Full wwPDB EM Validation Report ⓘ

Jul 31, 2024 – 12:40 PM JST

PDB ID	:	8I0R
EMDB ID	:	EMD-35107
Title	:	The cryo-EM structure of human Bact-I 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:

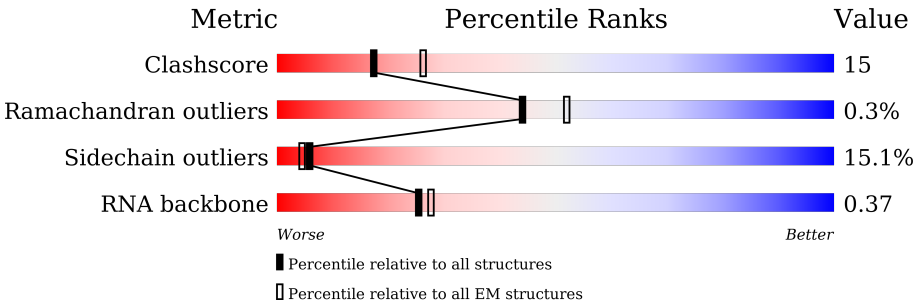
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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	58% 31% 6%
2	B	117	29% 39% 14% 16%
3	C	972	45% 36% 7% 12%
4	D	2136	20% 77% 19%
5	E	357	28% 38% 38% 8% 16%
6	F	107	7% 13% 41% 34% 9%
7	G	220	5% 10% 15% 68%

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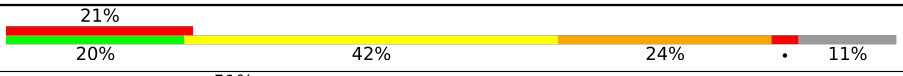
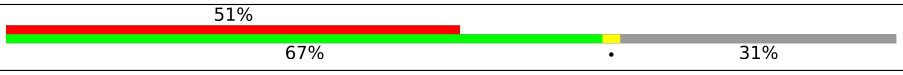
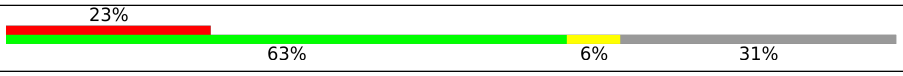
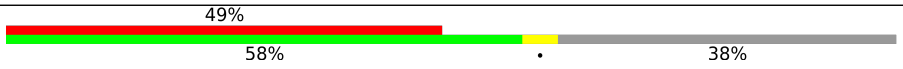
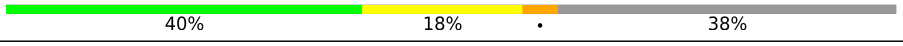
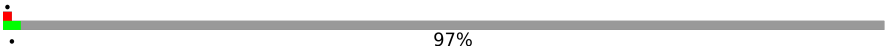
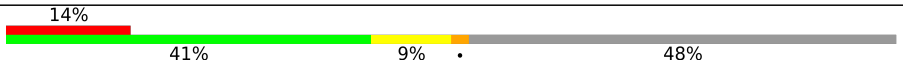
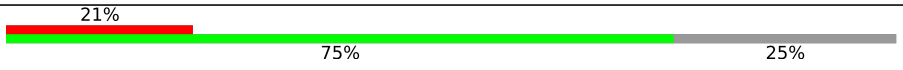
Mol	Chain	Length	Quality of chain
8	H	188	
9	I	855	
10	J	848	
11	K	343	
12	L	802	
13	N	144	
14	O	420	
15	P	229	
16	Q	1485	
17	R	536	
18	S	1041	
19	T	514	
20	U	2752	
21	V	908	
22	W	122	
23	X	396	
24	Y	322	
25	Z	619	
26	1	1304	
27	3	1217	
28	p	225	
29	w	501	
30	u	793	
31	2	895	
32	4	424	

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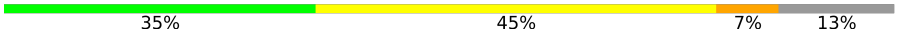
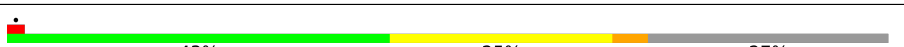
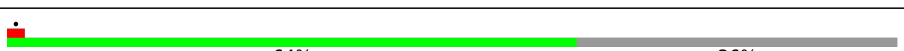
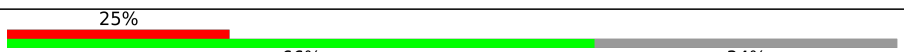
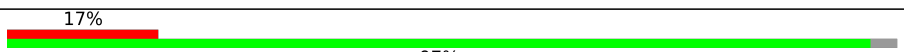
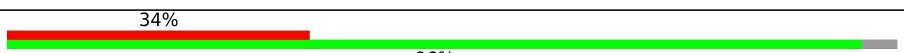
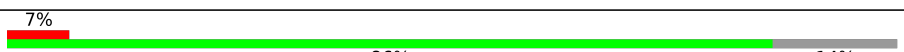
Mol	Chain	Length	Quality of chain
33	6	125	
34	7	110	
35	5	86	
36	9	520	
37	8	904	
38	y	301	
39	v	464	
40	o	255	
41	c	118	
41	h	118	
42	d	86	
42	i	86	
43	a	240	
43	m	240	
44	g	126	
44	l	126	
45	f	76	
45	k	76	
46	e	92	
46	j	92	
47	b	119	
47	n	119	
48	z	472	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 115060 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	2242	18543	11943	3241	3280	79	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 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	1722	8528	5084	1722	1722	0	0

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

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

- Molecule 6 is a RNA chain called U6 snRNA.

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

- Molecule 7 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	71	Total	C	N	O	P	0	0
			1481	663	243	504	71		

- Molecule 8 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	167	Total	C	N	O	P	0	0
			3539	1581	607	1184	167		

- Molecule 9 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	593	Total	C	N	O	0	0
			2991	1805	593	593		

- Molecule 10 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	249	Total	C	N	O	S	0	0
			2116	1355	380	375	6		

- Molecule 11 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	128	Total	C	N	O	S	0	0
			1059	660	190	204	5		

- Molecule 12 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	99	Total	C	N	O	S	0	0
			829	532	149	144	4		

- Molecule 13 is a protein called Protein BUD31 homolog.

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

- Molecule 14 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	290	Total 1433	C 853	N 290	O 290	0	0

- Molecule 15 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	42	Total 362	C 231	N 63	O 66	S 2	0	0

- Molecule 16 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	1329	Total 6730	C 4072	N 1329	O 1329	0	0

- Molecule 17 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	237	Total 1889	C 1171	N 347	O 360	S 11	0	0

- Molecule 18 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	643	Total 3180	C 1894	N 643	O 643	0	0

- Molecule 19 is a protein called Pleiotropic regulator 1.

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

- Molecule 20 is a protein called Serine/arginine repetitive matrix protein 2.

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

- Molecule 21 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	468	Total	C	N	O	S	0	0
			3008	1873	546	576	13		

- Molecule 22 is a protein called Unknown polymer.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	43	Total	C	N	O	0	0
			229	140	46	43		

- Molecule 23 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	154	Total	C	N	O	S	0	0
			1279	819	231	227	2		

- Molecule 24 is a protein called RNA-binding motif protein, X-linked 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	118	Total	C	N	O	S	0	0
			948	605	163	176	4		

- Molecule 25 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	137	Total	C	N	O	S	0	0
			1142	708	213	216	5		

- Molecule 26 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	1	993	Total	C	N	O	P	S	0	0
			7866	5018	1363	1438	1	46		

- Molecule 27 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	3	1177	Total	C	N	O	S	0	0
			9220	5854	1566	1755	45		

- Molecule 28 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
28	p	169	Total 851	C 513	N 169	O 169	0	0

- Molecule 29 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	434	Total 2275	C 1287	N 491	O 493	S 4	0	0

- Molecule 30 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	u	187	Total 834	C 460	N 187	O 187	0	0

- Molecule 31 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	2	250	Total 1807	C 1134	N 340	O 326	S 7	0	0

- Molecule 32 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	4	161	Total 792	C 470	N 161	O 161	0	0

- Molecule 33 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	109	Total 906	C 582	N 157	O 163	S 4	0	0

- Molecule 34 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	105	Total 811	C 502	N 145	O 151	S 13	0	0

- Molecule 35 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	5	81	Total	C	N	O	S	0	0
			669	422	117	124	6		

- Molecule 36 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	379	Total	C	N	O	S	0	0
			2636	1633	479	516	8		

- Molecule 37 is a protein called Serine/arginine repetitive matrix protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	8	115	Total	C	N	O	S	0	0
			931	602	154	170	5		

- Molecule 38 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	y	79	Total	C	N	O	0	0
			390	232	79	79		

- Molecule 39 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	v	173	Total	C	N	O	S	0	0
			1041	602	219	217	3		

- Molecule 40 is a protein called U2 small nuclear ribonucleoprotein A'.

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

- Molecule 41 is a protein called Small nuclear ribonucleoprotein Sm D2.

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

- Molecule 42 is a protein called Small nuclear ribonucleoprotein F.

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

- Molecule 43 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

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

- Molecule 44 is a protein called Small nuclear ribonucleoprotein Sm D3.

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

- Molecule 45 is a protein called Small nuclear ribonucleoprotein G.

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

- Molecule 46 is a protein called Small nuclear ribonucleoprotein E.

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

- Molecule 47 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	n	80	Total 402	C 242	N 80	O 80	0	0

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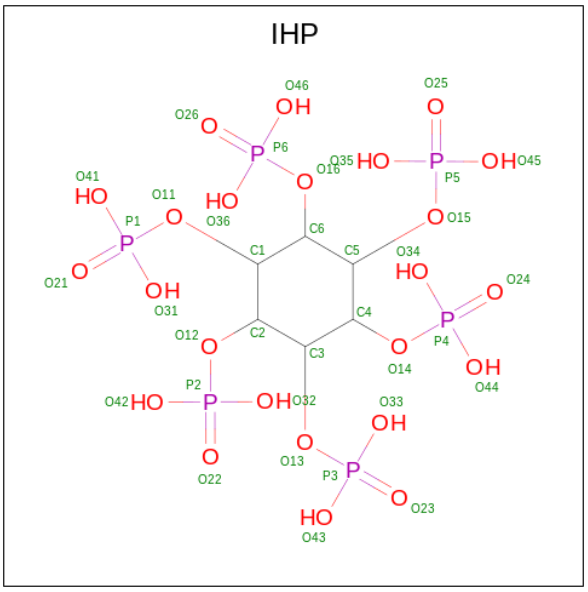
Mol	Chain	Residues	Atoms				AltConf	Trace
47	b	82	Total	C	N	O	0	0
			328	164	82	82		

- Molecule 48 is a protein called Peptidyl-prolyl cis-trans isomerase CWC27 homolog.

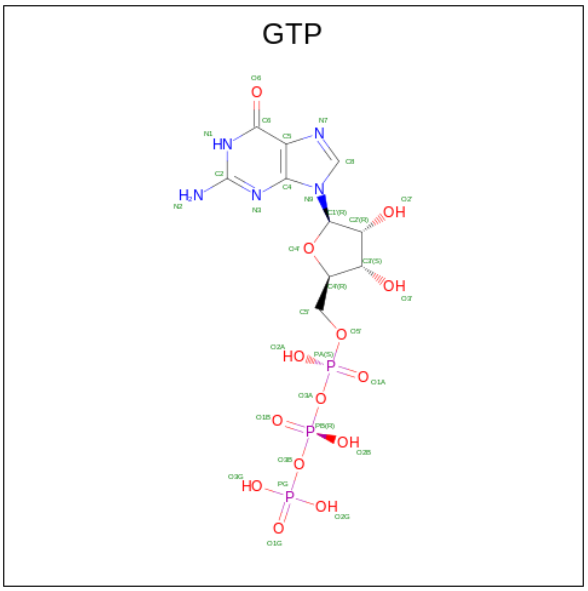
Mol	Chain	Residues	Atoms					AltConf	Trace
48	z	177	Total	C	N	O	S	1	0
			1402	884	243	270	5		

- Molecule 49 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 50 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 51 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

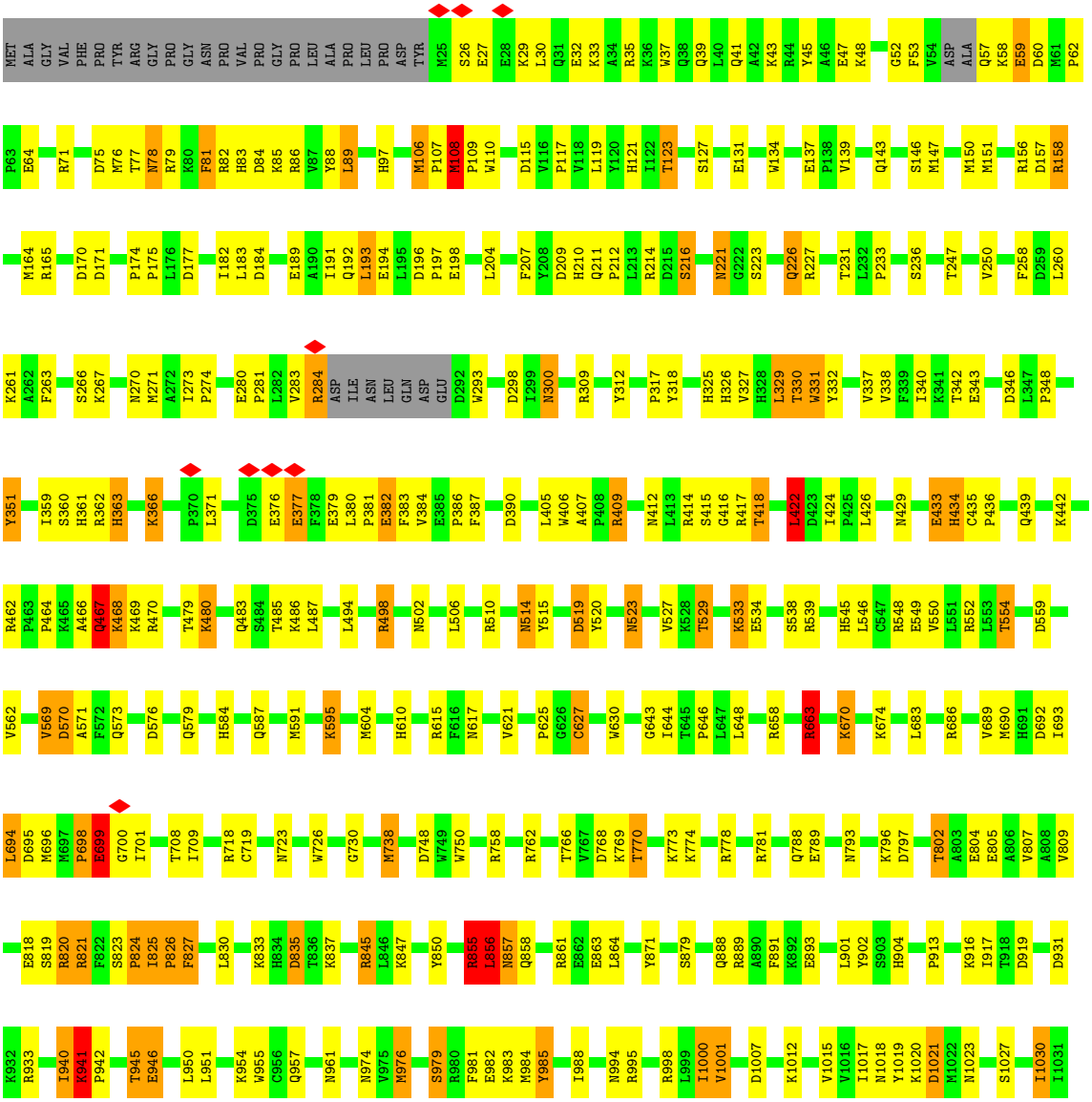
Mol	Chain	Residues	Atoms		AltConf
52	K	1	Total	Zn	0
			1	1	
52	N	3	Total	Zn	0
			3	3	
52	7	3	Total	Zn	0
			3	3	

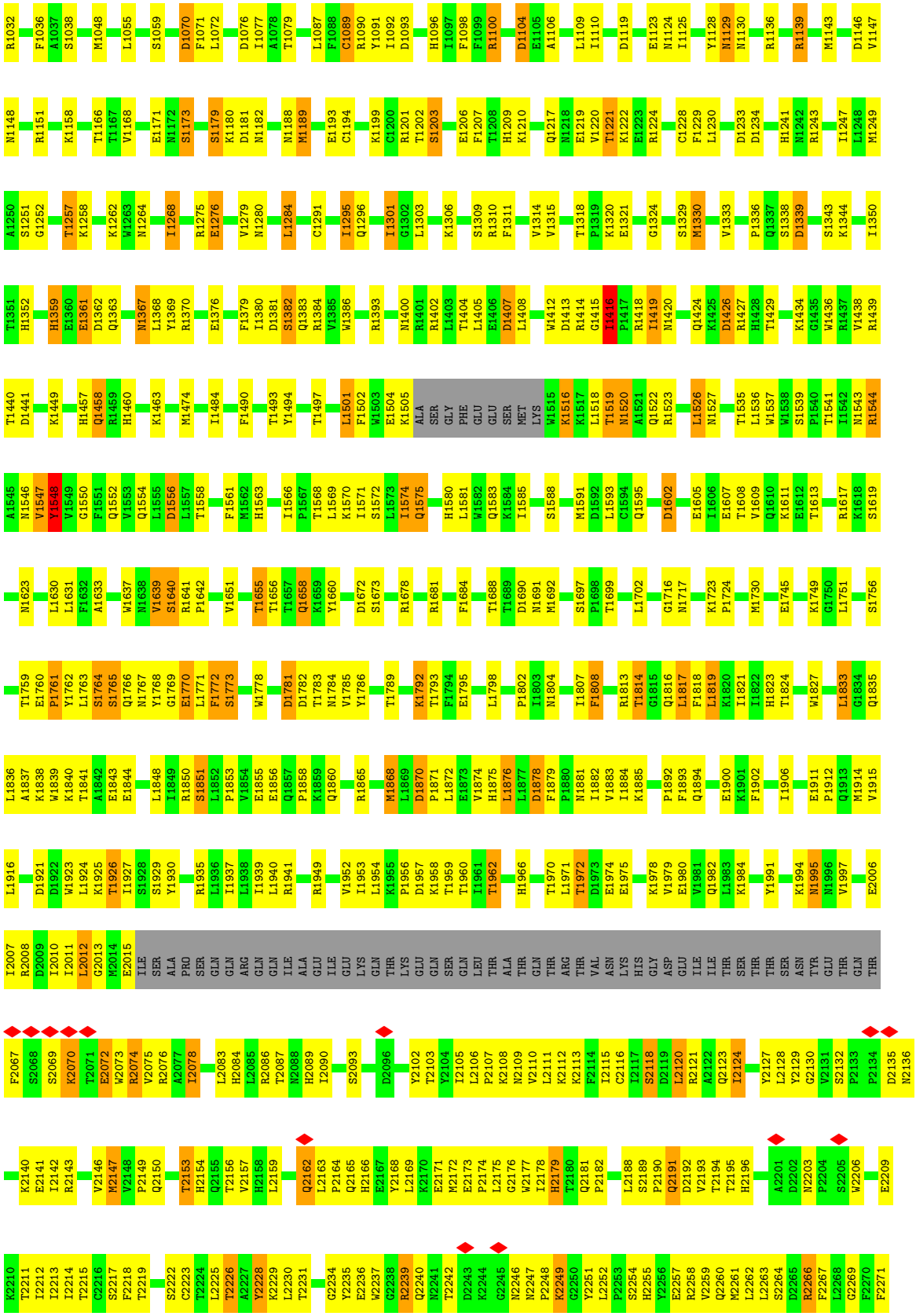
3 Residue-property plots (i)

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:

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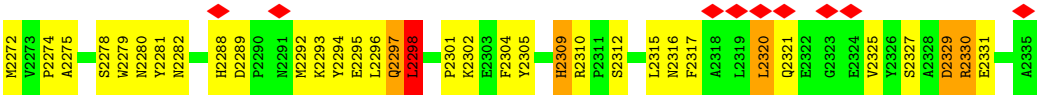
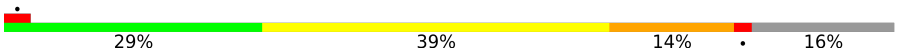
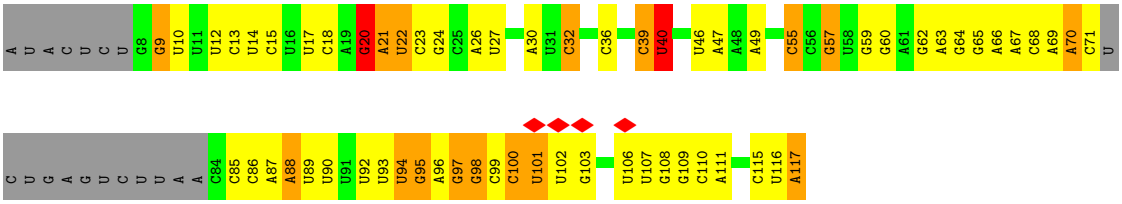


• Molecule 2: U5 snRNA

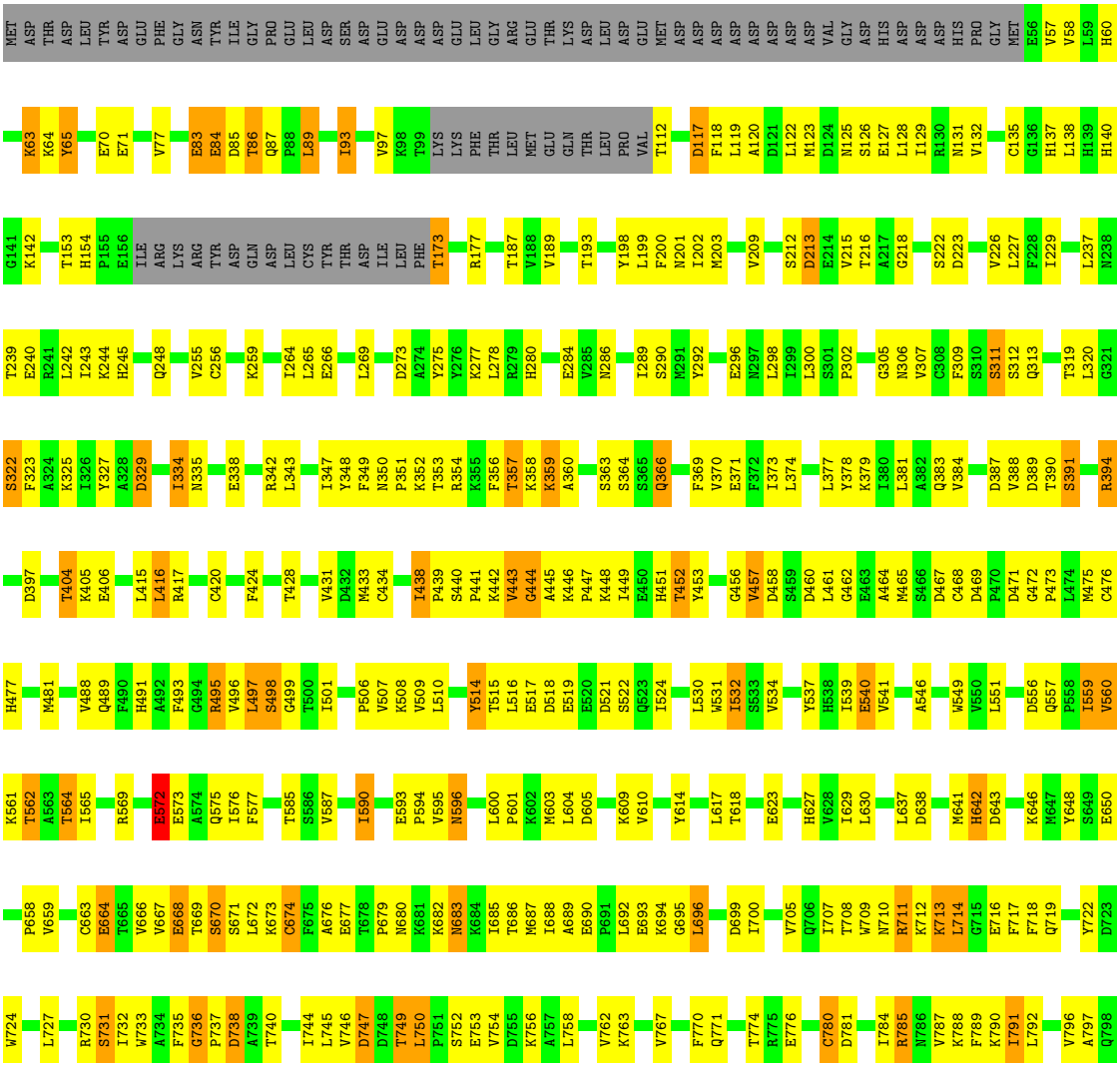
Chain B:





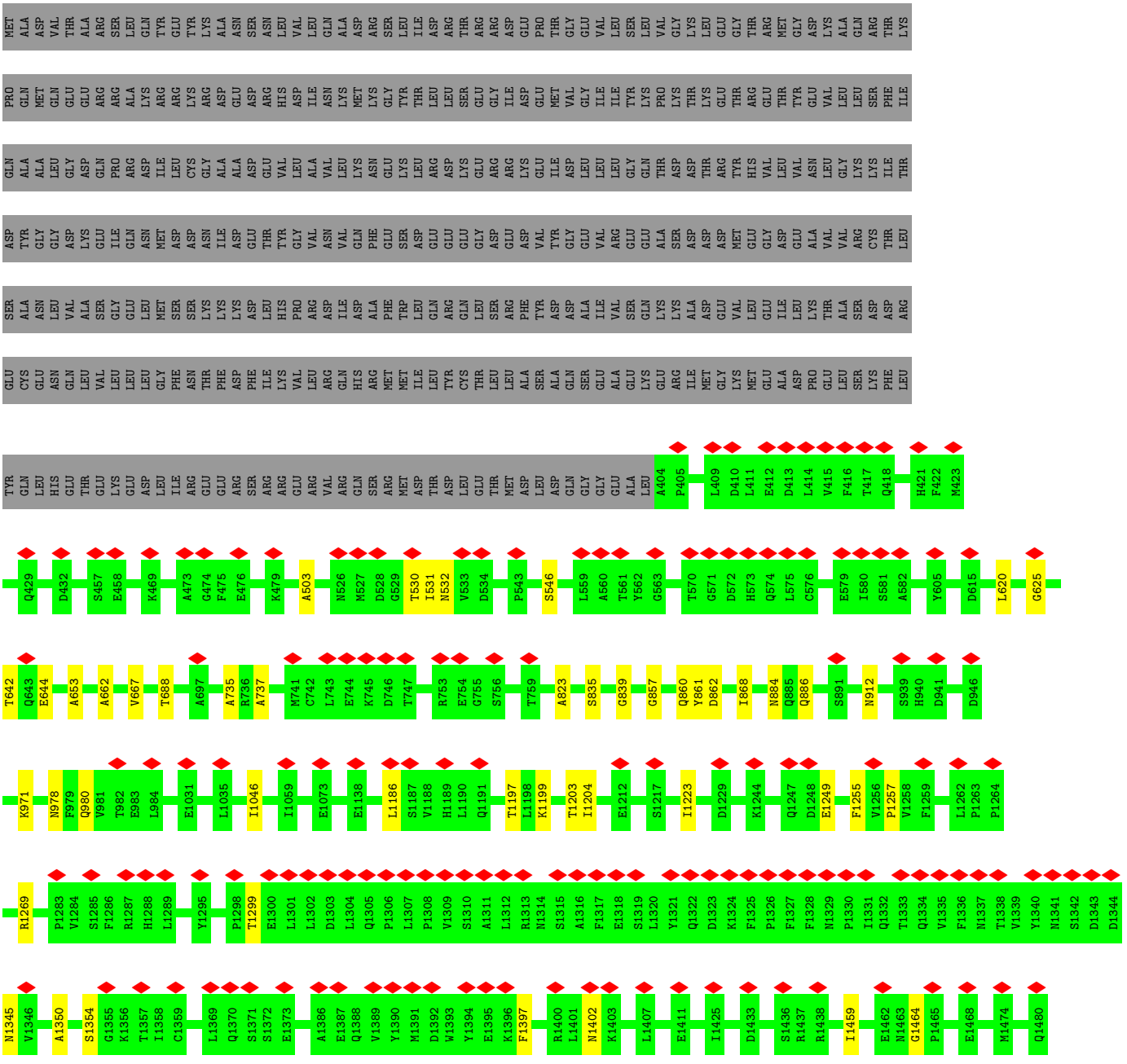
• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

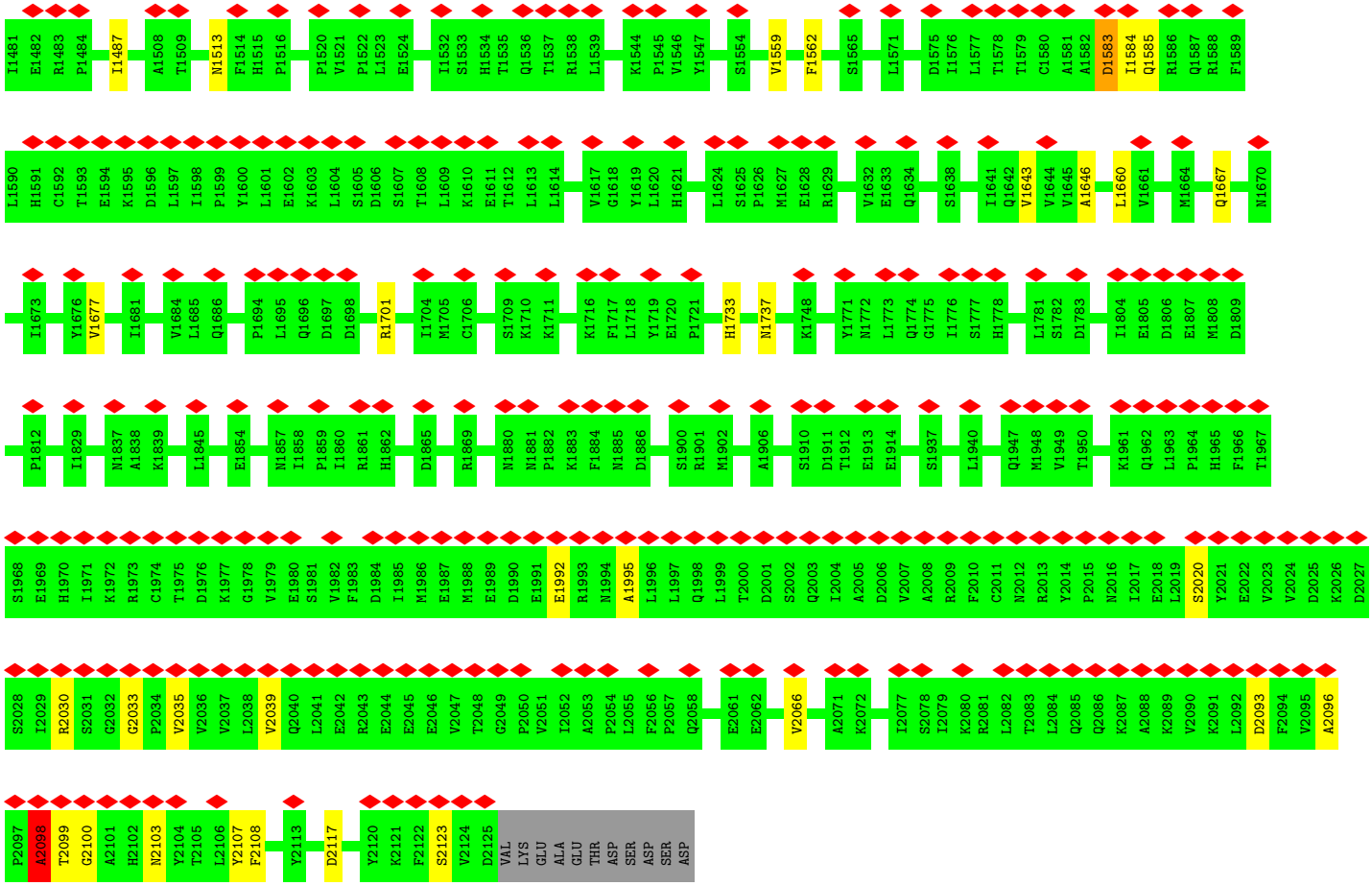
Chain C:



• Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

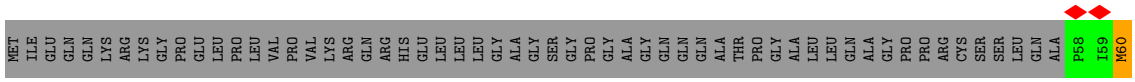
Chain D:

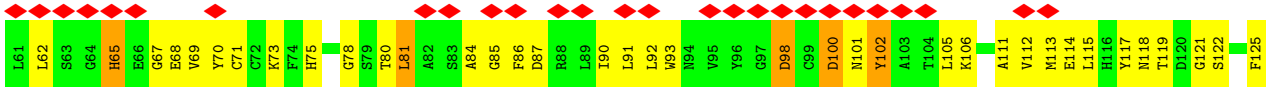


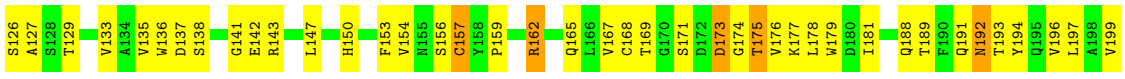


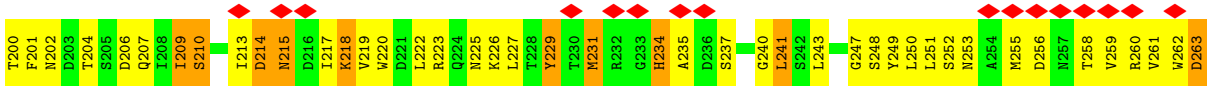
• Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

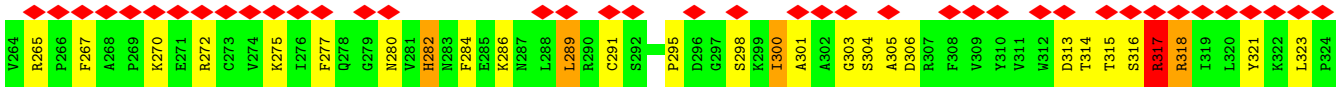
Chain E:

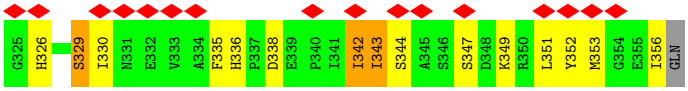




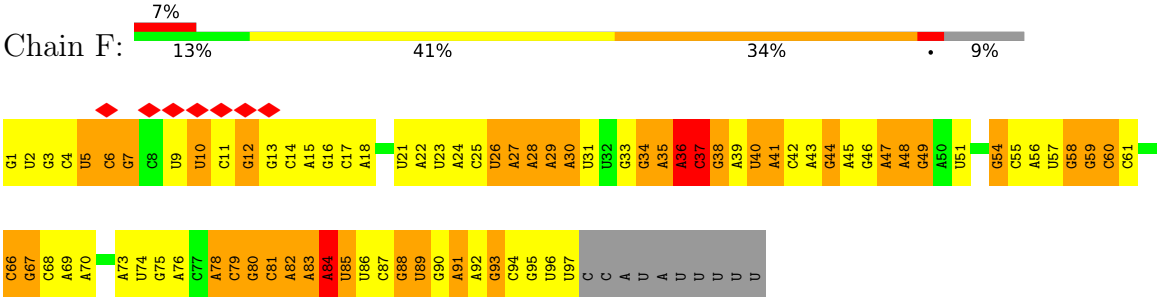




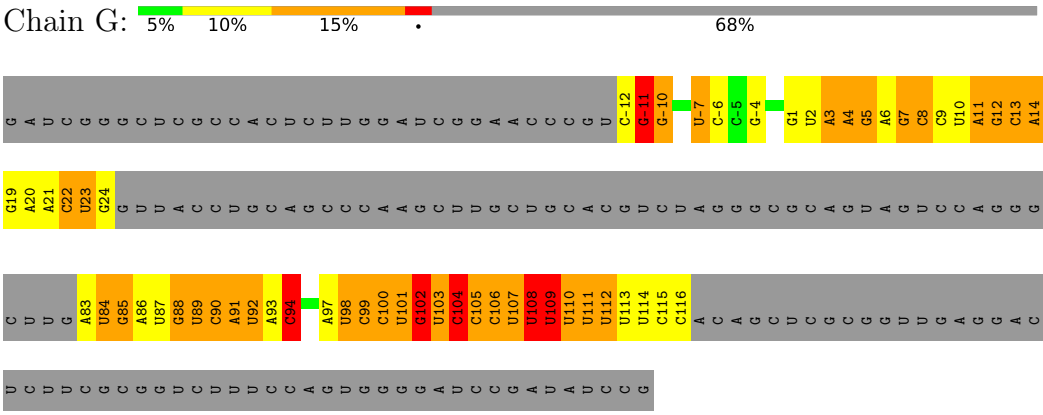




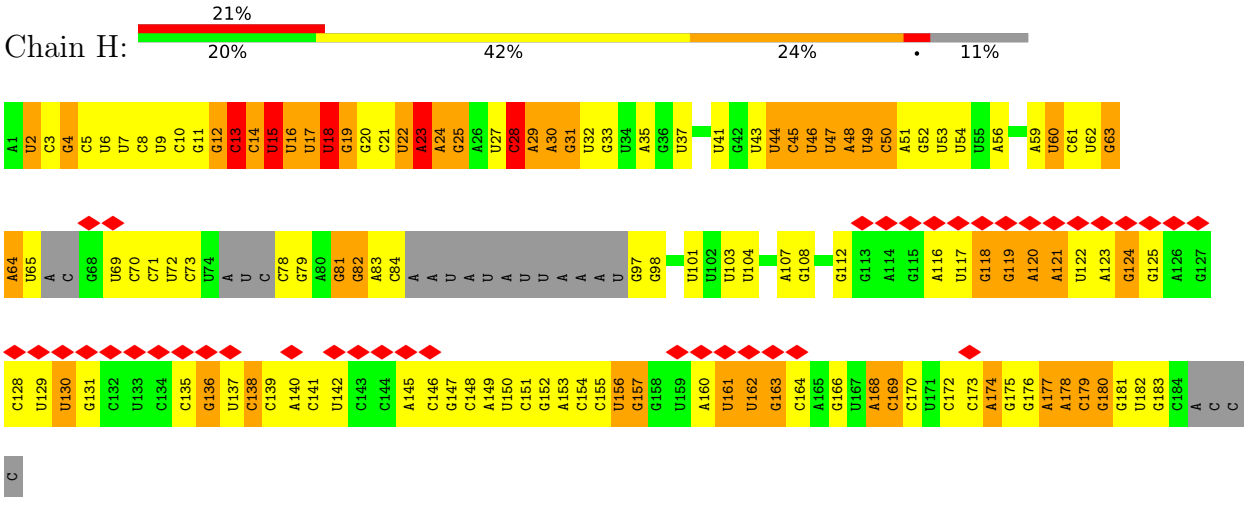
• Molecule 6: U6 snRNA



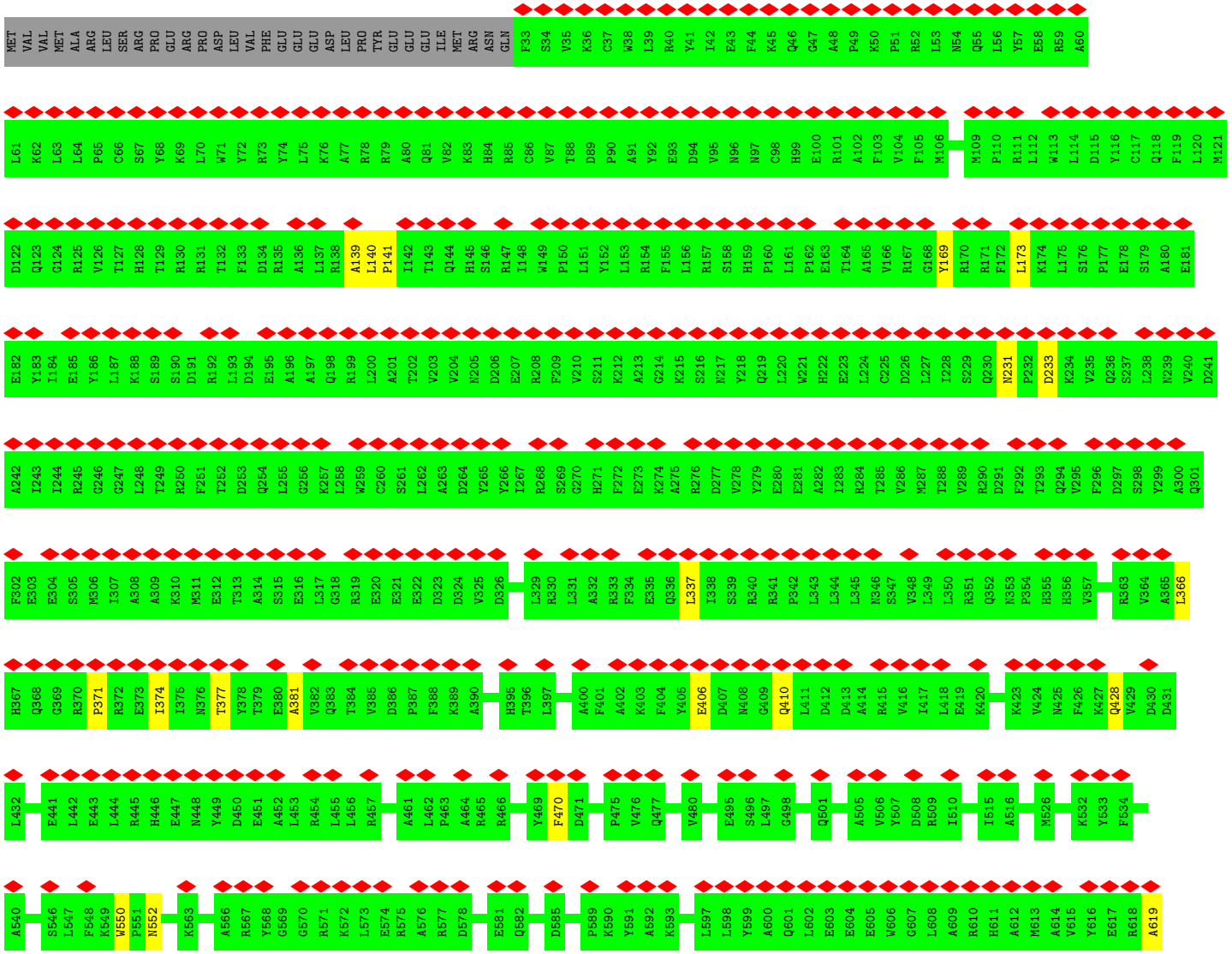
• Molecule 7: pre-mRNA



• Molecule 8: U2 snRNA

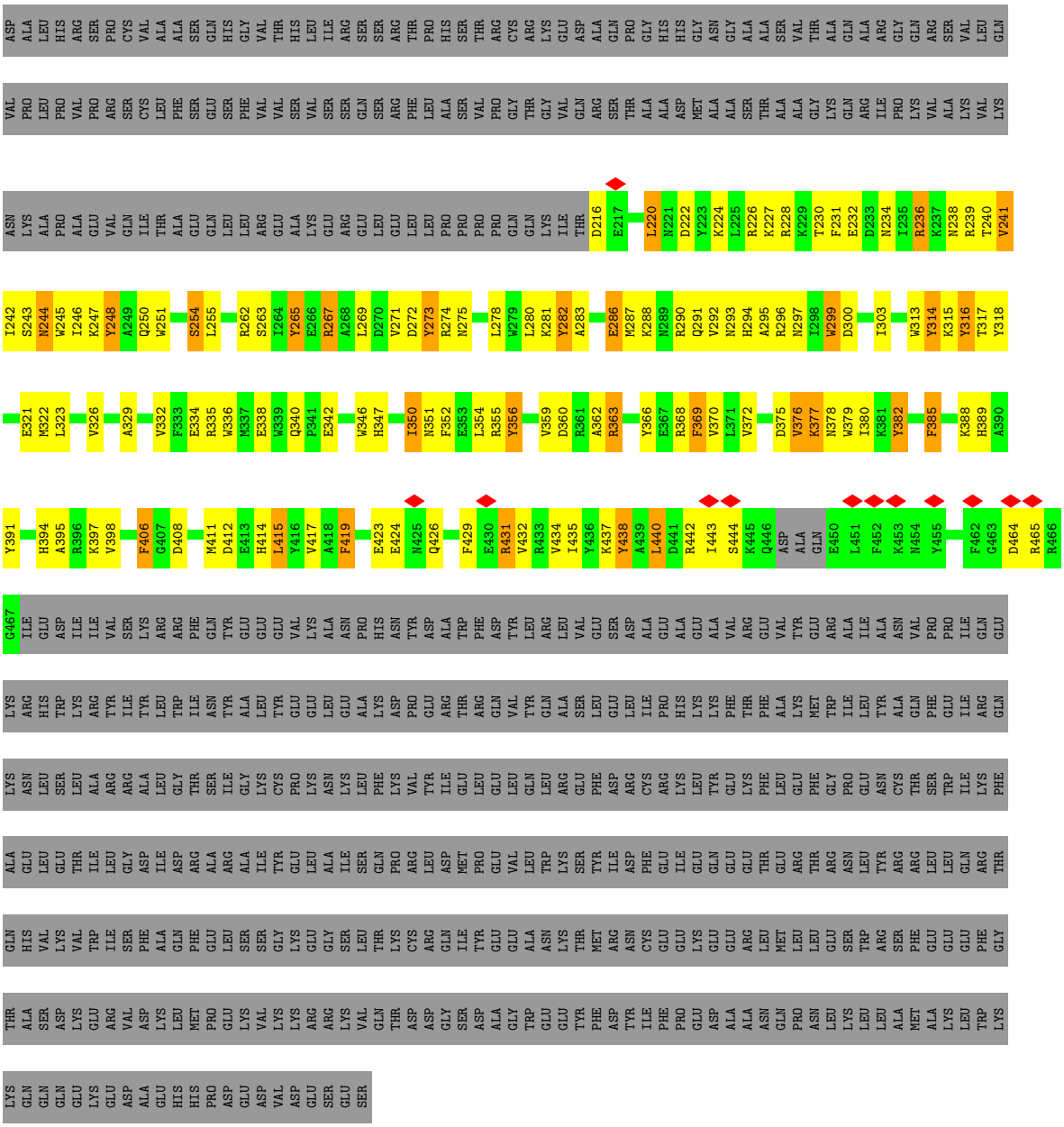


• Molecule 9: Pre-mRNA-splicing factor SYF1



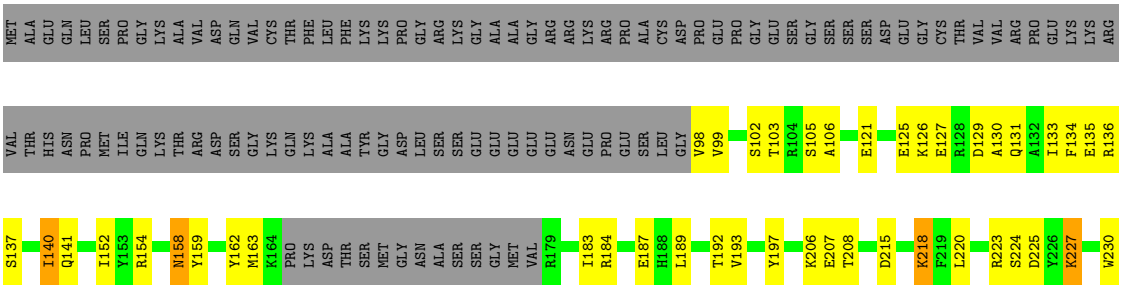
• Molecule 10: Crooked neck-like protein 1

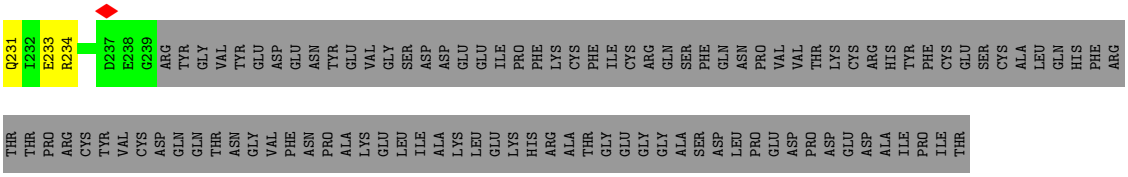
Chain J:

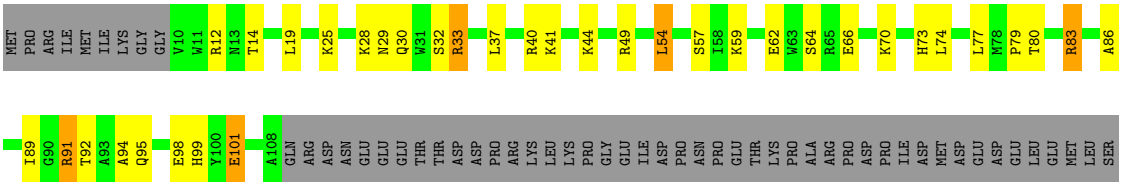


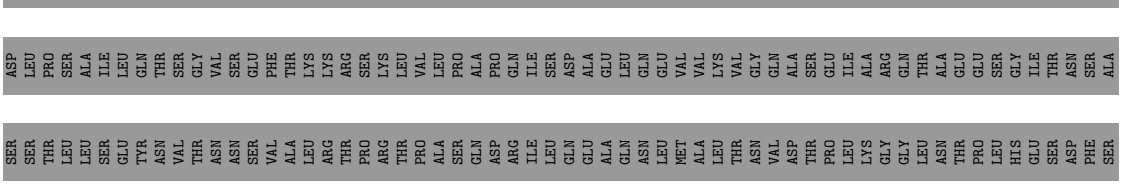
• Molecule 11: RING finger protein 113A

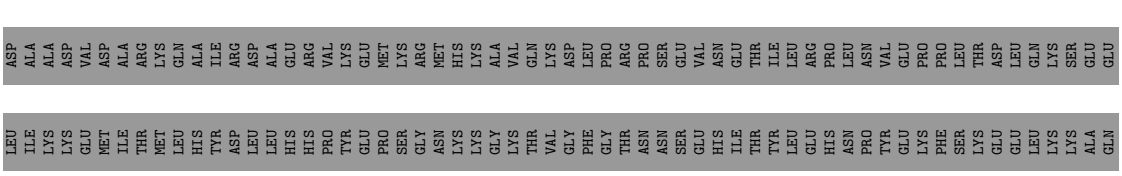
Chain K:

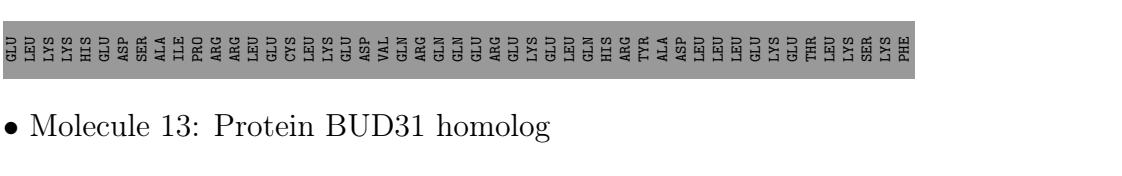










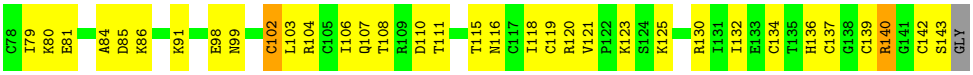


• Molecule 12: Cell division cycle 5-like protein

Chain L: 8% 88%

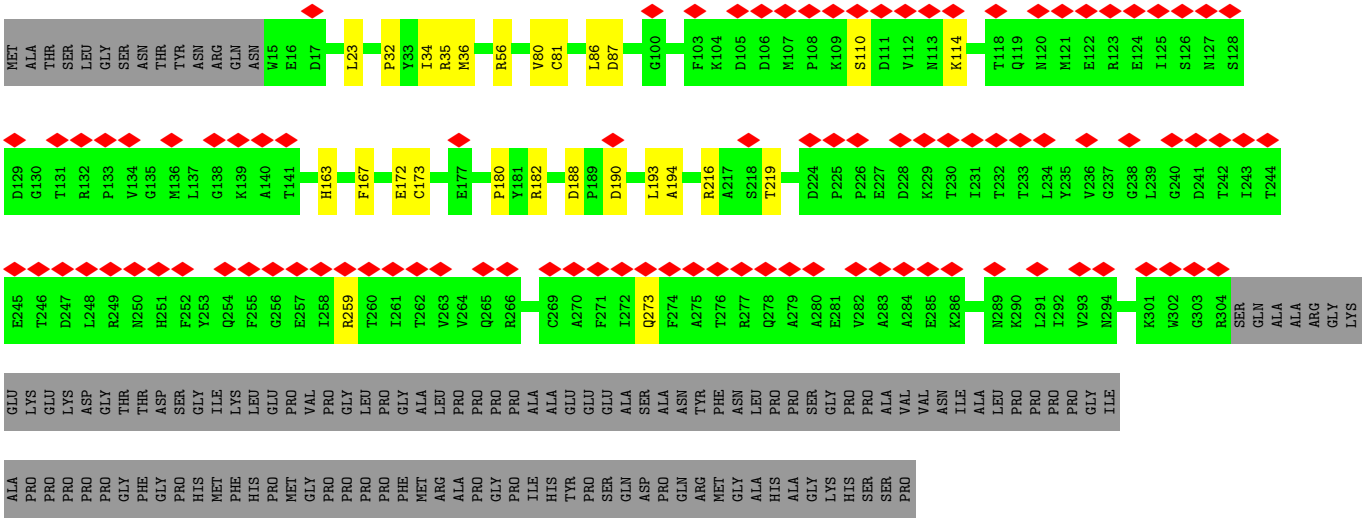
• Molecule 13: Protein BUD31 homolog

Chain N: 48% 47% 5%



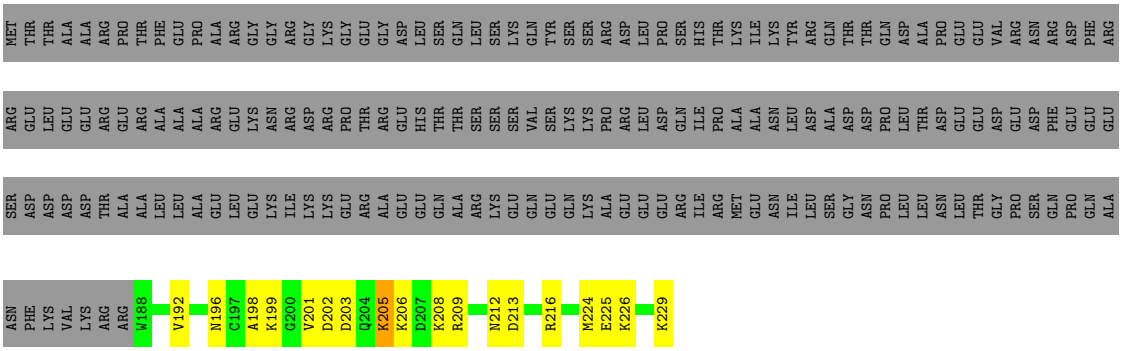
• Molecule 14: Pre-mRNA-splicing factor RBM22

Chain O:



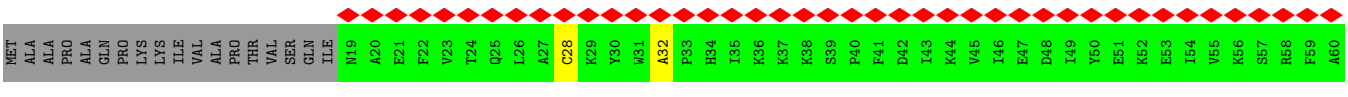
• Molecule 15: Spliceosome-associated protein CWC15 homolog

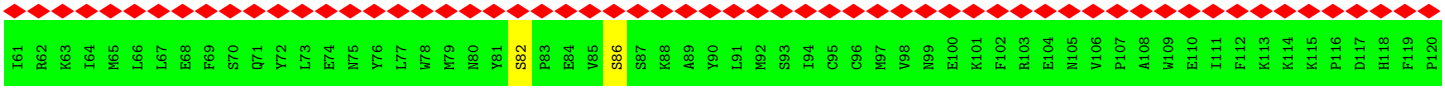
Chain P:

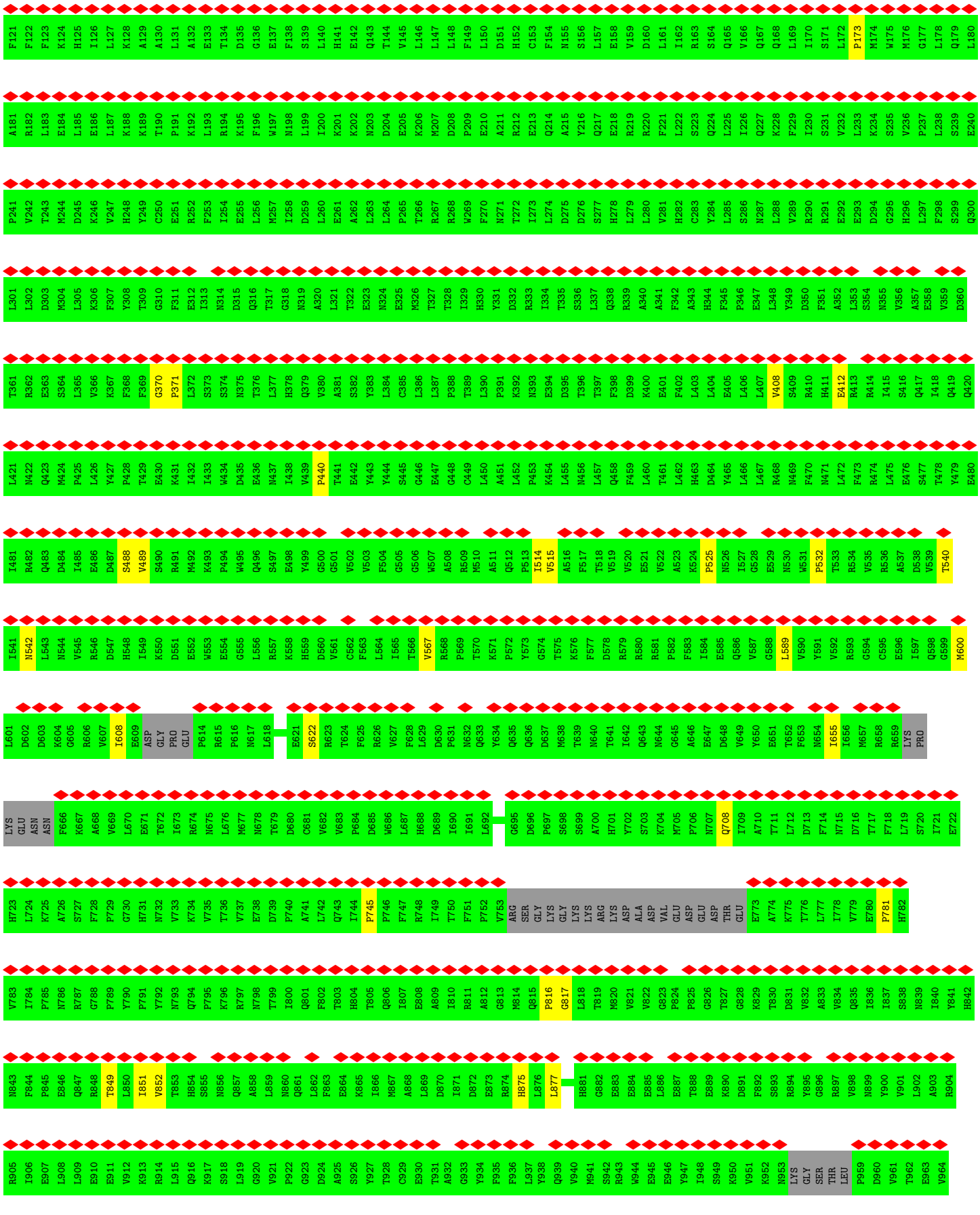


• Molecule 16: RNA helicase aquarius

Chain Q:



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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 L225 I226 Q227 K228 F229 I230 S231 V232 L233 K234 S235 Y236 P237 L238 S239 E240
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N843 P844 P845 E846 Q847 R848 T849 L850 I851 V852 T853 H854 S855 N856 Q857 A858 L859 N860 Q861 L862 F863 E864 K865 I866 M867 A868 L869 D870 I871 D872 E873 R874 H875 L876 L877 H881 G882 E883 E884 E885 L886 E887 T888 E889 K890 D891 F892 S893 R894 Y895 G896 R897 V898 N899 Y900 V901 L902 A903 R904
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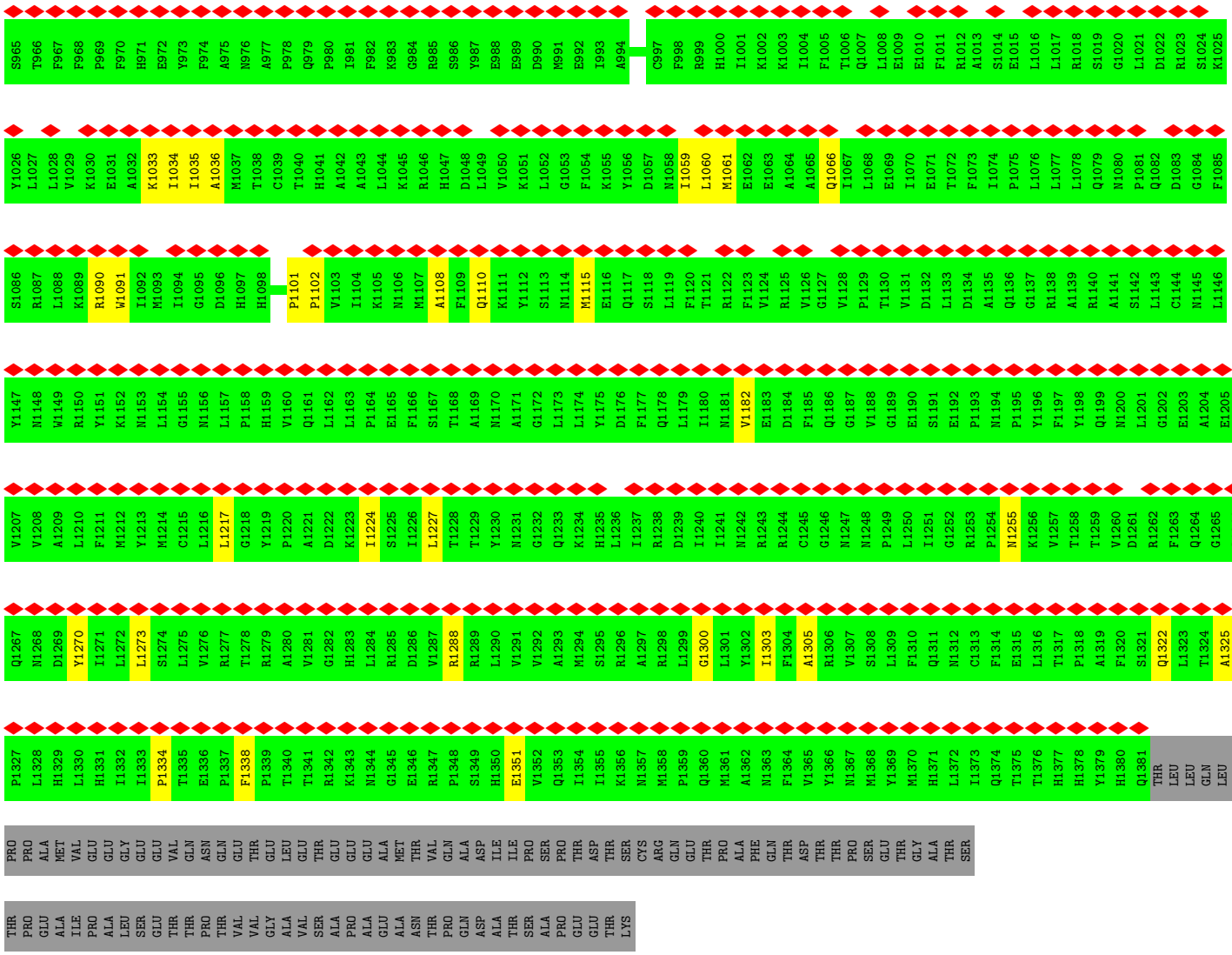
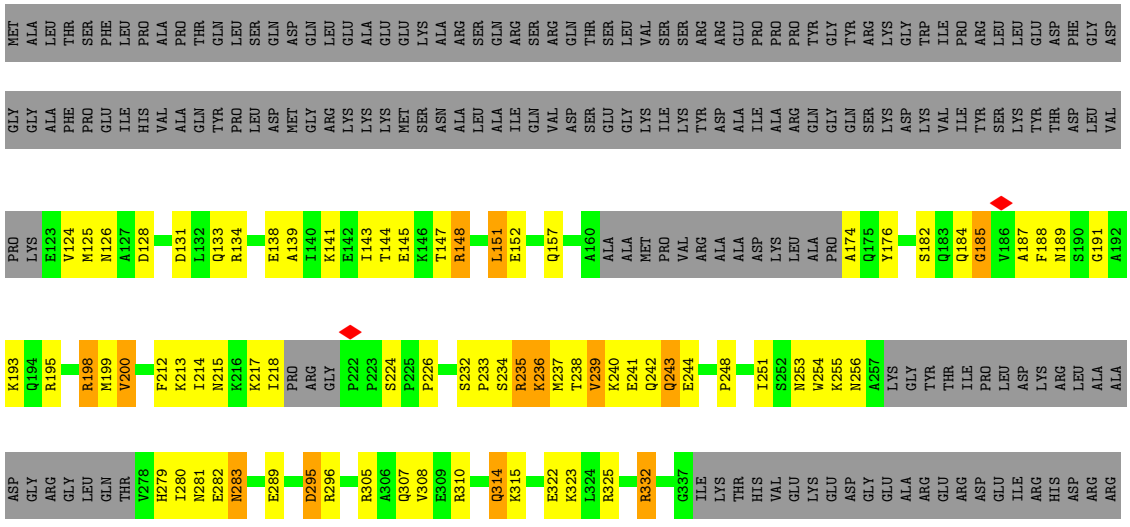
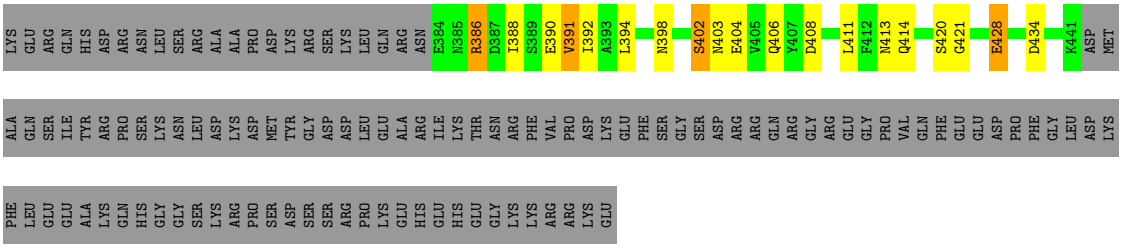


• Molecule 17: SNW domain-containing protein 1

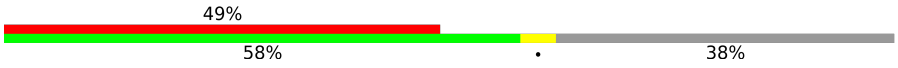
Chain R:

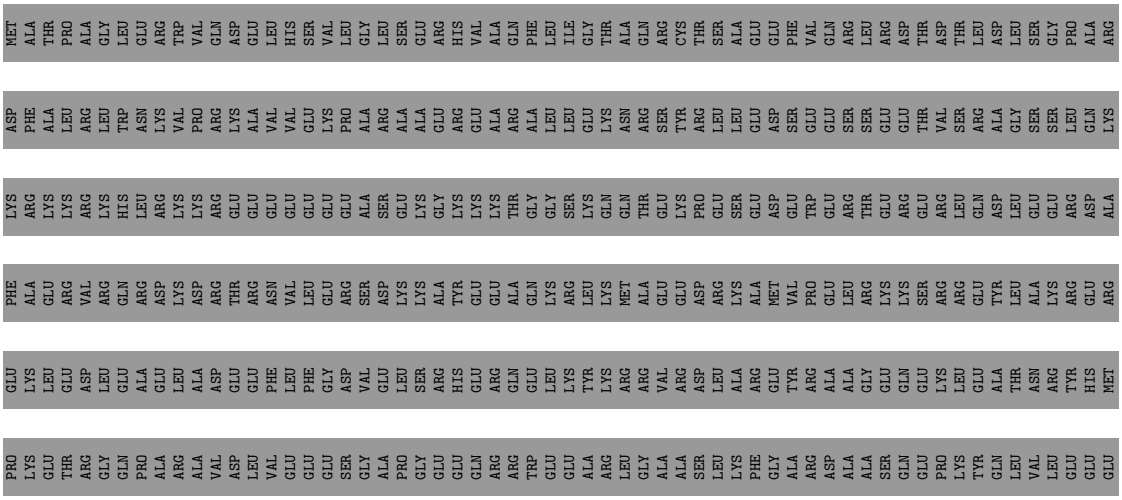


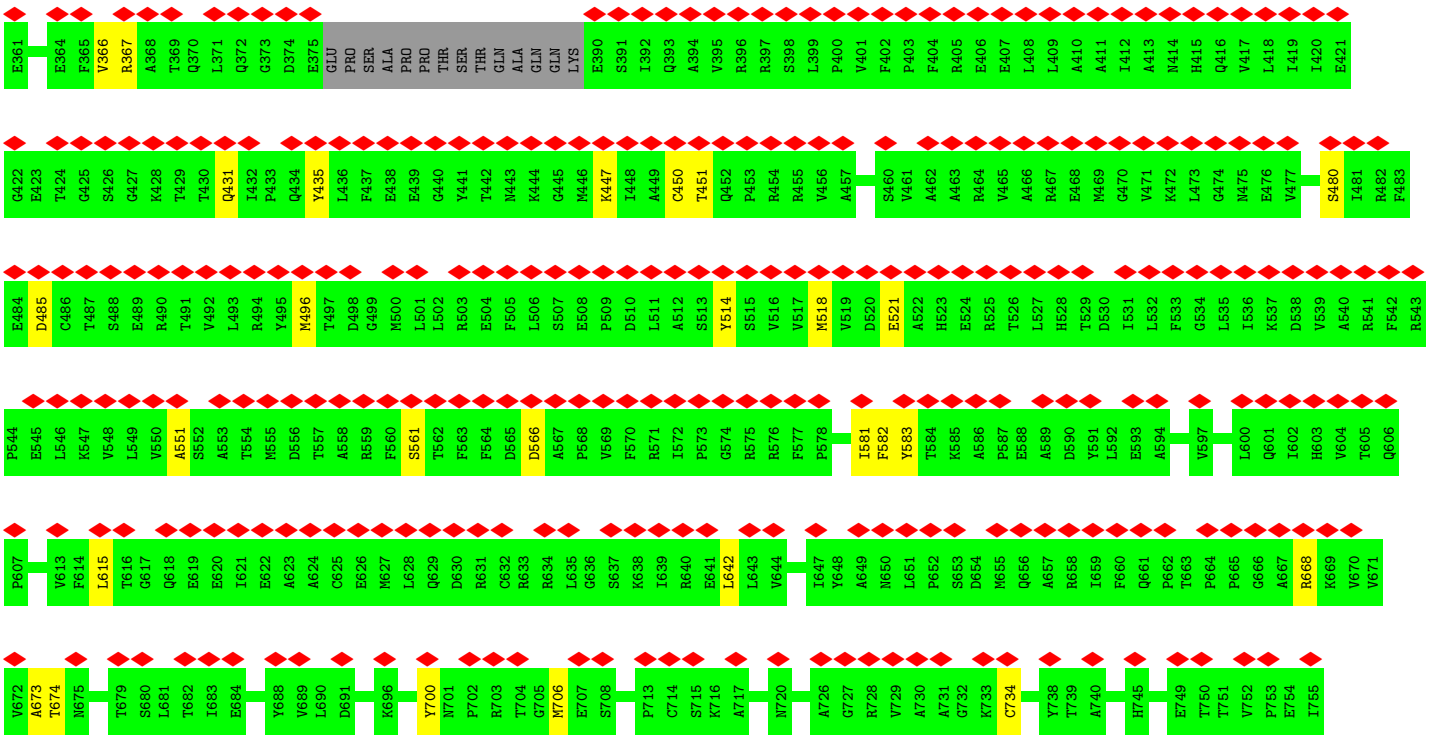


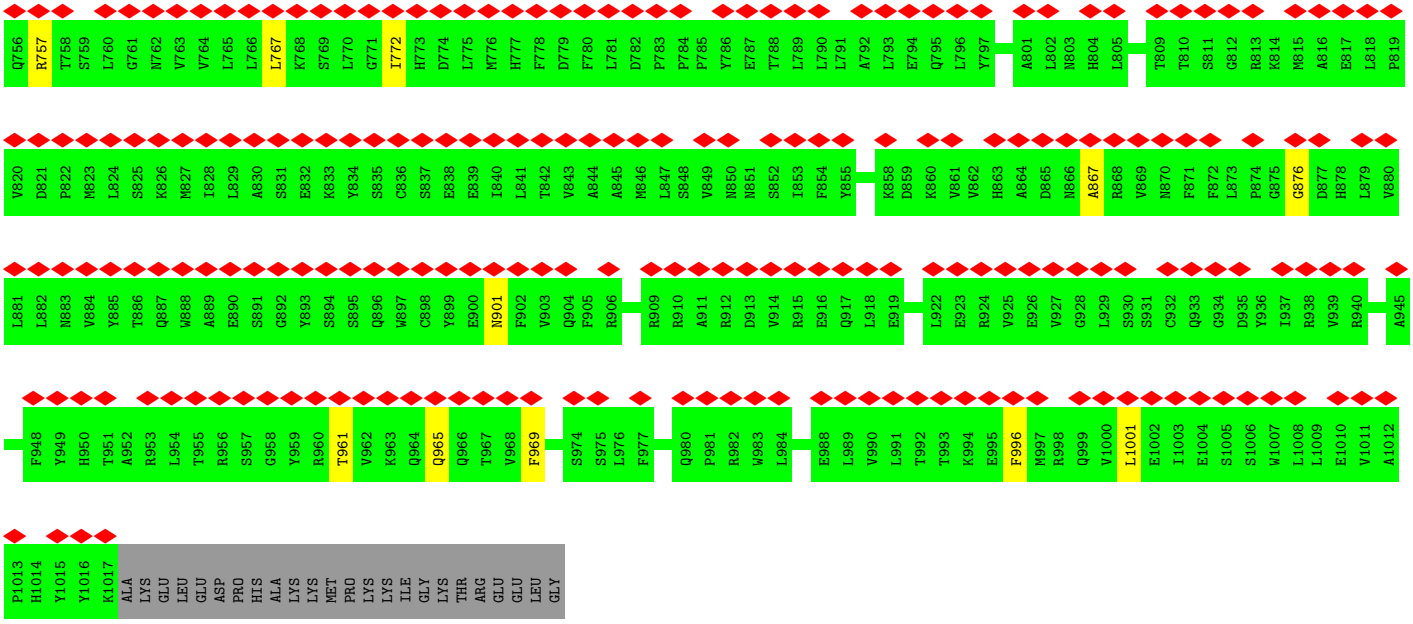
• Molecule 18: Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16

Chain S:



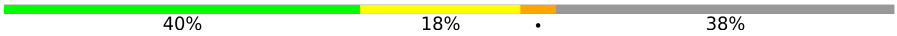


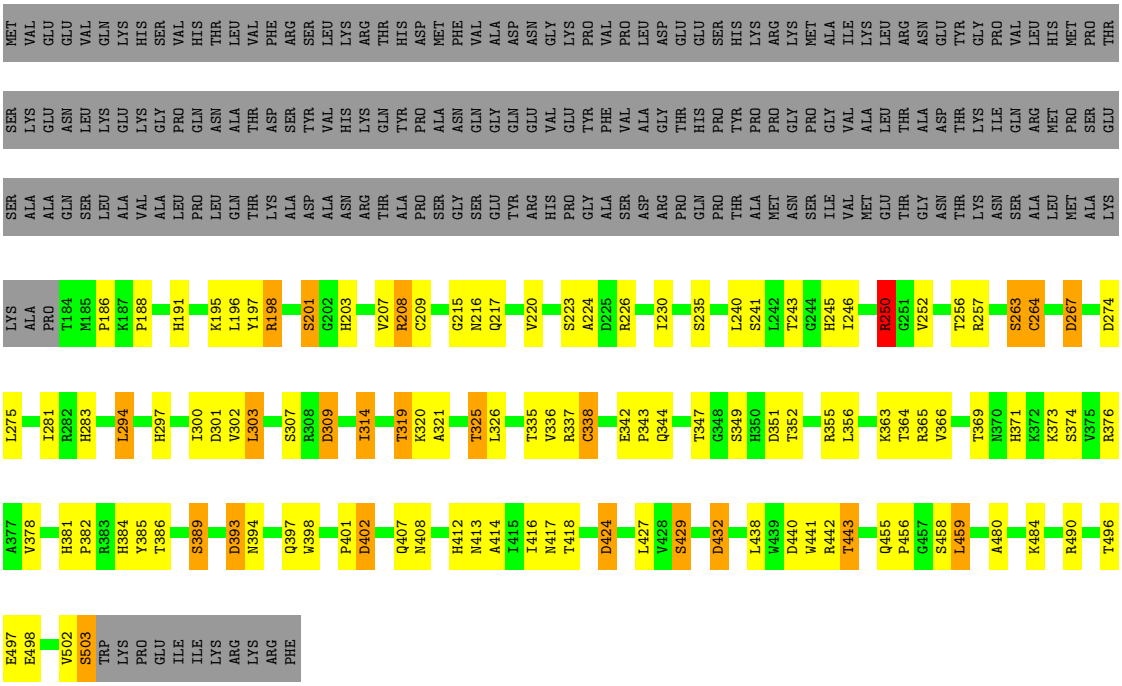




• Molecule 19: Pleiotropic regulator 1

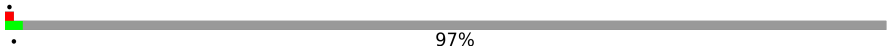
Chain T:

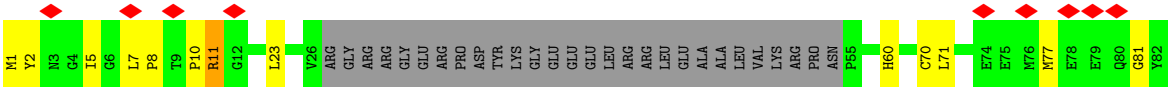


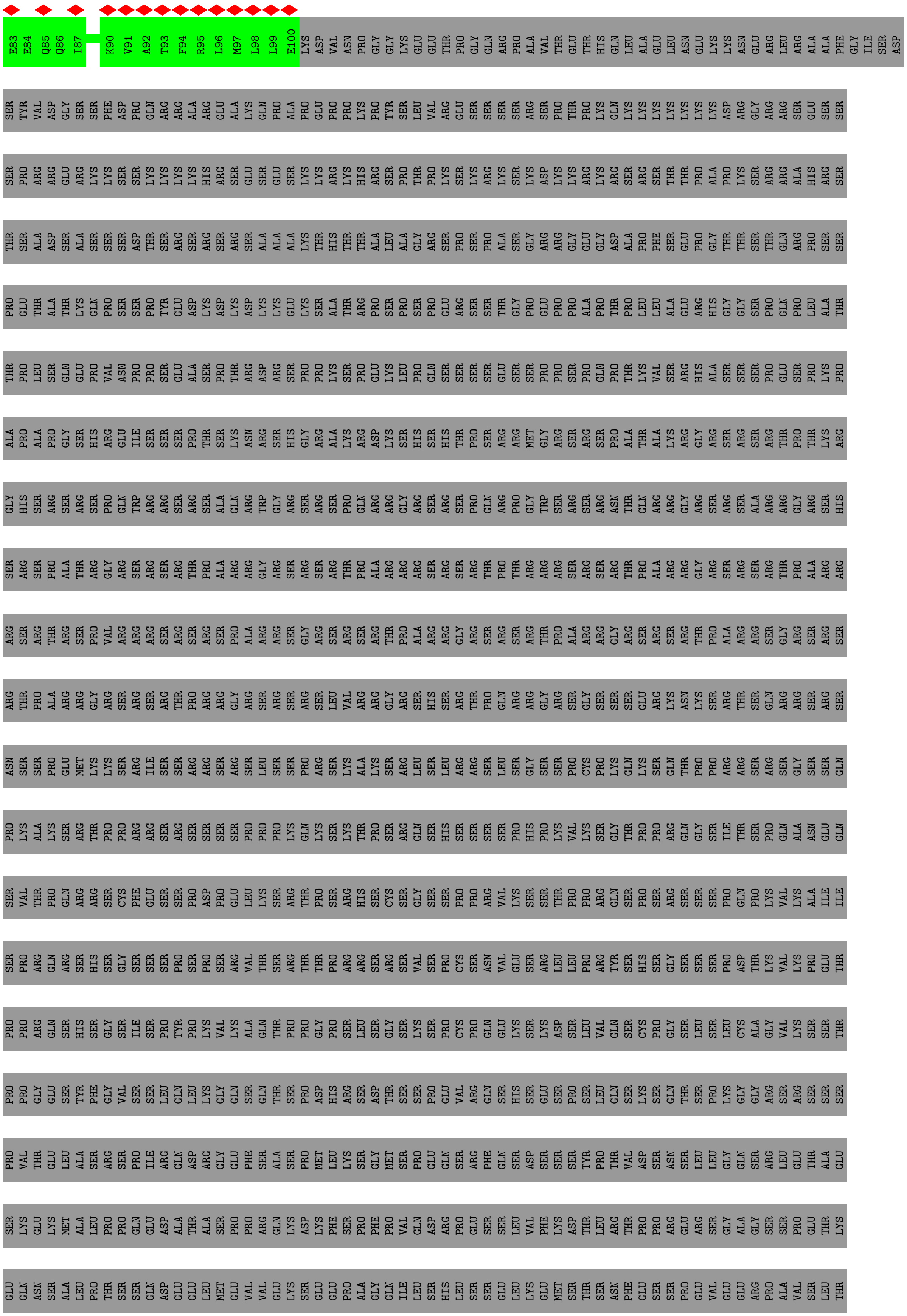


• Molecule 20: Serine/arginine repetitive matrix protein 2

Chain U:



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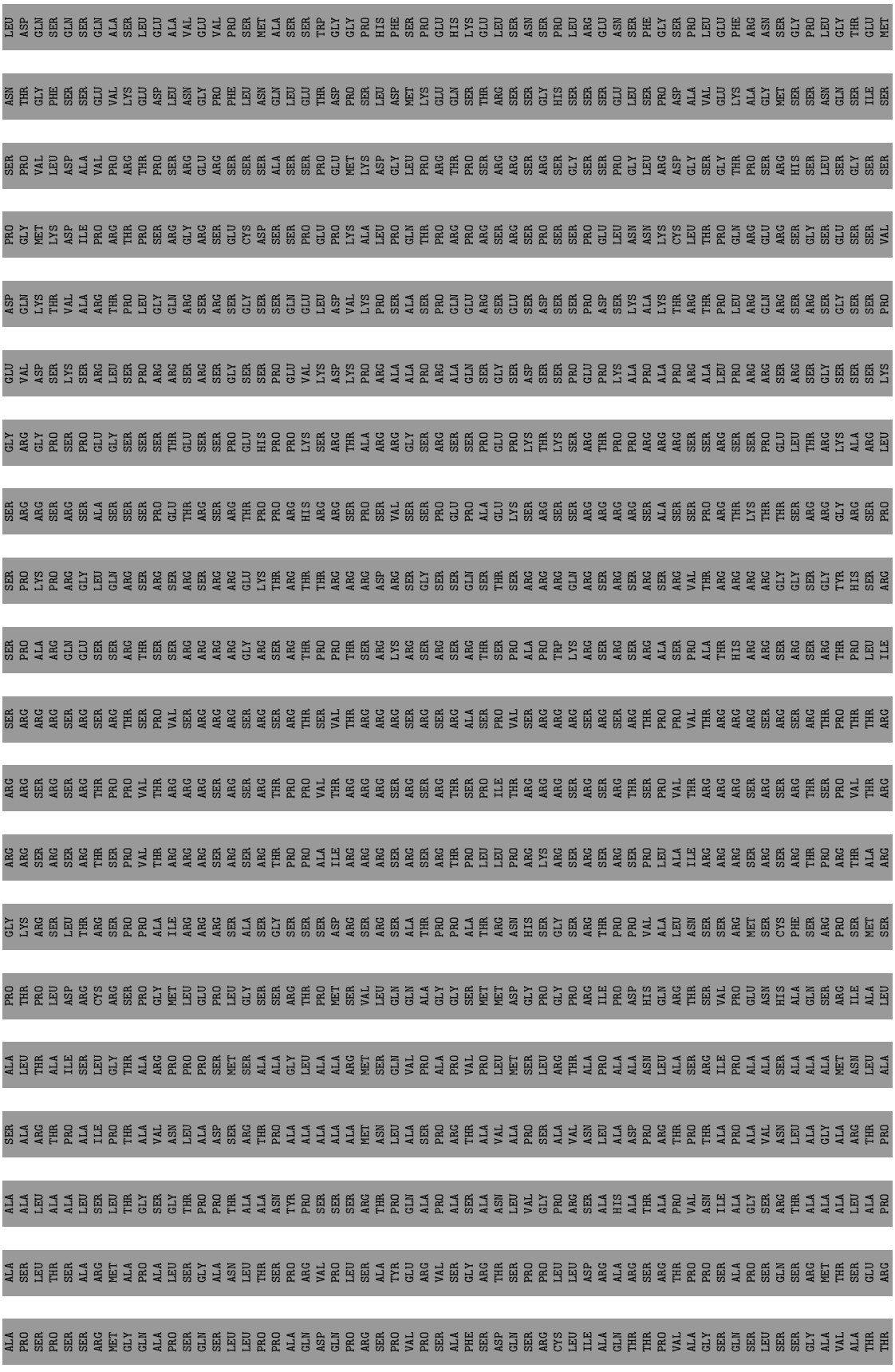
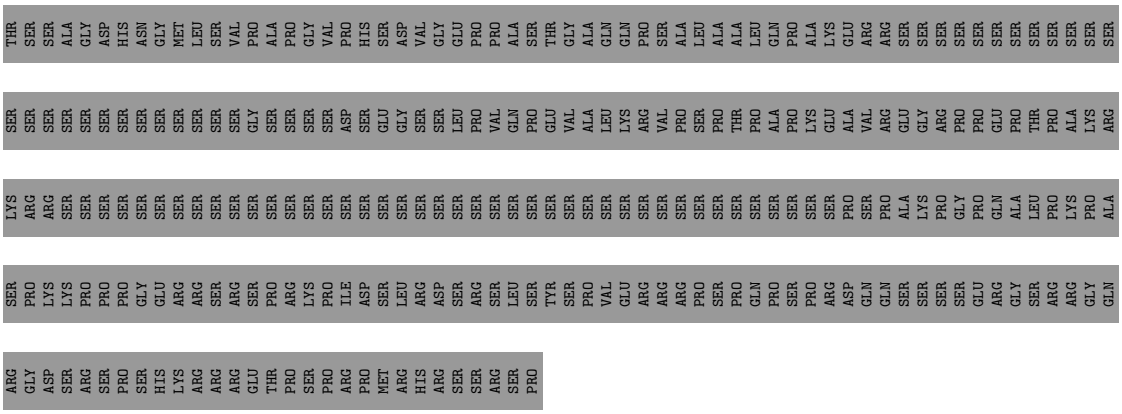
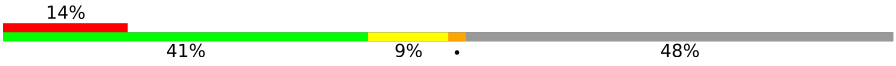
SER TYR VAL ASP GLY SER SER PHE ASP PRO GLN ARG ARG ALA ARG GLU ALA LYS GLN PRO ALA PRO GLU PRO PRO LYS PRO TYR SER LEU VAL ARG GLU SER SER SER SER ARG SER PRO THR PRO LYS GLN LYS LYS LYS LYS LYS LYS ASP ARG GLY ARG ARG SER GLU SER SER
SER PRO ARG ARG GLU ARG LYS LYS SER SER LYS LYS LYS LYS HIS ARG SER GLU SER GLU SER LYS LYS ARG LYS HIS ARG SER PRO THR PRO LYS SER LYS ARG LYS SER LYS ASP LYS LYS ARG LYS ARG SER ARG SER THR THR PRO ALA PRO LYS SER ARG ARG ALA HIS ARG SER
THR SER ALA ASP SER ALA SER SER SER ASP THR SER ARG SER ARG SER ARG SER ALA ALA ALA LYS THR HIS THR THR ALA LEU ALA GLY ARG SER PRO SER PRO ALA SER GLY ARG ARG GLY GLU GLY ASP ALA PRO PHE SER GLU PRO GLY THR THR SER THR GLN ARG PRO SER SER
PRO GLU THR ALA THR LYS GLN PRO SER SER PRO TYR GLU ASP LYS ASP LYS ASP LYS LYS GLU LYS SER ALA THR ARG PRO SER PRO SER PRO GLU ARG SER SER THR GLY PRO GLU PRO PRO ALA PRO THR PRO LEU LEU ALA GLU ARG HIS GLY GLY SER PRO GLN PRO LEU ALA THR
THR PRO LEU SER GLN GLU PRO VAL ASN PRO PRO SER GLU ALA SER PRO THR ARG ASP ARG SER PRO PRO LYS SER PRO GLU LYS LEU PRO GLN SER SER SER GLU SER SER PRO PRO SER PRO GLN PRO THR LYS VAL SER ARG HIS ALA SER SER SER PRO GLU SER PRO LYS PRO
ALA PRO ALA PRO GLY SER HIS ARG GLU ILE SER SER SER PRO THR SER LYS ASN ARG SER HIS GLY ARG ALA LYS ARG ASP LYS SER HIS SER HIS THR PRO SER ARG ARG MET GLY ARG SER ARG SER PRO ALA THR ALA LYS ARG GLY ARG SER ARG SER ARG THR PRO THR LYS ARG
GLY HIS SER ARG SER ARG SER PRO GLN TRP ARG ARG SER ARG SER ALA GLN ARG TRP GLY ARG SER ARG SER PRO GLN ARG ARG GLY ARG SER ARG SER PRO GLN ARG PRO GLY TRP SER ARG SER ARG ASN THR GLN ARG ARG GLY ARG SER ARG SER ALA ARG ARG GLY ARG SER HIS
SER ARG SER PRO ALA THR ARG GLY ARG SER ARG SER ARG THR PRO ALA ARG ARG GLY ARG SER ARG SER ARG THR PRO ALA ARG ARG ARG SER ARG SER ARG THR PRO THR ARG ARG SER ARG SER ARG THR PRO ALA ARG ARG GLY ARG SER ARG SER ARG THR PRO ALA ARG ARG
ARG SER ARG THR ARG SER PRO VAL ARG ARG ARG SER ARG SER ARG SER PRO ALA ARG ARG SER GLY ARG SER ARG SER ARG THR PRO ALA ARG ARG GLY ARG SER ARG SER ARG THR PRO ALA ARG ARG GLY ARG SER ARG SER ARG THR PRO ALA ARG ARG SER GLY ARG SER ARG SER
ARG THR PRO ALA ARG ARG GLY ARG SER ARG SER ARG THR PRO ARG ARG GLY ARG SER ARG SER ARG SER LEU VAL ARG ARG GLY ARG SER HIS SER ARG THR PRO GLN ARG ARG GLY ARG SER GLY SER SER SER GLU ARG LYS ASN LYS SER ARG THR SER GLN ARG ARG SER ARG SER
ASN SER SER PRO GLU MET LYS LYS SER ARG ILE SER SER ARG ARG SER ARG SER LEU SER SER PRO ARG SER LYS ALA LYS SER ARG LEU SER LEU ARG ARG SER LEU SER GLY SER SER PRO CYS PRO LYS GLN LYS SER GLN THR PRO PRO ARG ARG SER ARG SER GLY SER GLN
PRO LYS ALA LYS SER ARG THR PRO PRO ARG ARG SER ARG SER SER SER SER PRO PRO PRO LYS GLN LYS SER LYS THR PRO SER ARG GLN SER HIS SER SER SER SER PRO HIS PRO LYS VAL LYS SER GLY THR PRO PRO ARG GLN GLY SER ILE THR SER PRO GLN ALA ASN GLN GLN
SER VAL THR PRO GLN ARG ARG SER CYS PHE GLU SER SER PRO ASP PRO GLU LEU LYS SER ARG THR PRO SER ARG HIS SER CYS SER GLY SER SER PRO PRO ARG VAL LYS SER SER THR PRO PRO ARG GLN SER PRO SER ARG SER SER SER PRO GLN PRO LYS VAL LYS ALA ILE ILE
SER PRO ARG GLN ARG SER HIS SER GLY SER SER SER PRO SER PRO SER ARG VAL THR SER ARG THR THR PRO ARG ARG SER ARG SER VAL SER PRO CYS SER ASN VAL GLU SER ARG LEU LEU PRO ARG TYR SER HIS SER GLY SER SER SER PRO ASP THR LYS VAL LYS PRO GLU THR
PRO PRO ARG GLN SER HIS SER GLY SER ILE SER PRO TYR PRO LYS VAL LYS ALA GLN THR PRO PRO GLY PRO SER LEU SER GLY SER LYS SER PRO CYS PRO GLN GLU LYS SER LYS ASP SER LEU VAL GLN SER CYS PRO GLY SER LEU SER LEU CYS ALA GLY VAL LYS SER SER THR
PRO PRO GLY GLU SER TYR PHE GLY VAL SER SER LEU GLN LEU LYS GLY GLN SER GLN THR SER PRO ASP HIS ARG SER ASP THR SER SER PRO GLU VAL ARG GLN SER HIS SER GLU SER PRO SER LEU GLN SER LYS SER GLN THR SER PRO LYS GLY GLY ARG SER ARG SER SER SER
PRO VAL THR GLU LEU ALA SER ARG SER PRO ILE ARG GLN ASP ARG GLY GLU PHE SER ALA SER PRO MET LEU LYS SER GLY MET SER PRO GLU GLN SER ARG PHE GLN SER ASP SER SER SER TYR PRO THR VAL ASP SER ASN SER LEU LEU GLY GLN SER ARG LEU GLU THR ALA GLU
SER LYS GLU LYS MET ALA LEU PRO PRO GLN GLU ASP ALA THR ALA SER PRO PRO ARG GLN LYS ASP LYS PHE SER PRO PHE PRO VAL GLN ASP ARG PRO GLU SER SER LEU VAL PHE LYS ASP THR LEU ARG THR PRO PRO ARG GLU ARG SER GLY ALA GLY SER SER PRO GLU THR LYS
GLU GLN ASN SER ALA LEU PRO THR SER SER GLN ASP GLU GLU LEU MET GLU VAL VAL GLU LYS SER GLU GLU PRO ALA GLY GLN ILE LEU SER HIS LEU SER SER GLU LEU LYS GLU MET SER THR SER ASN PHE GLU SER SER PRO GLU VAL GLU GLU ARG PRO ALA VAL SER LEU THR

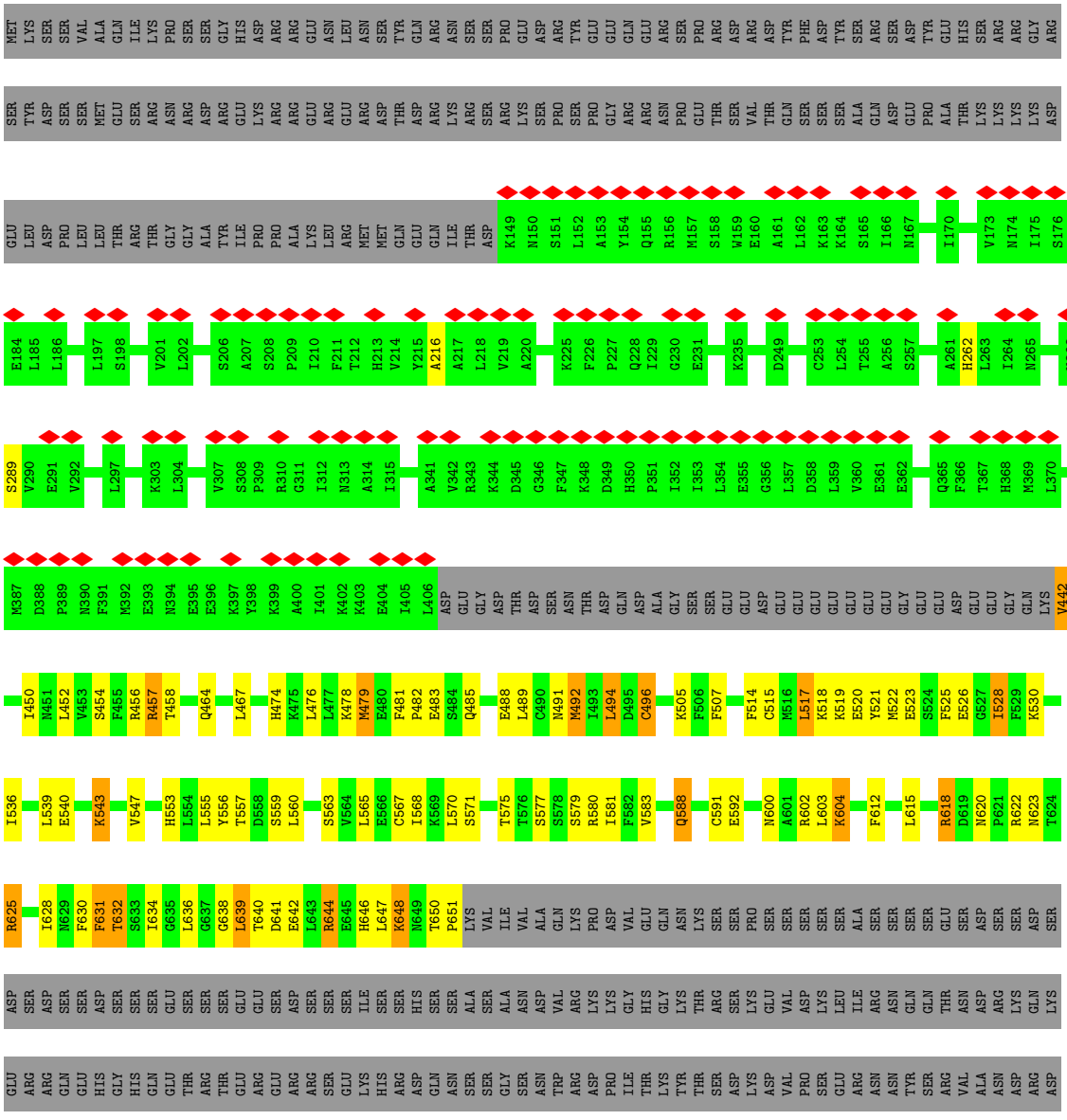


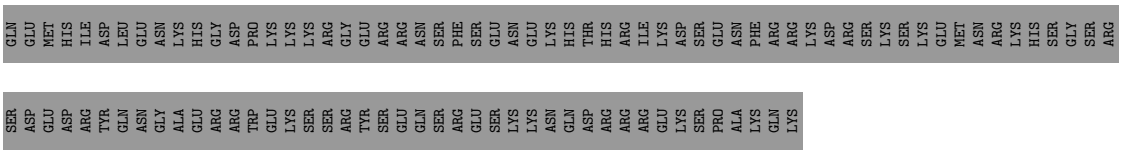


• Molecule 21: Pre-mRNA-splicing factor CWC22 homolog

Chain V:





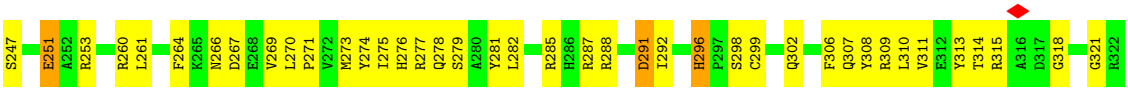


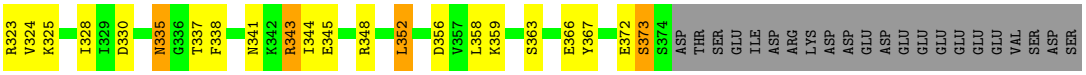
• Molecule 22: Unknown polymer

Chain W:

• Molecule 23: Smad nuclear-interacting protein 1

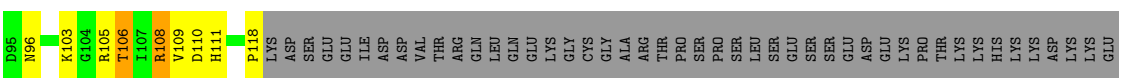
Chain X:

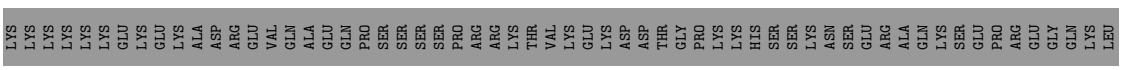


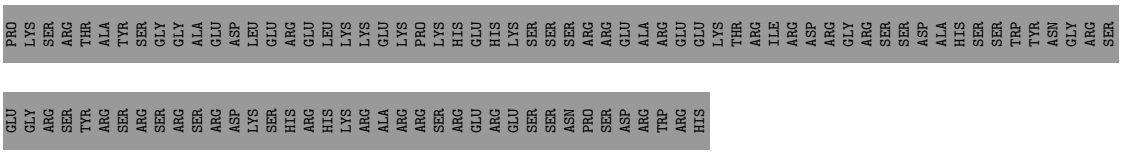


• Molecule 24: RNA-binding motif protein, X-linked 2

Chain Y:

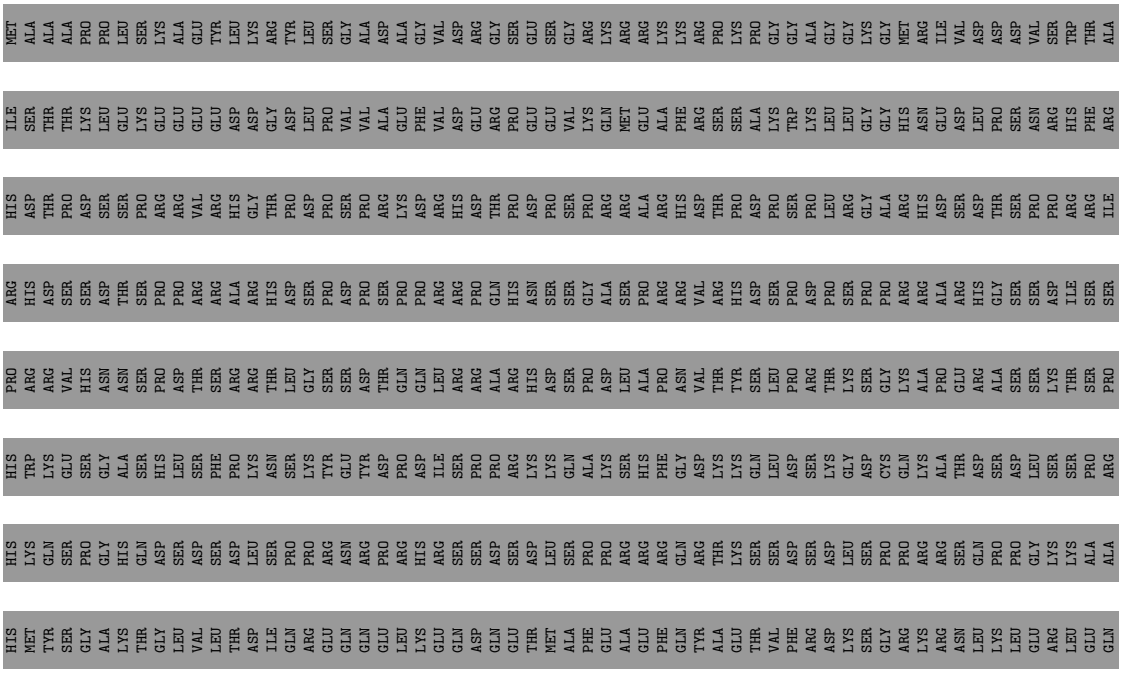






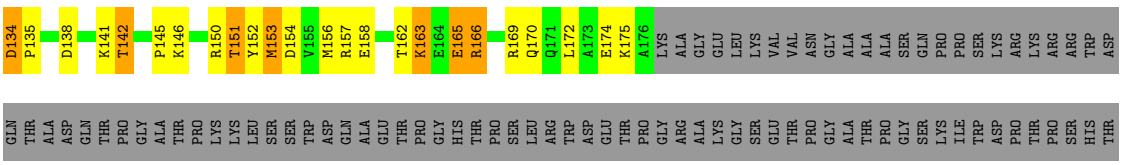
• Molecule 25: BUD13 homolog

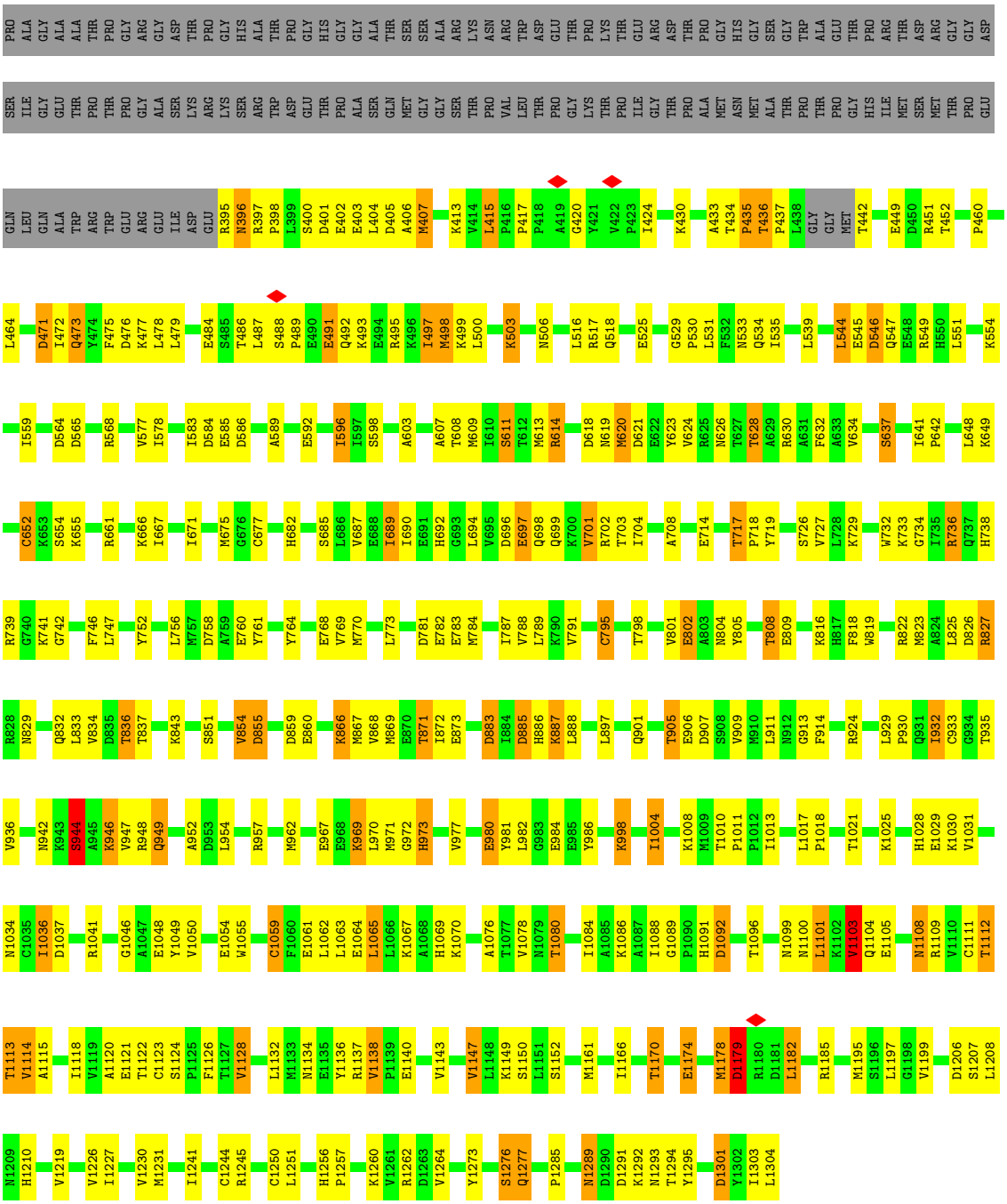
Chain Z:



• Molecule 26: Splicing factor 3B subunit 1

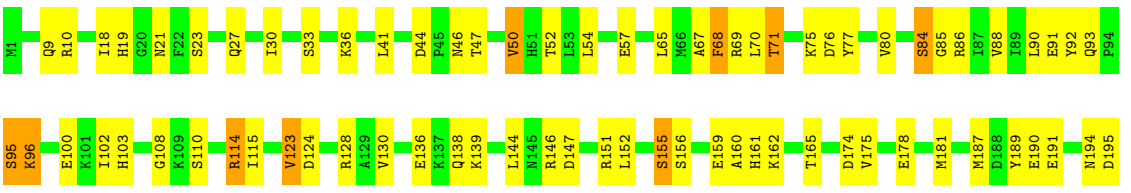
Chain 1:

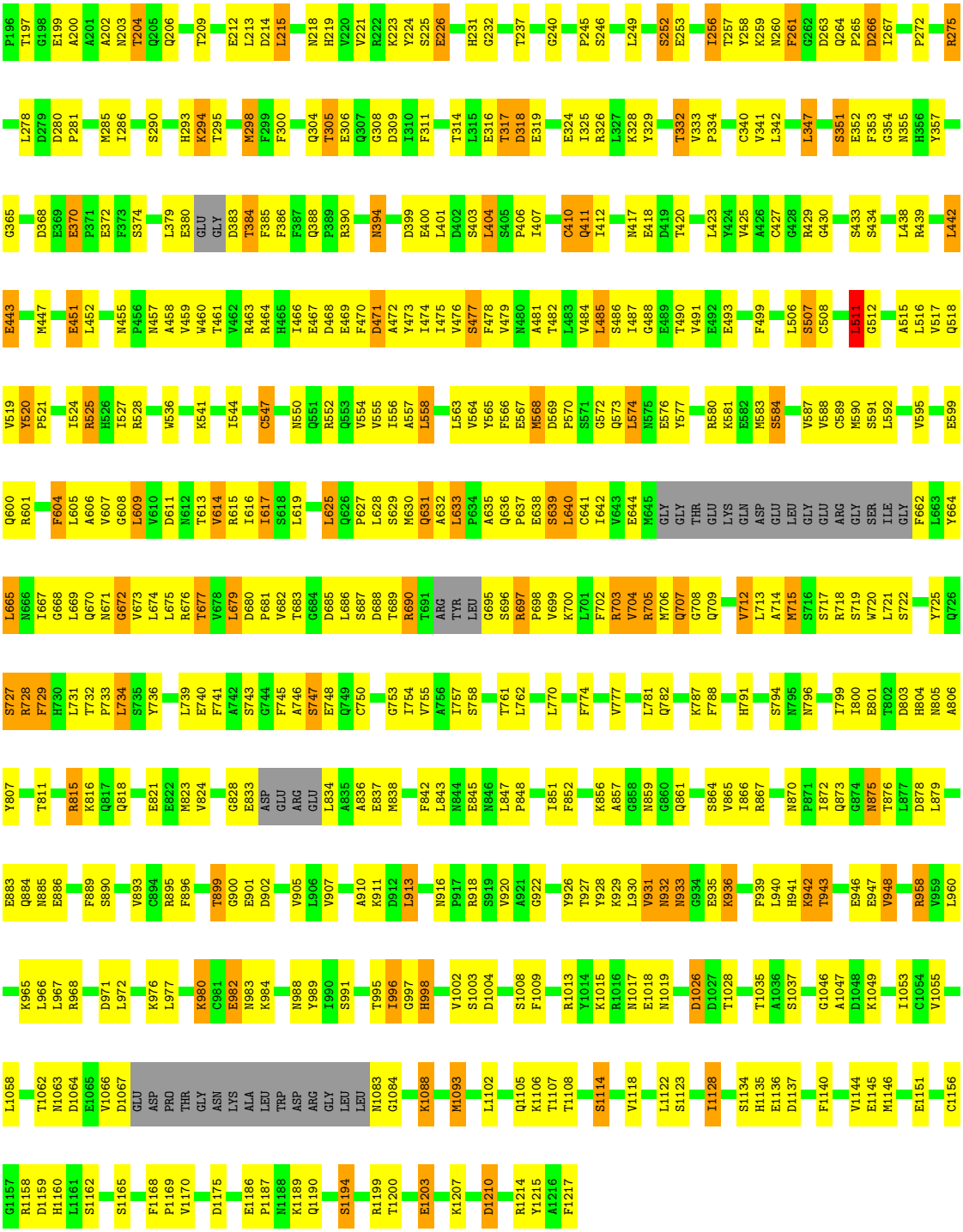




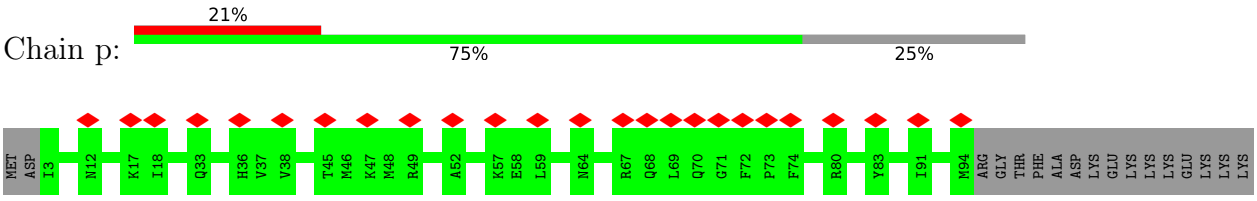
• Molecule 27: Splicing factor 3B subunit 3

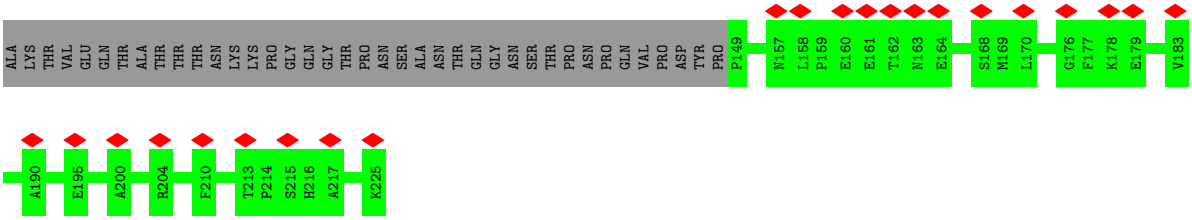
Chain 3:



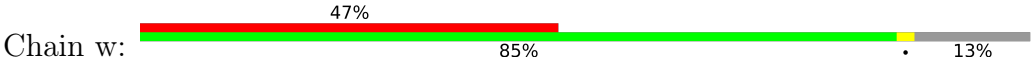


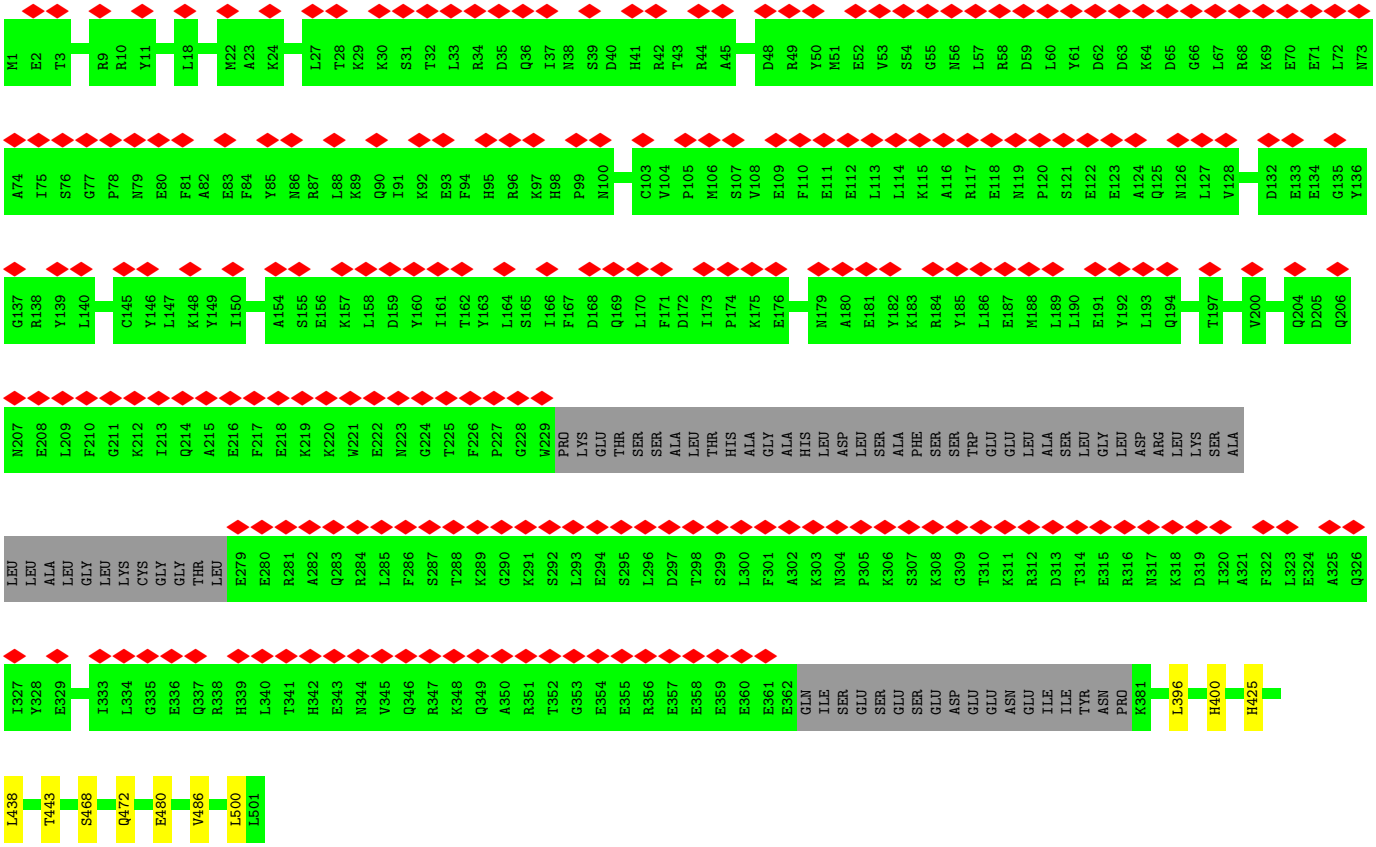
• Molecule 28: U2 small nuclear ribonucleoprotein B"



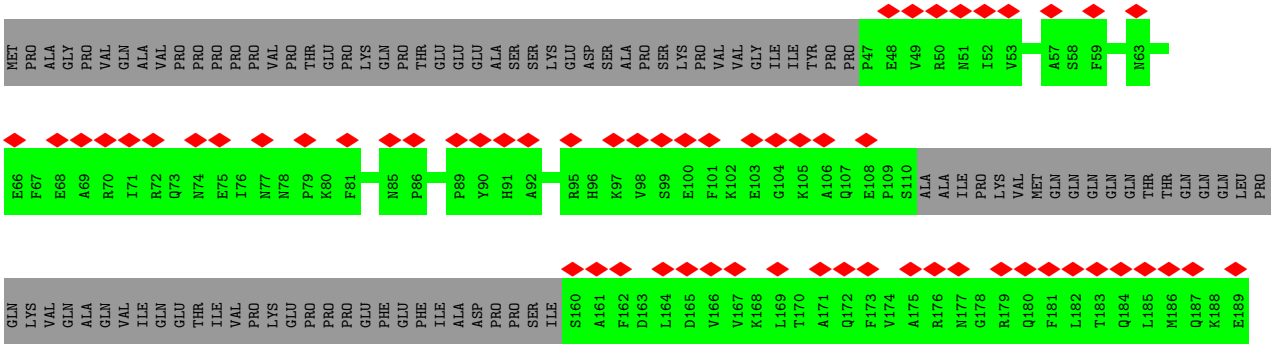


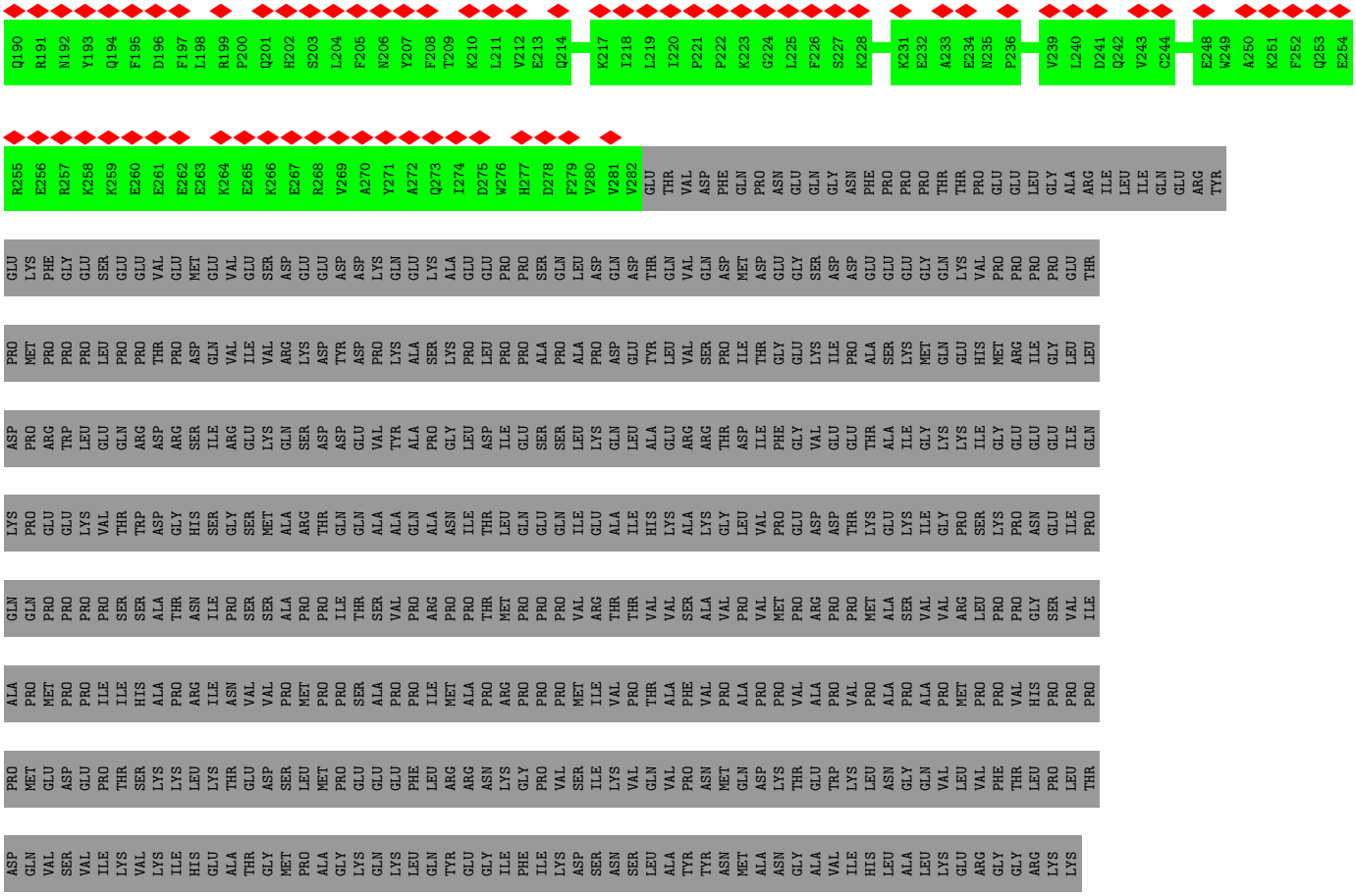
• Molecule 29: Splicing factor 3A subunit 3





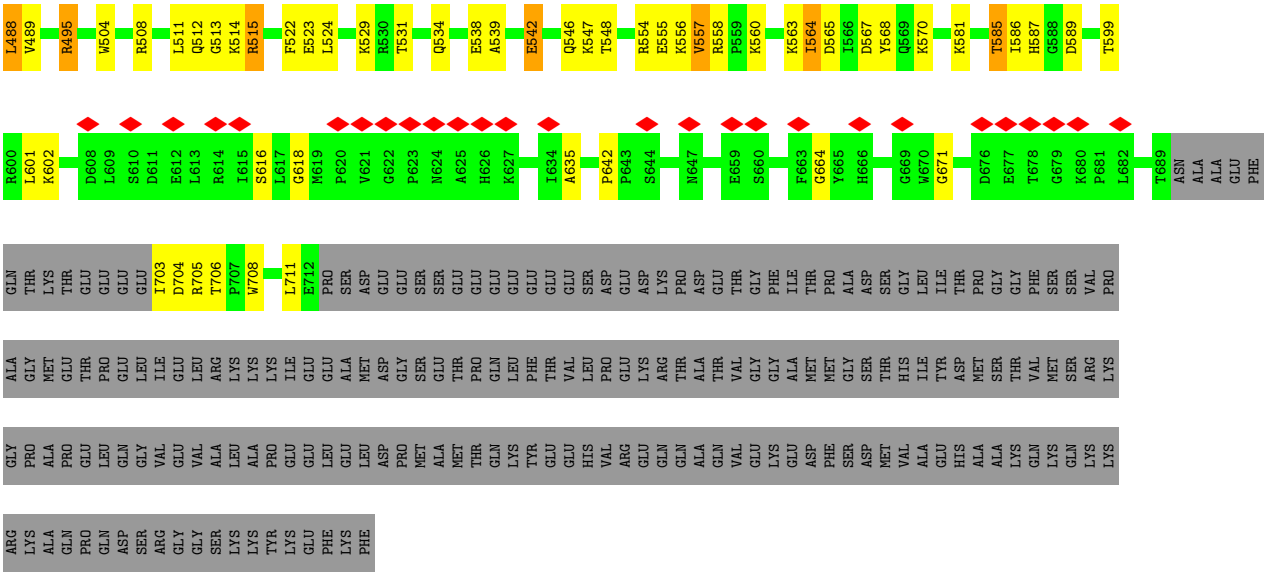
• Molecule 30: Splicing factor 3A subunit 1





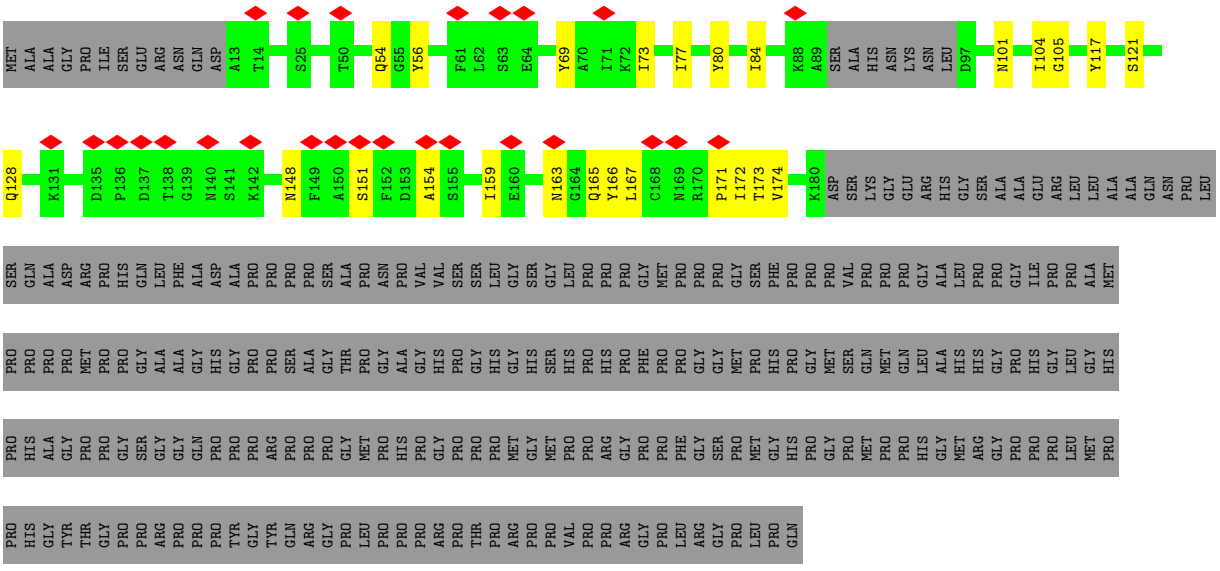
• Molecule 31: Splicing factor 3B subunit 2

Chain 2:



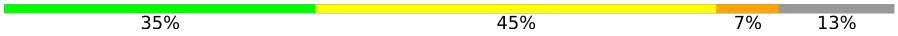
• Molecule 32: Splicing factor 3B subunit 4

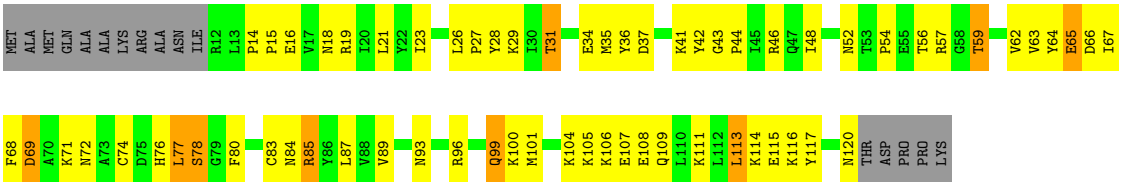
Chain 4:



• Molecule 33: Splicing factor 3B subunit 6

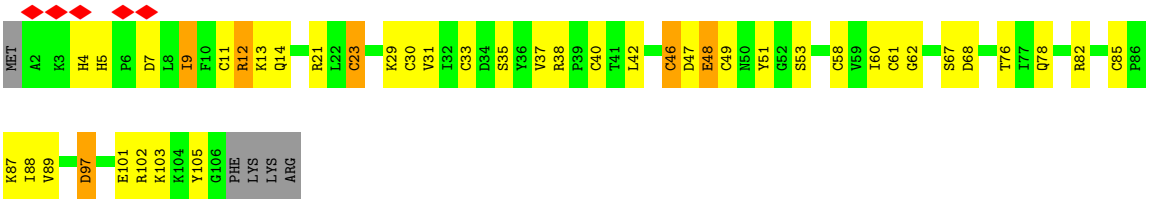
Chain 6:





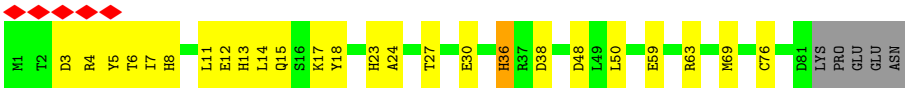
• Molecule 34: PHD finger-like domain-containing protein 5A

Chain 7:



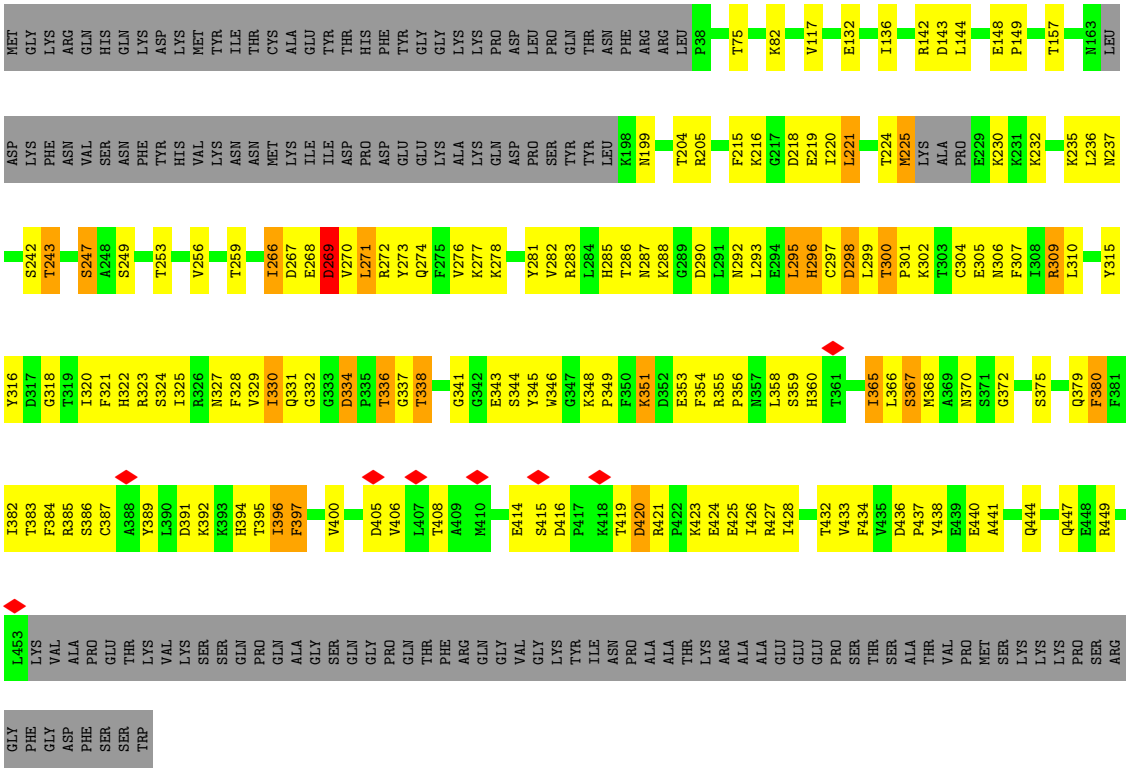
• Molecule 35: Splicing factor 3B subunit 5

Chain 5:



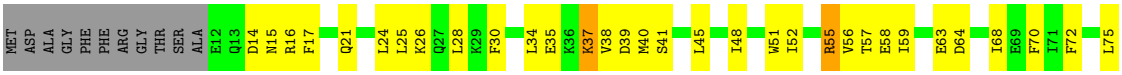
• Molecule 36: RING-type E3 ubiquitin-protein ligase PPIL2

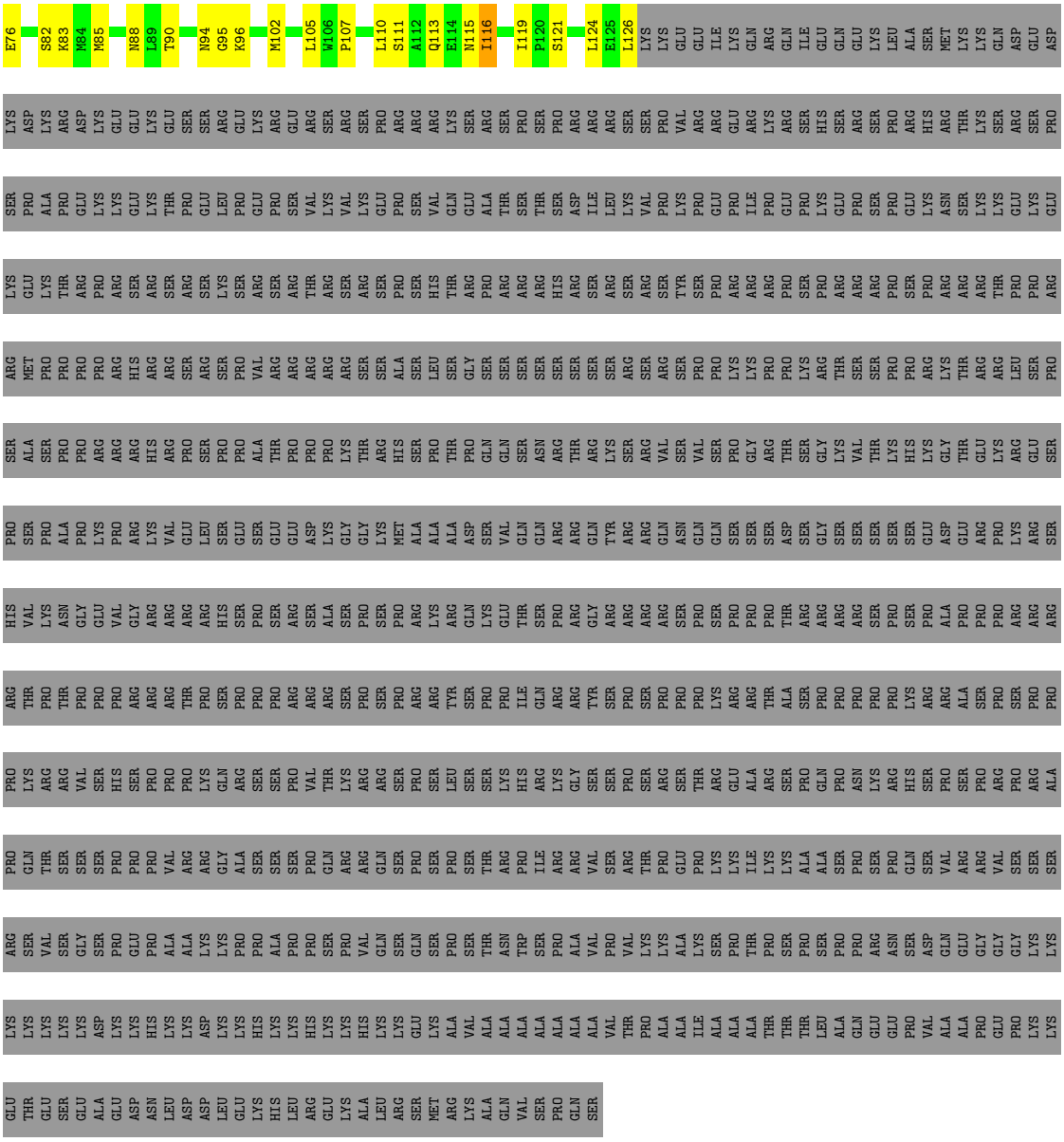
Chain 9:



• Molecule 37: Serine/arginine repetitive matrix protein 1

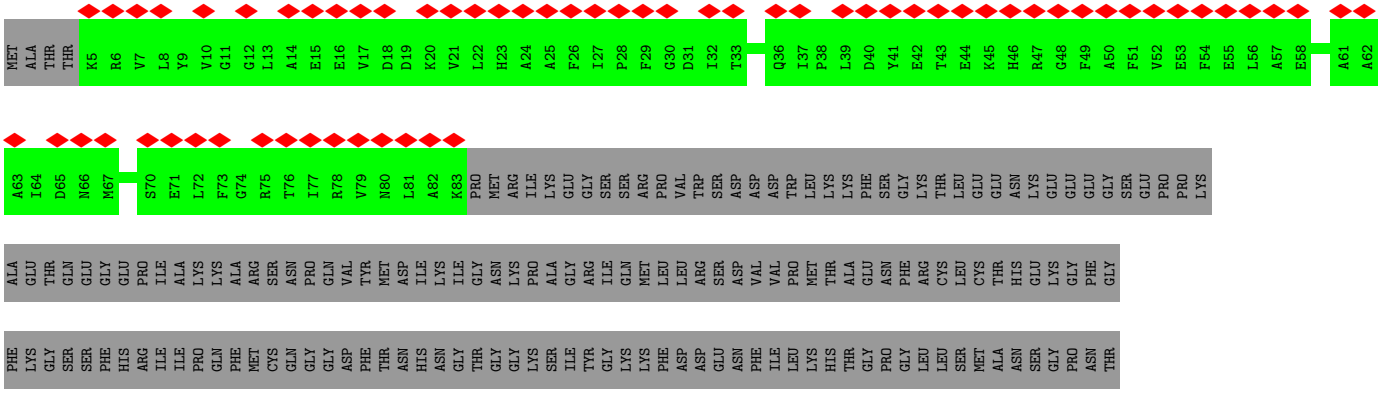
Chain 8:

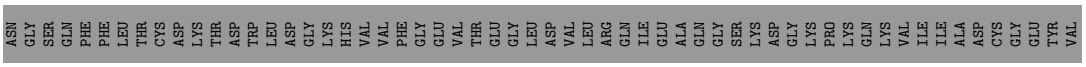




• Molecule 38: Peptidyl-prolyl cis-trans isomerase E

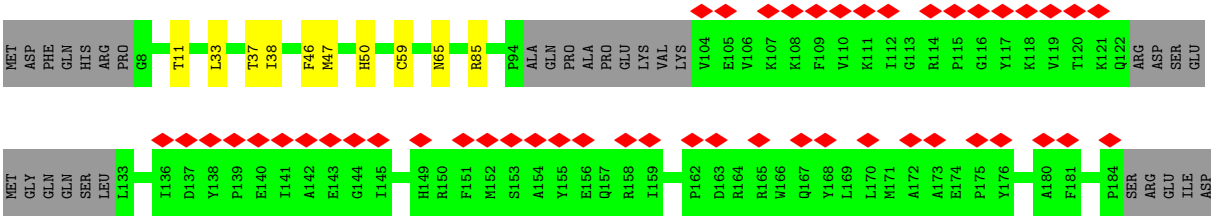
Chain y:

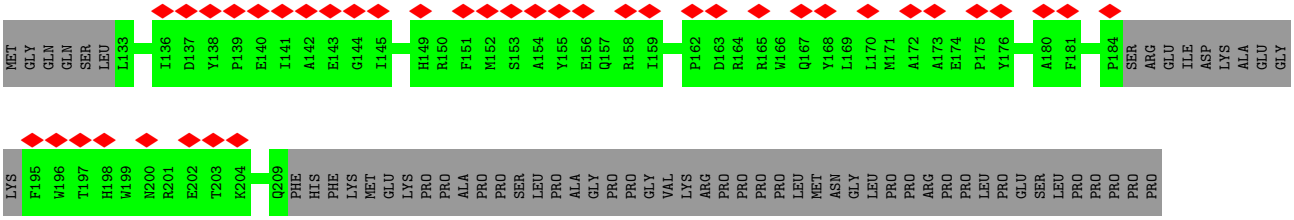




• Molecule 39: Splicing factor 3A subunit 2

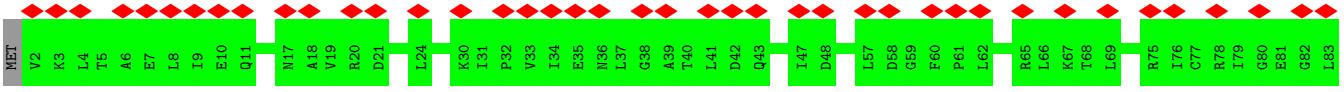
Chain v:

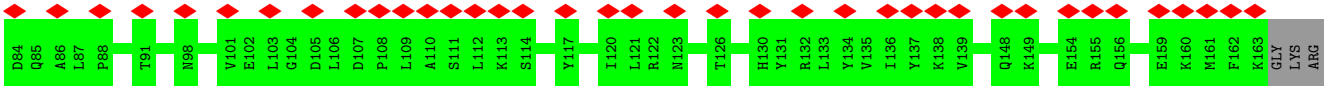


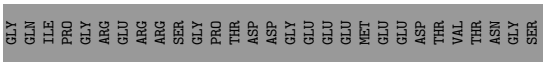


• Molecule 40: U2 small nuclear ribonucleoprotein A'

Chain o:

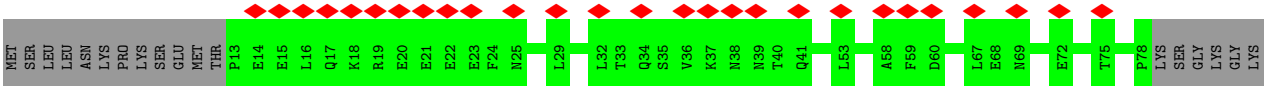


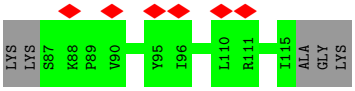




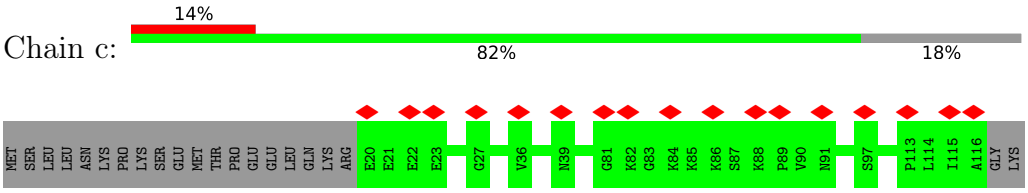
• Molecule 41: Small nuclear ribonucleoprotein Sm D2

Chain h:

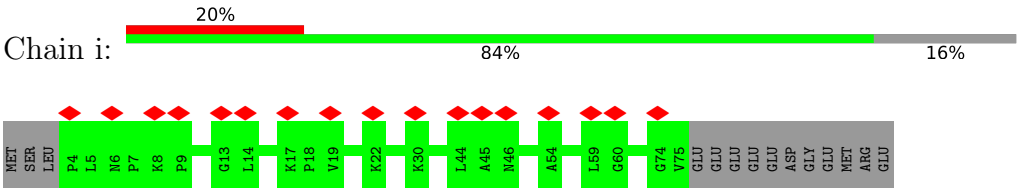




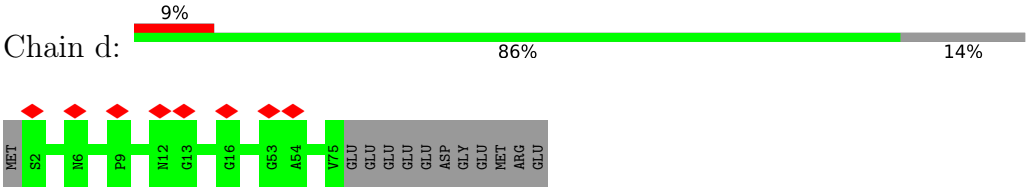
• Molecule 41: Small nuclear ribonucleoprotein Sm D2



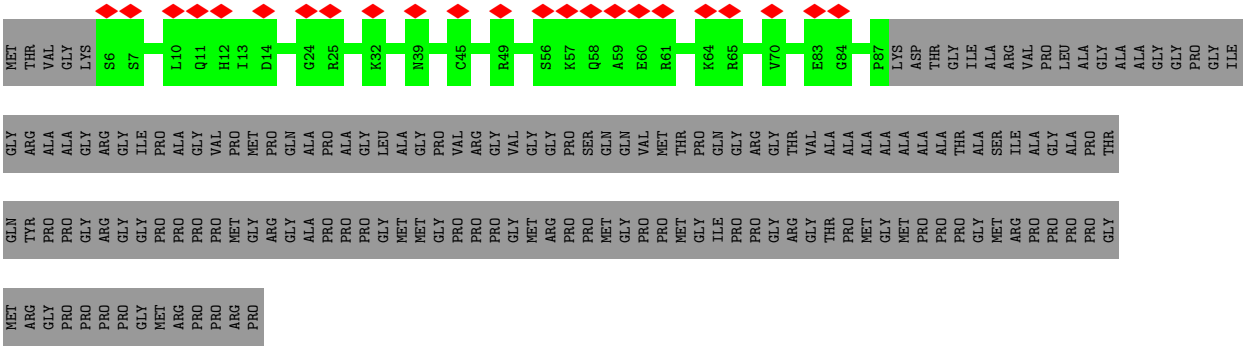
• Molecule 42: Small nuclear ribonucleoprotein F



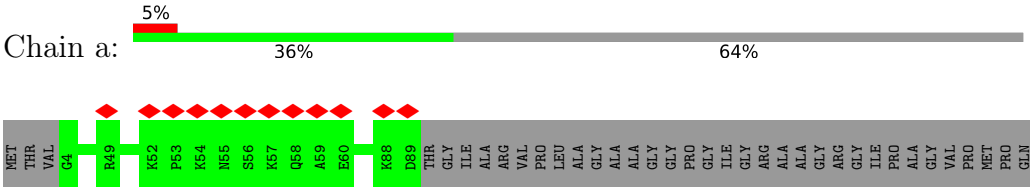
• Molecule 42: Small nuclear ribonucleoprotein F



• Molecule 43: Small nuclear ribonucleoprotein-associated proteins B and B'

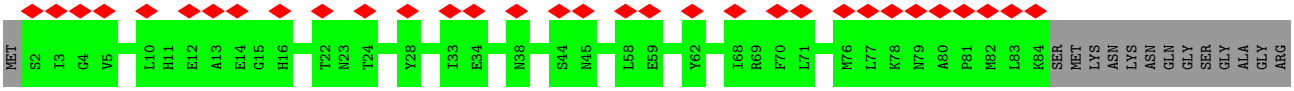


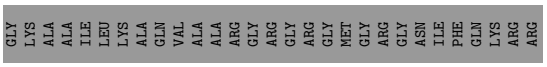
• Molecule 43: Small nuclear ribonucleoprotein-associated proteins B and B'



• Molecule 44: Small nuclear ribonucleoprotein Sm D3

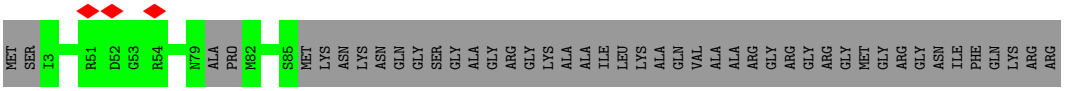
Chain l:





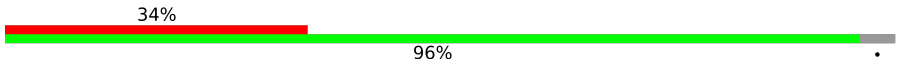
• Molecule 44: Small nuclear ribonucleoprotein Sm D3

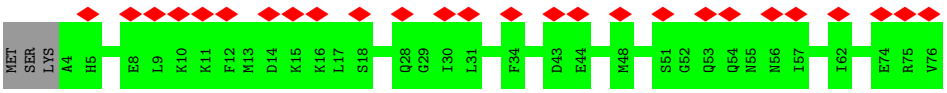
Chain g:



• Molecule 45: Small nuclear ribonucleoprotein G

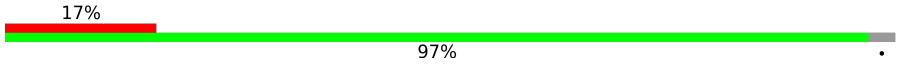
Chain k:

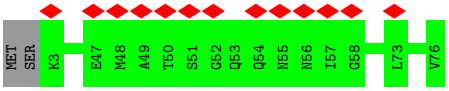




• Molecule 45: Small nuclear ribonucleoprotein G

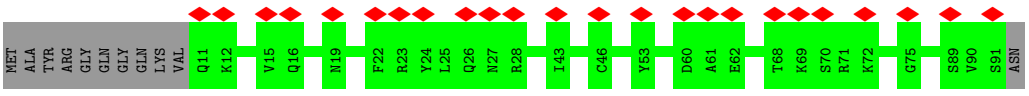
Chain f:





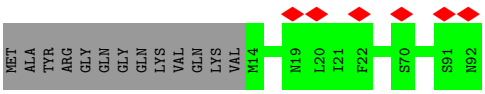
• Molecule 46: Small nuclear ribonucleoprotein E

Chain j:



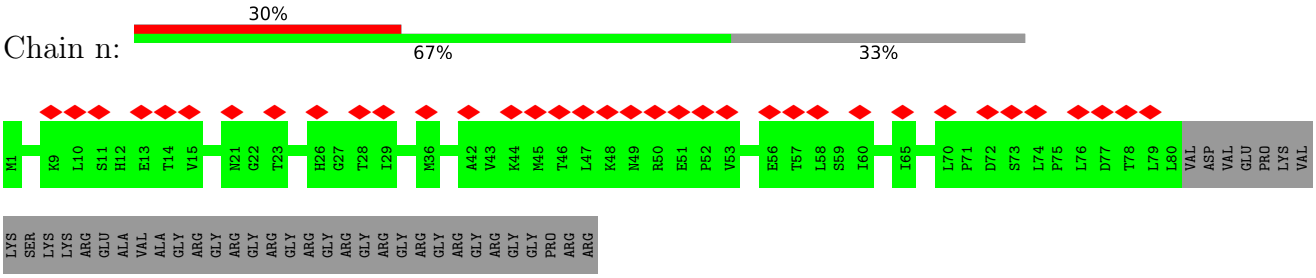
• Molecule 46: Small nuclear ribonucleoprotein E

Chain e:



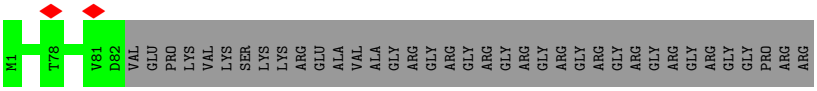
• Molecule 47: Small nuclear ribonucleoprotein Sm D1

Chain n:



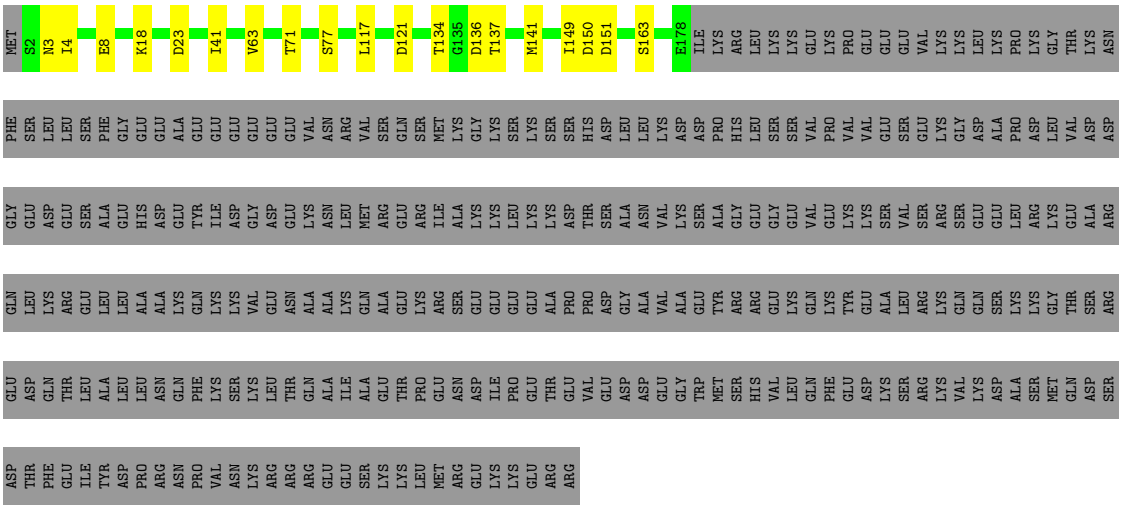
• Molecule 47: Small nuclear ribonucleoprotein Sm D1

Chain b:



• Molecule 48: Peptidyl-prolyl cis-trans isomerase CWC27 homolog

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136665	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	3.781	Depositor
Minimum map value	-1.945	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.24	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, ZN, SEP, GTP, 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	0.81	5/19056 (0.0%)	0.67	10/25857 (0.0%)
2	B	1.10	2/2303 (0.1%)	1.11	6/3579 (0.2%)
3	C	0.45	0/6873	0.59	1/9346 (0.0%)
4	D	0.25	0/8527	0.44	0/11887
5	E	0.29	0/2392	0.60	1/3242 (0.0%)
6	F	1.23	8/2323 (0.3%)	1.20	11/3619 (0.3%)
7	G	0.99	1/1648 (0.1%)	1.20	14/2558 (0.5%)
8	H	0.76	2/3947 (0.1%)	1.10	8/6138 (0.1%)
9	I	0.24	0/3013	0.45	0/4223
10	J	0.32	0/2171	0.54	0/2929
11	K	0.67	0/1081	0.60	0/1447
12	L	0.62	0/850	0.61	0/1146
13	N	0.34	0/1210	0.55	0/1622
14	O	0.25	0/1432	0.45	0/1993
15	P	0.83	0/369	0.68	0/489
16	Q	0.24	0/6796	0.43	0/9527
17	R	0.57	0/1920	0.59	1/2576 (0.0%)
18	S	0.25	0/3178	0.43	0/4425
19	T	0.91	4/2574 (0.2%)	0.72	2/3511 (0.1%)
20	U	0.36	0/424	0.53	0/582
21	V	0.38	0/3043	0.51	0/4156
22	W	0.63	0/33	0.78	0/42
23	X	0.42	0/1312	0.56	0/1769
24	Y	0.63	0/966	0.62	1/1303 (0.1%)
25	Z	0.46	0/1166	0.56	0/1559
26	1	0.74	7/8004 (0.1%)	0.69	10/10830 (0.1%)
27	3	0.61	0/9408	0.65	4/12767 (0.0%)
28	p	0.25	0/857	0.45	0/1196
29	w	0.30	0/2311	0.47	0/3008
30	u	0.23	0/842	0.41	0/1110
31	2	0.56	0/1837	0.64	1/2473 (0.0%)
32	4	0.26	0/790	0.46	0/1095

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	6	0.37	0/925	0.56	0/1247
34	7	0.54	0/825	0.54	0/1106
35	5	0.77	0/688	0.64	0/930
36	9	0.36	0/2675	0.56	0/3631
37	8	0.40	0/946	0.51	0/1270
38	y	0.25	0/389	0.44	0/540
39	v	0.47	0/1054	0.55	0/1385
40	o	0.24	0/821	0.48	0/1149
41	c	0.23	0/387	0.52	0/482
41	h	0.25	0/485	0.46	0/677
42	d	0.24	0/295	0.54	0/367
42	i	0.27	0/362	0.49	0/502
43	a	0.25	0/343	0.54	0/427
43	m	0.25	0/416	0.52	0/581
44	g	0.24	0/322	0.52	0/399
44	l	0.25	0/417	0.50	0/581
45	f	0.24	0/295	0.54	0/367
45	k	0.24	0/366	0.51	0/509
46	e	0.23	0/315	0.50	0/392
46	j	0.24	0/403	0.49	0/561
47	b	0.24	0/327	0.53	0/407
47	n	0.24	0/404	0.47	0/564
48	z	0.59	0/1436	0.58	0/1945
All	All	0.60	29/117552 (0.0%)	0.66	70/162023 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16
3	C	0	7
4	D	0	2
9	I	0	1
13	N	0	1
15	P	0	2
16	Q	0	2
17	R	0	1
23	X	0	1
26	1	0	5
27	3	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	2	0	1
48	z	0	1
All	All	0	42

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	827	PHE	C-N	8.64	1.50	1.34
19	T	307	SER	CA-CB	-8.22	1.40	1.52
19	T	349	SER	CA-CB	-7.69	1.41	1.52
1	A	826	PRO	C-O	-7.65	1.07	1.23
19	T	307	SER	C-O	-7.26	1.09	1.23
1	A	823	SER	CA-CB	-6.88	1.42	1.52
2	B	32	C	N1-C6	-6.23	1.33	1.37
6	F	67	G	C5-C4	-5.85	1.34	1.38
2	B	55	C	N3-C4	-5.79	1.29	1.33
6	F	84	A	N9-C4	-5.66	1.34	1.37
19	T	349	SER	C-O	-5.66	1.12	1.23
1	A	825	ILE	C-O	-5.61	1.12	1.23
1	A	824	PRO	C-O	-5.55	1.12	1.23
6	F	66	C	N1-C6	-5.53	1.33	1.37
8	H	25	G	C5-C4	-5.52	1.34	1.38
6	F	55	C	N1-C6	-5.51	1.33	1.37
26	1	944	SER	CA-CB	-5.47	1.44	1.52
26	1	1114	VAL	C-O	-5.45	1.13	1.23
26	1	1115	ALA	C-O	-5.35	1.13	1.23
6	F	67	G	N9-C4	-5.33	1.33	1.38
7	G	94	C	N1-C6	-5.33	1.33	1.37
26	1	1250	CYS	CB-SG	-5.32	1.73	1.81
6	F	70	A	C5-C4	-5.25	1.35	1.38
26	1	952	ALA	C-O	-5.17	1.13	1.23
8	H	21	C	N1-C6	-5.09	1.34	1.37
26	1	949	GLN	C-O	-5.09	1.13	1.23
26	1	1108	ASN	C-O	-5.08	1.13	1.23
6	F	75	G	C6-N1	-5.07	1.36	1.39
6	F	55	C	N3-C4	-5.04	1.30	1.33

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	1108	ASN	CB-CA-C	-9.45	91.49	110.40
8	H	15	U	C2-N1-C1'	-9.39	106.43	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	104	C	N1-C2-O2	8.48	123.99	118.90
8	H	15	U	C6-N1-C1'	8.47	133.06	121.20
26	1	942	ASN	CB-CA-C	-7.91	94.57	110.40
7	G	109	U	C2-N1-C1'	7.83	127.10	117.70
6	F	37	C	P-O5'-C5'	7.62	133.10	120.90
27	3	123	VAL	C-N-CA	-7.25	103.57	121.70
7	G	104	C	N3-C2-O2	-7.14	116.90	121.90
24	Y	40	LEU	CA-CB-CG	6.96	131.30	115.30
1	A	422	LEU	CA-CB-CG	6.95	131.27	115.30
6	F	84	A	N3-C4-N9	-6.91	121.88	127.40
2	B	40	U	C2-N1-C1'	6.79	125.85	117.70
19	T	303	LEU	CA-CB-CG	6.72	130.75	115.30
26	1	435	PRO	N-CA-C	-6.70	94.67	112.10
7	G	104	C	C2-N1-C1'	6.69	126.16	118.80
26	1	407	MET	C-N-CA	-6.69	104.98	121.70
1	A	694	LEU	CA-CB-CG	-6.64	100.02	115.30
1	A	1501	LEU	CA-CB-CG	6.57	130.42	115.30
1	A	820	ARG	CB-CA-C	-6.51	97.37	110.40
1	A	663	ARG	NE-CZ-NH1	6.42	123.51	120.30
7	G	102	G	C8-N9-C4	-6.42	103.83	106.40
5	E	289	LEU	CA-CB-CG	6.39	130.01	115.30
8	H	15	U	C5-C4-O4	6.37	129.72	125.90
6	F	84	A	C2-N3-C4	-6.25	107.48	110.60
8	H	18	U	P-O3'-C3'	6.24	127.19	119.70
26	1	935	THR	CA-CB-OG1	-6.11	96.17	109.00
7	G	108	U	OP2-P-O3'	5.99	118.37	105.20
6	F	54	G	O5'-P-OP2	-5.96	100.34	105.70
1	A	1230	LEU	CB-CG-CD1	-5.95	100.89	111.00
6	F	84	A	N1-C2-N3	5.92	132.26	129.30
7	G	85	G	C4-N9-C1'	-5.86	118.88	126.50
7	G	109	U	C6-N1-C1'	-5.86	113.00	121.20
26	1	935	THR	CB-CA-C	-5.83	95.85	111.60
8	H	28	C	C6-N1-C2	-5.76	118.00	120.30
6	F	84	A	C6-C5-N7	5.68	136.28	132.30
26	1	1101	LEU	O-C-N	-5.66	113.65	122.70
26	1	1111	CYS	CB-CA-C	5.65	121.71	110.40
2	B	101	U	C5-C6-N1	5.62	125.51	122.70
26	1	1112	THR	OG1-CB-CG2	-5.61	97.10	110.00
8	H	13	C	P-O3'-C3'	5.61	126.43	119.70
7	G	109	U	N1-C2-O2	5.57	126.70	122.80
27	3	485	LEU	CA-CB-CG	5.46	127.87	115.30
31	2	618	GLY	C-N-CA	5.46	135.36	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	821	ARG	CG-CD-NE	-5.45	100.36	111.80
19	T	250	ARG	NE-CZ-NH1	5.39	122.99	120.30
7	G	102	G	N7-C8-N9	5.34	115.77	113.10
6	F	84	A	C4-N9-C1'	-5.33	116.70	126.30
27	3	84	SER	C-N-CA	-5.28	111.21	122.30
7	G	-11	G	C3'-C2'-C1'	5.27	105.71	101.50
6	F	55	C	C6-N1-C2	-5.26	118.19	120.30
6	F	37	C	N1-C1'-C2'	5.23	120.80	114.00
1	A	1252	GLY	N-CA-C	-5.21	100.07	113.10
7	G	85	G	C8-N9-C1'	5.21	133.78	127.00
6	F	84	A	N3-C4-C5	5.17	130.42	126.80
26	1	948	ARG	CG-CD-NE	-5.17	100.95	111.80
8	H	28	C	C5-C6-N1	5.16	123.58	121.00
2	B	40	U	C6-N1-C1'	-5.16	113.98	121.20
2	B	100	C	C5-C6-N1	5.16	123.58	121.00
7	G	85	G	N3-C4-N9	-5.15	122.91	126.00
27	3	511	LEU	CA-CB-CG	5.08	126.99	115.30
8	H	23	A	O5'-P-OP1	-5.08	101.13	105.70
6	F	36	A	N1-C6-N6	5.07	121.64	118.60
7	G	-11	G	P-O3'-C3'	5.05	125.77	119.70
3	C	750	LEU	CA-CB-CG	5.04	126.88	115.30
1	A	2298	LEU	CA-CB-CG	5.03	126.86	115.30
2	B	95	G	C4-N9-C1'	5.03	133.03	126.50
2	B	20	G	C2-N3-C4	-5.02	109.39	111.90
1	A	1771	LEU	CA-CB-CG	5.02	126.84	115.30
17	R	151	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	1	1101	LEU	Mainchain
26	1	1178	MET	Peptide
26	1	1179	ASP	Peptide
26	1	717	THR	Peptide
26	1	944	SER	Mainchain
31	2	515	ARG	Peptide
27	3	916	ASN	Peptide
27	3	996	ILE	Peptide
1	A	1019	TYR	Peptide
1	A	1189	MET	Peptide
1	A	1416	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	A	1547	VAL	Peptide
1	A	1548	TYR	Peptide
1	A	1765	SER	Peptide
1	A	2320	LEU	Peptide
1	A	2329	ASP	Peptide
1	A	433	GLU	Peptide
1	A	467	GLN	Peptide
1	A	699	GLU	Peptide
1	A	700	GLY	Peptide
1	A	81	PHE	Peptide
1	A	855	ARG	Peptide
1	A	940	ILE	Peptide
1	A	941	LYS	Peptide
3	C	359	LYS	Peptide
3	C	360	ALA	Peptide
3	C	443	VAL	Peptide
3	C	560	VAL	Peptide
3	C	572	GLU	Peptide
3	C	736	GLY	Peptide
3	C	823	ALA	Peptide
4	D	1583	ASP	Peptide
4	D	2098	ALA	Peptide
9	I	337	LEU	Peptide
13	N	36	PRO	Peptide
15	P	202	ASP	Peptide
15	P	203	ASP	Peptide
16	Q	488	SER	Peptide
16	Q	489	VAL	Peptide
17	R	235	ARG	Peptide
23	X	296	HIS	Peptide
48	z	151	ASP	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	18543	0	18403	623	0
2	B	2066	0	1047	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	6724	0	6696	310	0
4	D	8528	0	3745	42	0
5	E	2338	0	2275	125	0
6	F	2075	0	1048	104	0
7	G	1481	0	755	81	0
8	H	3539	0	1791	123	0
9	I	2991	0	1473	11	0
10	J	2116	0	1977	100	0
11	K	1059	0	1012	36	0
12	L	829	0	837	22	0
13	N	1184	0	1193	50	0
14	O	1433	0	621	18	0
15	P	362	0	356	13	0
16	Q	6730	0	3268	32	0
17	R	1889	0	1866	73	0
18	S	3180	0	1441	20	0
19	T	2507	0	2451	80	0
20	U	422	0	291	15	0
21	V	3008	0	2288	89	0
22	W	229	0	85	3	0
23	X	1279	0	1284	66	0
24	Y	948	0	954	34	0
25	Z	1142	0	1112	35	0
26	1	7866	0	7964	285	0
27	3	9220	0	9139	407	0
28	p	851	0	423	0	0
29	w	2275	0	1347	0	0
30	u	834	0	325	0	0
31	2	1807	0	1622	57	0
32	4	792	0	367	16	0
33	6	906	0	913	49	0
34	7	811	0	790	29	0
35	5	669	0	631	16	0
36	9	2636	0	2228	125	0
37	8	931	0	960	39	0
38	y	390	0	190	0	0
39	v	1041	0	800	0	0
40	o	816	0	386	0	0
41	c	388	0	102	0	0
41	h	482	0	220	0	0
42	d	296	0	87	0	0
42	i	359	0	179	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	a	344	0	93	0	0
43	m	413	0	194	0	0
44	g	324	0	89	0	0
44	l	415	0	198	0	0
45	f	296	0	84	0	0
45	k	364	0	176	0	0
46	e	316	0	85	0	0
46	j	403	0	173	0	0
47	b	328	0	89	0	0
47	n	402	0	184	0	0
48	z	1402	0	1336	0	0
49	A	36	0	6	2	0
50	C	32	0	12	3	0
51	C	1	0	0	0	0
51	F	5	0	0	0	0
52	7	3	0	0	0	0
52	K	1	0	0	0	0
52	N	3	0	0	0	0
All	All	115060	0	89661	2901	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 15.

All (2901) 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)
26:1:933:CYS:SG	26:1:970:LEU:HD21	1.63	1.38
26:1:933:CYS:SG	26:1:970:LEU:HD11	1.74	1.27
26:1:933:CYS:SG	26:1:970:LEU:CD2	2.35	1.13
26:1:933:CYS:SG	26:1:970:LEU:CD1	2.43	1.06
21:V:580:ARG:HE	25:Z:545:MET:HB2	1.19	1.04
1:A:2087:THR:HG21	1:A:2112:LYS:HA	1.39	1.01
23:X:273:MET:HE1	26:1:433:ALA:HB1	1.38	1.01
27:3:642:ILE:H	27:3:703:ARG:HH21	1.09	0.99
23:X:273:MET:CE	26:1:433:ALA:HB1	1.93	0.98
5:E:91:LEU:HB3	5:E:101:ASN:HD21	1.28	0.98
1:A:59:GLU:HG3	13:N:103:LEU:HB3	1.45	0.97
26:1:933:CYS:HG	26:1:970:LEU:HD21	0.95	0.95
7:G:98:U:H3	8:H:33:G:H1	1.01	0.94
3:C:670:SER:HA	3:C:823:ALA:HB3	1.48	0.94
23:X:274:TYR:HE1	26:1:436:THR:N	1.64	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:54:U:O2	8:H:59:A:N6	2.02	0.91
6:F:38:G:H2'	6:F:39:A:H8	1.33	0.91
26:1:578:ILE:HG13	26:1:596:ILE:HD11	1.52	0.91
31:2:456:ARG:HA	31:2:459:ARG:HD3	1.51	0.90
2:B:17:U:O2	2:B:60:G:N1	2.05	0.90
6:F:79:C:H4'	6:F:80:G:H5"	1.50	0.90
7:G:85:G:N2	8:H:45:C:N3	2.19	0.89
26:1:933:CYS:SG	26:1:970:LEU:CG	2.61	0.89
23:X:274:TYR:CE1	26:1:436:THR:N	2.37	0.89
27:3:1026:ASP:OD2	31:2:495:ARG:NH2	2.04	0.89
1:A:1851:SER:HG	21:V:442:VAL:N	1.71	0.89
36:9:285:HIS:HE2	36:9:432:THR:HG1	1.03	0.88
19:T:343:PRO:HG3	19:T:356:LEU:HD23	1.56	0.87
23:X:352:LEU:HD21	23:X:358:LEU:HD11	1.57	0.87
36:9:370:ASN:ND2	36:9:372:GLY:O	2.07	0.87
1:A:2166:HIS:HB3	1:A:2169:LEU:H	1.40	0.87
8:H:19:G:N2	8:H:20:G:O6	2.09	0.85
21:V:644:ARG:NH2	22:W:114:UNK:O	2.10	0.85
27:3:552:ARG:HH11	27:3:600:GLN:HB3	1.42	0.84
23:X:277:ARG:HH22	26:1:437:PRO:CB	1.90	0.84
3:C:727:LEU:HD23	20:U:71:LEU:CB	2.08	0.84
1:A:226:GLN:OE1	1:A:417:ARG:NH2	2.11	0.84
21:V:580:ARG:NH2	25:Z:545:MET:SD	2.51	0.83
23:X:274:TYR:CE1	26:1:436:THR:HA	2.13	0.83
21:V:580:ARG:NE	25:Z:545:MET:HB2	1.94	0.83
5:E:90:ILE:HB	5:E:105:LEU:HB3	1.57	0.83
6:F:27:A:N6	7:G:17:U:OP1	2.12	0.82
10:J:354:LEU:HD11	10:J:362:ALA:HB2	1.60	0.82
27:3:870:ASN:HD21	27:3:872:ILE:HB	1.44	0.82
31:2:563:LYS:HG2	31:2:564:ILE:HG13	1.58	0.82
3:C:534:VAL:HB	3:C:537:TYR:HB2	1.58	0.82
13:N:120:ARG:NH1	13:N:142:CYS:SG	2.51	0.82
19:T:336:VAL:HG23	19:T:347:THR:HG22	1.62	0.82
27:3:472:ALA:HA	27:3:487:ILE:HG12	1.62	0.82
1:A:371:LEU:HD11	3:C:347:ILE:HD11	1.61	0.82
34:7:13:LYS:NZ	34:7:48:GLU:OE1	2.13	0.82
31:2:473:ASP:OD1	31:2:473:ASP:N	2.12	0.81
26:1:734:GLY:O	26:1:738:HIS:HB2	1.79	0.81
26:1:1260:LYS:NZ	31:2:504:TRP:O	2.14	0.81
34:7:58:CYS:HB3	34:7:62:GLY:H	1.45	0.81
3:C:750:LEU:HD11	20:U:70:CYS:CB	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:37:C:OP1	6:F:37:C:H3'	1.81	0.80
27:3:508:CYS:SG	27:3:518:GLN:NE2	2.54	0.80
6:F:59:G:H1	6:F:76:A:H61	1.30	0.80
11:K:127:GLU:O	11:K:136:ARG:NH2	2.15	0.80
27:3:932:ASN:O	27:3:933:ASN:ND2	2.14	0.80
19:T:274:ASP:HB2	19:T:281:ILE:HD13	1.63	0.80
1:A:1660:TYR:OH	1:A:1717:ASN:O	2.00	0.80
13:N:41:ARG:HB2	13:N:44:GLU:HG2	1.64	0.79
36:9:341:GLY:O	36:9:379:GLN:NE2	2.15	0.79
3:C:746:VAL:O	3:C:790:LYS:HA	1.81	0.79
2:B:18:C:N3	2:B:59:G:N1	2.27	0.79
21:V:575:THR:O	21:V:580:ARG:NH2	2.15	0.79
17:R:386:ARG:NH2	23:X:356:ASP:OD2	2.16	0.79
6:F:38:G:H2'	6:F:39:A:C8	2.18	0.79
3:C:457:VAL:HA	3:C:462:GLY:HA3	1.65	0.78
19:T:371:HIS:HE2	19:T:389:SER:HG	1.29	0.78
26:1:717:THR:HA	26:1:756:LEU:HD11	1.65	0.78
27:3:304:GLN:HE21	27:3:308:GLY:HA2	1.47	0.78
1:A:1870:ASP:N	1:A:1870:ASP:OD1	2.13	0.78
3:C:732:ILE:HA	3:C:746:VAL:HG22	1.65	0.78
26:1:802:GLU:OE1	26:1:805:TYR:N	2.15	0.78
1:A:57:GLN:O	13:N:107:GLN:NE2	2.15	0.78
5:E:214:ASP:N	5:E:214:ASP:OD1	2.17	0.78
31:2:523:GLU:OE1	31:2:529:LYS:NZ	2.16	0.78
3:C:593:GLU:HG2	3:C:594:PRO:HD2	1.65	0.78
1:A:850:TYR:OH	1:A:863:GLU:OE1	2.02	0.78
26:1:1257:PRO:HD3	31:2:488:LEU:HD11	1.66	0.78
1:A:821:ARG:HG2	1:A:821:ARG:NH1	1.97	0.78
5:E:81:LEU:O	5:E:92:LEU:HA	1.84	0.78
8:H:43:U:H2'	8:H:44:U:H6	1.49	0.78
36:9:397:PHE:H	36:9:397:PHE:HD1	1.30	0.77
19:T:371:HIS:NE2	19:T:389:SER:OG	2.14	0.77
27:3:1200:THR:N	27:3:1203:GLU:OE1	2.14	0.77
1:A:332:TYR:O	3:C:888:ARG:NH2	2.16	0.77
1:A:762:ARG:HH22	15:P:226:LYS:HZ3	1.31	0.77
26:1:1004:ILE:HD11	26:1:1008:LYS:HB2	1.66	0.77
1:A:380:LEU:HD22	1:A:384:VAL:HG21	1.67	0.77
1:A:1146:ASP:OD2	1:A:1182:ASN:ND2	2.18	0.77
3:C:122:LEU:HD23	3:C:128:LEU:HD23	1.65	0.77
27:3:352:GLU:OE2	27:3:429:ARG:NH1	2.18	0.77
1:A:835:ASP:N	1:A:835:ASP:OD1	2.11	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:317:THR:OG1	27:3:318:ASP:O	2.03	0.77
7:G:111:U:H3	24:Y:105:ARG:HG2	1.48	0.77
26:1:804:ASN:O	26:1:808:THR:OG1	2.02	0.77
1:A:1124:ASN:ND2	1:A:1148:ASN:OD1	2.15	0.77
3:C:853:ARG:NH1	3:C:879:ASP:O	2.17	0.77
27:3:114:ARG:NH1	35:5:38:ASP:OD1	2.17	0.77
1:A:1690:ASP:OD1	1:A:1691:ASN:N	2.18	0.76
1:A:519:ASP:OD2	1:A:523:ASN:ND2	2.16	0.76
1:A:1804:ASN:HD22	1:A:1823:HIS:HA	1.50	0.76
1:A:2146:VAL:HA	1:A:2272:MET:HB3	1.65	0.76
27:3:200:ALA:O	27:3:204:THR:OG1	2.04	0.76
36:9:268:GLU:O	36:9:271:LEU:N	2.18	0.76
2:B:18:C:N4	2:B:59:G:O6	2.18	0.76
12:L:77:LEU:HD12	36:9:221:LEU:HD21	1.65	0.76
26:1:138:ASP:HB3	26:1:141:LYS:HB2	1.66	0.76
2:B:20:G:O6	2:B:57:G:N1	2.15	0.76
3:C:666:VAL:HG12	3:C:668:GLU:H	1.49	0.76
8:H:151:C:H2'	8:H:152:G:C8	2.21	0.76
19:T:220:VAL:HG22	19:T:230:ILE:HD13	1.66	0.76
27:3:316:GLU:OE2	27:3:326:ARG:NH2	2.19	0.76
27:3:199:GLU:O	27:3:203:ASN:ND2	2.19	0.76
36:9:321:PHE:HA	36:9:332:GLY:HA3	1.67	0.76
26:1:420:GLY:O	26:1:424:ILE:N	2.17	0.76
7:G:85:G:H1	8:H:45:C:H42	1.32	0.76
8:H:14:C:H1'	8:H:15:U:H5'	1.68	0.76
13:N:58:ARG:NH2	13:N:98:GLU:O	2.18	0.76
26:1:883:ASP:OD2	26:1:883:ASP:N	2.14	0.76
27:3:639:SER:OG	27:3:699:VAL:O	2.03	0.76
4:D:835:SER:O	4:D:839:GLY:N	2.18	0.75
1:A:584:HIS:HE1	49:A:2401:IHP:O26	1.69	0.75
26:1:714:GLU:O	34:7:51:TYR:OH	2.03	0.75
36:9:360:HIS:HB3	36:9:365:ILE:HG21	1.67	0.75
1:A:548:ARG:NH2	1:A:549:GLU:OE2	2.20	0.75
36:9:269:ASP:HA	36:9:272:ARG:HE	1.49	0.75
1:A:766:THR:HG22	1:A:768:ASP:H	1.51	0.75
14:O:259:ARG:N	14:O:273:GLN:O	2.18	0.75
16:Q:514:ILE:H	16:Q:655:ILE:HA	1.51	0.75
27:3:613:THR:HG22	27:3:632:ALA:HA	1.69	0.75
23:X:277:ARG:NH2	26:1:434:THR:CB	2.49	0.74
27:3:705:ARG:HH22	27:3:708:GLY:H	1.34	0.74
36:9:219:GLU:HG2	36:9:220:ILE:HD12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2191:GLN:O	1:A:2195:THR:OG1	2.05	0.74
26:1:471:ASP:OD1	26:1:471:ASP:N	2.19	0.74
27:3:128:ARG:NH2	27:3:178:GLU:O	2.20	0.74
1:A:1314:VAL:O	1:A:1318:THR:OG1	2.04	0.74
5:E:90:ILE:HD12	5:E:105:LEU:HD13	1.69	0.74
24:Y:86:ASP:OD1	24:Y:86:ASP:N	2.16	0.74
7:G:-11:G:O2'	7:G:-10:G:O4'	2.06	0.74
1:A:821:ARG:HG2	1:A:821:ARG:HH11	1.51	0.74
8:H:46:U:O2'	8:H:47:U:OP2	2.05	0.74
1:A:891:PHE:O	12:L:83:ARG:NH2	2.21	0.74
3:C:846:VAL:HG22	3:C:887:LEU:HD11	1.70	0.74
6:F:40:U:H3	7:G:7:G:H1	1.36	0.74
23:X:273:MET:CE	26:1:433:ALA:CB	2.65	0.74
5:E:261:VAL:HB	5:E:275:LYS:HB2	1.68	0.73
27:3:718:ARG:HB2	27:3:720:TRP:HE1	1.52	0.73
17:R:403:ASN:OD1	23:X:253:ARG:NH2	2.22	0.73
6:F:92:A:H2'	6:F:93:G:C8	2.24	0.73
23:X:298:SER:O	23:X:335:ASN:ND2	2.22	0.73
5:E:251:LEU:HD22	5:E:300:ILE:HG12	1.68	0.73
6:F:30:A:H61	7:G:16:G:H1'	1.53	0.73
6:F:83:A:O2'	6:F:84:A:N7	2.21	0.73
26:1:866:LYS:NZ	26:1:907:ASP:OD2	2.22	0.73
36:9:298:ASP:OD1	36:9:298:ASP:N	2.16	0.73
10:J:438:TYR:O	10:J:442:ARG:HB2	1.88	0.73
24:Y:32:TYR:OH	26:1:822:ARG:NH2	2.19	0.73
8:H:161:U:O2	8:H:163:G:N2	2.20	0.73
26:1:826:ASP:OD2	26:1:829:ASN:ND2	2.22	0.73
27:3:576:GLU:OE1	27:3:580:ARG:NH2	2.20	0.73
17:R:174:ALA:HA	17:R:199:MET:O	1.88	0.73
27:3:473:TYR:HB3	27:3:475:ILE:HD11	1.71	0.73
33:6:74:CYS:O	33:6:78:SER:OG	2.07	0.73
6:F:36:A:N1	7:G:10:U:C4	2.57	0.73
6:F:48:A:O2'	12:L:33:ARG:NH1	2.21	0.73
19:T:497:GLU:OE1	19:T:497:GLU:N	2.19	0.73
27:3:285:MET:SD	27:3:305:THR:OG1	2.47	0.73
27:3:326:ARG:NH1	27:3:372:GLU:OE2	2.21	0.73
1:A:1104:ASP:OD1	1:A:1104:ASP:N	2.18	0.72
7:G:92:U:OP1	12:L:40:ARG:NH2	2.20	0.72
15:P:205:LYS:HG2	15:P:208:LYS:HD3	1.68	0.72
23:X:274:TYR:CE1	26:1:436:THR:CA	2.71	0.72
27:3:280:ASP:H	27:3:857:ALA:HB3	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1991:TYR:OH	1:A:2015:GLU:OE2	2.07	0.72
5:E:300:ILE:HD12	5:E:314:THR:HG22	1.70	0.72
4:D:1992:GLU:HA	4:D:1995:ALA:HB3	1.71	0.72
1:A:2189:SER:HB3	1:A:2191:GLN:HE21	1.53	0.72
26:1:1301:ASP:N	26:1:1301:ASP:OD1	2.21	0.72
4:D:2098:ALA:O	4:D:2100:GLY:N	2.23	0.72
1:A:1762:TYR:O	1:A:1768:TYR:OH	2.03	0.72
5:E:250:LEU:O	5:E:261:VAL:HA	1.90	0.72
20:U:23:LEU:H	21:V:474:HIS:HD2	1.38	0.72
24:Y:44:PRO:HG2	24:Y:47:LEU:HD13	1.70	0.72
26:1:699:GLN:OE1	26:1:702:ARG:NH2	2.22	0.72
27:3:484:VAL:HG11	27:3:499:PHE:HD2	1.55	0.72
1:A:858:GLN:HE22	8:H:30:A:H5"	1.55	0.72
3:C:187:THR:OG1	3:C:201:ASN:OD1	2.07	0.71
8:H:43:U:H2'	8:H:44:U:C6	2.25	0.71
10:J:231:PHE:HE1	10:J:247:LYS:HG3	1.55	0.71
27:3:864:SER:OG	27:3:886:GLU:O	2.08	0.71
6:F:36:A:H2'	6:F:37:C:H5"	1.72	0.71
7:G:16:G:H5"	7:G:17:U:O4'	1.91	0.71
17:R:332:ARG:HH22	23:X:267:ASP:H	1.38	0.71
19:T:216:ASN:O	19:T:216:ASN:ND2	2.23	0.71
2:B:97:G:H1	2:B:116:U:H3	1.37	0.71
10:J:230:THR:O	10:J:234:ASN:ND2	2.23	0.71
4:D:862:ASP:HA	27:3:599:GLU:HA	1.73	0.71
6:F:34:G:H2'	6:F:35:A:O4'	1.90	0.71
1:A:1761:PRO:O	1:A:1763:LEU:N	2.23	0.71
3:C:445:ALA:HB1	3:C:449:ILE:HD11	1.73	0.71
7:G:8:C:H2'	7:G:9:C:C6	2.25	0.71
10:J:242:ILE:HA	10:J:245:TRP:HD1	1.55	0.71
21:V:536:ILE:HG13	21:V:539:LEU:HD12	1.72	0.71
27:3:696:SER:O	27:3:696:SER:OG	2.08	0.71
27:3:878:ASP:OD1	27:3:879:LEU:N	2.24	0.71
26:1:967:GLU:O	26:1:971:MET:CB	2.38	0.71
1:A:182:ILE:HD11	1:A:562:VAL:HG13	1.73	0.71
1:A:1188:ASN:ND2	1:A:1193:GLU:OE1	2.22	0.71
31:2:616:SER:O	32:4:80:TYR:N	2.22	0.71
36:9:310:LEU:HD21	36:9:345:TYR:HA	1.72	0.71
1:A:211:GLN:OE1	1:A:214:ARG:NH1	2.24	0.71
1:A:1546:ASN:ND2	11:K:183:ILE:O	2.18	0.71
19:T:424:ASP:OD1	19:T:424:ASP:N	2.20	0.71
27:3:412:ILE:HG12	27:3:423:LEU:HG	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:8:38:VAL:HG22	37:8:113:GLN:HE22	1.55	0.71
23:X:345:GLU:OE2	23:X:348:ARG:NH1	2.24	0.70
5:E:80:THR:HA	5:E:93:TRP:O	1.91	0.70
3:C:300:LEU:HA	3:C:306:ASN:HD22	1.57	0.70
1:A:298:ASP:OD1	1:A:300:ASN:ND2	2.24	0.70
1:A:2275:ALA:HA	1:A:2297:GLN:HG2	1.73	0.70
5:E:60:MET:HB2	5:E:353:MET:HB3	1.73	0.70
7:G:91:A:OP1	12:L:12:ARG:NH2	2.24	0.70
27:3:260:ASN:OD1	27:3:261:PHE:N	2.24	0.70
2:B:46:U:O2	20:U:11:ARG:NH2	2.19	0.70
7:G:85:G:H2'	7:G:86:A:C8	2.26	0.70
10:J:414:HIS:HA	10:J:417:VAL:HG22	1.74	0.70
27:3:246:SER:O	27:3:258:TYR:OH	2.09	0.70
36:9:360:HIS:ND1	36:9:391:ASP:OD1	2.25	0.70
1:A:1941:ARG:NH2	1:A:2012:LEU:O	2.18	0.70
3:C:677:GLU:HA	3:C:683:ASN:O	1.91	0.70
35:5:36:HIS:ND1	35:5:76:CYS:SG	2.65	0.70
10:J:220:LEU:HD13	10:J:224:LYS:HD2	1.72	0.70
26:1:460:PRO:HB2	26:1:464:LEU:HD12	1.74	0.70
2:B:100:C:H2'	2:B:101:U:C6	2.27	0.70
23:X:296:HIS:O	23:X:298:SER:N	2.25	0.70
27:3:442:LEU:H	27:3:734:LEU:HA	1.57	0.70
27:3:461:THR:HA	27:3:473:TYR:O	1.92	0.70
5:E:295:PRO:HD3	5:E:335:PHE:HB3	1.72	0.70
6:F:84:A:H1'	6:F:85:U:H5'	1.74	0.70
8:H:78:C:H2'	8:H:79:G:H8	1.57	0.69
1:A:2105:ILE:HD11	1:A:2141:GLU:HG3	1.72	0.69
19:T:496:THR:OG1	19:T:498:GLU:OE2	2.10	0.69
24:Y:87:GLN:O	24:Y:90:THR:OG1	2.09	0.69
26:1:544:LEU:HD21	26:1:549:ARG:HB2	1.74	0.69
3:C:453:TYR:OH	3:C:575:GLN:HB2	1.92	0.69
1:A:78:ASN:HD22	1:A:79:ARG:N	1.91	0.69
6:F:37:C:H3'	6:F:37:C:P	2.33	0.69
3:C:826:ARG:HA	3:C:911:PRO:HG3	1.73	0.69
26:1:967:GLU:O	26:1:971:MET:HB2	1.93	0.69
27:3:806:ALA:HA	27:3:856:LYS:HB3	1.75	0.69
27:3:388:GLN:NE2	27:3:845:GLU:OE2	2.25	0.69
27:3:499:PHE:O	27:3:525:ARG:NH1	2.18	0.69
27:3:875:ASN:HD22	27:3:875:ASN:H	1.39	0.69
1:A:2330:ARG:H	1:A:2330:ARG:HD3	1.57	0.69
27:3:640:LEU:HD22	27:3:667:ILE:HG23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1764:SER:O	1:A:1766:GLN:N	2.26	0.68
1:A:2259:VAL:HG12	1:A:2260:GLN:H	1.58	0.68
5:E:262:TRP:HB3	5:E:272:ARG:HG3	1.74	0.68
27:3:115:ILE:O	27:3:138:GLN:NE2	2.26	0.68
27:3:266:ASP:OD1	27:3:266:ASP:N	2.22	0.68
27:3:452:LEU:HD21	27:3:476:VAL:HG11	1.76	0.68
36:9:75:THR:HA	36:9:82:LYS:HA	1.73	0.68
1:A:41:GLN:O	1:A:45:TYR:HB2	1.93	0.68
9:I:169:TYR:O	9:I:173:LEU:CB	2.41	0.68
25:Z:601:LEU:O	25:Z:604:LYS:HG3	1.93	0.68
32:4:101:ASN:HA	32:4:148:ASN:HA	1.74	0.68
34:7:30:CYS:SG	34:7:31:VAL:N	2.66	0.68
36:9:300:THR:O	36:9:300:THR:OG1	2.06	0.68
5:E:259:VAL:HB	5:E:277:PHE:HB2	1.75	0.68
7:G:7:G:H2'	7:G:8:C:C6	2.28	0.68
10:J:242:ILE:HA	10:J:245:TRP:CD1	2.27	0.68
26:1:614:ARG:NH2	26:1:618:ASP:OD2	2.26	0.68
27:3:528:ARG:NH1	27:3:572:GLY:O	2.26	0.68
5:E:241:LEU:HD23	5:E:250:LEU:HD21	1.75	0.68
16:Q:1066:GLN:HA	16:Q:1102:PRO:HD3	1.75	0.68
27:3:275:ARG:HG2	27:3:388:GLN:HB2	1.75	0.68
34:7:46:CYS:HB3	34:7:85:CYS:HB2	1.76	0.68
6:F:92:A:H2'	6:F:93:G:H8	1.57	0.68
26:1:624:VAL:O	26:1:628:THR:OG1	2.09	0.68
3:C:682:LYS:HB3	3:C:797:ALA:HB2	1.76	0.68
1:A:270:ASN:HD21	20:U:8:PRO:HB3	1.58	0.68
1:A:1201:ARG:O	1:A:1203:SER:N	2.26	0.68
2:B:98:G:H2'	2:B:99:C:C6	2.28	0.68
27:3:429:ARG:NH2	35:5:59:GLU:O	2.22	0.68
1:A:1855:GLU:OE1	11:K:136:ARG:NH1	2.27	0.68
8:H:107:A:H2'	8:H:108:G:C8	2.29	0.68
36:9:132:GLU:O	36:9:136:ILE:N	2.22	0.68
1:A:1792:LYS:HB3	1:A:1798:LEU:HG	1.74	0.68
1:A:2106:LEU:HB2	1:A:2142:ILE:HD12	1.76	0.68
31:2:450:SER:HB3	31:2:453:LYS:HG2	1.76	0.68
6:F:41:A:H2'	6:F:42:C:C6	2.29	0.68
1:A:330:THR:O	3:C:177:ARG:NH1	2.27	0.67
8:H:151:C:H2'	8:H:152:G:H8	1.57	0.67
17:R:174:ALA:HB2	17:R:200:VAL:HG23	1.75	0.67
23:X:274:TYR:HE1	26:1:436:THR:CA	2.06	0.67
1:A:979:SER:HB3	1:A:1173:SER:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1217:GLN:OE1	1:A:1224:ARG:NE	2.27	0.67
3:C:674:CYS:HB3	3:C:818:SER:HB2	1.75	0.67
13:N:70:ILE:HG23	13:N:74:LEU:HD23	1.75	0.67
3:C:509:VAL:HG12	3:C:565:ILE:HG12	1.75	0.67
4:D:1559:VAL:O	4:D:1643:VAL:HA	1.94	0.67
5:E:214:ASP:OD2	5:E:218:LYS:NZ	2.26	0.67
6:F:80:G:H1'	6:F:81:C:H2'	1.77	0.67
27:3:782:GLN:HG3	27:3:867:ARG:HH22	1.60	0.67
1:A:2076:ARG:NH1	1:A:2305:TYR:OH	2.27	0.67
10:J:370:VAL:HG22	10:J:378:ASN:HB3	1.76	0.67
21:V:517:LEU:HD23	21:V:518:LYS:HG3	1.75	0.67
27:3:353:PHE:HD1	27:3:406:PRO:HD3	1.59	0.67
1:A:1000:ILE:HG22	1:A:1001:VAL:HG22	1.76	0.67
1:A:863:GLU:HG3	1:A:913:PRO:HB3	1.77	0.67
1:A:1925:LYS:HE2	21:V:457:ARG:NH2	2.09	0.67
27:3:326:ARG:HE	27:3:372:GLU:HG2	1.59	0.67
1:A:1786:TYR:CE1	1:A:1837:ALA:HB2	2.30	0.67
3:C:731:SER:HB2	3:C:746:VAL:HG13	1.76	0.67
8:H:70:C:H2'	8:H:71:C:C6	2.30	0.67
27:3:430:GLY:O	27:3:433:SER:OG	2.11	0.67
1:A:2067:PHE:HB2	1:A:2072:GLU:HB3	1.77	0.67
1:A:2086:ARG:O	1:A:2089:HIS:N	2.22	0.67
27:3:616:ILE:HB	27:3:629:SER:O	1.95	0.67
27:3:672:GLY:H	27:3:696:SER:HA	1.58	0.67
27:3:806:ALA:HB1	27:3:856:LYS:HD3	1.75	0.67
1:A:1199:LYS:NZ	1:A:1206:GLU:OE2	2.22	0.66
12:L:64:SER:OG	12:L:66:GLU:OE1	2.12	0.66
7:G:13:C:H2'	7:G:14:A:H8	1.60	0.66
10:J:234:ASN:O	10:J:238:ASN:ND2	2.17	0.66
10:J:240:THR:OG1	10:J:241:VAL:N	2.26	0.66
26:1:1210:HIS:ND1	31:2:585:THR:OG1	2.29	0.66
27:3:41:LEU:HD22	27:3:52:THR:HG22	1.77	0.66
27:3:195:ASP:OD2	27:3:200:ALA:N	2.21	0.66
1:A:52:GLY:O	2:B:64:G:O2'	2.12	0.66
3:C:561:LYS:NZ	3:C:614:TYR:O	2.27	0.66
1:A:1412:TRP:O	1:A:1420:ASN:ND2	2.21	0.66
16:Q:515:VAL:N	16:Q:540:THR:O	2.28	0.66
16:Q:1227:LEU:O	16:Q:1273:LEU:HA	1.95	0.66
1:A:1106:ALA:O	1:A:1110:ILE:HG13	1.95	0.66
1:A:2312:SER:O	1:A:2316:ASN:ND2	2.27	0.66
3:C:690:GLU:HG3	3:C:788:LYS:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:108:U:H4'	7:G:109:U:OP2	1.96	0.66
24:Y:3:PRO:HA	24:Y:6:LYS:HG3	1.75	0.66
27:3:464:ARG:HG3	27:3:516:LEU:HD11	1.76	0.66
36:9:324:SER:OG	36:9:415:SER:OG	2.13	0.66
37:8:115:ASN:OD1	37:8:116:ILE:N	2.28	0.66
2:B:99:C:H2'	2:B:100:C:C6	2.31	0.66
26:1:477:LYS:HB3	26:1:499:LYS:NZ	2.11	0.66
1:A:982:GLU:O	1:A:983:LYS:HG3	1.96	0.66
33:6:48:ILE:HG12	33:6:62:VAL:HG12	1.76	0.66
36:9:267:ASP:OD1	36:9:268:GLU:N	2.29	0.66
5:E:175:THR:HA	5:E:191:GLN:HA	1.77	0.66
16:Q:1182:VAL:N	16:Q:1305:ALA:O	2.28	0.66
1:A:533:LYS:HZ2	1:A:533:LYS:HB3	1.61	0.66
1:A:1957:ASP:OD2	1:A:1959:THR:OG1	2.14	0.66
8:H:50:C:H2'	8:H:51:A:H8	1.61	0.66
26:1:1166:ILE:O	26:1:1170:THR:HG22	1.95	0.66
6:F:17:C:H2'	6:F:18:A:H8	1.61	0.65
23:X:273:MET:HE1	26:1:433:ALA:CB	2.22	0.65
1:A:325:HIS:HD2	1:A:326:HIS:HD2	1.43	0.65
27:3:552:ARG:NH2	27:3:568:MET:O	2.27	0.65
1:A:552:ARG:HG2	1:A:552:ARG:HH11	1.62	0.65
3:C:323:PHE:CD2	3:C:373:ILE:HG12	2.32	0.65
3:C:560:VAL:HG12	3:C:561:LYS:H	1.59	0.65
10:J:408:ASP:OD1	10:J:408:ASP:N	2.30	0.65
27:3:507:SER:HB2	27:3:547:CYS:SG	2.35	0.65
36:9:368:MET:O	36:9:394:HIS:ND1	2.30	0.65
1:A:1384:ARG:HH22	1:A:1414:ARG:HH22	1.45	0.65
1:A:1591:MET:SD	1:A:1611:LYS:NZ	2.61	0.65
3:C:727:LEU:O	3:C:731:SER:OG	2.13	0.65
25:Z:547:ASN:OD1	25:Z:547:ASN:N	2.20	0.65
27:3:670:GLN:HA	27:3:698:PRO:HA	1.79	0.65
36:9:337:GLY:O	36:9:421:ARG:NH2	2.28	0.65
17:R:295:ASP:OD2	17:R:296:ARG:N	2.30	0.65
21:V:618:ARG:HB3	21:V:646:HIS:HE1	1.62	0.65
3:C:925:PRO:HG2	3:C:928:HIS:CE1	2.31	0.65
15:P:198:ALA:HB1	15:P:201:VAL:HG21	1.77	0.65
27:3:715:MET:HE2	27:3:739:LEU:H	1.59	0.65
27:3:351:SER:OG	27:3:355:ASN:O	2.13	0.65
27:3:1187:PRO:HA	27:3:1190:GLN:HB2	1.78	0.65
36:9:299:LEU:HD12	36:9:300:THR:HG22	1.79	0.65
1:A:2105:ILE:HG22	1:A:2262:LEU:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:TRP:HB2	3:C:177:ARG:HH11	1.62	0.65
1:A:1076:ASP:OD1	1:A:1077:ILE:N	2.30	0.65
1:A:2164:PRO:HB3	1:A:2296:LEU:HD11	1.78	0.65
27:3:556:ILE:HG13	27:3:564:VAL:HB	1.78	0.65
27:3:223:LYS:NZ	27:3:224:TYR:OH	2.22	0.64
1:A:529:THR:HG22	11:K:197:TYR:HB3	1.79	0.64
3:C:441:PRO:O	3:C:444:GLY:HA3	1.97	0.64
19:T:257:ARG:NH2	19:T:300:ILE:O	2.30	0.64
1:A:1760:GLU:HG2	1:A:1760:GLU:O	1.98	0.64
3:C:836:VAL:HG22	3:C:897:SER:HB2	1.78	0.64
8:H:12:G:O2'	8:H:13:C:O4'	2.11	0.64
26:1:607:ALA:O	26:1:611:SER:OG	2.14	0.64
18:S:366:VAL:N	18:S:583:TYR:O	2.26	0.64
3:C:338:GLU:OE2	3:C:342:ARG:NH1	2.29	0.64
6:F:43:A:H2	7:G:4:A:H61	1.46	0.64
17:R:134:ARG:NH2	19:T:385:TYR:H	1.95	0.64
18:S:431:GLN:O	18:S:435:TYR:N	2.26	0.64
4:D:2020:SER:O	4:D:2039:VAL:HA	1.97	0.64
19:T:245:HIS:NE2	19:T:263:SER:OG	2.28	0.64
23:X:275:ILE:O	23:X:308:TYR:OH	2.11	0.64
26:1:1262:ARG:NH1	35:5:24:ALA:O	2.30	0.64
27:3:84:SER:OG	27:3:85:GLY:N	2.31	0.64
27:3:604:PHE:HD1	27:3:628:LEU:HD23	1.62	0.64
3:C:60:HIS:O	3:C:63:LYS:HB2	1.98	0.64
5:E:125:PHE:HE1	5:E:159:PRO:HB3	1.63	0.64
10:J:251:TRP:CE2	10:J:255:LEU:HD11	2.33	0.64
33:6:68:PHE:HA	33:6:71:LYS:HG2	1.80	0.64
21:V:515:CYS:HA	21:V:521:TYR:HB2	1.79	0.64
27:3:583:MET:HG3	27:3:584:SER:H	1.63	0.64
5:E:90:ILE:HD11	5:E:112:VAL:HG11	1.79	0.64
7:G:-12:C:O2'	7:G:-11:G:N7	2.31	0.64
26:1:531:LEU:HD23	26:1:559:ILE:HD12	1.79	0.64
8:H:28:C:O2'	8:H:29:A:O5'	2.16	0.63
25:Z:509:GLN:NE2	25:Z:510:ASN:OD1	2.31	0.63
27:3:875:ASN:HD22	27:3:875:ASN:N	1.95	0.63
35:5:3:ASP:O	35:5:7:ILE:HG12	1.98	0.63
1:A:146:SER:HB2	1:A:193:LEU:HD22	1.80	0.63
1:A:781:ARG:HH21	8:H:24:A:H5"	1.63	0.63
21:V:640:THR:O	21:V:644:ARG:HG3	1.98	0.63
26:1:1100:ASN:O	26:1:1103:VAL:HG22	1.98	0.63
26:1:1289:ASN:HB3	26:1:1295:TYR:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:215:LEU:H	27:3:215:LEU:HD12	1.63	0.63
1:A:78:ASN:HD22	1:A:79:ARG:H	1.46	0.63
1:A:2229:LYS:O	1:A:2257:GLU:N	2.32	0.63
5:E:304:SER:O	5:E:330:ILE:N	2.31	0.63
1:A:658:ARG:NH1	6:F:67:G:OP2	2.32	0.63
3:C:496:VAL:HG23	3:C:546:ALA:HA	1.79	0.63
26:1:1120:ALA:HB2	26:1:1128:VAL:HG21	1.80	0.63
27:3:511:LEU:HD23	27:3:512:GLY:H	1.63	0.63
3:C:489:GLN:OE1	3:C:489:GLN:N	2.32	0.63
13:N:8:ARG:HB2	13:N:9:LYS:HE2	1.81	0.63
21:V:646:HIS:O	21:V:650:THR:OG1	2.14	0.63
25:Z:575:ARG:NH1	25:Z:594:GLU:OE1	2.32	0.63
26:1:1030:LYS:O	26:1:1034:ASN:ND2	2.32	0.63
27:3:93:GLN:NE2	27:3:100:GLU:OE1	2.31	0.63
36:9:360:HIS:NE2	36:9:394:HIS:O	2.32	0.63
1:A:617:ASN:HA	1:A:621:VAL:HG23	1.78	0.63
1:A:1021:ASP:N	1:A:1021:ASP:OD1	2.31	0.63
5:E:118:ASN:HD21	5:E:122:SER:H	1.47	0.63
10:J:280:LEU:HD21	10:J:315:LYS:HD2	1.80	0.63
21:V:525:PHE:HB3	21:V:560:LEU:HD21	1.80	0.63
26:1:150:ARG:NH1	26:1:158:GLU:OE1	2.31	0.63
27:3:399:ASP:OD1	27:3:400:GLU:N	2.32	0.63
33:6:111:LYS:HZ2	33:6:115:GLU:HG3	1.63	0.63
1:A:1407:ASP:OD1	1:A:1407:ASP:N	2.20	0.63
1:A:1655:THR:OG1	1:A:1656:THR:N	2.31	0.63
5:E:73:LYS:HE3	5:E:117:TYR:H	1.63	0.63
13:N:26:ASP:O	13:N:30:ARG:HG2	1.98	0.63
17:R:240:LYS:O	17:R:244:GLU:HG3	1.99	0.63
23:X:366:GLU:N	23:X:366:GLU:OE2	2.32	0.63
27:3:911:LYS:HB3	27:3:922:GLY:O	1.98	0.63
32:4:117:TYR:O	32:4:121:SER:CB	2.47	0.63
21:V:641:ASP:HA	21:V:644:ARG:HD2	1.81	0.63
23:X:279:SER:O	23:X:307:GLN:NE2	2.31	0.63
1:A:266:SER:OG	1:A:271:MET:O	2.16	0.63
6:F:82:A:HO2'	6:F:83:A:H8	1.47	0.63
8:H:27:U:C2'	8:H:28:C:H5'	2.29	0.63
9:I:374:ILE:O	9:I:377:THR:N	2.31	0.63
10:J:350:ILE:HD11	10:J:362:ALA:HA	1.81	0.63
1:A:382:GLU:HB3	3:C:354:ARG:HD2	1.79	0.62
6:F:93:G:OP1	10:J:318:TYR:OH	2.15	0.62
12:L:79:PRO:O	12:L:80:THR:OG1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:209:ILE:HG12	5:E:219:VAL:HG22	1.79	0.62
10:J:431:ARG:O	10:J:435:ILE:HD12	1.99	0.62
27:3:1160:HIS:NE2	27:3:1175:ASP:OD2	2.23	0.62
1:A:1816:GLN:HG2	1:A:1916:LEU:HD11	1.81	0.62
3:C:604:LEU:HD21	3:C:627:HIS:CE1	2.34	0.62
3:C:937:THR:HG22	3:C:941:LYS:HD3	1.81	0.62
21:V:488:GLU:O	21:V:492:MET:HB2	2.00	0.62
27:3:511:LEU:HD21	27:3:574:LEU:HD11	1.81	0.62
27:3:918:ARG:HG2	27:3:918:ARG:HH11	1.64	0.62
1:A:837:LYS:NZ	26:1:101:TYR:HB3	2.14	0.62
3:C:534:VAL:HG23	3:C:539:ILE:HD11	1.80	0.62
23:X:335:ASN:O	23:X:343:ARG:NE	2.32	0.62
27:3:895:ARG:NE	27:3:901:GLU:OE1	2.32	0.62
36:9:271:LEU:HA	36:9:274:GLN:NE2	2.15	0.62
36:9:366:LEU:HD13	36:9:382:ILE:HG13	1.79	0.62
1:A:2181:GLN:O	1:A:2217:SER:HA	1.99	0.62
16:Q:875:HIS:O	16:Q:1033:LYS:N	2.32	0.62
23:X:273:MET:HE2	26:1:433:ALA:CB	2.30	0.62
27:3:1009:PHE:HZ	27:3:1046:GLY:HA3	1.62	0.62
3:C:770:PHE:HE1	3:C:789:PHE:CD1	2.18	0.62
8:H:182:U:H2'	8:H:183:G:C8	2.34	0.62
21:V:647:LEU:O	21:V:651:PRO:HD2	2.00	0.62
23:X:338:PHE:HB3	23:X:341:ASN:HA	1.80	0.62
27:3:341:VAL:HG22	27:3:347:LEU:HD12	1.81	0.62
27:3:1140:PHE:O	27:3:1144:VAL:HG23	2.00	0.62
1:A:698:PRO:HG2	19:T:373:LYS:HZ1	1.64	0.62
4:D:860:GLN:O	27:3:601:ARG:NH1	2.33	0.62
7:G:98:U:H4'	34:7:4:HIS:HD2	1.64	0.62
8:H:53:U:OP1	31:2:450:SER:OG	2.15	0.62
10:J:347:HIS:O	10:J:351:ASN:ND2	2.33	0.62
19:T:215:GLY:O	19:T:217:GLN:NE2	2.28	0.62
19:T:394:ASN:ND2	19:T:408:ASN:OD1	2.32	0.62
36:9:449:ARG:HA	36:9:452:GLN:HE21	1.65	0.62
4:D:1583:ASP:O	4:D:1585:GLN:N	2.33	0.62
1:A:699:GLU:HA	1:A:701:ILE:HG13	1.82	0.62
26:1:583:ILE:HD11	26:1:623:TYR:HE1	1.64	0.62
27:3:718:ARG:HB2	27:3:720:TRP:NE1	2.15	0.62
36:9:277:LYS:HA	36:9:298:ASP:HB3	1.80	0.62
3:C:685:ILE:HD11	3:C:808:ILE:HD11	1.81	0.61
5:E:90:ILE:HG13	5:E:105:LEU:HD22	1.80	0.61
10:J:220:LEU:O	10:J:224:LYS:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:23:LEU:H	21:V:474:HIS:CD2	2.16	0.61
2:B:99:C:H2'	2:B:100:C:H6	1.64	0.61
5:E:217:ILE:HB	5:E:231:MET:HG2	1.82	0.61
23:X:314:THR:HG22	23:X:318:GLY:HA2	1.82	0.61
1:A:693:ILE:HG22	1:A:694:LEU:HD23	1.83	0.61
3:C:453:TYR:CZ	3:C:575:GLN:HB2	2.36	0.61
5:E:91:LEU:HB3	5:E:101:ASN:ND2	2.09	0.61
8:H:50:C:H2'	8:H:51:A:C8	2.36	0.61
21:V:481:PHE:HD2	21:V:485:GLN:HB2	1.65	0.61
1:A:2178:ILE:HB	1:A:2214:ILE:HD13	1.80	0.61
1:A:2264:SER:HG	1:A:2267:PHE:HD2	1.48	0.61
6:F:42:C:H2'	6:F:43:A:O4'	2.00	0.61
1:A:1384:ARG:HH22	1:A:1414:ARG:NH2	1.97	0.61
3:C:495:ARG:HB2	3:C:495:ARG:HH11	1.64	0.61
6:F:81:C:H42	8:H:18:U:H3	1.49	0.61
14:O:163:HIS:O	14:O:182:ARG:N	2.34	0.61
27:3:412:ILE:HB	27:3:1105:GLN:HE21	1.65	0.61
27:3:511:LEU:HD23	27:3:512:GLY:N	2.15	0.61
27:3:675:LEU:HB3	27:3:686:LEU:HD12	1.81	0.61
3:C:679:PRO:HD2	3:C:807:GLN:HB3	1.82	0.61
5:E:133:VAL:HG22	5:E:154:VAL:HG11	1.82	0.61
14:O:23:LEU:HA	14:O:81:CYS:HA	1.82	0.61
27:3:933:ASN:ND2	27:3:935:GLU:OE2	2.33	0.61
1:A:546:LEU:HD11	1:A:595:LYS:HG3	1.81	0.61
1:A:1018:ASN:ND2	1:A:1023:ASN:OD1	2.34	0.61
5:E:222:LEU:HB3	5:E:223:ARG:HH11	1.64	0.61
23:X:273:MET:HE2	26:1:433:ALA:HB1	1.78	0.61
3:C:269:LEU:O	3:C:378:TYR:OH	2.09	0.61
3:C:559:ILE:HD12	3:C:560:VAL:O	2.00	0.61
3:C:737:PRO:HG3	3:C:774:THR:HB	1.82	0.61
7:G:111:U:O2	24:Y:105:ARG:NE	2.32	0.61
1:A:1502:PHE:HE2	1:A:1505:LYS:HB2	1.66	0.61
3:C:809:ILE:HB	3:C:810:PRO:HD3	1.81	0.61
3:C:931:ARG:HE	3:C:935:ILE:HD11	1.64	0.61
7:G:88:G:N2	8:H:41:U:H3	1.98	0.61
27:3:946:GLU:OE1	27:3:946:GLU:N	2.33	0.61
31:2:471:ARG:HH21	31:2:474:VAL:HG23	1.66	0.61
37:8:39:ASP:OD2	37:8:41:SER:OG	2.19	0.61
19:T:503:SER:O	19:T:503:SER:OG	2.16	0.60
24:Y:86:ASP:O	24:Y:89:SER:OG	2.19	0.60
27:3:260:ASN:HB3	27:3:264:GLN:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1769:GLY:HA2	1:A:1772:PHE:CZ	2.36	0.60
13:N:102:CYS:SG	13:N:137:CYS:HB2	2.41	0.60
1:A:1994:LYS:O	1:A:1995:ASN:ND2	2.27	0.60
3:C:843:VAL:HG22	3:C:871:ILE:HD11	1.82	0.60
10:J:246:ILE:HG23	10:J:281:LYS:HE3	1.84	0.60
10:J:262:ARG:NH2	10:J:286:GLU:OE1	2.34	0.60
13:N:30:ARG:O	13:N:34:THR:OG1	2.19	0.60
26:1:151:THR:N	26:1:154:ASP:OD2	2.32	0.60
26:1:477:LYS:HB3	26:1:499:LYS:HZ1	1.65	0.60
27:3:138:GLN:HG2	27:3:161:HIS:ND1	2.15	0.60
27:3:893:VAL:HG22	27:3:905:VAL:HG22	1.84	0.60
1:A:858:GLN:OE1	1:A:861:ARG:NH2	2.34	0.60
3:C:118:PHE:O	3:C:122:LEU:HD12	2.01	0.60
5:E:171:SER:OG	5:E:173:ASP:OD2	2.19	0.60
24:Y:62:ILE:HD13	24:Y:82:LEU:HD21	1.83	0.60
26:1:128:ILE:HB	33:6:96:ARG:HB3	1.83	0.60
26:1:400:SER:N	26:1:403:GLU:OE1	2.32	0.60
26:1:690:ILE:HD11	26:1:708:ALA:HB3	1.83	0.60
26:1:866:LYS:HG3	26:1:909:VAL:HG11	1.81	0.60
27:3:70:LEU:HD11	27:3:152:LEU:HD13	1.84	0.60
27:3:697:ARG:NH2	27:3:717:SER:HB3	2.16	0.60
36:9:425:GLU:OE1	36:9:427:ARG:NH1	2.34	0.60
1:A:216:SER:O	1:A:216:SER:OG	2.16	0.60
1:A:274:PRO:HG3	20:U:1:MET:HG3	1.83	0.60
1:A:2128:LEU:HD23	1:A:2142:ILE:HG21	1.83	0.60
18:S:451:THR:HA	18:S:496:MET:O	2.02	0.60
24:Y:7:VAL:HG22	24:Y:108:ARG:HB2	1.84	0.60
37:8:110:LEU:HA	37:8:113:GLN:HE21	1.66	0.60
1:A:1878:ASP:OD1	1:A:1878:ASP:N	2.34	0.60
1:A:2121:ARG:HA	1:A:2182:PRO:HB3	1.84	0.60
3:C:488:VAL:HG13	3:C:609:LYS:HE2	1.84	0.60
6:F:29:A:N6	7:G:16:G:O2'	2.34	0.60
21:V:491:ASN:HA	21:V:528:ILE:HD11	1.83	0.60
27:3:206:GLN:HE21	27:3:231:HIS:HA	1.66	0.60
27:3:249:LEU:HD22	27:3:256:ILE:HD11	1.83	0.60
3:C:286:ASN:OD1	3:C:300:LEU:N	2.26	0.60
6:F:36:A:N6	7:G:10:U:O4	2.34	0.60
8:H:72:U:H2'	8:H:73:C:C6	2.36	0.60
17:R:434:ASP:N	17:R:434:ASP:OD1	2.35	0.60
21:V:489:LEU:HD23	21:V:521:TYR:HE1	1.67	0.60
27:3:407:ILE:HG23	27:3:425:VAL:HG13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:637:PRO:HB3	27:3:640:LEU:HD21	1.84	0.60
27:3:899:THR:OG1	27:3:900:GLY:N	2.33	0.60
1:A:43:LYS:HZ3	6:F:21:U:H3	1.50	0.60
27:3:525:ARG:NE	27:3:527:ILE:HD11	2.16	0.60
27:3:1136:GLU:OE1	27:3:1136:GLU:N	2.23	0.60
1:A:1850:ARG:NH1	1:A:1878:ASP:OD2	2.34	0.60
3:C:352:LYS:H	3:C:352:LYS:HD3	1.67	0.60
5:E:69:VAL:HG23	5:E:349:LYS:HA	1.82	0.60
5:E:175:THR:HG22	5:E:191:GLN:HB3	1.83	0.60
7:G:98:U:H4'	34:7:4:HIS:CD2	2.37	0.60
8:H:37:U:OP2	26:1:517:ARG:NH1	2.35	0.60
36:9:296:HIS:H	36:9:296:HIS:CD2	2.18	0.60
37:8:115:ASN:ND2	37:8:119:ILE:O	2.29	0.60
1:A:1535:THR:HG22	1:A:1569:LEU:HD13	1.84	0.60
1:A:2177:TRP:HZ3	1:A:2179:HIS:HB3	1.66	0.60
9:I:231:ASN:O	9:I:233:ASP:N	2.27	0.60
27:3:725:TYR:O	27:3:728:ARG:HB2	2.02	0.60
32:4:105:GLY:N	32:4:173:THR:O	2.29	0.60
1:A:485:THR:OG1	1:A:486:LYS:N	2.35	0.59
1:A:1548:TYR:CE2	1:A:1550:GLY:HA2	2.36	0.59
5:E:305:ALA:HA	5:E:329:SER:HB3	1.84	0.59
23:X:231:ALA:HA	24:Y:103:LYS:HE3	1.84	0.59
27:3:475:ILE:HG21	27:3:508:CYS:SG	2.42	0.59
1:A:2275:ALA:HB3	1:A:2295:GLU:HB2	1.83	0.59
3:C:86:THR:OG1	3:C:87:GLN:N	2.35	0.59
3:C:642:HIS:HE1	3:C:646:LYS:HD3	1.65	0.59
5:E:215:ASN:ND2	5:E:235:ALA:O	2.35	0.59
11:K:159:TYR:CE2	21:V:450:ILE:HG21	2.36	0.59
1:A:529:THR:HG23	11:K:230:TRP:NE1	2.16	0.59
1:A:692:ASP:HA	19:T:376:ARG:HH22	1.67	0.59
1:A:1581:LEU:O	1:A:1585:ILE:HG13	2.02	0.59
5:E:344:SER:O	5:E:351:LEU:HA	2.01	0.59
26:1:1291:ASP:OD1	26:1:1292:LYS:N	2.34	0.59
19:T:267:ASP:OD1	19:T:267:ASP:N	2.17	0.59
21:V:579:SER:O	21:V:583:VAL:HG23	2.03	0.59
24:Y:110:ASP:OD1	24:Y:111:HIS:N	2.35	0.59
26:1:907:ASP:OD1	26:1:907:ASP:N	2.35	0.59
36:9:436:ASP:O	36:9:440:GLU:HG3	2.01	0.59
1:A:1808:PHE:CE2	1:A:1893:PHE:HB3	2.37	0.59
6:F:39:A:H2'	6:F:40:U:O4'	2.03	0.59
7:G:98:U:O2'	34:7:5:HIS:NE2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:622:ARG:HA	21:V:625:ARG:HE	1.67	0.59
3:C:774:THR:HG22	3:C:784:ILE:HD11	1.84	0.59
14:O:110:SER:O	14:O:114:LYS:CB	2.51	0.59
27:3:485:LEU:HB3	27:3:491:VAL:HG12	1.83	0.59
31:2:567:ASP:OD2	31:2:570:LYS:NZ	2.26	0.59
1:A:1502:PHE:CE2	1:A:1505:LYS:HB2	2.38	0.59
4:D:884:ASN:O	4:D:886:GLN:N	2.31	0.59
6:F:87:C:H4'	36:9:356:PRO:HG3	1.85	0.59
26:1:701:VAL:HA	26:1:704:ILE:HG22	1.83	0.59
27:3:947:GLU:HG3	27:3:948:VAL:H	1.68	0.59
3:C:514:TYR:CE2	3:C:522:SER:HB2	2.38	0.59
8:H:2:U:H2'	8:H:3:C:C6	2.38	0.59
11:K:136:ARG:O	11:K:140:ILE:HG12	2.02	0.59
27:3:547:CYS:HA	27:3:555:VAL:HG12	1.85	0.59
1:A:2106:LEU:O	1:A:2264:SER:N	2.36	0.59
3:C:922:GLU:O	3:C:924:GLN:NE2	2.35	0.59
5:E:318:ARG:HB3	5:E:318:ARG:HH11	1.67	0.59
27:3:520:TYR:HB2	27:3:521:PRO:HD2	1.85	0.59
1:A:37:TRP:O	1:A:41:GLN:HG2	2.03	0.58
2:B:97:G:H2'	2:B:98:G:C8	2.38	0.58
7:G:19:G:N2	14:O:193:LEU:O	2.30	0.58
26:1:652:CYS:SG	26:1:692:HIS:HE1	2.26	0.58
26:1:1078:VAL:HG12	26:1:1118:ILE:HD12	1.83	0.58
27:3:108:GLY:O	34:7:82:ARG:NH1	2.35	0.58
31:2:451:LYS:O	31:2:455:ARG:NH1	2.35	0.58
1:A:1251:SER:O	1:A:1251:SER:OG	2.15	0.58
1:A:1838:LYS:O	1:A:1841:THR:OG1	2.19	0.58
3:C:731:SER:HB3	3:C:747:ASP:O	2.03	0.58
6:F:85:U:H1'	6:F:86:U:C5	2.38	0.58
10:J:251:TRP:CZ2	10:J:255:LEU:HD11	2.39	0.58
13:N:18:ILE:HG21	13:N:70:ILE:HD11	1.84	0.58
27:3:547:CYS:HB2	27:3:556:ILE:HG22	1.85	0.58
37:8:64:ASP:O	37:8:68:ILE:HG12	2.03	0.58
6:F:38:G:P	6:F:38:G:H8	2.26	0.58
10:J:326:VAL:HG13	10:J:352:PHE:HZ	1.68	0.58
31:2:511:LEU:O	31:2:514:LYS:N	2.36	0.58
1:A:280:GLU:OE2	2:B:47:A:H1'	2.04	0.58
1:A:2076:ARG:HD3	1:A:2121:ARG:HE	1.68	0.58
1:A:2190:PRO:O	1:A:2194:THR:HG22	2.03	0.58
5:E:202:ASN:HD21	5:E:206:ASP:H	1.51	0.58
18:S:447:LYS:H	18:S:514:TYR:HA	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1208:LEU:HB2	26:1:1241:ILE:HD11	1.85	0.58
27:3:442:LEU:HB2	27:3:734:LEU:HB3	1.84	0.58
27:3:739:LEU:HD23	27:3:758:SER:HB3	1.86	0.58
6:F:88:G:H2'	6:F:89:U:H5"	1.86	0.58
26:1:962:MET:O	26:1:967:GLU:HB2	2.03	0.58
27:3:939:PHE:HZ	27:3:942:LYS:HG2	1.68	0.58
1:A:663:ARG:CB	1:A:663:ARG:HH11	2.16	0.58
6:F:59:G:H1	6:F:76:A:N6	1.98	0.58
8:H:27:U:H2'	8:H:28:C:H5'	1.86	0.58
10:J:267:ARG:O	10:J:271:VAL:HG23	2.04	0.58
10:J:376:VAL:HA	10:J:379:TRP:HD1	1.68	0.58
16:Q:1224:ILE:O	16:Q:1255:ASN:N	2.34	0.58
17:R:176:TYR:CE2	17:R:198:ARG:HB3	2.38	0.58
18:S:367:ARG:HA	18:S:582:PHE:HA	1.86	0.58
26:1:493:LYS:O	26:1:497:ILE:HG23	2.04	0.58
27:3:1019:ASN:O	27:3:1019:ASN:ND2	2.36	0.58
36:9:143:ASP:N	36:9:148:GLU:O	2.35	0.58
1:A:2174:PRO:HB2	1:A:2206:TRP:CD1	2.39	0.58
3:C:540:GLU:H	3:C:540:GLU:CD	2.05	0.58
3:C:785:ARG:HB2	3:C:785:ARG:HH11	1.69	0.58
3:C:928:HIS:ND1	3:C:928:HIS:N	2.52	0.58
27:3:458:ALA:HB1	27:3:460:TRP:HZ3	1.68	0.58
1:A:134:TRP:HB3	1:A:418:THR:HG21	1.85	0.58
1:A:267:LYS:NZ	2:B:49:A:OP1	2.26	0.58
1:A:1436:TRP:O	1:A:1440:THR:HG23	2.03	0.58
1:A:2093:SER:HB2	1:A:2226:THR:HG23	1.85	0.58
3:C:670:SER:HB3	3:C:688:ILE:HB	1.85	0.58
3:C:925:PRO:HG2	3:C:928:HIS:HE1	1.69	0.58
10:J:232:GLU:O	10:J:236:ARG:HB2	2.03	0.58
19:T:394:ASN:N	19:T:394:ASN:OD1	2.35	0.58
24:Y:106:THR:O	24:Y:106:THR:OG1	2.22	0.58
25:Z:532:ASP:O	25:Z:536:ARG:HG3	2.03	0.58
36:9:310:LEU:HB2	36:9:316:TYR:CE2	2.39	0.58
37:8:14:ASP:OD1	37:8:15:ASN:N	2.37	0.58
1:A:331:TRP:HB2	3:C:177:ARG:HD3	1.85	0.58
1:A:693:ILE:HG13	1:A:738:MET:HB2	1.84	0.58
1:A:1617:ARG:HD3	11:K:233:GLU:HG2	1.86	0.58
8:H:156:U:H2'	8:H:157:G:C8	2.38	0.58
27:3:544:ILE:HD11	27:3:556:ILE:HB	1.85	0.58
27:3:615:ARG:CZ	27:3:630:MET:HB3	2.34	0.58
27:3:848:PRO:HG2	27:3:851:ILE:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:7:23:CYS:HB3	34:7:58:CYS:HB2	1.84	0.58
36:9:366:LEU:HD11	36:9:380:PHE:CD2	2.39	0.58
1:A:1949:ARG:O	1:A:1953:ILE:HG13	2.04	0.58
3:C:117:ASP:N	3:C:117:ASP:OD1	2.37	0.58
3:C:618:THR:HB	3:C:630:LEU:HB2	1.85	0.58
5:E:253:ASN:ND2	5:E:291:CYS:HB3	2.18	0.58
18:S:969:PHE:O	18:S:996:PHE:HA	2.04	0.58
24:Y:58:GLN:NE2	25:Z:588:ASP:OD1	2.37	0.58
26:1:1092:ASP:O	26:1:1096:THR:HG23	2.03	0.58
27:3:685:ASP:OD1	27:3:686:LEU:N	2.37	0.58
31:2:460:PHE:HB3	31:2:464:GLU:HB3	1.86	0.58
3:C:434:CYS:O	3:C:438:ILE:HB	2.03	0.57
3:C:692:LEU:HD22	3:C:696:LEU:HD11	1.85	0.57
7:G:88:G:H22	8:H:41:U:H3	1.51	0.57
19:T:412:HIS:ND1	19:T:429:SER:OG	2.31	0.57
27:3:614:VAL:HB	27:3:633:LEU:HD11	1.86	0.57
36:9:351:LYS:H	36:9:351:LYS:HD2	1.68	0.57
1:A:595:LYS:NZ	2:B:30:A:OP1	2.34	0.57
3:C:812:ALA:O	3:C:816:VAL:HG23	2.04	0.57
8:H:13:C:H1’	8:H:14:C:H5’	1.85	0.57
26:1:122:HIS:ND1	26:1:125:THR:OG1	2.37	0.57
26:1:826:ASP:OD1	26:1:827:ARG:N	2.37	0.57
26:1:1010:THR:OG1	26:1:1011:PRO:HD3	2.04	0.57
33:6:42:TYR:OH	33:6:76:HIS:HB3	2.04	0.57
34:7:21:ARG:NH2	34:7:68:ASP:OD1	2.36	0.57
2:B:66:A:H2’	2:B:67:A:C8	2.40	0.57
3:C:514:TYR:HE2	3:C:522:SER:HB2	1.69	0.57
3:C:719:GLN:HG3	3:C:724:TRP:O	2.04	0.57
5:E:125:PHE:CE1	5:E:159:PRO:HB3	2.39	0.57
7:G:22:C:O2’	7:G:23:U:OP1	2.20	0.57
16:Q:852:VAL:O	16:Q:1061:MET:HA	2.04	0.57
23:X:230:GLY:O	23:X:234:GLU:HB2	2.04	0.57
31:2:478:HIS:O	31:2:481:THR:OG1	2.20	0.57
1:A:1352:HIS:CD2	20:U:5:ILE:HG21	2.39	0.57
19:T:195:LYS:HE3	19:T:490:ARG:NH2	2.19	0.57
23:X:328:ILE:HB	23:X:352:LEU:HD11	1.86	0.57
27:3:960:LEU:HD22	27:3:967:LEU:HD11	1.87	0.57
3:C:335:ASN:ND2	3:C:338:GLU:H	2.03	0.57
23:X:222:GLU:OE1	23:X:222:GLU:N	2.38	0.57
26:1:529:GLY:O	26:1:533:ASN:ND2	2.37	0.57
27:3:1159:ASP:HB3	27:3:1162:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:9:440:GLU:O	36:9:444:GLN:HG3	2.03	0.57
3:C:390:THR:OG1	3:C:391:SER:N	2.38	0.57
3:C:491:HIS:HB3	3:C:551:LEU:HD22	1.86	0.57
3:C:673:LYS:HB3	3:C:686:THR:HG23	1.87	0.57
3:C:774:THR:HA	3:C:784:ILE:HD11	1.86	0.57
9:I:406:GLU:HA	9:I:410:GLN:HA	1.87	0.57
27:3:636:GLN:HB3	27:3:670:GLN:HE22	1.69	0.57
36:9:306:ASN:OD1	36:9:345:TYR:N	2.32	0.57
1:A:2150:GLN:HG2	1:A:2279:TRP:O	2.05	0.57
3:C:687:MET:HE2	3:C:791:ILE:HG12	1.86	0.57
5:E:156:SER:HB2	5:E:199:VAL:HG12	1.87	0.57
8:H:181:G:H2'	8:H:182:U:C6	2.39	0.57
9:I:139:ALA:C	9:I:141:PRO:HD3	2.25	0.57
10:J:263:SER:O	10:J:267:ARG:NE	2.37	0.57
16:Q:851:ILE:O	16:Q:1036:ALA:HA	2.05	0.57
26:1:696:ASP:OD1	26:1:697:GLU:N	2.36	0.57
27:3:720:TRP:HE3	27:3:731:LEU:HG	1.69	0.57
37:8:45:LEU:O	37:8:48:ILE:N	2.37	0.57
1:A:2173:GLU:HG2	1:A:2174:PRO:HD2	1.87	0.57
3:C:343:LEU:HD13	3:C:373:ILE:HD11	1.87	0.57
13:N:53:HIS:NE2	13:N:85:ASP:OD2	2.35	0.57
27:3:206:GLN:NE2	27:3:232:GLY:H	2.02	0.57
27:3:475:ILE:HG23	27:3:484:VAL:HG22	1.85	0.57
36:9:281:TYR:HA	36:9:293:LEU:O	2.05	0.57
1:A:1089:CYS:SG	1:A:1096:HIS:HD2	2.28	0.57
1:A:2142:ILE:HG12	1:A:2175:LEU:HD23	1.85	0.57
1:A:2271:PHE:O	1:A:2298:LEU:HD23	2.05	0.57
10:J:360:ASP:OD1	10:J:360:ASP:N	2.33	0.57
27:3:1017:ASN:OD1	27:3:1018:GLU:HG3	2.04	0.57
3:C:465:MET:HA	3:C:498:SER:OG	2.05	0.57
7:G:101:U:C2	7:G:102:G:H8	2.22	0.57
8:H:69:U:H2'	8:H:70:C:C6	2.40	0.57
14:O:81:CYS:N	14:O:86:LEU:O	2.30	0.57
17:R:256:ASN:OD1	17:R:256:ASN:N	2.38	0.57
19:T:319:THR:O	19:T:321:ALA:N	2.38	0.57
26:1:1276:SER:O	26:1:1276:SER:OG	2.17	0.57
27:3:1199:ARG:NH2	27:3:1207:LYS:HE3	2.20	0.57
1:A:1318:THR:HB	1:A:1324:GLY:HA3	1.87	0.56
3:C:669:THR:HG22	3:C:690:GLU:HB3	1.86	0.56
6:F:49:G:N7	12:L:33:ARG:NH1	2.53	0.56
10:J:245:TRP:O	10:J:248:TYR:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:476:LEU:O	21:V:479:MET:HG3	2.06	0.56
27:3:554:VAL:HB	27:3:566:PHE:HB2	1.87	0.56
1:A:247:THR:OG1	1:A:429:ASN:OD1	2.21	0.56
1:A:837:LYS:HZ1	26:1:101:TYR:HB3	1.70	0.56
1:A:1868:MET:HE1	1:A:1872:LEU:HG	1.85	0.56
17:R:390:GLU:H	17:R:390:GLU:CD	2.09	0.56
25:Z:493:LEU:O	25:Z:496:GLN:HG2	2.06	0.56
27:3:719:SER:OG	27:3:734:LEU:HG	2.05	0.56
31:2:635:ALA:HB3	32:4:73:ILE:HA	1.86	0.56
1:A:1960:THR:O	25:Z:524:ARG:NH1	2.38	0.56
1:A:2121:ARG:O	1:A:2182:PRO:HG3	2.05	0.56
3:C:137:HIS:O	3:C:142:LYS:NZ	2.26	0.56
3:C:749:THR:HB	3:C:792:LEU:O	2.06	0.56
5:E:73:LYS:HE3	5:E:117:TYR:N	2.20	0.56
6:F:60:C:H4'	17:R:217:LYS:HD2	1.87	0.56
8:H:9:U:H2'	8:H:10:C:H6	1.70	0.56
20:U:7:LEU:HD13	20:U:10:PRO:HA	1.87	0.56
21:V:648:LYS:O	21:V:648:LYS:NZ	2.21	0.56
23:X:359:LYS:NZ	23:X:366:GLU:HB3	2.21	0.56
26:1:1076:ALA:O	26:1:1080:THR:HG22	2.05	0.56
27:3:1083:ASN:OD1	27:3:1084:GLY:N	2.39	0.56
37:8:34:LEU:HG	37:8:82:SER:HB2	1.87	0.56
1:A:1843:GLU:HB3	1:A:1875:HIS:ND1	2.20	0.56
1:A:1957:ASP:OD1	1:A:1958:LYS:N	2.38	0.56
2:B:21:A:O3'	2:B:22:U:H4'	2.06	0.56
10:J:224:LYS:HE2	10:J:255:LEU:HD13	1.87	0.56
26:1:609:MET:O	26:1:613:MET:HG2	2.04	0.56
27:3:671:ASN:O	27:3:673:VAL:HG23	2.05	0.56
36:9:237:ASN:O	36:9:266:ILE:HG22	2.06	0.56
36:9:416:ASP:O	36:9:420:ASP:N	2.27	0.56
1:A:312:TYR:OH	3:C:886:ASP:OD2	2.13	0.56
1:A:826:PRO:HG2	1:A:826:PRO:O	2.05	0.56
8:H:118:G:O2'	8:H:119:G:H5'	2.05	0.56
10:J:231:PHE:CE1	10:J:247:LYS:HG3	2.40	0.56
25:Z:507:GLN:O	25:Z:511:VAL:HG23	2.06	0.56
26:1:781:ASP:OD1	26:1:783:GLU:N	2.38	0.56
34:7:46:CYS:SG	34:7:49:CYS:N	2.66	0.56
3:C:464:ALA:HB1	3:C:473:PRO:HG3	1.88	0.56
6:F:94:C:OP1	10:J:355:ARG:NH2	2.39	0.56
27:3:931:VAL:HG23	27:3:936:LYS:HD2	1.87	0.56
1:A:796:LYS:HG3	17:R:279:HIS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:471:ASP:H	3:C:499:GLY:HA2	1.70	0.56
19:T:207:VAL:HG12	19:T:480:ALA:HB1	1.88	0.56
20:U:23:LEU:HD12	21:V:478:LYS:HB2	1.88	0.56
21:V:577:SER:O	21:V:581:ILE:HG13	2.05	0.56
1:A:191:ILE:HG13	1:A:571:ALA:HB1	1.86	0.56
1:A:1257:THR:HG22	1:A:1320:LYS:HE3	1.87	0.56
1:A:1853:PRO:HB2	1:A:1856:GLU:OE2	2.06	0.56
3:C:187:THR:HA	3:C:200:PHE:O	2.06	0.56
10:J:326:VAL:HG13	10:J:352:PHE:CZ	2.41	0.56
19:T:402:ASP:OD1	19:T:402:ASP:N	2.37	0.56
21:V:618:ARG:HB3	21:V:646:HIS:CE1	2.41	0.56
26:1:492:GLN:NE2	26:1:495:ARG:HE	2.04	0.56
27:3:226:GLU:OE1	27:3:259:LYS:HD3	2.06	0.56
32:4:77:ILE:O	32:4:84:ILE:N	2.21	0.56
1:A:698:PRO:HG2	19:T:373:LYS:NZ	2.20	0.56
1:A:770:THR:O	1:A:774:LYS:HG3	2.05	0.56
2:B:98:G:H2'	2:B:99:C:H6	1.71	0.56
21:V:543:LYS:O	21:V:547:VAL:HG23	2.05	0.56
26:1:1273:TYR:O	26:1:1277:GLN:HB3	2.06	0.56
27:3:404:LEU:HD21	27:3:438:LEU:HD11	1.87	0.56
27:3:794:SER:O	27:3:796:ASN:ND2	2.39	0.56
33:6:28:TYR:CE1	33:6:57:ARG:HG3	2.41	0.56
1:A:283:VAL:HG13	1:A:284:ARG:H	1.71	0.56
1:A:1539:SER:HB2	1:A:1569:LEU:HD11	1.88	0.56
26:1:117:ASP:OD1	26:1:120:LYS:N	2.23	0.56
1:A:1301:ILE:HD11	1:A:1306:LYS:HD3	1.87	0.55
1:A:2193:VAL:HG11	1:A:2251:TYR:HE1	1.70	0.55
5:E:65:HIS:CD2	5:E:91:LEU:HD23	2.41	0.55
26:1:153:MET:O	26:1:157:ARG:HG3	2.05	0.55
36:9:334:ASP:HB3	36:9:337:GLY:H	1.70	0.55
1:A:533:LYS:HD3	6:F:37:C:H6	1.71	0.55
8:H:63:G:N1	8:H:64:A:N6	2.52	0.55
17:R:148:ARG:HH22	17:R:152:GLU:HB2	1.71	0.55
27:3:605:LEU:HB3	27:3:617:ILE:O	2.06	0.55
1:A:701:ILE:H	1:A:701:ILE:HD12	1.71	0.55
1:A:974:ASN:OD1	1:A:1100:ARG:NH1	2.36	0.55
3:C:351:PRO:O	3:C:354:ARG:HG2	2.06	0.55
7:G:13:C:H2'	7:G:14:A:C8	2.39	0.55
8:H:63:G:H1	8:H:64:A:N6	2.04	0.55
23:X:282:LEU:N	23:X:291:ASP:OD2	2.38	0.55
27:3:240:GLY:HA2	27:3:245:PRO:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:9:370:ASN:H	36:9:394:HIS:HE1	1.53	0.55
1:A:117:PRO:HD2	1:A:131:GLU:OE1	2.06	0.55
2:B:69:A:H3'	2:B:70:A:H8	1.71	0.55
6:F:41:A:C2	7:G:7:G:C2	2.94	0.55
19:T:257:ARG:NH1	19:T:301:ASP:OD1	2.28	0.55
20:U:77:MET:O	20:U:81:GLY:N	2.40	0.55
27:3:452:LEU:HD22	27:3:762:LEU:HD22	1.87	0.55
27:3:473:TYR:CE1	27:3:486:SER:HB2	2.42	0.55
27:3:617:ILE:HG12	27:3:627:PRO:HA	1.86	0.55
36:9:282:VAL:HB	36:9:293:LEU:HD12	1.89	0.55
36:9:366:LEU:HD11	36:9:380:PHE:HD2	1.69	0.55
1:A:422:LEU:HD23	1:A:422:LEU:H	1.72	0.55
2:B:64:G:H2'	2:B:65:G:C8	2.41	0.55
3:C:227:LEU:HD22	3:C:243:ILE:HD13	1.89	0.55
3:C:811:THR:O	3:C:815:VAL:HG23	2.05	0.55
33:6:66:ASP:OD2	33:6:69:ASP:N	2.32	0.55
1:A:81:PHE:O	1:A:83:HIS:N	2.40	0.55
1:A:1258:LYS:O	1:A:1262:LYS:HG3	2.06	0.55
5:E:133:VAL:HB	5:E:147:LEU:HB2	1.89	0.55
10:J:300:ASP:HA	10:J:303:ILE:HG12	1.89	0.55
13:N:118:ILE:HD11	13:N:132:ILE:HG21	1.88	0.55
26:1:905:THR:HG22	26:1:906:GLU:H	1.71	0.55
27:3:380:GLU:O	27:3:383:ASP:N	2.39	0.55
27:3:511:LEU:HD22	27:3:517:VAL:HG23	1.89	0.55
27:3:565:TYR:OH	27:3:567:GLU:OE1	2.20	0.55
27:3:996:ILE:O	27:3:998:HIS:N	2.39	0.55
27:3:1013:ARG:HD3	27:3:1064:ASP:OD1	2.07	0.55
1:A:762:ARG:NH2	15:P:226:LYS:HZ3	2.02	0.55
1:A:957:GLN:O	1:A:961:ASN:ND2	2.37	0.55
1:A:1419:ILE:HG13	1:A:1419:ILE:O	2.05	0.55
1:A:2083:LEU:HD22	1:A:2116:CYS:HA	1.89	0.55
1:A:2113:LYS:HA	1:A:2116:CYS:SG	2.46	0.55
1:A:2127:TYR:HD2	1:A:2164:PRO:HG2	1.71	0.55
1:A:2330:ARG:NH2	1:A:2331:GLU:HG2	2.22	0.55
5:E:127:ALA:HB2	5:E:157:CYS:SG	2.47	0.55
6:F:45:A:OP2	31:2:554:ARG:NH1	2.40	0.55
11:K:207:GLU:OE2	31:2:558:ARG:NH1	2.35	0.55
17:R:198:ARG:HD2	17:R:198:ARG:O	2.07	0.55
19:T:343:PRO:HB3	19:T:365:ARG:NH1	2.21	0.55
27:3:123:VAL:HG23	27:3:130:VAL:HG12	1.88	0.55
27:3:459:VAL:HA	27:3:475:ILE:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:4:165:GLN:O	32:4:172:ILE:N	2.39	0.55
37:8:107:PRO:HA	37:8:110:LEU:HD12	1.88	0.55
1:A:1505:LYS:HG3	25:Z:615:SER:HB3	1.89	0.55
1:A:2075:VAL:O	1:A:2078:ILE:HD13	2.06	0.55
3:C:319:THR:H	3:C:322:SER:HG	1.53	0.55
14:O:167:PHE:O	14:O:172:GLU:N	2.29	0.55
27:3:720:TRP:CZ2	27:3:733:PRO:HG3	2.42	0.55
36:9:322:HIS:HB3	36:9:337:GLY:O	2.06	0.55
37:8:52:ILE:O	37:8:56:VAL:HG22	2.06	0.55
3:C:129:ILE:HD11	3:C:441:PRO:HG3	1.88	0.55
3:C:515:THR:H	3:C:518:ASP:HB3	1.70	0.55
27:3:425:VAL:HG12	27:3:427:CYS:HB2	1.89	0.55
27:3:451:GLU:HG2	27:3:761:THR:HG22	1.88	0.55
37:8:90:THR:HG23	37:8:95:GLY:HA2	1.89	0.55
21:V:525:PHE:HA	21:V:528:ILE:HB	1.89	0.55
1:A:726:TRP:O	36:9:247:SER:OG	2.24	0.54
3:C:119:LEU:HD23	3:C:123:MET:HG3	1.89	0.54
5:E:121:GLY:O	5:E:138:SER:OG	2.19	0.54
7:G:102:G:N2	7:G:103:U:H2'	2.21	0.54
8:H:135:C:H2'	8:H:136:G:C8	2.42	0.54
10:J:241:VAL:HG22	10:J:243:SER:H	1.72	0.54
10:J:391:TYR:HB3	10:J:394:HIS:ND1	2.22	0.54
26:1:972:GLY:HA2	26:1:1010:THR:HG21	1.88	0.54
27:3:77:TYR:HD1	27:3:91:GLU:HB2	1.71	0.54
1:A:436:PRO:HB2	1:A:439:GLN:CD	2.27	0.54
1:A:1339:ASP:OD1	1:A:1339:ASP:N	2.40	0.54
1:A:2108:LYS:N	1:A:2264:SER:O	2.37	0.54
1:A:2236:GLU:O	1:A:2239:ARG:HD3	2.08	0.54
10:J:332:VAL:HA	10:J:335:ARG:HD2	1.89	0.54
11:K:163:MET:SD	21:V:479:MET:HB3	2.48	0.54
14:O:35:ARG:HA	17:R:198:ARG:NH1	2.23	0.54
16:Q:408:VAL:O	16:Q:412:GLU:CB	2.56	0.54
19:T:335:THR:HG21	19:T:378:VAL:HG13	1.88	0.54
26:1:565:ASP:O	26:1:568:ARG:HG3	2.07	0.54
1:A:1379:PHE:O	1:A:1383:GLN:HG2	2.07	0.54
2:B:63:A:H2'	2:B:64:G:H8	1.71	0.54
3:C:85:ASP:OD1	3:C:85:ASP:N	2.33	0.54
6:F:84:A:C1'	6:F:85:U:H5'	2.37	0.54
8:H:8:C:H2'	8:H:9:U:H6	1.73	0.54
16:Q:1270:TYR:HA	16:Q:1300:GLY:O	2.07	0.54
19:T:342:GLU:HG2	19:T:343:PRO:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1140:GLU:HB2	26:1:1143:VAL:HG13	1.89	0.54
26:1:1303:ILE:HD11	27:3:989:TYR:HE2	1.72	0.54
27:3:727:SER:O	27:3:728:ARG:HD2	2.07	0.54
31:2:664:GLY:H	31:2:671:GLY:N	2.05	0.54
15:P:196:ASN:OD1	15:P:198:ALA:N	2.34	0.54
17:R:253:ASN:HB3	17:R:254:TRP:CE3	2.43	0.54
27:3:418:GLU:HG3	27:3:420:THR:H	1.73	0.54
27:3:587:VAL:HA	27:3:608:GLY:O	2.08	0.54
1:A:985:TYR:CD1	1:A:985:TYR:N	2.75	0.54
3:C:595:VAL:HG23	3:C:596:ASN:ND2	2.22	0.54
8:H:15:U:O2'	8:H:16:U:H5'	2.07	0.54
8:H:69:U:H2'	8:H:70:C:H6	1.72	0.54
11:K:154:ARG:O	11:K:158:ASN:ND2	2.35	0.54
19:T:198:ARG:HH12	19:T:235:SER:HA	1.73	0.54
27:3:488:GLY:H	27:3:491:VAL:HG22	1.72	0.54
27:3:1210:ASP:O	27:3:1214:ARG:HG2	2.07	0.54
33:6:111:LYS:NZ	33:6:115:GLU:HG3	2.22	0.54
4:D:2066:VAL:HA	4:D:2107:TYR:O	2.07	0.54
8:H:162:U:H4'	8:H:163:G:H5'	1.89	0.54
23:X:239:PHE:CE2	23:X:240:ARG:HG3	2.42	0.54
27:3:895:ARG:HH21	27:3:895:ARG:HG3	1.73	0.54
37:8:30:PHE:CE1	37:8:83:LYS:HD2	2.43	0.54
1:A:134:TRP:HB3	1:A:418:THR:CG2	2.37	0.54
1:A:893:GLU:OE1	1:A:893:GLU:N	2.40	0.54
1:A:1206:GLU:HG2	1:A:1207:PHE:N	2.23	0.54
4:D:530:THR:C	4:D:532:ASN:H	2.10	0.54
27:3:458:ALA:HB1	27:3:460:TRP:CZ3	2.43	0.54
1:A:1318:THR:HG23	1:A:1484:ILE:HD13	1.89	0.54
1:A:1554:GLN:HG3	1:A:1561:PHE:CE1	2.42	0.54
1:A:2229:LYS:N	1:A:2257:GLU:O	2.31	0.54
6:F:30:A:N6	7:G:16:G:H1'	2.21	0.54
6:F:81:C:N4	8:H:18:U:H3	2.04	0.54
26:1:977:VAL:O	26:1:981:TYR:HD2	1.91	0.54
31:2:547:LYS:NZ	31:2:555:GLU:OE2	2.20	0.54
1:A:545:HIS:O	1:A:549:GLU:HG2	2.08	0.54
8:H:7:U:H2'	8:H:8:C:H6	1.73	0.54
26:1:1185:ARG:HH11	31:2:511:LEU:HD12	1.73	0.54
27:3:68:PHE:HB2	27:3:123:VAL:HG21	1.90	0.54
37:8:28:LEU:HB3	37:8:30:PHE:CE2	2.43	0.54
1:A:1640:SER:OG	1:A:1641:ARG:N	2.41	0.54
1:A:1953:ILE:HD13	1:A:1982:GLN:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2006:GLU:O	1:A:2010:ILE:HG13	2.08	0.54
1:A:2188:LEU:O	1:A:2251:TYR:OH	2.26	0.54
3:C:213:ASP:OD1	3:C:213:ASP:N	2.39	0.54
3:C:350:ASN:O	3:C:353:THR:OG1	2.25	0.54
7:G:99:C:H42	8:H:32:U:H3	1.55	0.54
8:H:70:C:H2'	8:H:71:C:C5	2.43	0.54
8:H:182:U:H2'	8:H:183:G:H8	1.72	0.54
21:V:494:LEU:HD12	21:V:528:ILE:HD13	1.89	0.54
26:1:967:GLU:O	26:1:971:MET:HB3	2.08	0.54
27:3:943:THR:HG21	27:3:977:LEU:HB2	1.89	0.54
31:2:451:LYS:O	31:2:455:ARG:HD2	2.07	0.54
1:A:467:GLN:HG2	2:B:20:G:H21	1.73	0.53
1:A:919:ASP:OD2	1:A:1012:LYS:NZ	2.40	0.53
3:C:93:ILE:HD12	19:T:275:LEU:HD22	1.89	0.53
17:R:322:GLU:OE2	17:R:325:ARG:NH1	2.41	0.53
26:1:1118:ILE:O	26:1:1122:THR:HG23	2.08	0.53
27:3:1058:LEU:HD22	27:3:1062:THR:HG21	1.90	0.53
1:A:109:PRO:HD3	1:A:630:TRP:CZ2	2.43	0.53
1:A:533:LYS:HZ2	1:A:533:LYS:CB	2.21	0.53
3:C:508:LYS:HG3	3:C:524:ILE:HG22	1.89	0.53
3:C:696:LEU:O	3:C:699:ASP:N	2.41	0.53
7:G:12:G:H3'	7:G:13:C:C5	2.43	0.53
17:R:139:ALA:O	17:R:143:ILE:HG13	2.07	0.53
26:1:949:GLN:O	26:1:949:GLN:HG2	2.06	0.53
36:9:338:THR:HA	36:9:421:ARG:NH2	2.22	0.53
1:A:533:LYS:CB	1:A:533:LYS:NZ	2.72	0.53
3:C:496:VAL:HG11	3:C:501:ILE:HD12	1.90	0.53
4:D:620:LEU:HA	4:D:625:GLY:HA3	1.89	0.53
6:F:1:G:H2'	6:F:2:U:C6	2.43	0.53
8:H:47:U:H4'	8:H:48:A:OP1	2.08	0.53
10:J:294:HIS:HA	10:J:297:ASN:HD22	1.73	0.53
17:R:279:HIS:HB3	36:9:225:MET:HG2	1.89	0.53
25:Z:590:SER:OG	25:Z:591:ASN:N	2.39	0.53
36:9:296:HIS:HB2	36:9:299:LEU:HG	1.91	0.53
36:9:322:HIS:CE1	36:9:332:GLY:HA2	2.43	0.53
1:A:60:ASP:OD1	1:A:60:ASP:N	2.42	0.53
1:A:807:VAL:HG12	36:9:204:THR:HG23	1.90	0.53
1:A:1309:SER:OG	1:A:1547:VAL:HG11	2.07	0.53
1:A:2072:GLU:HA	1:A:2075:VAL:HG22	1.91	0.53
1:A:2130:GLY:H	1:A:2172:MET:HB3	1.73	0.53
3:C:465:MET:HE2	3:C:475:MET:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:393:ASP:OD1	19:T:393:ASP:N	2.41	0.53
21:V:481:PHE:CD2	21:V:485:GLN:HB2	2.44	0.53
21:V:628:ILE:O	21:V:632:THR:OG1	2.27	0.53
26:1:1113:THR:HG21	26:1:1149:LYS:HG2	1.90	0.53
33:6:46:ARG:HB3	33:6:63:VAL:HG12	1.89	0.53
1:A:191:ILE:O	1:A:191:ILE:HG22	2.09	0.53
1:A:1217:GLN:HE21	1:A:1222:LYS:HD2	1.72	0.53
3:C:605:ASP:O	3:C:609:LYS:HG3	2.09	0.53
5:E:234:HIS:ND1	5:E:256:ASP:OD2	2.41	0.53
10:J:250:GLN:O	10:J:254:SER:HB2	2.09	0.53
11:K:125:GLU:OE2	11:K:127:GLU:HB2	2.09	0.53
24:Y:87:GLN:HE22	24:Y:91:ILE:HD11	1.73	0.53
1:A:1258:LYS:HG2	17:R:428:GLU:HB2	1.90	0.53
3:C:724:TRP:HE1	3:C:732:ILE:HD11	1.74	0.53
6:F:3:G:H2'	6:F:4:C:C6	2.43	0.53
11:K:129:ASP:OD1	11:K:130:ALA:N	2.41	0.53
11:K:162:TYR:OH	21:V:485:GLN:NE2	2.42	0.53
14:O:36:MET:HA	14:O:56:ARG:O	2.09	0.53
21:V:581:ILE:HG12	25:Z:543:ASP:HB2	1.90	0.53
26:1:1091:HIS:HE2	31:2:568:TYR:HH	1.57	0.53
27:3:232:GLY:HA2	27:3:252:SER:HA	1.91	0.53
27:3:565:TYR:HB3	27:3:577:TYR:HB3	1.90	0.53
27:3:607:VAL:HB	27:3:615:ARG:HB3	1.89	0.53
27:3:804:HIS:NE2	27:3:859:ASN:O	2.42	0.53
1:A:985:TYR:HD2	1:A:1032:ARG:HE	1.55	0.53
1:A:2177:TRP:CZ3	1:A:2179:HIS:HB3	2.44	0.53
2:B:39:C:H4'	2:B:40:U:OP1	2.07	0.53
4:D:1459:ILE:HA	4:D:1464:GLY:HA3	1.89	0.53
7:G:12:G:H3'	7:G:13:C:C6	2.43	0.53
8:H:9:U:H2'	8:H:10:C:C6	2.44	0.53
9:I:550:TRP:O	9:I:552:ASN:N	2.42	0.53
26:1:1134:ASN:ND2	31:2:534:GLN:HA	2.24	0.53
27:3:278:LEU:HD23	27:3:815:ARG:HD3	1.91	0.53
36:9:285:HIS:NE2	36:9:432:THR:OG1	2.15	0.53
36:9:360:HIS:NE2	36:9:396:ILE:HG12	2.24	0.53
1:A:1783:THR:HG22	1:A:1865:ARG:HG3	1.91	0.53
8:H:8:C:H2'	8:H:9:U:C6	2.44	0.53
23:X:372:GLU:HG2	23:X:373:SER:N	2.23	0.53
27:3:68:PHE:CZ	27:3:144:LEU:HD13	2.43	0.53
36:9:330:ILE:HB	36:9:384:PHE:HZ	1.74	0.53
1:A:58:LYS:HA	13:N:107:GLN:NE2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1641:ARG:NH1	1:A:1651:VAL:O	2.42	0.53
11:K:137:SER:O	11:K:141:GLN:HG2	2.09	0.53
13:N:118:ILE:HA	13:N:121:VAL:HG23	1.90	0.53
26:1:130:PRO:HG2	26:1:150:ARG:HD2	1.90	0.53
1:A:1119:ASP:OD1	1:A:1123:GLU:HG3	2.08	0.53
1:A:2163:LEU:HD22	1:A:2164:PRO:HD2	1.91	0.53
1:A:2274:PRO:HA	1:A:2296:LEU:HA	1.90	0.53
1:A:2289:ASP:HB3	1:A:2292:MET:HG2	1.89	0.53
5:E:335:PHE:CE2	5:E:342:ILE:HD11	2.44	0.53
10:J:265:TYR:HB3	10:J:282:TYR:CZ	2.43	0.53
11:K:131:GLN:NE2	11:K:184:ARG:H	2.07	0.53
26:1:1114:VAL:O	26:1:1114:VAL:HG12	2.09	0.53
1:A:325:HIS:HD2	1:A:326:HIS:CD2	2.26	0.52
1:A:1552:GLN:HE21	11:K:193:VAL:HG22	1.73	0.52
3:C:302:PRO:HA	3:C:307:VAL:HB	1.90	0.52
6:F:43:A:N6	6:F:44:G:O6	2.41	0.52
6:F:59:G:N2	6:F:76:A:N1	2.51	0.52
24:Y:2:ASN:HD22	24:Y:2:ASN:H	1.56	0.52
27:3:214:ASP:O	27:3:218:ASN:N	2.35	0.52
27:3:1102:LEU:HD12	27:3:1122:LEU:HD12	1.90	0.52
36:9:320:ILE:HG22	36:9:427:ARG:HB2	1.91	0.52
5:E:316:SER:O	5:E:317:ARG:HG3	2.08	0.52
19:T:243:THR:O	19:T:243:THR:OG1	2.24	0.52
21:V:641:ASP:HA	21:V:644:ARG:CD	2.38	0.52
27:3:383:ASP:OD1	27:3:384:THR:N	2.42	0.52
27:3:947:GLU:HG3	27:3:948:VAL:N	2.24	0.52
1:A:363:HIS:CD2	3:C:284:GLU:HA	2.44	0.52
3:C:369:PHE:CD1	3:C:373:ILE:HD12	2.43	0.52
6:F:36:A:C6	7:G:10:U:O4	2.63	0.52
27:3:91:GLU:HB3	27:3:102:ILE:HD11	1.91	0.52
27:3:569:ASP:N	27:3:573:GLN:O	2.39	0.52
27:3:983:ASN:OD1	27:3:984:LYS:N	2.43	0.52
1:A:2146:VAL:HG13	1:A:2272:MET:HG2	1.90	0.52
1:A:2330:ARG:HD3	1:A:2330:ARG:N	2.24	0.52
3:C:177:ARG:NH2	3:C:638:ASP:OD2	2.42	0.52
3:C:841:ASP:OD2	3:C:841:ASP:N	2.39	0.52
10:J:238:ASN:C	10:J:240:THR:H	2.12	0.52
10:J:244:ASN:HA	10:J:247:LYS:NZ	2.24	0.52
26:1:1103:VAL:HG23	26:1:1109:ARG:HG3	1.91	0.52
34:7:46:CYS:HB3	34:7:85:CYS:CB	2.38	0.52
1:A:1376:GLU:O	1:A:1380:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1527:ASN:HD22	11:K:215:ASP:HB3	1.73	0.52
1:A:2196:HIS:CG	1:A:2213:ILE:HD11	2.43	0.52
1:A:2280:ASN:OD1	1:A:2282:ASN:ND2	2.32	0.52
3:C:264:ILE:HG12	3:C:378:TYR:CE1	2.44	0.52
16:Q:1059:ILE:O	16:Q:1091:TRP:HA	2.10	0.52
23:X:270:LEU:HB3	23:X:271:PRO:HD2	1.91	0.52
26:1:1260:LYS:O	26:1:1264:VAL:HG23	2.09	0.52
27:3:463:ARG:HG3	27:3:471:ASP:HA	1.90	0.52
27:3:727:SER:O	27:3:727:SER:OG	2.22	0.52
36:9:287:ASN:HD21	36:9:426:ILE:HG12	1.74	0.52
1:A:1541:THR:O	1:A:1544:ARG:HG2	2.10	0.52
1:A:1548:TYR:HE2	1:A:1550:GLY:HA2	1.73	0.52
1:A:1570:LYS:HZ3	1:A:1574:ILE:HD12	1.74	0.52
1:A:2106:LEU:HD21	1:A:2111:LEU:HB2	1.91	0.52
1:A:2304:PHE:HB3	1:A:2305:TYR:CD2	2.45	0.52
3:C:614:TYR:OH	3:C:643:ASP:OD2	2.10	0.52
5:E:86:PHE:HA	5:E:111:ALA:HB1	1.91	0.52
8:H:162:U:H4'	8:H:163:G:C5'	2.38	0.52
10:J:293:ASN:HA	10:J:296:ARG:HD2	1.91	0.52
12:L:98:GLU:O	12:L:101:GLU:HG3	2.09	0.52
13:N:29:MET:HB2	13:N:52:ILE:HG21	1.91	0.52
1:A:359:ILE:HA	3:C:864:PRO:HB2	1.92	0.52
1:A:1802:PRO:HB3	1:A:1827:TRP:CZ3	2.45	0.52
1:A:2228:TYR:CD1	1:A:2228:TYR:N	2.78	0.52
3:C:370:VAL:HA	3:C:374:LEU:HB2	1.90	0.52
6:F:10:U:C2	6:F:11:C:H1'	2.44	0.52
8:H:7:U:H2'	8:H:8:C:C6	2.45	0.52
8:H:12:G:H2'	8:H:13:C:C2	2.45	0.52
19:T:381:HIS:HD2	19:T:441:TRP:NE1	2.08	0.52
27:3:162:LYS:HG2	27:3:165:THR:HG21	1.92	0.52
27:3:705:ARG:NH2	27:3:708:GLY:H	2.05	0.52
27:3:707:GLN:HB2	27:3:770:LEU:HD12	1.91	0.52
35:5:3:ASP:HA	35:5:6:THR:HG22	1.92	0.52
36:9:292:ASN:O	36:9:400:VAL:HA	2.09	0.52
36:9:295:LEU:HD22	36:9:397:PHE:O	2.09	0.52
1:A:158:ARG:HH12	1:A:573:GLN:HE21	1.58	0.52
1:A:1393:ARG:NH1	26:1:90:LEU:HD22	2.25	0.52
3:C:215:VAL:HG11	3:C:242:LEU:CD2	2.40	0.52
6:F:87:C:H2'	6:F:88:G:O4'	2.10	0.52
6:F:93:G:H2'	6:F:94:C:C6	2.44	0.52
10:J:375:ASP:HB3	10:J:377:LYS:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:191:HIS:NE2	19:T:440:ASP:OD1	2.43	0.52
27:3:263:ASP:OD1	27:3:263:ASP:N	2.43	0.52
1:A:1147:VAL:O	1:A:1151:ARG:HG3	2.10	0.52
1:A:1602:ASP:O	1:A:1605:GLU:N	2.39	0.52
1:A:1972:THR:N	1:A:1975:GLU:OE1	2.18	0.52
3:C:112:THR:O	3:C:112:THR:OG1	2.20	0.52
3:C:758:LEU:O	3:C:762:VAL:HG22	2.10	0.52
6:F:84:A:H4'	6:F:85:U:OP1	2.09	0.52
21:V:620:ASN:ND2	21:V:623:ASN:OD1	2.33	0.52
21:V:630:PHE:HE2	25:Z:544:PRO:HD2	1.75	0.52
1:A:1136:ARG:HA	1:A:1139:ARG:HH11	1.75	0.52
1:A:1833:LEU:HD23	1:A:1833:LEU:H	1.74	0.52
1:A:1876:LEU:HD12	1:A:1884:ILE:HD11	1.92	0.52
1:A:2109:ASN:O	1:A:2112:LYS:HB2	2.09	0.52
2:B:97:G:N2	2:B:117:A:H62	2.07	0.52
3:C:218:GLY:O	3:C:222:SER:HB3	2.10	0.52
8:H:155:C:N3	8:H:176:G:N2	2.57	0.52
10:J:434:VAL:O	10:J:438:TYR:HB3	2.10	0.52
18:S:767:LEU:O	18:S:772:ILE:N	2.38	0.52
26:1:1179:ASP:H	31:2:511:LEU:HD13	1.74	0.52
27:3:485:LEU:HG	27:3:493:GLU:HA	1.92	0.52
1:A:1209:HIS:CG	1:A:1210:LYS:N	2.78	0.51
1:A:1792:LYS:HA	1:A:1798:LEU:HA	1.91	0.51
1:A:2305:TYR:HD1	1:A:2310:ARG:NH1	2.08	0.51
3:C:801:LEU:HB2	3:C:803:ARG:HD3	1.91	0.51
3:C:919:ARG:HD2	3:C:922:GLU:OE1	2.10	0.51
5:E:150:HIS:CE1	5:E:177:LYS:HG3	2.45	0.51
8:H:50:C:C2	8:H:64:A:N6	2.75	0.51
26:1:770:MET:HE2	26:1:795:CYS:SG	2.50	0.51
27:3:463:ARG:NE	27:3:468:ASP:O	2.42	0.51
27:3:697:ARG:HH21	27:3:717:SER:HB3	1.75	0.51
27:3:712:VAL:HG22	27:3:722:SER:HB3	1.91	0.51
27:3:828:GLY:O	27:3:834:LEU:N	2.43	0.51
33:6:43:GLY:HA3	33:6:69:ASP:OD2	2.09	0.51
36:9:285:HIS:ND1	36:9:290:ASP:OD1	2.43	0.51
36:9:318:GLY:HA2	36:9:427:ARG:HD2	1.93	0.51
37:8:57:THR:HG22	37:8:63:GLU:HA	1.91	0.51
1:A:309:ARG:HG2	1:A:309:ARG:HH11	1.75	0.51
1:A:348:PRO:HG2	1:A:351:TYR:HB2	1.92	0.51
2:B:107:U:H2'	2:B:108:G:O4'	2.10	0.51
3:C:223:ASP:OD1	3:C:495:ARG:NH2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1199:LYS:HA	4:D:1255:PHE:HA	1.92	0.51
7:G:22:C:HO2'	7:G:23:U:P	2.32	0.51
8:H:179:C:N4	8:H:180:G:O6	2.43	0.51
10:J:272:ASP:OD1	10:J:274:ARG:N	2.39	0.51
24:Y:96:ASN:HD21	25:Z:594:GLU:HG2	1.76	0.51
26:1:584:ASP:OD1	26:1:585:GLU:N	2.42	0.51
33:6:104:LYS:O	33:6:107:GLU:HG2	2.09	0.51
1:A:1129:ASN:N	1:A:1129:ASN:OD1	2.44	0.51
3:C:674:CYS:HB2	3:C:822:MET:SD	2.51	0.51
5:E:133:VAL:HG21	5:E:169:THR:HG21	1.93	0.51
14:O:32:PRO:HA	17:R:195:ARG:HH12	1.76	0.51
27:3:19:HIS:HD2	27:3:340:CYS:SG	2.34	0.51
27:3:902:ASP:OD2	27:3:929:LYS:NZ	2.41	0.51
31:2:539:ALA:O	31:2:542:GLU:HG3	2.10	0.51
31:2:635:ALA:CB	32:4:73:ILE:HA	2.40	0.51
36:9:358:LEU:HD13	36:9:396:ILE:HG13	1.91	0.51
1:A:143:GLN:NE2	1:A:207:PHE:O	2.43	0.51
3:C:126:SER:O	3:C:126:SER:OG	2.24	0.51
3:C:931:ARG:NE	3:C:935:ILE:HD11	2.25	0.51
27:3:675:LEU:HA	27:3:687:SER:O	2.11	0.51
36:9:329:VAL:HG12	36:9:383:THR:HG22	1.92	0.51
1:A:156:ARG:NE	1:A:157:ASP:OD1	2.42	0.51
1:A:750:TRP:CZ2	1:A:778:ARG:HG2	2.45	0.51
5:E:165:GLN:HB3	5:E:181:ILE:HD11	1.93	0.51
10:J:329:ALA:O	10:J:332:VAL:HG22	2.11	0.51
11:K:159:TYR:CZ	21:V:450:ILE:HG21	2.46	0.51
13:N:6:ARG:HG2	13:N:6:ARG:HH11	1.76	0.51
13:N:38:GLU:C	13:N:40:LYS:H	2.13	0.51
26:1:475:PHE:HB3	26:1:478:LEU:HD12	1.93	0.51
27:3:574:LEU:H	27:3:574:LEU:HD22	1.75	0.51
27:3:609:LEU:HB2	27:3:611:ASP:HB3	1.92	0.51
27:3:943:THR:HB	27:3:976:LYS:HB2	1.91	0.51
1:A:467:GLN:HG2	2:B:20:G:N2	2.25	0.51
3:C:277:LYS:HD2	3:C:865:GLY:HA3	1.92	0.51
3:C:481:MET:SD	3:C:559:ILE:HD11	2.51	0.51
5:E:234:HIS:CE1	5:E:260:ARG:HG2	2.45	0.51
6:F:35:A:C6	6:F:36:A:N6	2.79	0.51
17:R:195:ARG:HH11	17:R:195:ARG:HG2	1.76	0.51
17:R:332:ARG:NH2	23:X:366:GLU:OE1	2.44	0.51
27:3:695:GLY:HA3	27:3:717:SER:OG	2.11	0.51
27:3:876:THR:O	27:3:876:THR:OG1	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:4:167:LEU:H	32:4:171:PRO:HA	1.75	0.51
1:A:170:ASP:OD1	1:A:171:ASP:N	2.42	0.51
1:A:227:ARG:NH2	1:A:415:SER:OG	2.44	0.51
1:A:381:PRO:HG2	3:C:334:ILE:HG22	1.92	0.51
1:A:1458:GLN:OE1	17:R:421:GLY:HA3	2.10	0.51
1:A:1520:ASN:ND2	6:F:51:U:O2	2.44	0.51
1:A:1835:GLN:O	1:A:1839:TRP:HD1	1.93	0.51
1:A:2222:SER:OG	1:A:2223:CYS:N	2.43	0.51
3:C:350:ASN:HD22	3:C:353:THR:HG23	1.75	0.51
3:C:677:GLU:N	3:C:677:GLU:OE2	2.43	0.51
3:C:933:PHE:O	3:C:937:THR:OG1	2.27	0.51
5:E:192:ASN:HB3	5:E:220:TRP:CH2	2.46	0.51
26:1:592:GLU:O	26:1:596:ILE:HG23	2.11	0.51
26:1:718:PRO:O	26:1:719:TYR:CG	2.64	0.51
27:3:75:LYS:NZ	27:3:92:TYR:O	2.44	0.51
27:3:745:PHE:HE2	27:3:750:CYS:HB3	1.75	0.51
27:3:910:ALA:HB2	27:3:948:VAL:HB	1.92	0.51
1:A:1591:MET:O	1:A:1595:GLN:HG3	2.11	0.51
2:B:115:C:H2'	2:B:116:U:O4'	2.11	0.51
5:E:259:VAL:O	5:E:260:ARG:HD3	2.11	0.51
7:G:-7:U:H2'	7:G:-6:C:O4'	2.10	0.51
10:J:411:MET:HG3	10:J:415:LEU:HD23	1.93	0.51
21:V:622:ARG:HA	21:V:625:ARG:HH21	1.76	0.51
27:3:155:SER:OG	27:3:156:SER:N	2.40	0.51
27:3:873:GLN:O	27:3:875:ASN:ND2	2.43	0.51
1:A:409:ARG:HD2	1:A:409:ARG:C	2.30	0.51
1:A:1209:HIS:ND1	1:A:1210:LYS:N	2.58	0.51
1:A:1766:GLN:HG3	1:A:1767:ASN:H	1.76	0.51
1:A:1926:THR:O	1:A:1926:THR:OG1	2.26	0.51
1:A:2237:TRP:CH2	1:A:2251:TYR:HB2	2.46	0.51
6:F:38:G:H8	6:F:38:G:OP2	1.94	0.51
36:9:307:PHE:CD1	36:9:397:PHE:HE2	2.29	0.51
37:8:68:ILE:HG22	37:8:72:PHE:CE2	2.46	0.51
10:J:232:GLU:O	10:J:236:ARG:CB	2.58	0.51
27:3:664:TYR:HA	27:3:677:THR:O	2.11	0.51
27:3:946:GLU:OE2	27:3:968:ARG:NH1	2.44	0.51
1:A:1609:VAL:HG22	1:A:1631:LEU:HD22	1.93	0.50
1:A:2228:TYR:HA	1:A:2258:ARG:HA	1.94	0.50
2:B:20:G:H4'	2:B:20:G:OP1	2.11	0.50
3:C:209:VAL:HG21	3:C:237:LEU:HD23	1.92	0.50
3:C:829:GLU:HB3	3:C:907:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:961:THR:O	18:S:965:GLN:N	2.43	0.50
21:V:636:LEU:O	21:V:640:THR:OG1	2.24	0.50
26:1:967:GLU:HB3	26:1:970:LEU:HB3	1.92	0.50
27:3:1158:ARG:HG3	27:3:1159:ASP:H	1.75	0.50
31:2:485:PRO:O	31:2:489:VAL:HG23	2.10	0.50
36:9:242:SER:OG	36:9:243:THR:N	2.44	0.50
36:9:283:ARG:HG2	36:9:434:PHE:CE1	2.46	0.50
1:A:550:VAL:O	1:A:554:THR:HG22	2.12	0.50
1:A:789:GLU:HB2	36:9:253:THR:HB	1.92	0.50
1:A:1570:LYS:NZ	1:A:1574:ILE:HD12	2.26	0.50
1:A:1819:LEU:HD11	1:A:1906:ILE:HD11	1.94	0.50
21:V:588:GLN:O	21:V:592:GLU:HG2	2.10	0.50
27:3:328:LYS:NZ	27:3:365:GLY:O	2.43	0.50
1:A:123:THR:O	1:A:123:THR:OG1	2.23	0.50
1:A:464:PRO:O	1:A:466:ALA:N	2.43	0.50
4:D:1223:ILE:HA	4:D:1269:ARG:O	2.11	0.50
5:E:342:ILE:HG13	5:E:356:ILE:HD11	1.94	0.50
8:H:5:C:H2'	8:H:6:U:C6	2.46	0.50
17:R:402:SER:OG	17:R:403:ASN:N	2.44	0.50
26:1:473:GLN:NE2	33:6:93:ASN:HB2	2.27	0.50
27:3:705:ARG:HH12	27:3:709:GLN:H	1.59	0.50
33:6:28:TYR:CD1	33:6:57:ARG:HG3	2.47	0.50
36:9:323:ARG:HB3	36:9:331:GLN:HB3	1.93	0.50
1:A:1575:GLN:HB2	11:K:220:LEU:HD11	1.93	0.50
1:A:1843:GLU:HB3	1:A:1875:HIS:CE1	2.47	0.50
1:A:2176:GLY:HA2	1:A:2206:TRP:CZ2	2.46	0.50
2:B:67:A:H2'	2:B:68:C:C6	2.46	0.50
3:C:352:LYS:HD3	3:C:352:LYS:N	2.27	0.50
10:J:220:LEU:CD1	10:J:224:LYS:HD2	2.41	0.50
10:J:406:PHE:HB3	10:J:411:MET:HB2	1.93	0.50
13:N:72:ARG:HH11	13:N:72:ARG:HG3	1.77	0.50
19:T:297:HIS:HB2	19:T:302:VAL:HG22	1.92	0.50
26:1:911:LEU:HD23	26:1:957:ARG:HE	1.76	0.50
26:1:969:LYS:O	26:1:973:HIS:HB2	2.11	0.50
27:3:1035:THR:HG22	27:3:1047:ALA:HB3	1.92	0.50
1:A:43:LYS:NZ	6:F:21:U:H3	2.09	0.50
1:A:147:MET:O	1:A:151:MET:HG3	2.10	0.50
1:A:945:THR:OG1	1:A:946:GLU:HG3	2.11	0.50
1:A:2191:GLN:NE2	1:A:2246:ASN:OD1	2.39	0.50
1:A:2206:TRP:CG	1:A:2211:THR:HG21	2.46	0.50
1:A:2249:LYS:H	1:A:2249:LYS:HD2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:240:GLU:O	3:C:243:ILE:HG22	2.12	0.50
5:E:318:ARG:HB3	5:E:318:ARG:NH1	2.26	0.50
8:H:22:U:O2'	8:H:23:A:H8	1.95	0.50
10:J:303:ILE:HD12	10:J:313:TRP:CZ3	2.46	0.50
23:X:277:ARG:NH2	26:1:437:PRO:CB	2.67	0.50
26:1:699:GLN:HE22	26:1:738:HIS:CE1	2.29	0.50
26:1:1179:ASP:HB2	26:1:1185:ARG:NH1	2.26	0.50
27:3:478:PHE:HB2	27:3:481:ALA:H	1.76	0.50
27:3:515:ALA:HB2	27:3:528:ARG:NH2	2.27	0.50
27:3:704:VAL:HG21	27:3:754:ILE:HD11	1.93	0.50
3:C:753:GLU:O	3:C:756:LYS:HG3	2.11	0.50
8:H:11:G:C2	8:H:12:G:N7	2.80	0.50
10:J:326:VAL:HA	10:J:329:ALA:HB3	1.94	0.50
11:K:208:THR:HB	31:2:557:VAL:HG22	1.94	0.50
26:1:1195:MET:O	26:1:1199:VAL:HG23	2.10	0.50
35:5:15:GLN:O	35:5:18:TYR:C	2.50	0.50
36:9:282:VAL:HG22	36:9:433:VAL:HA	1.94	0.50
36:9:367:SER:HB2	36:9:394:HIS:HB3	1.94	0.50
1:A:1424:GLN:O	1:A:1427:ARG:NH2	2.44	0.50
1:A:1962:THR:HG21	25:Z:523:ALA:HB1	1.93	0.50
3:C:916:ILE:HB	3:C:931:ARG:HG2	1.93	0.50
4:D:1197:THR:HA	4:D:1257:PRO:HA	1.93	0.50
5:E:84:ALA:HB2	5:E:90:ILE:HG12	1.94	0.50
8:H:140:A:H2'	8:H:141:C:C6	2.46	0.50
27:3:50:VAL:HG21	27:3:401:LEU:HD11	1.94	0.50
27:3:80:VAL:HG11	27:3:1156:CYS:SG	2.51	0.50
36:9:323:ARG:HE	36:9:325:ILE:HD11	1.75	0.50
1:A:2209:GLU:O	1:A:2209:GLU:HG2	2.10	0.50
5:E:192:ASN:HB3	5:E:220:TRP:HH2	1.77	0.50
7:G:-11:G:HO2'	7:G:-10:G:C1'	2.24	0.50
7:G:19:G:H2'	7:G:20:A:C8	2.47	0.50
16:Q:1273:LEU:O	16:Q:1303:ILE:HA	2.11	0.50
18:S:615:LEU:N	18:S:673:ALA:O	2.41	0.50
21:V:518:LYS:HE2	21:V:520:GLU:OE1	2.11	0.50
27:3:940:LEU:HB3	27:3:941:HIS:ND1	2.27	0.50
33:6:44:PRO:HB2	33:6:65:GLU:HG3	1.93	0.50
36:9:415:SER:HB3	36:9:420:ASP:HA	1.94	0.50
3:C:129:ILE:HA	3:C:199:LEU:O	2.11	0.50
3:C:495:ARG:HB3	3:C:549:TRP:CD1	2.47	0.50
4:D:688:THR:O	4:D:868:ILE:HA	2.12	0.50
6:F:21:U:C4	13:N:125:LYS:HE3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:188:PRO:HG2	19:T:502:VAL:HG11	1.93	0.50
26:1:732:TRP:HE1	26:1:768:GLU:HG2	1.77	0.50
27:3:147:ASP:OD1	27:3:151:ARG:N	2.41	0.50
27:3:635:ALA:HB3	27:3:669:LEU:HD13	1.93	0.50
1:A:643:GLY:O	1:A:646:PRO:HD2	2.11	0.49
1:A:748:ASP:OD2	19:T:484:LYS:NZ	2.37	0.49
1:A:1361:GLU:HG2	1:A:1362:ASP:H	1.77	0.49
1:A:1814:THR:OG1	1:A:1816:GLN:HB2	2.12	0.49
1:A:2111:LEU:HG	1:A:2115:ILE:HD12	1.94	0.49
7:G:8:C:C4	7:G:9:C:N4	2.80	0.49
10:J:291:GLN:HB3	10:J:294:HIS:ND1	2.26	0.49
27:3:394:ASN:OD1	27:3:394:ASN:N	2.45	0.49
1:A:793:ASN:HD22	3:C:60:HIS:CE1	2.30	0.49
1:A:1333:VAL:HG11	21:V:467:LEU:HD22	1.93	0.49
16:Q:28:CYS:HA	16:Q:32:ALA:HB3	1.94	0.49
26:1:626:ASN:OD1	26:1:630:ARG:NH1	2.45	0.49
27:3:673:VAL:HA	27:3:690:ARG:HA	1.94	0.49
31:2:601:LEU:HD12	31:2:602:LYS:H	1.77	0.49
1:A:325:HIS:CD2	1:A:326:HIS:HD2	2.28	0.49
1:A:406:TRP:HH2	3:C:265:LEU:O	1.95	0.49
1:A:1607:GLU:HG2	1:A:1608:THR:OG1	2.13	0.49
1:A:1745:GLU:OE2	26:1:980:GLU:HB3	2.12	0.49
2:B:64:G:H2'	2:B:65:G:H8	1.77	0.49
3:C:125:ASN:ND2	3:C:128:LEU:HD13	2.27	0.49
3:C:131:ASN:HB2	3:C:223:ASP:OD2	2.12	0.49
16:Q:851:ILE:HA	16:Q:1060:LEU:O	2.12	0.49
26:1:741:LYS:HG3	26:1:742:GLY:N	2.27	0.49
26:1:854:VAL:HG23	26:1:855:ASP:OD1	2.12	0.49
36:9:419:THR:HG23	36:9:421:ARG:HG3	1.94	0.49
1:A:1519:THR:HG22	1:A:1522:GLN:HG3	1.93	0.49
3:C:587:VAL:HG11	3:C:830:PRO:HG3	1.93	0.49
7:G:106:C:H4'	7:G:107:U:OP2	2.11	0.49
8:H:148:C:H2'	8:H:149:A:C8	2.48	0.49
13:N:25:LEU:HD23	13:N:28:LYS:HE2	1.94	0.49
17:R:185:GLY:O	17:R:187:ALA:N	2.45	0.49
24:Y:26:VAL:HG11	26:1:860:GLU:HB2	1.93	0.49
26:1:819:TRP:HH2	26:1:871:THR:HG21	1.77	0.49
27:3:316:GLU:HB2	27:3:324:GLU:HG2	1.94	0.49
27:3:791:HIS:ND1	27:3:930:LEU:HD21	2.28	0.49
3:C:118:PHE:CZ	3:C:122:LEU:HD11	2.47	0.49
6:F:12:G:H2'	6:F:13:G:C8	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:575:THR:OG1	21:V:580:ARG:NH1	2.41	0.49
33:6:31:THR:OG1	33:6:34:GLU:HB2	2.12	0.49
33:6:78:SER:HB3	33:6:89:VAL:HG22	1.94	0.49
1:A:1055:LEU:HB3	22:W:18:LEU:HD11	1.95	0.49
5:E:229:TYR:OH	5:E:270:LYS:HA	2.12	0.49
17:R:124:VAL:HG13	19:T:407:GLN:NE2	2.27	0.49
18:S:581:ILE:HA	18:S:734:CYS:O	2.12	0.49
19:T:264:CYS:HB3	19:T:294:LEU:HD13	1.94	0.49
26:1:577:VAL:HG12	26:1:578:ILE:HD13	1.93	0.49
27:3:745:PHE:HB2	27:3:755:VAL:HG23	1.93	0.49
1:A:502:ASN:O	1:A:506:LEU:HG	2.11	0.49
1:A:1416:ILE:O	1:A:1416:ILE:HG23	2.12	0.49
3:C:465:MET:O	3:C:468:CYS:N	2.45	0.49
5:E:255:MET:HB3	5:E:282:HIS:ND1	2.27	0.49
10:J:395:ALA:HA	10:J:398:VAL:HG12	1.95	0.49
21:V:519:LYS:O	21:V:522:MET:N	2.46	0.49
26:1:738:HIS:CE1	26:1:742:GLY:HA3	2.48	0.49
26:1:1138:VAL:HG22	26:1:1143:VAL:HG21	1.94	0.49
27:3:190:GLU:O	27:3:194:ASN:ND2	2.46	0.49
37:8:28:LEU:HB3	37:8:30:PHE:HE2	1.78	0.49
1:A:533:LYS:HE3	6:F:37:C:C5	2.48	0.49
1:A:984:MET:O	1:A:988:ILE:HG13	2.13	0.49
1:A:994:ASN:O	1:A:998:ARG:HG3	2.13	0.49
5:E:255:MET:SD	5:E:286:LYS:HG2	2.53	0.49
6:F:58:G:O2'	6:F:59:G:OP1	2.27	0.49
18:S:700:TYR:HA	18:S:706:MET:O	2.13	0.49
26:1:855:ASP:OD1	26:1:855:ASP:N	2.45	0.49
27:3:258:TYR:HB2	27:3:325:ILE:HD11	1.94	0.49
27:3:787:LYS:HB3	27:3:800:ILE:HD11	1.95	0.49
27:3:1217:PHE:CD1	27:3:1217:PHE:N	2.80	0.49
3:C:832:TYR:HD2	3:C:899:SER:HG	1.57	0.49
11:K:131:GLN:O	11:K:135:GLU:HG3	2.13	0.49
15:P:206:LYS:HA	15:P:209:ARG:HG3	1.94	0.49
21:V:568:ILE:HG22	21:V:570:LEU:HD13	1.95	0.49
24:Y:27:SER:OG	24:Y:29:HIS:HD2	1.95	0.49
27:3:590:MET:HG2	27:3:606:ALA:O	2.12	0.49
27:3:741:PHE:HB3	27:3:757:ILE:HD11	1.93	0.49
1:A:84:ASP:O	1:A:85:LYS:C	2.51	0.49
1:A:1770:GLU:O	1:A:1773:SER:HB3	2.12	0.49
3:C:275:TYR:HD1	3:C:369:PHE:HD2	1.61	0.49
3:C:776:GLU:O	3:C:781:ASP:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:99:ASN:O	13:N:142:CYS:HB2	2.13	0.49
19:T:201:SER:HB3	19:T:455:GLN:HE22	1.78	0.49
23:X:278:GLN:HB2	23:X:281:TYR:CZ	2.48	0.49
26:1:834:VAL:HG22	26:1:871:THR:HG22	1.94	0.49
27:3:616:ILE:O	27:3:628:LEU:N	2.37	0.49
27:3:718:ARG:O	27:3:720:TRP:HD1	1.96	0.49
36:9:441:ALA:HA	36:9:444:GLN:OE1	2.12	0.49
1:A:27:GLU:HA	1:A:30:LEU:HG	1.95	0.48
3:C:767:VAL:O	3:C:771:GLN:HG3	2.13	0.48
3:C:831:TYR:HB2	3:C:903:HIS:O	2.13	0.48
5:E:98:ASP:N	5:E:98:ASP:OD1	2.46	0.48
5:E:249:TYR:CE2	5:E:263:ASP:HB3	2.48	0.48
10:J:286:GLU:OE1	10:J:291:GLN:HB2	2.13	0.48
10:J:294:HIS:HA	10:J:297:ASN:ND2	2.28	0.48
16:Q:82:SER:O	16:Q:86:SER:N	2.45	0.48
17:R:310:ARG:HH11	17:R:310:ARG:HG3	1.78	0.48
23:X:285:ARG:HB2	23:X:299:CYS:HB2	1.95	0.48
26:1:652:CYS:O	26:1:661:ARG:HG2	2.13	0.48
26:1:1036:ILE:HD11	26:1:1062:LEU:HD22	1.95	0.48
27:3:155:SER:OG	27:3:156:SER:O	2.31	0.48
27:3:443:GLU:CD	27:3:443:GLU:H	2.15	0.48
31:2:586:ILE:H	31:2:586:ILE:HD12	1.78	0.48
37:8:48:ILE:O	37:8:51:TRP:N	2.46	0.48
1:A:360:SER:O	1:A:360:SER:OG	2.27	0.48
2:B:101:U:H2'	2:B:102:U:H6	1.78	0.48
4:D:2108:PHE:O	4:D:2117:ASP:HA	2.13	0.48
5:E:329:SER:N	5:E:347:SER:OG	2.39	0.48
7:G:89:U:H3	26:1:503:LYS:CD	2.27	0.48
13:N:104:ARG:HD3	13:N:136:HIS:HB3	1.95	0.48
15:P:213:ASP:OD2	15:P:216:ARG:HD2	2.13	0.48
23:X:245:LYS:NZ	23:X:302:GLN:O	2.46	0.48
26:1:697:GLU:OE2	26:1:698:GLN:N	2.46	0.48
26:1:944:SER:O	26:1:944:SER:OG	2.20	0.48
27:3:457:ASN:ND2	27:3:479:VAL:HA	2.27	0.48
33:6:19:ARG:HG2	33:6:67:ILE:HA	1.95	0.48
36:9:327:ASN:O	36:9:385:ARG:HD3	2.13	0.48
1:A:2156:THR:OG1	1:A:2157:VAL:N	2.45	0.48
3:C:212:SER:O	3:C:216:THR:HG23	2.13	0.48
5:E:253:ASN:HD21	5:E:291:CYS:HB3	1.77	0.48
6:F:7:G:C6	6:F:15:A:C6	3.02	0.48
6:F:89:U:H3'	6:F:90:G:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:369:PHE:HA	10:J:372:VAL:HG22	1.96	0.48
16:Q:542:ASN:HA	16:Q:622:SER:HA	1.94	0.48
25:Z:619:MET:HG3	25:Z:619:MET:O	2.12	0.48
26:1:1210:HIS:HD1	31:2:585:THR:H	1.61	0.48
36:9:282:VAL:HG22	36:9:433:VAL:HG22	1.94	0.48
1:A:137:GLU:HG3	1:A:424:ILE:HD13	1.94	0.48
3:C:670:SER:HB2	3:C:689:ALA:H	1.78	0.48
3:C:676:ALA:HB3	3:C:811:THR:HG23	1.94	0.48
3:C:710:ASN:OD1	3:C:712:LYS:HB3	2.13	0.48
8:H:148:C:N4	8:H:149:A:N6	2.62	0.48
27:3:757:ILE:HG22	27:3:762:LEU:HB3	1.95	0.48
27:3:918:ARG:HG2	27:3:918:ARG:NH1	2.28	0.48
1:A:221:ASN:HB3	1:A:226:GLN:O	2.13	0.48
1:A:683:LEU:HD11	6:F:57:U:H4'	1.94	0.48
1:A:1840:LYS:HE3	1:A:1840:LYS:HB3	1.58	0.48
3:C:305:GLY:O	3:C:433:MET:HG3	2.14	0.48
3:C:497:LEU:HD13	3:C:577:PHE:CZ	2.48	0.48
3:C:916:ILE:HG21	3:C:928:HIS:HB3	1.96	0.48
4:D:1397:PHE:O	4:D:1402:ASN:N	2.47	0.48
4:D:1660:LEU:HA	4:D:1701:ARG:O	2.13	0.48
6:F:89:U:H3'	6:F:90:G:C8	2.48	0.48
8:H:48:A:C2	8:H:65:U:H2'	2.49	0.48
25:Z:566:TYR:HD1	25:Z:579:TRP:HZ3	1.61	0.48
26:1:586:ASP:OD1	26:1:589:ALA:N	2.43	0.48
27:3:353:PHE:CD1	27:3:406:PRO:HD3	2.43	0.48
1:A:293:TRP:HE1	1:A:1136:ARG:CZ	2.26	0.48
1:A:2107:PRO:HG2	1:A:2110:VAL:HG22	1.95	0.48
2:B:63:A:H2'	2:B:64:G:C8	2.47	0.48
3:C:680:ASN:O	3:C:682:LYS:N	2.46	0.48
7:G:102:G:H21	7:G:103:U:H5'	1.79	0.48
12:L:41:LYS:HA	12:L:41:LYS:HD3	1.58	0.48
12:L:92:THR:OG1	12:L:95:GLN:HG3	2.13	0.48
23:X:253:ARG:HB3	23:X:324:VAL:HG11	1.95	0.48
26:1:472:ILE:O	26:1:476:ASP:HB3	2.13	0.48
26:1:867:MET:O	26:1:871:THR:HG23	2.14	0.48
27:3:175:VAL:HB	27:3:178:GLU:OE1	2.14	0.48
27:3:485:LEU:HB3	27:3:491:VAL:CG1	2.42	0.48
27:3:565:TYR:HE1	27:3:619:LEU:HD22	1.79	0.48
36:9:370:ASN:H	36:9:394:HIS:CE1	2.31	0.48
1:A:569:VAL:O	1:A:570:ASP:HB2	2.13	0.48
1:A:1561:PHE:HE1	11:K:193:VAL:HG11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1808:PHE:CZ	1:A:1893:PHE:HB3	2.48	0.48
1:A:2228:TYR:N	1:A:2228:TYR:HD1	2.12	0.48
1:A:2252:LEU:H	1:A:2255:HIS:HD1	1.62	0.48
3:C:441:PRO:HA	3:C:444:GLY:HA3	1.96	0.48
4:D:735:ALA:C	4:D:737:ALA:H	2.16	0.48
4:D:2035:VAL:O	4:D:2093:ASP:HA	2.14	0.48
6:F:40:U:H2'	6:F:41:A:C8	2.48	0.48
10:J:368:ARG:HA	10:J:368:ARG:NE	2.29	0.48
26:1:498:MET:HE1	26:1:530:PRO:HB2	1.95	0.48
27:3:328:LYS:NZ	27:3:370:GLU:OE1	2.47	0.48
33:6:116:LYS:HG2	33:6:117:TYR:CD1	2.49	0.48
1:A:1361:GLU:OE1	1:A:1363:GLN:HB2	2.12	0.48
1:A:1782:ASP:O	1:A:1785:VAL:HG23	2.14	0.48
5:E:243:LEU:HD21	5:E:247:GLY:HA2	1.96	0.48
7:G:11:A:H2'	7:G:12:G:O4'	2.13	0.48
8:H:19:G:O2'	8:H:20:G:OP2	2.26	0.48
13:N:79:ILE:HA	13:N:84:ALA:HB3	1.96	0.48
26:1:413:LYS:HB2	33:6:52:ASN:HD21	1.78	0.48
26:1:489:PRO:HB2	26:1:492:GLN:HB2	1.96	0.48
27:3:665:LEU:HD23	27:3:677:THR:HB	1.94	0.48
27:3:791:HIS:CD2	27:3:794:SER:H	2.31	0.48
1:A:2274:PRO:HG2	1:A:2278:SER:O	2.14	0.48
3:C:131:ASN:HB3	3:C:549:TRP:CZ2	2.48	0.48
3:C:663:CYS:HB2	3:C:828:MET:HB2	1.96	0.48
10:J:366:TYR:HB3	10:J:382:TYR:CD2	2.48	0.48
21:V:522:MET:O	21:V:526:GLU:HG3	2.14	0.48
27:3:866:ILE:HD13	27:3:907:VAL:HG21	1.96	0.48
37:8:115:ASN:HD21	37:8:124:LEU:HD21	1.79	0.48
1:A:569:VAL:HG12	1:A:573:GLN:HB2	1.96	0.48
3:C:711:ARG:NE	3:C:730:ARG:O	2.46	0.48
5:E:174:GLY:HA2	5:E:194:TYR:O	2.13	0.48
8:H:119:G:N2	8:H:139:C:O2	2.47	0.48
10:J:292:VAL:HG11	10:J:323:LEU:HD13	1.96	0.48
13:N:58:ARG:NH2	13:N:99:ASN:HA	2.29	0.48
13:N:139:CYS:SG	13:N:140:ARG:N	2.87	0.48
26:1:406:ALA:HA	33:6:99:GLN:HE22	1.79	0.48
27:3:958:ARG:NH1	27:3:980:LYS:HG2	2.29	0.48
33:6:18:ASN:OD1	33:6:19:ARG:N	2.47	0.48
36:9:142:ARG:HA	36:9:149:PRO:HA	1.96	0.48
1:A:197:PRO:HG3	1:A:204:LEU:HD21	1.95	0.47
1:A:1233:ASP:OD1	1:A:1234:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2150:GLN:HA	1:A:2288:HIS:CE1	2.49	0.47
2:B:101:U:H2'	2:B:102:U:C6	2.48	0.47
3:C:296:GLU:H	3:C:296:GLU:CD	2.17	0.47
3:C:366:GLN:HG3	3:C:371:GLU:HG3	1.96	0.47
3:C:515:THR:O	3:C:518:ASP:N	2.47	0.47
6:F:84:A:N6	8:H:14:C:N4	2.62	0.47
6:F:90:G:H2'	6:F:91:A:H8	1.79	0.47
21:V:603:LEU:HA	21:V:612:PHE:CE2	2.49	0.47
23:X:296:HIS:ND1	23:X:298:SER:OG	2.46	0.47
24:Y:17:GLU:HG3	24:Y:22:VAL:HB	1.96	0.47
26:1:984:GLU:HG3	26:1:986:TYR:H	1.78	0.47
27:3:65:LEU:HD12	27:3:80:VAL:HG22	1.95	0.47
27:3:676:ARG:HD2	27:3:729:PHE:CE2	2.49	0.47
1:A:766:THR:CG2	1:A:768:ASP:H	2.26	0.47
3:C:693:GLU:OE1	3:C:695:GLY:N	2.40	0.47
6:F:35:A:N7	7:G:11:A:N1	2.62	0.47
8:H:11:G:O2'	8:H:12:G:H5'	2.15	0.47
10:J:286:GLU:HB3	10:J:295:ALA:HB2	1.96	0.47
10:J:299:TRP:HA	10:J:299:TRP:CE3	2.48	0.47
14:O:80:VAL:HA	14:O:87:ASP:HA	1.96	0.47
26:1:145:PRO:HB2	26:1:146:LYS:NZ	2.29	0.47
26:1:1143:VAL:O	26:1:1147:VAL:HG13	2.14	0.47
1:A:1264:ASN:O	1:A:1268:ILE:HG13	2.14	0.47
1:A:1575:GLN:HB2	11:K:220:LEU:CD1	2.44	0.47
1:A:1762:TYR:HB3	1:A:2008:ARG:HD2	1.96	0.47
1:A:2171:GLU:O	1:A:2171:GLU:HG2	2.14	0.47
3:C:439:PRO:O	3:C:443:VAL:HB	2.14	0.47
4:D:823:ALA:O	4:D:857:GLY:N	2.30	0.47
10:J:275:ASN:HB3	10:J:278:LEU:HB2	1.95	0.47
13:N:108:THR:O	13:N:111:THR:HG22	2.15	0.47
19:T:440:ASP:OD2	19:T:443:THR:HG23	2.14	0.47
21:V:648:LYS:HA	21:V:648:LYS:HD2	1.63	0.47
23:X:274:TYR:CD1	26:1:436:THR:N	2.72	0.47
26:1:1037:ASP:O	26:1:1041:ARG:HG2	2.14	0.47
1:A:1405:LEU:HD13	17:R:411:LEU:HD23	1.96	0.47
1:A:1490:PHE:O	1:A:1493:THR:OG1	2.30	0.47
1:A:2190:PRO:HG3	1:A:2251:TYR:CE2	2.49	0.47
8:H:60:U:H2'	8:H:61:C:C6	2.49	0.47
8:H:154:C:H1'	8:H:178:A:H61	1.80	0.47
10:J:429:PHE:CE1	10:J:465:ARG:HA	2.49	0.47
19:T:319:THR:O	19:T:319:THR:OG1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:381:HIS:ND1	19:T:382:PRO:HD2	2.30	0.47
27:3:484:VAL:HG11	27:3:499:PHE:CD2	2.43	0.47
27:3:700:LYS:O	27:3:714:ALA:HA	2.14	0.47
1:A:318:TYR:HB2	3:C:638:ASP:OD1	2.14	0.47
1:A:552:ARG:HG2	1:A:552:ARG:NH1	2.29	0.47
1:A:856:LEU:O	1:A:857:ASN:HB3	2.15	0.47
3:C:244:LYS:HE3	3:C:248:GLN:HE22	1.79	0.47
3:C:514:TYR:HB2	3:C:521:ASP:HB3	1.95	0.47
3:C:600:LEU:HD12	3:C:600:LEU:HA	1.68	0.47
3:C:718:PHE:HB3	3:C:724:TRP:CD1	2.50	0.47
4:D:662:ALA:O	4:D:667:VAL:N	2.47	0.47
5:E:298:SER:O	5:E:314:THR:HG23	2.14	0.47
6:F:23:U:H2'	6:F:24:A:O4'	2.15	0.47
8:H:130:U:H2'	8:H:131:G:H8	1.79	0.47
10:J:354:LEU:HA	10:J:356:TYR:O	2.14	0.47
10:J:359:VAL:O	10:J:363:ARG:HG2	2.15	0.47
16:Q:877:LEU:O	16:Q:1035:ILE:HA	2.15	0.47
21:V:482:PRO:HD2	21:V:485:GLN:OE1	2.14	0.47
26:1:885:ASP:OD1	26:1:886:HIS:N	2.47	0.47
26:1:1137:ARG:HD2	31:2:522:PHE:O	2.15	0.47
1:A:150:MET:CG	1:A:193:LEU:HB2	2.45	0.47
1:A:1673:SER:O	1:A:1673:SER:OG	2.30	0.47
1:A:2294:TYR:HE2	1:A:2296:LEU:HD21	1.80	0.47
3:C:129:ILE:HG22	3:C:199:LEU:HB3	1.96	0.47
3:C:369:PHE:HD1	3:C:373:ILE:HD12	1.80	0.47
3:C:384:VAL:HG11	3:C:416:LEU:HD23	1.96	0.47
3:C:711:ARG:HG2	3:C:730:ARG:HD2	1.97	0.47
5:E:75:HIS:O	5:E:78:GLY:N	2.48	0.47
9:I:366:LEU:HA	9:I:381:ALA:HB1	1.97	0.47
19:T:337:ARG:HG3	19:T:378:VAL:HG23	1.95	0.47
21:V:602:ARG:HD3	21:V:602:ARG:HA	1.67	0.47
26:1:397:ARG:HD2	26:1:398:PRO:HD2	1.97	0.47
34:7:49:CYS:HB3	34:7:87:LYS:HD3	1.95	0.47
37:8:26:LYS:HA	37:8:26:LYS:HD3	1.66	0.47
1:A:480:LYS:HB2	13:N:110:ASP:HA	1.97	0.47
1:A:985:TYR:HD2	1:A:1032:ARG:NE	2.11	0.47
1:A:1527:ASN:ND2	11:K:215:ASP:HB3	2.30	0.47
1:A:1690:ASP:OD1	1:A:1692:MET:N	2.39	0.47
1:A:2174:PRO:HB2	1:A:2206:TRP:NE1	2.30	0.47
1:A:2304:PHE:HB3	1:A:2305:TYR:HD2	1.79	0.47
2:B:62:G:H2'	2:B:63:A:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:216:THR:HG22	3:C:245:HIS:CE1	2.50	0.47
3:C:319:THR:O	3:C:322:SER:N	2.47	0.47
3:C:446:LYS:HB3	3:C:447:PRO:HD3	1.96	0.47
3:C:938:ARG:HG2	3:C:938:ARG:HH11	1.80	0.47
4:D:1299:THR:N	4:D:1513:ASN:O	2.48	0.47
4:D:1667:GLN:HA	4:D:1677:VAL:O	2.14	0.47
16:Q:370:GLY:H	16:Q:371:PRO:HD2	1.79	0.47
19:T:417:ASN:HD21	19:T:432:ASP:HB2	1.80	0.47
25:Z:548:PHE:O	25:Z:551:LYS:HB3	2.14	0.47
26:1:152:TYR:CE2	26:1:156:MET:HG3	2.49	0.47
26:1:781:ASP:HB3	26:1:784:MET:HB2	1.95	0.47
26:1:1122:THR:OG1	26:1:1123:CYS:N	2.47	0.47
27:3:518:GLN:HG2	27:3:520:TYR:CE2	2.50	0.47
27:3:1026:ASP:OD1	27:3:1088:LYS:HE2	2.15	0.47
31:2:601:LEU:O	31:2:602:LYS:HB2	2.15	0.47
31:2:703:ILE:HG22	31:2:704:ASP:H	1.80	0.47
32:4:128:GLN:CB	32:4:148:ASN:H	2.28	0.47
36:9:269:ASP:CG	36:9:272:ARG:HH21	2.18	0.47
3:C:65:TYR:CD2	3:C:65:TYR:N	2.81	0.47
3:C:349:PHE:HB2	3:C:356:PHE:CE1	2.49	0.47
3:C:448:LYS:O	3:C:452:THR:OG1	2.33	0.47
3:C:530:LEU:HD23	3:C:530:LEU:HA	1.68	0.47
3:C:799:GLU:HG3	3:C:801:LEU:HG	1.96	0.47
3:C:913:ASP:H	3:C:931:ARG:NH1	2.13	0.47
5:E:73:LYS:NZ	5:E:115:LEU:HB3	2.29	0.47
5:E:78:GLY:HA3	5:E:336:HIS:CE1	2.50	0.47
17:R:398:ASN:HB2	23:X:237:ASN:HD21	1.79	0.47
18:S:450:CYS:HA	18:S:518:MET:O	2.15	0.47
19:T:343:PRO:HB3	19:T:365:ARG:HH12	1.80	0.47
26:1:478:LEU:HG	26:1:499:LYS:HE3	1.97	0.47
26:1:1067:LYS:HB2	26:1:1067:LYS:NZ	2.29	0.47
27:3:488:GLY:C	27:3:490:THR:H	2.17	0.47
27:3:519:VAL:HB	27:3:524:ILE:HG23	1.97	0.47
27:3:720:TRP:CE2	27:3:733:PRO:HG3	2.49	0.47
27:3:833:GLU:HA	27:3:834:LEU:HB2	1.96	0.47
33:6:37:ASP:O	33:6:41:LYS:HG2	2.15	0.47
36:9:328:PHE:CD2	36:9:329:VAL:HG13	2.49	0.47
1:A:494:LEU:HD21	1:A:562:VAL:HG21	1.96	0.47
1:A:663:ARG:HH11	1:A:663:ARG:CG	2.28	0.47
1:A:1840:LYS:O	1:A:1844:GLU:HG2	2.15	0.47
1:A:2107:PRO:HA	1:A:2264:SER:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:193:THR:HG23	3:C:428:THR:HB	1.97	0.47
5:E:193:THR:HG23	5:E:194:TYR:CG	2.50	0.47
6:F:78:A:H3'	6:F:79:C:C6	2.49	0.47
21:V:565:LEU:HD12	21:V:612:PHE:HE1	1.80	0.47
24:Y:71:LYS:HB2	24:Y:71:LYS:NZ	2.29	0.47
26:1:1185:ARG:NH1	31:2:511:LEU:HD12	2.30	0.47
26:1:1251:LEU:HD11	26:1:1285:PRO:HG3	1.97	0.47
27:3:544:ILE:HD12	27:3:558:LEU:HG	1.97	0.47
35:5:11:LEU:HD22	35:5:23:HIS:HB3	1.95	0.47
37:8:72:PHE:O	37:8:76:GLU:HG2	2.15	0.47
1:A:468:LYS:HD3	1:A:469:LYS:H	1.80	0.47
1:A:1923:TRP:HB3	1:A:1927:ILE:HD11	1.97	0.47
6:F:16:G:H2'	6:F:17:C:C6	2.50	0.47
6:F:84:A:H2	8:H:15:U:O2	1.98	0.47
8:H:6:U:H2'	8:H:7:U:C6	2.49	0.47
16:Q:525:PRO:HA	16:Q:532:PRO:HA	1.96	0.47
17:R:125:MET:HG3	19:T:186:PRO:HD2	1.97	0.47
17:R:233:PRO:O	17:R:235:ARG:NH1	2.47	0.47
19:T:226:ARG:HD3	19:T:246:ILE:O	2.15	0.47
21:V:600:ASN:O	21:V:604:LYS:HB2	2.15	0.47
21:V:650:THR:HB	21:V:651:PRO:CD	2.45	0.47
27:3:272:PRO:HG2	27:3:311:PHE:HE1	1.80	0.47
27:3:411:GLN:HE21	27:3:411:GLN:HB2	1.42	0.47
33:6:116:LYS:HZ2	33:6:116:LYS:HB3	1.80	0.47
36:9:266:ILE:HG23	36:9:267:ASP:H	1.79	0.47
36:9:321:PHE:HA	36:9:332:GLY:CA	2.39	0.47
1:A:988:ILE:HD12	1:A:1030:ILE:HD12	1.97	0.46
1:A:1833:LEU:O	1:A:1836:LEU:HB3	2.15	0.46
1:A:2107:PRO:HG2	1:A:2110:VAL:CG2	2.45	0.46
1:A:2176:GLY:HA2	1:A:2206:TRP:CE2	2.51	0.46
1:A:2309:HIS:CD2	1:A:2309:HIS:N	2.83	0.46
3:C:264:ILE:HG21	3:C:381:LEU:HD12	1.98	0.46
3:C:278:LEU:HD13	3:C:309:PHE:CE1	2.50	0.46
3:C:709:TRP:HZ3	3:C:717:PHE:HB2	1.80	0.46
6:F:13:G:H2'	6:F:14:C:C6	2.51	0.46
8:H:81:G:H2'	8:H:82:G:O4'	2.14	0.46
13:N:9:LYS:HA	13:N:9:LYS:HD3	1.77	0.46
23:X:261:LEU:HG	23:X:367:TYR:HB3	1.96	0.46
26:1:170:GLN:O	26:1:174:GLU:HG2	2.15	0.46
26:1:843:LYS:HA	26:1:843:LYS:HD2	1.62	0.46
27:3:705:ARG:HH12	27:3:709:GLN:N	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:6:26:LEU:HD12	33:6:87:LEU:HD11	1.96	0.46
1:A:382:GLU:HA	3:C:354:ARG:NH1	2.30	0.46
1:A:758:ARG:HA	1:A:758:ARG:HD2	1.62	0.46
1:A:1881:ASN:OD1	1:A:1881:ASN:N	2.47	0.46
3:C:120:ALA:O	3:C:123:MET:HB2	2.15	0.46
5:E:129:THR:O	5:E:153:PHE:HA	2.14	0.46
11:K:140:ILE:HG12	11:K:140:ILE:H	1.49	0.46
13:N:91:LYS:HD2	13:N:91:LYS:HA	1.64	0.46
19:T:250:ARG:HH11	19:T:250:ARG:CG	2.29	0.46
23:X:310:LEU:HB2	23:X:324:VAL:HG12	1.96	0.46
26:1:967:GLU:HG2	26:1:970:LEU:HD23	1.96	0.46
31:2:557:VAL:HG13	31:2:558:ARG:HG3	1.96	0.46
31:2:642:PRO:HA	32:4:69:TYR:CB	2.45	0.46
32:4:166:TYR:HA	32:4:171:PRO:HA	1.96	0.46
1:A:514:ASN:ND2	1:A:514:ASN:H	2.13	0.46
1:A:820:ARG:HA	1:A:820:ARG:HD2	1.58	0.46
3:C:313:GLN:HB2	50:C:1500:GTP:C5	2.50	0.46
3:C:342:ARG:O	3:C:347:ILE:HD12	2.15	0.46
25:Z:546:ALA:O	25:Z:550:LYS:HG2	2.15	0.46
26:1:1256:HIS:CD2	26:1:1257:PRO:HD2	2.50	0.46
27:3:71:THR:O	27:3:146:ARG:NH2	2.49	0.46
27:3:896:PHE:CD1	27:3:972:LEU:HB2	2.50	0.46
1:A:1975:GLU:O	1:A:1979:VAL:HG13	2.16	0.46
3:C:273:ASP:N	3:C:273:ASP:OD1	2.46	0.46
3:C:420:CYS:O	3:C:424:PHE:HB2	2.16	0.46
3:C:711:ARG:NH2	3:C:730:ARG:O	2.48	0.46
8:H:28:C:H4'	8:H:29:A:OP1	2.16	0.46
8:H:138:C:H2'	8:H:139:C:C6	2.50	0.46
8:H:175:G:H2'	8:H:176:G:C4	2.49	0.46
26:1:733:LYS:HE2	26:1:733:LYS:HB3	1.70	0.46
37:8:30:PHE:HE1	37:8:83:LYS:HA	1.80	0.46
1:A:325:HIS:CD2	1:A:326:HIS:CD2	3.03	0.46
1:A:363:HIS:NE2	3:C:284:GLU:HA	2.31	0.46
1:A:1860:GLN:OE1	1:A:1885:LYS:NZ	2.47	0.46
1:A:2259:VAL:HG12	1:A:2260:GLN:N	2.30	0.46
2:B:110:C:H2'	2:B:111:A:C8	2.49	0.46
3:C:201:ASN:HB3	3:C:549:TRP:CE3	2.50	0.46
3:C:286:ASN:ND2	3:C:300:LEU:O	2.37	0.46
3:C:453:TYR:HD2	3:C:456:GLY:H	1.64	0.46
6:F:84:A:O2'	6:F:85:U:H2'	2.16	0.46
7:G:104:C:O2	7:G:104:C:H2'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:168:A:H5”	8:H:169:C:H5	1.80	0.46
8:H:172:C:H2’	8:H:173:C:C6	2.50	0.46
10:J:236:ARG:HE	10:J:236:ARG:HB3	1.57	0.46
10:J:338:GLU:O	10:J:340:GLN:NE2	2.49	0.46
23:X:291:ASP:HB2	23:X:292:ILE:HG13	1.98	0.46
26:1:484:GLU:O	26:1:487:LEU:N	2.49	0.46
26:1:694:LEU:HA	26:1:694:LEU:HD23	1.64	0.46
27:3:552:ARG:HH12	27:3:601:ARG:NH2	2.12	0.46
1:A:1807:ILE:HG12	1:A:1841:THR:HG22	1.96	0.46
1:A:2129:TYR:CZ	1:A:2169:LEU:HD13	2.51	0.46
3:C:384:VAL:HG13	3:C:415:LEU:HD23	1.97	0.46
4:D:1562:PHE:HA	4:D:1646:ALA:O	2.16	0.46
8:H:2:U:H2’	8:H:3:C:H6	1.77	0.46
8:H:3:C:H2’	8:H:4:G:H8	1.81	0.46
8:H:16:U:H1’	8:H:17:U:H5’	1.98	0.46
17:R:295:ASP:OD2	17:R:295:ASP:C	2.53	0.46
25:Z:533:ARG:O	25:Z:537:GLU:HG2	2.16	0.46
26:1:400:SER:O	26:1:404:LEU:HG	2.15	0.46
26:1:495:ARG:HB3	26:1:495:ARG:CZ	2.44	0.46
26:1:773:LEU:HD11	26:1:791:VAL:HG12	1.98	0.46
26:1:1013:ILE:HG22	26:1:1049:TYR:HB2	1.97	0.46
27:3:608:GLY:HA2	27:3:614:VAL:HG22	1.98	0.46
36:9:276:VAL:HG21	36:9:438:TYR:CD1	2.50	0.46
1:A:47:GLU:H	1:A:47:GLU:CD	2.19	0.46
1:A:361:HIS:O	1:A:362:ARG:NE	2.48	0.46
1:A:570:ASP:HB3	1:A:573:GLN:HG3	1.97	0.46
1:A:845:ARG:HH22	1:A:1440:THR:HG22	1.80	0.46
1:A:2278:SER:HG	1:A:2309:HIS:CD2	2.34	0.46
2:B:100:C:H2’	2:B:101:U:C5	2.50	0.46
3:C:696:LEU:O	3:C:700:ILE:HD12	2.16	0.46
3:C:750:LEU:O	3:C:754:VAL:HG23	2.15	0.46
7:G:9:C:H2’	7:G:10:U:N1	2.31	0.46
17:R:283:ASN:N	17:R:283:ASN:OD1	2.46	0.46
23:X:296:HIS:HB3	23:X:363:SER:OG	2.16	0.46
25:Z:560:LYS:HD3	25:Z:561:LYS:H	1.80	0.46
26:1:531:LEU:O	26:1:535:ILE:HG13	2.16	0.46
27:3:565:TYR:CE2	27:3:567:GLU:HB2	2.51	0.46
34:7:11:CYS:SG	34:7:13:LYS:NZ	2.76	0.46
1:A:82:ARG:HG2	1:A:82:ARG:O	2.15	0.46
1:A:1393:ARG:HH11	26:1:90:LEU:HD22	1.81	0.46
2:B:108:G:H3’	2:B:109:G:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:HIS:HB2	3:C:239:THR:HG23	1.98	0.46
5:E:248:SER:O	5:E:263:ASP:HA	2.16	0.46
8:H:168:A:N3	8:H:168:A:H2'	2.29	0.46
10:J:236:ARG:HA	10:J:239:ARG:CZ	2.45	0.46
12:L:49:ARG:HG3	12:L:54:LEU:HD22	1.97	0.46
15:P:199:LYS:HA	15:P:199:LYS:HD2	1.61	0.46
15:P:212:ASN:OD1	19:T:458:SER:HB3	2.16	0.46
26:1:675:MET:HE3	26:1:675:MET:HB3	1.88	0.46
27:3:102:ILE:HG22	27:3:103:HIS:CD2	2.50	0.46
27:3:429:ARG:HG2	27:3:430:GLY:N	2.31	0.46
27:3:550:ASN:HD21	27:3:595:VAL:N	2.14	0.46
27:3:788:PHE:HB2	27:3:799:ILE:HG12	1.97	0.46
27:3:818:GLN:O	27:3:821:GLU:HB2	2.16	0.46
33:6:104:LYS:HA	33:6:107:GLU:OE2	2.16	0.46
1:A:260:LEU:O	1:A:263:PHE:N	2.49	0.46
1:A:1684:PHE:O	1:A:1688:THR:HG23	2.16	0.46
3:C:712:LYS:O	3:C:716:GLU:HG3	2.16	0.46
5:E:226:LYS:HD2	5:E:226:LYS:HA	1.73	0.46
7:G:88:G:H4'	7:G:89:U:OP1	2.15	0.46
10:J:423:GLU:HA	10:J:426:GLN:HG2	1.98	0.46
26:1:933:CYS:CB	26:1:970:LEU:HD11	2.45	0.46
31:2:568:TYR:C	31:2:570:LYS:H	2.19	0.46
32:4:159:ILE:O	32:4:163:ASN:CB	2.63	0.46
33:6:106:LYS:O	33:6:109:GLN:HG2	2.16	0.46
36:9:293:LEU:HD11	36:9:295:LEU:HG	1.98	0.46
36:9:315:TYR:OH	36:9:343:GLU:HB2	2.16	0.46
1:A:693:ILE:HB	1:A:738:MET:SD	2.56	0.46
1:A:902:TYR:OH	1:A:1249:MET:SD	2.68	0.46
1:A:1291:CYS:O	1:A:1295:ILE:HG23	2.15	0.46
1:A:2150:GLN:O	1:A:2281:TYR:N	2.49	0.46
2:B:12:U:H2'	2:B:13:C:H6	1.81	0.46
3:C:357:THR:OG1	3:C:358:LYS:O	2.33	0.46
8:H:2:U:C2	8:H:3:C:C5	3.04	0.46
8:H:154:C:N3	8:H:155:C:N4	2.64	0.46
10:J:313:TRP:O	10:J:317:THR:HG23	2.15	0.46
17:R:141:LYS:O	17:R:145:GLU:HG2	2.15	0.46
27:3:636:GLN:HB3	27:3:670:GLN:NE2	2.30	0.46
27:3:1106:LYS:HD2	31:2:708:TRP:NE1	2.31	0.46
27:3:1199:ARG:HH22	27:3:1207:LYS:HE3	1.80	0.46
1:A:83:HIS:NE2	7:G:16:G:O6	2.49	0.45
1:A:1784:ASN:ND2	1:A:1894:GLN:HB2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:110:U:OP2	24:Y:2:ASN:ND2	2.49	0.45
11:K:129:ASP:O	11:K:133:ILE:HD12	2.16	0.45
16:Q:1217:LEU:O	16:Q:1338:PHE:N	2.49	0.45
26:1:547:GLN:NE2	34:7:101:GLU:OE2	2.49	0.45
26:1:805:TYR:CE1	26:1:809:GLU:HG3	2.51	0.45
26:1:826:ASP:HB3	26:1:829:ASN:HB2	1.96	0.45
27:3:333:VAL:HB	27:3:334:PRO:HD2	1.98	0.45
27:3:354:GLY:O	27:3:403:SER:OG	2.33	0.45
27:3:370:GLU:H	27:3:370:GLU:HG2	1.41	0.45
27:3:1063:ASN:ND2	27:3:1066:VAL:HG12	2.31	0.45
27:3:1123:SER:OG	35:5:48:ASP:OD1	2.34	0.45
33:6:77:LEU:O	33:6:80:PHE:HB2	2.15	0.45
34:7:12:ARG:HD3	34:7:12:ARG:HA	1.46	0.45
36:9:219:GLU:CG	36:9:220:ILE:HD12	2.43	0.45
1:A:64:GLU:CD	1:A:64:GLU:H	2.20	0.45
1:A:1386:TRP:CH2	26:1:91:LEU:HD21	2.51	0.45
4:D:1186:LEU:HA	4:D:1203:THR:O	2.17	0.45
5:E:114:GLU:OE2	5:E:156:SER:HA	2.16	0.45
7:G:87:U:H2'	7:G:88:G:O4'	2.16	0.45
7:G:109:U:OP1	24:Y:2:ASN:ND2	2.49	0.45
25:Z:489:GLU:O	25:Z:492:GLU:HG2	2.16	0.45
26:1:568:ARG:HH11	26:1:608:THR:HG21	1.81	0.45
27:3:1114:SER:HB2	27:3:1215:TYR:CE1	2.51	0.45
27:3:1158:ARG:HG3	27:3:1159:ASP:N	2.30	0.45
33:6:29:LYS:HE3	33:6:29:LYS:HB3	1.54	0.45
36:9:199:ASN:HD21	36:9:205:ARG:HD3	1.81	0.45
1:A:818:GLU:OE2	17:R:305:ARG:NH1	2.47	0.45
1:A:1382:SER:HA	1:A:1415:GLY:HA2	1.97	0.45
1:A:1570:LYS:O	1:A:1574:ILE:HB	2.17	0.45
1:A:2189:SER:HB3	1:A:2191:GLN:HG2	1.99	0.45
4:D:912:ASN:HA	4:D:978:ASN:HA	1.99	0.45
5:E:301:ALA:HB2	5:E:335:PHE:HE2	1.81	0.45
6:F:49:G:H8	6:F:49:G:OP1	1.98	0.45
7:G:19:G:N2	14:O:194:ALA:HA	2.31	0.45
9:I:619:ALA:O	9:I:623:VAL:CA	2.65	0.45
26:1:413:LYS:HB3	26:1:413:LYS:HE2	1.59	0.45
33:6:66:ASP:HB3	33:6:69:ASP:HB2	1.97	0.45
36:9:301:PRO:O	36:9:305:GLU:HB2	2.17	0.45
1:A:689:VAL:HG13	1:A:738:MET:SD	2.57	0.45
1:A:1841:THR:HB	1:A:1868:MET:HE3	1.96	0.45
3:C:227:LEU:HD12	3:C:227:LEU:HA	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:178:LEU:HD11	5:E:222:LEU:HD22	1.98	0.45
8:H:79:G:H2'	8:H:79:G:N3	2.30	0.45
10:J:299:TRP:HB3	10:J:316:TYR:CD2	2.51	0.45
10:J:332:VAL:HA	10:J:335:ARG:CD	2.46	0.45
17:R:144:THR:O	17:R:148:ARG:HB2	2.16	0.45
17:R:332:ARG:HH22	23:X:267:ASP:N	2.10	0.45
21:V:555:LEU:HD23	21:V:555:LEU:HA	1.66	0.45
27:3:971:ASP:OD1	27:3:972:LEU:N	2.43	0.45
1:A:646:PRO:HG3	2:B:55:C:H4'	1.98	0.45
1:A:1457:HIS:ND1	1:A:1460:HIS:HD2	2.14	0.45
1:A:1642:PRO:HA	1:A:1716:GLY:O	2.17	0.45
2:B:88:A:H4'	2:B:94:U:O4	2.15	0.45
5:E:84:ALA:HB1	5:E:112:VAL:HB	1.97	0.45
8:H:31:G:C6	26:1:1069:HIS:NE2	2.85	0.45
8:H:154:C:H1'	8:H:178:A:N6	2.30	0.45
10:J:313:TRP:HB3	10:J:336:TRP:CE3	2.52	0.45
12:L:30:GLN:HG2	12:L:33:ARG:HE	1.82	0.45
13:N:77:TYR:CE2	13:N:81:GLU:HG3	2.52	0.45
17:R:189:ASN:HB3	17:R:191:GLY:H	1.81	0.45
18:S:480:SER:HA	18:S:485:ASP:HA	1.98	0.45
18:S:521:GLU:N	18:S:551:ALA:O	2.50	0.45
21:V:514:PHE:HB3	21:V:521:TYR:CD1	2.51	0.45
24:Y:48:THR:OG1	24:Y:49:GLU:N	2.47	0.45
26:1:742:GLY:O	26:1:746:PHE:HD2	2.00	0.45
27:3:365:GLY:HA3	27:3:394:ASN:HD21	1.80	0.45
35:5:59:GLU:OE1	35:5:63:ARG:HG2	2.17	0.45
1:A:109:PRO:HD3	1:A:630:TRP:HZ2	1.80	0.45
1:A:338:VAL:HG21	3:C:867:PRO:HD2	1.98	0.45
1:A:1386:TRP:HB3	26:1:87:PRO:HG2	1.97	0.45
1:A:2234:GLY:HA2	1:A:2255:HIS:CD2	2.52	0.45
6:F:15:A:H2'	6:F:16:G:C8	2.52	0.45
7:G:109:U:H1'	26:1:626:ASN:ND2	2.32	0.45
13:N:44:GLU:HB2	13:N:47:TRP:CZ3	2.52	0.45
26:1:619:ASN:OD1	26:1:620:MET:N	2.50	0.45
26:1:637:SER:HA	26:1:675:MET:SD	2.56	0.45
26:1:699:GLN:HE22	26:1:738:HIS:HE1	1.65	0.45
26:1:1046:GLY:O	26:1:1048:GLU:N	2.48	0.45
27:3:544:ILE:HG13	27:3:557:ALA:O	2.17	0.45
27:3:680:ASP:CG	27:3:681:PRO:HD2	2.36	0.45
31:2:469:VAL:HG11	31:2:489:VAL:CG1	2.46	0.45
36:9:348:LYS:HE3	36:9:348:LYS:HB3	1.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LYS:HA	1:A:53:PHE:CE1	2.52	0.45
1:A:196:ASP:OD2	1:A:198:GLU:HB2	2.16	0.45
1:A:1699:THR:HA	1:A:1717:ASN:HD22	1.81	0.45
1:A:2188:LEU:HD12	1:A:2188:LEU:HA	1.79	0.45
2:B:66:A:H2'	2:B:67:A:H8	1.80	0.45
3:C:300:LEU:HA	3:C:306:ASN:ND2	2.29	0.45
5:E:113:MET:HA	5:E:113:MET:HE2	1.98	0.45
6:F:47:A:H2'	6:F:48:A:C5	2.50	0.45
7:G:-11:G:H2'	7:G:-10:G:C8	2.52	0.45
21:V:555:LEU:HD23	21:V:560:LEU:HB2	1.99	0.45
24:Y:64:ASN:HB3	24:Y:83:CYS:HB3	1.99	0.45
24:Y:66:ASN:HD21	24:Y:118:PRO:HG3	1.82	0.45
26:1:153:MET:HE2	26:1:153:MET:HB2	1.86	0.45
26:1:932:ILE:N	26:1:932:ILE:CD1	2.79	0.45
26:1:946:LYS:HA	26:1:946:LYS:HD3	1.51	0.45
27:3:410:CYS:SG	27:3:411:GLN:N	2.89	0.45
27:3:1145:GLU:HG3	27:3:1146:MET:N	2.31	0.45
31:2:556:LYS:HB2	31:2:556:LYS:HZ3	1.81	0.45
36:9:268:GLU:OE1	36:9:268:GLU:HA	2.16	0.45
1:A:226:GLN:HA	1:A:418:THR:HB	1.98	0.45
1:A:1935:ARG:O	1:A:1939:ILE:HG13	2.17	0.45
1:A:2129:TYR:CE2	1:A:2169:LEU:HB3	2.52	0.45
1:A:2279:TRP:NE1	1:A:2301:PRO:HB3	2.30	0.45
3:C:153:THR:OG1	3:C:154:HIS:N	2.50	0.45
3:C:594:PRO:HD3	3:C:603:MET:SD	2.57	0.45
3:C:673:LYS:HE2	20:U:60:HIS:CB	2.47	0.45
3:C:750:LEU:HD23	3:C:750:LEU:H	1.82	0.45
7:G:89:U:H4'	7:G:90:C:OP2	2.16	0.45
10:J:231:PHE:HA	10:J:234:ASN:HD22	1.82	0.45
17:R:233:PRO:HG2	17:R:235:ARG:NH1	2.32	0.45
21:V:620:ASN:HB3	21:V:623:ASN:OD1	2.17	0.45
24:Y:88:ARG:NH1	25:Z:503:GLN:OE1	2.49	0.45
27:3:525:ARG:O	27:3:525:ARG:HG2	2.16	0.45
27:3:720:TRP:CE3	27:3:731:LEU:HG	2.49	0.45
27:3:884:GLN:HG3	27:3:885:ASN:OD1	2.17	0.45
1:A:913:PRO:HA	1:A:916:LYS:HB2	1.99	0.45
1:A:1678:ARG:HD3	1:A:1678:ARG:HA	1.70	0.45
1:A:2280:ASN:HD22	1:A:2304:PHE:HA	1.81	0.45
3:C:275:TYR:CD1	3:C:369:PHE:HD2	2.35	0.45
3:C:709:TRP:HB2	3:C:714:LEU:HD12	1.98	0.45
3:C:735:PHE:CE1	3:C:744:ILE:HG12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:139:C:H2'	8:H:140:A:C8	2.52	0.45
13:N:72:ARG:HG3	13:N:72:ARG:NH1	2.31	0.45
13:N:118:ILE:CD1	13:N:132:ILE:HG21	2.46	0.45
19:T:195:LYS:HE3	19:T:490:ARG:CZ	2.47	0.45
21:V:530:LYS:HD3	21:V:567:CYS:SG	2.57	0.45
26:1:866:LYS:HB2	26:1:866:LYS:HE2	1.50	0.45
27:3:298:MET:N	27:3:298:MET:SD	2.90	0.45
31:2:555:GLU:OE1	31:2:560:LYS:HB2	2.16	0.45
34:7:21:ARG:HA	34:7:67:SER:O	2.17	0.45
1:A:2163:LEU:HG	1:A:2203:ASN:ND2	2.31	0.45
2:B:88:A:H2'	2:B:88:A:N3	2.32	0.45
3:C:416:LEU:HD23	3:C:416:LEU:HA	1.65	0.45
3:C:495:ARG:HD2	3:C:497:LEU:HG	1.98	0.45
3:C:564:THR:HG21	3:C:576:ILE:HA	1.99	0.45
3:C:854:ARG:NH1	3:C:879:ASP:OD2	2.50	0.45
6:F:26:U:H2'	14:O:180:PRO:CB	2.47	0.45
7:G:90:C:H2'	7:G:91:A:C8	2.52	0.45
8:H:157:G:C6	8:H:174:A:N1	2.85	0.45
11:K:230:TRP:HA	11:K:233:GLU:HG3	1.98	0.45
12:L:19:LEU:HD23	12:L:54:LEU:HD23	1.99	0.45
13:N:16:GLU:CD	13:N:16:GLU:H	2.20	0.45
19:T:355:ARG:HD3	19:T:364:THR:HG21	1.99	0.45
26:1:405:ASP:C	33:6:99:GLN:HE22	2.21	0.45
27:3:206:GLN:NE2	27:3:232:GLY:N	2.65	0.45
27:3:614:VAL:HG12	27:3:631:GLN:OE1	2.17	0.45
27:3:870:ASN:ND2	27:3:872:ILE:H	2.14	0.45
27:3:1194:SER:HB2	27:3:1199:ARG:O	2.16	0.45
36:9:268:GLU:O	36:9:270:VAL:N	2.50	0.45
36:9:354:PHE:HB3	36:9:392:LYS:NZ	2.32	0.45
37:8:51:TRP:HZ3	37:8:105:LEU:HD12	1.82	0.45
1:A:1971:LEU:HB3	1:A:1975:GLU:HB2	1.99	0.44
1:A:2070:LYS:O	1:A:2074:ARG:HG2	2.17	0.44
1:A:2113:LYS:HB3	1:A:2271:PHE:CE2	2.52	0.44
1:A:2147:MET:HB3	1:A:2279:TRP:HB3	1.99	0.44
2:B:14:U:H2'	2:B:15:C:H6	1.82	0.44
3:C:311:SER:O	3:C:311:SER:OG	2.31	0.44
3:C:687:MET:HB3	3:C:815:VAL:HG11	1.99	0.44
3:C:807:GLN:NE2	36:9:144:LEU:O	2.49	0.44
5:E:243:LEU:HD11	5:E:247:GLY:O	2.17	0.44
8:H:123:A:N3	8:H:123:A:H2'	2.31	0.44
8:H:156:U:C2	8:H:175:G:N2	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:1322:GLN:HA	16:Q:1325:ALA:HB2	2.00	0.44
24:Y:64:ASN:OD1	24:Y:65:ILE:N	2.50	0.44
26:1:123:ARG:NH2	26:1:124:ARG:HG3	2.31	0.44
27:3:614:VAL:O	27:3:630:MET:HB2	2.17	0.44
37:8:30:PHE:CD1	37:8:83:LYS:HD2	2.52	0.44
1:A:110:TRP:O	1:A:192:GLN:NE2	2.48	0.44
1:A:183:LEU:HD23	13:N:30:ARG:NH2	2.32	0.44
1:A:231:THR:OG1	1:A:233:PRO:HD2	2.18	0.44
1:A:670:LYS:HE2	1:A:670:LYS:HB3	1.35	0.44
1:A:1870:ASP:O	1:A:1874:VAL:HG23	2.17	0.44
1:A:2107:PRO:HD3	1:A:2267:PHE:CZ	2.53	0.44
3:C:495:ARG:HB3	3:C:549:TRP:HD1	1.82	0.44
5:E:73:LYS:HZ1	5:E:115:LEU:HD12	1.83	0.44
5:E:326:HIS:CE1	5:E:352:TYR:HD2	2.36	0.44
8:H:177:A:O2'	8:H:178:A:H5'	2.16	0.44
19:T:455:GLN:HG3	19:T:456:PRO:HD2	2.00	0.44
23:X:359:LYS:HZ1	23:X:366:GLU:HB3	1.82	0.44
26:1:406:ALA:HA	33:6:99:GLN:NE2	2.32	0.44
26:1:869:MET:SD	26:1:913:GLY:HA3	2.57	0.44
26:1:1108:ASN:N	26:1:1108:ASN:OD1	2.50	0.44
33:6:21:LEU:HD21	33:6:64:TYR:HE2	1.82	0.44
1:A:888:GLN:O	1:A:889:ARG:HD3	2.16	0.44
1:A:1681:ARG:HE	1:A:1681:ARG:HB2	1.52	0.44
1:A:2237:TRP:O	1:A:2240:GLN:HB3	2.17	0.44
13:N:12:PRO:HB2	13:N:74:LEU:HB2	2.00	0.44
16:Q:1110:GLN:HA	16:Q:1115:MET:H	1.82	0.44
19:T:223:SER:OG	19:T:224:ALA:N	2.48	0.44
21:V:520:GLU:HA	21:V:523:GLU:OE2	2.17	0.44
24:Y:44:PRO:HA	24:Y:105:ARG:HD2	1.99	0.44
26:1:682:HIS:O	26:1:685:SER:OG	2.26	0.44
26:1:1036:ILE:HD12	26:1:1065:LEU:HD22	1.98	0.44
26:1:1055:TRP:HA	26:1:1055:TRP:CE3	2.52	0.44
27:3:69:ARG:HB2	27:3:76:ASP:OD1	2.16	0.44
27:3:581:LYS:HB2	27:3:625:LEU:HD22	1.98	0.44
27:3:847:LEU:HB3	27:3:852:PHE:CD2	2.53	0.44
27:3:966:LEU:HD22	27:3:982:GLU:OE2	2.18	0.44
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.78	0.44
1:A:329:LEU:HD12	3:C:177:ARG:HG3	1.98	0.44
1:A:1556:ASP:OD1	1:A:1556:ASP:N	2.51	0.44
1:A:1974:GLU:O	1:A:1978:LYS:HG3	2.18	0.44
1:A:2162:GLN:HB3	1:A:2294:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:43:A:H1'	7:G:5:G:N2	2.33	0.44
8:H:118:G:O6	8:H:140:A:N6	2.50	0.44
13:N:64:PHE:HE1	13:N:72:ARG:HA	1.81	0.44
14:O:216:ARG:O	14:O:219:THR:N	2.51	0.44
17:R:134:ARG:HH22	19:T:385:TYR:H	1.63	0.44
26:1:162:THR:HA	26:1:165:GLU:HB2	2.00	0.44
26:1:1103:VAL:HB	26:1:1104:GLN:H	1.75	0.44
27:3:212:GLU:OE1	27:3:223:LYS:HD2	2.16	0.44
27:3:550:ASN:HD21	27:3:595:VAL:H	1.63	0.44
27:3:615:ARG:NE	27:3:627:PRO:HB3	2.33	0.44
27:3:842:PHE:HD2	27:3:843:LEU:HD12	1.81	0.44
27:3:870:ASN:ND2	27:3:872:ILE:HB	2.21	0.44
27:3:965:LYS:HG2	27:3:988:ASN:O	2.17	0.44
1:A:617:ASN:HA	1:A:621:VAL:CG2	2.46	0.44
1:A:2118:SER:HB3	1:A:2124:ILE:HD13	1.98	0.44
1:A:2295:GLU:O	1:A:2296:LEU:HD23	2.18	0.44
2:B:36:C:O2	20:U:11:ARG:NH2	2.50	0.44
3:C:493:PHE:HB2	3:C:551:LEU:HD23	1.98	0.44
3:C:902:HIS:ND1	3:C:903:HIS:HD2	2.16	0.44
5:E:343:ILE:HG23	5:E:351:LEU:HD13	2.00	0.44
6:F:28:A:N1	14:O:173:CYS:HA	2.32	0.44
8:H:46:U:HO2'	8:H:47:U:P	2.36	0.44
10:J:227:LYS:HB3	10:J:251:TRP:CZ2	2.53	0.44
13:N:15:TRP:O	13:N:18:ILE:HG12	2.17	0.44
17:R:138:GLU:HG3	17:R:139:ALA:H	1.83	0.44
26:1:630:ARG:O	26:1:634:VAL:HG23	2.17	0.44
26:1:1182:LEU:HG	26:1:1226:VAL:HG21	2.00	0.44
27:3:91:GLU:OE1	27:3:102:ILE:HD11	2.18	0.44
27:3:608:GLY:HA2	27:3:614:VAL:CG2	2.48	0.44
1:A:281:PRO:HG2	1:A:284:ARG:NH1	2.33	0.44
1:A:719:CYS:HG	17:R:254:TRP:HZ3	1.62	0.44
1:A:1091:TYR:O	1:A:1092:ILE:C	2.56	0.44
1:A:1303:LEU:HD13	1:A:1311:PHE:CE1	2.53	0.44
2:B:106:U:H2'	2:B:107:U:C6	2.53	0.44
7:G:104:C:H1'	7:G:105:C:OP1	2.18	0.44
10:J:350:ILE:HD12	10:J:350:ILE:HA	1.66	0.44
19:T:314:ILE:HD11	19:T:326:LEU:HD11	1.99	0.44
21:V:641:ASP:OD2	21:V:642:GLU:N	2.51	0.44
26:1:166:ARG:O	26:1:170:GLN:HG2	2.16	0.44
26:1:667:ILE:O	26:1:671:ILE:HG13	2.18	0.44
26:1:1091:HIS:NE2	31:2:568:TYR:OH	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:365:GLY:HA3	27:3:394:ASN:ND2	2.32	0.44
27:3:607:VAL:O	27:3:614:VAL:HG22	2.17	0.44
37:8:35:GLU:OE1	37:8:35:GLU:N	2.51	0.44
1:A:39:GLN:O	1:A:43:LYS:HD2	2.17	0.44
1:A:436:PRO:HB2	1:A:439:GLN:NE2	2.32	0.44
1:A:468:LYS:HE2	1:A:468:LYS:HA	2.00	0.44
1:A:1879:PHE:HB3	1:A:1882:ILE:HG13	2.00	0.44
3:C:89:LEU:HG	19:T:240:LEU:HD11	1.98	0.44
3:C:531:TRP:O	3:C:532:ILE:HD13	2.17	0.44
5:E:67:GLY:C	5:E:349:LYS:HG2	2.38	0.44
6:F:10:U:H2'	6:F:11:C:O4'	2.17	0.44
7:G:7:G:C2	7:G:8:C:N3	2.86	0.44
10:J:318:TYR:O	10:J:322:MET:HG2	2.18	0.44
10:J:424:GLU:OE1	10:J:464:ASP:HA	2.18	0.44
17:R:185:GLY:O	17:R:188:PHE:N	2.26	0.44
19:T:417:ASN:ND2	19:T:432:ASP:HB2	2.32	0.44
23:X:277:ARG:HH21	26:1:434:THR:CB	2.27	0.44
24:Y:2:ASN:HB2	24:Y:3:PRO:HD2	1.99	0.44
26:1:897:LEU:O	26:1:901:GLN:HG3	2.18	0.44
27:3:324:GLU:OE1	27:3:374:SER:HB2	2.18	0.44
27:3:384:THR:OG1	27:3:385:PHE:O	2.35	0.44
31:2:464:GLU:O	31:2:468:LEU:HG	2.18	0.44
31:2:586:ILE:HG22	31:2:587:HIS:N	2.33	0.44
36:9:288:LYS:HB2	36:9:406:VAL:HG13	1.99	0.44
1:A:769:LYS:HE2	1:A:1249:MET:O	2.18	0.44
1:A:1275:ARG:C	1:A:1276:GLU:HG3	2.37	0.44
1:A:1876:LEU:CD1	1:A:1884:ILE:HD11	2.48	0.44
1:A:2074:ARG:HG2	1:A:2074:ARG:H	1.45	0.44
5:E:85:GLY:O	5:E:112:VAL:N	2.51	0.44
5:E:202:ASN:ND2	5:E:204:THR:OG1	2.51	0.44
8:H:160:A:H2'	8:H:161:U:C6	2.52	0.44
11:K:105:SER:OG	11:K:106:ALA:N	2.51	0.44
12:L:74:LEU:O	12:L:77:LEU:N	2.50	0.44
19:T:338:CYS:HA	19:T:344:GLN:O	2.17	0.44
23:X:251:GLU:H	23:X:251:GLU:HG3	1.52	0.44
23:X:323:ARG:HE	23:X:325:LYS:HG3	1.82	0.44
26:1:1055:TRP:HB2	26:1:1088:ILE:HD11	2.00	0.44
27:3:165:THR:O	27:3:165:THR:OG1	2.31	0.44
27:3:293:HIS:HD1	27:3:300:PHE:HZ	1.66	0.44
27:3:982:GLU:HG3	27:3:983:ASN:N	2.32	0.44
33:6:56:THR:O	33:6:59:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:9:353:GLU:HG3	36:9:355:ARG:HH21	1.82	0.44
1:A:75:ASP:O	1:A:77:THR:N	2.51	0.44
1:A:381:PRO:O	1:A:383:PHE:N	2.49	0.44
1:A:730:GLY:O	17:R:248:PRO:HG3	2.18	0.44
1:A:827:PHE:CD2	1:A:827:PHE:C	2.90	0.44
1:A:1361:GLU:HG2	1:A:1362:ASP:N	2.33	0.44
1:A:1434:LYS:O	1:A:1439:ARG:NH2	2.50	0.44
1:A:2153:THR:HG22	1:A:2154:HIS:H	1.82	0.44
4:D:971:LYS:N	4:D:980:GLN:O	2.33	0.44
6:F:94:C:H5"	10:J:351:ASN:HD22	1.83	0.44
6:F:96:U:H2'	6:F:97:U:C6	2.53	0.44
8:H:155:C:H2'	8:H:156:U:C6	2.53	0.44
15:P:205:LYS:HE3	15:P:205:LYS:HB3	1.66	0.44
21:V:632:THR:HG22	22:W:115:UNK:HA	2.00	0.44
26:1:1289:ASN:HD22	26:1:1294:THR:HG23	1.82	0.44
27:3:21:ASN:OD1	27:3:69:ARG:NH2	2.50	0.44
27:3:77:TYR:CD1	27:3:91:GLU:HB2	2.52	0.44
27:3:782:GLN:HG3	27:3:867:ARG:NH2	2.29	0.44
36:9:295:LEU:HD22	36:9:397:PHE:C	2.37	0.44
36:9:320:ILE:HA	36:9:427:ARG:HA	2.00	0.44
1:A:486:LYS:O	1:A:487:LEU:HD23	2.18	0.43
1:A:913:PRO:O	1:A:917:ILE:HG13	2.18	0.43
1:A:976:MET:HE2	1:A:1098:PHE:HD1	1.82	0.43
1:A:2111:LEU:HD22	1:A:2263:LEU:HD11	1.99	0.43
1:A:2192:ASP:HB3	1:A:2213:ILE:HG21	2.00	0.43
3:C:444:GLY:O	3:C:447:PRO:HD2	2.18	0.43
3:C:569:ARG:O	3:C:569:ARG:HG2	2.17	0.43
5:E:68:GLU:HB3	5:E:70:TYR:CE1	2.53	0.43
5:E:200:THR:O	5:E:209:ILE:HB	2.19	0.43
10:J:342:GLU:O	10:J:346:TRP:HD1	2.01	0.43
26:1:112:ILE:HD11	26:1:546:ASP:HA	1.99	0.43
27:3:457:ASN:OD1	27:3:477:SER:OG	2.28	0.43
1:A:467:GLN:OE1	1:A:467:GLN:HA	2.16	0.43
1:A:805:GLU:O	1:A:809:VAL:HG23	2.18	0.43
1:A:1359:HIS:HB2	1:A:1361:GLU:O	2.17	0.43
1:A:1941:ARG:HH12	1:A:2013:GLY:N	2.16	0.43
1:A:2120:LEU:O	1:A:2182:PRO:HB3	2.18	0.43
1:A:2149:PRO:HB3	1:A:2281:TYR:CE1	2.53	0.43
5:E:217:ILE:HB	5:E:231:MET:CG	2.48	0.43
5:E:304:SER:H	5:E:330:ILE:HB	1.84	0.43
5:E:343:ILE:HD13	5:E:343:ILE:HA	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:13:C:C1’	8:H:14:C:H5’	2.48	0.43
8:H:59:A:C2’	8:H:60:U:H5’	2.48	0.43
10:J:437:LYS:O	10:J:440:LEU:N	2.51	0.43
18:S:615:LEU:O	18:S:674:THR:HA	2.18	0.43
24:Y:17:GLU:HB2	26:1:825:LEU:HD21	1.99	0.43
26:1:1197:LEU:HD11	34:7:78:GLN:NE2	2.33	0.43
27:3:637:PRO:HB3	27:3:640:LEU:CD2	2.48	0.43
27:3:644:GLU:HG3	27:3:662:PHE:HB3	1.99	0.43
37:8:37:LYS:HG2	37:8:38:VAL:N	2.33	0.43
1:A:950:LEU:O	1:A:954:LYS:HG3	2.17	0.43
5:E:168:CYS:HB2	5:E:201:PHE:CE1	2.53	0.43
5:E:321:TYR:HD1	5:E:323:LEU:HD21	1.83	0.43
7:G:17:U:H3’	7:G:18:A:H8	1.83	0.43
15:P:206:LYS:HA	15:P:209:ARG:HD2	2.00	0.43
16:Q:567:VAL:HA	16:Q:589:LEU:HA	2.00	0.43
17:R:148:ARG:O	17:R:148:ARG:NH2	2.51	0.43
19:T:283:HIS:O	19:T:320:LYS:HD3	2.19	0.43
23:X:315:ARG:CZ	23:X:321:GLY:HA3	2.48	0.43
26:1:1080:THR:O	26:1:1084:ILE:HG23	2.18	0.43
27:3:226:GLU:HG2	27:3:261:PHE:CZ	2.53	0.43
27:3:286:ILE:HG12	27:3:306:GLU:OE2	2.18	0.43
27:3:558:LEU:HD12	27:3:558:LEU:N	2.33	0.43
27:3:704:VAL:HG22	27:3:706:MET:HG2	2.00	0.43
31:2:495:ARG:HE	31:2:495:ARG:HB3	1.36	0.43
35:5:14:LEU:HA	35:5:14:LEU:HD23	1.60	0.43
36:9:273:TYR:CG	36:9:301:PRO:HB2	2.53	0.43
1:A:1089:CYS:SG	1:A:1096:HIS:CD2	3.11	0.43
1:A:2067:PHE:CE2	1:A:2069:SER:HA	2.53	0.43
3:C:173:THR:O	3:C:177:ARG:HB2	2.18	0.43
3:C:572:GLU:H	3:C:572:GLU:HG3	1.60	0.43
5:E:277:PHE:HE2	5:E:300:ILE:HD13	1.82	0.43
17:R:195:ARG:HG2	17:R:195:ARG:NH1	2.33	0.43
18:S:867:ALA:HB1	18:S:901:ASN:HA	2.00	0.43
21:V:581:ILE:HD11	25:Z:540:ARG:HG3	2.01	0.43
23:X:253:ARG:HD3	23:X:253:ARG:HA	1.73	0.43
27:3:257:THR:HG23	27:3:267:ILE:O	2.18	0.43
27:3:458:ALA:O	27:3:459:VAL:HG23	2.18	0.43
27:3:536:TRP:CE2	27:3:576:GLU:HG3	2.54	0.43
27:3:636:GLN:H	27:3:670:GLN:HE22	1.66	0.43
27:3:700:LYS:HE2	27:3:715:MET:O	2.18	0.43
27:3:939:PHE:CZ	27:3:942:LYS:HG2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:4:151:SER:H	32:4:154:ALA:HB3	1.82	0.43
33:6:27:PRO:HG3	33:6:83:CYS:CB	2.48	0.43
36:9:360:HIS:HB2	36:9:387:CYS:O	2.18	0.43
37:8:55:ARG:HA	37:8:55:ARG:HD2	1.39	0.43
1:A:533:LYS:HE3	6:F:37:C:H5	1.83	0.43
1:A:718:ARG:NH2	17:R:255:LYS:HE2	2.34	0.43
1:A:1310:ARG:NH2	1:A:1563:HIS:O	2.51	0.43
1:A:1821:ILE:HG12	1:A:1906:ILE:HG12	2.01	0.43
1:A:1980:GLU:O	1:A:1984:LYS:HG3	2.19	0.43
1:A:2074:ARG:NH2	4:D:1046:ILE:O	2.51	0.43
2:B:18:C:O2	2:B:59:G:N2	2.26	0.43
3:C:733:TRP:NE1	3:C:747:ASP:OD2	2.52	0.43
8:H:97:G:H2'	8:H:97:G:N3	2.34	0.43
8:H:124:G:H2'	8:H:125:G:C8	2.54	0.43
26:1:564:ASP:OD1	26:1:564:ASP:N	2.44	0.43
26:1:649:LYS:HG2	26:1:689:ILE:HG12	2.00	0.43
26:1:1134:ASN:HD21	31:2:534:GLN:HA	1.84	0.43
36:9:423:LYS:HD2	36:9:423:LYS:HA	1.77	0.43
1:A:174:PRO:HA	1:A:520:TYR:CD1	2.54	0.43
1:A:1407:ASP:O	1:A:1408:LEU:HD23	2.19	0.43
1:A:1900:GLU:H	1:A:1900:GLU:CD	2.22	0.43
3:C:243:ILE:HD12	3:C:243:ILE:HA	1.65	0.43
3:C:244:LYS:HD2	3:C:292:TYR:CZ	2.54	0.43
3:C:477:HIS:HE1	3:C:562:THR:HG23	1.84	0.43
3:C:696:LEU:HD23	3:C:696:LEU:H	1.84	0.43
4:D:861:TYR:O	27:3:599:GLU:HG3	2.19	0.43
4:D:2103:ASN:HA	4:D:2123:SER:HA	2.00	0.43
5:E:62:LEU:HB3	5:E:93:TRP:CH2	2.54	0.43
6:F:23:U:C4	13:N:118:ILE:HD13	2.52	0.43
6:F:88:G:C2	8:H:11:G:C2	3.06	0.43
11:K:218:LYS:H	11:K:218:LYS:HG3	1.66	0.43
18:S:700:TYR:N	18:S:757:ARG:O	2.34	0.43
25:Z:497:TRP:CD1	25:Z:501:LEU:HD21	2.53	0.43
26:1:413:LYS:HB2	33:6:52:ASN:ND2	2.34	0.43
26:1:914:PHE:CG	26:1:954:LEU:HD11	2.54	0.43
26:1:929:LEU:N	26:1:930:PRO:HD2	2.34	0.43
27:3:325:ILE:O	27:3:374:SER:HA	2.19	0.43
27:3:615:ARG:NE	27:3:630:MET:HB3	2.33	0.43
33:6:21:LEU:HG	33:6:23:ILE:HD11	2.01	0.43
36:9:236:LEU:HB3	36:9:452:GLN:OE1	2.18	0.43
36:9:405:ASP:OD1	36:9:405:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:8:70:PHE:HZ	37:8:88:ASN:HD22	1.65	0.43
1:A:1593:LEU:HD23	1:A:1593:LEU:HA	1.66	0.43
1:A:1892:PRO:HG2	1:A:1940:LEU:HB3	2.00	0.43
2:B:12:U:H2'	2:B:13:C:C6	2.53	0.43
3:C:137:HIS:CD2	3:C:138:LEU:H	2.37	0.43
3:C:255:VAL:O	3:C:307:VAL:HA	2.18	0.43
3:C:650:GLU:H	3:C:650:GLU:CD	2.21	0.43
3:C:713:LYS:HA	3:C:716:GLU:OE1	2.19	0.43
4:D:1733:HIS:O	4:D:1737:ASN:CB	2.66	0.43
6:F:89:U:H2'	6:F:90:G:O4'	2.18	0.43
8:H:119:G:O2'	8:H:120:A:H5'	2.18	0.43
16:Q:849:THR:O	16:Q:1034:ILE:HA	2.17	0.43
19:T:208:ARG:HE	19:T:208:ARG:HB3	1.32	0.43
21:V:570:LEU:HD12	21:V:570:LEU:HA	1.77	0.43
23:X:337:THR:HB	23:X:344:ILE:HD11	2.00	0.43
26:1:818:PHE:O	26:1:823:MET:HG3	2.19	0.43
26:1:1091:HIS:CE1	31:2:568:TYR:HE1	2.36	0.43
27:3:412:ILE:H	27:3:1105:GLN:NE2	2.16	0.43
27:3:470:PHE:HA	27:3:746:ALA:HB3	2.01	0.43
27:3:807:TYR:O	27:3:856:LYS:HE2	2.18	0.43
27:3:1015:LYS:HZ3	27:3:1067:ASP:HB2	1.83	0.43
32:4:104:ILE:HA	32:4:174:VAL:HA	1.99	0.43
33:6:116:LYS:HG2	33:6:117:TYR:CE1	2.54	0.43
36:9:117:VAL:HA	36:9:157:THR:HA	2.00	0.43
36:9:273:TYR:OH	36:9:302:LYS:HA	2.19	0.43
3:C:404:THR:OG1	3:C:405:LYS:N	2.51	0.43
3:C:705:VAL:HG22	3:C:705:VAL:O	2.17	0.43
3:C:724:TRP:HH2	3:C:788:LYS:HE3	1.84	0.43
7:G:-10:G:N7	20:U:1:MET:HE3	2.32	0.43
14:O:34:ILE:O	17:R:198:ARG:NH1	2.51	0.43
17:R:184:GLN:NE2	17:R:193:LYS:HA	2.34	0.43
17:R:240:LYS:HA	17:R:240:LYS:HD2	1.78	0.43
25:Z:497:TRP:HD1	25:Z:501:LEU:HD21	1.84	0.43
25:Z:579:TRP:CE3	25:Z:580:PRO:HD2	2.53	0.43
27:3:278:LEU:HD21	27:3:816:LYS:HB2	2.00	0.43
27:3:280:ASP:HA	27:3:281:PRO:HD3	1.93	0.43
27:3:838:MET:N	27:3:838:MET:SD	2.92	0.43
37:8:39:ASP:OD2	37:8:40:MET:N	2.52	0.43
1:A:762:ARG:HH12	15:P:226:LYS:HZ1	1.67	0.43
1:A:1763:LEU:O	1:A:1764:SER:O	2.37	0.43
1:A:1764:SER:C	1:A:1766:GLN:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1872:LEU:HD13	1:A:1884:ILE:HD13	2.00	0.43
1:A:1911:GLU:HG2	1:A:1912:PRO:HD2	2.01	0.43
5:E:280:ASN:ND2	5:E:303:GLY:O	2.49	0.43
6:F:85:U:H1'	6:F:86:U:C4	2.54	0.43
7:G:12:G:P	7:G:13:C:H41	2.42	0.43
10:J:236:ARG:O	10:J:239:ARG:NE	2.51	0.43
16:Q:600:MET:O	16:Q:608:ILE:N	2.52	0.43
19:T:459:LEU:HA	36:9:259:THR:HB	2.01	0.43
21:V:577:SER:HB2	25:Z:543:ASP:OD2	2.19	0.43
21:V:638:GLY:HA2	21:V:641:ASP:OD1	2.19	0.43
26:1:396:ASN:HB2	33:6:67:ILE:HG23	2.00	0.43
26:1:539:LEU:HD12	26:1:539:LEU:HA	1.66	0.43
26:1:998:LYS:NZ	26:1:1041:ARG:HD3	2.33	0.43
27:3:264:GLN:OE1	27:3:265:PRO:HD2	2.18	0.43
27:3:1186:GLU:O	27:3:1189:LYS:N	2.51	0.43
31:2:524:LEU:HD23	31:2:524:LEU:HA	1.79	0.43
34:7:9:ILE:O	34:7:88:ILE:HA	2.19	0.43
1:A:139:VAL:HG11	1:A:212:PRO:HG2	2.01	0.43
1:A:386:PRO:HB3	3:C:371:GLU:O	2.19	0.43
1:A:1543:ASN:HB2	1:A:1569:LEU:HD21	2.01	0.43
1:A:2294:TYR:CE2	1:A:2296:LEU:HD21	2.54	0.43
3:C:319:THR:N	3:C:322:SER:HG	2.17	0.43
3:C:438:ILE:HD12	3:C:438:ILE:HA	1.70	0.43
9:I:140:LEU:N	9:I:141:PRO:HD3	2.34	0.43
10:J:394:HIS:HA	10:J:397:LYS:HD2	2.01	0.43
13:N:104:ARG:O	13:N:107:GLN:N	2.41	0.43
26:1:714:GLU:HB2	26:1:752:TYR:CE1	2.54	0.43
27:3:614:VAL:HG23	27:3:637:PRO:HG2	2.01	0.43
27:3:712:VAL:O	27:3:721:LEU:HD12	2.19	0.43
36:9:380:PHE:HZ	36:9:428:ILE:HD11	1.84	0.43
1:A:694:LEU:HD23	1:A:694:LEU:HA	1.84	0.42
1:A:1544:ARG:HB2	1:A:1672:ASP:OD2	2.19	0.42
1:A:2179:HIS:CD2	1:A:2215:THR:HA	2.54	0.42
3:C:699:ASP:OD2	3:C:722:TYR:OH	2.35	0.42
3:C:727:LEU:HD12	3:C:727:LEU:HA	1.79	0.42
5:E:100:ASP:OD1	5:E:100:ASP:N	2.52	0.42
5:E:263:ASP:OD1	5:E:263:ASP:N	2.52	0.42
10:J:226:ARG:O	10:J:230:THR:HG23	2.19	0.42
13:N:18:ILE:HG22	13:N:63:LEU:HD12	2.00	0.42
26:1:714:GLU:HB2	26:1:752:TYR:CD1	2.53	0.42
26:1:1017:LEU:HD23	26:1:1050:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:MET:HE3	1:A:76:MET:HB3	1.95	0.42
1:A:106:MET:HA	1:A:107:PRO:HD3	1.76	0.42
1:A:985:TYR:N	1:A:985:TYR:HD1	2.15	0.42
1:A:1330:MET:HE2	1:A:1330:MET:HB3	1.83	0.42
1:A:1458:GLN:HB2	17:R:421:GLY:H	1.83	0.42
3:C:718:PHE:HB3	3:C:724:TRP:HD1	1.84	0.42
3:C:770:PHE:CE1	3:C:789:PHE:CD1	3.03	0.42
3:C:818:SER:O	3:C:822:MET:HB2	2.19	0.42
7:G:2:U:H5"	7:G:3:A:H4'	2.01	0.42
8:H:3:C:H2'	8:H:4:G:C8	2.54	0.42
8:H:149:A:H2'	8:H:150:U:C6	2.54	0.42
10:J:273:TYR:CD1	17:R:226:PRO:HB2	2.54	0.42
26:1:415:LEU:HD23	26:1:415:LEU:HA	1.86	0.42
26:1:789:LEU:HD12	26:1:789:LEU:HA	1.88	0.42
26:1:1029:GLU:OE2	26:1:1070:LYS:HB2	2.19	0.42
26:1:1084:ILE:HG21	26:1:1084:ILE:HD13	1.69	0.42
26:1:1289:ASN:HB3	26:1:1294:THR:HA	2.01	0.42
27:3:50:VAL:CG2	27:3:401:LEU:HD11	2.49	0.42
27:3:1118:VAL:HG22	27:3:1128:ILE:HG22	2.00	0.42
33:6:114:LYS:HE3	33:6:114:LYS:HB3	1.73	0.42
35:5:11:LEU:HD12	35:5:12:GLU:N	2.34	0.42
36:9:365:ILE:HG23	36:9:396:ILE:CG2	2.49	0.42
1:A:762:ARG:NH2	15:P:226:LYS:NZ	2.67	0.42
1:A:1072:LEU:HD22	1:A:1087:LEU:HB3	2.01	0.42
1:A:1855:GLU:HG2	11:K:133:ILE:HG12	2.00	0.42
3:C:736:GLY:O	3:C:738:ASP:N	2.52	0.42
5:E:70:TYR:HB2	5:E:85:GLY:HA2	2.01	0.42
7:G:7:G:C2	7:G:8:C:C2	3.06	0.42
7:G:99:C:C2'	7:G:100:C:H5'	2.50	0.42
19:T:414:ALA:O	19:T:416:ILE:HG13	2.19	0.42
21:V:580:ARG:HG2	21:V:630:PHE:CE2	2.55	0.42
26:1:1059:CYS:SG	26:1:1084:ILE:HD11	2.58	0.42
26:1:1182:LEU:HA	26:1:1182:LEU:HD12	1.64	0.42
27:3:275:ARG:HA	27:3:386:PHE:CD2	2.55	0.42
27:3:294:LYS:HB3	27:3:294:LYS:HE3	1.73	0.42
27:3:488:GLY:N	27:3:491:VAL:HG22	2.33	0.42
27:3:740:GLU:HB2	27:3:757:ILE:HD12	2.01	0.42
27:3:781:LEU:HB3	27:3:801:GLU:OE1	2.18	0.42
27:3:1015:LYS:NZ	27:3:1066:VAL:O	2.49	0.42
36:9:235:LYS:HD3	36:9:452:GLN:HB2	2.01	0.42
36:9:278:LYS:HE3	36:9:278:LYS:HB3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:9:405:ASP:HA	36:9:408:THR:OG1	2.19	0.42
1:A:1571:ILE:HD13	11:K:218:LYS:O	2.19	0.42
1:A:2275:ALA:HB2	1:A:2296:LEU:O	2.19	0.42
3:C:745:LEU:HB2	3:C:770:PHE:CE2	2.55	0.42
6:F:35:A:H1'	7:G:12:G:O6	2.19	0.42
6:F:57:U:C2'	6:F:58:G:H5'	2.49	0.42
7:G:85:G:H1	8:H:44:U:H3	1.66	0.42
8:H:46:U:H1'	8:H:47:U:H5"	2.00	0.42
10:J:334:GLU:O	10:J:338:GLU:HG3	2.20	0.42
10:J:419:PHE:HD1	10:J:419:PHE:HA	1.74	0.42
16:Q:708:GLN:HA	16:Q:816:PRO:HD2	2.02	0.42
19:T:297:HIS:HA	19:T:338:CYS:SG	2.60	0.42
21:V:491:ASN:O	21:V:494:LEU:HB3	2.19	0.42
21:V:639:LEU:HA	21:V:642:GLU:OE2	2.20	0.42
23:X:261:LEU:HA	23:X:261:LEU:HD12	1.76	0.42
26:1:402:GLU:OE1	26:1:402:GLU:HA	2.16	0.42
26:1:687:VAL:HA	26:1:690:ILE:HG22	2.00	0.42
27:3:139:LYS:HB2	27:3:160:ALA:HB3	2.01	0.42
27:3:488:GLY:H	27:3:491:VAL:HG13	1.84	0.42
31:2:534:GLN:O	31:2:538:GLU:HG3	2.20	0.42
35:5:17:LYS:HA	35:5:17:LYS:HD2	1.58	0.42
37:8:75:LEU:HA	37:8:75:LEU:HD23	1.83	0.42
1:A:648:LEU:HA	1:A:648:LEU:HD23	1.79	0.42
1:A:1295:ILE:HG13	1:A:1296:GLN:N	2.35	0.42
1:A:1457:HIS:CD2	17:R:420:SER:HB3	2.54	0.42
1:A:2166:HIS:CG	1:A:2168:TYR:HB2	2.54	0.42
1:A:2188:LEU:HD13	1:A:2228:TYR:CG	2.55	0.42
3:C:796:VAL:HG12	3:C:800:PRO:HB3	2.01	0.42
5:E:102:TYR:HD1	5:E:102:TYR:H	1.67	0.42
7:G:99:C:H2'	7:G:100:C:C6	2.54	0.42
8:H:11:G:C2	8:H:12:G:C8	3.07	0.42
8:H:13:C:H1'	8:H:14:C:OP2	2.20	0.42
8:H:18:U:H1'	8:H:19:G:OP1	2.20	0.42
13:N:106:ILE:HG22	13:N:116:ASN:HD22	1.85	0.42
16:Q:440:PRO:HG2	16:Q:1108:ALA:HB1	2.01	0.42
17:R:236:LYS:HD3	17:R:236:LYS:HA	1.53	0.42
17:R:251:ILE:HD12	17:R:251:ILE:HA	1.79	0.42
18:S:876:GLY:HA3	18:S:1001:LEU:HA	2.02	0.42
19:T:191:HIS:CD2	19:T:440:ASP:OD1	2.73	0.42
19:T:443:THR:O	19:T:443:THR:OG1	2.35	0.42
21:V:456:ARG:HG2	21:V:492:MET:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:505:LYS:HE3	21:V:553:HIS:NE2	2.34	0.42
26:1:163:LYS:HD2	26:1:166:ARG:NH1	2.35	0.42
27:3:319:GLU:H	27:3:319:GLU:CD	2.21	0.42
32:4:54:GLN:C	32:4:56:TYR:H	2.23	0.42
33:6:54:PRO:HA	33:6:57:ARG:HB2	2.01	0.42
34:7:37:VAL:HB	34:7:38:ARG:HG3	2.00	0.42
34:7:58:CYS:HB3	34:7:62:GLY:N	2.23	0.42
1:A:75:ASP:HB3	1:A:498:ARG:HH12	1.85	0.42
1:A:366:LYS:HE2	1:A:366:LYS:HB2	1.77	0.42
1:A:1516:LYS:H	1:A:1516:LYS:HG2	1.60	0.42
1:A:1639:VAL:HG11	1:A:1699:THR:CG2	2.50	0.42
1:A:2007:ILE:O	1:A:2011:ILE:HG13	2.19	0.42
1:A:2315:LEU:HA	1:A:2317:PHE:CE1	2.54	0.42
3:C:335:ASN:HD22	3:C:338:GLU:HB2	1.83	0.42
4:D:1350:ALA:HB1	4:D:1354:SER:CB	2.49	0.42
5:E:262:TRP:HA	5:E:272:ARG:O	2.20	0.42
7:G:112:U:H2'	7:G:113:U:O4'	2.20	0.42
8:H:52:G:H2'	8:H:53:U:C6	2.55	0.42
10:J:423:GLU:HB3	10:J:432:VAL:HG23	2.01	0.42
13:N:19:GLU:HG3	13:N:23:ASP:OD2	2.19	0.42
26:1:122:HIS:CE1	26:1:125:THR:HG1	2.37	0.42
26:1:1132:LEU:HD23	26:1:1132:LEU:HA	1.84	0.42
26:1:1174:GLU:O	26:1:1178:MET:HG3	2.20	0.42
27:3:568:MET:HE1	27:3:570:PRO:HA	2.01	0.42
27:3:875:ASN:N	27:3:875:ASN:ND2	2.65	0.42
27:3:1055:VAL:HG23	27:3:1093:MET:HG2	2.01	0.42
37:8:34:LEU:HG	37:8:82:SER:CB	2.48	0.42
1:A:462:ARG:HA	1:A:462:ARG:HE	1.85	0.42
1:A:781:ARG:NH2	8:H:24:A:H5"	2.34	0.42
1:A:1723:LYS:HB3	1:A:1724:PRO:HD3	2.02	0.42
1:A:1939:ILE:HG23	1:A:1954:LEU:HD11	2.01	0.42
1:A:2129:TYR:CG	1:A:2169:LEU:HD22	2.54	0.42
1:A:2252:LEU:H	1:A:2255:HIS:CE1	2.38	0.42
3:C:491:HIS:CD2	3:C:551:LEU:HD13	2.55	0.42
3:C:658:PRO:HB2	3:C:881:PHE:CZ	2.55	0.42
3:C:872:LYS:HE3	3:C:872:LYS:HB2	1.92	0.42
12:L:62:GLU:OE2	12:L:62:GLU:N	2.53	0.42
17:R:253:ASN:HB3	17:R:254:TRP:CZ3	2.54	0.42
19:T:245:HIS:HE2	19:T:263:SER:HG	1.58	0.42
19:T:351:ASP:OD1	19:T:351:ASP:N	2.47	0.42
21:V:286:THR:H	21:V:289:SER:CB	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:519:LYS:HA	21:V:522:MET:HG3	2.01	0.42
23:X:315:ARG:NH2	23:X:321:GLY:HA3	2.35	0.42
26:1:141:LYS:HG2	26:1:142:THR:O	2.19	0.42
27:3:811:THR:O	27:3:815:ARG:HG3	2.20	0.42
34:7:46:CYS:H	34:7:85:CYS:HB2	1.84	0.42
37:8:70:PHE:HZ	37:8:88:ASN:ND2	2.18	0.42
1:A:62:PRO:HB2	1:A:64:GLU:OE1	2.19	0.42
1:A:1189:MET:HE2	1:A:1189:MET:HB2	1.78	0.42
1:A:2189:SER:HB2	1:A:2192:ASP:CG	2.40	0.42
1:A:2237:TRP:CZ2	1:A:2248:PRO:HB2	2.55	0.42
1:A:2330:ARG:NH1	4:D:546:SER:H	2.17	0.42
5:E:202:ASN:ND2	5:E:207:GLN:OE1	2.53	0.42
5:E:251:LEU:HD23	5:E:291:CYS:HB2	2.01	0.42
5:E:282:HIS:H	5:E:282:HIS:CD2	2.38	0.42
6:F:87:C:C2	6:F:88:G:C8	3.08	0.42
7:G:101:U:O4	34:7:102:ARG:HD2	2.19	0.42
9:I:428:GLN:CB	9:I:470:PHE:H	2.33	0.42
10:J:385:PHE:CE1	10:J:389:HIS:HD2	2.37	0.42
17:R:314:GLN:OE1	17:R:315:LYS:N	2.52	0.42
24:Y:69:ARG:HE	24:Y:69:ARG:HB3	1.47	0.42
26:1:648:LEU:O	26:1:649:LYS:C	2.58	0.42
26:1:747:LEU:HD12	26:1:747:LEU:HA	1.67	0.42
26:1:833:LEU:O	26:1:837:THR:OG1	2.29	0.42
26:1:1028:HIS:HB3	26:1:1031:VAL:HG13	2.02	0.42
27:3:187:MET:CE	27:3:206:GLN:HG2	2.49	0.42
27:3:805:ASN:N	27:3:861:GLN:O	2.50	0.42
36:9:336:THR:HG21	36:9:341:GLY:HA3	2.00	0.42
1:A:549:GLU:HB2	1:A:591:MET:HG3	2.02	0.42
1:A:693:ILE:HG22	1:A:694:LEU:CD2	2.50	0.42
1:A:825:ILE:HD13	1:A:825:ILE:HG21	1.89	0.42
1:A:981:PHE:O	1:A:1166:THR:OG1	2.38	0.42
1:A:1093:ASP:OD1	1:A:1093:ASP:N	2.51	0.42
1:A:1923:TRP:O	1:A:1927:ILE:HG12	2.20	0.42
3:C:600:LEU:N	3:C:601:PRO:HD2	2.34	0.42
3:C:610:VAL:HG12	3:C:648:TYR:HD2	1.85	0.42
3:C:850:LEU:HD23	3:C:850:LEU:HA	1.73	0.42
10:J:411:MET:O	10:J:443:ILE:HD12	2.20	0.42
13:N:28:LYS:NZ	13:N:28:LYS:HB2	2.35	0.42
27:3:982:GLU:OE2	27:3:984:LYS:HE3	2.20	0.42
36:9:269:ASP:OD2	36:9:269:ASP:N	2.43	0.42
1:A:150:MET:HG3	1:A:193:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PRO:HD3	1:A:520:TYR:CD1	2.55	0.42
1:A:312:TYR:CD1	1:A:312:TYR:N	2.88	0.42
1:A:988:ILE:HG21	1:A:1030:ILE:HD12	2.02	0.42
1:A:1020:LYS:H	1:A:1020:LYS:HG3	1.68	0.42
1:A:1179:SER:HB3	1:A:1181:ASP:H	1.85	0.42
1:A:1220:VAL:HG12	1:A:1221:THR:HG22	2.02	0.42
1:A:1284:LEU:HD23	1:A:1284:LEU:HA	1.86	0.42
1:A:1426:ASP:OD2	1:A:1426:ASP:N	2.53	0.42
1:A:1921:ASP:HB3	1:A:1966:HIS:CE1	2.55	0.42
1:A:2115:ILE:HG23	1:A:2218:PHE:CE1	2.54	0.42
3:C:244:LYS:HB2	3:C:292:TYR:CE2	2.55	0.42
3:C:519:GLU:O	3:C:522:SER:HB3	2.19	0.42
14:O:32:PRO:HA	17:R:195:ARG:NH1	2.34	0.42
17:R:332:ARG:HH12	23:X:267:ASP:HA	1.85	0.42
19:T:209:CYS:SG	19:T:252:VAL:HG22	2.60	0.42
21:V:615:LEU:HA	21:V:615:LEU:HD23	1.76	0.42
24:Y:53:ILE:O	24:Y:57:SER:HB2	2.20	0.42
26:1:145:PRO:HB2	26:1:146:LYS:HZ2	1.84	0.42
26:1:1088:ILE:HG22	26:1:1089:GLY:H	1.85	0.42
27:3:305:THR:CG2	27:3:309:ASP:HB2	2.50	0.42
27:3:507:SER:O	27:3:518:GLN:HA	2.20	0.42
27:3:563:LEU:HB3	27:3:581:LYS:H	1.84	0.42
27:3:889:PHE:HE2	27:3:913:LEU:HD12	1.84	0.42
27:3:1049:LYS:HB2	27:3:1049:LYS:HE3	1.64	0.42
34:7:102:ARG:O	34:7:105:TYR:N	2.53	0.42
36:9:273:TYR:CD2	36:9:301:PRO:HB2	2.53	0.42
36:9:397:PHE:CD1	36:9:397:PHE:N	2.74	0.42
37:8:55:ARG:O	37:8:59:ILE:HG13	2.20	0.42
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.83	0.41
1:A:534:GLU:O	1:A:538:SER:OG	2.28	0.41
1:A:1818:PHE:CE1	1:A:1916:LEU:HD13	2.55	0.41
1:A:2102:TYR:CD2	1:A:2140:LYS:HG2	2.55	0.41
2:B:9:G:H2'	2:B:10:U:C6	2.55	0.41
3:C:313:GLN:HB2	50:C:1500:GTP:C6	2.54	0.41
3:C:801:LEU:O	3:C:803:ARG:N	2.52	0.41
6:F:58:G:O2'	6:F:59:G:H5'	2.19	0.41
8:H:11:G:N1	8:H:12:G:N7	2.68	0.41
8:H:121:A:N3	8:H:121:A:H2'	2.35	0.41
17:R:282:GLU:HA	36:9:221:LEU:HD13	2.01	0.41
19:T:207:VAL:CG1	19:T:480:ALA:HB1	2.49	0.41
21:V:604:LYS:HD3	21:V:604:LYS:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:94:VAL:HG22	24:Y:109:VAL:HG12	2.02	0.41
26:1:758:ASP:N	26:1:758:ASP:OD1	2.41	0.41
26:1:832:GLN:O	26:1:836:THR:HG23	2.20	0.41
26:1:871:THR:OG1	26:1:872:ILE:N	2.53	0.41
26:1:1018:PRO:HG3	26:1:1054:GLU:OE2	2.18	0.41
27:3:136:GLU:OE2	27:3:189:TYR:OH	2.18	0.41
27:3:202:ALA:O	27:3:203:ASN:ND2	2.53	0.41
27:3:506:LEU:HD23	27:3:547:CYS:SG	2.59	0.41
1:A:119:LEU:HD12	1:A:483:GLN:O	2.20	0.41
1:A:338:VAL:O	3:C:266:GLU:HG2	2.19	0.41
1:A:376:GLU:O	1:A:377:GLU:HB3	2.20	0.41
1:A:723:ASN:ND2	36:9:253:THR:OG1	2.42	0.41
1:A:1658:GLN:HB2	11:K:98:VAL:HG11	2.02	0.41
1:A:2109:ASN:HA	1:A:2112:LYS:HD3	2.01	0.41
1:A:2213:ILE:N	1:A:2213:ILE:HD12	2.35	0.41
1:A:2264:SER:HA	1:A:2266:ARG:NH1	2.35	0.41
1:A:2327:SER:O	1:A:2327:SER:OG	2.33	0.41
3:C:137:HIS:HB3	3:C:140:HIS:CE1	2.55	0.41
3:C:556:ASP:OD1	3:C:557:GLN:N	2.51	0.41
3:C:674:CYS:CB	3:C:818:SER:HB2	2.46	0.41
3:C:780:CYS:O	3:C:941:LYS:NZ	2.46	0.41
5:E:136:TRP:HA	5:E:142:GLU:O	2.20	0.41
11:K:126:LYS:HD3	11:K:187:GLU:OE2	2.19	0.41
12:L:94:ALA:O	12:L:98:GLU:HG2	2.20	0.41
13:N:32:ALA:HA	13:N:35:GLU:HG3	2.01	0.41
21:V:216:ALA:HB2	21:V:262:HIS:CB	2.51	0.41
21:V:452:LEU:HD23	21:V:452:LEU:HA	1.72	0.41
27:3:544:ILE:CD1	27:3:556:ILE:HB	2.49	0.41
27:3:604:PHE:CD1	27:3:628:LEU:HD23	2.50	0.41
27:3:641:CYS:HB3	27:3:703:ARG:NE	2.35	0.41
27:3:715:MET:HG3	27:3:739:LEU:HB2	2.02	0.41
1:A:261:LYS:NZ	1:A:261:LYS:H	2.19	0.41
1:A:1275:ARG:O	1:A:1369:TYR:HE1	2.03	0.41
1:A:1778:TRP:CE2	1:A:1858:PRO:HG3	2.56	0.41
2:B:97:G:H2'	2:B:98:G:H8	1.82	0.41
3:C:590:ILE:HG13	3:C:637:LEU:HD13	2.02	0.41
5:E:73:LYS:NZ	5:E:73:LYS:HB2	2.33	0.41
5:E:126:SER:OG	5:E:136:TRP:NE1	2.53	0.41
5:E:240:GLY:O	5:E:252:SER:HA	2.20	0.41
6:F:85:U:C2	6:F:86:U:C4	3.08	0.41
6:F:90:G:H2'	6:F:91:A:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:118:G:N1	8:H:140:A:C6	2.88	0.41
10:J:269:LEU:HD12	10:J:269:LEU:HA	1.72	0.41
13:N:38:GLU:OE2	13:N:40:LYS:HD2	2.20	0.41
17:R:289:GLU:OE2	36:9:215:PHE:CD1	2.73	0.41
19:T:309:ASP:OD1	19:T:309:ASP:N	2.39	0.41
19:T:343:PRO:HD3	19:T:365:ARG:HH22	1.85	0.41
19:T:385:TYR:HE2	19:T:401:PRO:HD3	1.85	0.41
21:V:496:CYS:HB3	21:V:507:PHE:CE1	2.55	0.41
21:V:641:ASP:O	21:V:642:GLU:C	2.58	0.41
26:1:982:LEU:HA	26:1:982:LEU:HD12	1.79	0.41
26:1:1226:VAL:O	26:1:1230:VAL:HG23	2.20	0.41
27:3:174:ASP:HB3	27:3:240:GLY:H	1.85	0.41
27:3:747:SER:N	27:3:750:CYS:O	2.53	0.41
27:3:967:LEU:HD22	27:3:1002:VAL:HG21	2.02	0.41
27:3:1015:LYS:NZ	27:3:1067:ASP:HB2	2.35	0.41
31:2:469:VAL:HG11	31:2:489:VAL:HG11	2.03	0.41
35:5:15:GLN:O	35:5:18:TYR:O	2.39	0.41
36:9:282:VAL:O	36:9:293:LEU:HB3	2.21	0.41
1:A:380:LEU:HD12	3:C:349:PHE:CE1	2.55	0.41
1:A:407:ALA:O	1:A:412:ASN:ND2	2.54	0.41
1:A:464:PRO:HG2	2:B:20:G:C4	2.54	0.41
1:A:1194:CYS:HB3	1:A:1228:CYS:SG	2.60	0.41
1:A:1952:VAL:HA	25:Z:517:GLU:OE1	2.21	0.41
1:A:2143:ARG:O	1:A:2269:GLY:HA2	2.21	0.41
1:A:2178:ILE:HG13	1:A:2214:ILE:HB	2.02	0.41
3:C:83:GLU:HB2	3:C:84:GLU:H	1.71	0.41
3:C:491:HIS:HD2	3:C:551:LEU:HD13	1.85	0.41
3:C:687:MET:HB3	3:C:815:VAL:CG1	2.50	0.41
3:C:941:LYS:HG2	3:C:942:GLY:N	2.36	0.41
6:F:41:A:C2	7:G:6:A:N1	2.88	0.41
6:F:43:A:OP2	31:2:560:LYS:HE3	2.21	0.41
8:H:139:C:N4	8:H:140:A:H62	2.18	0.41
13:N:21:THR:O	13:N:24:GLU:HG3	2.19	0.41
14:O:188:ASP:O	14:O:190:ASP:N	2.53	0.41
16:Q:745:PRO:HG2	16:Q:781:PRO:HA	2.03	0.41
16:Q:817:GLY:O	16:Q:1090:ARG:HA	2.20	0.41
16:Q:1334:PRO:HD2	16:Q:1351:GLU:O	2.20	0.41
17:R:394:LEU:HD11	23:X:246:TYR:HA	2.03	0.41
19:T:325:THR:O	19:T:325:THR:OG1	2.38	0.41
21:V:600:ASN:OD1	21:V:604:LYS:HE3	2.20	0.41
23:X:338:PHE:HB2	23:X:359:LYS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1206:ASP:OD1	26:1:1207:SER:N	2.52	0.41
26:1:1227:ILE:HD12	26:1:1227:ILE:HA	1.79	0.41
26:1:1241:ILE:HD12	26:1:1241:ILE:HG23	1.67	0.41
27:3:472:ALA:O	27:3:487:ILE:N	2.54	0.41
27:3:667:ILE:HD12	27:3:675:LEU:O	2.21	0.41
27:3:672:GLY:O	27:3:690:ARG:HD3	2.20	0.41
27:3:720:TRP:HB3	27:3:731:LEU:HD11	2.02	0.41
27:3:1165:SER:HB3	27:3:1169:PRO:HA	2.02	0.41
36:9:268:GLU:O	36:9:269:ASP:C	2.58	0.41
36:9:287:ASN:ND2	36:9:426:ILE:HA	2.36	0.41
36:9:297:CYS:HA	36:9:304:CYS:SG	2.61	0.41
37:8:94:ASN:N	37:8:94:ASN:OD1	2.54	0.41
1:A:227:ARG:HA	1:A:416:GLY:O	2.20	0.41
1:A:361:HIS:HB2	3:C:280:HIS:ND1	2.35	0.41
1:A:1072:LEU:HD22	1:A:1087:LEU:HD22	2.01	0.41
1:A:1537:TRP:CE3	1:A:1751:LEU:HD13	2.56	0.41
1:A:1639:VAL:HG11	1:A:1699:THR:HG21	2.02	0.41
1:A:1781:ASP:OD2	1:A:1893:PHE:HB2	2.20	0.41
1:A:2249:LYS:HD2	1:A:2249:LYS:N	2.34	0.41
1:A:2320:LEU:HD13	1:A:2320:LEU:HA	1.77	0.41
2:B:62:G:H2'	2:B:63:A:C8	2.55	0.41
3:C:364:SER:OG	3:C:364:SER:O	2.37	0.41
3:C:441:PRO:C	3:C:444:GLY:HA3	2.40	0.41
4:D:1345:ASN:HA	4:D:1487:ILE:O	2.21	0.41
5:E:196:VAL:HG11	5:E:210:SER:OG	2.21	0.41
10:J:283:ALA:O	10:J:287:MET:HG2	2.20	0.41
10:J:377:LYS:HE3	10:J:377:LYS:HB3	1.89	0.41
10:J:408:ASP:HA	10:J:443:ILE:HG22	2.03	0.41
12:L:86:ALA:HB1	12:L:91:ARG:O	2.21	0.41
13:N:23:ASP:O	13:N:26:ASP:N	2.52	0.41
19:T:203:HIS:CD2	19:T:207:VAL:HG22	2.56	0.41
19:T:351:ASP:O	19:T:352:THR:OG1	2.28	0.41
23:X:264:PHE:CD1	23:X:269:VAL:HG22	2.55	0.41
26:1:1227:ILE:O	26:1:1231:MET:HG2	2.20	0.41
27:3:275:ARG:HA	27:3:386:PHE:HD2	1.85	0.41
27:3:590:MET:SD	27:3:607:VAL:HG22	2.60	0.41
31:2:513:GLY:C	31:2:515:ARG:H	2.23	0.41
33:6:14:PRO:HA	33:6:15:PRO:HD3	1.92	0.41
1:A:610:HIS:NE2	49:A:2401:IHP:O31	2.47	0.41
1:A:1838:LYS:HB3	1:A:1871:PRO:HG2	2.02	0.41
3:C:855:GLY:O	3:C:874:PHE:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2033:GLY:O	4:D:2096:ALA:N	2.48	0.41
5:E:125:PHE:HE2	5:E:135:VAL:HG13	1.85	0.41
7:G:7:G:C6	7:G:8:C:N4	2.89	0.41
8:H:48:A:H2'	8:H:49:U:C6	2.55	0.41
12:L:44:LYS:HB3	12:L:44:LYS:HE3	1.54	0.41
12:L:73:HIS:NE2	36:9:218:ASP:OD1	2.50	0.41
18:S:561:SER:O	18:S:566:ASP:N	2.48	0.41
25:Z:592:GLY:O	25:Z:596:LYS:HG3	2.21	0.41
26:1:151:THR:OG1	26:1:154:ASP:OD2	2.32	0.41
26:1:618:ASP:OD1	26:1:618:ASP:N	2.53	0.41
26:1:1062:LEU:O	26:1:1064:GLU:N	2.53	0.41
33:6:113:LEU:HD13	33:6:113:LEU:HA	1.89	0.41
37:8:96:LYS:HE2	37:8:96:LYS:HB3	1.55	0.41
1:A:47:GLU:OE1	1:A:47:GLU:N	2.40	0.41
1:A:696:MET:C	1:A:698:PRO:HD3	2.40	0.41
1:A:1526:LEU:H	1:A:1526:LEU:HD12	1.86	0.41
3:C:442:LYS:HA	3:C:442:LYS:HD3	1.63	0.41
4:D:642:THR:C	4:D:644:GLU:H	2.23	0.41
5:E:137:ASP:O	5:E:141:GLY:N	2.48	0.41
5:E:258:THR:HG22	5:E:260:ARG:HE	1.85	0.41
10:J:437:LYS:HA	10:J:437:LYS:HD2	1.62	0.41
12:L:98:GLU:HG3	12:L:99:HIS:N	2.36	0.41
17:R:234:SER:HB3	17:R:236:LYS:NZ	2.36	0.41
26:1:489:PRO:HB3	26:1:491:GLU:HG3	2.02	0.41
26:1:492:GLN:CD	26:1:495:ARG:HH11	2.24	0.41
26:1:641:ILE:N	26:1:642:PRO:HD2	2.36	0.41
26:1:888:LEU:HA	26:1:888:LEU:HD12	1.76	0.41
26:1:911:LEU:HG	26:1:957:ARG:HD2	2.02	0.41
26:1:969:LYS:H	26:1:969:LYS:HD2	1.86	0.41
27:3:329:TYR:OH	27:3:332:THR:HG22	2.21	0.41
27:3:511:LEU:HD13	27:3:517:VAL:HG21	2.02	0.41
27:3:580:ARG:HH11	27:3:580:ARG:HG3	1.85	0.41
27:3:679:LEU:HD13	27:3:679:LEU:HA	1.86	0.41
36:9:287:ASN:HD21	36:9:426:ILE:HA	1.86	0.41
1:A:261:LYS:H	1:A:261:LYS:HZ3	1.68	0.41
1:A:559:ASP:N	1:A:559:ASP:OD1	2.52	0.41
1:A:701:ILE:HD13	17:R:237:MET:SD	2.61	0.41
1:A:2012:LEU:HD13	1:A:2012:LEU:HA	1.79	0.41
3:C:323:PHE:CZ	3:C:373:ILE:HG23	2.56	0.41
3:C:394:ARG:O	3:C:397:ASP:HB2	2.21	0.41
5:E:119:THR:HG21	5:E:162:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:191:GLN:H	5:E:191:GLN:CD	2.23	0.41
7:G:83:A:N3	7:G:84:U:C5	2.88	0.41
7:G:91:A:H2'	7:G:92:U:C6	2.55	0.41
7:G:93:A:H2'	7:G:94:C:O4'	2.21	0.41
17:R:307:GLN:HG3	17:R:308:VAL:N	2.36	0.41
21:V:631:PHE:HD1	21:V:634:ILE:HD11	1.84	0.41
26:1:102:ASP:HA	26:1:103:PRO:HD3	1.86	0.41
26:1:1124:SER:HB2	26:1:1126:PHE:CE1	2.55	0.41
27:3:18:ILE:HD12	27:3:67:ALA:HB2	2.02	0.41
27:3:753:GLY:O	27:3:754:ILE:HD13	2.20	0.41
27:3:833:GLU:OE1	27:3:833:GLU:N	2.47	0.41
27:3:1053:ILE:HD13	27:3:1053:ILE:HG21	1.83	0.41
27:3:1190:GLN:O	27:3:1194:SER:OG	2.31	0.41
34:7:23:CYS:N	34:7:58:CYS:SG	2.73	0.41
35:5:50:LEU:HA	35:5:50:LEU:HD12	1.73	0.41
1:A:407:ALA:HB3	1:A:412:ASN:HB3	2.03	0.41
1:A:1817:LEU:HD22	1:A:1902:PHE:HE1	1.86	0.41
1:A:1924:LEU:HD23	1:A:1924:LEU:HA	1.67	0.41
1:A:2179:HIS:HD2	1:A:2214:ILE:O	2.03	0.41
2:B:64:G:C2	2:B:65:G:C4	3.09	0.41
3:C:278:LEU:HD23	3:C:278:LEU:HA	1.86	0.41
3:C:350:ASN:HD21	3:C:352:LYS:HB2	1.86	0.41
3:C:379:LYS:O	3:C:383:GLN:HG2	2.20	0.41
3:C:467:ASP:O	3:C:468:CYS:HB2	2.20	0.41
3:C:666:VAL:HG12	3:C:667:VAL:N	2.35	0.41
3:C:745:LEU:HD22	3:C:770:PHE:CG	2.56	0.41
4:D:503:ALA:O	4:D:653:ALA:HA	2.20	0.41
5:E:169:THR:HG1	5:E:179:TRP:HE1	1.64	0.41
5:E:174:GLY:HA2	5:E:194:TYR:C	2.42	0.41
6:F:5:U:H2'	6:F:7:G:H5'	2.02	0.41
6:F:5:U:H4'	6:F:6:C:OP2	2.20	0.41
6:F:78:A:H3'	6:F:79:C:H6	1.85	0.41
9:I:619:ALA:O	9:I:623:VAL:HA	2.21	0.41
11:K:231:GLN:HG2	11:K:234:ARG:HH21	1.85	0.41
12:L:37:LEU:HD12	12:L:37:LEU:HA	1.87	0.41
17:R:126:ASN:HD22	19:T:442:ARG:HD2	1.86	0.41
17:R:280:ILE:HG22	17:R:281:ASN:O	2.21	0.41
19:T:393:ASP:HB2	19:T:394:ASN:OD1	2.20	0.41
25:Z:543:ASP:OD2	25:Z:546:ALA:N	2.50	0.41
26:1:477:LYS:HB3	26:1:499:LYS:HZ3	1.86	0.41
26:1:1088:ILE:HG22	26:1:1089:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:206:GLN:HE21	27:3:231:HIS:CA	2.32	0.41
27:3:219:HIS:CE1	27:3:221:VAL:HG12	2.56	0.41
27:3:334:PRO:HG3	27:3:357:TYR:HE2	1.86	0.41
27:3:438:LEU:HB3	27:3:774:PHE:HB3	2.02	0.41
27:3:552:ARG:HH12	27:3:601:ARG:HH22	1.68	0.41
27:3:638:GLU:HB3	27:3:668:GLY:O	2.21	0.41
33:6:57:ARG:HD3	33:6:57:ARG:HA	1.82	0.41
33:6:85:ARG:HE	33:6:85:ARG:HB3	1.61	0.41
36:9:327:ASN:HD22	36:9:385:ARG:CD	2.34	0.41
37:8:21:GLN:HA	37:8:24:LEU:HD12	2.03	0.41
37:8:121:SER:HA	37:8:124:LEU:HD12	2.03	0.41
1:A:108:MET:HG3	1:A:110:TRP:CZ2	2.56	0.41
1:A:284:ARG:HH11	1:A:284:ARG:HG2	1.86	0.41
1:A:317:PRO:HB2	1:A:327:VAL:HG11	2.03	0.41
1:A:694:LEU:HD22	1:A:709:ILE:HD12	2.02	0.41
1:A:955:TRP:HE1	1:A:976:MET:HE1	1.86	0.41
1:A:1012:LYS:HG2	1:A:1036:PHE:HZ	1.85	0.41
1:A:1994:LYS:C	1:A:1995:ASN:HD22	2.17	0.41
1:A:2226:THR:HB	1:A:2228:TYR:CE1	2.56	0.41
3:C:259:LYS:HG2	50:C:1500:GTP:C6	2.56	0.41
3:C:731:SER:HB2	3:C:746:VAL:CG1	2.47	0.41
5:E:71:CYS:SG	5:E:114:GLU:HA	2.61	0.41
16:Q:1101:PRO:HD3	16:Q:1288:ARG:CB	2.51	0.41
21:V:553:HIS:O	21:V:557:THR:HG23	2.21	0.41
23:X:230:GLY:O	23:X:234:GLU:CB	2.68	0.41
26:1:405:ASP:O	33:6:99:GLN:NE2	2.53	0.41
27:3:275:ARG:O	27:3:275:ARG:HG3	2.20	0.41
27:3:455:ASN:HB2	27:3:479:VAL:CG2	2.51	0.41
33:6:34:GLU:O	33:6:35:MET:C	2.59	0.41
36:9:309:ARG:N	36:9:309:ARG:HD2	2.34	0.41
1:A:1000:ILE:HD12	1:A:1000:ILE:HA	1.51	0.40
1:A:1367:ASN:HD22	1:A:1367:ASN:HA	1.53	0.40
1:A:1956:PRO:HD2	1:A:1960:THR:HG21	2.03	0.40
3:C:83:GLU:H	3:C:83:GLU:HG2	1.55	0.40
3:C:189:VAL:HA	3:C:198:TYR:O	2.21	0.40
3:C:506:PRO:HG3	3:C:569:ARG:HH12	1.86	0.40
3:C:617:LEU:HD11	3:C:629:ILE:HG23	2.02	0.40
3:C:664:GLU:HB2	3:C:784:ILE:HG22	2.03	0.40
6:F:86:U:C4	8:H:12:G:O6	2.74	0.40
8:H:118:G:H2'	8:H:119:G:C8	2.56	0.40
21:V:565:LEU:HD12	21:V:612:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:529:GLU:O	25:Z:533:ARG:HG3	2.21	0.40
26:1:153:MET:HE2	26:1:153:MET:H	1.86	0.40
26:1:396:ASN:HB2	33:6:67:ILE:CG2	2.50	0.40
26:1:827:ARG:HE	26:1:827:ARG:HB2	1.67	0.40
26:1:1025:LYS:HB3	26:1:1025:LYS:HE3	1.61	0.40
26:1:1136:TYR:HB2	26:1:1147:VAL:HG21	2.02	0.40
27:3:181:MET:HE3	27:3:212:GLU:HB2	2.03	0.40
27:3:474:ILE:HD12	27:3:485:LEU:O	2.21	0.40
36:9:276:VAL:HG13	36:9:437:PRO:HB2	2.02	0.40
37:8:38:VAL:HG22	37:8:113:GLN:NE2	2.29	0.40
1:A:210:HIS:CD2	1:A:210:HIS:C	2.95	0.40
1:A:1762:TYR:O	1:A:1768:TYR:CZ	2.74	0.40
1:A:2261:MET:O	1:A:2262:LEU:HD23	2.21	0.40
3:C:516:LEU:HB3	3:C:517:GLU:OE2	2.20	0.40
3:C:727:LEU:CD2	20:U:71:LEU:CB	2.90	0.40
4:D:1204:ILE:O	4:D:1249:GLU:HA	2.21	0.40
5:E:313:ASP:O	5:E:317:ARG:HA	2.20	0.40
7:G:98:U:H3’	7:G:99:C:H5”	2.03	0.40
8:H:63:G:H1	8:H:64:A:H62	1.58	0.40
10:J:411:MET:HG2	10:J:412:ASP:N	2.35	0.40
13:N:58:ARG:HA	13:N:58:ARG:HD3	1.91	0.40
21:V:444:ILE:H	21:V:444:ILE:HD12	1.86	0.40
26:1:134:ASP:HA	26:1:135:PRO:HD3	1.90	0.40
26:1:172:LEU:HA	26:1:175:LYS:HG3	2.03	0.40
26:1:885:ASP:OD1	26:1:887:LYS:N	2.53	0.40
27:3:609:LEU:HG	27:3:613:THR:O	2.21	0.40
27:3:680:ASP:O	27:3:682:VAL:N	2.54	0.40
27:3:942:LYS:HE3	27:3:942:LYS:HB2	1.92	0.40
31:2:512:GLN:OE1	31:2:512:GLN:N	2.54	0.40
33:6:71:LYS:HG3	33:6:72:ASN:N	2.35	0.40
1:A:108:MET:O	1:A:110:TRP:N	2.54	0.40
1:A:434:HIS:C	1:A:434:HIS:ND1	2.75	0.40
1:A:976:MET:HE2	1:A:976:MET:HB2	1.86	0.40
1:A:1336:PRO:HB3	1:A:1350:ILE:HD13	2.02	0.40
1:A:1633:ALA:HB2	1:A:1637:TRP:CZ3	2.56	0.40
1:A:1848:LEU:HD13	1:A:1914:MET:HE3	2.03	0.40
1:A:2188:LEU:HD13	1:A:2228:TYR:CD2	2.56	0.40
2:B:103:G:N1	2:B:111:A:C6	2.89	0.40
3:C:476:CYS:SG	3:C:477:HIS:N	2.95	0.40
5:E:90:ILE:CD1	5:E:112:VAL:HG11	2.48	0.40
5:E:323:LEU:HD23	5:E:323:LEU:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:103:U:O2'	7:G:104:C:H5"	2.22	0.40
10:J:314:TYR:HD1	10:J:314:TYR:HA	1.67	0.40
23:X:225:SER:O	23:X:226:PHE:HD2	2.04	0.40
23:X:330:ASP:OD1	23:X:337:THR:OG1	2.40	0.40
27:3:833:GLU:C	27:3:836:ALA:H	2.21	0.40
27:3:1107:THR:OG1	27:3:1108:THR:N	2.54	0.40
34:7:58:CYS:CB	34:7:61:CYS:HB3	2.50	0.40
1:A:422:LEU:HD23	1:A:422:LEU:N	2.36	0.40
1:A:693:ILE:HG13	1:A:738:MET:CB	2.50	0.40
1:A:901:LEU:HD12	1:A:904:HIS:CE1	2.57	0.40
3:C:237:LEU:HB2	3:C:835:GLU:OE1	2.22	0.40
3:C:325:LYS:O	3:C:329:ASP:HB2	2.20	0.40
4:D:2030:ARG:O	4:D:2096:ALA:HB3	2.22	0.40
5:E:321:TYR:HB3	5:E:323:LEU:HG	2.02	0.40
6:F:15:A:C6	6:F:16:G:C6	3.08	0.40
6:F:85:U:O2	6:F:86:U:N3	2.55	0.40
6:F:88:G:N3	8:H:11:G:C2	2.89	0.40
8:H:18:U:O2'	8:H:19:G:O5'	2.38	0.40
10:J:415:LEU:O	10:J:415:LEU:HD12	2.22	0.40
11:K:227:LYS:HD2	11:K:227:LYS:HA	1.74	0.40
18:S:642:LEU:HA	18:S:668:ARG:O	2.21	0.40
21:V:447:LYS:HE2	21:V:447:LYS:HB3	1.48	0.40
23:X:276:HIS:CD2	23:X:276:HIS:H	2.39	0.40
26:1:564:ASP:O	26:1:603:ALA:HB1	2.22	0.40
26:1:736:ARG:HH21	26:1:736:ARG:HG2	1.86	0.40
27:3:95:SER:OG	27:3:96:LYS:HG3	2.22	0.40
36:9:444:GLN:O	36:9:447:GLN:HB3	2.21	0.40
37:8:56:VAL:O	37:8:59:ILE:N	2.54	0.40
1:A:26:SER:O	1:A:30:LEU:HG	2.21	0.40
1:A:32:GLU:HG3	1:A:33:LYS:N	2.36	0.40
1:A:121:HIS:ND1	1:A:123:THR:HG23	2.37	0.40
1:A:156:ARG:HH21	1:A:157:ASP:CG	2.25	0.40
1:A:625:PRO:O	1:A:627:CYS:N	2.51	0.40
1:A:940:ILE:HG21	1:A:940:ILE:HD13	1.86	0.40
1:A:941:LYS:HG2	1:A:951:LEU:HD11	2.04	0.40
1:A:1070:ASP:O	1:A:1071:PHE:C	2.58	0.40
1:A:1179:SER:O	1:A:1201:ARG:NH1	2.47	0.40
1:A:1247:ILE:O	1:A:1251:SER:HB3	2.21	0.40
1:A:2228:TYR:CG	1:A:2258:ARG:HG3	2.57	0.40
2:B:97:G:C2	2:B:98:G:C5	3.09	0.40
3:C:461:LEU:HD11	3:C:573:GLU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:519:GLU:N	3:C:519:GLU:OE1	2.55	0.40
5:E:65:HIS:NE2	5:E:91:LEU:HD23	2.36	0.40
5:E:197:LEU:HD11	5:E:213:ILE:HD13	2.03	0.40
5:E:315:THR:OG1	5:E:316:SER:N	2.54	0.40
17:R:128:ASP:HB3	17:R:131:ASP:HB3	2.04	0.40
17:R:239:VAL:O	17:R:243:GLN:HG3	2.21	0.40
17:R:391:VAL:O	17:R:392:ILE:HD13	2.22	0.40
26:1:554:LYS:NZ	34:7:97:ASP:OD1	2.49	0.40
26:1:729:LYS:HA	26:1:729:LYS:HD3	1.57	0.40
26:1:781:ASP:OD1	26:1:782:GLU:N	2.55	0.40
27:3:159:GLU:OE2	34:7:14:GLN:HB2	2.21	0.40
27:3:459:VAL:HG22	27:3:476:VAL:HA	2.03	0.40
27:3:592:LEU:HD13	27:3:605:LEU:HD13	2.03	0.40
27:3:791:HIS:HD2	27:3:794:SER:H	1.67	0.40
27:3:926:TYR:HB3	27:3:928:TYR:CE2	2.57	0.40
35:5:8:HIS:CD2	35:5:11:LEU:HD11	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2232/2335 (96%)	2012 (90%)	205 (9%)	15 (1%)	22	60
3	C	854/972 (88%)	748 (88%)	99 (12%)	7 (1%)	19	57
4	D	1720/2136 (80%)	1598 (93%)	118 (7%)	4 (0%)	47	82
5	E	297/357 (83%)	268 (90%)	28 (9%)	1 (0%)	41	76
9	I	591/855 (69%)	492 (83%)	98 (17%)	1 (0%)	47	82
10	J	245/848 (29%)	229 (94%)	15 (6%)	1 (0%)	34	72
11	K	124/343 (36%)	115 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	97/802 (12%)	89 (92%)	8 (8%)	0	100	100
13	N	141/144 (98%)	119 (84%)	20 (14%)	2 (1%)	11	43
14	O	288/420 (69%)	271 (94%)	17 (6%)	0	100	100
15	P	40/229 (18%)	30 (75%)	9 (22%)	1 (2%)	5	28
16	Q	1319/1485 (89%)	1237 (94%)	82 (6%)	0	100	100
17	R	227/536 (42%)	208 (92%)	18 (8%)	1 (0%)	34	72
18	S	639/1041 (61%)	600 (94%)	39 (6%)	0	100	100
19	T	318/514 (62%)	295 (93%)	23 (7%)	0	100	100
20	U	68/2752 (2%)	59 (87%)	9 (13%)	0	100	100
21	V	464/908 (51%)	438 (94%)	26 (6%)	0	100	100
22	W	4/122 (3%)	4 (100%)	0	0	100	100
23	X	152/396 (38%)	136 (90%)	16 (10%)	0	100	100
24	Y	116/322 (36%)	111 (96%)	5 (4%)	0	100	100
25	Z	135/619 (22%)	126 (93%)	8 (6%)	1 (1%)	22	60
26	1	984/1304 (76%)	910 (92%)	68 (7%)	6 (1%)	25	64
27	3	1165/1217 (96%)	1058 (91%)	104 (9%)	3 (0%)	41	76
28	p	165/225 (73%)	155 (94%)	10 (6%)	0	100	100
29	w	428/501 (85%)	393 (92%)	35 (8%)	0	100	100
30	u	183/793 (23%)	175 (96%)	8 (4%)	0	100	100
31	2	246/895 (28%)	221 (90%)	25 (10%)	0	100	100
32	4	157/424 (37%)	143 (91%)	14 (9%)	0	100	100
33	6	107/125 (86%)	99 (92%)	8 (8%)	0	100	100
34	7	103/110 (94%)	95 (92%)	8 (8%)	0	100	100
35	5	79/86 (92%)	69 (87%)	10 (13%)	0	100	100
36	9	373/520 (72%)	336 (90%)	35 (9%)	2 (0%)	29	68
37	8	113/904 (12%)	106 (94%)	7 (6%)	0	100	100
38	y	77/301 (26%)	73 (95%)	4 (5%)	0	100	100
39	v	165/464 (36%)	156 (94%)	9 (6%)	0	100	100
40	o	160/255 (63%)	145 (91%)	15 (9%)	0	100	100
41	c	95/118 (80%)	84 (88%)	11 (12%)	0	100	100
41	h	91/118 (77%)	85 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	d	72/86 (84%)	66 (92%)	6 (8%)	0	100	100
42	i	70/86 (81%)	66 (94%)	4 (6%)	0	100	100
43	a	84/240 (35%)	78 (93%)	6 (7%)	0	100	100
43	m	80/240 (33%)	74 (92%)	6 (8%)	0	100	100
44	g	77/126 (61%)	70 (91%)	7 (9%)	0	100	100
44	l	81/126 (64%)	74 (91%)	7 (9%)	0	100	100
45	f	72/76 (95%)	67 (93%)	5 (7%)	0	100	100
45	k	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
46	e	77/92 (84%)	70 (91%)	7 (9%)	0	100	100
46	j	79/92 (86%)	71 (90%)	8 (10%)	0	100	100
47	b	80/119 (67%)	75 (94%)	5 (6%)	0	100	100
47	n	78/119 (66%)	70 (90%)	8 (10%)	0	100	100
48	z	176/472 (37%)	163 (93%)	13 (7%)	0	100	100
All	All	15859/28446 (56%)	14501 (91%)	1313 (8%)	45 (0%)	44	76

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	802	THR
1	A	856	LEU
3	C	801	LEU
3	C	824	THR
13	N	40	LYS
36	9	269	ASP
1	A	189	GLU
1	A	1764	SER
1	A	1765	SER
3	C	802	HIS
4	D	531	ILE
4	D	1584	ILE
4	D	2098	ALA
4	D	2099	THR
1	A	377	GLU
1	A	855	ARG
1	A	1202	THR
1	A	570	ASP
1	A	699	GLU

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Mol	Chain	Res	Type
3	C	440	SER
15	P	205	LYS
26	1	436	THR
26	1	1063	LEU
27	3	672	GLY
1	A	108	MET
1	A	857	ASN
25	Z	500	GLY
26	1	430	LYS
26	1	435	PRO
1	A	698	PRO
1	A	942	PRO
1	A	1761	PRO
3	C	444	GLY
3	C	472	GLY
5	E	317	ARG
26	1	417	PRO
27	3	1008	SER
17	R	185	GLY
27	3	997	GLY
9	I	371	PRO
3	C	93	ILE
10	J	241	VAL
26	1	1103	VAL
36	9	349	PRO
13	N	36	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	2012/2108 (95%)	1706 (85%)	306 (15%)	3 14
3	C	747/866 (86%)	633 (85%)	114 (15%)	2 13
5	E	256/300 (85%)	212 (83%)	44 (17%)	2 10
9	I	23/749 (3%)	23 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	J	205/751 (27%)	169 (82%)	36 (18%)	2 10
11	K	111/294 (38%)	95 (86%)	16 (14%)	3 15
12	L	86/709 (12%)	72 (84%)	14 (16%)	2 11
13	N	130/130 (100%)	111 (85%)	19 (15%)	3 15
15	P	40/203 (20%)	36 (90%)	4 (10%)	7 29
16	Q	71/1336 (5%)	70 (99%)	1 (1%)	67 88
17	R	200/459 (44%)	164 (82%)	36 (18%)	1 9
19	T	273/441 (62%)	234 (86%)	39 (14%)	3 15
20	U	21/2432 (1%)	19 (90%)	2 (10%)	8 32
21	V	194/838 (23%)	166 (86%)	28 (14%)	3 15
22	W	4/4 (100%)	4 (100%)	0	100 100
23	X	139/349 (40%)	119 (86%)	20 (14%)	3 15
24	Y	105/291 (36%)	88 (84%)	17 (16%)	2 12
25	Z	118/545 (22%)	100 (85%)	18 (15%)	2 13
26	1	840/1103 (76%)	709 (84%)	131 (16%)	2 13
27	3	1018/1051 (97%)	852 (84%)	166 (16%)	2 11
28	p	8/195 (4%)	8 (100%)	0	100 100
29	w	112/446 (25%)	102 (91%)	10 (9%)	9 35
30	u	10/709 (1%)	10 (100%)	0	100 100
31	2	152/776 (20%)	126 (83%)	26 (17%)	2 10
33	6	97/109 (89%)	80 (82%)	17 (18%)	2 10
34	7	90/95 (95%)	72 (80%)	18 (20%)	1 7
35	5	72/77 (94%)	65 (90%)	7 (10%)	8 31
36	9	218/456 (48%)	179 (82%)	39 (18%)	2 9
37	8	104/831 (12%)	93 (89%)	11 (11%)	6 26
39	v	78/382 (20%)	68 (87%)	10 (13%)	4 19
40	o	6/218 (3%)	6 (100%)	0	100 100
41	h	5/110 (4%)	5 (100%)	0	100 100
42	i	4/74 (5%)	4 (100%)	0	100 100
43	m	4/177 (2%)	4 (100%)	0	100 100
44	l	3/101 (3%)	3 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
45	k	3/66 (4%)	3 (100%)	0	100 100
46	j	1/84 (1%)	1 (100%)	0	100 100
47	n	3/101 (3%)	3 (100%)	0	100 100
48	z	152/416 (36%)	133 (88%)	19 (12%)	4 20
All	All	7715/20382 (38%)	6547 (85%)	1168 (15%)	6 14

All (1168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	35	ARG
1	A	59	GLU
1	A	71	ARG
1	A	78	ASN
1	A	86	ARG
1	A	88	TYR
1	A	89	LEU
1	A	97	HIS
1	A	106	MET
1	A	108	MET
1	A	115	ASP
1	A	123	THR
1	A	127	SER
1	A	158	ARG
1	A	164	MET
1	A	165	ARG
1	A	177	ASP
1	A	184	ASP
1	A	193	LEU
1	A	194	GLU
1	A	209	ASP
1	A	216	SER
1	A	221	ASN
1	A	223	SER
1	A	226	GLN
1	A	236	SER
1	A	250	VAL
1	A	258	PHE
1	A	273	ILE
1	A	284	ARG
1	A	300	ASN

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Mol	Chain	Res	Type
1	A	329	LEU
1	A	330	THR
1	A	331	TRP
1	A	337	VAL
1	A	340	ILE
1	A	342	THR
1	A	343	GLU
1	A	346	ASP
1	A	351	TYR
1	A	363	HIS
1	A	366	LYS
1	A	379	GLU
1	A	382	GLU
1	A	387	PHE
1	A	390	ASP
1	A	409	ARG
1	A	414	ARG
1	A	418	THR
1	A	422	LEU
1	A	426	LEU
1	A	433	GLU
1	A	434	HIS
1	A	435	CYS
1	A	442	LYS
1	A	467	GLN
1	A	468	LYS
1	A	470	ARG
1	A	479	THR
1	A	480	LYS
1	A	498	ARG
1	A	510	ARG
1	A	514	ASN
1	A	515	TYR
1	A	519	ASP
1	A	523	ASN
1	A	527	VAL
1	A	529	THR
1	A	533	LYS
1	A	539	ARG
1	A	554	THR
1	A	569	VAL
1	A	576	ASP

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Mol	Chain	Res	Type
1	A	579	GLN
1	A	587	GLN
1	A	595	LYS
1	A	604	MET
1	A	615	ARG
1	A	627	CYS
1	A	644	ILE
1	A	663	ARG
1	A	670	LYS
1	A	674	LYS
1	A	686	ARG
1	A	690	MET
1	A	695	ASP
1	A	708	THR
1	A	738	MET
1	A	770	THR
1	A	773	LYS
1	A	788	GLN
1	A	797	ASP
1	A	802	THR
1	A	804	GLU
1	A	819	SER
1	A	824	PRO
1	A	830	LEU
1	A	833	LYS
1	A	835	ASP
1	A	845	ARG
1	A	847	LYS
1	A	855	ARG
1	A	856	LEU
1	A	864	LEU
1	A	871	TYR
1	A	879	SER
1	A	931	ASP
1	A	933	ARG
1	A	941	LYS
1	A	945	THR
1	A	946	GLU
1	A	976	MET
1	A	979	SER
1	A	985	TYR
1	A	995	ARG

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Mol	Chain	Res	Type
1	A	1000	ILE
1	A	1001	VAL
1	A	1007	ASP
1	A	1015	VAL
1	A	1017	ILE
1	A	1021	ASP
1	A	1027	SER
1	A	1030	ILE
1	A	1038	SER
1	A	1048	MET
1	A	1059	SER
1	A	1070	ASP
1	A	1079	THR
1	A	1089	CYS
1	A	1090	ARG
1	A	1100	ARG
1	A	1104	ASP
1	A	1109	LEU
1	A	1125	ILE
1	A	1128	TYR
1	A	1129	ASN
1	A	1130	ASN
1	A	1139	ARG
1	A	1143	MET
1	A	1158	LYS
1	A	1168	VAL
1	A	1171	GLU
1	A	1173	SER
1	A	1179	SER
1	A	1180	LYS
1	A	1203	SER
1	A	1219	GLU
1	A	1221	THR
1	A	1229	PHE
1	A	1241	HIS
1	A	1243	ARG
1	A	1257	THR
1	A	1268	ILE
1	A	1276	GLU
1	A	1279	VAL
1	A	1280	ASN
1	A	1284	LEU

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Mol	Chain	Res	Type
1	A	1295	ILE
1	A	1301	ILE
1	A	1315	VAL
1	A	1321	GLU
1	A	1329	SER
1	A	1330	MET
1	A	1338	SER
1	A	1339	ASP
1	A	1343	SER
1	A	1344	LYS
1	A	1359	HIS
1	A	1361	GLU
1	A	1367	ASN
1	A	1368	LEU
1	A	1370	ARG
1	A	1381	ASP
1	A	1382	SER
1	A	1400	ASN
1	A	1402	ARG
1	A	1404	THR
1	A	1407	ASP
1	A	1413	ASP
1	A	1416	ILE
1	A	1418	ARG
1	A	1419	ILE
1	A	1426	ASP
1	A	1429	THR
1	A	1438	VAL
1	A	1441	ASP
1	A	1449	LYS
1	A	1458	GLN
1	A	1463	LYS
1	A	1474	MET
1	A	1494	TYR
1	A	1497	THR
1	A	1501	LEU
1	A	1504	GLU
1	A	1516	LYS
1	A	1518	LEU
1	A	1519	THR
1	A	1520	ASN
1	A	1523	ARG

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Mol	Chain	Res	Type
1	A	1526	LEU
1	A	1536	LEU
1	A	1544	ARG
1	A	1548	TYR
1	A	1556	ASP
1	A	1558	THR
1	A	1566	ILE
1	A	1568	THR
1	A	1572	SER
1	A	1574	ILE
1	A	1575	GLN
1	A	1580	HIS
1	A	1583	GLN
1	A	1588	SER
1	A	1602	ASP
1	A	1613	THR
1	A	1619	SER
1	A	1623	ASN
1	A	1630	LEU
1	A	1639	VAL
1	A	1640	SER
1	A	1655	THR
1	A	1658	GLN
1	A	1697	SER
1	A	1702	LEU
1	A	1730	MET
1	A	1749	LYS
1	A	1756	SER
1	A	1759	THR
1	A	1770	GLU
1	A	1772	PHE
1	A	1773	SER
1	A	1781	ASP
1	A	1789	THR
1	A	1792	LYS
1	A	1793	THR
1	A	1795	GLU
1	A	1808	PHE
1	A	1813	ARG
1	A	1814	THR
1	A	1817	LEU
1	A	1819	LEU

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Mol	Chain	Res	Type
1	A	1824	THR
1	A	1833	LEU
1	A	1851	SER
1	A	1868	MET
1	A	1870	ASP
1	A	1876	LEU
1	A	1878	ASP
1	A	1883	VAL
1	A	1915	VAL
1	A	1926	THR
1	A	1929	SER
1	A	1930	TYR
1	A	1937	ILE
1	A	1962	THR
1	A	1970	THR
1	A	1972	THR
1	A	1995	ASN
1	A	1997	VAL
1	A	2012	LEU
1	A	2070	LYS
1	A	2072	GLU
1	A	2073	TRP
1	A	2074	ARG
1	A	2078	ILE
1	A	2084	HIS
1	A	2090	ILE
1	A	2103	THR
1	A	2118	SER
1	A	2120	LEU
1	A	2123	GLN
1	A	2124	ILE
1	A	2132	SER
1	A	2135	ASP
1	A	2136	ASN
1	A	2147	MET
1	A	2153	THR
1	A	2159	LEU
1	A	2162	GLN
1	A	2165	GLN
1	A	2179	HIS
1	A	2191	GLN
1	A	2212	ILE

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Mol	Chain	Res	Type
1	A	2219	THR
1	A	2225	LEU
1	A	2226	THR
1	A	2228	TYR
1	A	2230	LEU
1	A	2231	THR
1	A	2235	TYR
1	A	2239	ARG
1	A	2242	THR
1	A	2247	ASN
1	A	2249	LYS
1	A	2254	SER
1	A	2266	ARG
1	A	2293	LYS
1	A	2297	GLN
1	A	2298	LEU
1	A	2302	LYS
1	A	2309	HIS
1	A	2321	GLN
1	A	2325	VAL
1	A	2329	ASP
1	A	2330	ARG
3	C	57	VAL
3	C	58	VAL
3	C	63	LYS
3	C	64	LYS
3	C	65	TYR
3	C	70	GLU
3	C	71	GLU
3	C	77	VAL
3	C	83	GLU
3	C	84	GLU
3	C	86	THR
3	C	89	LEU
3	C	97	VAL
3	C	117	ASP
3	C	127	GLU
3	C	132	VAL
3	C	135	CYS
3	C	173	THR
3	C	202	ILE
3	C	203	MET

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Mol	Chain	Res	Type
3	C	213	ASP
3	C	226	VAL
3	C	229	ILE
3	C	256	CYS
3	C	289	ILE
3	C	290	SER
3	C	298	LEU
3	C	311	SER
3	C	312	SER
3	C	320	LEU
3	C	322	SER
3	C	327	TYR
3	C	329	ASP
3	C	334	ILE
3	C	348	TYR
3	C	357	THR
3	C	359	LYS
3	C	363	SER
3	C	366	GLN
3	C	377	LEU
3	C	387	ASP
3	C	388	VAL
3	C	389	ASP
3	C	391	SER
3	C	394	ARG
3	C	404	THR
3	C	406	GLU
3	C	416	LEU
3	C	417	ARG
3	C	431	VAL
3	C	438	ILE
3	C	451	HIS
3	C	452	THR
3	C	457	VAL
3	C	458	ASP
3	C	460	ASP
3	C	469	ASP
3	C	495	ARG
3	C	497	LEU
3	C	498	SER
3	C	507	VAL
3	C	510	LEU

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Mol	Chain	Res	Type
3	C	514	TYR
3	C	532	ILE
3	C	540	GLU
3	C	541	VAL
3	C	559	ILE
3	C	562	THR
3	C	564	THR
3	C	572	GLU
3	C	585	THR
3	C	590	ILE
3	C	596	ASN
3	C	623	GLU
3	C	641	MET
3	C	642	HIS
3	C	659	VAL
3	C	664	GLU
3	C	668	GLU
3	C	670	SER
3	C	671	SER
3	C	672	LEU
3	C	674	CYS
3	C	683	ASN
3	C	694	LYS
3	C	696	LEU
3	C	707	ILE
3	C	708	THR
3	C	711	ARG
3	C	713	LYS
3	C	714	LEU
3	C	731	SER
3	C	738	ASP
3	C	740	THR
3	C	747	ASP
3	C	749	THR
3	C	752	SER
3	C	763	LYS
3	C	780	CYS
3	C	785	ARG
3	C	787	VAL
3	C	791	ILE
3	C	803	ARG
3	C	811	THR

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Mol	Chain	Res	Type
3	C	841	ASP
3	C	875	ILE
3	C	878	ILE
3	C	890	HIS
3	C	914	LYS
3	C	916	ILE
3	C	922	GLU
3	C	928	HIS
3	C	941	LYS
3	C	943	LEU
5	E	60	MET
5	E	65	HIS
5	E	81	LEU
5	E	87	ASP
5	E	98	ASP
5	E	100	ASP
5	E	102	TYR
5	E	106	LYS
5	E	143	ARG
5	E	157	CYS
5	E	162	ARG
5	E	167	VAL
5	E	173	ASP
5	E	175	THR
5	E	176	VAL
5	E	188	GLN
5	E	189	THR
5	E	192	ASN
5	E	209	ILE
5	E	210	SER
5	E	214	ASP
5	E	215	ASN
5	E	218	LYS
5	E	225	ASN
5	E	227	LEU
5	E	229	TYR
5	E	231	MET
5	E	234	HIS
5	E	237	SER
5	E	241	LEU
5	E	263	ASP
5	E	265	ARG

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Mol	Chain	Res	Type
5	E	267	PHE
5	E	282	HIS
5	E	284	PHE
5	E	289	LEU
5	E	300	ILE
5	E	306	ASP
5	E	317	ARG
5	E	318	ARG
5	E	329	SER
5	E	338	ASP
5	E	342	ILE
5	E	343	ILE
10	J	216	ASP
10	J	220	LEU
10	J	222	ASP
10	J	228	ARG
10	J	236	ARG
10	J	244	ASN
10	J	248	TYR
10	J	254	SER
10	J	265	TYR
10	J	267	ARG
10	J	273	TYR
10	J	282	TYR
10	J	286	GLU
10	J	288	LYS
10	J	290	ARG
10	J	299	TRP
10	J	314	TYR
10	J	316	TYR
10	J	321	GLU
10	J	350	ILE
10	J	356	TYR
10	J	363	ARG
10	J	369	PHE
10	J	376	VAL
10	J	377	LYS
10	J	380	ILE
10	J	382	TYR
10	J	385	PHE
10	J	388	LYS
10	J	406	PHE

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Mol	Chain	Res	Type
10	J	415	LEU
10	J	419	PHE
10	J	431	ARG
10	J	438	TYR
10	J	440	LEU
10	J	444	SER
11	K	99	VAL
11	K	102	SER
11	K	103	THR
11	K	121	GLU
11	K	134	PHE
11	K	140	ILE
11	K	152	ILE
11	K	158	ASN
11	K	189	LEU
11	K	192	THR
11	K	206	LYS
11	K	218	LYS
11	K	223	ARG
11	K	224	SER
11	K	225	ASP
11	K	227	LYS
12	L	14	THR
12	L	25	LYS
12	L	28	LYS
12	L	29	ASN
12	L	32	SER
12	L	33	ARG
12	L	54	LEU
12	L	57	SER
12	L	59	LYS
12	L	70	LYS
12	L	83	ARG
12	L	89	ILE
12	L	91	ARG
12	L	101	GLU
13	N	1	MET
13	N	13	ASP
13	N	17	LEU
13	N	21	THR
13	N	34	THR
13	N	44	GLU

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Mol	Chain	Res	Type
13	N	45	SER
13	N	56	LYS
13	N	71	SER
13	N	80	LYS
13	N	86	LYS
13	N	102	CYS
13	N	115	THR
13	N	119	CYS
13	N	123	LYS
13	N	130	ARG
13	N	134	CYS
13	N	140	ARG
13	N	143	SER
15	P	192	VAL
15	P	224	MET
15	P	225	GLU
15	P	229	LYS
16	Q	173	PRO
17	R	133	GLN
17	R	147	THR
17	R	148	ARG
17	R	151	LEU
17	R	157	GLN
17	R	182	SER
17	R	198	ARG
17	R	200	VAL
17	R	212	PHE
17	R	213	LYS
17	R	214	ILE
17	R	215	ASN
17	R	218	ILE
17	R	224	SER
17	R	232	SER
17	R	236	LYS
17	R	238	THR
17	R	239	VAL
17	R	241	GLU
17	R	242	GLN
17	R	243	GLN
17	R	283	ASN
17	R	295	ASP
17	R	314	GLN

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Mol	Chain	Res	Type
17	R	323	LYS
17	R	332	ARG
17	R	386	ARG
17	R	388	ILE
17	R	391	VAL
17	R	402	SER
17	R	404	GLU
17	R	406	GLN
17	R	408	ASP
17	R	413	ASN
17	R	414	GLN
17	R	428	GLU
19	T	196	LEU
19	T	197	TYR
19	T	198	ARG
19	T	201	SER
19	T	208	ARG
19	T	241	SER
19	T	250	ARG
19	T	256	THR
19	T	263	SER
19	T	264	CYS
19	T	267	ASP
19	T	294	LEU
19	T	303	LEU
19	T	309	ASP
19	T	314	ILE
19	T	319	THR
19	T	325	THR
19	T	338	CYS
19	T	363	LYS
19	T	366	VAL
19	T	369	THR
19	T	374	SER
19	T	384	HIS
19	T	386	THR
19	T	389	SER
19	T	393	ASP
19	T	397	GLN
19	T	398	TRP
19	T	402	ASP
19	T	413	ASN

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Mol	Chain	Res	Type
19	T	418	THR
19	T	424	ASP
19	T	427	LEU
19	T	429	SER
19	T	432	ASP
19	T	438	LEU
19	T	443	THR
19	T	459	LEU
19	T	503	SER
20	U	2	TYR
20	U	11	ARG
21	V	442	VAL
21	V	454	SER
21	V	457	ARG
21	V	458	THR
21	V	464	GLN
21	V	479	MET
21	V	483	GLU
21	V	492	MET
21	V	494	LEU
21	V	496	CYS
21	V	517	LEU
21	V	528	ILE
21	V	540	GLU
21	V	543	LYS
21	V	556	TYR
21	V	559	SER
21	V	563	SER
21	V	571	SER
21	V	588	GLN
21	V	591	CYS
21	V	604	LYS
21	V	618	ARG
21	V	625	ARG
21	V	631	PHE
21	V	632	THR
21	V	639	LEU
21	V	644	ARG
21	V	648	LYS
23	X	221	LYS
23	X	225	SER
23	X	226	PHE

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Mol	Chain	Res	Type
23	X	228	LEU
23	X	229	SER
23	X	247	SER
23	X	251	GLU
23	X	260	ARG
23	X	266	ASN
23	X	287	ARG
23	X	288	ARG
23	X	291	ASP
23	X	306	PHE
23	X	309	ARG
23	X	311	VAL
23	X	313	TYR
23	X	335	ASN
23	X	343	ARG
23	X	352	LEU
23	X	373	SER
24	Y	2	ASN
24	Y	15	GLU
24	Y	16	ARG
24	Y	25	LYS
24	Y	26	VAL
24	Y	33	LYS
24	Y	34	ASP
24	Y	35	SER
24	Y	40	LEU
24	Y	48	THR
24	Y	57	SER
24	Y	69	ARG
24	Y	73	THR
24	Y	86	ASP
24	Y	89	SER
24	Y	106	THR
24	Y	108	ARG
25	Z	488	SER
25	Z	490	ARG
25	Z	526	ILE
25	Z	527	ASP
25	Z	532	ASP
25	Z	540	ARG
25	Z	543	ASP
25	Z	547	ASN

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Mol	Chain	Res	Type
25	Z	559	ASN
25	Z	563	ARG
25	Z	575	ARG
25	Z	583	ARG
25	Z	597	ARG
25	Z	604	LYS
25	Z	610	LEU
25	Z	615	SER
25	Z	617	GLU
25	Z	619	MET
26	1	102	ASP
26	1	111	LYS
26	1	115	ARG
26	1	127	ILE
26	1	134	ASP
26	1	142	THR
26	1	151	THR
26	1	153	MET
26	1	163	LYS
26	1	165	GLU
26	1	166	ARG
26	1	169	ARG
26	1	395	ARG
26	1	396	ASN
26	1	401	ASP
26	1	407	MET
26	1	415	LEU
26	1	442	THR
26	1	449	GLU
26	1	451	ARG
26	1	452	THR
26	1	471	ASP
26	1	473	GLN
26	1	479	LEU
26	1	486	THR
26	1	488	SER
26	1	491	GLU
26	1	497	ILE
26	1	498	MET
26	1	500	LEU
26	1	503	LYS
26	1	506	ASN

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Mol	Chain	Res	Type
26	1	516	LEU
26	1	518	GLN
26	1	525	GLU
26	1	534	GLN
26	1	544	LEU
26	1	545	GLU
26	1	546	ASP
26	1	551	LEU
26	1	596	ILE
26	1	598	SER
26	1	611	SER
26	1	614	ARG
26	1	620	MET
26	1	621	ASP
26	1	628	THR
26	1	632	PHE
26	1	637	SER
26	1	652	CYS
26	1	654	SER
26	1	655	LYS
26	1	666	LYS
26	1	677	CYS
26	1	689	ILE
26	1	697	GLU
26	1	701	VAL
26	1	703	THR
26	1	726	SER
26	1	727	VAL
26	1	736	ARG
26	1	739	ARG
26	1	760	GLU
26	1	761	TYR
26	1	764	TYR
26	1	769	VAL
26	1	787	ILE
26	1	788	VAL
26	1	795	CYS
26	1	798	THR
26	1	801	VAL
26	1	802	GLU
26	1	808	THR
26	1	816	LYS

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Mol	Chain	Res	Type
26	1	827	ARG
26	1	836	THR
26	1	851	SER
26	1	854	VAL
26	1	855	ASP
26	1	859	ASP
26	1	866	LYS
26	1	868	VAL
26	1	871	THR
26	1	873	GLU
26	1	883	ASP
26	1	885	ASP
26	1	887	LYS
26	1	905	THR
26	1	924	ARG
26	1	932	ILE
26	1	936	VAL
26	1	946	LYS
26	1	947	VAL
26	1	969	LYS
26	1	973	HIS
26	1	980	GLU
26	1	998	LYS
26	1	1004	ILE
26	1	1021	THR
26	1	1036	ILE
26	1	1059	CYS
26	1	1061	GLU
26	1	1065	LEU
26	1	1080	THR
26	1	1086	LYS
26	1	1092	ASP
26	1	1099	ASN
26	1	1103	VAL
26	1	1105	GLU
26	1	1112	THR
26	1	1113	THR
26	1	1121	GLU
26	1	1128	VAL
26	1	1138	VAL
26	1	1147	VAL
26	1	1150	SER

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Mol	Chain	Res	Type
26	1	1152	SER
26	1	1161	MET
26	1	1170	THR
26	1	1174	GLU
26	1	1179	ASP
26	1	1182	LEU
26	1	1219	VAL
26	1	1244	CYS
26	1	1245	ARG
26	1	1276	SER
26	1	1277	GLN
26	1	1289	ASN
26	1	1293	ASN
26	1	1301	ASP
26	1	1304	LEU
27	3	9	GLN
27	3	10	ARG
27	3	23	SER
27	3	27	GLN
27	3	30	ILE
27	3	33	SER
27	3	36	LYS
27	3	44	ASP
27	3	46	ASN
27	3	47	THR
27	3	50	VAL
27	3	54	LEU
27	3	57	GLU
27	3	68	PHE
27	3	71	THR
27	3	86	ARG
27	3	88	VAL
27	3	90	LEU
27	3	95	SER
27	3	96	LYS
27	3	110	SER
27	3	114	ARG
27	3	124	ASP
27	3	155	SER
27	3	191	GLU
27	3	197	THR
27	3	204	THR

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Mol	Chain	Res	Type
27	3	209	THR
27	3	213	LEU
27	3	215	LEU
27	3	225	SER
27	3	226	GLU
27	3	237	THR
27	3	252	SER
27	3	253	GLU
27	3	256	ILE
27	3	261	PHE
27	3	266	ASP
27	3	275	ARG
27	3	290	SER
27	3	294	LYS
27	3	295	THR
27	3	298	MET
27	3	305	THR
27	3	314	THR
27	3	317	THR
27	3	318	ASP
27	3	332	THR
27	3	342	LEU
27	3	347	LEU
27	3	351	SER
27	3	368	ASP
27	3	370	GLU
27	3	379	LEU
27	3	384	THR
27	3	390	ARG
27	3	394	ASN
27	3	404	LEU
27	3	410	CYS
27	3	411	GLN
27	3	417	ASN
27	3	434	SER
27	3	439	ARG
27	3	442	LEU
27	3	443	GLU
27	3	447	MET
27	3	451	GLU
27	3	466	ILE
27	3	467	GLU

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Mol	Chain	Res	Type
27	3	469	GLU
27	3	471	ASP
27	3	477	SER
27	3	482	THR
27	3	507	SER
27	3	511	LEU
27	3	520	TYR
27	3	525	ARG
27	3	541	LYS
27	3	547	CYS
27	3	558	LEU
27	3	568	MET
27	3	574	LEU
27	3	584	SER
27	3	588	VAL
27	3	589	CYS
27	3	591	SER
27	3	604	PHE
27	3	609	LEU
27	3	614	VAL
27	3	617	ILE
27	3	625	LEU
27	3	631	GLN
27	3	633	LEU
27	3	639	SER
27	3	640	LEU
27	3	665	LEU
27	3	674	LEU
27	3	677	THR
27	3	679	LEU
27	3	683	THR
27	3	688	ASP
27	3	689	THR
27	3	690	ARG
27	3	697	ARG
27	3	702	PHE
27	3	703	ARG
27	3	704	VAL
27	3	705	ARG
27	3	707	GLN
27	3	712	VAL
27	3	713	LEU

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Mol	Chain	Res	Type
27	3	715	MET
27	3	727	SER
27	3	728	ARG
27	3	729	PHE
27	3	732	THR
27	3	734	LEU
27	3	736	TYR
27	3	743	SER
27	3	747	SER
27	3	748	GLU
27	3	777	VAL
27	3	803	ASP
27	3	815	ARG
27	3	823	MET
27	3	824	VAL
27	3	837	GLU
27	3	865	VAL
27	3	875	ASN
27	3	883	GLU
27	3	890	SER
27	3	899	THR
27	3	913	LEU
27	3	920	VAL
27	3	927	THR
27	3	931	VAL
27	3	932	ASN
27	3	933	ASN
27	3	936	LYS
27	3	942	LYS
27	3	943	THR
27	3	948	VAL
27	3	958	ARG
27	3	980	LYS
27	3	982	GLU
27	3	991	SER
27	3	995	THR
27	3	998	HIS
27	3	1003	SER
27	3	1004	ASP
27	3	1026	ASP
27	3	1028	THR
27	3	1037	SER

Continued on next page...

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Mol	Chain	Res	Type
27	3	1088	LYS
27	3	1093	MET
27	3	1114	SER
27	3	1128	ILE
27	3	1134	SER
27	3	1135	HIS
27	3	1137	ASP
27	3	1151	GLU
27	3	1168	PHE
27	3	1170	VAL
27	3	1194	SER
27	3	1203	GLU
27	3	1210	ASP
29	w	396	LEU
29	w	400	HIS
29	w	425	HIS
29	w	438	LEU
29	w	443	THR
29	w	468	SER
29	w	472	GLN
29	w	480	GLU
29	w	486	VAL
29	w	500	LEU
31	2	455	ARG
31	2	465	LEU
31	2	467	GLN
31	2	471	ARG
31	2	473	ASP
31	2	477	MET
31	2	478	HIS
31	2	481	THR
31	2	484	ASP
31	2	488	LEU
31	2	495	ARG
31	2	508	ARG
31	2	531	THR
31	2	542	GLU
31	2	546	GLN
31	2	548	THR
31	2	557	VAL
31	2	564	ILE
31	2	565	ASP

Continued on next page...

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Mol	Chain	Res	Type
31	2	581	LYS
31	2	585	THR
31	2	589	ASP
31	2	599	THR
31	2	705	ARG
31	2	706	THR
31	2	711	LEU
33	6	16	GLU
33	6	31	THR
33	6	36	TYR
33	6	59	THR
33	6	65	GLU
33	6	69	ASP
33	6	77	LEU
33	6	78	SER
33	6	84	ASN
33	6	85	ARG
33	6	99	GLN
33	6	100	LYS
33	6	101	MET
33	6	105	LYS
33	6	108	GLU
33	6	113	LEU
33	6	120	ASN
34	7	7	ASP
34	7	9	ILE
34	7	12	ARG
34	7	23	CYS
34	7	29	LYS
34	7	33	CYS
34	7	35	SER
34	7	40	CYS
34	7	42	LEU
34	7	46	CYS
34	7	47	ASP
34	7	48	GLU
34	7	53	SER
34	7	60	ILE
34	7	76	THR
34	7	89	VAL
34	7	97	ASP
34	7	103	LYS

Continued on next page...

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Mol	Chain	Res	Type
35	5	4	ARG
35	5	5	TYR
35	5	13	HIS
35	5	27	THR
35	5	30	GLU
35	5	36	HIS
35	5	69	MET
36	9	216	LYS
36	9	221	LEU
36	9	224	THR
36	9	225	MET
36	9	230	LYS
36	9	232	LYS
36	9	243	THR
36	9	247	SER
36	9	249	SER
36	9	256	VAL
36	9	266	ILE
36	9	269	ASP
36	9	271	LEU
36	9	286	THR
36	9	295	LEU
36	9	296	HIS
36	9	298	ASP
36	9	300	THR
36	9	309	ARG
36	9	330	ILE
36	9	334	ASP
36	9	336	THR
36	9	338	THR
36	9	344	SER
36	9	346	TRP
36	9	351	LYS
36	9	359	SER
36	9	365	ILE
36	9	367	SER
36	9	375	SER
36	9	380	PHE
36	9	386	SER
36	9	389	TYR
36	9	395	THR
36	9	396	ILE

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Mol	Chain	Res	Type
36	9	397	PHE
36	9	414	GLU
36	9	420	ASP
36	9	424	GLU
37	8	16	ARG
37	8	17	PHE
37	8	25	LEU
37	8	37	LYS
37	8	55	ARG
37	8	58	GLU
37	8	85	MET
37	8	102	MET
37	8	111	SER
37	8	116	ILE
37	8	126	LEU
39	v	11	THR
39	v	33	LEU
39	v	37	THR
39	v	38	ILE
39	v	46	PHE
39	v	47	MET
39	v	50	HIS
39	v	59	CYS
39	v	65	ASN
39	v	85	ARG
48	z	3	ASN
48	z	4	ILE
48	z	8	GLU
48	z	18	LYS
48	z	23	ASP
48	z	41	ILE
48	z	63	VAL
48	z	71	THR
48	z	77	SER
48	z	117	LEU
48	z	121	ASP
48	z	134	THR
48	z	136[A]	ASP
48	z	136[B]	ASP
48	z	137	THR
48	z	141	MET
48	z	149	ILE

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Mol	Chain	Res	Type
48	z	150	ASP
48	z	163	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	160	HIS
1	A	181	ASN
1	A	210	HIS
1	A	221	ASN
1	A	270	ASN
1	A	300	ASN
1	A	325	HIS
1	A	326	HIS
1	A	328	HIS
1	A	514	ASN
1	A	584	HIS
1	A	675	GLN
1	A	755	HIS
1	A	775	ASN
1	A	792	HIS
1	A	815	HIS
1	A	873	ASN
1	A	1014	ASN
1	A	1096	HIS
1	A	1111	GLN
1	A	1117	HIS
1	A	1121	ASN
1	A	1367	ASN
1	A	1424	GLN
1	A	1460	HIS
1	A	1527	ASN
1	A	1552	GLN
1	A	1623	ASN
1	A	1717	ASN
1	A	1784	ASN
1	A	1804	ASN
1	A	1890	GLN
1	A	1894	GLN
1	A	1944	HIS
1	A	1966	HIS

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Mol	Chain	Res	Type
1	A	2082	ASN
1	A	2155	GLN
1	A	2162	GLN
1	A	2179	HIS
1	A	2240	GLN
1	A	2247	ASN
1	A	2260	GLN
1	A	2297	GLN
1	A	2306	HIS
1	A	2316	ASN
3	C	87	GLN
3	C	140	HIS
3	C	154	HIS
3	C	245	HIS
3	C	335	ASN
3	C	505	GLN
3	C	575	GLN
3	C	596	ASN
3	C	627	HIS
3	C	706	GLN
3	C	859	GLN
3	C	903	HIS
5	E	101	ASN
5	E	165	GLN
10	J	234	ASN
10	J	297	ASN
10	J	331	GLN
10	J	351	ASN
10	J	373	HIS
11	K	131	GLN
12	L	29	ASN
12	L	45	GLN
15	P	212	ASN
17	R	215	ASN
17	R	279	HIS
17	R	385	ASN
19	T	269	GLN
19	T	407	GLN
19	T	413	ASN
20	U	20	GLN
21	V	474	HIS
21	V	646	HIS

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Mol	Chain	Res	Type
23	X	286	HIS
23	X	303	HIS
23	X	307	GLN
23	X	347	GLN
24	Y	2	ASN
24	Y	19	GLN
24	Y	29	HIS
24	Y	87	GLN
24	Y	96	ASN
24	Y	114	ASN
25	Z	559	ASN
25	Z	595	GLN
26	1	447	GLN
26	1	534	GLN
26	1	670	GLN
26	1	692	HIS
26	1	738	HIS
26	1	820	GLN
26	1	949	GLN
26	1	1100	ASN
26	1	1104	GLN
26	1	1142	ASN
26	1	1194	HIS
27	3	19	HIS
27	3	138	GLN
27	3	203	ASN
27	3	206	GLN
27	3	218	ASN
27	3	304	GLN
27	3	411	GLN
27	3	417	ASN
27	3	480	ASN
27	3	518	GLN
27	3	666	ASN
27	3	775	ASN
27	3	796	ASN
27	3	814	GLN
27	3	817	GLN
27	3	861	GLN
27	3	870	ASN
27	3	875	ASN
27	3	932	ASN

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Mol	Chain	Res	Type
27	3	985	HIS
27	3	1105	GLN
29	w	445	HIS
33	6	84	ASN
33	6	99	GLN
33	6	109	GLN
34	7	4	HIS
35	5	10	GLN
36	9	199	ASN
36	9	296	HIS
36	9	327	ASN
36	9	394	HIS
36	9	412	ASN
37	8	88	ASN
37	8	113	GLN
48	z	3	ASN
48	z	51	ASN
48	z	107	HIS
48	z	112	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/117 (82%)	27 (28%)	3 (3%)
6	F	96/107 (89%)	49 (51%)	6 (6%)
7	G	69/220 (31%)	43 (62%)	9 (13%)
8	H	163/188 (86%)	72 (44%)	7 (4%)
All	All	424/632 (67%)	191 (45%)	25 (5%)

All (191) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C
2	B	24	G
2	B	26	A
2	B	27	U
2	B	32	C

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Mol	Chain	Res	Type
2	B	40	U
2	B	57	G
2	B	70	A
2	B	71	C
2	B	85	C
2	B	86	C
2	B	87	A
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	117	A
6	F	6	C
6	F	7	G
6	F	9	U
6	F	10	U
6	F	12	G
6	F	22	A
6	F	25	C
6	F	26	U
6	F	27	A
6	F	28	A
6	F	29	A
6	F	30	A
6	F	31	U
6	F	33	G
6	F	34	G
6	F	36	A
6	F	37	C
6	F	38	G
6	F	40	U
6	F	41	A
6	F	44	G
6	F	46	G
6	F	47	A
6	F	48	A

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Mol	Chain	Res	Type
6	F	49	G
6	F	54	G
6	F	56	A
6	F	58	G
6	F	59	G
6	F	60	C
6	F	61	C
6	F	66	C
6	F	68	C
6	F	69	A
6	F	73	A
6	F	74	U
6	F	78	A
6	F	79	C
6	F	80	G
6	F	81	C
6	F	82	A
6	F	83	A
6	F	84	A
6	F	85	U
6	F	88	G
6	F	89	U
6	F	91	A
6	F	93	G
6	F	95	G
7	G	-11	G
7	G	-10	G
7	G	-7	U
7	G	-4	G
7	G	1	G
7	G	3	A
7	G	4	A
7	G	5	G
7	G	7	G
7	G	8	C
7	G	11	A
7	G	12	G
7	G	13	C
7	G	14	A
7	G	17	U
7	G	22	C
7	G	23	U

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Mol	Chain	Res	Type
7	G	24	G
7	G	84	U
7	G	88	G
7	G	89	U
7	G	90	C
7	G	91	A
7	G	92	U
7	G	94	C
7	G	97	A
7	G	98	U
7	G	99	C
7	G	100	C
7	G	101	U
7	G	102	G
7	G	103	U
7	G	104	C
7	G	105	C
7	G	106	C
7	G	107	U
7	G	109	U
7	G	110	U
7	G	111	U
7	G	112	U
7	G	114	U
7	G	115	C
7	G	116	C
8	H	2	U
8	H	4	G
8	H	13	C
8	H	14	C
8	H	15	U
8	H	16	U
8	H	17	U
8	H	18	U
8	H	19	G
8	H	23	A
8	H	24	A
8	H	25	G
8	H	28	C
8	H	29	A
8	H	30	A
8	H	31	G

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Mol	Chain	Res	Type
8	H	35	A
8	H	44	U
8	H	45	C
8	H	46	U
8	H	47	U
8	H	48	A
8	H	49	U
8	H	50	C
8	H	56	A
8	H	60	U
8	H	62	U
8	H	63	G
8	H	64	A
8	H	81	G
8	H	82	G
8	H	83	A
8	H	84	C
8	H	98	G
8	H	101	U
8	H	103	U
8	H	104	U
8	H	112	G
8	H	116	A
8	H	117	U
8	H	118	G
8	H	119	G
8	H	120	A
8	H	121	A
8	H	122	U
8	H	124	G
8	H	128	C
8	H	129	U
8	H	130	U
8	H	136	G
8	H	137	U
8	H	138	C
8	H	142	U
8	H	145	A
8	H	146	C
8	H	147	G
8	H	153	A
8	H	156	U

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Mol	Chain	Res	Type
8	H	157	G
8	H	161	U
8	H	162	U
8	H	163	G
8	H	164	C
8	H	166	G
8	H	168	A
8	H	169	C
8	H	170	C
8	H	174	A
8	H	177	A
8	H	178	A
8	H	179	C
8	H	180	G

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	20	G
2	B	39	C
2	B	94	U
6	F	5	U
6	F	35	A
6	F	37	C
6	F	47	A
6	F	58	G
6	F	84	A
7	G	-11	G
7	G	21	A
7	G	22	C
7	G	88	G
7	G	89	U
7	G	101	U
7	G	104	C
7	G	106	C
7	G	108	U
8	H	12	G
8	H	13	C
8	H	18	U
8	H	22	U
8	H	24	A
8	H	28	C

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Mol	Chain	Res	Type
8	H	47	U

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
26	SEP	1	129	26	8,9,10	1.46	1 (12%)	8,12,14	1.21	0

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
26	SEP	1	129	26	-	1/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	129	SEP	P-O1P	3.13	1.60	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	1	129	SEP	N-CA-CB-OG

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	$\#\|Z\| > 2$
50	GTP	C	1500	51	26,34,34	1.34	2 (7%)	32,54,54	1.82	8 (25%)
49	IHP	A	2401	-	36,36,36	1.41	6 (16%)	54,60,60	1.80	12 (22%)

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
50	GTP	C	1500	51	-	6/18/38/38	0/3/3/3
49	IHP	A	2401	-	-	3/30/54/54	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C	1500	GTP	C5-C6	-4.65	1.38	1.47
49	A	2401	IHP	P1-O31	-2.81	1.44	1.54
49	A	2401	IHP	P5-O35	-2.54	1.45	1.54
49	A	2401	IHP	P5-O45	-2.32	1.45	1.54
50	C	1500	GTP	C5-C4	-2.23	1.37	1.43
49	A	2401	IHP	P6-O46	-2.11	1.46	1.54
49	A	2401	IHP	P4-O44	-2.11	1.46	1.54
49	A	2401	IHP	P1-O41	-2.06	1.46	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C	1500	GTP	PB-O3B-PG	-5.17	115.10	132.83
49	A	2401	IHP	O15-C5-C4	4.72	119.81	108.69
49	A	2401	IHP	C5-C4-C3	4.49	120.24	110.41
49	A	2401	IHP	O14-C4-C5	3.86	117.80	108.69
49	A	2401	IHP	C5-C6-C1	3.85	118.84	110.41
50	C	1500	GTP	C5-C6-N1	3.58	120.27	113.95
49	A	2401	IHP	O44-P4-O34	3.46	120.85	107.64
50	C	1500	GTP	C2-N1-C6	-3.23	119.14	125.10
50	C	1500	GTP	C8-N7-C5	3.23	109.15	102.99
50	C	1500	GTP	PA-O3A-PB	-3.11	122.16	132.83
49	A	2401	IHP	O15-C5-C6	3.11	116.01	108.69
50	C	1500	GTP	C3'-C2'-C1'	2.99	105.48	100.98
49	A	2401	IHP	O43-P3-O33	2.86	118.55	107.64
49	A	2401	IHP	O11-C1-C6	2.67	114.99	108.69
49	A	2401	IHP	O13-C3-C4	2.65	114.93	108.69
49	A	2401	IHP	C4-C3-C2	2.63	116.17	110.41
50	C	1500	GTP	O6-C6-C5	-2.37	119.75	124.37
50	C	1500	GTP	O2G-PG-O3B	2.17	111.93	104.64
49	A	2401	IHP	O13-C3-C2	2.14	113.72	108.69
49	A	2401	IHP	O43-P3-O13	-2.05	96.82	105.99

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	A	2401	IHP	C2-O12-P2-O22
49	A	2401	IHP	C3-O13-P3-O43
50	C	1500	GTP	C5'-O5'-PA-O3A
50	C	1500	GTP	C5'-O5'-PA-O1A
50	C	1500	GTP	O4'-C4'-C5'-O5'
50	C	1500	GTP	C3'-C4'-C5'-O5'
49	A	2401	IHP	C5-O15-P5-O35
50	C	1500	GTP	PB-O3A-PA-O2A
50	C	1500	GTP	C5'-O5'-PA-O2A

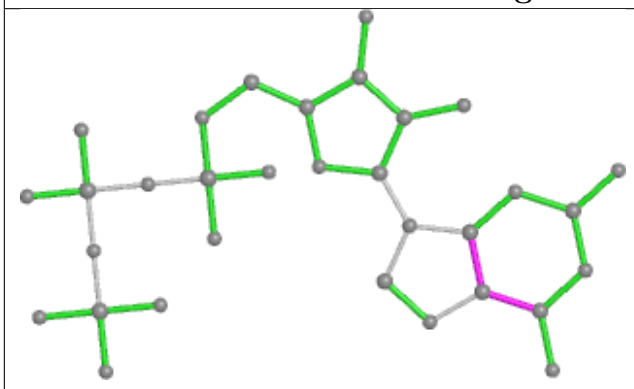
There are no ring outliers.

2 monomers are involved in 5 short contacts:

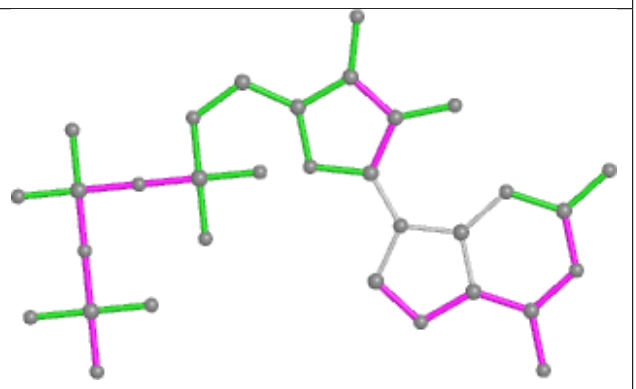
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	C	1500	GTP	3	0
49	A	2401	IHP	2	0

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.

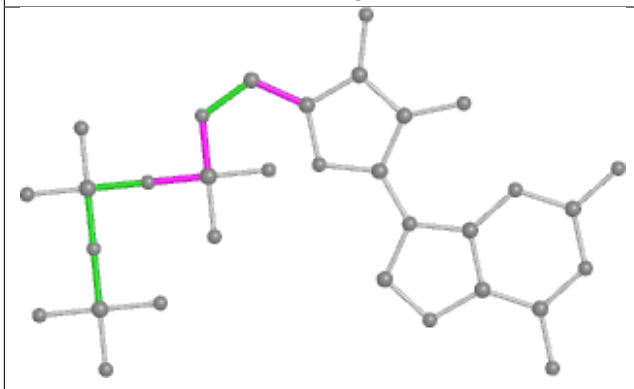
Ligand GTP C 1500



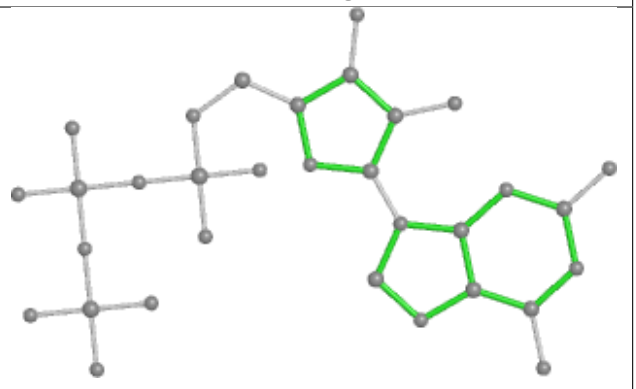
Bond lengths



Bond angles

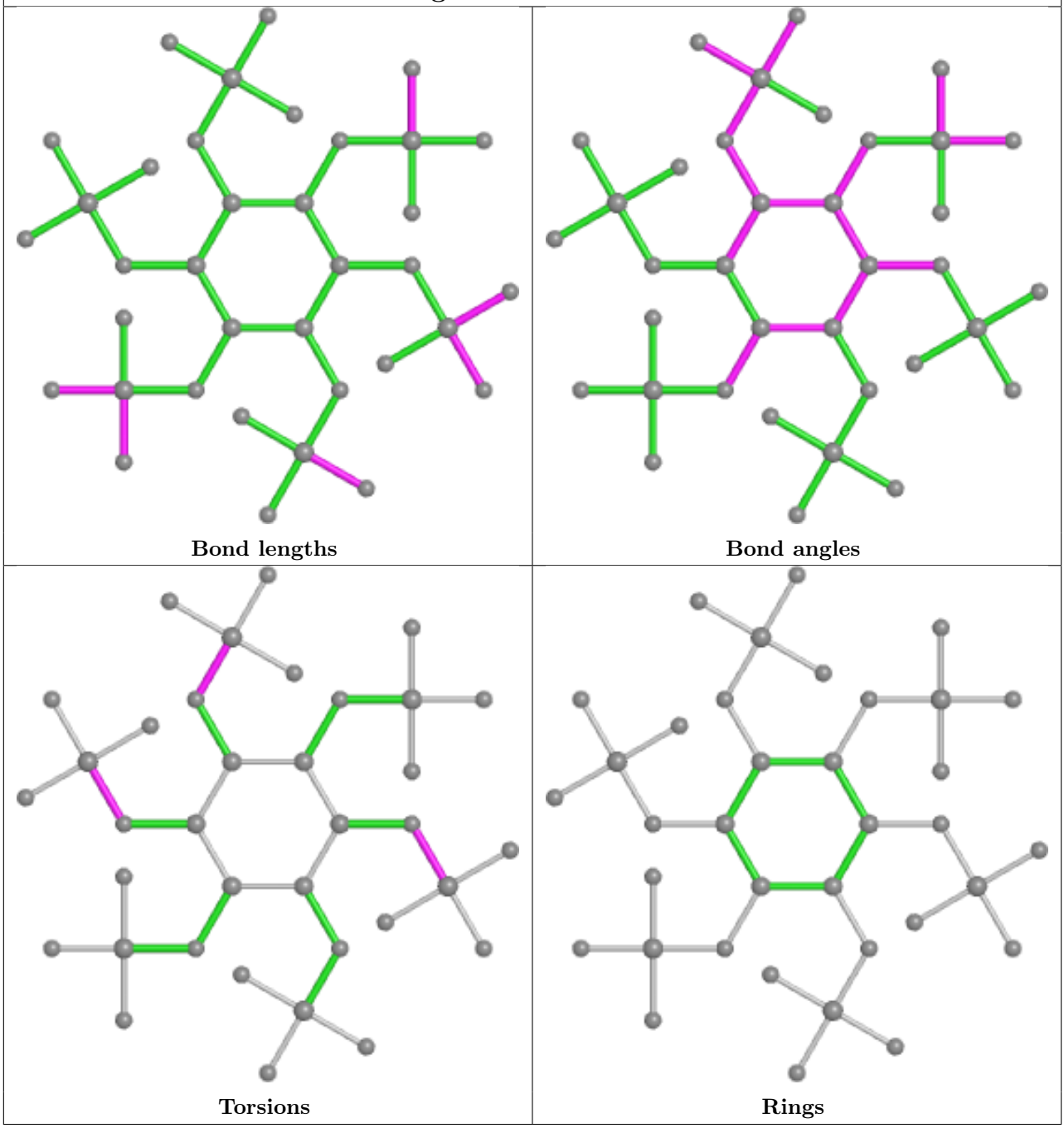


Torsions



Rings

Ligand IHP A 2401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

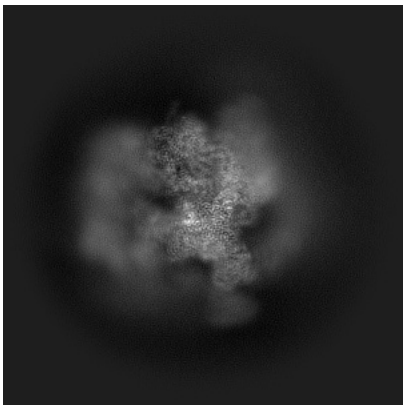
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35107. These allow visual inspection of the internal detail of the map and identification of artifacts.

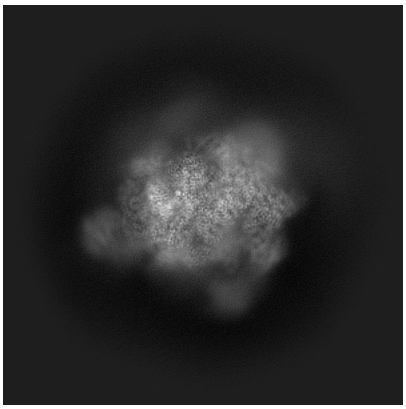
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

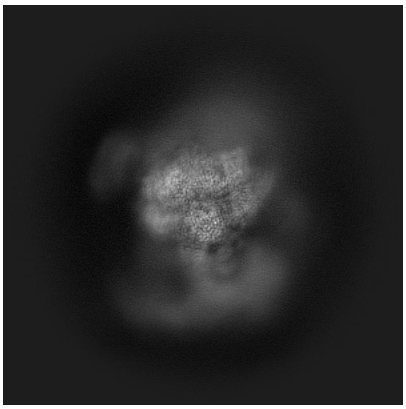
6.1.1 Primary map



X

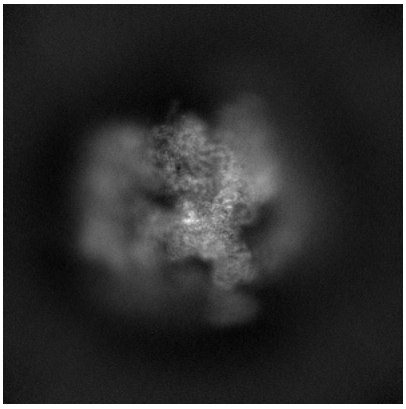


Y

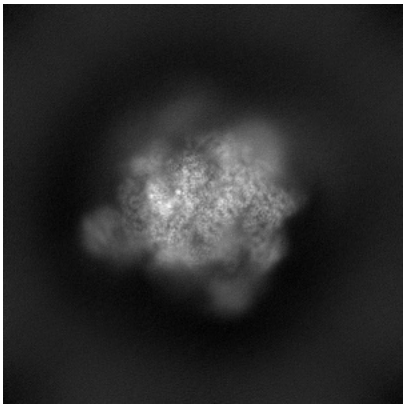


Z

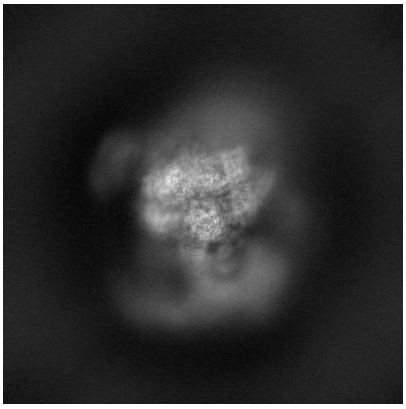
6.1.2 Raw map



X



Y

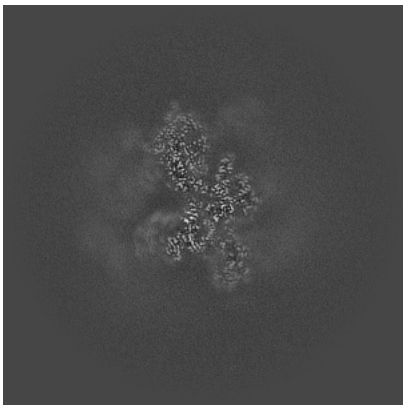


Z

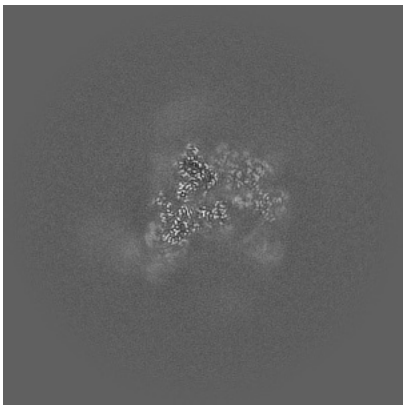
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

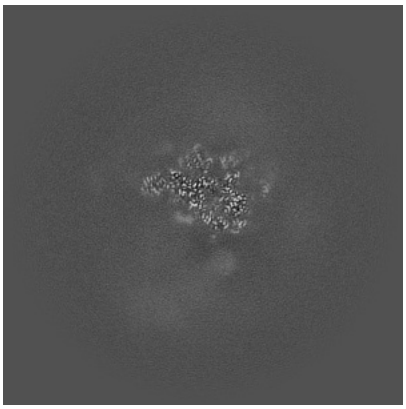
6.2.1 Primary map



X Index: 240

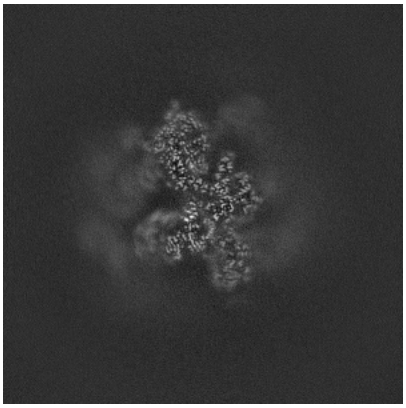


Y Index: 240

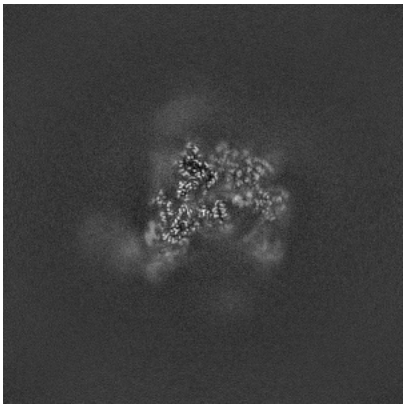


Z Index: 240

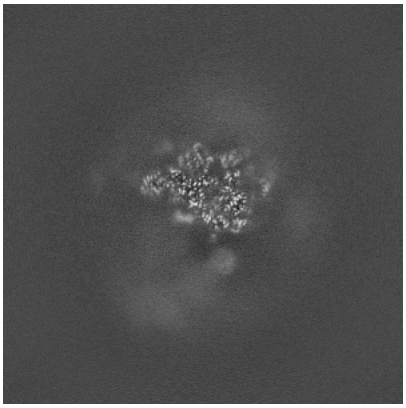
6.2.2 Raw map



X Index: 240



Y Index: 240

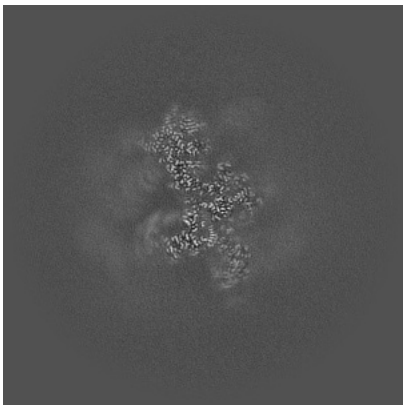


Z Index: 240

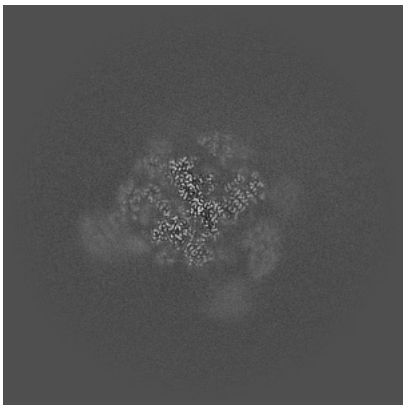
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

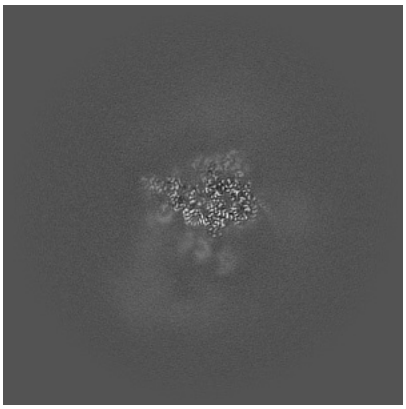
6.3.1 Primary map



X Index: 237

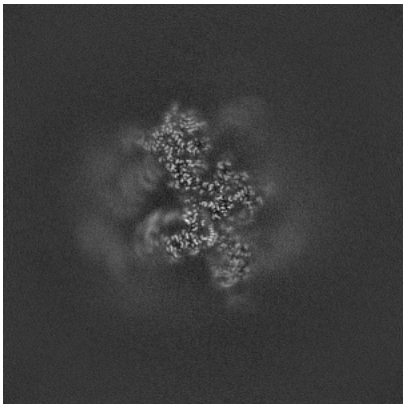


Y Index: 262

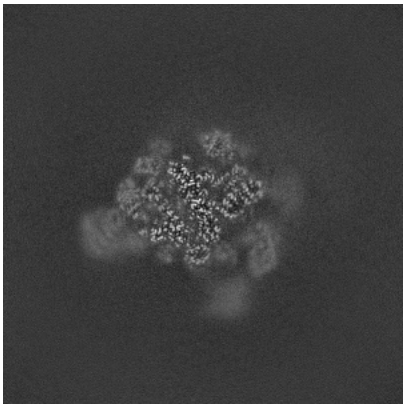


Z Index: 220

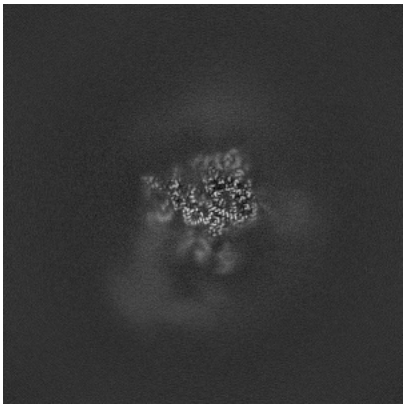
6.3.2 Raw map



X Index: 237



Y Index: 266

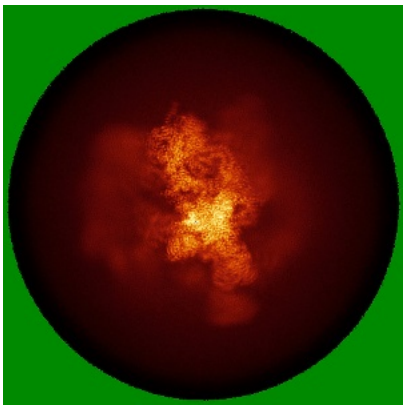


Z Index: 219

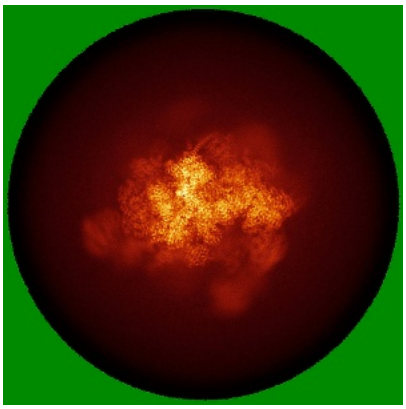
The images above show the largest variance slices of the map in three orthogonal directions.

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

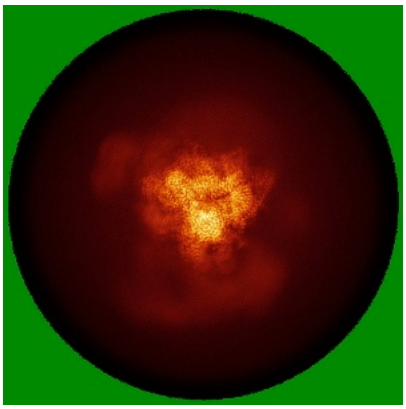
6.4.1 Primary map



X

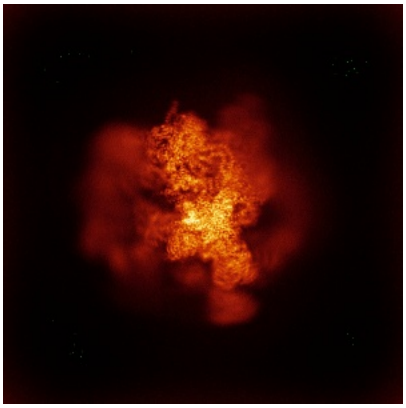


Y

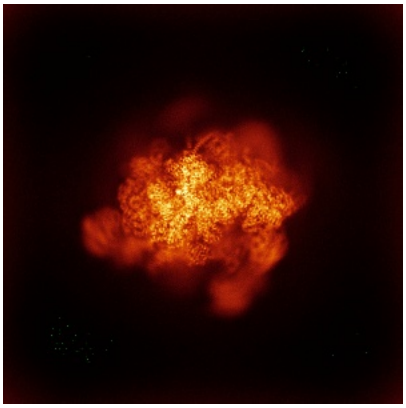


Z

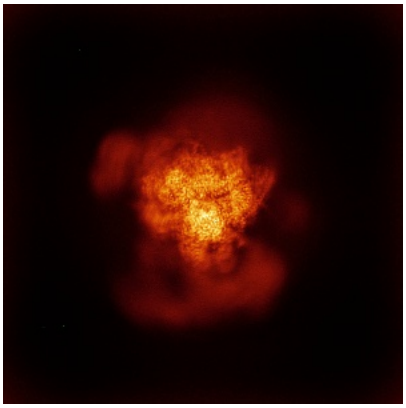
6.4.2 Raw map



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 0.24. 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.

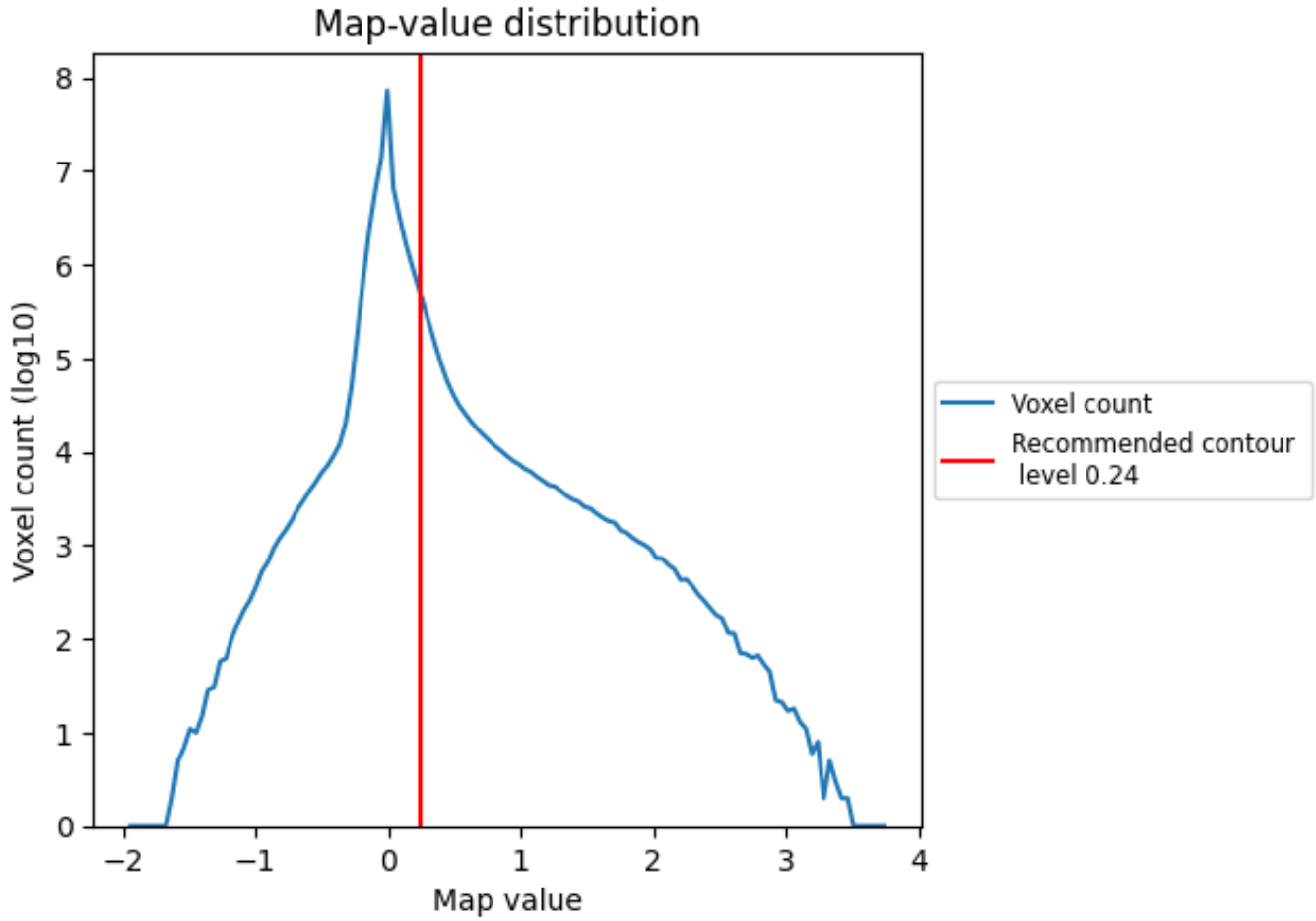
6.6 Mask visualisation (i)

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

7 Map analysis

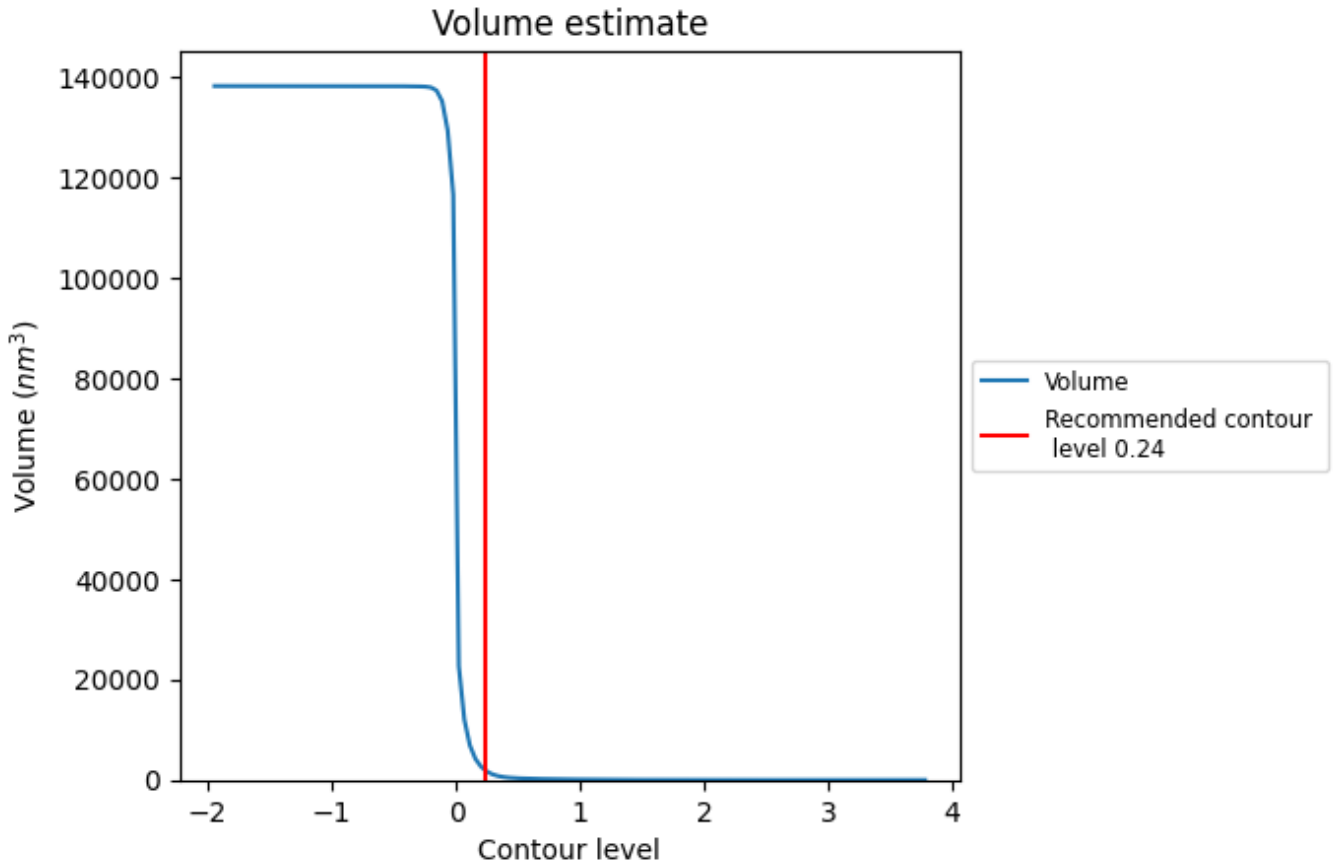
This section contains the results of statistical analysis of the map.

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.

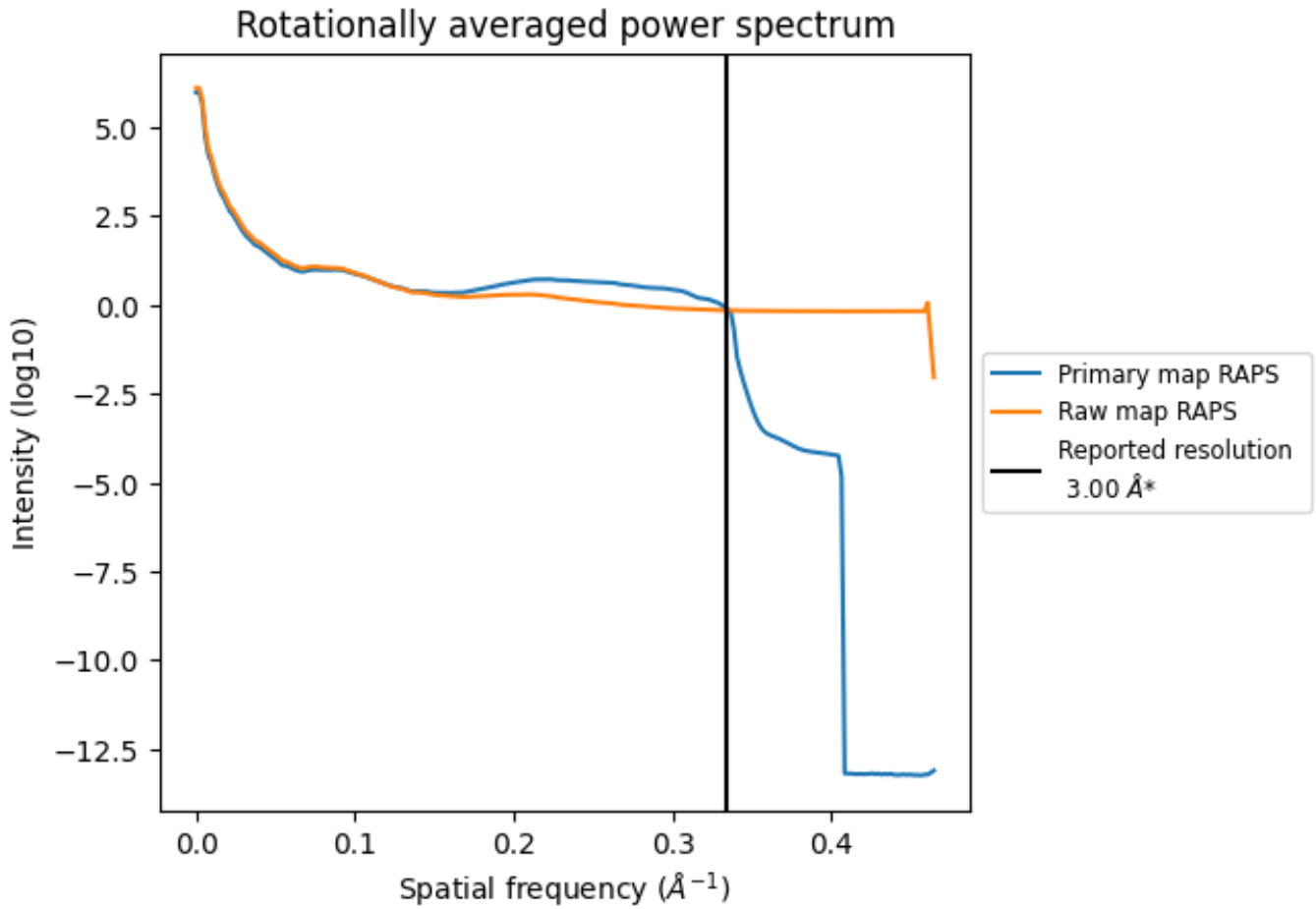
7.2 Volume estimate



The volume at the recommended contour level is 1878 nm^3; this corresponds to an approximate mass of 1697 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)

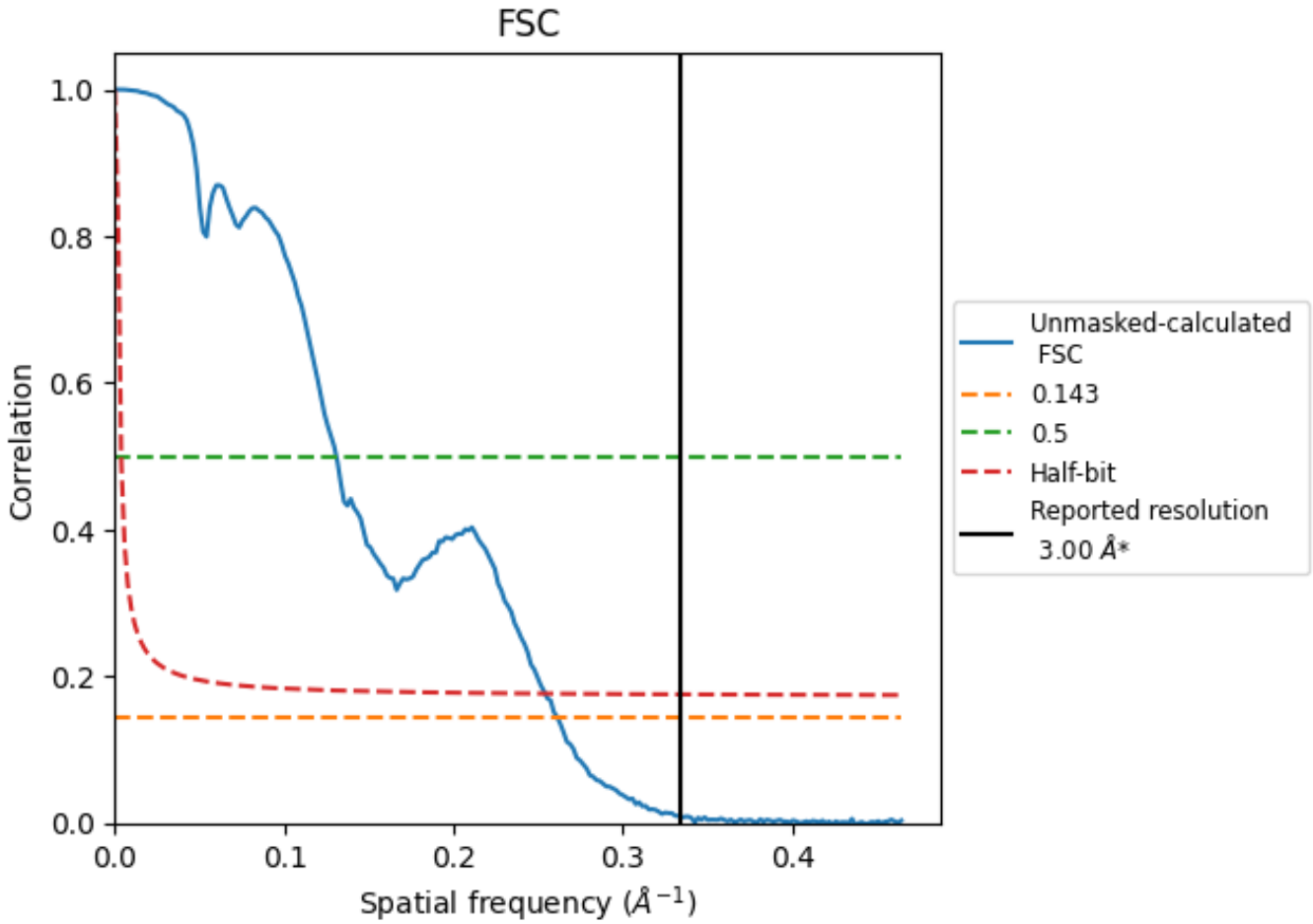


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

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)

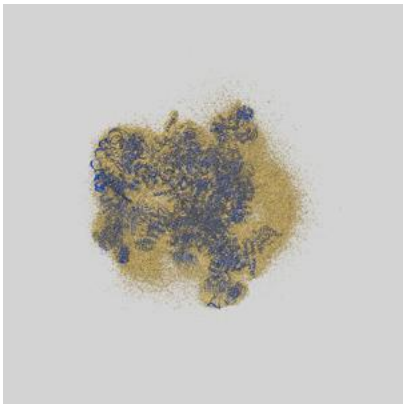
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	7.65	3.94

*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 3.83 differs from the reported value 3.0 by more than 10 %

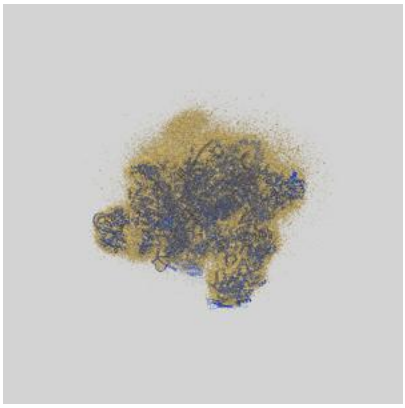
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35107 and PDB model 8I0R. Per-residue inclusion information can be found in section 3 on page 14.

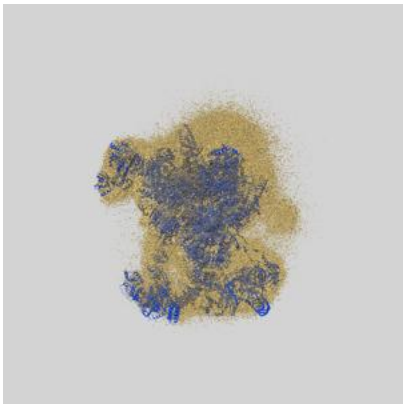
9.1 Map-model overlay



X



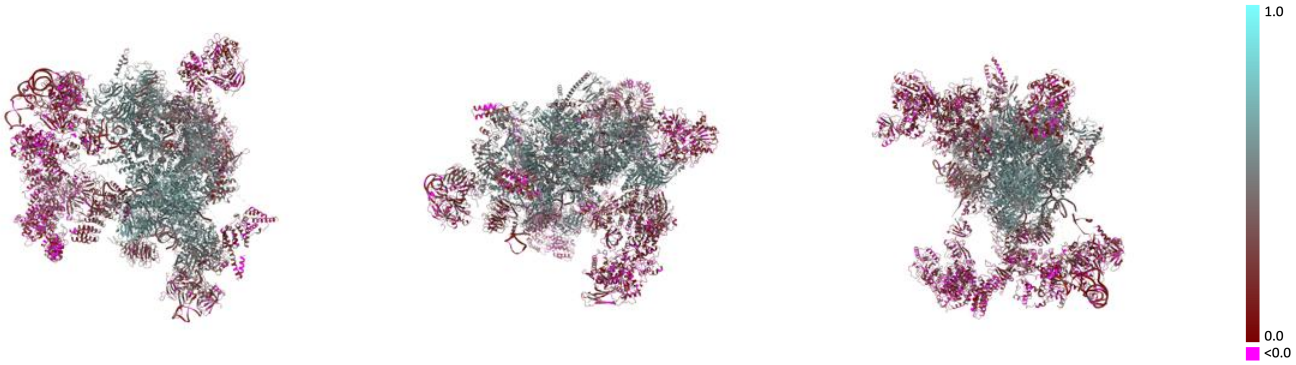
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.24 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.

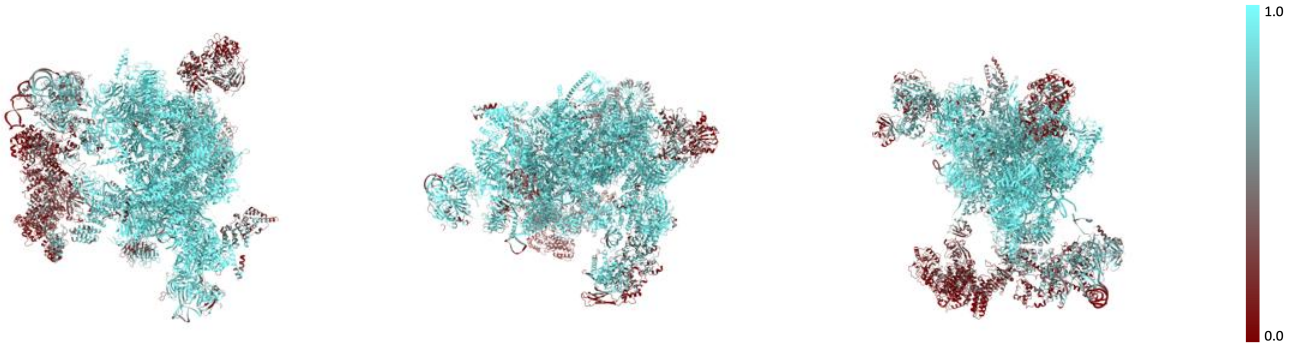
9.2 Q-score mapped to coordinate model (i)



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.

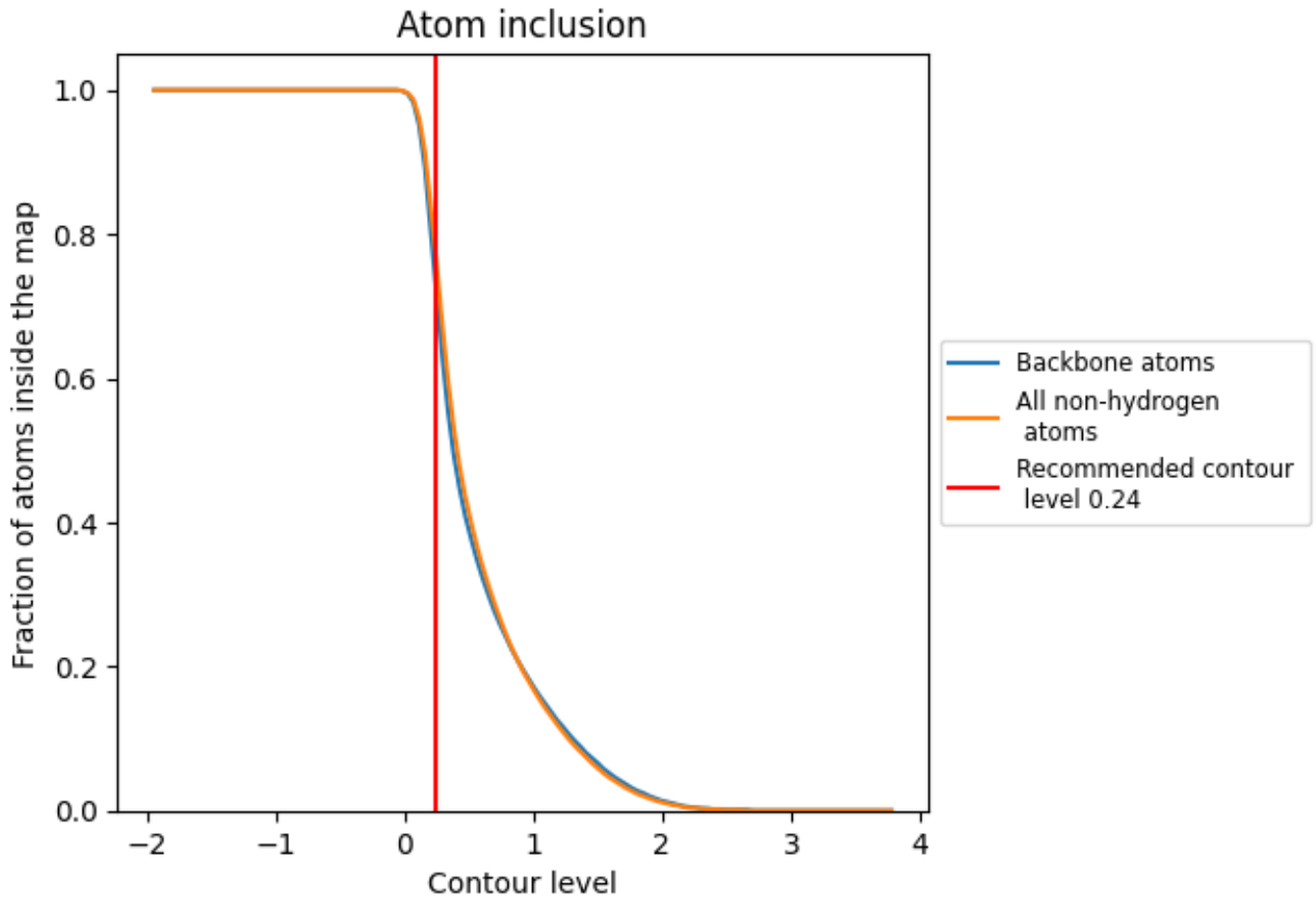
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.24).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 78% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7770	0.3880
1	0.9580	0.5450
2	0.8750	0.4670
3	0.9680	0.4970
4	0.7370	0.2210
5	0.9130	0.5330
6	0.9390	0.4230
7	0.9170	0.5070
8	0.9470	0.4500
9	0.8880	0.3600
A	0.9370	0.5370
B	0.9000	0.3820
C	0.9660	0.4770
D	0.6980	0.2090
E	0.5950	0.2590
F	0.8920	0.3750
G	0.9370	0.3900
H	0.6720	0.2550
I	0.3100	0.1380
J	0.8480	0.2900
K	0.9090	0.5550
L	0.9780	0.5670
N	0.9300	0.4500
O	0.6680	0.2620
P	0.9550	0.5210
Q	0.1020	0.1460
R	0.9300	0.4930
S	0.2830	0.1640
T	0.9920	0.6000
U	0.6610	0.2900
V	0.7560	0.3430
W	0.8680	0.4140
X	0.9540	0.4960
Y	0.9690	0.5740
Z	0.8500	0.4850

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Chain	Atom inclusion	Q-score
a	0.7670	0.2450
b	0.8720	0.2450
c	0.7420	0.2020
d	0.8040	0.2300
e	0.8130	0.2130
f	0.7330	0.3120
g	0.8980	0.3170
h	0.6140	0.1890
i	0.6680	0.1730
j	0.6650	0.2140
k	0.5880	0.1740
l	0.5570	0.1680
m	0.6370	0.2450
n	0.5450	0.1990
o	0.4720	0.1700
p	0.6100	0.1980
u	0.2810	0.1830
v	0.7100	0.4520
w	0.5330	0.2690
y	0.2800	0.1760
z	0.9840	0.5600