:E:328:GLY:O	4:E:346:SER:OG	2.31	0.48
10:L:164:GLY:N	10:L:167:ALA:HB3	2.28	0.48
14:P:186:ARG:HA	23:Y:49:PHE:CE1	2.49	0.48
22:X:461:VAL:O	22:X:465:VAL:HG23	2.14	0.48
22:X:461:VAL:HA	22:X:464:ARG:HE	1.78	0.48
22:X:618:GLN:HG2	22:X:648:TYR:CE2	2.48	0.48
34:1:558:ARG:NH1	35:3:217:LEU:HD21	2.24	0.48
34:1:563:LEU:HB2	34:1:567:VAL:HG13	1.95	0.48
35:3:22:PHE:HA	35:3:76:ASP:HB2	1.95	0.48
35:3:24:GLY:HA2	35:3:74:THR:O	2.14	0.48
35:3:302:LEU:HA	35:3:311:PHE:O	2.14	0.48
35:3:604:PHE:HA	35:3:618:SER:HA	1.96	0.48
1:A:1019:TYR:O	1:A:1020:LYS:C	2.52	0.48
1:A:1210:LYS:HD3	1:A:1210:LYS:N	2.29	0.48
1:A:1303:LEU:HD12	1:A:1311:PHE:HE1	1.78	0.48
1:A:1684:PHE:HD1	1:A:1702:LEU:HG	1.78	0.48
7:H:106:G:H1'	7:H:107:A:N7	2.29	0.48
7:H:107:A:C6	7:H:108:G:C6	3.02	0.48
10:L:19:LEU:HD23	10:L:54:LEU:CD2	2.44	0.48
10:L:201:LYS:HD2	10:L:202:ARG:N	2.28	0.48
13:O:155:PRO:N	16:R:188:PHE:HE1	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:235:ARG:HB3	16:R:235:ARG:CZ	2.43	0.48
23:Y:241:VAL:HA	23:Y:286:ILE:O	2.12	0.48
34:1:974:LEU:HG	34:1:974:LEU:H	1.46	0.48
34:1:1179:ASP:N	36:2:511:LEU:CD1	2.76	0.48
35:3:143:ILE:H	35:3:143:ILE:HD12	1.79	0.48
35:3:449:VAL:HG11	35:3:763:ARG:NH1	2.29	0.48
35:3:457:ASN:ND2	35:3:479:VAL:HG12	2.29	0.48
35:3:605:LEU:HD23	35:3:617:ILE:HG22	1.95	0.48
35:3:926:TYR:CZ	35:3:942:LYS:HD2	2.48	0.48
36:2:518:GLU:OE1	36:2:518:GLU:HA	2.14	0.48
37:4:102:ILE:C	37:4:177:ALA:HB2	2.33	0.48
1:A:1776:ILE:HD11	1:A:1778:TRP:NE1	2.29	0.48
1:A:1935:ARG:O	1:A:1939:ILE:HG13	2.14	0.48
5:F:13:G:H8	5:F:13:G:O5'	1.97	0.48
6:G:116:C:OP1	23:Y:309:ARG:HD3	2.14	0.48
10:L:774:VAL:O	10:L:778:GLN:N	2.46	0.48
12:N:132:ILE:O	12:N:140:ARG:HG3	2.13	0.48
20:V:606:GLU:HA	20:V:609:GLN:HG2	1.96	0.48
22:X:224:PRO:O	22:X:228:LYS:HD2	2.14	0.48
22:X:878:HIS:CE1	22:X:1001:LEU:HB2	2.48	0.48
34:1:914:PHE:O	34:1:918:VAL:HG23	2.14	0.48
34:1:1140:GLU:HB2	34:1:1143:VAL:CG1	2.44	0.48
34:1:1193:GLN:HE21	38:7:78:GLN:HE21	1.60	0.48
34:1:1287:ILE:HG23	36:2:490:HIS:CD2	2.49	0.48
35:3:415:LEU:HB2	35:3:424:TYR:CE2	2.49	0.48
35:3:664:TYR:CG	35:3:729:PHE:HZ	2.32	0.48
35:3:674:LEU:C	35:3:675:LEU:HD12	2.34	0.48
1:A:41:GLN:NE2	1:A:45:TYR:HB2	2.28	0.48
1:A:137:GLU:HG2	1:A:419:ARG:HD3	1.96	0.48
1:A:278:LYS:NZ	6:G:-8:C:OP1	2.47	0.48
1:A:384:VAL:HA	3:C:331:PHE:CD2	2.48	0.48
1:A:1664:ILE:HG13	1:A:1664:ILE:O	2.13	0.48
3:C:118:PHE:HA	3:C:121:ASP:OD2	2.14	0.48
3:C:592:VAL:O	3:C:593:GLU:HG2	2.14	0.48
3:C:826:ARG:NH1	3:C:911:PRO:HD2	2.29	0.48
3:C:918:ILE:HG23	3:C:924:GLN:NE2	2.29	0.48
7:H:176:G:H8	7:H:176:G:O5'	1.97	0.48
11:M:200:ARG:HD2	11:M:200:ARG:N	2.28	0.48
22:X:285:ALA:HA	22:X:288:GLU:OE2	2.13	0.48
22:X:503:ARG:O	22:X:506:LEU:HB3	2.14	0.48
22:X:835:SER:OG	22:X:835:SER:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:777:PHE:CZ	34:1:814:PHE:HB2	2.39	0.48
34:1:1251:LEU:CD1	36:2:497:SER:CB	2.75	0.48
35:3:839:ALA:O	35:3:843:LEU:HD12	2.14	0.48
37:4:103:PHE:N	37:4:177:ALA:HB2	2.29	0.48
1:A:845:ARG:NH1	1:A:1440:THR:HG22	2.29	0.47
3:C:181:ILE:O	3:C:206:PRO:HG3	2.14	0.47
3:C:192:ASP:CG	3:C:193:THR:N	2.67	0.47
10:L:206:ARG:HD2	10:L:206:ARG:O	2.13	0.47
11:M:222:ALA:HB1	16:R:266:LYS:HE3	1.96	0.47
14:P:186:ARG:NH1	14:P:186:ARG:HB2	2.28	0.47
20:V:471:GLU:OE1	20:V:475:LYS:NZ	2.33	0.47
22:X:166:ARG:HH22	22:X:773:HIS:CD2	2.31	0.47
22:X:234:TYR:CE1	23:Y:317:GLN:HB3	2.48	0.47
22:X:503:ARG:NH2	22:X:817:GLU:O	2.47	0.47
34:1:929:LEU:O	34:1:970:LEU:CD2	2.62	0.47
35:3:286:ILE:HD12	39:5:63:ARG:N	2.29	0.47
35:3:357:TYR:HE1	35:3:400:GLU:HG3	1.77	0.47
35:3:373:PHE:CE1	35:3:385:PHE:HB3	2.48	0.47
35:3:617:ILE:HG12	35:3:627:PRO:HA	1.95	0.47
38:7:47:ASP:HA	38:7:50:ASN:HB3	1.96	0.47
38:7:73:LYS:HA	38:7:76:THR:HG22	1.95	0.47
1:A:1352:HIS:HD1	19:U:21:ARG:HA	1.79	0.47
1:A:1491:LYS:HE3	1:A:1491:LYS:HB2	1.49	0.47
1:A:1838:LYS:HE2	1:A:1868:MET:CE	2.44	0.47
2:B:15:C:H2'	2:B:16:U:C6	2.49	0.47
4:E:308:PHE:CE1	4:E:324:PRO:HB3	2.49	0.47
34:1:570:TYR:HA	34:1:573:LYS:HD3	1.96	0.47
34:1:594:ARG:CD	34:1:674:LEU:HD11	2.27	0.47
34:1:823:MET:O	34:1:829:ASN:HB2	2.14	0.47
35:3:19:HIS:ND1	35:3:19:HIS:O	2.46	0.47
35:3:169:HIS:HD2	35:3:170:VAL:N	2.09	0.47
35:3:563:LEU:O	35:3:580:ARG:HB3	2.14	0.47
35:3:945:VAL:HG23	35:3:968:ARG:HH12	1.80	0.47
1:A:123:THR:O	1:A:123:THR:OG1	2.30	0.47
1:A:1953:ILE:O	1:A:1956:PRO:HD3	2.13	0.47
3:C:116:MET:HA	3:C:119:LEU:HD12	1.95	0.47
7:H:6:U:H2'	7:H:7:U:C6	2.48	0.47
10:L:204:ARG:HE	10:L:207:GLY:HA3	1.78	0.47
11:M:222:ALA:CB	16:R:266:LYS:HE3	2.44	0.47
13:O:233:THR:O	13:O:303:GLY:N	2.41	0.47
14:P:184:VAL:HG13	14:P:184:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:493:ASP:OD1	18:T:493:ASP:N	2.34	0.47
20:V:549:LYS:O	20:V:549:LYS:HD3	2.13	0.47
22:X:698:LYS:HZ1	22:X:758:THR:HA	1.79	0.47
34:1:582:LEU:HA	34:1:590:ARG:HA	1.97	0.47
35:3:592:LEU:HD11	35:3:619:LEU:HD11	1.97	0.47
35:3:642:ILE:H	35:3:703:ARG:HH21	1.61	0.47
1:A:1211:ASP:C	1:A:1213:VAL:H	2.18	0.47
1:A:1391:LEU:O	1:A:1394:GLN:HG3	2.13	0.47
1:A:1630:LEU:HA	1:A:1660:TYR:O	2.14	0.47
3:C:153:THR:O	3:C:155:PRO:HD3	2.14	0.47
3:C:352:LYS:HE2	3:C:352:LYS:H	1.80	0.47
3:C:441:PRO:HA	3:C:444:GLY:HA3	1.96	0.47
3:C:737:PRO:HD3	3:C:743:ASN:HD22	1.80	0.47
4:E:124:LEU:O	4:E:135:VAL:HA	2.14	0.47
6:G:97:A:H8	6:G:97:A:H2'	1.59	0.47
9:J:189:ILE:HD12	10:L:140:ASP:OD2	2.13	0.47
10:L:764:PRO:O	10:L:768:GLU:N	2.41	0.47
20:V:497:CYS:HB3	20:V:507:PHE:CB	2.43	0.47
23:Y:27:ASN:OD1	23:Y:66:ILE:N	2.36	0.47
34:1:529:GLY:HA2	34:1:570:TYR:CZ	2.49	0.47
34:1:666:LYS:HB3	34:1:704:ILE:HD13	1.96	0.47
34:1:1255:PHE:HE1	39:5:26:THR:O	1.97	0.47
35:3:347:LEU:CD2	35:3:359:TYR:HB2	2.44	0.47
35:3:594:ASN:OD1	35:3:594:ASN:N	2.46	0.47
38:7:58:CYS:HB3	38:7:62:GLY:H	1.79	0.47
39:5:13:HIS:ND1	39:5:17:LYS:HE3	2.30	0.47
1:A:171:ASP:O	1:A:520:TYR:HB2	2.14	0.47
1:A:179:ALA:HA	1:A:183:LEU:HB2	1.96	0.47
1:A:1779:PHE:CG	1:A:1862:ILE:HD11	2.50	0.47
4:E:60:MET:HB3	4:E:353:MET:HB3	1.96	0.47
5:F:49:G:H2'	5:F:50:A:C8	2.47	0.47
6:G:106:C:N3	22:X:851:ASN:ND2	2.63	0.47
7:H:171:U:N3	7:H:172:C:C4	2.83	0.47
12:N:44:GLU:HB2	12:N:47:TRP:CE3	2.49	0.47
16:R:235:ARG:H	16:R:235:ARG:HE	1.62	0.47
18:T:213:GLU:HG2	18:T:214:PRO:HD2	1.97	0.47
18:T:295:ASP:OD1	18:T:296:LEU:N	2.40	0.47
20:V:556:TYR:HB2	20:V:594:MET:SD	2.53	0.47
34:1:684:ARG:CZ	34:1:723:SER:HB2	2.44	0.47
34:1:1070:LYS:HE3	34:1:1070:LYS:HB2	1.72	0.47
34:1:1158:ILE:HG22	34:1:1161:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:168:TYR:OH	35:3:187:MET:SD	2.63	0.47
35:3:442:LEU:HD23	35:3:442:LEU:HA	1.71	0.47
35:3:679:LEU:HD22	35:3:679:LEU:HA	1.78	0.47
35:3:1015:LYS:HZ2	35:3:1016:ARG:N	2.12	0.47
1:A:182:ILE:HD11	1:A:562:VAL:HG13	1.95	0.47
1:A:464:PRO:O	1:A:466:ALA:N	2.47	0.47
1:A:762:ARG:HA	1:A:902:TYR:O	2.15	0.47
1:A:1624:SER:OG	1:A:1625:SER:N	2.47	0.47
3:C:496:VAL:HG23	3:C:546:ALA:HA	1.97	0.47
3:C:667:VAL:HG13	3:C:826:ARG:HG3	1.97	0.47
4:E:150:HIS:HA	4:E:177:LYS:NZ	2.29	0.47
10:L:633:GLN:O	10:L:637:VAL:N	2.46	0.47
20:V:577:SER:O	20:V:581:ILE:HG12	2.14	0.47
22:X:291:LYS:O	22:X:295:THR:HG22	2.15	0.47
22:X:597:VAL:HA	22:X:600:LEU:HD12	1.97	0.47
22:X:618:GLN:HA	22:X:648:TYR:CE1	2.50	0.47
23:Y:44:ASN:OD1	23:Y:52:GLN:HB3	2.13	0.47
23:Y:212:LYS:O	23:Y:216:GLU:HG3	2.15	0.47
34:1:949:GLN:HA	34:1:989:VAL:HG11	1.93	0.47
35:3:169:HIS:CD2	35:3:170:VAL:N	2.82	0.47
35:3:636:GLN:HG2	35:3:637:PRO:HD2	1.96	0.47
35:3:665:LEU:CB	35:3:679:LEU:HD23	2.45	0.47
35:3:700:LYS:HB3	35:3:702:PHE:HZ	1.74	0.47
35:3:1125:GLY:C	35:3:1126:ILE:HG13	2.35	0.47
1:A:608:LEU:HD13	1:A:632:ALA:HB1	1.96	0.47
1:A:697:MET:N	1:A:698:PRO:HD3	2.29	0.47
1:A:833:LYS:O	1:A:833:LYS:HD3	2.14	0.47
1:A:1852:LEU:HD23	1:A:1857:GLN:HA	1.97	0.47
1:A:1919:LEU:N	1:A:1919:LEU:HD23	2.29	0.47
3:C:320:LEU:HD11	3:C:344:TRP:HB2	1.96	0.47
3:C:801:LEU:HD13	3:C:802:HIS:NE2	2.30	0.47
4:E:131:LYS:HA	4:E:152:SER:O	2.15	0.47
4:E:343:ILE:HA	4:E:352:TYR:O	2.14	0.47
6:G:88:G:O2'	6:G:89:U:H5'	2.15	0.47
8:I:564:PHE:O	8:I:568:TYR:N	2.44	0.47
10:L:98:GLU:O	10:L:101:GLU:HG3	2.15	0.47
11:M:165:ASN:ND2	16:R:95:LYS:HE2	2.28	0.47
22:X:702:PRO:HG2	22:X:788:THR:HB	1.96	0.47
22:X:718:SER:OG	22:X:719:ALA:N	2.47	0.47
22:X:811:SER:HA	22:X:814:LYS:HZ2	1.80	0.47
22:X:824:LEU:O	22:X:828:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:911:ALA:HA	22:X:914:VAL:HG22	1.97	0.47
22:X:970:ILE:HD12	22:X:977:PHE:O	2.14	0.47
23:Y:65:SER:N	23:Y:76:SER:O	2.27	0.47
34:1:908:SER:OG	34:1:912:ASN:OD1	2.28	0.47
34:1:1178:MET:CA	36:2:511:LEU:HD13	2.37	0.47
34:1:1205:GLU:CD	35:3:1171:LYS:HD2	2.35	0.47
34:1:1243:PRO:CG	35:3:1167:TYR:O	2.63	0.47
35:3:569:ASP:O	35:3:572:GLY:N	2.45	0.47
35:3:612:ASN:HA	35:3:636:GLN:HA	1.95	0.47
35:3:1041:TYR:CG	36:2:705:ARG:HG3	2.46	0.47
1:A:376:GLU:H	1:A:376:GLU:HG3	1.50	0.47
1:A:693:ILE:HB	1:A:738:MET:SD	2.55	0.47
1:A:1413:ASP:O	1:A:1414:ARG:HG3	2.14	0.47
1:A:1836:LEU:HA	1:A:1839:TRP:HD1	1.79	0.47
1:A:1901:LYS:NZ	1:A:1967:ILE:HA	2.30	0.47
1:A:1998:ASN:OD1	1:A:2001:SER:N	2.48	0.47
3:C:311:SER:HB2	3:C:316:ILE:HG23	1.96	0.47
3:C:804:GLY:O	3:C:808:ILE:HG12	2.15	0.47
4:E:241:LEU:HA	4:E:251:LEU:O	2.14	0.47
4:E:259:VAL:HG22	4:E:277:PHE:HB2	1.97	0.47
6:G:88:G:N1	7:H:41:U:N3	2.46	0.47
11:M:121:ASP:OD2	11:M:122:LEU:N	2.47	0.47
16:R:434:ASP:OD2	16:R:434:ASP:N	2.48	0.47
22:X:183:GLU:HA	22:X:186:ARG:HD2	1.96	0.47
22:X:842:THR:O	22:X:846:MET:HG2	2.15	0.47
34:1:860:GLU:O	34:1:865:ARG:NH2	2.48	0.47
34:1:929:LEU:N	34:1:930:PRO:HD2	2.30	0.47
34:1:1295:TYR:OH	39:5:29:TRP:HD1	1.98	0.47
34:1:1300:LEU:HD13	35:3:1032:TRP:CZ3	2.43	0.47
35:3:35:GLY:HA3	39:5:47:PHE:HZ	1.79	0.47
35:3:484:VAL:C	35:3:485:LEU:HD12	2.34	0.47
35:3:558:LEU:HG	35:3:559:THR:N	2.30	0.47
35:3:864:SER:O	35:3:865:VAL:HG23	2.15	0.47
35:3:867:ARG:NH1	35:3:879:LEU:HD13	2.30	0.47
38:7:12:ARG:NH1	38:7:84:GLY:O	2.48	0.47
1:A:682:ASP:O	1:A:686:ARG:HG2	2.14	0.47
1:A:1090:ARG:HG2	1:A:1091:TYR:O	2.15	0.47
3:C:200:PHE:HE1	3:C:434:CYS:SG	2.37	0.47
3:C:219:LEU:HD23	3:C:219:LEU:HA	1.68	0.47
3:C:350:ASN:HD22	3:C:353:THR:H	1.63	0.47
4:E:161:ARG:HH12	4:E:203:ASP:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:325:ASN:HB2	11:M:172:HIS:HD2	1.80	0.47
14:P:53:GLU:HB3	14:P:57:ARG:HH12	1.80	0.47
22:X:267:ARG:O	22:X:271:LYS:HD3	2.14	0.47
22:X:606:GLN:HG3	22:X:688:TYR:CE1	2.50	0.47
34:1:568:ARG:HG3	34:1:568:ARG:HH11	1.80	0.47
34:1:770:MET:O	34:1:774:ILE:HG12	2.14	0.47
34:1:826:ASP:OD1	34:1:828:ARG:N	2.42	0.47
35:3:304:GLN:HE21	35:3:308:GLY:HA2	1.80	0.47
35:3:477:SER:HA	35:3:482:THR:HG23	1.95	0.47
36:2:466:LYS:HG2	36:2:475:VAL:HG21	1.97	0.47
1:A:874:PRO:CG	22:X:866:ASN:HD21	2.28	0.47
3:C:239:THR:O	3:C:243:ILE:HG23	2.14	0.47
3:C:284:GLU:O	3:C:288:LEU:HG	2.14	0.47
3:C:702:ASN:HB2	3:C:704:VAL:HG23	1.95	0.47
4:E:345:ALA:HA	4:E:351:LEU:HD23	1.96	0.47
5:F:3:G:H2'	5:F:4:C:C6	2.50	0.47
20:V:479:MET:HE3	20:V:479:MET:HB3	1.84	0.47
22:X:189:ASP:O	22:X:193:THR:HG22	2.15	0.47
22:X:871:PHE:HZ	22:X:901:ASN:HB3	1.80	0.47
34:1:647:PHE:O	34:1:651:VAL:HG13	2.15	0.47
34:1:1178:MET:HG2	36:2:591:TYR:CE1	2.49	0.47
35:3:272:PRO:HD3	35:3:327:LEU:HD13	1.97	0.47
35:3:1181:GLN:O	35:3:1185:MET:HG3	2.14	0.47
35:3:1204:VAL:HG23	35:3:1205:SER:N	2.30	0.47
1:A:1000:ILE:HD12	1:A:1000:ILE:HA	1.59	0.46
1:A:1943:LEU:HD12	1:A:1950:ALA:HB1	1.97	0.46
3:C:668:GLU:HG3	3:C:824:THR:HG21	1.97	0.46
3:C:693:GLU:OE1	3:C:695:GLY:N	2.38	0.46
12:N:1:MET:N	12:N:2:PRO:HD2	2.30	0.46
12:N:117:CYS:SG	12:N:136:HIS:ND1	2.87	0.46
13:O:167:PHE:O	13:O:171:GLY:N	2.48	0.46
18:T:221:THR:OG1	18:T:231:TRP:NE1	2.46	0.46
20:V:562:TRP:CE2	20:V:602:ARG:HD3	2.50	0.46
22:X:591:TYR:HB2	22:X:737:LEU:HD23	1.97	0.46
34:1:554:LYS:HD2	34:1:558:ARG:HE	1.80	0.46
34:1:1216:TRP:HD1	36:2:590:LEU:CD1	2.26	0.46
34:1:1243:PRO:HD2	35:3:1167:TYR:O	2.10	0.46
34:1:1279:ALA:O	34:1:1281:ILE:N	2.48	0.46
35:3:524:ILE:O	35:3:535:GLU:HA	2.15	0.46
35:3:1085:ALA:HB3	35:3:1088:LYS:HE2	1.97	0.46
39:5:69:MET:HE2	39:5:69:MET:HB2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:HD22	4:E:214:ASP:HA	1.97	0.46
1:A:296:PHE:O	1:A:302:ILE:HD11	2.14	0.46
1:A:362:ARG:HH22	20:V:320:ARG:HA	1.80	0.46
1:A:497:CYS:SG	1:A:558:VAL:HG11	2.55	0.46
2:B:21:A:H2'	2:B:21:A:N3	2.31	0.46
3:C:137:HIS:CG	3:C:138:LEU:H	2.33	0.46
3:C:243:ILE:O	3:C:247:VAL:HG13	2.15	0.46
3:C:514:TYR:CD1	3:C:514:TYR:C	2.89	0.46
3:C:514:TYR:C	3:C:514:TYR:HD1	2.19	0.46
4:E:124:LEU:HD21	4:E:138:SER:HB3	1.97	0.46
4:E:137:ASP:HB2	4:E:140:THR:OG1	2.14	0.46
5:F:29:A:H2'	5:F:30:A:O4'	2.14	0.46
5:F:86:U:H5"	11:M:134:GLN:NE2	2.30	0.46
11:M:125:SER:HA	16:R:242:GLN:OE1	2.14	0.46
18:T:315:TRP:CZ3	18:T:322:SER:HB2	2.51	0.46
18:T:393:ASP:OD2	18:T:393:ASP:N	2.40	0.46
20:V:540:GLU:HG3	20:V:541:THR:N	2.28	0.46
34:1:898:TYR:HA	34:1:901:GLN:OE1	2.15	0.46
34:1:1248:GLN:O	36:2:498:VAL:N	2.47	0.46
35:3:1131:PRO:HG3	36:2:709:GLY:HA2	1.96	0.46
35:3:1158:ARG:HG3	35:3:1159:ASP:H	1.79	0.46
38:7:13:LYS:HD2	38:7:48:GLU:OE2	2.15	0.46
1:A:362:ARG:HD3	1:A:362:ARG:HA	1.69	0.46
1:A:781:ARG:O	1:A:785:LYS:HG3	2.14	0.46
1:A:1019:TYR:CG	1:A:1020:LYS:N	2.83	0.46
3:C:749:THR:O	3:C:753:GLU:HB2	2.16	0.46
3:C:916:ILE:HG21	3:C:928:HIS:HB3	1.97	0.46
7:H:18:U:C5	11:M:218:PHE:CE2	3.02	0.46
7:H:173:C:H2'	7:H:174:A:H8	1.76	0.46
12:N:38:GLU:CD	12:N:38:GLU:H	2.18	0.46
21:W:579:ASP:C	36:2:623:PRO:CB	2.83	0.46
22:X:941:LYS:HE2	22:X:1007:TRP:NE1	2.31	0.46
22:X:998:ARG:O	22:X:999:GLN:HG2	2.16	0.46
23:Y:21:ARG:NH1	23:Y:83:VAL:O	2.48	0.46
34:1:625:ARG:HH21	34:1:662:HIS:HB3	1.79	0.46
34:1:962:MET:CE	34:1:974:LEU:CD1	2.94	0.46
34:1:1178:MET:CG	36:2:591:TYR:CE2	2.96	0.46
35:3:69:ARG:HG3	35:3:75:LYS:O	2.15	0.46
35:3:232:GLY:HA3	35:3:252:SER:HA	1.97	0.46
35:3:334:PRO:HB3	35:3:432:ARG:NH1	2.30	0.46
35:3:511:LEU:HD21	35:3:517:VAL:CG2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:565:TYR:HE1	35:3:619:LEU:HD12	1.80	0.46
1:A:468:LYS:HA	1:A:468:LYS:HZ2	1.80	0.46
1:A:1091:TYR:O	1:A:1092:ILE:C	2.52	0.46
1:A:1799:THR:O	1:A:1801:LYS:NZ	2.42	0.46
3:C:622:GLU:O	3:C:625:GLY:N	2.41	0.46
5:F:41:A:H2	6:G:6:A:N1	2.13	0.46
12:N:25:LEU:HD23	12:N:25:LEU:HA	1.70	0.46
20:V:594:MET:O	20:V:598:LYS:HE3	2.15	0.46
22:X:172:LEU:HD12	22:X:173:GLN:N	2.31	0.46
34:1:871:THR:O	34:1:875:ILE:HG13	2.15	0.46
34:1:1167:TYR:CE2	36:2:581:LYS:CA	2.82	0.46
34:1:1233:ALA:O	34:1:1237:LEU:HB2	2.15	0.46
35:3:226:GLU:HB3	35:3:261:PHE:CE2	2.51	0.46
35:3:601:ARG:HD3	35:3:620:ASP:HB3	1.98	0.46
35:3:1210:ASP:HA	35:3:1213:THR:OG1	2.15	0.46
36:2:450:SER:HB2	36:2:453:LYS:HD3	1.98	0.46
1:A:81:PHE:C	1:A:83:HIS:H	2.19	0.46
1:A:371:LEU:HD22	1:A:371:LEU:HA	1.74	0.46
3:C:281:ILE:O	3:C:285:VAL:HG12	2.15	0.46
9:J:191:ALA:O	9:J:194:LEU:N	2.49	0.46
9:J:199:LYS:O	9:J:199:LYS:NZ	2.46	0.46
9:J:297:ASN:OD1	10:L:225:TYR:HB2	2.15	0.46
9:J:325:ASN:HB2	11:M:172:HIS:CD2	2.51	0.46
22:X:249:GLU:CB	22:X:273:LYS:HE2	2.45	0.46
22:X:663:THR:HG23	22:X:669:LYS:HB2	1.98	0.46
22:X:818:LEU:HD12	22:X:825:SER:OG	2.15	0.46
34:1:573:LYS:O	34:1:577:VAL:HG23	2.15	0.46
34:1:778:GLN:HG3	34:1:817:HIS:CB	2.36	0.46
34:1:830:TYR:CG	34:1:867:MET:HG3	2.51	0.46
34:1:864:TYR:O	34:1:868:VAL:HG13	2.15	0.46
34:1:869:MET:O	34:1:873:GLU:HB3	2.15	0.46
34:1:1244:CYS:HB3	35:3:1029:TYR:CD1	2.51	0.46
34:1:1292:LYS:HZ3	39:5:78:PRO:HG2	1.75	0.46
35:3:233:ASN:ND2	35:3:233:ASN:N	2.59	0.46
35:3:1199:ARG:HH21	35:3:1207:LYS:HD3	1.80	0.46
38:7:12:ARG:HD2	38:7:12:ARG:HA	1.67	0.46
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.70	0.46
1:A:1382:SER:HA	1:A:1415:GLY:HA2	1.96	0.46
1:A:1629:ILE:O	1:A:1661:TRP:HA	2.15	0.46
3:C:532:ILE:HB	3:C:539:ILE:HD11	1.97	0.46
3:C:841:ASP:OD1	3:C:842:CYS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:166:G:N3	7:H:166:G:H2'	2.30	0.46
11:M:175:SER:N	11:M:178:GLU:OE2	2.49	0.46
14:P:186:ARG:HH11	14:P:186:ARG:HB2	1.77	0.46
22:X:474:GLY:HA2	22:X:486:CYS:O	2.15	0.46
34:1:848:GLU:O	34:1:852:ARG:HG3	2.15	0.46
35:3:114:ARG:CZ	39:5:37:ARG:CB	2.93	0.46
35:3:451:GLU:HG3	35:3:760:ASN:O	2.16	0.46
35:3:592:LEU:HA	35:3:592:LEU:HD13	1.64	0.46
1:A:1275:ARG:O	1:A:1369:TYR:HE1	1.99	0.46
2:B:8:G:N2	2:B:70:A:H1'	2.26	0.46
3:C:283:ASP:OD2	3:C:284:GLU:N	2.48	0.46
4:E:143:ARG:CZ	4:E:146:ARG:HE	2.28	0.46
5:F:23:U:H2'	5:F:24:A:O4'	2.15	0.46
9:J:199:LYS:HA	9:J:199:LYS:CE	2.29	0.46
11:M:214:ARG:HB3	16:R:260:TYR:OH	2.14	0.46
14:P:205:LYS:CB	14:P:208:LYS:HB3	2.46	0.46
16:R:251:ILE:O	16:R:251:ILE:HG12	2.15	0.46
18:T:412:HIS:ND1	18:T:429:SER:OG	2.47	0.46
20:V:609:GLN:HE21	20:V:612:PHE:HD2	1.64	0.46
20:V:618:ARG:HB3	20:V:646:HIS:CE1	2.50	0.46
22:X:257:PHE:CZ	22:X:266:GLU:HG3	2.50	0.46
34:1:884:ILE:CD1	34:1:889:GLU:CB	2.88	0.46
34:1:1135:GLU:HG3	34:1:1135:GLU:O	2.15	0.46
34:1:1277:GLN:NE2	34:1:1277:GLN:O	2.48	0.46
35:3:642:ILE:H	35:3:703:ARG:NH2	2.14	0.46
39:5:8:HIS:HA	39:5:11:LEU:HB2	1.97	0.46
1:A:1638:ASN:O	1:A:1652:MET:HB3	2.15	0.46
1:A:1660:TYR:CE1	1:A:1699:THR:HG22	2.51	0.46
3:C:604:LEU:HD21	3:C:627:HIS:HE1	1.80	0.46
3:C:710:ASN:O	3:C:714:LEU:HD13	2.16	0.46
4:E:62:LEU:HD21	4:E:99:CYS:HB2	1.98	0.46
7:H:56:A:N6	36:2:505:CYS:CB	2.78	0.46
16:R:328:ALA:CB	23:Y:226:MET:HA	2.46	0.46
22:X:953:ARG:HB3	22:X:983:TRP:CZ3	2.51	0.46
34:1:606:LEU:HG	34:1:639:LEU:HD11	1.81	0.46
34:1:702:ARG:HG2	34:1:738:HIS:CD2	2.51	0.46
34:1:1027:ARG:HD3	34:1:1027:ARG:HA	1.82	0.46
35:3:147:ASP:OD2	35:3:151:ARG:HG2	2.16	0.46
35:3:159:GLU:CD	35:3:161:HIS:H	2.19	0.46
35:3:817:GLN:HG3	35:3:818:GLN:OE1	2.15	0.46
35:3:1034:THR:HG22	35:3:1049:LYS:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ILE:O	1:A:191:ILE:HG22	2.16	0.46
1:A:361:HIS:HD1	1:A:361:HIS:N	2.14	0.46
1:A:1199:LYS:HE2	1:A:1206:GLU:HG3	1.97	0.46
3:C:465:MET:O	3:C:468:CYS:N	2.46	0.46
4:E:147:LEU:HD23	4:E:147:LEU:HA	1.72	0.46
5:F:38:G:OP2	5:F:38:G:H8	1.99	0.46
6:G:9:C:O2'	6:G:10:U:O4'	2.25	0.46
16:R:91:ASP:HA	16:R:97:LYS:NZ	2.31	0.46
22:X:487:THR:HG21	22:X:494:ARG:HD2	1.98	0.46
22:X:520:ASP:HB3	22:X:521:GLU:OE1	2.16	0.46
22:X:640:ARG:HG3	22:X:640:ARG:NH1	2.30	0.46
34:1:516:LEU:HD12	34:1:516:LEU:HA	1.69	0.46
34:1:586:ASP:O	34:1:590:ARG:HG3	2.16	0.46
34:1:907:ASP:OD2	34:1:909:VAL:HB	2.16	0.46
34:1:1000:ILE:O	34:1:1003:VAL:HG13	2.16	0.46
34:1:1015:ASP:OD1	34:1:1015:ASP:N	2.49	0.46
34:1:1135:GLU:O	34:1:1138:VAL:HG12	2.16	0.46
34:1:1195:MET:O	34:1:1199:VAL:HG23	2.16	0.46
34:1:1216:TRP:O	34:1:1219:VAL:HB	2.16	0.46
35:3:184:CYS:SG	35:3:211:TYR:HE1	2.39	0.46
35:3:565:TYR:CE1	35:3:619:LEU:HD12	2.51	0.46
35:3:910:ALA:CB	35:3:913:LEU:HD11	2.45	0.46
36:2:548:THR:C	36:2:550:LYS:N	2.70	0.46
1:A:1868:MET:O	1:A:1871:PRO:HD2	2.15	0.46
1:A:1870:ASP:HA	1:A:1873:GLU:OE1	2.16	0.46
3:C:673:LYS:NZ	19:U:57:ILE:HA	2.31	0.46
3:C:921:LEU:HD23	3:C:921:LEU:HA	1.78	0.46
4:E:117:TYR:CD1	4:E:121:GLY:HA2	2.51	0.46
5:F:31:U:H3'	5:F:32:U:C6	2.51	0.46
6:G:86:A:H2'	6:G:87:U:C6	2.51	0.46
7:H:51:A:H2'	7:H:52:G:O4'	2.15	0.46
9:J:537:TRP:O	9:J:541:ALA:N	2.48	0.46
10:L:94:ALA:O	10:L:98:GLU:HG3	2.16	0.46
11:M:217:LYS:HZ2	11:M:224:ARG:HH12	1.63	0.46
12:N:15:TRP:NE1	12:N:19:GLU:OE1	2.49	0.46
12:N:122:PRO:HB2	12:N:125:LYS:HD3	1.98	0.46
16:R:382:ARG:NH2	16:R:385:ASN:HB2	2.31	0.46
23:Y:73:ASP:OD1	23:Y:73:ASP:N	2.48	0.46
34:1:497:ILE:CG2	34:1:526:PHE:HE1	2.21	0.46
34:1:1178:MET:CG	36:2:514:LYS:NZ	2.79	0.46
34:1:1279:ALA:HB1	35:3:1167:TYR:CA	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:93:GLN:O	35:3:97:ASN:N	2.49	0.46
35:3:676:ARG:HD2	35:3:729:PHE:CD2	2.51	0.46
35:3:809:GLU:O	35:3:812:LYS:HB2	2.15	0.46
1:A:67:ARG:HE	1:A:67:ARG:HB2	1.47	0.45
1:A:198:GLU:HG2	1:A:199:GLU:H	1.82	0.45
1:A:468:LYS:NZ	1:A:469:LYS:H	2.14	0.45
1:A:1361:GLU:HG3	1:A:1362:ASP:OD2	2.17	0.45
1:A:1391:LEU:O	1:A:1395:GLU:HG2	2.16	0.45
1:A:1552:GLN:OE1	1:A:1563:HIS:NE2	2.48	0.45
1:A:1892:PRO:HG2	1:A:1940:LEU:CB	2.45	0.45
3:C:350:ASN:HD21	3:C:352:LYS:HB2	1.80	0.45
3:C:510:LEU:HB3	3:C:576:ILE:HG22	1.98	0.45
3:C:711:ARG:HB3	3:C:730:ARG:NH2	2.31	0.45
4:E:118:ASN:ND2	4:E:122:SER:H	2.10	0.45
10:L:223:GLY:HA2	16:R:86:LEU:HD21	1.98	0.45
20:V:562:TRP:CD2	20:V:602:ARG:HD3	2.51	0.45
22:X:228:LYS:HA	22:X:231:ARG:HD3	1.99	0.45
22:X:576:ARG:HB3	22:X:577:PHE:CD2	2.51	0.45
22:X:624:ALA:O	22:X:628:LEU:HG	2.16	0.45
22:X:715:SER:HB3	22:X:718:SER:HB3	1.98	0.45
22:X:997:MET:HE2	22:X:997:MET:HB3	1.65	0.45
22:X:1008:LEU:HB3	22:X:1016:TYR:CD2	2.50	0.45
23:Y:198:ASP:CG	23:Y:199:ASP:H	2.19	0.45
34:1:1158:ILE:HD12	34:1:1162:GLY:CA	2.46	0.45
34:1:1167:TYR:CD2	36:2:581:LYS:HA	2.46	0.45
35:3:164:ASN:HA	35:3:189:TYR:OH	2.15	0.45
35:3:485:LEU:HA	35:3:494:VAL:HB	1.99	0.45
35:3:604:PHE:CE1	35:3:681:PRO:HD3	2.51	0.45
1:A:84:ASP:O	1:A:88:TYR:HB2	2.16	0.45
1:A:101:LYS:HD3	1:A:101:LYS:HA	1.76	0.45
1:A:1127:GLY:HA3	1:A:1151:ARG:HH22	1.81	0.45
1:A:1144:LYS:O	1:A:1148:ASN:HB2	2.16	0.45
1:A:1359:HIS:HD2	1:A:1361:GLU:O	1.99	0.45
3:C:351:PRO:O	3:C:354:ARG:HD3	2.16	0.45
5:F:36:A:N1	6:G:10:U:C4	2.84	0.45
6:G:13:C:C2	6:G:14:A:C8	3.04	0.45
7:H:28:C:O2'	7:H:29:A:O4'	2.35	0.45
7:H:158:G:H2'	7:H:159:U:O4'	2.17	0.45
8:I:569:GLY:HA3	8:I:576:ALA:HB2	1.97	0.45
11:M:160:PHE:HB3	11:M:161:PHE:CD1	2.51	0.45
18:T:341:ALA:O	18:T:344:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:790:LEU:O	22:X:794:GLU:HG2	2.16	0.45
35:3:234:PHE:HE1	35:3:236:ILE:HG12	1.81	0.45
35:3:333:VAL:HG21	35:3:349:VAL:HG21	1.97	0.45
35:3:528:ARG:NH1	35:3:572:GLY:O	2.49	0.45
35:3:558:LEU:HD23	35:3:562:GLU:HB3	1.99	0.45
1:A:977:LEU:HG	1:A:978:GLU:N	2.31	0.45
3:C:845:ALA:O	3:C:848:THR:OG1	2.31	0.45
4:E:171:SER:H	4:E:196:VAL:HG13	1.81	0.45
4:E:207:GLN:HB3	4:E:219:VAL:HG12	1.99	0.45
7:H:43:U:HO2'	7:H:44:U:P	2.36	0.45
9:J:199:LYS:CA	9:J:199:LYS:CE	2.85	0.45
16:R:377:ARG:HH21	16:R:377:ARG:HG2	1.81	0.45
20:V:569:LYS:HD2	20:V:614:GLY:HA3	1.98	0.45
34:1:747:LEU:HA	34:1:750:ILE:HG13	1.98	0.45
34:1:856:ASP:HB3	34:1:864:TYR:CE2	2.51	0.45
34:1:1154:LEU:O	34:1:1158:ILE:CG1	2.29	0.45
35:3:249:LEU:HD23	35:3:256:ILE:HD11	1.98	0.45
35:3:353:PHE:CZ	39:5:55:ILE:HG13	2.51	0.45
35:3:717:SER:HB2	35:3:718:ARG:HH12	1.81	0.45
35:3:745:PHE:CG	35:3:755:VAL:HG23	2.51	0.45
35:3:769:LYS:HD3	35:3:769:LYS:H	1.81	0.45
1:A:1275:ARG:C	1:A:1276:GLU:HG3	2.35	0.45
1:A:1670:ASP:N	1:A:1670:ASP:OD1	2.48	0.45
1:A:1785:VAL:HG11	1:A:1807:ILE:HD13	1.99	0.45
1:A:1820:LYS:NZ	1:A:1914:MET:HB2	2.32	0.45
2:B:103:G:C6	2:B:104:C:C4	3.04	0.45
3:C:860:ASP:N	3:C:860:ASP:OD1	2.49	0.45
5:F:33:G:C2	5:F:34:G:C8	3.05	0.45
7:H:150:U:H3	7:H:181:G:H22	1.64	0.45
18:T:203:HIS:CE1	18:T:223:SER:HB3	2.51	0.45
18:T:329:HIS:CE1	18:T:349:SER:HB3	2.51	0.45
22:X:807:GLU:HA	22:X:807:GLU:OE2	2.17	0.45
34:1:850:ILE:CB	34:1:888:LEU:HD21	2.46	0.45
34:1:903:GLN:HG2	34:1:910:MET:HG3	1.98	0.45
34:1:946:LYS:O	34:1:950:GLN:HG3	2.17	0.45
34:1:1193:GLN:HE22	38:7:78:GLN:HE22	1.60	0.45
34:1:1263:ASP:CB	39:5:24:ALA:HB2	2.40	0.45
35:3:515:ALA:HA	35:3:528:ARG:HA	1.97	0.45
35:3:696:SER:O	35:3:696:SER:OG	2.32	0.45
35:3:704:VAL:C	35:3:710:GLU:HG3	2.37	0.45
35:3:725:TYR:O	35:3:728:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2:456:ARG:C	36:2:456:ARG:CD	2.85	0.45
36:2:557:VAL:O	36:2:559:PRO:N	2.49	0.45
1:A:542:ASN:O	1:A:546:LEU:HB2	2.17	0.45
1:A:699:GLU:OE1	1:A:699:GLU:HA	2.14	0.45
1:A:845:ARG:HA	1:A:845:ARG:HD2	1.61	0.45
1:A:1526:LEU:HD22	1:A:1527:ASN:H	1.82	0.45
1:A:1854:VAL:HA	1:A:1857:GLN:OE1	2.17	0.45
3:C:662:PHE:CE1	3:C:829:GLU:HB3	2.51	0.45
3:C:755:ASP:O	3:C:758:LEU:N	2.47	0.45
3:C:918:ILE:HG21	3:C:932:GLU:OE2	2.16	0.45
4:E:209:ILE:HG23	4:E:219:VAL:HG22	1.99	0.45
4:E:299:LYS:HE2	4:E:299:LYS:HB2	1.79	0.45
6:G:15:U:C2	6:G:16:G:C8	3.05	0.45
9:J:199:LYS:C	9:J:199:LYS:CD	2.85	0.45
11:M:139:THR:O	11:M:142:ILE:HG22	2.17	0.45
15:Q:263:LEU:O	15:Q:267:ARG:N	2.47	0.45
16:R:309:GLU:OE1	16:R:309:GLU:HA	2.17	0.45
16:R:351:GLU:HG3	22:X:260:VAL:HG21	1.99	0.45
18:T:391:SER:OG	18:T:393:ASP:OD2	2.26	0.45
20:V:476:LEU:HD23	20:V:476:LEU:HA	1.83	0.45
23:Y:117:ASP:N	23:Y:117:ASP:OD1	2.48	0.45
34:1:644:LEU:HB3	34:1:648:LEU:CD1	2.46	0.45
34:1:668:VAL:HG22	34:1:686:LEU:HD23	1.99	0.45
34:1:802:GLU:OE1	34:1:802:GLU:HA	2.16	0.45
34:1:1203:GLY:HA2	35:3:1171:LYS:CD	2.45	0.45
34:1:1226:VAL:O	34:1:1230:VAL:HG23	2.17	0.45
35:3:278:LEU:HD21	35:3:816:LYS:NZ	2.32	0.45
35:3:412:ILE:H	35:3:1105:GLN:NE2	2.09	0.45
1:A:235:MET:HB3	1:A:404:LEU:HD11	1.98	0.45
1:A:292:ASP:CG	1:A:293:TRP:H	2.20	0.45
1:A:727:LYS:HE2	1:A:727:LYS:HB3	1.70	0.45
1:A:832:TYR:HB3	1:A:835:ASP:OD1	2.17	0.45
2:B:97:G:O6	2:B:116:U:O4	2.35	0.45
13:O:249:ARG:O	13:O:253:TYR:N	2.50	0.45
16:R:331:ALA:HA	22:X:275:ARG:HH12	1.81	0.45
16:R:335:ARG:CB	22:X:272:TYR:HB2	2.47	0.45
22:X:774:ASP:CG	22:X:777:HIS:HD1	2.18	0.45
23:Y:186:LEU:HD23	23:Y:186:LEU:HA	1.71	0.45
23:Y:236:LYS:HA	23:Y:236:LYS:HD3	1.69	0.45
34:1:869:MET:HE1	34:1:896:ILE:CA	2.31	0.45
34:1:1041:ARG:HD2	34:1:1041:ARG:HA	1.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:1148:LEU:HD12	34:1:1187:THR:HB	1.80	0.45
35:3:185:LEU:O	35:3:186:GLU:HG3	2.16	0.45
35:3:1211:ILE:HD12	35:3:1214:ARG:HE	1.82	0.45
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.80	0.45
1:A:1458:GLN:NE2	1:A:1463:LYS:HD3	2.32	0.45
1:A:1969:PRO:HB2	1:A:1971:LEU:CD2	2.47	0.45
3:C:137:HIS:HB3	3:C:140:HIS:CE1	2.51	0.45
3:C:188:VAL:HG23	3:C:190:LEU:HD11	1.97	0.45
3:C:685:ILE:HB	3:C:815:VAL:HG21	1.99	0.45
4:E:108:HIS:CE1	4:E:128:SER:HB2	2.52	0.45
5:F:10:U:H2'	5:F:11:C:H4'	1.99	0.45
14:P:51:PRO:HA	14:P:54:VAL:HG22	1.99	0.45
14:P:73:GLU:HG2	14:P:76:ARG:HH21	1.81	0.45
14:P:78:ARG:HD3	14:P:78:ARG:HA	1.72	0.45
18:T:478:LEU:HD23	18:T:488:VAL:HG22	1.98	0.45
22:X:592:LEU:O	22:X:596:VAL:HG23	2.16	0.45
22:X:725:ARG:HD3	22:X:728:ARG:HH12	1.82	0.45
34:1:532:PHE:HD2	34:1:570:TYR:CD2	2.35	0.45
34:1:702:ARG:CG	34:1:738:HIS:NE2	2.80	0.45
34:1:761:TYR:O	34:1:765:TYR:HB2	2.17	0.45
34:1:857:LEU:HA	34:1:865:ARG:HB3	1.98	0.45
34:1:1142:ASN:H	34:1:1142:ASN:HD22	1.64	0.45
34:1:1300:LEU:CB	35:3:1032:TRP:CH2	2.98	0.45
35:3:49:LYS:HD3	35:3:49:LYS:HA	1.59	0.45
35:3:294:LYS:HZ2	35:3:294:LYS:C	2.20	0.45
35:3:528:ARG:HG3	35:3:529:ALA:N	2.32	0.45
35:3:788:PHE:HB2	35:3:799:ILE:HA	1.98	0.45
1:A:1402:ARG:NH2	22:X:641:GLU:OE2	2.47	0.45
1:A:1812:PRO:O	1:A:1920:TYR:OH	2.22	0.45
3:C:678:THR:HB	3:C:680:ASN:O	2.17	0.45
3:C:803:ARG:O	3:C:807:GLN:HG3	2.17	0.45
9:J:357:LYS:N	9:J:357:LYS:HD2	2.31	0.45
10:L:14:THR:HG23	10:L:152:LEU:HD21	1.99	0.45
16:R:147:THR:O	16:R:151:LEU:HB2	2.17	0.45
20:V:490:CYS:HA	20:V:493:ILE:HD12	1.99	0.45
20:V:503:TYR:CE2	20:V:550:MET:HG2	2.52	0.45
20:V:647:LEU:O	20:V:651:PRO:HD3	2.17	0.45
22:X:182:ALA:HB1	22:X:186:ARG:HH21	1.82	0.45
22:X:475:ASN:ND2	22:X:490:ARG:HD3	2.32	0.45
22:X:871:PHE:HB3	22:X:883:ASN:HD22	1.82	0.45
34:1:503:LYS:HE2	34:1:511:MET:CG	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:536:LEU:O	34:1:540:MET:HG2	2.16	0.45
34:1:560:LEU:HD11	34:1:600:LEU:HD12	1.99	0.45
34:1:658:TRP:CZ3	34:1:698:GLN:HG2	2.52	0.45
34:1:1080:THR:HA	34:1:1083:TYR:CD2	2.52	0.45
35:3:125:PRO:HG2	35:3:174:ASP:HA	1.98	0.45
35:3:1159:ASP:OD1	35:3:1160:HIS:N	2.50	0.45
1:A:108:MET:O	1:A:110:TRP:N	2.50	0.45
1:A:1359:HIS:CD2	1:A:1361:GLU:O	2.70	0.45
1:A:1661:TRP:HH2	1:A:1684:PHE:CE1	2.35	0.45
1:A:1977:ILE:HG22	1:A:1978:LYS:HD2	1.98	0.45
3:C:530:LEU:HD23	3:C:530:LEU:HA	1.70	0.45
4:E:263:ASP:O	4:E:272:ARG:HD2	2.16	0.45
7:H:160:A:C2	7:H:171:U:C2	3.05	0.45
22:X:172:LEU:HA	22:X:175:LEU:HD23	1.99	0.45
22:X:502:LEU:O	22:X:505:PHE:HB2	2.17	0.45
22:X:674:THR:HG22	22:X:675:ASN:N	2.32	0.45
22:X:984:LEU:HD21	22:X:1000:VAL:HG21	1.97	0.45
34:1:1217:PRO:HB2	36:2:510:TYR:CE2	2.41	0.45
35:3:14:ILE:HD11	35:3:356:HIS:CD2	2.52	0.45
35:3:52:THR:O	35:3:52:THR:OG1	2.34	0.45
35:3:164:ASN:HD22	35:3:190:GLU:HG2	1.82	0.45
35:3:996:ILE:HG21	35:3:1041:TYR:CD1	2.52	0.45
38:7:23:CYS:N	38:7:58:CYS:SG	2.73	0.45
1:A:64:GLU:OE1	1:A:64:GLU:N	2.35	0.45
1:A:995:ARG:HH11	1:A:998:ARG:HH11	1.64	0.45
1:A:1402:ARG:HH22	22:X:641:GLU:CD	2.20	0.45
1:A:1554:GLN:HG3	1:A:1561:PHE:HE1	1.82	0.45
1:A:1914:MET:HE3	1:A:1916:LEU:HD23	1.98	0.45
2:B:26:A:H2'	2:B:27:U:O4'	2.17	0.45
3:C:177:ARG:C	3:C:179:VAL:H	2.20	0.45
3:C:719:GLN:HG3	3:C:724:TRP:O	2.17	0.45
3:C:774:THR:HG22	3:C:784:ILE:HD11	1.99	0.45
4:E:181:ILE:HD12	4:E:181:ILE:N	2.32	0.45
10:L:162:THR:HG23	11:M:211:ILE:HG21	1.98	0.45
12:N:9:LYS:HE2	12:N:9:LYS:HB3	1.58	0.45
18:T:399:LYS:HB2	18:T:406:ILE:HD11	1.98	0.45
20:V:539:LEU:HB3	20:V:543:LYS:HB2	1.99	0.45
20:V:560:LEU:HA	20:V:560:LEU:HD23	1.80	0.45
22:X:171:ARG:NH1	22:X:509:PRO:HB3	2.32	0.45
34:1:606:LEU:O	34:1:610:ILE:HG13	2.17	0.45
35:3:910:ALA:HB2	35:3:948:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:1117:LEU:HD12	35:3:1117:LEU:HA	1.60	0.45
36:2:512:GLN:O	36:2:515:ARG:HB3	2.17	0.45
1:A:367:SER:OG	1:A:368:GLN:N	2.50	0.44
1:A:1189:MET:CG	1:A:1190:CYS:H	2.30	0.44
1:A:1397:ILE:CG1	16:R:405:VAL:HG22	2.47	0.44
7:H:105:G:N2	7:H:107:A:H5'	2.32	0.44
9:J:367:GLU:OE1	9:J:382:TYR:CZ	2.70	0.44
10:L:233:GLN:H	10:L:233:GLN:CD	2.19	0.44
14:P:205:LYS:HG2	14:P:208:LYS:HB3	1.98	0.44
22:X:719:ALA:HB1	22:X:736:ARG:HE	1.82	0.44
34:1:662:HIS:HB2	34:1:701:VAL:HB	1.98	0.44
34:1:685:SER:O	34:1:689:ILE:HG12	2.18	0.44
34:1:834:VAL:HG22	34:1:871:THR:CG2	2.44	0.44
34:1:1248:GLN:HB3	36:2:496:ASN:O	2.17	0.44
35:3:5:ASN:O	35:3:1176:GLY:HA3	2.16	0.44
35:3:259:LYS:HB2	35:3:259:LYS:HE3	1.69	0.44
35:3:292:THR:HG1	35:3:301:PHE:HD1	1.61	0.44
35:3:595:VAL:HG22	35:3:596:PRO:O	2.17	0.44
35:3:611:ASP:O	35:3:612:ASN:HB2	2.17	0.44
35:3:639:SER:OG	35:3:699:VAL:O	2.13	0.44
1:A:1498:TRP:O	1:A:1501:LEU:HG	2.16	0.44
1:A:1813:ARG:HA	1:A:1929:SER:HB2	1.99	0.44
2:B:67:A:H2'	2:B:68:C:O4'	2.18	0.44
3:C:260:ILE:CD1	3:C:309:PHE:HB3	2.47	0.44
4:E:176:VAL:O	4:E:189:THR:HA	2.17	0.44
9:J:187:VAL:CG1	9:J:188:GLN:H	2.22	0.44
11:M:215:ASN:ND2	16:R:261:THR:N	2.49	0.44
13:O:167:PHE:O	13:O:172:GLU:N	2.48	0.44
16:R:386:ARG:NE	16:R:386:ARG:HA	2.29	0.44
16:R:404:GLU:OE1	22:X:327:ARG:NE	2.42	0.44
20:V:551:PHE:HA	20:V:554:LEU:HD12	1.98	0.44
21:W:279:LYS:CB	36:2:622:GLY:C	2.78	0.44
22:X:388:GLN:O	22:X:392:ILE:HG13	2.17	0.44
22:X:698:LYS:HZ2	22:X:758:THR:HA	1.82	0.44
34:1:581:LEU:HD13	34:1:589:ALA:HB1	1.98	0.44
34:1:769:VAL:HG13	34:1:773:LEU:HD21	1.98	0.44
34:1:1158:ILE:HD12	34:1:1162:GLY:HA2	1.99	0.44
34:1:1178:MET:CB	36:2:514:LYS:HZ3	2.26	0.44
35:3:124:ASP:OD2	35:3:128:ARG:HG3	2.17	0.44
35:3:278:LEU:HD21	35:3:816:LYS:HZ3	1.82	0.44
35:3:745:PHE:CB	35:3:755:VAL:HG23	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:993:ILE:HG23	35:3:1002:VAL:HG23	1.99	0.44
1:A:106:MET:HE2	1:A:106:MET:HB2	1.74	0.44
1:A:159:ARG:HA	1:A:159:ARG:CZ	2.48	0.44
1:A:329:LEU:HD23	1:A:329:LEU:H	1.83	0.44
1:A:1164:SER:HB3	3:C:59:LEU:HD21	1.99	0.44
1:A:2007:ILE:HA	1:A:2010:ILE:HG22	1.99	0.44
2:B:97:G:H2'	2:B:97:G:N3	2.31	0.44
2:B:110:C:H2'	2:B:111:A:C8	2.52	0.44
3:C:304:LEU:H	3:C:304:LEU:HD12	1.82	0.44
3:C:585:THR:O	3:C:587:VAL:HG23	2.17	0.44
3:C:687:MET:HB3	3:C:815:VAL:CG1	2.47	0.44
3:C:711:ARG:HA	3:C:714:LEU:HD22	1.99	0.44
5:F:30:A:H2'	5:F:31:U:O4'	2.17	0.44
5:F:58:G:HO2'	5:F:59:G:P	2.38	0.44
5:F:93:G:H2'	5:F:94:C:C6	2.52	0.44
7:H:18:U:O2	16:R:258:LYS:HB2	2.17	0.44
9:J:194:LEU:HA	9:J:194:LEU:HD22	1.76	0.44
18:T:435:THR:HB	18:T:451:HIS:CE1	2.53	0.44
20:V:622:ARG:NH2	20:V:623:ASN:HB3	2.32	0.44
22:X:826:LYS:HZ3	22:X:948:PHE:HE1	1.66	0.44
23:Y:221:ALA:O	23:Y:225:GLU:HG2	2.17	0.44
34:1:645:LEU:HD13	34:1:682:HIS:CD2	2.52	0.44
34:1:1152:SER:OG	34:1:1194:HIS:CE1	2.70	0.44
35:3:27:GLN:OE1	35:3:42:ARG:NH1	2.50	0.44
35:3:243:ASP:OD1	35:3:244:GLY:N	2.50	0.44
35:3:331:ASP:CG	35:3:390:ARG:HH21	2.21	0.44
35:3:633:LEU:HD12	35:3:637:PRO:HG3	1.97	0.44
35:3:1183:ASN:OD1	35:3:1183:ASN:N	2.51	0.44
1:A:251:ASP:HB3	1:A:337:VAL:HG13	1.99	0.44
1:A:644:ILE:HD12	1:A:644:ILE:HA	1.80	0.44
1:A:1606:ILE:HD11	1:A:1631:LEU:HD13	1.98	0.44
7:H:106:G:N3	7:H:107:A:N6	2.65	0.44
11:M:125:SER:HB2	16:R:237:MET:O	2.18	0.44
16:R:411:LEU:HD13	16:R:411:LEU:HA	1.74	0.44
20:V:468:ASP:OD1	20:V:468:ASP:N	2.49	0.44
20:V:503:TYR:HE2	20:V:550:MET:HG2	1.82	0.44
22:X:289:GLN:HA	22:X:292:LEU:HD23	2.00	0.44
23:Y:246:LYS:HE3	23:Y:312:HIS:CB	2.40	0.44
34:1:524:ARG:HA	34:1:566:LEU:HD23	1.99	0.44
34:1:602:LYS:HD2	34:1:638:ALA:O	2.17	0.44
35:3:741:PHE:HB3	35:3:757:ILE:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:753:GLY:O	35:3:754:ILE:HD13	2.17	0.44
35:3:965:LYS:HB3	35:3:965:LYS:HE2	1.69	0.44
1:A:758:ARG:HD2	1:A:775:ASN:HD21	1.83	0.44
1:A:1817:LEU:O	1:A:1916:LEU:HA	2.17	0.44
3:C:118:PHE:O	3:C:122:LEU:HD12	2.18	0.44
3:C:461:LEU:HD21	3:C:572:GLU:OE2	2.18	0.44
3:C:485:ASP:OD2	3:C:485:ASP:N	2.47	0.44
3:C:642:HIS:O	3:C:646:LYS:HB2	2.18	0.44
5:F:44:G:H8	5:F:44:G:OP2	2.00	0.44
8:I:50:LYS:CB	8:I:51:PRO:HD3	2.47	0.44
10:L:223:GLY:O	10:L:225:TYR:N	2.51	0.44
14:P:218:GLU:HA	14:P:221:LYS:HG3	2.00	0.44
16:R:314:GLN:HA	22:X:290:GLU:OE1	2.17	0.44
16:R:325:ARG:NE	23:Y:222:ILE:HG23	2.26	0.44
20:V:497:CYS:HB3	20:V:507:PHE:HB2	1.99	0.44
20:V:532:GLN:HE22	20:V:539:LEU:HD11	1.82	0.44
22:X:461:VAL:HA	22:X:464:ARG:NE	2.33	0.44
22:X:461:VAL:HG22	22:X:464:ARG:HH21	1.83	0.44
22:X:620:GLU:CD	22:X:620:GLU:H	2.15	0.44
22:X:1017:LYS:HE2	22:X:1017:LYS:HB2	1.76	0.44
23:Y:126:PHE:C	23:Y:126:PHE:CD2	2.91	0.44
34:1:1205:GLU:CD	35:3:1171:LYS:CD	2.86	0.44
35:3:341:VAL:HG12	35:3:347:LEU:HB2	2.00	0.44
35:3:488:GLY:C	35:3:490:THR:H	2.20	0.44
35:3:543:THR:O	35:3:558:LEU:HD12	2.17	0.44
35:3:549:VAL:HG12	35:3:550:ASN:O	2.18	0.44
36:2:487:LEU:HD22	39:5:28:LYS:HB3	1.81	0.44
39:5:33:VAL:CG2	39:5:76:CYS:HB2	2.47	0.44
1:A:564:TYR:HA	1:A:569:VAL:HG23	1.99	0.44
1:A:1043:TYR:O	1:A:1046:LEU:HB3	2.18	0.44
1:A:1427:ARG:HB3	22:X:329:TRP:CE3	2.52	0.44
1:A:1503:TRP:HE3	1:A:1533:ARG:HH11	1.66	0.44
1:A:1963:GLU:O	1:A:1965:HIS:N	2.51	0.44
2:B:109:G:H2'	2:B:110:C:C6	2.52	0.44
3:C:349:PHE:HE1	3:C:354:ARG:HA	1.82	0.44
3:C:514:TYR:HB2	3:C:521:ASP:HB2	1.99	0.44
4:E:181:ILE:HG22	4:E:182:ARG:NH1	2.32	0.44
4:E:287:ASN:OD1	4:E:288:LEU:N	2.51	0.44
5:F:26:U:H3'	5:F:27:A:H5"	2.00	0.44
5:F:79:C:O2'	5:F:80:G:O5'	2.32	0.44
9:J:333:PHE:O	9:J:337:MET:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:160:PHE:C	11:M:161:PHE:HD1	2.20	0.44
12:N:120:ARG:HA	12:N:120:ARG:HD2	1.66	0.44
16:R:383:ASN:N	16:R:383:ASN:OD1	2.51	0.44
18:T:191:HIS:CD2	18:T:440:ASP:OD1	2.70	0.44
23:Y:39:TYR:HB3	23:Y:185:GLN:HE22	1.82	0.44
35:3:312:LYS:HB2	35:3:330:PHE:CD1	2.50	0.44
35:3:925:VAL:O	35:3:942:LYS:HA	2.18	0.44
35:3:955:PHE:HZ	35:3:1014:TYR:CD2	2.36	0.44
39:5:44:MET:HE2	39:5:44:MET:HB2	1.87	0.44
1:A:369:GLU:OE1	1:A:370:PRO:HD2	2.18	0.44
1:A:946:GLU:HG2	1:A:954:LYS:NZ	2.33	0.44
1:A:1635:TYR:CE2	1:A:1636:LYS:HB2	2.52	0.44
3:C:789:PHE:CE2	3:C:816:VAL:HG13	2.53	0.44
9:J:428:GLU:O	9:J:432:VAL:HG13	2.18	0.44
9:J:440:LEU:O	9:J:445:LYS:HD2	2.16	0.44
16:R:86:LEU:HD23	16:R:86:LEU:H	1.81	0.44
20:V:554:LEU:HA	20:V:559:SER:OG	2.18	0.44
20:V:617:PRO:HB3	20:V:623:ASN:ND2	2.32	0.44
22:X:659:ILE:O	22:X:669:LYS:NZ	2.50	0.44
34:1:508:THR:HB	34:1:510:PRO:CD	2.46	0.44
34:1:774:ILE:HG23	34:1:813:PRO:CB	2.45	0.44
34:1:1262:ARG:C	39:5:24:ALA:HB2	2.27	0.44
35:3:1:MET:CA	36:2:709:GLY:O	2.66	0.44
35:3:404:LEU:HB3	35:3:407:ILE:HG12	1.99	0.44
35:3:503:THR:OG1	35:3:522:ASP:OD2	2.21	0.44
35:3:728:ARG:HD3	35:3:728:ARG:HA	1.88	0.44
35:3:988:ASN:ND2	35:3:1004:ASP:OD1	2.50	0.44
36:2:707:PRO:HG2	36:2:710:GLU:HG2	2.00	0.44
36:2:711:LEU:HD22	36:2:712:GLU:N	2.32	0.44
38:7:9:ILE:O	38:7:88:ILE:HG22	2.17	0.44
1:A:1284:LEU:HA	1:A:1284:LEU:HD23	1.72	0.44
3:C:470:PRO:HA	3:C:499:GLY:O	2.18	0.44
3:C:587:VAL:HG11	3:C:830:PRO:HG3	1.99	0.44
3:C:902:HIS:ND1	3:C:903:HIS:HD2	2.16	0.44
5:F:32:U:H2'	5:F:33:G:C8	2.53	0.44
6:G:99:C:C4	7:H:33:G:C5	3.06	0.44
6:G:110:U:H4'	22:X:497:THR:HG21	1.99	0.44
7:H:57:A:H5'	36:2:477:MET:CB	2.47	0.44
16:R:63:ALA:H	17:S:131:ARG:CB	2.31	0.44
22:X:824:LEU:HA	22:X:827:MET:HG2	1.99	0.44
23:Y:194:ASP:N	23:Y:194:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:770:MET:SD	34:1:810:ILE:CG1	3.06	0.44
34:1:1178:MET:HB3	36:2:514:LYS:CE	2.48	0.44
34:1:1256:HIS:CG	34:1:1257:PRO:CD	2.72	0.44
34:1:1279:ALA:C	35:3:1167:TYR:HD1	2.20	0.44
34:1:1281:ILE:HG21	35:3:1050:PHE:CE1	2.33	0.44
35:3:184:CYS:HG	35:3:211:TYR:HE1	1.66	0.44
35:3:458:ALA:O	35:3:459:VAL:HG23	2.17	0.44
36:2:526:ASP:O	36:2:528:ILE:N	2.50	0.44
39:5:20:GLY:HA2	39:5:34:ASN:ND2	2.33	0.44
1:A:599:MET:O	1:A:603:ARG:HG3	2.17	0.44
1:A:929:GLU:OE1	1:A:933:ARG:NH2	2.51	0.44
1:A:1427:ARG:HE	22:X:326:GLN:CD	2.15	0.44
1:A:1857:GLN:HE21	1:A:1857:GLN:HB2	1.54	0.44
3:C:78:GLU:HG3	3:C:79:THR:N	2.33	0.44
3:C:305:GLY:O	3:C:433:MET:HG3	2.18	0.44
5:F:80:G:C6	9:J:206:LEU:HD12	2.53	0.44
5:F:87:C:OP2	11:M:193:ARG:HA	2.17	0.44
6:G:91:A:H2'	6:G:92:U:H6	1.83	0.44
6:G:111:U:O2	22:X:503:ARG:NH1	2.50	0.44
10:L:163:GLN:HA	10:L:163:GLN:NE2	2.31	0.44
18:T:333:VAL:HA	18:T:349:SER:HB2	1.99	0.44
20:V:570:LEU:HD23	20:V:570:LEU:HA	1.86	0.44
23:Y:28:PHE:O	23:Y:32:CYS:HB2	2.18	0.44
34:1:582:LEU:HD23	34:1:631:ALA:N	2.32	0.44
34:1:1300:LEU:HD13	35:3:1032:TRP:CE2	2.48	0.44
35:3:924:PHE:HA	35:3:943:THR:O	2.18	0.44
1:A:253:ASN:O	3:C:893:GLY:HA3	2.18	0.43
1:A:1527:ASN:O	1:A:1529:ILE:HD12	2.17	0.43
5:F:13:G:H2'	5:F:14:C:C6	2.53	0.43
5:F:36:A:C3'	5:F:37:C:H5"	2.37	0.43
5:F:58:G:O2'	5:F:59:G:H5'	2.17	0.43
7:H:114:A:H2'	7:H:115:G:C8	2.53	0.43
12:N:124:SER:OG	12:N:125:LYS:HD2	2.18	0.43
20:V:515:CYS:HA	20:V:521:TYR:HB2	2.00	0.43
34:1:548:GLU:O	34:1:552:LEU:HG	2.18	0.43
34:1:1149:LYS:O	34:1:1152:SER:HB3	2.17	0.43
34:1:1197:LEU:HD22	38:7:77:ILE:HG22	1.99	0.43
34:1:1287:ILE:HG23	36:2:490:HIS:HD2	1.81	0.43
35:3:206:GLN:HE22	35:3:232:GLY:H	1.66	0.43
35:3:1098:GLY:C	35:3:1099:GLU:HG3	2.37	0.43
36:2:517:ILE:C	36:2:517:ILE:CD1	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TYR:HE1	1:A:485:THR:OG1	2.01	0.43
1:A:1865:ARG:HD2	1:A:1865:ARG:HA	1.76	0.43
2:B:100:C:H2'	2:B:101:U:C6	2.52	0.43
3:C:267:LEU:HD23	3:C:267:LEU:HA	1.81	0.43
3:C:750:LEU:HD13	19:U:67:GLU:HA	2.00	0.43
7:H:162:U:H4'	7:H:163:G:O4'	2.18	0.43
14:P:188:TRP:O	14:P:188:TRP:CD1	2.71	0.43
16:R:320:HIS:HA	16:R:323:LYS:CE	2.48	0.43
18:T:266:GLU:HG2	18:T:290:ALA:HB1	2.00	0.43
22:X:297:ARG:HE	22:X:297:ARG:HB3	1.60	0.43
22:X:681:LEU:O	22:X:725:ARG:NH2	2.50	0.43
22:X:915:ARG:O	22:X:919:GLU:HG3	2.18	0.43
22:X:1003:ILE:HG13	22:X:1004:GLU:N	2.33	0.43
34:1:739:ARG:CA	34:1:743:LEU:HD21	2.48	0.43
34:1:806:ILE:HA	34:1:810:ILE:HD12	2.00	0.43
34:1:830:TYR:HA	34:1:867:MET:SD	2.57	0.43
34:1:873:GLU:HG3	34:1:916:THR:OG1	2.19	0.43
35:3:112:CYS:SG	39:5:46:HIS:CD2	3.10	0.43
35:3:169:HIS:HD2	35:3:170:VAL:O	2.02	0.43
35:3:424:TYR:HD1	35:3:437:VAL:HG22	1.82	0.43
35:3:526:HIS:HB2	35:3:574:LEU:CD2	2.48	0.43
35:3:604:PHE:CZ	35:3:681:PRO:HD3	2.53	0.43
35:3:833:GLU:C	35:3:836:ALA:H	2.14	0.43
35:3:986:ILE:HG21	35:3:990:ILE:HG12	1.99	0.43
1:A:1401:ARG:HG2	1:A:1401:ARG:HH11	1.82	0.43
1:A:1580:HIS:HB3	1:A:1583:GLN:NE2	2.33	0.43
3:C:436:GLN:HB3	3:C:437:HIS:HD2	1.82	0.43
4:E:283:ASN:O	4:E:286:LYS:HD2	2.19	0.43
4:E:304:SER:O	4:E:330:ILE:HD12	2.17	0.43
4:E:326:HIS:CE1	4:E:346:SER:HB2	2.52	0.43
5:F:34:G:H2'	5:F:35:A:C8	2.54	0.43
7:H:161:U:H2'	7:H:163:G:N2	2.32	0.43
17:S:96:GLY:O	17:S:131:ARG:HA	2.19	0.43
18:T:288:LEU:O	18:T:289:SER:OG	2.34	0.43
20:V:496:CYS:HA	20:V:499:GLN:OE1	2.17	0.43
22:X:192:ARG:HG2	22:X:192:ARG:NH1	2.30	0.43
22:X:871:PHE:HB3	22:X:883:ASN:ND2	2.33	0.43
34:1:551:LEU:O	34:1:555:VAL:HG23	2.18	0.43
34:1:673:ILE:HD13	34:1:673:ILE:HA	1.76	0.43
34:1:748:LYS:HB2	34:1:787:ILE:CB	2.49	0.43
34:1:1153:PHE:C	34:1:1157:TYR:HD2	2.08	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:1217:PRO:O	36:2:503:HIS:HE1	1.98	0.43
35:3:407:ILE:HD11	35:3:1124:GLY:HA2	1.99	0.43
35:3:543:THR:C	35:3:558:LEU:HD12	2.38	0.43
35:3:576:GLU:OE1	35:3:580:ARG:NH2	2.52	0.43
35:3:705:ARG:NH2	35:3:746:ALA:HB2	2.33	0.43
38:7:74:GLU:O	38:7:78:GLN:HG3	2.18	0.43
1:A:1838:LYS:HE2	1:A:1868:MET:HE2	2.00	0.43
3:C:660:VAL:HG22	3:C:878:ILE:HD11	2.01	0.43
3:C:682:LYS:HB3	3:C:797:ALA:CB	2.45	0.43
4:E:301:ALA:HB2	4:E:335:PHE:CZ	2.53	0.43
12:N:7:SER:O	12:N:8:ARG:HB2	2.18	0.43
17:S:103:ALA:HB2	21:W:93:PHE:HA	2.01	0.43
20:V:546:ASN:OD1	20:V:547:VAL:N	2.51	0.43
23:Y:225:GLU:OE1	23:Y:233:ALA:HA	2.18	0.43
34:1:733:LYS:HE3	34:1:733:LYS:HB3	1.80	0.43
35:3:329:TYR:HB3	35:3:370:GLU:CD	2.39	0.43
35:3:595:VAL:HG21	35:3:600:GLN:C	2.39	0.43
35:3:1106:LYS:HG3	36:2:708:TRP:CD1	2.54	0.43
36:2:512:GLN:N	36:2:512:GLN:OE1	2.51	0.43
1:A:41:GLN:NE2	1:A:45:TYR:HD2	2.09	0.43
1:A:59:GLU:CD	12:N:87:ASN:HB2	2.38	0.43
1:A:699:GLU:HB3	16:R:237:MET:HE2	2.00	0.43
1:A:1586:HIS:NE2	1:A:1664:ILE:HG13	2.34	0.43
3:C:173:THR:O	3:C:177:ARG:HB2	2.18	0.43
3:C:279:ARG:HH12	20:V:324:HIS:CB	2.31	0.43
4:E:335:PHE:CE1	4:E:342:ILE:HD12	2.54	0.43
10:L:177:GLU:O	10:L:180:ARG:N	2.51	0.43
16:R:325:ARG:NH1	23:Y:225:GLU:HB2	2.32	0.43
20:V:547:VAL:HA	20:V:550:MET:HG3	2.00	0.43
22:X:399:LEU:HD23	22:X:399:LEU:HA	1.84	0.43
22:X:888:TRP:O	22:X:891:SER:OG	2.24	0.43
23:Y:147:ASP:OD2	23:Y:147:ASP:N	2.51	0.43
34:1:630:ARG:O	34:1:634:VAL:HG23	2.19	0.43
34:1:956:SER:HB3	34:1:996:ALA:HB2	1.99	0.43
34:1:969:LYS:HD2	34:1:969:LYS:H	1.83	0.43
34:1:1154:LEU:HD12	34:1:1158:ILE:HG23	2.01	0.43
34:1:1251:LEU:HD23	34:1:1251:LEU:HA	1.68	0.43
35:3:123:VAL:HG22	35:3:124:ASP:H	1.83	0.43
35:3:234:PHE:CD1	35:3:235:LEU:N	2.86	0.43
35:3:275:ARG:HH21	35:3:275:ARG:CB	2.31	0.43
35:3:554:VAL:HG12	35:3:556:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:1116:SER:C	36:2:708:TRP:CH2	2.83	0.43
1:A:191:ILE:HD13	1:A:191:ILE:HG21	1.69	0.43
1:A:1109:LEU:HG	1:A:1152:ALA:HB1	2.00	0.43
1:A:1623:ASN:H	1:A:1623:ASN:ND2	2.17	0.43
1:A:1661:TRP:HH2	1:A:1684:PHE:HE1	1.67	0.43
3:C:154:HIS:C	3:C:156:GLU:H	2.22	0.43
3:C:231:ALA:O	3:C:277:LYS:HE3	2.18	0.43
3:C:392:LEU:HB3	3:C:393:PRO:HD3	2.01	0.43
9:J:202:GLU:HG2	9:J:205:LEU:HD11	2.01	0.43
9:J:400:GLU:O	9:J:404:GLU:HG2	2.19	0.43
16:R:353:ASP:O	16:R:357:HIS:HB2	2.19	0.43
18:T:269:GLN:HE21	18:T:269:GLN:HB3	1.60	0.43
22:X:523:HIS:O	22:X:525:ARG:HG2	2.18	0.43
22:X:654:ASP:OD1	22:X:655:MET:N	2.52	0.43
22:X:743:TYR:HA	22:X:747:LEU:HD23	2.00	0.43
23:Y:183:ARG:HA	23:Y:183:ARG:CZ	2.48	0.43
34:1:592:GLU:O	34:1:596:ILE:HG23	2.18	0.43
34:1:601:ALA:HB1	34:1:639:LEU:HG	2.00	0.43
34:1:1155:PHE:CD1	34:1:1158:ILE:HD11	2.53	0.43
34:1:1179:ASP:N	36:2:511:LEU:HD13	2.34	0.43
35:3:373:PHE:HD1	35:3:385:PHE:CD2	2.36	0.43
35:3:1041:TYR:HD2	36:2:705:ARG:NE	1.98	0.43
35:3:1158:ARG:HG3	35:3:1159:ASP:N	2.34	0.43
36:2:461:THR:OG1	36:2:464:GLU:N	2.26	0.43
36:2:472:PRO:O	36:2:475:VAL:HG23	2.19	0.43
1:A:65:HIS:CD2	12:N:46:LEU:HD13	2.54	0.43
1:A:1213:VAL:HG22	1:A:1229:PHE:CD1	2.53	0.43
1:A:1690:ASP:OD1	1:A:1693:SER:OG	2.29	0.43
1:A:1865:ARG:HA	1:A:1865:ARG:NH2	2.33	0.43
3:C:177:ARG:HG3	3:C:179:VAL:HB	2.01	0.43
3:C:665:THR:HG21	3:C:828:MET:HG3	2.00	0.43
6:G:90:C:H2'	6:G:91:A:C8	2.54	0.43
9:J:240:THR:HG22	9:J:241:VAL:N	2.33	0.43
10:L:92:THR:OG1	10:L:95:GLN:HG3	2.19	0.43
11:M:153:ARG:HB2	11:M:160:PHE:HE2	1.84	0.43
16:R:428:GLU:O	16:R:429:ILE:HD13	2.19	0.43
18:T:213:GLU:HG2	18:T:214:PRO:CD	2.48	0.43
20:V:609:GLN:N	20:V:610:PRO:HD2	2.33	0.43
22:X:268:GLN:HA	22:X:271:LYS:HE2	2.00	0.43
22:X:289:GLN:NE2	22:X:293:GLU:OE2	2.51	0.43
34:1:666:LYS:HB3	34:1:704:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:873:GLU:HB2	34:1:913:GLY:HA2	2.00	0.43
34:1:1292:LYS:HZ2	39:5:78:PRO:CG	2.20	0.43
35:3:325:ILE:HB	35:3:375:SER:HB3	1.99	0.43
35:3:565:TYR:HB3	35:3:577:TYR:CB	2.46	0.43
36:2:469:VAL:HG12	36:2:471:ARG:N	2.31	0.43
1:A:64:GLU:H	1:A:64:GLU:CD	2.21	0.43
1:A:388:LEU:HD23	3:C:399:LEU:HD21	2.01	0.43
1:A:1050:LEU:HD23	1:A:1050:LEU:HA	1.83	0.43
1:A:1555:LEU:HD22	1:A:1555:LEU:HA	1.71	0.43
1:A:1799:THR:O	1:A:1801:LYS:HG3	2.19	0.43
1:A:1975:GLU:HG2	1:A:1979:VAL:HG13	2.00	0.43
2:B:109:G:H2'	2:B:110:C:H6	1.83	0.43
3:C:242:LEU:HD23	3:C:242:LEU:HA	1.68	0.43
3:C:300:LEU:HA	3:C:306:ASN:HD22	1.84	0.43
4:E:133:VAL:HG22	4:E:154:VAL:HG21	2.00	0.43
5:F:80:G:N2	9:J:209:PRO:HD3	2.34	0.43
6:G:111:U:OP2	22:X:482:ARG:HB2	2.19	0.43
9:J:206:LEU:HA	9:J:206:LEU:HD23	1.55	0.43
9:J:354:LEU:HA	9:J:354:LEU:HD23	1.81	0.43
9:J:429:PHE:HA	9:J:432:VAL:HG22	1.99	0.43
11:M:224:ARG:HE	11:M:224:ARG:HB2	1.54	0.43
34:1:948:ARG:NH2	34:1:984:GLU:OE2	2.51	0.43
34:1:1270:ASN:OD1	39:5:22:GLY:N	2.49	0.43
35:3:192:ALA:HA	35:3:200:ALA:HB3	2.01	0.43
35:3:514:ASP:OD1	35:3:514:ASP:N	2.52	0.43
35:3:779:PHE:N	35:3:779:PHE:CD1	2.86	0.43
35:3:791:HIS:NE2	35:3:793:GLU:HB2	2.34	0.43
36:2:635:ALA:HB3	37:4:69:TYR:CB	2.49	0.43
1:A:1718:TRP:HZ3	1:A:1726:ILE:HD11	1.84	0.43
3:C:193:THR:HB	3:C:428:THR:CG2	2.49	0.43
4:E:96:TYR:OH	4:E:336:HIS:NE2	2.49	0.43
7:H:56:A:N6	36:2:505:CYS:HB2	2.34	0.43
12:N:7:SER:C	12:N:9:LYS:H	2.22	0.43
18:T:356:LEU:HD13	18:T:366:VAL:HB	2.00	0.43
18:T:394:ASN:OD1	18:T:394:ASN:N	2.51	0.43
20:V:502:THR:HG22	20:V:503:TYR:H	1.84	0.43
21:W:279:LYS:CB	36:2:622:GLY:N	2.73	0.43
22:X:232:ARG:HD2	23:Y:213:ALA:HB1	2.00	0.43
22:X:516:VAL:HG13	22:X:549:LEU:HD13	2.01	0.43
22:X:535:LEU:O	22:X:539:VAL:HG23	2.19	0.43
22:X:868:ARG:NH2	22:X:973:ASN:HD21	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:1106:ARG:H	34:1:1109:ARG:HG3	1.83	0.43
35:3:590:MET:HB2	35:3:606:ALA:O	2.18	0.43
35:3:641:CYS:H	35:3:701:LEU:HD23	1.83	0.43
35:3:1191:LYS:O	35:3:1192:ASN:C	2.57	0.43
39:5:57:GLU:H	39:5:57:GLU:HG2	1.71	0.43
39:5:61:LYS:HB3	39:5:65:ARG:HH22	1.83	0.43
1:A:82:ARG:HE	1:A:82:ARG:HB3	1.70	0.43
1:A:785:LYS:HB3	1:A:785:LYS:HE3	1.67	0.43
1:A:976:MET:HB2	1:A:976:MET:HE2	1.71	0.43
1:A:1581:LEU:HD22	1:A:1746:ARG:HH11	1.84	0.43
1:A:1719:PHE:HB2	1:A:1720:PRO:HD2	2.01	0.43
3:C:624:SER:OG	3:C:941:LYS:HA	2.19	0.43
3:C:658:PRO:HB2	3:C:881:PHE:CZ	2.54	0.43
3:C:673:LYS:HB3	3:C:688:ILE:CG2	2.49	0.43
3:C:938:ARG:O	3:C:942:GLY:N	2.50	0.43
5:F:37:C:H6	5:F:37:C:H2'	1.48	0.43
5:F:97:U:O5'	5:F:97:U:H6	2.01	0.43
6:G:88:G:O2'	6:G:89:U:OP1	2.27	0.43
8:I:177:PRO:HB3	8:I:211:SER:HA	2.01	0.43
9:J:260:ARG:NH1	10:L:215:PRO:HD3	2.33	0.43
10:L:57:SER:O	10:L:57:SER:OG	2.36	0.43
11:M:165:ASN:O	16:R:95:LYS:HA	2.19	0.43
15:Q:514:ILE:N	15:Q:654:ASN:O	2.31	0.43
20:V:545:ARG:HG3	20:V:585:ILE:HD13	2.00	0.43
22:X:396:ARG:NE	22:X:431:GLN:HE22	2.17	0.43
23:Y:183:ARG:HH21	23:Y:187:ASP:CG	2.21	0.43
35:3:249:LEU:HD12	35:3:249:LEU:N	2.33	0.43
35:3:462:VAL:HG11	35:3:516:LEU:HD23	2.00	0.43
35:3:542:LYS:H	35:3:542:LYS:HG3	1.45	0.43
3:C:189:VAL:HA	3:C:198:TYR:O	2.19	0.42
3:C:200:PHE:CE1	3:C:434:CYS:SG	3.12	0.42
3:C:255:VAL:O	3:C:307:VAL:HA	2.19	0.42
3:C:933:PHE:O	3:C:937:THR:HG22	2.18	0.42
4:E:287:ASN:ND2	4:E:331:ASN:OD1	2.52	0.42
4:E:305:ALA:HA	4:E:329:SER:HB2	1.99	0.42
5:F:42:C:H3'	5:F:43:A:C8	2.54	0.42
7:H:63:G:N1	7:H:64:A:N6	2.67	0.42
18:T:253:ILE:O	18:T:261:LEU:HD12	2.19	0.42
18:T:394:ASN:ND2	18:T:408:ASN:HD22	2.17	0.42
18:T:471:ASP:OD2	18:T:472:GLN:N	2.48	0.42
20:V:584:LYS:HE2	20:V:584:LYS:HB2	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:257:PHE:CE2	22:X:262:LEU:HD21	2.54	0.42
22:X:397:ARG:HA	22:X:402:PHE:CD1	2.54	0.42
22:X:419:ILE:HG21	22:X:557:THR:OG1	2.19	0.42
22:X:913:ASP:O	22:X:916:GLU:HG3	2.19	0.42
22:X:991:LEU:HB2	22:X:995:GLU:OE1	2.19	0.42
23:Y:207:GLU:HA	23:Y:210:GLU:HB3	2.01	0.42
34:1:961:VAL:C	34:1:963:LYS:N	2.69	0.42
34:1:1199:VAL:HG12	34:1:1199:VAL:O	2.19	0.42
34:1:1255:PHE:CE2	36:2:487:LEU:HD21	2.54	0.42
35:3:16:PHE:HE2	35:3:63:ARG:C	2.22	0.42
35:3:665:LEU:HB2	35:3:679:LEU:HD23	2.00	0.42
35:3:671:ASN:HB3	35:3:696:SER:HA	2.01	0.42
35:3:822:GLU:H	35:3:822:GLU:HG3	1.64	0.42
35:3:1156:CYS:O	35:3:1158:ARG:N	2.50	0.42
39:5:12:GLU:HA	39:5:15:GLN:HB3	2.01	0.42
1:A:382:GLU:N	1:A:382:GLU:OE1	2.52	0.42
1:A:1169:GLN:O	1:A:1173:SER:OG	2.24	0.42
1:A:1965:HIS:N	1:A:1965:HIS:CD2	2.87	0.42
3:C:505:GLN:HG3	3:C:507:VAL:HG13	2.00	0.42
3:C:506:PRO:HB2	3:C:569:ARG:HH22	1.84	0.42
3:C:665:THR:OG1	3:C:666:VAL:N	2.52	0.42
7:H:152:G:C6	7:H:153:A:N6	2.87	0.42
11:M:186:LEU:HA	11:M:186:LEU:HD22	1.82	0.42
16:R:356:ARG:O	16:R:360:ARG:HB2	2.19	0.42
16:R:367:ARG:HD2	16:R:368:ASN:N	2.35	0.42
16:R:391:VAL:HG13	16:R:396:VAL:HB	2.01	0.42
22:X:431:GLN:HA	22:X:434:GLN:NE2	2.35	0.42
22:X:658:ARG:HE	22:X:658:ARG:HB3	1.73	0.42
34:1:501:LEU:HD23	34:1:501:LEU:HA	1.72	0.42
34:1:1249:TYR:CD2	36:2:587:HIS:CE1	3.06	0.42
34:1:1252:GLN:OE1	36:2:499:PRO:HB3	2.19	0.42
34:1:1273:TYR:O	34:1:1277:GLN:HB3	2.19	0.42
35:3:896:PHE:H	35:3:896:PHE:HD2	1.67	0.42
35:3:1151:GLU:OE2	35:3:1193:VAL:HG21	2.18	0.42
36:2:477:MET:HA	36:2:480:VAL:CG1	2.44	0.42
36:2:598:GLU:HA	36:2:598:GLU:OE2	2.19	0.42
1:A:435:CYS:SG	6:G:-10:G:N1	2.70	0.42
1:A:623:LYS:O	42:A:3000:IHP:O44	2.37	0.42
1:A:800:TYR:HB3	3:C:59:LEU:HD23	2.00	0.42
1:A:1489:LEU:HD12	1:A:1489:LEU:HA	1.77	0.42
1:A:1779:PHE:CD2	1:A:1862:ILE:HD11	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:U:C2'	2:B:47:A:H5'	2.49	0.42
3:C:193:THR:HB	3:C:428:THR:HG21	2.01	0.42
5:F:35:A:C5	6:G:11:A:N1	2.87	0.42
5:F:35:A:H2	5:F:36:A:N6	2.16	0.42
5:F:36:A:H5"	5:F:37:C:OP2	2.20	0.42
5:F:92:A:H2'	5:F:93:G:C8	2.54	0.42
7:H:182:U:H2'	7:H:183:G:H8	1.85	0.42
9:J:183:ALA:O	10:L:142:ILE:HG12	2.19	0.42
10:L:201:LYS:HZ2	10:L:203:LYS:HG2	1.84	0.42
16:R:155:VAL:O	16:R:159:VAL:HG12	2.18	0.42
22:X:218:ASP:O	22:X:222:MET:HG2	2.19	0.42
34:1:497:ILE:CG1	34:1:526:PHE:CZ	2.94	0.42
34:1:550:HIS:CD2	34:1:551:LEU:HD22	2.49	0.42
34:1:679:ILE:O	34:1:682:HIS:N	2.46	0.42
34:1:936:VAL:HG12	34:1:937:LEU:HD12	2.01	0.42
34:1:1270:ASN:OD1	39:5:21:THR:CB	2.67	0.42
35:3:356:HIS:CE1	35:3:403:SER:HG	2.34	0.42
35:3:484:VAL:O	35:3:494:VAL:HB	2.19	0.42
35:3:568:MET:H	35:3:568:MET:HG2	1.58	0.42
35:3:1114:SER:HB2	35:3:1215:TYR:HE1	1.83	0.42
38:7:48:GLU:H	38:7:48:GLU:HG3	1.32	0.42
1:A:57:GLN:O	1:A:57:GLN:NE2	2.52	0.42
1:A:299:ILE:HD12	3:C:920:PRO:HB2	2.00	0.42
1:A:364:SER:O	1:A:366:LYS:HD3	2.19	0.42
1:A:758:ARG:NH2	1:A:775:ASN:HD22	2.15	0.42
1:A:1076:ASP:N	1:A:1076:ASP:OD1	2.52	0.42
1:A:1436:TRP:CZ3	1:A:1457:HIS:HB2	2.54	0.42
3:C:80:ILE:HG22	3:C:82:GLN:HG2	2.01	0.42
3:C:668:GLU:O	3:C:824:THR:OG1	2.37	0.42
3:C:763:LYS:O	3:C:767:VAL:HG22	2.20	0.42
5:F:73:A:OP1	5:F:75:G:O2'	2.33	0.42
10:L:131:ASN:O	10:L:135:LYS:NZ	2.53	0.42
12:N:37:HIS:O	12:N:37:HIS:CG	2.72	0.42
12:N:75:TYR:CZ	12:N:79:ILE:HD11	2.54	0.42
14:P:72:ARG:HA	14:P:75:ASN:HD21	1.83	0.42
22:X:277:ARG:O	22:X:281:ARG:HG2	2.20	0.42
22:X:419:ILE:HG21	22:X:569:VAL:HG22	2.02	0.42
22:X:787:GLU:O	22:X:790:LEU:HB3	2.19	0.42
22:X:862:VAL:HG13	22:X:863:HIS:CD2	2.54	0.42
23:Y:267:ARG:HB3	23:Y:287:GLU:HG2	2.02	0.42
34:1:666:LYS:O	34:1:670:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:823:MET:SD	34:1:829:ASN:ND2	2.92	0.42
34:1:972:GLY:CA	34:1:1010:THR:HG21	2.40	0.42
35:3:114:ARG:CZ	39:5:37:ARG:HD2	2.49	0.42
35:3:199:GLU:OE2	35:3:199:GLU:HA	2.19	0.42
35:3:436:ARG:HG2	35:3:778:ALA:CB	2.49	0.42
35:3:595:VAL:HG21	35:3:601:ARG:N	2.34	0.42
35:3:996:ILE:O	35:3:998:HIS:N	2.53	0.42
35:3:1116:SER:O	36:2:708:TRP:CZ2	2.69	0.42
36:2:458:ASN:ND2	36:2:458:ASN:C	2.72	0.42
36:2:465:LEU:HB3	36:2:475:VAL:HG11	2.01	0.42
1:A:711:GLN:HE22	7:H:18:U:C5'	2.30	0.42
1:A:856:LEU:H	1:A:856:LEU:HG	1.36	0.42
1:A:1802:PRO:HB3	1:A:1827:TRP:CZ3	2.55	0.42
1:A:1826:VAL:HB	1:A:1830:GLN:HE22	1.85	0.42
3:C:603:MET:O	3:C:607:LEU:HD12	2.18	0.42
3:C:762:VAL:HG23	3:C:808:ILE:HD12	2.02	0.42
9:J:256:LYS:HG3	10:L:235:LEU:HD23	2.01	0.42
10:L:168:LYS:O	10:L:172:ARG:HG3	2.20	0.42
10:L:205:LYS:H	10:L:205:LYS:CD	2.33	0.42
23:Y:224:LEU:CD1	23:Y:230:LEU:HD23	2.50	0.42
34:1:747:LEU:HD23	34:1:788:VAL:CB	2.49	0.42
34:1:754:ILE:HD12	34:1:754:ILE:HA	1.81	0.42
34:1:1244:CYS:HB3	35:3:1029:TYR:HE1	1.81	0.42
35:3:131:MET:HB2	35:3:141:VAL:HG22	2.01	0.42
35:3:185:LEU:HD23	35:3:185:LEU:HA	1.69	0.42
35:3:483:LEU:HD11	35:3:493:GLU:OE2	2.19	0.42
35:3:1175:ASP:OD1	35:3:1178:LEU:N	2.52	0.42
36:2:548:THR:O	36:2:551:SER:N	2.48	0.42
1:A:110:TRP:O	1:A:192:GLN:NE2	2.53	0.42
1:A:1503:TRP:HE3	1:A:1533:ARG:NH1	2.18	0.42
1:A:1963:GLU:O	1:A:1966:HIS:N	2.50	0.42
4:E:74:PHE:CZ	4:E:343:ILE:HG13	2.55	0.42
4:E:251:LEU:HB2	4:E:293:TRP:NE1	2.34	0.42
4:E:308:PHE:N	4:E:330:ILE:HD11	2.35	0.42
7:H:56:A:N6	36:2:505:CYS:HB3	2.35	0.42
8:I:213:ALA:HA	8:I:216:SER:O	2.20	0.42
8:I:512:ASP:O	8:I:514:ARG:N	2.52	0.42
9:J:299:TRP:O	9:J:303:ILE:HG23	2.18	0.42
10:L:164:GLY:O	10:L:167:ALA:CB	2.67	0.42
10:L:787:ARG:O	10:L:791:LEU:N	2.48	0.42
20:V:590:LEU:HB3	20:V:599:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:898:CYS:HB3	22:X:903:VAL:O	2.19	0.42
23:Y:30:LYS:O	23:Y:34:ILE:HG23	2.19	0.42
23:Y:35:LYS:NZ	23:Y:159:THR:O	2.50	0.42
35:3:182:PHE:O	35:3:210:PHE:HA	2.19	0.42
35:3:638:GLU:O	35:3:638:GLU:HG3	2.19	0.42
35:3:855:PRO:O	35:3:856:LYS:HD3	2.20	0.42
35:3:914:ILE:HG22	35:3:917:PRO:HD2	2.02	0.42
35:3:1199:ARG:HH21	35:3:1207:LYS:NZ	2.18	0.42
36:2:471:ARG:HE	36:2:471:ARG:HB3	1.49	0.42
36:2:506:PHE:N	36:2:506:PHE:CD1	2.88	0.42
38:7:30:CYS:SG	38:7:32:ILE:N	2.90	0.42
39:5:11:LEU:O	39:5:14:LEU:HB2	2.19	0.42
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.82	0.42
1:A:1000:ILE:HG22	1:A:1001:VAL:HG13	2.00	0.42
1:A:1633:ALA:HB2	1:A:1637:TRP:CZ3	2.55	0.42
1:A:1640:SER:HB3	1:A:1652:MET:HA	2.01	0.42
3:C:522:SER:O	3:C:522:SER:OG	2.36	0.42
3:C:736:GLY:HA2	3:C:771:GLN:HG2	2.02	0.42
3:C:809:ILE:CG1	3:C:810:PRO:HD3	2.49	0.42
3:C:810:PRO:HA	3:C:813:ARG:HG2	2.01	0.42
9:J:268:ALA:HB1	9:J:278:LEU:HD21	2.01	0.42
16:R:352:ARG:HA	16:R:355:ILE:HD12	2.02	0.42
18:T:309:ASP:O	18:T:310:SER:OG	2.26	0.42
20:V:452:LEU:HD11	20:V:456:ARG:CZ	2.49	0.42
20:V:487:LYS:H	20:V:487:LYS:HD3	1.85	0.42
22:X:814:LYS:NZ	22:X:814:LYS:HB2	2.34	0.42
22:X:1004:GLU:HB2	22:X:1007:TRP:CD2	2.55	0.42
23:Y:31:LEU:HD11	23:Y:66:ILE:N	2.35	0.42
34:1:493:LYS:O	34:1:496:LYS:N	2.52	0.42
34:1:551:LEU:O	34:1:554:LYS:HB3	2.19	0.42
34:1:612:THR:HB	34:1:613:MET:HE2	2.01	0.42
34:1:740:GLY:H	34:1:743:LEU:HD22	1.84	0.42
34:1:816:LYS:HB3	34:1:816:LYS:HE3	1.82	0.42
35:3:58:VAL:HG21	35:3:62:ILE:CD1	2.49	0.42
35:3:288:VAL:HG12	39:5:62:ALA:HB3	2.02	0.42
35:3:408:LEU:HD12	35:3:427:CYS:HA	2.02	0.42
35:3:947:GLU:HG3	35:3:948:VAL:H	1.84	0.42
35:3:969:VAL:HB	35:3:981:CYS:CB	2.45	0.42
1:A:35:ARG:HG2	1:A:35:ARG:HH11	1.84	0.42
1:A:525:LYS:HB2	1:A:525:LYS:NZ	2.34	0.42
1:A:1217:GLN:OE1	1:A:1224:ARG:NE	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1397:ILE:HD13	1:A:1397:ILE:HA	1.72	0.42
3:C:440:SER:O	3:C:442:LYS:N	2.52	0.42
3:C:907:VAL:HA	3:C:908:PRO:HD3	1.83	0.42
4:E:313:ASP:OD1	4:E:316:SER:OG	2.32	0.42
4:E:341:ILE:C	4:E:342:ILE:HD13	2.39	0.42
6:G:100:C:H4'	6:G:101:U:O2	2.19	0.42
9:J:238:ASN:O	9:J:239:ARG:HB3	2.20	0.42
22:X:450:CYS:O	22:X:495:TYR:HA	2.20	0.42
22:X:595:CYS:O	22:X:599:VAL:HG22	2.20	0.42
22:X:887:GLN:O	22:X:890:GLU:HB3	2.19	0.42
23:Y:24:ALA:HA	23:Y:78:PHE:CZ	2.53	0.42
34:1:594:ARG:O	34:1:634:VAL:HG13	2.20	0.42
34:1:632:PHE:HA	34:1:635:VAL:HG22	2.02	0.42
34:1:739:ARG:NH1	34:1:740:GLY:HA2	2.33	0.42
34:1:796:CYS:O	34:1:843:LYS:HG3	2.20	0.42
34:1:815:PHE:HA	34:1:819:TRP:HD1	1.83	0.42
34:1:949:GLN:OE1	34:1:989:VAL:CG2	2.58	0.42
34:1:1179:ASP:H	36:2:511:LEU:CB	2.33	0.42
34:1:1243:PRO:HD3	35:3:1167:TYR:O	2.16	0.42
35:3:541:LYS:HD3	35:3:541:LYS:HA	1.87	0.42
35:3:675:LEU:HB3	35:3:686:LEU:HD12	2.02	0.42
35:3:1083:ASN:O	35:3:1085:ALA:N	2.48	0.42
1:A:1776:ILE:HG23	1:A:1859:LYS:HG3	2.02	0.42
3:C:243:ILE:HG13	3:C:244:LYS:N	2.33	0.42
3:C:381:LEU:CD2	3:C:416:LEU:HD21	2.49	0.42
3:C:602:LYS:HE2	3:C:602:LYS:HB3	1.84	0.42
5:F:45:A:N6	6:G:3:A:C8	2.88	0.42
6:G:88:G:N2	7:H:41:U:O2	2.46	0.42
6:G:105:C:H41	22:X:856:ARG:NH1	2.18	0.42
12:N:2:PRO:O	12:N:4:VAL:N	2.53	0.42
14:P:73:GLU:HG2	14:P:76:ARG:NH2	2.34	0.42
16:R:352:ARG:HG2	16:R:356:ARG:HH21	1.85	0.42
16:R:352:ARG:HG2	16:R:356:ARG:NH2	2.35	0.42
20:V:617:PRO:HB2	20:V:624:THR:OG1	2.19	0.42
22:X:406:GLU:HA	22:X:409:LEU:CD2	2.48	0.42
22:X:480:SER:HB3	22:X:500:MET:HE1	2.02	0.42
22:X:692:PRO:HA	22:X:737:LEU:HB2	2.02	0.42
34:1:664:GLY:O	34:1:668:VAL:HG23	2.20	0.42
34:1:1109:ARG:O	34:1:1112:THR:HG23	2.20	0.42
34:1:1137:ARG:HH12	36:2:522:PHE:H	1.67	0.42
34:1:1227:ILE:O	34:1:1231:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:3:1:MET:HG3	35:3:1092:ILE:HD12	2.02	0.42
35:3:91:GLU:OE1	35:3:102:ILE:HD11	2.20	0.42
35:3:164:ASN:ND2	35:3:190:GLU:HG2	2.35	0.42
35:3:275:ARG:HB3	35:3:386:PHE:HB3	2.02	0.42
35:3:605:LEU:HB3	35:3:619:LEU:HD22	2.02	0.42
1:A:1604:LEU:HB3	1:A:1606:ILE:CD1	2.49	0.42
42:A:3000:IHP:O12	42:A:3000:IHP:P1	2.78	0.42
3:C:299:ILE:HD13	3:C:299:ILE:HA	1.79	0.42
5:F:92:A:H2'	5:F:93:G:H8	1.85	0.42
7:H:36:G:H2'	7:H:37:U:H6	1.84	0.42
7:H:118:G:C6	7:H:140:A:N6	2.87	0.42
9:J:278:LEU:HD12	9:J:278:LEU:HA	1.69	0.42
18:T:423:SER:HB3	18:T:474:GLU:OE1	2.20	0.42
22:X:832:GLU:HG2	22:X:927:VAL:HG22	2.02	0.42
23:Y:41:LEU:HD23	23:Y:155:ARG:HH12	1.85	0.42
34:1:750:ILE:O	34:1:754:ILE:N	2.53	0.42
34:1:892:LEU:HA	34:1:892:LEU:HD22	1.70	0.42
35:3:43:PRO:HA	35:3:50:VAL:HA	2.01	0.42
35:3:128:ARG:HH21	35:3:180:PRO:HG3	1.85	0.42
35:3:228:LEU:HD12	35:3:229:GLU:N	2.28	0.42
35:3:789:VAL:HG13	35:3:891:VAL:HG13	2.01	0.42
1:A:47:GLU:OE1	1:A:47:GLU:N	2.52	0.41
1:A:120:TYR:HE1	1:A:485:THR:HG1	1.68	0.41
1:A:599:MET:HA	1:A:602:ILE:HB	2.01	0.41
1:A:1661:TRP:CD2	1:A:1700:GLY:HA3	2.55	0.41
3:C:420:CYS:O	3:C:424:PHE:HB2	2.20	0.41
3:C:662:PHE:HE1	3:C:829:GLU:HB3	1.84	0.41
3:C:809:ILE:H	3:C:809:ILE:HG12	1.46	0.41
5:F:10:U:H2'	5:F:11:C:C4'	2.50	0.41
8:I:374:ILE:O	8:I:376:ASN:N	2.52	0.41
11:M:160:PHE:O	11:M:162:PRO:HD3	2.19	0.41
12:N:41:ARG:HB3	12:N:44:GLU:HG2	2.02	0.41
13:O:34:ILE:O	16:R:197:ILE:HA	2.20	0.41
16:R:387:ASP:OD1	16:R:388:ILE:N	2.53	0.41
20:V:600:ASN:OD1	20:V:639:LEU:HB2	2.20	0.41
22:X:932:CYS:HB2	22:X:938:ARG:HD2	2.01	0.41
23:Y:204:SER:OG	23:Y:207:GLU:HG2	2.20	0.41
23:Y:317:GLN:NE2	23:Y:317:GLN:HA	2.35	0.41
34:1:777:PHE:CG	34:1:814:PHE:HA	2.55	0.41
34:1:903:GLN:OE1	34:1:910:MET:HB2	2.19	0.41
35:3:274:ARG:NH1	35:3:309:ASP:OD1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2:548:THR:O	36:2:550:LYS:N	2.52	0.41
1:A:79:ARG:HG2	1:A:82:ARG:HG3	2.02	0.41
1:A:119:LEU:HD11	1:A:482:PHE:HB3	2.03	0.41
1:A:265:THR:OG1	1:A:328:HIS:O	2.38	0.41
1:A:451:LEU:HA	1:A:451:LEU:HD23	1.86	0.41
1:A:857:ASN:OD1	1:A:859:SER:N	2.53	0.41
1:A:1122:ASN:OD1	1:A:1122:ASN:N	2.53	0.41
1:A:1310:ARG:NH1	1:A:1566:ILE:HD11	2.35	0.41
1:A:1385:VAL:HG12	1:A:1419:ILE:HD11	2.01	0.41
1:A:1633:ALA:HB3	1:A:1658:GLN:HA	2.02	0.41
42:A:3000:IHP:P3	42:A:3000:IHP:O24	2.79	0.41
2:B:9:G:H2'	2:B:10:U:C6	2.55	0.41
3:C:121:ASP:OD1	3:C:122:LEU:N	2.53	0.41
3:C:801:LEU:HD13	3:C:802:HIS:CE1	2.56	0.41
3:C:940:ARG:H	3:C:940:ARG:HG2	1.71	0.41
4:E:179:TRP:HA	4:E:187:ILE:HG12	2.02	0.41
4:E:321:TYR:HB3	4:E:323:LEU:HG	2.02	0.41
9:J:189:ILE:HG21	10:L:152:LEU:HD22	2.02	0.41
10:L:146:GLU:HA	10:L:149:LEU:HD12	2.02	0.41
11:M:153:ARG:HA	11:M:160:PHE:CE2	2.55	0.41
20:V:603:LEU:HA	20:V:603:LEU:HD12	1.79	0.41
22:X:169:ARG:O	22:X:173:GLN:HG3	2.20	0.41
23:Y:18:THR:HB	23:Y:166:PHE:CE2	2.55	0.41
23:Y:241:VAL:O	23:Y:316:SER:HB3	2.20	0.41
34:1:1257:PRO:HD3	36:2:488:LEU:HD11	2.02	0.41
35:3:311:PHE:HZ	35:3:387:PHE:CE2	2.38	0.41
35:3:791:HIS:CB	35:3:796:ASN:O	2.68	0.41
38:7:58:CYS:N	38:7:63:GLY:O	2.52	0.41
38:7:85:CYS:HA	38:7:86:PRO:HD3	1.89	0.41
1:A:1352:HIS:CD2	19:U:5:ILE:HG12	2.55	0.41
1:A:1684:PHE:HB2	1:A:1702:LEU:HD11	2.03	0.41
1:A:1781:ASP:HB2	1:A:1808:PHE:HB3	2.01	0.41
1:A:1847:ALA:O	1:A:1850:ARG:HB3	2.21	0.41
1:A:1868:MET:C	1:A:1871:PRO:HD2	2.41	0.41
2:B:101:U:H2'	2:B:102:U:H6	1.85	0.41
3:C:174:GLU:OE1	3:C:182:LYS:NZ	2.53	0.41
3:C:529:ARG:HH12	3:C:540:GLU:HG3	1.86	0.41
4:E:313:ASP:HB3	4:E:320:LEU:HD11	2.02	0.41
9:J:400:GLU:OE2	9:J:401:ARG:HG3	2.20	0.41
16:R:377:ARG:HG2	16:R:377:ARG:NH2	2.35	0.41
20:V:612:PHE:O	20:V:616:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:610:ASP:HB2	22:X:686:ILE:HA	2.02	0.41
23:Y:41:LEU:HD23	23:Y:155:ARG:NH1	2.34	0.41
34:1:504:ILE:HG13	34:1:515:ALA:HB3	2.03	0.41
34:1:933:CYS:O	34:1:934:GLY:C	2.58	0.41
34:1:949:GLN:HB2	34:1:989:VAL:HG21	1.93	0.41
34:1:967:GLU:O	34:1:971:MET:N	2.36	0.41
34:1:1216:TRP:CH2	34:1:1268:ILE:HD13	2.56	0.41
35:3:423:LEU:HB2	35:3:438:LEU:HB2	2.02	0.41
35:3:577:TYR:HE2	35:3:579:GLU:HB3	1.85	0.41
35:3:610:VAL:HA	35:3:636:GLN:HE21	1.85	0.41
35:3:615:ARG:C	35:3:616:ILE:HD12	2.41	0.41
35:3:715:MET:HE3	35:3:739:LEU:H	1.85	0.41
35:3:1035:THR:HG21	35:3:1103:SER:HA	2.01	0.41
35:3:1147:HIS:O	35:3:1150:SER:OG	2.33	0.41
1:A:456:LEU:HD22	1:A:460:LYS:NZ	2.35	0.41
1:A:569:VAL:O	1:A:570:ASP:HB2	2.19	0.41
1:A:1019:TYR:O	1:A:1021:ASP:N	2.53	0.41
2:B:93:U:O2’	2:B:94:U:O4’	2.38	0.41
3:C:286:ASN:ND2	3:C:299:ILE:HG23	2.35	0.41
3:C:493:PHE:CD2	3:C:551:LEU:HG	2.50	0.41
3:C:696:LEU:O	3:C:700:ILE:HG12	2.20	0.41
3:C:833:PHE:O	3:C:899:SER:HA	2.20	0.41
4:E:290:ARG:HG3	4:E:331:ASN:O	2.20	0.41
10:L:130:PRO:HB2	10:L:131:ASN:H	1.62	0.41
13:O:165:CYS:O	13:O:169:VAL:N	2.52	0.41
16:R:265:ASP:OD1	16:R:265:ASP:N	2.53	0.41
20:V:469:PHE:CZ	20:V:509:LEU:HD22	2.55	0.41
20:V:630:PHE:HD1	20:V:631:PHE:HD2	1.68	0.41
22:X:832:GLU:CD	22:X:928:GLY:H	2.23	0.41
34:1:646:PRO:O	34:1:649:LYS:HB2	2.20	0.41
34:1:850:ILE:CG2	34:1:888:LEU:CD2	2.92	0.41
35:3:66:MET:HE1	35:3:122:ALA:HA	2.02	0.41
35:3:180:PRO:HD2	35:3:215:LEU:HD11	2.03	0.41
35:3:212:GLU:CB	35:3:223:LYS:HG3	2.49	0.41
35:3:343:LYS:C	35:3:345:GLY:H	2.24	0.41
35:3:528:ARG:HG3	35:3:529:ALA:H	1.83	0.41
35:3:690:ARG:HH12	35:3:696:SER:H	1.67	0.41
35:3:1135:HIS:HA	35:3:1138:HIS:HB3	2.03	0.41
36:2:478:HIS:C	36:2:481:THR:HG22	2.39	0.41
1:A:55:ASP:O	12:N:109:ARG:NH2	2.53	0.41
1:A:300:ASN:OD1	1:A:300:ASN:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:LYS:HB3	1:A:796:LYS:HE3	1.80	0.41
1:A:1117:HIS:CE1	14:P:199:LYS:HG3	2.56	0.41
1:A:1636:LYS:HE3	1:A:1656:THR:HG23	2.01	0.41
1:A:1638:ASN:HA	1:A:1655:THR:O	2.20	0.41
3:C:480:LYS:C	3:C:481:MET:HG3	2.40	0.41
4:E:81:LEU:O	4:E:92:LEU:HA	2.21	0.41
5:F:23:U:C4	12:N:118:ILE:HD13	2.55	0.41
9:J:323:LEU:HA	9:J:323:LEU:HD23	1.77	0.41
12:N:55:GLN:HE21	12:N:55:GLN:HB2	1.75	0.41
18:T:423:SER:N	18:T:474:GLU:OE2	2.52	0.41
22:X:411:ALA:HA	22:X:414:ASN:ND2	2.36	0.41
22:X:535:LEU:HA	22:X:535:LEU:HD23	1.78	0.41
22:X:969:PHE:CD2	22:X:994:LYS:HG2	2.55	0.41
34:1:641:ILE:H	34:1:641:ILE:HG13	1.56	0.41
34:1:717:THR:CB	34:1:718:PRO:CD	2.94	0.41
34:1:769:VAL:O	34:1:772:ILE:HB	2.21	0.41
34:1:862:GLU:O	34:1:866:LYS:HB2	2.21	0.41
34:1:1292:LYS:CE	39:5:78:PRO:HG2	2.47	0.41
35:3:212:GLU:HG2	35:3:213:LEU:N	2.35	0.41
35:3:724:SER:HB2	35:3:727:SER:HA	2.01	0.41
35:3:1041:TYR:CB	36:2:705:ARG:CG	2.75	0.41
35:3:1096:HIS:ND1	35:3:1166:TYR:HB2	2.36	0.41
38:7:23:CYS:HB3	38:7:58:CYS:HB2	2.03	0.41
1:A:442:LYS:NZ	42:A:3000:IHP:O33	2.53	0.41
3:C:406:GLU:H	3:C:406:GLU:CD	2.21	0.41
3:C:736:GLY:O	3:C:738:ASP:N	2.53	0.41
3:C:828:MET:HG2	3:C:906:ILE:HD13	2.03	0.41
3:C:846:VAL:HB	3:C:887:LEU:HD11	2.02	0.41
20:V:476:LEU:O	20:V:479:MET:HB2	2.21	0.41
22:X:910:ARG:HA	22:X:913:ASP:OD2	2.20	0.41
34:1:686:LEU:HA	34:1:689:ILE:HG12	2.02	0.41
34:1:770:MET:SD	34:1:810:ILE:CD1	3.07	0.41
34:1:1245:ARG:CZ	36:2:587:HIS:HB2	2.50	0.41
34:1:1281:ILE:CG2	35:3:1050:PHE:CZ	2.87	0.41
35:3:941:HIS:CE1	35:3:974:LYS:HA	2.56	0.41
35:3:1015:LYS:NZ	35:3:1016:ARG:H	2.18	0.41
35:3:1200:THR:N	35:3:1203:GLU:OE1	2.38	0.41
1:A:57:GLN:HE21	1:A:57:GLN:C	2.23	0.41
1:A:305:ARG:HG3	3:C:878:ILE:HG21	2.01	0.41
1:A:611:LEU:HD12	1:A:611:LEU:HA	1.90	0.41
1:A:874:PRO:HB2	22:X:866:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:ASN:HD21	1:A:1140:MET:CB	2.33	0.41
1:A:1184:ASN:OD1	1:A:1195:ARG:NH1	2.51	0.41
1:A:1482:GLU:N	1:A:1482:GLU:OE2	2.53	0.41
3:C:353:THR:HG23	3:C:355:LYS:H	1.84	0.41
3:C:759:LEU:HA	3:C:759:LEU:HD12	1.83	0.41
7:H:168:A:H5"	7:H:169:C:C6	2.56	0.41
16:R:159:VAL:O	16:R:162:ALA:N	2.54	0.41
18:T:223:SER:OG	18:T:224:ALA:N	2.52	0.41
20:V:650:THR:HB	20:V:651:PRO:HD3	2.03	0.41
22:X:173:GLN:HA	22:X:176:GLU:OE2	2.21	0.41
22:X:483:PHE:HB2	22:X:484:GLU:OE1	2.20	0.41
22:X:981:PRO:HD2	22:X:984:LEU:HD13	2.02	0.41
23:Y:2:ALA:O	23:Y:162:LEU:HB3	2.20	0.41
34:1:556:ILE:O	34:1:560:LEU:HB2	2.21	0.41
34:1:662:HIS:HE1	34:1:700:LYS:HB3	1.81	0.41
34:1:854:VAL:HG23	34:1:855:ASP:N	2.34	0.41
34:1:933:CYS:SG	34:1:970:LEU:CG	3.08	0.41
35:3:66:MET:HE3	35:3:123:VAL:HG12	2.03	0.41
35:3:224:TYR:HB3	35:3:261:PHE:CD1	2.56	0.41
35:3:499:PHE:CZ	35:3:516:LEU:HD22	2.46	0.41
35:3:1131:PRO:CB	36:2:709:GLY:HA2	2.51	0.41
39:5:74:GLN:NE2	39:5:78:PRO:HA	2.36	0.41
1:A:296:PHE:HZ	3:C:593:GLU:HB2	1.85	0.41
1:A:1402:ARG:HD2	16:R:406:GLN:OE1	2.20	0.41
1:A:1885:LYS:HG2	1:A:1886:GLY:N	2.35	0.41
3:C:177:ARG:HA	3:C:177:ARG:HE	1.86	0.41
3:C:705:VAL:HB	3:C:717:PHE:CZ	2.55	0.41
4:E:168:CYS:SG	4:E:208:ILE:HD11	2.60	0.41
7:H:7:U:H2'	7:H:8:C:H6	1.82	0.41
7:H:36:G:H2'	7:H:37:U:C6	2.55	0.41
7:H:160:A:H2'	7:H:161:U:O4'	2.20	0.41
9:J:201:ARG:HH21	9:J:203:LEU:HD21	1.86	0.41
9:J:294:HIS:CE1	10:L:227:THR:OG1	2.73	0.41
10:L:26:TYR:CE1	10:L:33:ARG:HB3	2.56	0.41
10:L:749:LEU:O	10:L:753:GLU:N	2.48	0.41
14:P:66:ARG:HE	14:P:66:ARG:HB2	1.49	0.41
22:X:246:LEU:HG	22:X:277:ARG:CZ	2.51	0.41
22:X:393:GLN:HA	22:X:396:ARG:HB2	2.02	0.41
22:X:533:PHE:HE1	22:X:550:VAL:HG11	1.86	0.41
22:X:614:PHE:O	22:X:615:LEU:HD12	2.21	0.41
22:X:645:LEU:HB3	22:X:659:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:790:LEU:HD23	22:X:791:LEU:N	2.35	0.41
34:1:510:PRO:HA	34:1:513:LYS:HE2	2.03	0.41
34:1:777:PHE:CD2	34:1:814:PHE:N	2.89	0.41
35:3:164:ASN:N	35:3:164:ASN:OD1	2.53	0.41
35:3:289:CYS:SG	35:3:290:SER:N	2.94	0.41
35:3:968:ARG:HB2	35:3:970:TYR:CE2	2.47	0.41
1:A:62:PRO:HB2	1:A:64:GLU:OE1	2.20	0.41
1:A:131:GLU:HG2	1:A:132:ILE:N	2.35	0.41
1:A:631:ALA:O	1:A:635:ARG:HG3	2.21	0.41
1:A:888:GLN:C	1:A:889:ARG:HG2	2.41	0.41
1:A:962:LEU:HD23	1:A:962:LEU:HA	1.80	0.41
1:A:1012:LYS:O	1:A:1012:LYS:HG3	2.20	0.41
1:A:1194:CYS:HB3	1:A:1228:CYS:SG	2.60	0.41
1:A:1457:HIS:O	1:A:1461:ASP:HB2	2.20	0.41
1:A:1581:LEU:O	1:A:1585:ILE:HG13	2.20	0.41
1:A:1933:PHE:O	1:A:1937:ILE:HG13	2.21	0.41
1:A:2002:LEU:HD22	1:A:2006:GLU:OE1	2.21	0.41
3:C:95:LYS:HA	3:C:96:PRO:HD3	1.90	0.41
3:C:129:ILE:HA	3:C:199:LEU:O	2.21	0.41
3:C:501:ILE:HG22	3:C:530:LEU:HD11	2.01	0.41
3:C:516:LEU:HD23	3:C:516:LEU:H	1.86	0.41
4:E:125:PHE:CD2	4:E:125:PHE:N	2.89	0.41
4:E:197:LEU:HD21	4:E:213:ILE:HD11	2.03	0.41
6:G:99:C:N4	6:G:100:C:H42	2.19	0.41
7:H:15:U:O3’	7:H:16:U:H2’	2.21	0.41
7:H:28:C:O2’	7:H:29:A:C4	2.69	0.41
7:H:38:A:H2’	7:H:39:U:C6	2.56	0.41
7:H:55:U:H2’	7:H:57:A:OP2	2.21	0.41
10:L:161:ASN:OD1	10:L:168:LYS:CD	2.53	0.41
10:L:170:LYS:HA	10:L:173:GLU:HG2	2.03	0.41
10:L:173:GLU:HA	10:L:176:LEU:HB3	2.02	0.41
16:R:114:SER:HB3	16:R:228:PRO:HG2	2.02	0.41
16:R:213:LYS:NZ	16:R:215:ASN:OD1	2.48	0.41
16:R:238:THR:OG1	16:R:239:VAL:N	2.53	0.41
16:R:408:ASP:HB3	16:R:411:LEU:HD23	2.02	0.41
18:T:207:VAL:HG12	18:T:480:ALA:HB1	2.03	0.41
18:T:297:HIS:CG	18:T:298:PRO:HD2	2.56	0.41
18:T:306:CYS:HB2	18:T:333:VAL:HG12	2.02	0.41
20:V:495:ASP:O	20:V:498:ALA:HB3	2.21	0.41
20:V:617:PRO:HB3	20:V:623:ASN:HD22	1.86	0.41
22:X:246:LEU:HG	22:X:277:ARG:HE	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:389:LYS:NZ	22:X:390:GLU:HG3	2.35	0.41
22:X:422:GLY:O	22:X:553:ALA:HA	2.20	0.41
22:X:595:CYS:SG	22:X:613:VAL:HG11	2.61	0.41
22:X:674:THR:HG22	22:X:675:ASN:H	1.86	0.41
22:X:716:LYS:HB2	22:X:748:GLU:O	2.21	0.41
23:Y:255:ASP:OD2	23:Y:259:ILE:HD11	2.21	0.41
34:1:555:VAL:HG12	34:1:559:ILE:HD13	2.02	0.41
34:1:702:ARG:CG	34:1:738:HIS:CD2	3.03	0.41
34:1:777:PHE:CA	34:1:818:PHE:HE2	2.30	0.41
34:1:914:PHE:O	34:1:917:VAL:HG12	2.21	0.41
34:1:1262:ARG:CA	39:5:24:ALA:HB1	2.49	0.41
34:1:1300:LEU:HD22	35:3:1032:TRP:CD2	2.56	0.41
35:3:280:ASP:H	35:3:857:ALA:CB	2.33	0.41
35:3:610:VAL:HG23	35:3:636:GLN:NE2	2.36	0.41
35:3:1022:ILE:HD13	35:3:1022:ILE:HA	1.77	0.41
35:3:1188:ASN:HA	35:3:1191:LYS:HZ3	1.85	0.41
36:2:510:TYR:O	36:2:511:LEU:HD23	2.20	0.41
1:A:27:GLU:O	1:A:31:GLN:HG2	2.21	0.41
1:A:76:MET:HE3	1:A:76:MET:HB3	1.73	0.41
1:A:387:PHE:HZ	3:C:330:THR:HG21	1.85	0.41
1:A:615:ARG:HE	1:A:615:ARG:HB2	1.69	0.41
1:A:1636:LYS:HE3	1:A:1656:THR:CG2	2.51	0.41
1:A:1831:LYS:HZ3	1:A:1832:ARG:HB2	1.85	0.41
5:F:8:C:H3'	5:F:9:U:O4'	2.20	0.41
5:F:33:G:C2	5:F:34:G:H8	2.39	0.41
6:G:7:G:C2	6:G:8:C:C2	3.09	0.41
9:J:200:GLU:OE1	9:J:200:GLU:CA	2.69	0.41
9:J:394:HIS:O	9:J:398:VAL:HG23	2.21	0.41
12:N:91:LYS:HA	12:N:91:LYS:HD3	1.80	0.41
13:O:200:ASP:O	13:O:204:GLY:N	2.46	0.41
18:T:320:LYS:HE2	18:T:320:LYS:HB2	1.64	0.41
20:V:402:LYS:O	20:V:406:LEU:N	2.53	0.41
20:V:458:THR:HG21	20:V:479:MET:HE1	2.03	0.41
22:X:387:GLN:NE2	22:X:391:SER:OG	2.54	0.41
22:X:466:ALA:HA	22:X:469:MET:HB2	2.03	0.41
22:X:856:ARG:HB3	22:X:856:ARG:CZ	2.51	0.41
22:X:931:SER:O	22:X:933:GLN:NE2	2.54	0.41
22:X:955:THR:OG1	22:X:958:GLY:O	2.24	0.41
23:Y:41:LEU:HA	23:Y:155:ARG:HA	2.02	0.41
23:Y:47:ARG:HA	23:Y:140:ASN:HD21	1.85	0.41
23:Y:55:ASP:OD1	23:Y:57:THR:OG1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:729:LYS:O	34:1:733:LYS:HG2	2.21	0.41
34:1:961:VAL:O	34:1:964:THR:N	2.54	0.41
34:1:1145:ASN:HD21	34:1:1183:VAL:CG1	2.27	0.41
34:1:1208:LEU:HB3	34:1:1237:LEU:HD21	2.03	0.41
35:3:334:PRO:HG2	35:3:357:TYR:CD2	2.56	0.41
35:3:469:GLU:OE1	35:3:469:GLU:N	2.53	0.41
35:3:1001:ILE:HG21	35:3:1044:VAL:HG21	2.02	0.41
35:3:1004:ASP:OD2	35:3:1007:GLU:HB2	2.21	0.41
1:A:519:ASP:OD2	1:A:523:ASN:HB2	2.20	0.40
2:B:13:C:H2'	2:B:14:U:H6	1.85	0.40
3:C:415:LEU:HD12	3:C:415:LEU:HA	1.83	0.40
3:C:572:GLU:HG3	3:C:573:GLU:H	1.86	0.40
3:C:680:ASN:O	3:C:682:LYS:N	2.53	0.40
3:C:717:PHE:CE1	3:C:721:LYS:HE2	2.55	0.40
4:E:136:TRP:CZ3	4:E:143:ARG:HG2	2.56	0.40
4:E:208:ILE:HA	4:E:208:ILE:HD12	1.81	0.40
5:F:94:C:H2'	5:F:95:G:C8	2.56	0.40
6:G:-8:C:O4'	19:U:18:TYR:HB2	2.22	0.40
6:G:8:C:H2'	6:G:9:C:C4	2.57	0.40
10:L:186:GLN:HG3	10:L:189:ARG:HH12	1.87	0.40
16:R:376:LYS:CA	16:R:379:LYS:HB2	2.42	0.40
16:R:412:PHE:HE2	22:X:326:GLN:HE22	1.68	0.40
20:V:529:PHE:CE1	20:V:564:VAL:HB	2.56	0.40
21:W:279:LYS:CB	36:2:623:PRO:N	2.84	0.40
22:X:832:GLU:OE1	22:X:927:VAL:HG13	2.21	0.40
22:X:909:ARG:HG2	22:X:909:ARG:HH11	1.85	0.40
23:Y:26:LEU:HB2	23:Y:166:PHE:CG	2.56	0.40
23:Y:212:LYS:HA	23:Y:212:LYS:HD2	1.80	0.40
34:1:534:GLN:O	34:1:538:LEU:HD12	2.20	0.40
34:1:702:ARG:HG2	34:1:738:HIS:NE2	2.35	0.40
34:1:881:ALA:HB1	34:1:921:LEU:HD23	2.03	0.40
34:1:1244:CYS:O	34:1:1245:ARG:C	2.60	0.40
35:3:226:GLU:HG3	35:3:226:GLU:O	2.22	0.40
35:3:328:LYS:NZ	35:3:370:GLU:HB3	2.36	0.40
35:3:637:PRO:HB3	35:3:640:LEU:HD21	2.03	0.40
35:3:820:ALA:HA	35:3:823:MET:HE1	2.02	0.40
35:3:911:LYS:HG3	35:3:912:ASP:CG	2.42	0.40
35:3:1001:ILE:HD12	35:3:1011:TRP:NE1	2.36	0.40
1:A:83:HIS:NE2	6:G:16:G:C6	2.89	0.40
1:A:461:HIS:O	1:A:462:ARG:NH1	2.54	0.40
1:A:578:LEU:HD23	1:A:578:LEU:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:ASN:HA	1:A:621:VAL:HB	2.02	0.40
1:A:850:TYR:HD2	1:A:864:LEU:HD21	1.85	0.40
1:A:1409:GLU:OE2	1:A:1409:GLU:HA	2.20	0.40
1:A:1821:ILE:HD11	1:A:1911:GLU:O	2.22	0.40
1:A:1865:ARG:HA	1:A:1865:ARG:HH21	1.86	0.40
4:E:145:LYS:NZ	4:E:181:ILE:O	2.44	0.40
7:H:13:C:H5"	7:H:14:C:C5	2.56	0.40
7:H:142:U:C2	7:H:143:C:C5	3.09	0.40
18:T:405:PHE:HZ	18:T:408:ASN:OD1	2.04	0.40
22:X:723:ALA:HA	22:X:734:CYS:SG	2.61	0.40
23:Y:33:LYS:HA	23:Y:33:LYS:HD3	1.67	0.40
34:1:699:GLN:NE2	34:1:739:ARG:O	2.54	0.40
34:1:949:GLN:CA	34:1:989:VAL:CG1	2.88	0.40
34:1:1055:TRP:CE3	34:1:1055:TRP:HA	2.56	0.40
34:1:1185:ARG:HE	34:1:1185:ARG:HB2	1.43	0.40
34:1:1304:LEU:HD21	35:3:786:ARG:CZ	2.50	0.40
35:3:459:VAL:HA	35:3:475:ILE:O	2.21	0.40
35:3:485:LEU:CD2	35:3:491:VAL:HG12	2.46	0.40
35:3:615:ARG:O	35:3:616:ILE:HD12	2.21	0.40
35:3:998:HIS:CE1	35:3:1041:TYR:OH	2.75	0.40
35:3:1057:ARG:O	35:3:1090:GLU:HG3	2.22	0.40
35:3:1115:GLU:HG3	36:2:708:TRP:HE1	1.85	0.40
35:3:1165:SER:CB	35:3:1169:PRO:HA	2.52	0.40
1:A:229:GLN:O	1:A:230:PHE:HD1	2.03	0.40
1:A:264:PHE:CD1	1:A:459:LEU:HD13	2.57	0.40
1:A:1130:ASN:HD21	1:A:1140:MET:HB2	1.87	0.40
1:A:1776:ILE:HG22	1:A:1859:LYS:NZ	2.35	0.40
1:A:1776:ILE:CG2	1:A:1859:LYS:HG3	2.51	0.40
1:A:1777:ILE:HA	1:A:1860:GLN:O	2.21	0.40
3:C:183:SER:HG	3:C:480:LYS:HZ1	1.61	0.40
4:E:219:VAL:O	4:E:228:THR:N	2.54	0.40
6:G:5:G:N1	6:G:6:A:N6	2.69	0.40
6:G:7:G:C5	6:G:8:C:C4	3.10	0.40
7:H:56:A:N7	36:2:505:CYS:SG	2.94	0.40
10:L:169:ARG:O	10:L:173:GLU:HG2	2.22	0.40
11:M:114:LYS:HA	11:M:114:LYS:HD3	1.88	0.40
14:P:206:LYS:O	14:P:209:ARG:O	2.39	0.40
16:R:325:ARG:HH12	23:Y:226:MET:N	2.19	0.40
16:R:376:LYS:HA	16:R:379:LYS:CB	2.44	0.40
22:X:681:LEU:H	22:X:725:ARG:NH2	2.19	0.40
22:X:716:LYS:N	22:X:747:LEU:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:868:ARG:HH22	22:X:973:ASN:HD21	1.69	0.40
22:X:929:LEU:HD23	22:X:929:LEU:HA	1.89	0.40
23:Y:145:ASP:OD2	23:Y:190:ARG:NH2	2.54	0.40
23:Y:247:LEU:HG	23:Y:248:ASN:N	2.36	0.40
34:1:513:LYS:HE2	34:1:513:LYS:HB2	1.91	0.40
34:1:601:ALA:HB3	34:1:638:ALA:HB3	2.02	0.40
34:1:606:LEU:O	34:1:610:ILE:CG1	2.70	0.40
34:1:739:ARG:CA	34:1:743:LEU:CD2	2.94	0.40
34:1:777:PHE:HZ	34:1:810:ILE:HG23	1.86	0.40
34:1:897:LEU:HD21	34:1:932:ILE:HG13	2.04	0.40
34:1:1028:HIS:HB3	34:1:1031:VAL:HG13	2.02	0.40
34:1:1297:ARG:HH21	35:3:1032:TRP:HZ2	1.68	0.40
35:3:77:TYR:HE2	35:3:152:LEU:HD22	1.85	0.40
35:3:139:LYS:O	35:3:140:LEU:HD23	2.21	0.40
35:3:288:VAL:HG23	35:3:289:CYS:N	2.30	0.40
35:3:605:LEU:N	35:3:617:ILE:O	2.55	0.40
35:3:779:PHE:HA	35:3:780:PRO:HD3	1.95	0.40
38:7:26:CYS:SG	38:7:60:ILE:HG13	2.61	0.40
39:5:53:PHE:O	39:5:57:GLU:HG2	2.21	0.40
1:A:545:HIS:O	1:A:549:GLU:HG2	2.21	0.40
1:A:1131:LYS:HE2	1:A:1174:PHE:CE2	2.55	0.40
1:A:1215:ASN:HB3	1:A:1224:ARG:HH11	1.86	0.40
1:A:1342:TRP:HB2	1:A:1348:VAL:HG21	2.03	0.40
1:A:1362:ASP:O	1:A:1364:LEU:N	2.49	0.40
3:C:368:SER:O	3:C:372:PHE:HB2	2.21	0.40
5:F:39:A:C2'	5:F:40:U:H5'	2.51	0.40
5:F:47:A:H4'	5:F:48:A:OP1	2.21	0.40
10:L:11:TRP:CD2	10:L:49:ARG:HD3	2.56	0.40
10:L:55:ASP:OD2	10:L:57:SER:HB3	2.22	0.40
10:L:141:PRO:HG2	10:L:144:MET:HA	2.03	0.40
10:L:154:GLU:HG3	10:L:155:ALA:N	2.35	0.40
12:N:66:LYS:HD2	12:N:66:LYS:HA	1.84	0.40
16:R:178:ARG:HD3	16:R:194:GLN:OE1	2.21	0.40
19:U:5:ILE:O	19:U:5:ILE:HD12	2.21	0.40
20:V:461:LEU:HA	20:V:461:LEU:HD23	1.88	0.40
22:X:216:GLU:HG2	22:X:217:GLU:N	2.37	0.40
22:X:423:GLU:HB2	22:X:574:GLY:O	2.22	0.40
22:X:753:PRO:HG2	22:X:782:ASP:OD2	2.22	0.40
34:1:549:ARG:O	34:1:553:VAL:HG22	2.22	0.40
34:1:596:ILE:HA	34:1:599:ASN:HD22	1.86	0.40
34:1:846:ALA:HB2	34:1:883:ASP:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:912:ASN:OD1	34:1:912:ASN:N	2.53	0.40
34:1:1255:PHE:CD2	36:2:491:LEU:CD1	3.04	0.40
35:3:258:TYR:CG	35:3:259:LYS:N	2.90	0.40
35:3:373:PHE:HD1	35:3:385:PHE:CG	2.40	0.40
35:3:497:SER:OG	35:3:499:PHE:HB2	2.21	0.40
35:3:719:SER:OG	35:3:734:LEU:HB2	2.22	0.40
35:3:895:ARG:HG2	35:3:903:TRP:HA	2.04	0.40
35:3:926:TYR:CD1	35:3:942:LYS:HB3	2.56	0.40
36:2:487:LEU:HA	36:2:487:LEU:HD12	1.85	0.40
38:7:51:TYR:CG	38:7:52:GLY:N	2.90	0.40
1:A:366:LYS:HG3	20:V:324:HIS:O	2.21	0.40
1:A:1651:VAL:O	1:A:1651:VAL:HG23	2.21	0.40
3:C:823:ALA:O	3:C:824:THR:OG1	2.35	0.40
4:E:96:TYR:HH	4:E:336:HIS:HE2	1.68	0.40
7:H:30:A:H3'	7:H:31:G:H5"	2.04	0.40
10:L:186:GLN:HG3	10:L:189:ARG:NH1	2.37	0.40
16:R:124:VAL:O	16:R:124:VAL:CG1	2.69	0.40
18:T:412:HIS:NE2	18:T:431:ALA:HB2	2.37	0.40
20:V:553:HIS:HA	20:V:556:TYR:CD1	2.56	0.40
22:X:173:GLN:O	22:X:176:GLU:HG2	2.22	0.40
22:X:404:PHE:O	22:X:408:LEU:HD23	2.22	0.40
22:X:480:SER:HB3	22:X:500:MET:HE2	2.03	0.40
23:Y:136:ILE:O	23:Y:140:ASN:HB2	2.22	0.40
34:1:669:GLN:NE2	34:1:707:LEU:HD22	2.37	0.40
34:1:747:LEU:HD11	34:1:773:LEU:CD2	2.52	0.40
34:1:835:ASP:O	34:1:839:GLU:HG2	2.22	0.40
34:1:893:ILE:HG22	34:1:894:ASP:OD2	2.22	0.40
34:1:921:LEU:HD23	34:1:921:LEU:HA	1.86	0.40
34:1:1108:ASN:OD1	34:1:1108:ASN:N	2.51	0.40
34:1:1160:GLU:CD	34:1:1160:GLU:N	2.73	0.40
34:1:1179:ASP:H	36:2:511:LEU:HB3	1.86	0.40
35:3:70:LEU:HA	35:3:70:LEU:HD23	1.78	0.40
35:3:174:ASP:HB3	35:3:240:GLY:H	1.86	0.40
35:3:184:CYS:SG	35:3:211:TYR:CE1	3.14	0.40
35:3:278:LEU:HA	35:3:815:ARG:NH1	2.37	0.40
35:3:316:GLU:HG3	35:3:324:GLU:OE1	2.22	0.40
35:3:553:GLN:OE1	35:3:553:GLN:N	2.47	0.40
35:3:601:ARG:HB2	35:3:620:ASP:OD2	2.22	0.40
35:3:755:VAL:HG22	35:3:764:ILE:CD1	2.52	0.40
35:3:998:HIS:HE1	35:3:1041:TYR:OH	2.04	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	1961/2335 (84%)	1760 (90%)	186 (10%)	15 (1%)	19 57
3	C	854/972 (88%)	751 (88%)	100 (12%)	3 (0%)	34 72
4	E	297/357 (83%)	270 (91%)	27 (9%)	0	100 100
8	I	662/855 (77%)	575 (87%)	86 (13%)	1 (0%)	47 82
9	J	527/848 (62%)	487 (92%)	36 (7%)	4 (1%)	19 57
10	L	375/802 (47%)	360 (96%)	15 (4%)	0	100 100
11	M	112/243 (46%)	105 (94%)	5 (4%)	2 (2%)	8 37
12	N	141/144 (98%)	124 (88%)	17 (12%)	0	100 100
13	O	288/420 (69%)	262 (91%)	26 (9%)	0	100 100
14	P	97/229 (42%)	90 (93%)	6 (6%)	1 (1%)	15 53
15	Q	1304/1485 (88%)	1279 (98%)	25 (2%)	0	100 100
16	R	370/536 (69%)	337 (91%)	30 (8%)	3 (1%)	19 57
17	S	156/166 (94%)	144 (92%)	12 (8%)	0	100 100
18	T	318/514 (62%)	301 (95%)	17 (5%)	0	100 100
19	U	68/2752 (2%)	63 (93%)	4 (6%)	1 (2%)	10 42
20	V	458/908 (50%)	433 (94%)	25 (6%)	0	100 100
21	W	497/579 (86%)	473 (95%)	24 (5%)	0	100 100
22	X	778/1041 (75%)	730 (94%)	48 (6%)	0	100 100
23	Y	318/492 (65%)	296 (93%)	22 (7%)	0	100 100
24	Z	147/225 (65%)	138 (94%)	6 (4%)	3 (2%)	7 34
25	a	84/240 (35%)	76 (90%)	8 (10%)	0	100 100
25	m	80/240 (33%)	72 (90%)	8 (10%)	0	100 100
26	b	80/119 (67%)	73 (91%)	7 (9%)	0	100 100
26	n	78/119 (66%)	67 (86%)	11 (14%)	0	100 100
27	c	95/118 (80%)	87 (92%)	8 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	h	91/118 (77%)	82 (90%)	9 (10%)	0	100	100
28	d	72/86 (84%)	67 (93%)	5 (7%)	0	100	100
28	i	70/86 (81%)	64 (91%)	6 (9%)	0	100	100
29	e	77/92 (84%)	73 (95%)	4 (5%)	0	100	100
29	j	79/92 (86%)	73 (92%)	6 (8%)	0	100	100
30	f	72/76 (95%)	66 (92%)	6 (8%)	0	100	100
30	k	71/76 (93%)	63 (89%)	8 (11%)	0	100	100
31	g	77/126 (61%)	72 (94%)	5 (6%)	0	100	100
31	l	81/126 (64%)	70 (86%)	11 (14%)	0	100	100
32	q	130/504 (26%)	122 (94%)	8 (6%)	0	100	100
32	r	129/504 (26%)	122 (95%)	7 (5%)	0	100	100
32	s	130/504 (26%)	113 (87%)	12 (9%)	5 (4%)	3	18
32	t	129/504 (26%)	122 (95%)	7 (5%)	0	100	100
33	y	77/301 (26%)	76 (99%)	1 (1%)	0	100	100
34	1	814/1304 (62%)	709 (87%)	100 (12%)	5 (1%)	25	64
35	3	1165/1217 (96%)	992 (85%)	172 (15%)	1 (0%)	51	85
36	2	246/895 (28%)	217 (88%)	24 (10%)	5 (2%)	7	34
37	4	157/424 (37%)	138 (88%)	19 (12%)	0	100	100
38	7	79/110 (72%)	65 (82%)	14 (18%)	0	100	100
39	5	75/86 (87%)	64 (85%)	11 (15%)	0	100	100
40	p	88/225 (39%)	81 (92%)	7 (8%)	0	100	100
41	o	160/255 (63%)	137 (86%)	23 (14%)	0	100	100
All	All	14214/24450 (58%)	12941 (91%)	1224 (9%)	49 (0%)	44	76

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1417	PRO
16	R	164	PRO
32	s	59	HIS
32	s	60	PRO
34	1	718	PRO
34	1	1047	ALA
36	2	549	MET

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Mol	Chain	Res	Type
36	2	557	VAL
36	2	558	ARG
36	2	569	GLN
1	A	699	GLU
1	A	856	LEU
1	A	1517	LYS
3	C	84	GLU
9	J	241	VAL
11	M	202	TYR
14	P	199	LYS
24	Z	66	MET
34	1	1107	GLN
36	2	521	PRO
1	A	1418	ARG
1	A	1528	GLN
11	M	124	PHE
32	s	72	PRO
34	1	1106	ARG
1	A	378	PHE
1	A	570	ASP
1	A	698	PRO
3	C	358	LYS
9	J	188	GLN
16	R	428	GLU
19	U	2	TYR
24	Z	78	PRO
34	1	724	PHE
1	A	188	LEU
9	J	205	LEU
9	J	341	PRO
24	Z	79	ILE
32	s	56	LYS
1	A	108	MET
1	A	227	ARG
16	R	223	PRO
32	s	71	ILE
1	A	942	PRO
3	C	440	SER
1	A	109	PRO
8	I	51	PRO
35	3	672	GLY
1	A	729	PRO

5.3.2 Protein sidechains (i)

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	1768/2108 (84%)	1580 (89%)	188 (11%)	6 26
3	C	747/866 (86%)	654 (88%)	93 (12%)	4 20
4	E	256/300 (85%)	213 (83%)	43 (17%)	2 11
8	I	24/749 (3%)	24 (100%)	0	100 100
9	J	241/751 (32%)	223 (92%)	18 (8%)	13 43
10	L	171/709 (24%)	150 (88%)	21 (12%)	4 21
11	M	104/209 (50%)	89 (86%)	15 (14%)	3 15
12	N	130/130 (100%)	116 (89%)	14 (11%)	6 26
13	O	3/361 (1%)	3 (100%)	0	100 100
14	P	95/203 (47%)	80 (84%)	15 (16%)	2 12
16	R	282/457 (62%)	238 (84%)	44 (16%)	2 13
18	T	273/441 (62%)	248 (91%)	25 (9%)	9 34
19	U	21/2432 (1%)	19 (90%)	2 (10%)	8 32
20	V	188/838 (22%)	156 (83%)	32 (17%)	2 10
22	X	682/897 (76%)	599 (88%)	83 (12%)	5 21
23	Y	286/451 (63%)	246 (86%)	40 (14%)	3 16
25	m	4/177 (2%)	4 (100%)	0	100 100
26	n	3/101 (3%)	3 (100%)	0	100 100
27	h	5/110 (4%)	5 (100%)	0	100 100
28	i	4/74 (5%)	4 (100%)	0	100 100
29	j	1/84 (1%)	1 (100%)	0	100 100
30	k	3/66 (4%)	3 (100%)	0	100 100
31	l	3/101 (3%)	3 (100%)	0	100 100
34	1	675/1104 (61%)	574 (85%)	101 (15%)	3 14
35	3	1016/1051 (97%)	808 (80%)	208 (20%)	1 6
36	2	92/776 (12%)	68 (74%)	24 (26%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	7	69/95 (73%)	47 (68%)	22 (32%)	0 1
39	5	68/77 (88%)	53 (78%)	15 (22%)	1 4
40	p	3/195 (2%)	3 (100%)	0	100 100
41	o	6/218 (3%)	6 (100%)	0	100 100
All	All	7223/16131 (45%)	6220 (86%)	1003 (14%)	7 16

All (1003) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	43	LYS
1	A	47	GLU
1	A	55	ASP
1	A	57	GLN
1	A	59	GLU
1	A	60	ASP
1	A	82	ARG
1	A	88	TYR
1	A	95	MET
1	A	97	HIS
1	A	123	THR
1	A	137	GLU
1	A	146	SER
1	A	155	LYS
1	A	161	PHE
1	A	163	ARG
1	A	188	LEU
1	A	189	GLU
1	A	193	LEU
1	A	205	ASP
1	A	214	ARG
1	A	216	SER
1	A	258	PHE
1	A	261	LYS
1	A	284	ARG
1	A	295	GLU
1	A	329	LEU
1	A	330	THR
1	A	337	VAL
1	A	343	GLU
1	A	360	SER

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Mol	Chain	Res	Type
1	A	361	HIS
1	A	371	LEU
1	A	376	GLU
1	A	387	PHE
1	A	388	LEU
1	A	404	LEU
1	A	422	LEU
1	A	431	TYR
1	A	467	GLN
1	A	480	LYS
1	A	518	LEU
1	A	530	LEU
1	A	546	LEU
1	A	554	THR
1	A	560	SER
1	A	569	VAL
1	A	576	ASP
1	A	579	GLN
1	A	600	ARG
1	A	644	ILE
1	A	670	LYS
1	A	683	LEU
1	A	693	ILE
1	A	694	LEU
1	A	708	THR
1	A	714	SER
1	A	727	LYS
1	A	751	THR
1	A	769	LYS
1	A	789	GLU
1	A	815	HIS
1	A	819	SER
1	A	830	LEU
1	A	831	SER
1	A	836	THR
1	A	845	ARG
1	A	850	TYR
1	A	856	LEU
1	A	866	LEU
1	A	869	GLN
1	A	871	TYR
1	A	885	LEU

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Mol	Chain	Res	Type
1	A	893	GLU
1	A	931	ASP
1	A	933	ARG
1	A	941	LYS
1	A	946	GLU
1	A	968	THR
1	A	977	LEU
1	A	978	GLU
1	A	979	SER
1	A	983	LYS
1	A	995	ARG
1	A	1000	ILE
1	A	1038	SER
1	A	1075	GLN
1	A	1076	ASP
1	A	1079	THR
1	A	1091	TYR
1	A	1104	ASP
1	A	1122	ASN
1	A	1128	TYR
1	A	1144	LYS
1	A	1158	LYS
1	A	1166	THR
1	A	1176	SER
1	A	1181	ASP
1	A	1186	LEU
1	A	1199	LYS
1	A	1205	GLU
1	A	1210	LYS
1	A	1235	GLU
1	A	1243	ARG
1	A	1253	SER
1	A	1276	GLU
1	A	1293	ASN
1	A	1298	ARG
1	A	1327	MET
1	A	1329	SER
1	A	1343	SER
1	A	1344	LYS
1	A	1348	VAL
1	A	1359	HIS
1	A	1362	ASP

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Mol	Chain	Res	Type
1	A	1368	LEU
1	A	1370	ARG
1	A	1376	GLU
1	A	1377	SER
1	A	1382	SER
1	A	1394	GLN
1	A	1404	THR
1	A	1407	ASP
1	A	1427	ARG
1	A	1437	ARG
1	A	1449	LYS
1	A	1459	ARG
1	A	1517	LYS
1	A	1519	THR
1	A	1520	ASN
1	A	1523	ARG
1	A	1524	SER
1	A	1529	ILE
1	A	1548	TYR
1	A	1554	GLN
1	A	1555	LEU
1	A	1558	THR
1	A	1568	THR
1	A	1601	LEU
1	A	1606	ILE
1	A	1608	THR
1	A	1615	HIS
1	A	1623	ASN
1	A	1624	SER
1	A	1628	ASP
1	A	1635	TYR
1	A	1644	LEU
1	A	1648	SER
1	A	1649	LYS
1	A	1667	ARG
1	A	1672	ASP
1	A	1692	MET
1	A	1697	SER
1	A	1702	LEU
1	A	1723	LYS
1	A	1772	PHE
1	A	1773	SER

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Mol	Chain	Res	Type
1	A	1783	THR
1	A	1800	THR
1	A	1813	ARG
1	A	1818	PHE
1	A	1825	SER
1	A	1830	GLN
1	A	1831	LYS
1	A	1833	LEU
1	A	1836	LEU
1	A	1850	ARG
1	A	1852	LEU
1	A	1857	GLN
1	A	1870	ASP
1	A	1878	ASP
1	A	1887	SER
1	A	1910	THR
1	A	1914	MET
1	A	1919	LEU
1	A	1924	LEU
1	A	1926	THR
1	A	1930	TYR
1	A	1944	HIS
1	A	1970	THR
1	A	1973	ASP
1	A	1976	TRP
1	A	1977	ILE
1	A	1986	LEU
1	A	1997	VAL
1	A	2005	SER
1	A	2012	LEU
3	C	58	VAL
3	C	65	TYR
3	C	68	THR
3	C	86	THR
3	C	90	THR
3	C	117	ASP
3	C	135	CYS
3	C	197	SER
3	C	213	ASP
3	C	223	ASP
3	C	233	GLU
3	C	240	GLU

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Mol	Chain	Res	Type
3	C	248	GLN
3	C	256	CYS
3	C	283	ASP
3	C	290	SER
3	C	293	SER
3	C	295	ASP
3	C	296	GLU
3	C	308	CYS
3	C	312	SER
3	C	316	ILE
3	C	322	SER
3	C	326	ILE
3	C	327	TYR
3	C	333	ASP
3	C	359	LYS
3	C	363	SER
3	C	372	PHE
3	C	399	LEU
3	C	408	LEU
3	C	417	ARG
3	C	422	LYS
3	C	436	GLN
3	C	440	SER
3	C	450	GLU
3	C	454	THR
3	C	457	VAL
3	C	458	ASP
3	C	483	SER
3	C	485	ASP
3	C	498	SER
3	C	500	THR
3	C	507	VAL
3	C	510	LEU
3	C	514	TYR
3	C	536	ARG
3	C	538	HIS
3	C	543	ARG
3	C	559	ILE
3	C	562	THR
3	C	567	GLU
3	C	572	GLU
3	C	573	GLU

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Mol	Chain	Res	Type
3	C	578	ARG
3	C	608	ARG
3	C	612	LYS
3	C	616	SER
3	C	622	GLU
3	C	632	THR
3	C	639	CYS
3	C	642	HIS
3	C	657	ASP
3	C	661	THR
3	C	673	LYS
3	C	675	PHE
3	C	678	THR
3	C	696	LEU
3	C	698	GLU
3	C	716	GLU
3	C	722	TYR
3	C	723	ASP
3	C	724	TRP
3	C	749	THR
3	C	750	LEU
3	C	753	GLU
3	C	759	LEU
3	C	766	ILE
3	C	802	HIS
3	C	803	ARG
3	C	809	ILE
3	C	822	MET
3	C	824	THR
3	C	829	GLU
3	C	837	GLN
3	C	846	VAL
3	C	879	ASP
3	C	885	THR
3	C	900	VAL
3	C	916	ILE
3	C	922	GLU
3	C	928	HIS
3	C	940	ARG
4	E	61	LEU
4	E	71	CYS
4	E	73	LYS

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Mol	Chain	Res	Type
4	E	86	PHE
4	E	87	ASP
4	E	100	ASP
4	E	104	THR
4	E	106	LYS
4	E	108	HIS
4	E	117	TYR
4	E	119	THR
4	E	123	MET
4	E	125	PHE
4	E	137	ASP
4	E	143	ARG
4	E	144	VAL
4	E	155	ASN
4	E	162	ARG
4	E	167	VAL
4	E	175	THR
4	E	176	VAL
4	E	189	THR
4	E	205	SER
4	E	206	ASP
4	E	210	SER
4	E	226	LYS
4	E	227	LEU
4	E	232	ARG
4	E	234	HIS
4	E	243	LEU
4	E	258	THR
4	E	265	ARG
4	E	267	PHE
4	E	282	HIS
4	E	284	PHE
4	E	286	LYS
4	E	290	ARG
4	E	300	ILE
4	E	307	ARG
4	E	330	ILE
4	E	333	VAL
4	E	338	ASP
4	E	344	SER
9	J	180	LYS
9	J	186	GLU

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Mol	Chain	Res	Type
9	J	188	GLN
9	J	192	GLU
9	J	193	GLN
9	J	194	LEU
9	J	199	LYS
9	J	200	GLU
9	J	214	ILE
9	J	217	GLU
9	J	220	LEU
9	J	238	ASN
9	J	258	ILE
9	J	276	ILE
9	J	367	GLU
9	J	400	GLU
9	J	408	ASP
9	J	419	PHE
10	L	18	ILE
10	L	24	MET
10	L	25	LYS
10	L	63	TRP
10	L	64	SER
10	L	89	ILE
10	L	91	ARG
10	L	138	ARG
10	L	154	GLU
10	L	158	ARG
10	L	161	ASN
10	L	162	THR
10	L	163	GLN
10	L	181	ARG
10	L	182	LEU
10	L	201	LYS
10	L	203	LYS
10	L	205	LYS
10	L	206	ARG
10	L	218	LYS
10	L	222	LEU
11	M	122	LEU
11	M	126	ASP
11	M	151	ARG
11	M	160	PHE
11	M	163	THR

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Mol	Chain	Res	Type
11	M	166	SER
11	M	186	LEU
11	M	200	ARG
11	M	202	TYR
11	M	204	ASP
11	M	208	ILE
11	M	209	ASP
11	M	212	ASN
11	M	218	PHE
11	M	224	ARG
12	N	3	LYS
12	N	5	LYS
12	N	7	SER
12	N	24	GLU
12	N	41	ARG
12	N	57	THR
12	N	71	SER
12	N	72	ARG
12	N	99	ASN
12	N	112	ASN
12	N	125	LYS
12	N	128	VAL
12	N	134	CYS
12	N	140	ARG
14	P	31	SER
14	P	32	SER
14	P	47	THR
14	P	57	ARG
14	P	74	LYS
14	P	78	ARG
14	P	186	ARG
14	P	196	ASN
14	P	201	VAL
14	P	205	LYS
14	P	207	ASP
14	P	209	ARG
14	P	214	THR
14	P	217	SER
14	P	221	LYS
16	R	107	SER
16	R	108	LYS
16	R	125	MET

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Mol	Chain	Res	Type
16	R	128	ASP
16	R	131	ASP
16	R	132	LEU
16	R	136	ASP
16	R	151	LEU
16	R	153	LYS
16	R	166	ARG
16	R	170	LYS
16	R	180	THR
16	R	184	GLN
16	R	193	LYS
16	R	202	MET
16	R	218	ILE
16	R	220	ARG
16	R	235	ARG
16	R	238	THR
16	R	243	GLN
16	R	246	LYS
16	R	251	ILE
16	R	258	LYS
16	R	289	GLU
16	R	295	ASP
16	R	300	GLU
16	R	311	LYS
16	R	322	GLU
16	R	325	ARG
16	R	326	GLU
16	R	329	GLN
16	R	332	ARG
16	R	352	ARG
16	R	360	ARG
16	R	367	ARG
16	R	370	SER
16	R	382	ARG
16	R	383	ASN
16	R	386	ARG
16	R	398	ASN
16	R	406	GLN
16	R	407	TYR
16	R	409	GLN
16	R	416	LYS
18	T	221	THR

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Mol	Chain	Res	Type
18	T	223	SER
18	T	235	SER
18	T	247	SER
18	T	257	ARG
18	T	258	SER
18	T	263	SER
18	T	264	CYS
18	T	267	ASP
18	T	294	LEU
18	T	307	SER
18	T	319	THR
18	T	338	CYS
18	T	349	SER
18	T	383	ARG
18	T	384	HIS
18	T	385	TYR
18	T	389	SER
18	T	393	ASP
18	T	394	ASN
18	T	424	ASP
18	T	429	SER
18	T	443	THR
18	T	460	ASP
18	T	478	LEU
19	U	1	MET
19	U	2	TYR
20	V	457	ARG
20	V	458	THR
20	V	465	SER
20	V	481	PHE
20	V	483	GLU
20	V	486	THR
20	V	487	LYS
20	V	494	LEU
20	V	504	GLU
20	V	528	ILE
20	V	530	LYS
20	V	538	ARG
20	V	544	LEU
20	V	556	TYR
20	V	571	SER
20	V	576	THR

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Mol	Chain	Res	Type
20	V	578	SER
20	V	579	SER
20	V	584	LYS
20	V	588	GLN
20	V	590	LEU
20	V	593	TYR
20	V	606	GLU
20	V	616	LEU
20	V	619	ASP
20	V	622	ARG
20	V	625	ARG
20	V	628	ILE
20	V	633	SER
20	V	640	THR
20	V	646	HIS
20	V	648	LYS
22	X	163	GLU
22	X	194	ARG
22	X	216	GLU
22	X	225	GLU
22	X	228	LYS
22	X	232	ARG
22	X	237	LYS
22	X	252	ASP
22	X	254	GLU
22	X	257	PHE
22	X	276	VAL
22	X	277	ARG
22	X	278	ASP
22	X	282	GLU
22	X	292	LEU
22	X	293	GLU
22	X	329	TRP
22	X	338	SER
22	X	339	LEU
22	X	383	SER
22	X	387	GLN
22	X	389	LYS
22	X	393	GLN
22	X	408	LEU
22	X	409	LEU
22	X	436	LEU

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Mol	Chain	Res	Type
22	X	437	PHE
22	X	442	THR
22	X	452	GLN
22	X	476	GLU
22	X	482	ARG
22	X	494	ARG
22	X	503	ARG
22	X	510	ASP
22	X	511	LEU
22	X	513	SER
22	X	515	SER
22	X	517	VAL
22	X	518	MET
22	X	533	PHE
22	X	547	LYS
22	X	562	THR
22	X	575	ARG
22	X	590	ASP
22	X	599	VAL
22	X	621	ILE
22	X	625	CYS
22	X	633	ARG
22	X	643	LEU
22	X	648	TYR
22	X	682	THR
22	X	683	ILE
22	X	698	LYS
22	X	712	THR
22	X	714	CYS
22	X	715	SER
22	X	748	GLU
22	X	749	GLU
22	X	757	ARG
22	X	767	LEU
22	X	788	THR
22	X	789	LEU
22	X	795	GLN
22	X	796	LEU
22	X	808	LEU
22	X	809	THR
22	X	836	CYS
22	X	847	LEU

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Mol	Chain	Res	Type
22	X	895	SER
22	X	896	GLN
22	X	913	ASP
22	X	915	ARG
22	X	916	GLU
22	X	922	LEU
22	X	923	GLU
22	X	932	CYS
22	X	943	ILE
22	X	954	LEU
22	X	956	ARG
22	X	994	LYS
22	X	1014	HIS
22	X	1019	LYS
22	X	1021	LEU
23	Y	1	MET
23	Y	9	LEU
23	Y	14	ILE
23	Y	18	THR
23	Y	19	GLU
23	Y	26	LEU
23	Y	38	ASN
23	Y	61	ARG
23	Y	64	GLU
23	Y	73	ASP
23	Y	81	GLU
23	Y	85	ARG
23	Y	106	SER
23	Y	118	TYR
23	Y	126	PHE
23	Y	133	MET
23	Y	138	LYS
23	Y	140	ASN
23	Y	159	THR
23	Y	177	ARG
23	Y	182	THR
23	Y	188	SER
23	Y	194	ASP
23	Y	199	ASP
23	Y	200	PHE
23	Y	211	ILE
23	Y	219	THR

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Mol	Chain	Res	Type
23	Y	232	ASP
23	Y	245	CYS
23	Y	251	THR
23	Y	253	ASP
23	Y	255	ASP
23	Y	257	GLU
23	Y	274	ASP
23	Y	276	LYS
23	Y	279	GLU
23	Y	280	SER
23	Y	305	LEU
23	Y	312	HIS
23	Y	319	VAL
34	1	493	LYS
34	1	512	ARG
34	1	526	PHE
34	1	544	LEU
34	1	545	GLU
34	1	554	LYS
34	1	558	ARG
34	1	560	LEU
34	1	562	LYS
34	1	563	LEU
34	1	564	ASP
34	1	566	LEU
34	1	568	ARG
34	1	571	VAL
34	1	573	LYS
34	1	581	LEU
34	1	582	LEU
34	1	585	GLU
34	1	610	ILE
34	1	623	TYR
34	1	630	ARG
34	1	673	ILE
34	1	685	SER
34	1	686	LEU
34	1	698	GLN
34	1	707	LEU
34	1	718	PRO
34	1	719	TYR
34	1	721	ILE

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Mol	Chain	Res	Type
34	1	724	PHE
34	1	736	ARG
34	1	739	ARG
34	1	741	LYS
34	1	754	ILE
34	1	756	LEU
34	1	760	GLU
34	1	768	GLU
34	1	779	SER
34	1	794	GLN
34	1	795	CYS
34	1	827	ARG
34	1	836	THR
34	1	844	VAL
34	1	858	LYS
34	1	873	GLU
34	1	890	GLU
34	1	892	LEU
34	1	893	ILE
34	1	901	GLN
34	1	904	THR
34	1	925	VAL
34	1	926	LYS
34	1	928	TYR
34	1	943	LYS
34	1	946	LYS
34	1	947	VAL
34	1	958	THR
34	1	968	GLU
34	1	971	MET
34	1	973	HIS
34	1	982	LEU
34	1	1003	VAL
34	1	1009	MET
34	1	1010	THR
34	1	1014	LYS
34	1	1015	ASP
34	1	1019	ARG
34	1	1021	THR
34	1	1028	HIS
34	1	1029	GLU
34	1	1030	LYS

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Mol	Chain	Res	Type
34	1	1031	VAL
34	1	1032	GLN
34	1	1041	ARG
34	1	1065	LEU
34	1	1067	LYS
34	1	1080	THR
34	1	1092	ASP
34	1	1104	GLN
34	1	1106	ARG
34	1	1112	THR
34	1	1113	THR
34	1	1122	THR
34	1	1138	VAL
34	1	1143	VAL
34	1	1150	SER
34	1	1156	GLU
34	1	1170	THR
34	1	1174	GLU
34	1	1182	LEU
34	1	1196	SER
34	1	1219	VAL
34	1	1245	ARG
34	1	1250	CYS
34	1	1260	LYS
34	1	1276	SER
34	1	1277	GLN
34	1	1281	ILE
34	1	1292	LYS
34	1	1296	ILE
34	1	1304	LEU
35	3	1	MET
35	3	9	GLN
35	3	18	ILE
35	3	25	THR
35	3	33	SER
35	3	36	LYS
35	3	41	LEU
35	3	44	ASP
35	3	52	THR
35	3	56	VAL
35	3	66	MET
35	3	68	PHE

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Mol	Chain	Res	Type
35	3	74	THR
35	3	76	ASP
35	3	78	ILE
35	3	90	LEU
35	3	92	TYR
35	3	98	MET
35	3	106	THR
35	3	110	SER
35	3	116	VAL
35	3	121	LEU
35	3	124	ASP
35	3	126	LYS
35	3	130	VAL
35	3	131	MET
35	3	133	SER
35	3	139	LYS
35	3	143	ILE
35	3	153	THR
35	3	164	ASN
35	3	170	VAL
35	3	173	VAL
35	3	184	CYS
35	3	188	ASP
35	3	195	ASP
35	3	203	ASN
35	3	204	THR
35	3	207	THR
35	3	209	THR
35	3	221	VAL
35	3	222	ARG
35	3	225	SER
35	3	226	GLU
35	3	230	GLU
35	3	233	ASN
35	3	242	SER
35	3	256	ILE
35	3	261	PHE
35	3	263	ASP
35	3	264	GLN
35	3	266	ASP
35	3	271	ILE
35	3	273	ARG

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Mol	Chain	Res	Type
35	3	275	ARG
35	3	282	GLU
35	3	286	ILE
35	3	287	PHE
35	3	294	LYS
35	3	300	PHE
35	3	315	LEU
35	3	317	THR
35	3	318	ASP
35	3	320	ASP
35	3	327	LEU
35	3	330	PHE
35	3	331	ASP
35	3	332	THR
35	3	340	CYS
35	3	343	LYS
35	3	344	THR
35	3	347	LEU
35	3	355	ASN
35	3	356	HIS
35	3	364	LEU
35	3	384	THR
35	3	390	ARG
35	3	392	LEU
35	3	403	SER
35	3	404	LEU
35	3	408	LEU
35	3	411	GLN
35	3	417	ASN
35	3	419	ASP
35	3	427	CYS
35	3	433	SER
35	3	435	LEU
35	3	439	ARG
35	3	443	GLU
35	3	455	ASN
35	3	461	THR
35	3	464	ARG
35	3	465	HIS
35	3	469	GLU
35	3	471	ASP
35	3	475	ILE

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Mol	Chain	Res	Type
35	3	477	SER
35	3	482	THR
35	3	492	GLU
35	3	510	LEU
35	3	511	LEU
35	3	514	ASP
35	3	526	HIS
35	3	527	ILE
35	3	537	LYS
35	3	543	THR
35	3	544	ILE
35	3	547	CYS
35	3	568	MET
35	3	573	GLN
35	3	574	LEU
35	3	580	ARG
35	3	584	SER
35	3	592	LEU
35	3	594	ASN
35	3	595	VAL
35	3	604	PHE
35	3	605	LEU
35	3	612	ASN
35	3	617	ILE
35	3	620	ASP
35	3	630	MET
35	3	638	GLU
35	3	665	LEU
35	3	669	LEU
35	3	676	ARG
35	3	677	THR
35	3	679	LEU
35	3	685	ASP
35	3	689	THR
35	3	697	ARG
35	3	703	ARG
35	3	704	VAL
35	3	715	MET
35	3	727	SER
35	3	732	THR
35	3	738	THR
35	3	743	SER

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Mol	Chain	Res	Type
35	3	758	SER
35	3	768	GLU
35	3	775	ASN
35	3	776	GLN
35	3	786	ARG
35	3	797	LEU
35	3	798	ILE
35	3	802	THR
35	3	814	GLN
35	3	815	ARG
35	3	822	GLU
35	3	834	LEU
35	3	837	GLU
35	3	842	PHE
35	3	850	SER
35	3	851	ILE
35	3	867	ARG
35	3	876	THR
35	3	882	LEU
35	3	883	GLU
35	3	901	GLU
35	3	902	ASP
35	3	904	TYR
35	3	906	LEU
35	3	927	THR
35	3	931	VAL
35	3	936	LYS
35	3	937	LEU
35	3	941	HIS
35	3	942	LYS
35	3	958	ARG
35	3	961	ILE
35	3	966	LEU
35	3	978	LEU
35	3	981	CYS
35	3	988	ASN
35	3	991	SER
35	3	993	ILE
35	3	995	THR
35	3	996	ILE
35	3	998	HIS
35	3	1002	VAL

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Mol	Chain	Res	Type
35	3	1004	ASP
35	3	1012	VAL
35	3	1022	ILE
35	3	1026	ASP
35	3	1028	THR
35	3	1035	THR
35	3	1042	ASP
35	3	1062	THR
35	3	1066	VAL
35	3	1090	GLU
35	3	1093	MET
35	3	1094	ASN
35	3	1099	GLU
35	3	1103	SER
35	3	1107	THR
35	3	1114	SER
35	3	1116	SER
35	3	1118	VAL
35	3	1120	THR
35	3	1121	THR
35	3	1148	LEU
35	3	1150	SER
35	3	1151	GLU
35	3	1166	TYR
35	3	1168	PHE
35	3	1170	VAL
35	3	1183	ASN
35	3	1217	PHE
36	2	452	LYS
36	2	453	LYS
36	2	454	LEU
36	2	456	ARG
36	2	458	ASN
36	2	460	PHE
36	2	461	THR
36	2	464	GLU
36	2	465	LEU
36	2	471	ARG
36	2	475	VAL
36	2	476	GLU
36	2	479	ASP
36	2	480	VAL

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Mol	Chain	Res	Type
36	2	488	LEU
36	2	494	THR
36	2	497	SER
36	2	502	ARG
36	2	509	LYS
36	2	512	GLN
36	2	590	LEU
36	2	705	ARG
36	2	710	GLU
36	2	711	LEU
38	7	9	ILE
38	7	11	CYS
38	7	12	ARG
38	7	14	GLN
38	7	23	CYS
38	7	25	LYS
38	7	29	LYS
38	7	30	CYS
38	7	33	CYS
38	7	35	SER
38	7	37	VAL
38	7	40	CYS
38	7	45	ILE
38	7	48	GLU
38	7	60	ILE
38	7	68	ASP
38	7	70	TYR
38	7	71	TYR
38	7	72	CYS
38	7	74	GLU
38	7	81	ASP
38	7	89	VAL
39	5	5	TYR
39	5	18	TYR
39	5	23	HIS
39	5	25	ASP
39	5	27	THR
39	5	32	LEU
39	5	35	GLN
39	5	36	HIS
39	5	42	SER
39	5	51	ASN

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Mol	Chain	Res	Type
39	5	60	SER
39	5	63	ARG
39	5	65	ARG
39	5	69	MET
39	5	74	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	41	GLN
1	A	57	GLN
1	A	73	HIS
1	A	78	ASN
1	A	105	ASN
1	A	112	GLN
1	A	229	GLN
1	A	321	ASN
1	A	322	ASN
1	A	325	HIS
1	A	326	HIS
1	A	357	ASN
1	A	495	GLN
1	A	502	ASN
1	A	654	ASN
1	A	659	GLN
1	A	664	HIS
1	A	711	GLN
1	A	755	HIS
1	A	775	ASN
1	A	788	GLN
1	A	834	HIS
1	A	1014	ASN
1	A	1121	ASN
1	A	1400	ASN
1	A	1424	GLN
1	A	1460	HIS
1	A	1546	ASN
1	A	1552	GLN
1	A	1554	GLN
1	A	1583	GLN
1	A	1623	ASN

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Mol	Chain	Res	Type
1	A	1658	GLN
1	A	1774	ASN
1	A	1804	ASN
1	A	1823	HIS
1	A	1830	GLN
1	A	1857	GLN
1	A	1944	HIS
1	A	1965	HIS
3	C	82	GLN
3	C	139	HIS
3	C	245	HIS
3	C	306	ASN
3	C	313	GLN
3	C	350	ASN
3	C	402	HIS
3	C	437	HIS
3	C	505	GLN
3	C	538	HIS
3	C	627	HIS
3	C	903	HIS
3	C	924	GLN
4	E	188	GLN
4	E	225	ASN
4	E	257	ASN
4	E	280	ASN
9	J	193	GLN
9	J	238	ASN
9	J	410	HIS
10	L	45	GLN
10	L	81	GLN
10	L	163	GLN
10	L	175	GLN
10	L	233	GLN
11	M	134	GLN
11	M	172	HIS
11	M	189	GLN
11	M	215	ASN
11	M	219	ASN
12	N	54	HIS
12	N	95	GLN
14	P	45	GLN
14	P	212	ASN

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Mol	Chain	Res	Type
16	R	104	GLN
16	R	243	GLN
16	R	279	HIS
16	R	357	HIS
16	R	381	GLN
16	R	398	ASN
18	T	203	HIS
18	T	269	GLN
18	T	407	GLN
18	T	408	ASN
18	T	446	ASN
20	V	451	ASN
20	V	532	GLN
20	V	553	HIS
20	V	609	GLN
22	X	387	GLN
22	X	414	ASN
22	X	475	ASN
22	X	523	HIS
22	X	697	GLN
22	X	745	HIS
22	X	803	ASN
22	X	863	HIS
22	X	904	GLN
23	Y	52	GLN
23	Y	115	ASN
23	Y	123	HIS
23	Y	140	ASN
23	Y	312	HIS
34	1	550	HIS
34	1	599	ASN
34	1	682	HIS
34	1	692	HIS
34	1	738	HIS
34	1	763	ASN
34	1	817	HIS
34	1	829	ASN
34	1	886	HIS
34	1	891	GLN
34	1	973	HIS
34	1	1028	HIS
34	1	1032	GLN

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Mol	Chain	Res	Type
34	1	1145	ASN
34	1	1193	GLN
34	1	1277	GLN
34	1	1283	HIS
35	3	5	ASN
35	3	19	HIS
35	3	145	ASN
35	3	169	HIS
35	3	179	ASN
35	3	194	ASN
35	3	205	GLN
35	3	206	GLN
35	3	231	HIS
35	3	233	ASN
35	3	264	GLN
35	3	411	GLN
35	3	480	ASN
35	3	550	ASN
35	3	573	GLN
35	3	612	ASN
35	3	636	GLN
35	3	709	GLN
35	3	730	HIS
35	3	775	ASN
35	3	791	HIS
35	3	796	ASN
35	3	817	GLN
35	3	844	ASN
35	3	861	GLN
35	3	994	GLN
35	3	1019	ASN
35	3	1052	ASN
35	3	1105	GLN
36	2	458	ASN
36	2	483	GLN
38	7	14	GLN
38	7	55	GLN

5.3.3 RNA

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/117 (82%)	31 (32%)	1 (1%)
5	F	96/107 (89%)	42 (43%)	6 (6%)
6	G	77/220 (35%)	41 (53%)	7 (9%)
7	H	149/188 (79%)	60 (40%)	5 (3%)
All	All	418/632 (66%)	174 (41%)	19 (4%)

All (174) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	10	U
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C
2	B	24	G
2	B	25	C
2	B	26	A
2	B	40	U
2	B	43	U
2	B	45	C
2	B	47	A
2	B	48	A
2	B	52	U
2	B	65	G
2	B	70	A
2	B	71	C
2	B	88	A
2	B	89	U
2	B	90	U
2	B	92	U
2	B	93	U
2	B	94	U
2	B	95	G
2	B	96	A
2	B	97	G
2	B	98	G
2	B	102	U
2	B	116	U
2	B	117	A
5	F	6	C

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Mol	Chain	Res	Type
5	F	7	G
5	F	9	U
5	F	10	U
5	F	11	C
5	F	12	G
5	F	14	C
5	F	16	G
5	F	25	C
5	F	26	U
5	F	27	A
5	F	28	A
5	F	29	A
5	F	30	A
5	F	33	G
5	F	34	G
5	F	35	A
5	F	37	C
5	F	38	G
5	F	40	U
5	F	44	G
5	F	45	A
5	F	48	A
5	F	54	G
5	F	59	G
5	F	60	C
5	F	61	C
5	F	65	G
5	F	66	C
5	F	68	C
5	F	73	A
5	F	74	U
5	F	75	G
5	F	79	C
5	F	80	G
5	F	81	C
5	F	82	A
5	F	83	A
5	F	84	A
5	F	85	U
5	F	86	U
5	F	87	C
6	G	-10	G

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Mol	Chain	Res	Type
6	G	-9	C
6	G	-8	C
6	G	-7	U
6	G	-5	C
6	G	-4	G
6	G	1	G
6	G	2	U
6	G	3	A
6	G	4	A
6	G	8	C
6	G	9	C
6	G	11	A
6	G	13	C
6	G	17	U
6	G	21	A
6	G	22	C
6	G	23	U
6	G	25	G
6	G	26	U
6	G	27	U
6	G	30	C
6	G	84	U
6	G	88	G
6	G	89	U
6	G	90	C
6	G	97	A
6	G	98	U
6	G	100	C
6	G	101	U
6	G	103	U
6	G	104	C
6	G	106	C
6	G	107	U
6	G	111	U
6	G	112	U
6	G	113	U
6	G	114	U
6	G	115	C
6	G	116	C
6	G	117	A
7	H	15	U
7	H	16	U

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Mol	Chain	Res	Type
7	H	17	U
7	H	19	G
7	H	23	A
7	H	24	A
7	H	29	A
7	H	30	A
7	H	31	G
7	H	32	U
7	H	35	A
7	H	40	C
7	H	44	U
7	H	48	A
7	H	49	U
7	H	53	U
7	H	63	G
7	H	64	A
7	H	65	U
7	H	98	G
7	H	99	A
7	H	100	U
7	H	101	U
7	H	102	U
7	H	103	U
7	H	106	G
7	H	107	A
7	H	110	A
7	H	111	G
7	H	112	G
7	H	113	G
7	H	116	A
7	H	117	U
7	H	121	A
7	H	122	U
7	H	123	A
7	H	124	G
7	H	128	C
7	H	129	U
7	H	133	U
7	H	136	G
7	H	137	U
7	H	141	C
7	H	144	C

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Mol	Chain	Res	Type
7	H	145	A
7	H	146	C
7	H	147	G
7	H	149	A
7	H	157	G
7	H	162	U
7	H	164	C
7	H	165	A
7	H	166	G
7	H	168	A
7	H	169	C
7	H	171	U
7	H	177	A
7	H	178	A
7	H	179	C
7	H	180	G

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	39	C
5	F	37	C
5	F	47	A
5	F	58	G
5	F	79	C
5	F	84	A
5	F	86	U
6	G	21	A
6	G	88	G
6	G	89	U
6	G	102	G
6	G	105	C
6	G	111	U
6	G	113	U
7	H	15	U
7	H	16	U
7	H	43	U
7	H	47	U
7	H	165	A

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	SEP	R	224	16	8,9,10	1.41	1 (12%)	8,12,14	1.63	2 (25%)
16	SEP	R	232	16	8,9,10	1.50	1 (12%)	8,12,14	1.30	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SEP	R	224	16	-	1/5/8/10	-
16	SEP	R	232	16	-	2/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	R	232	SEP	P-O1P	3.20	1.60	1.50
16	R	224	SEP	P-O1P	3.11	1.60	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	R	224	SEP	P-OG-CB	-3.28	109.25	118.30
16	R	224	SEP	OG-CB-CA	2.41	110.50	108.14
16	R	232	SEP	P-OG-CB	-2.26	112.07	118.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	R	224	SEP	N-CA-CB-OG
16	R	232	SEP	CB-OG-P-O2P
16	R	232	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 13 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
42	IHP	A	3000	-	36,36,36	1.00	1 (2%)	54,60,60	1.84	12 (22%)
43	GTP	C	1500	44	26,34,34	1.60	4 (15%)	32,54,54	2.02	9 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	IHP	A	3000	-	-	5/30/54/54	0/1/1/1
43	GTP	C	1500	44	-	4/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	C	1500	GTP	C5-C6	-5.10	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	C	1500	GTP	C2'-C1'	-2.98	1.49	1.53
43	C	1500	GTP	C5-C4	-2.33	1.37	1.43
42	A	3000	IHP	P5-O15	2.16	1.63	1.59
43	C	1500	GTP	C2-N3	2.01	1.38	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	C	1500	GTP	PB-O3B-PG	-5.17	115.07	132.83
42	A	3000	IHP	O41-P1-O31	4.72	125.69	107.64
42	A	3000	IHP	C5-C4-C3	4.58	120.43	110.41
42	A	3000	IHP	C5-C6-C1	4.38	120.00	110.41
42	A	3000	IHP	O15-C5-C4	4.29	118.80	108.69
43	C	1500	GTP	C5-C6-N1	4.02	121.06	113.95
43	C	1500	GTP	PA-O3A-PB	-3.94	119.30	132.83
42	A	3000	IHP	O41-P1-O11	-3.91	88.46	105.99
43	C	1500	GTP	C2-N1-C6	-3.73	118.23	125.10
43	C	1500	GTP	C8-N7-C5	3.16	109.01	102.99
42	A	3000	IHP	C4-C3-C2	3.16	117.33	110.41
43	C	1500	GTP	O2G-PG-O3B	2.88	114.30	104.64
42	A	3000	IHP	O16-C6-C5	2.79	115.27	108.69
42	A	3000	IHP	C6-C1-C2	2.70	116.32	110.41
42	A	3000	IHP	O15-C5-C6	2.67	114.99	108.69
42	A	3000	IHP	O36-P6-O26	2.52	120.53	110.68
43	C	1500	GTP	O6-C6-C5	-2.42	119.65	124.37
42	A	3000	IHP	O12-P2-O22	-2.28	100.58	109.39
43	C	1500	GTP	O5'-C5'-C4'	2.26	116.76	108.99
43	C	1500	GTP	O2'-C2'-C1'	-2.09	103.14	110.85
42	A	3000	IHP	O34-P4-O24	2.02	118.57	110.68

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	A	3000	IHP	C3-C4-O14-P4
42	A	3000	IHP	C3-O13-P3-O23
42	A	3000	IHP	C5-O15-P5-O25
43	C	1500	GTP	C4'-C5'-O5'-PA
43	C	1500	GTP	C3'-C4'-C5'-O5'
43	C	1500	GTP	O4'-C4'-C5'-O5'
42	A	3000	IHP	C1-C6-O16-P6
42	A	3000	IHP	C3-O13-P3-O43

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Mol	Chain	Res	Type	Atoms
43	C	1500	GTP	C5'-O5'-PA-O1A

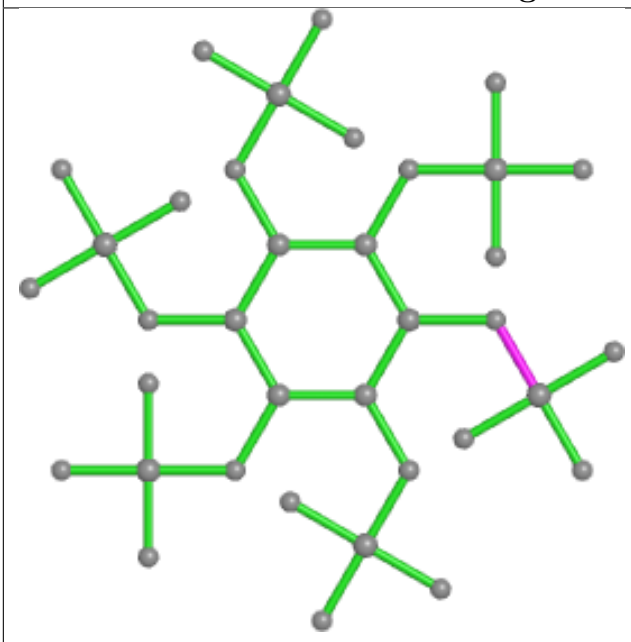
There are no ring outliers.

1 monomer is involved in 5 short contacts:

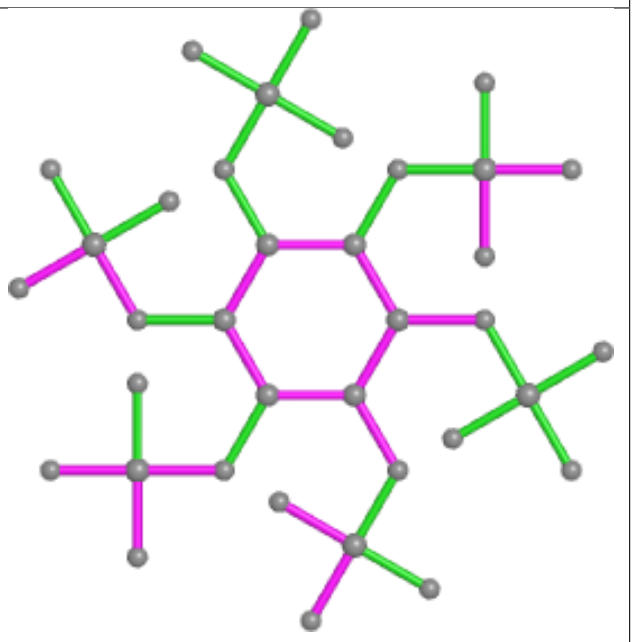
Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	A	3000	IHP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

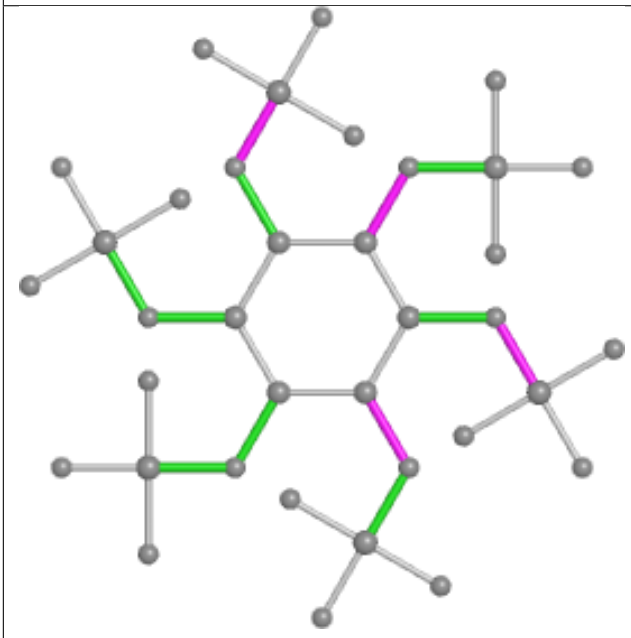
Ligand IHP A 3000



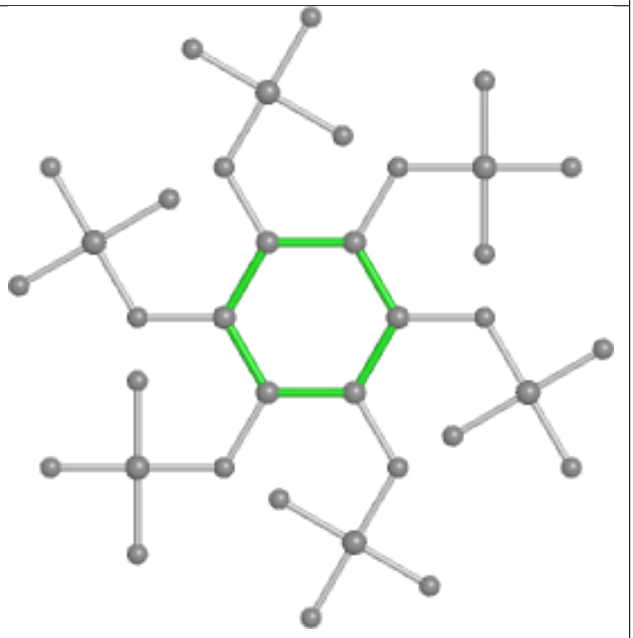
Bond lengths



Bond angles

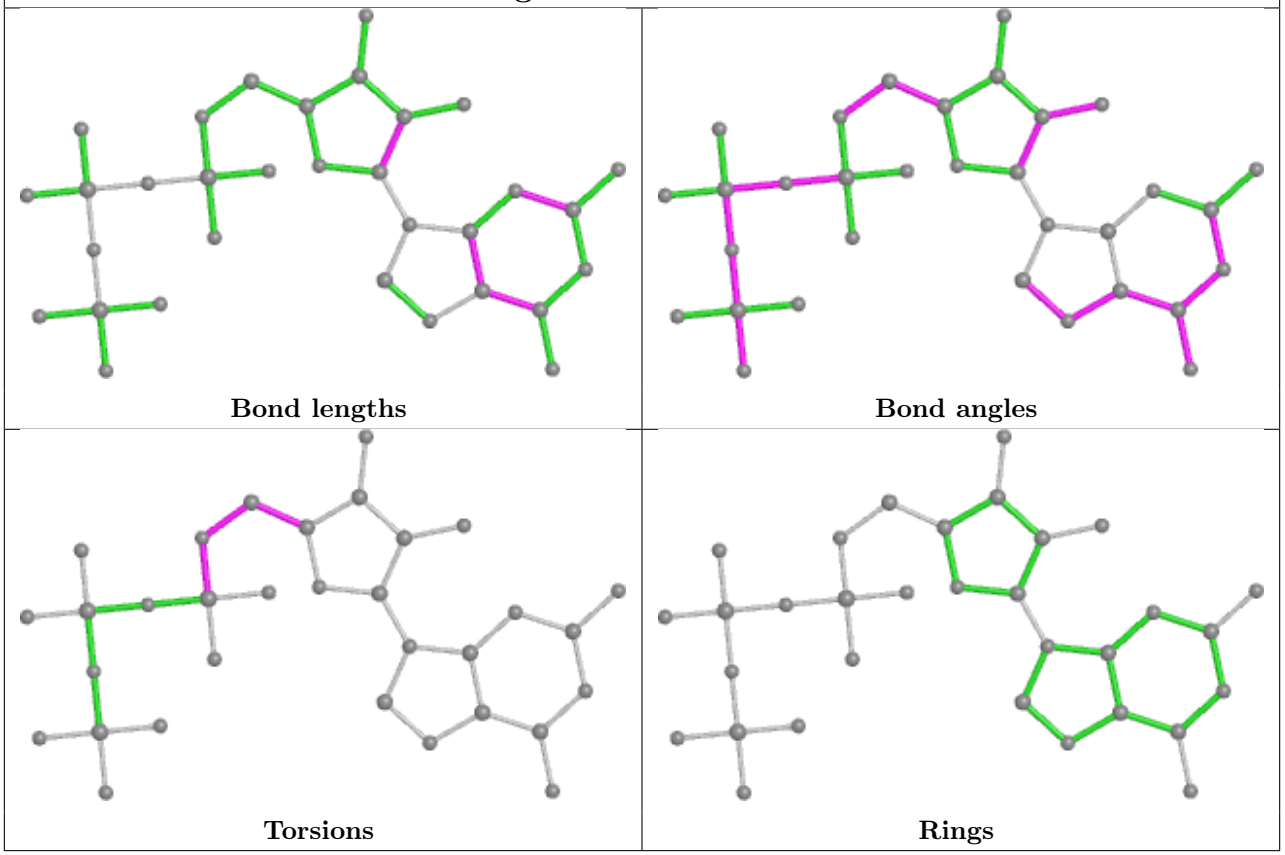


Torsions



Rings

Ligand GTP C 1500



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

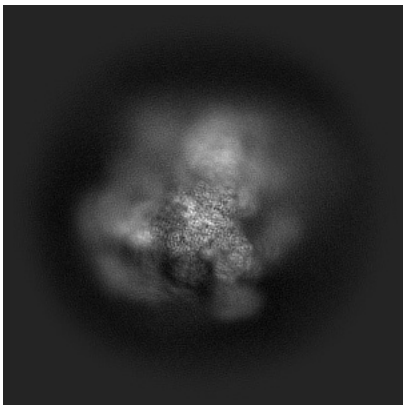
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35111. These allow visual inspection of the internal detail of the map and identification of artifacts.

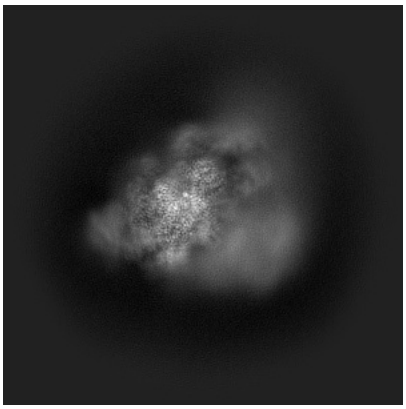
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

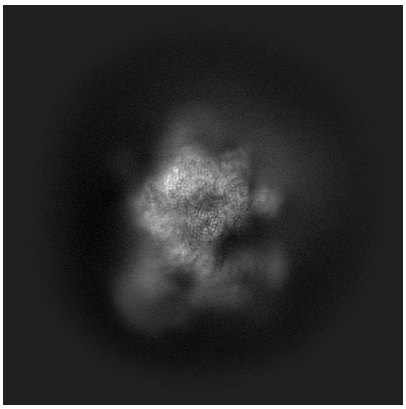
6.1.1 Primary map



X

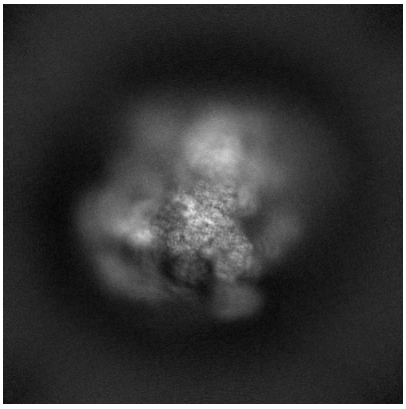


Y

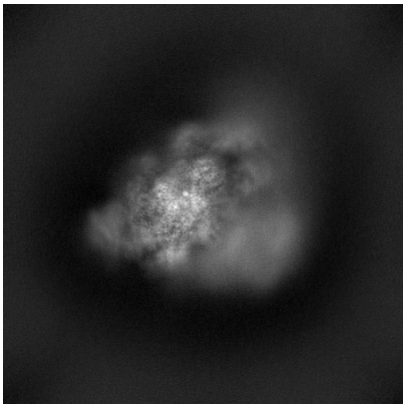


Z

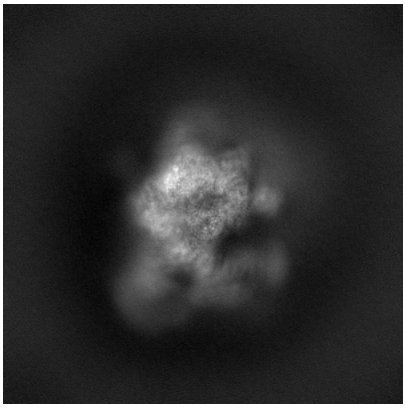
6.1.2 Raw map



X



Y

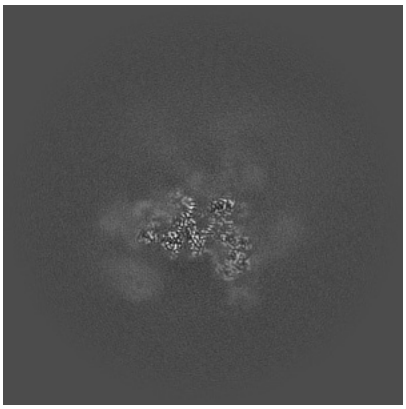


Z

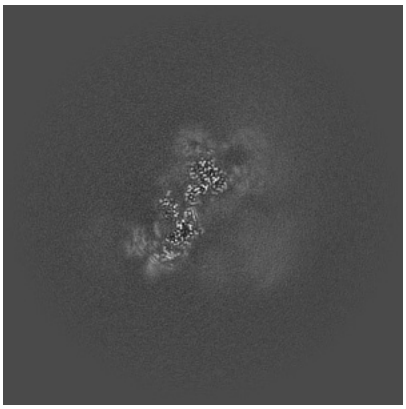
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

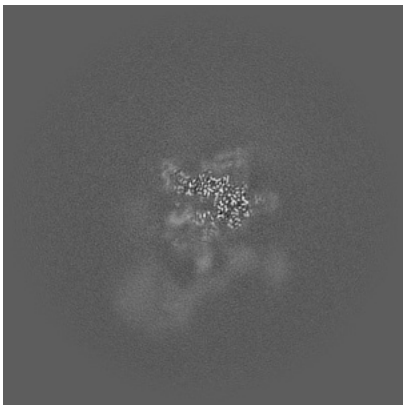
6.2.1 Primary map



X Index: 240

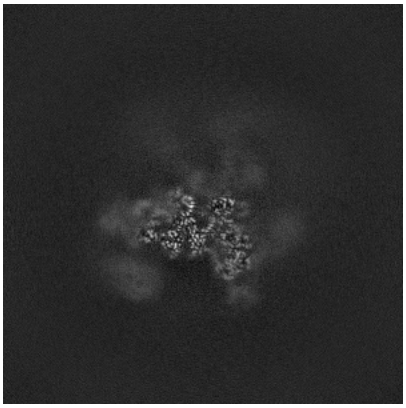


Y Index: 240

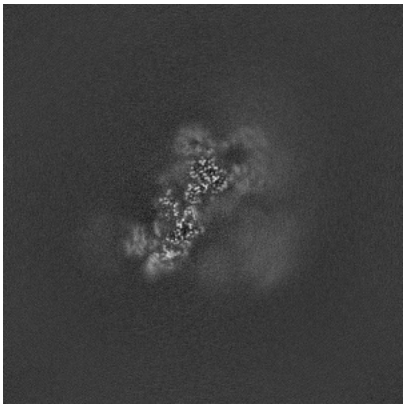


Z Index: 240

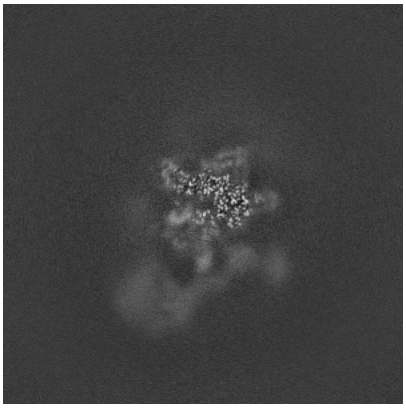
6.2.2 Raw map



X Index: 240



Y Index: 240

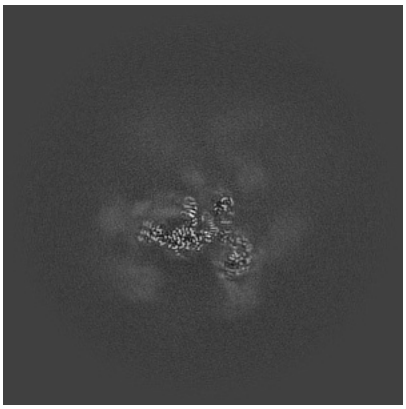


Z Index: 240

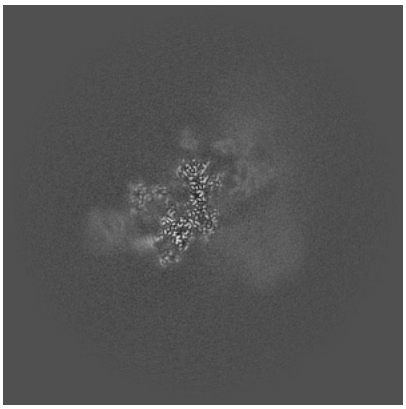
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

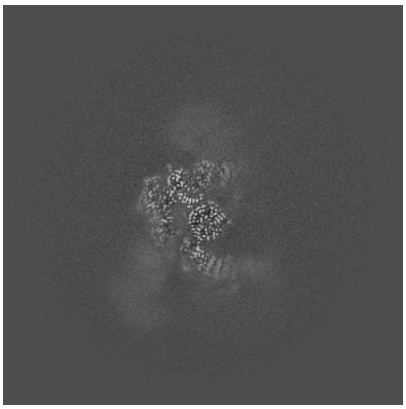
6.3.1 Primary map



X Index: 235

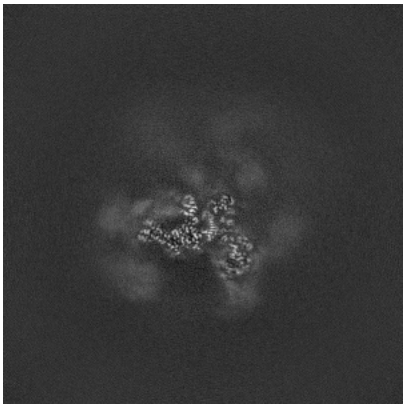


Y Index: 259

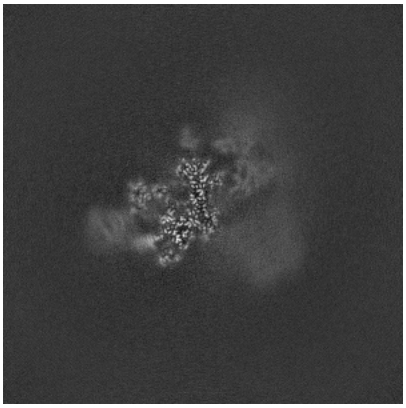


Z Index: 200

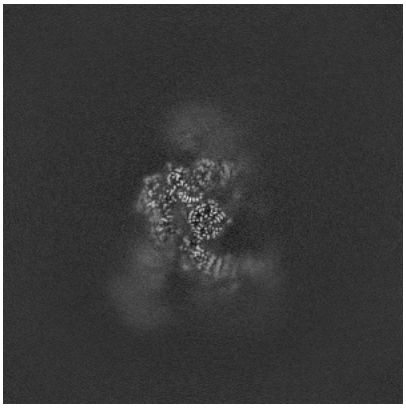
6.3.2 Raw map



X Index: 236



Y Index: 259

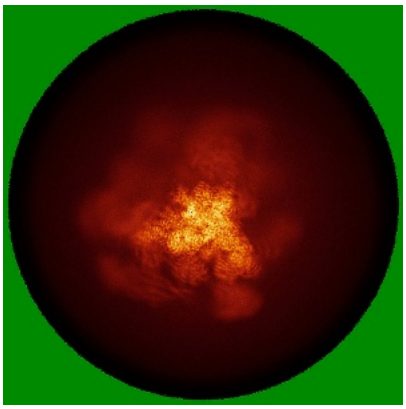


Z Index: 200

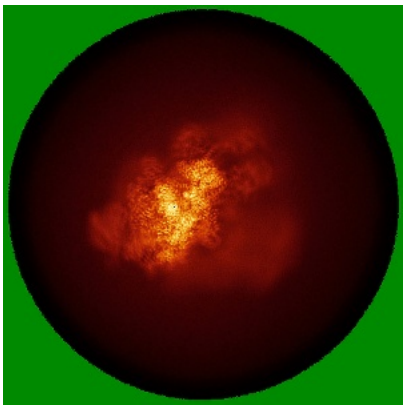
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

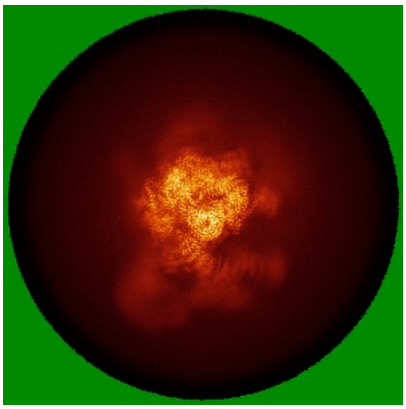
6.4.1 Primary map



X

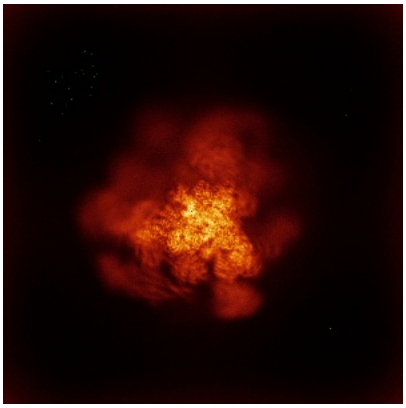


Y

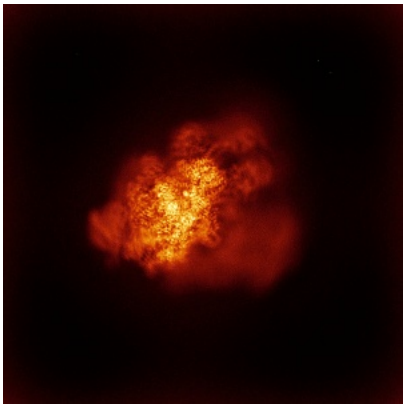


Z

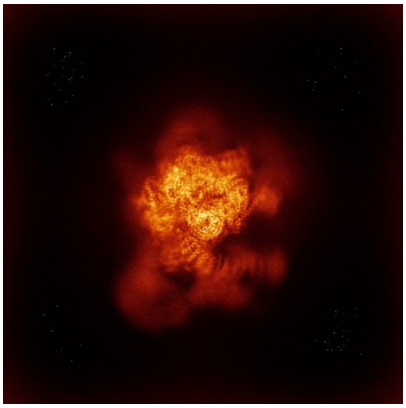
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

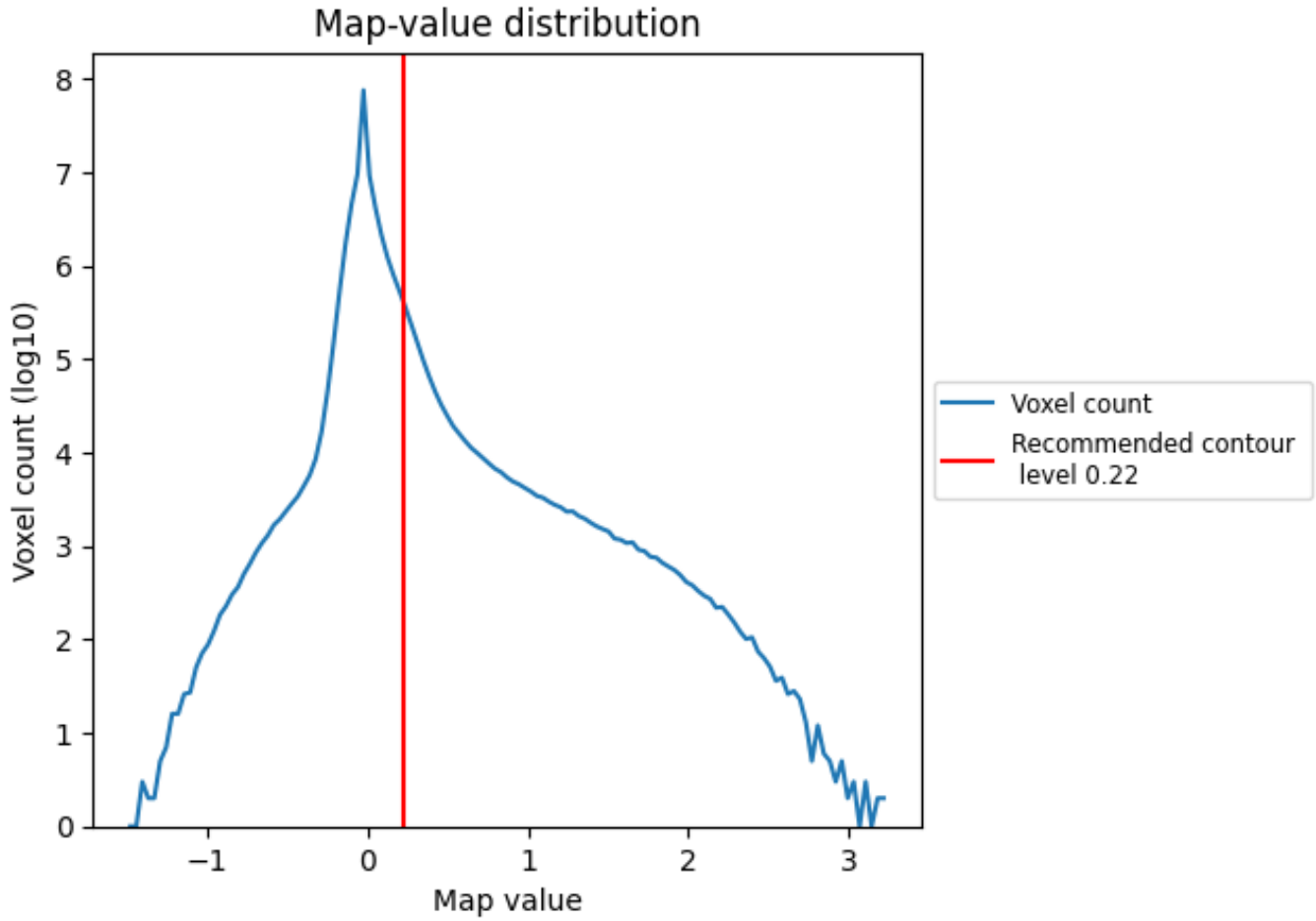
6.6 Mask visualisation (i)

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

7 Map analysis

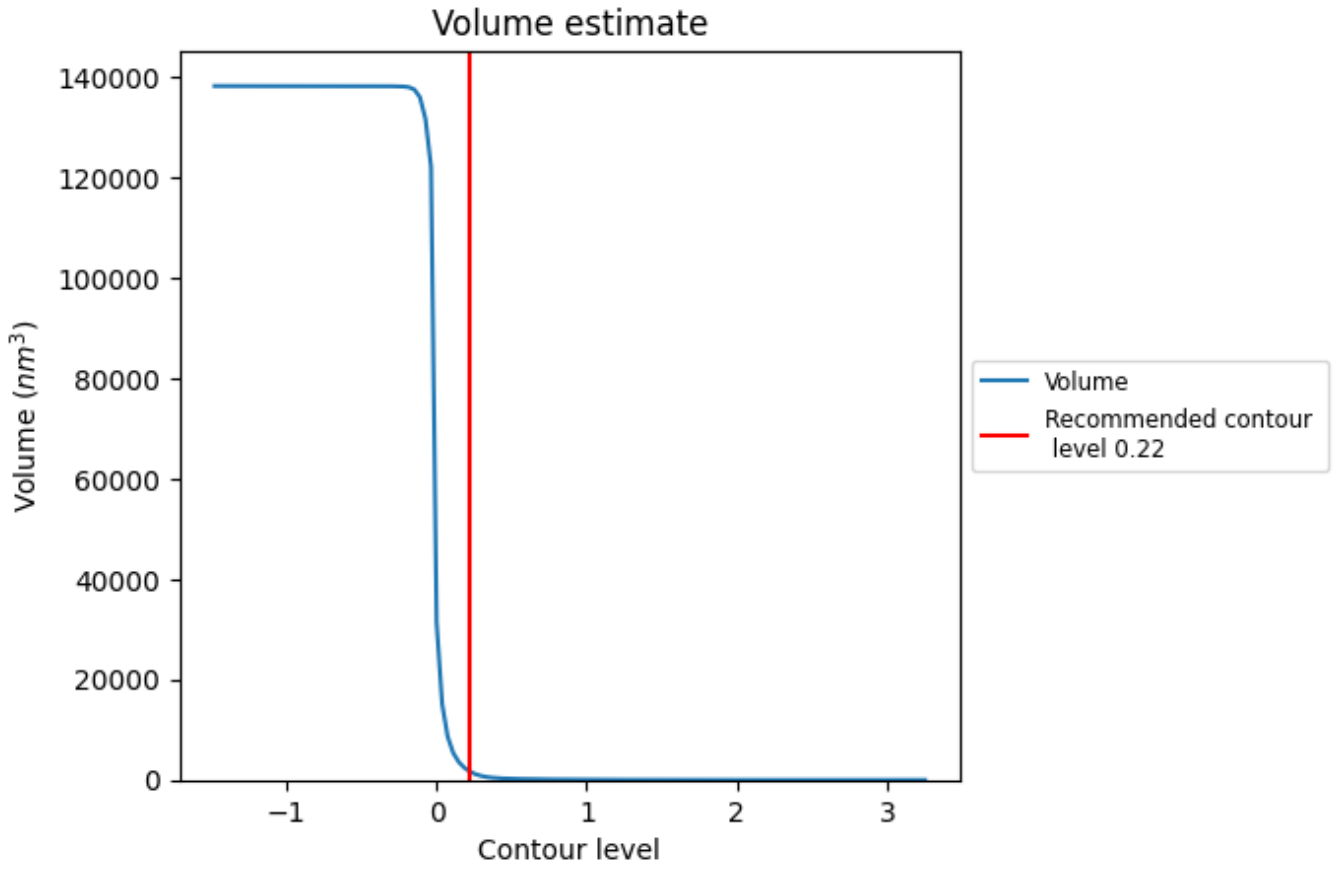
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

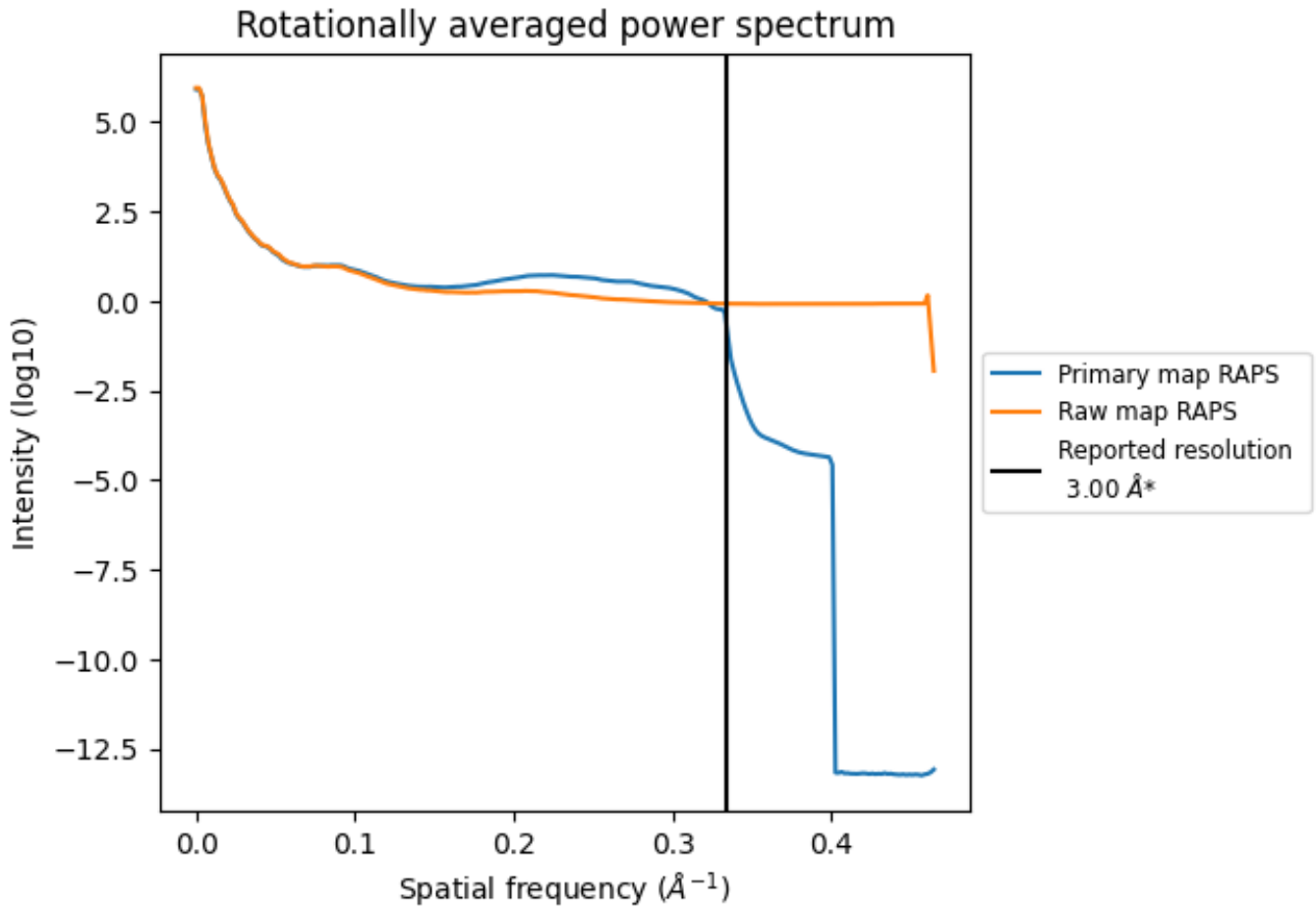
7.2 Volume estimate



The volume at the recommended contour level is 1755 nm^3; this corresponds to an approximate mass of 1586 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 (i)

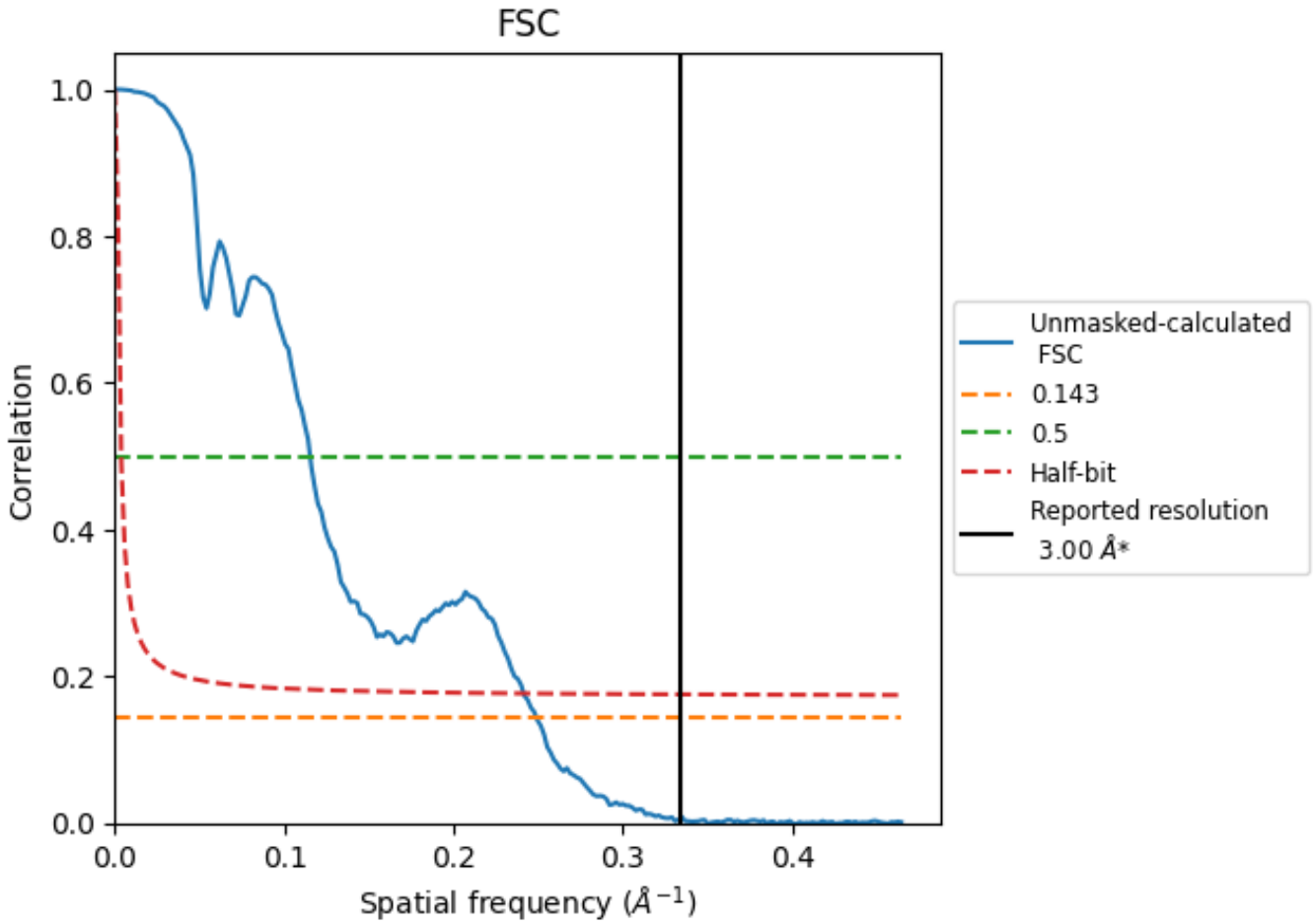


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

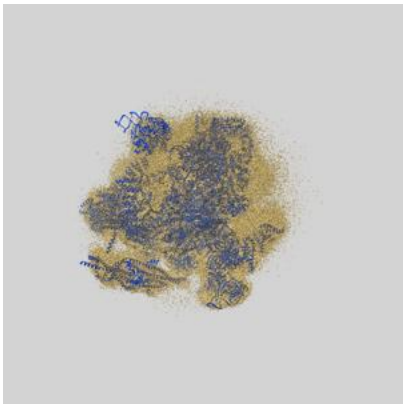
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.02	8.67	4.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 3.0 by more than 10 %

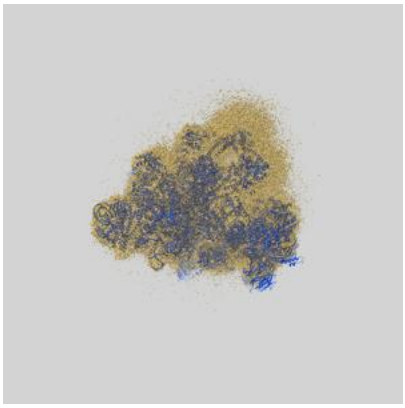
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35111 and PDB model 8I0V. Per-residue inclusion information can be found in section 3 on page 13.

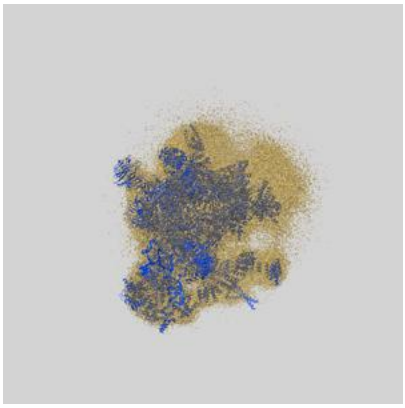
9.1 Map-model overlay



X



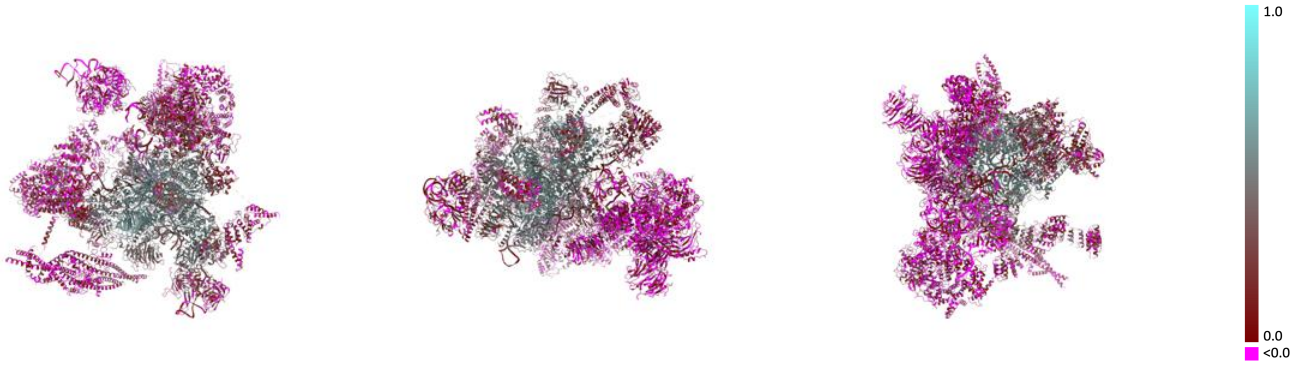
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

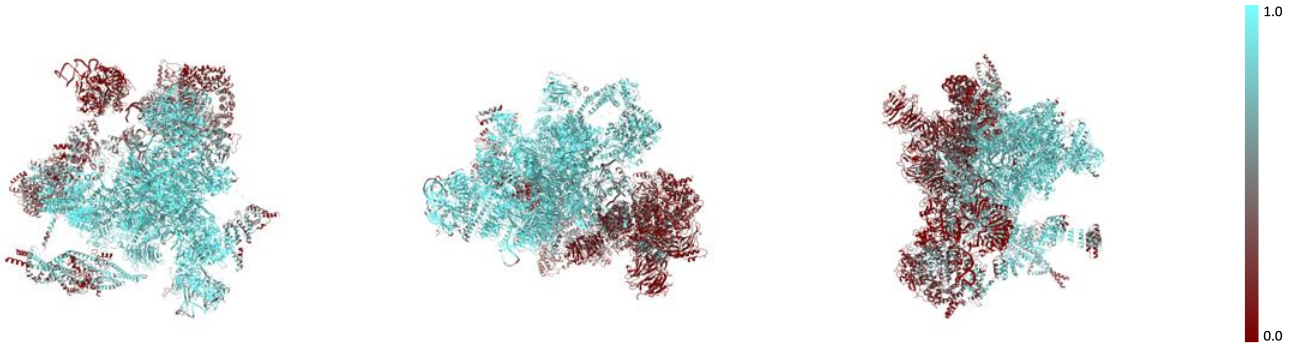
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

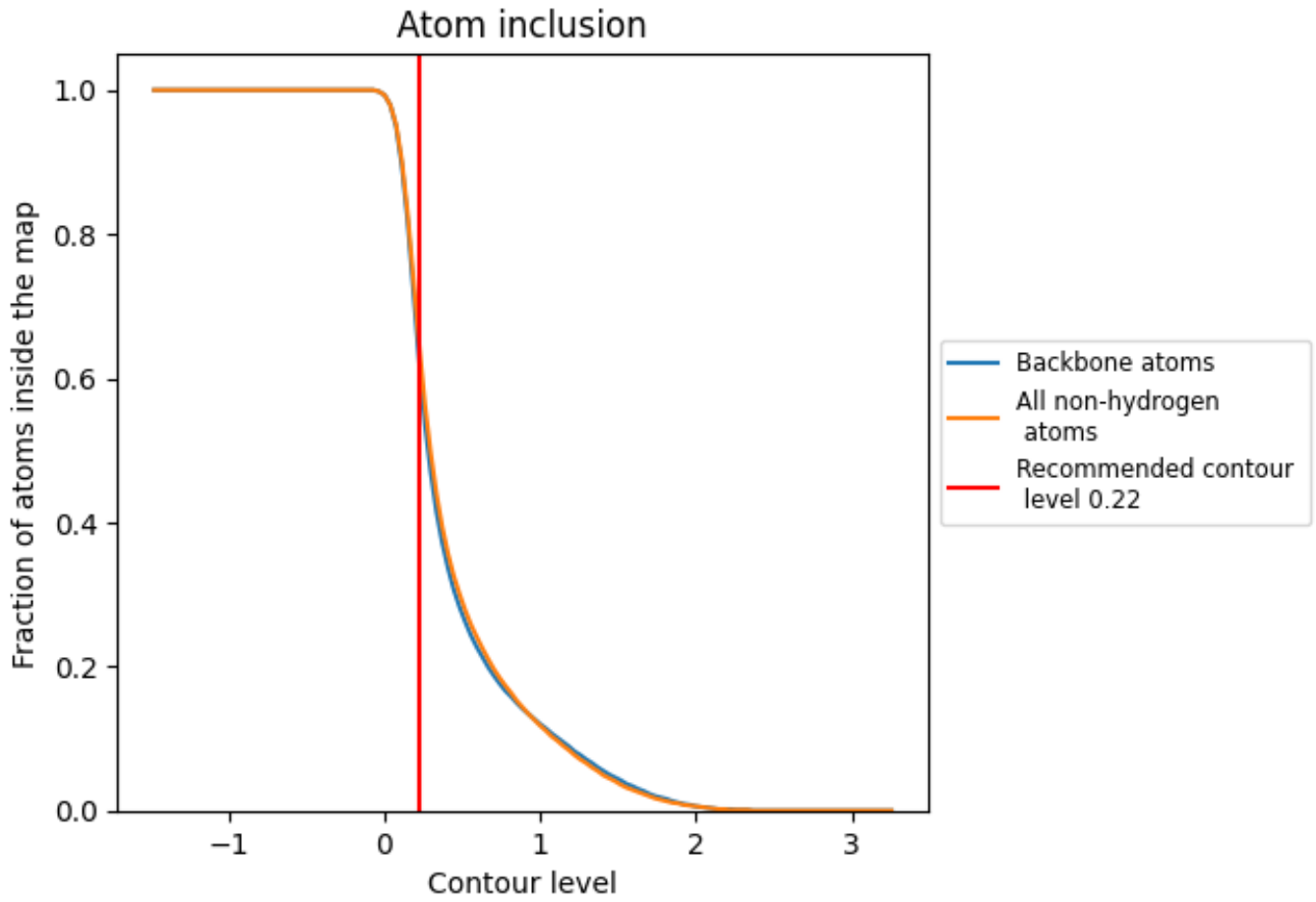
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.22).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 66% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6560	0.2460
1	0.2480	0.0090
2	0.2640	0.0420
3	0.1890	0.0020
4	0.3410	0.0300
5	0.3310	0.0080
7	0.2760	-0.0280
A	0.9260	0.4910
B	0.9280	0.3460
C	0.9700	0.4480
E	0.9600	0.3550
F	0.9400	0.3750
G	0.8110	0.2260
H	0.3280	0.0810
I	0.6230	0.0850
J	0.8550	0.3550
L	0.8380	0.3330
M	0.9220	0.3990
N	0.9740	0.5010
O	0.9330	0.3810
P	0.9530	0.4970
Q	0.3220	0.0740
R	0.9070	0.4050
S	0.9430	0.2510
T	0.9970	0.6080
U	0.7430	0.3070
V	0.7270	0.2130
W	0.3490	0.1250
X	0.8180	0.2260
Y	0.8710	0.2490
Z	0.6760	0.1220
a	0.7960	0.1420
b	0.8960	0.1690
c	0.7940	0.1090
d	0.8410	0.0950

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Chain	Atom inclusion	Q-score
e	0.8510	0.1010
f	0.8010	0.1390
g	0.9170	0.2400
h	0.0600	0.0340
i	0.0190	-0.0070
j	0.0200	-0.0000
k	0.0520	-0.0180
l	0.1610	-0.0180
m	0.1770	0.0080
n	0.1070	-0.0200
o	0.0370	-0.0200
p	0.0640	-0.0240
q	0.3500	0.0400
r	0.5180	0.0530
s	0.3980	0.0820
t	0.3260	0.0430
y	0.3230	0.0340