Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 05:35 PM JST

PDB ID	:	7D5S
EMDB ID	:	EMD-30584
Title	:	Cryo-EM structure of 90S preribosome with inactive Utp24 (state A2)
Authors	:	Du, Y.; Zhang, J.; An, W.; Ye, K.
Deposited on	:	2020-09-28
Resolution	:	4.60 Å(reported)
Based on initial model	:	6LQU

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:

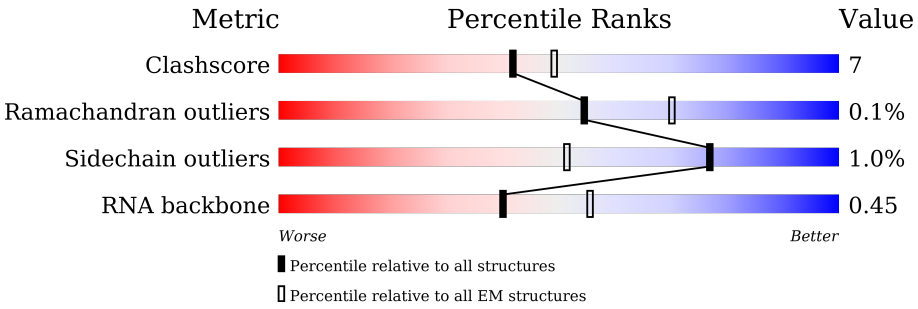
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 4.60 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	3A	333	33% 17% 47%
2	5A	700	10% 43% 25% 7% 25%
3	SA	1808	23% 23% 18% 6% 52%
4	SG	225	11% 82% 13% 5%
5	SK	197	57% 79% 7% 13%
6	SN	143	83% 66% 16% 17%
7	SO	151	89% 74% 13% 11%

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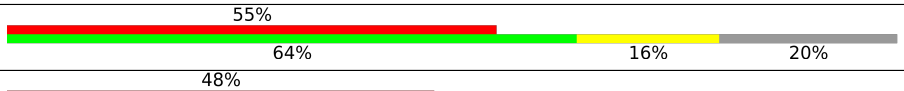
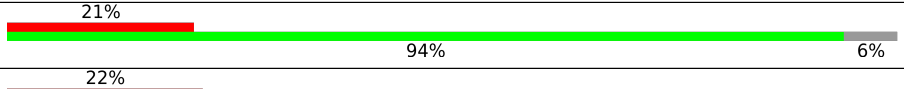
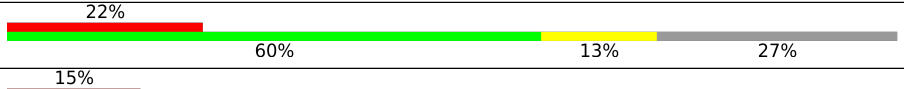
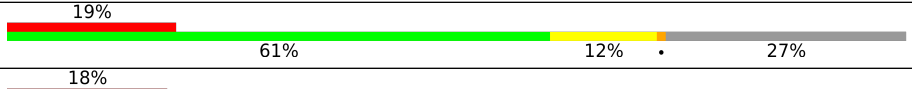
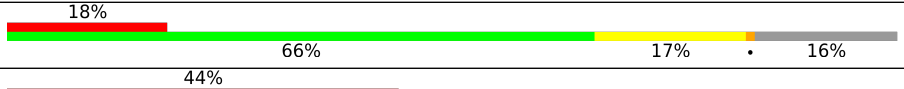
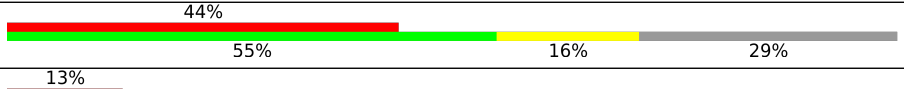
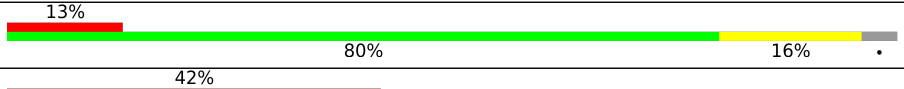
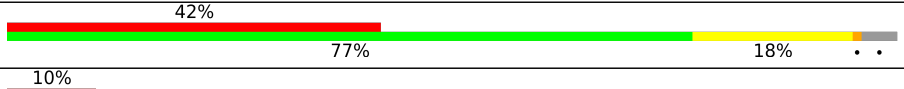
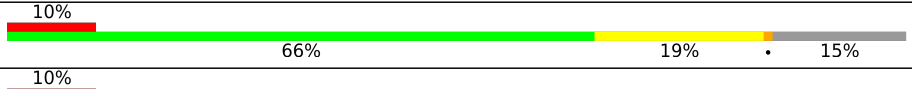
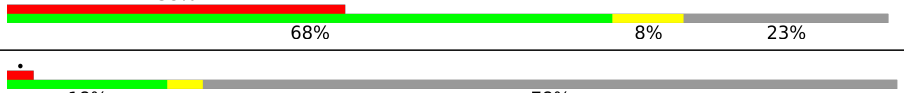
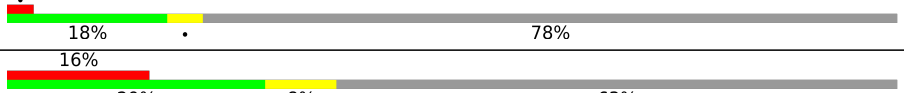
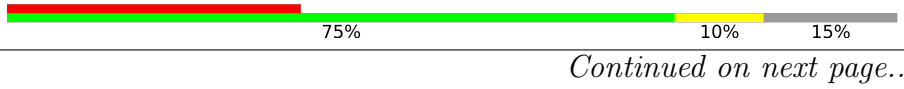
Mol	Chain	Length	Quality of chain
8	SP	137	
9	SR	143	
10	ST	146	
11	SY	145	
12	Sd	67	
13	3B	327	
13	3C	327	
14	3D	504	
15	3E	511	
16	3F	573	
17	3G	126	
17	3H	126	
18	A4	776	
19	A5	643	
20	A8	713	
21	A9	575	
22	AE	1769	
23	AF	513	
24	AG	896	
25	B1	923	
26	B2	943	
27	B3	817	
28	B8	594	
29	BE	939	
30	B6	440	

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Mol	Chain	Length	Quality of chain
31	5B	214	8% 20% 7% 72%
32	5C	554	28% 75% 18% 7%
33	5D	250	22% 82% 12% 6%
34	5E	593	11% 28% 6% 66%
35	5F	183	21% 80% 19%
36	5G	290	38% 79% 19%
37	5H	610	10% 20% 78%
38	5I	489	24% 71% 23% 6%
39	5J	217	33% 59% 11% 30%
40	5K	189	46% 77% 15% 7%
41	RC	316	55% 44% 11% 45%
42	RD	1729	15% 15% 85%
43	RE	1237	87% 66% 20% 13%
44	RF	297	59% 44% 13% 41%
45	RG	252	44% 62% 24% 14%
45	RH	252	37% 71% 20% 9%
46	RI	274	16% 73% 19% 8%
47	RJ	1183	18% 49% 12% 38%
48	RK	367	36% 74% 23%
49	RN	810	42% 62% 13% 25%
50	RO	552	26% 82% 13% 5%
51	RQ	899	17% 18% 78%
52	RS	483	49% 36% 16% 48%
53	RT	326	21% 43% 9% 48%
54	RW	206	24% 29% 69%

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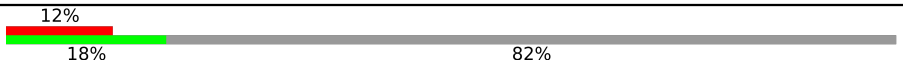
Mol	Chain	Length	Quality of chain
55	X1	347	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 179154 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 RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	3A	175	3711	1661	648	1227	175	0	0

- Molecule 2 is a RNA chain called 5' ETS.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5A	523	11163	4988	1984	3668	523	0	0

- Molecule 3 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	SA	859	18356	8201	3302	5994	859	0	0

- Molecule 4 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SG	213	1669	1045	307	314	3	0	0

- Molecule 5 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SK	171	1388	879	268	240	1	0	0

- Molecule 6 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SN	119	865	545	151	167	2	0	0

- Molecule 7 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SO	134	Total	C	N	O	S	0	0
			1087	698	202	186	1		

- Molecule 8 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SP	118	Total	C	N	O	S	0	0
			868	536	164	165	3		

- Molecule 9 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	SR	125	Total	C	N	O	0	0
			973	625	174	174		

- Molecule 10 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	ST	117	Total	C	N	O	S	0	0
			964	610	184	168	2		

- Molecule 11 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SY	103	Total	C	N	O	S	0	0
			786	503	144	137	2		

- Molecule 12 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Sd	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 13 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3B	240	Total	C	N	O	S	0	0
			1865	1184	333	338	10		
13	3C	225	Total	C	N	O	S	0	0
			1763	1120	316	317	10		

- Molecule 14 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3D	369	Total	C	N	O	S	0	0
			2848	1811	489	540	8		

- Molecule 15 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3E	431	Total	C	N	O	S	0	0
			3028	1888	543	588	9		

- Molecule 16 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3F	406	Total	C	N	O	S	0	0
			3248	2075	566	597	10		

- Molecule 17 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3G	121	Total	C	N	O	S	0	0
			916	583	158	171	4		
17	3H	121	Total	C	N	O	S	0	0
			916	583	158	171	4		

- Molecule 18 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A4	662	Total	C	N	O	S	0	0
			5226	3309	910	986	21		

- Molecule 19 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A5	514	Total	C	N	O	S	0	0
			3976	2520	688	755	13		

- Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	A8	548	Total	C	N	O	S	0	0
			3307	2054	608	642	3		

- Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A9	128	Total	C	N	O	S	0	0
			939	594	173	170	2		

- Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AE	649	Total	C	N	O	S	0	0
			5181	3355	849	960	17		

- Molecule 23 is a protein called U3 small nucleolar RNA-associated protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AF	493	Total	C	N	O	S	0	0
			3911	2462	702	735	12		

- Molecule 24 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AG	826	Total	C	N	O	S	0	0
			6570	4181	1111	1259	19		

- Molecule 25 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B1	834	Total	C	N	O	S	0	0
			6635	4223	1140	1253	19		

- Molecule 26 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B2	851	Total	C	N	O	S	0	0
			6723	4294	1133	1269	27		

- Molecule 27 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B3	752	Total	C	N	O	S	0	0
			5882	3746	987	1122	27		

- Molecule 28 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B8	477	Total	C	N	O	S	0	0
			3764	2387	662	705	10		

- Molecule 29 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BE	865	Total	C	N	O	S	0	0
			6810	4322	1175	1292	21		

- Molecule 30 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B6	374	Total	C	N	O	S	0	0
			2800	1782	501	505	12		

- Molecule 31 is a protein called Bud site selection protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	5B	60	Total	C	N	O	0	0
			495	310	101	84		

- Molecule 32 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5C	516	Total	C	N	O	S	0	0
			4084	2561	736	775	12		

- Molecule 33 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5D	235	Total	C	N	O	S	0	0
			1972	1226	380	359	7		

- Molecule 34 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	5E	204	Total	C	N	O	S	0	0
			1647	1021	294	328	4		

- Molecule 35 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	5F	182	Total	C	N	O	S	0	0
			1530	967	287	269	7		

- Molecule 36 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	5G	282	Total	C	N	O	S	0	0
			2296	1441	430	418	7		

- Molecule 37 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	5H	136	Total	C	N	O	0	0
			1065	658	211	196		

- Molecule 38 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5I	461	Total	C	N	O	S	0	0
			3765	2354	686	709	16		

- Molecule 39 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5J	151	Total	C	N	O	S	0	0
			1280	807	240	228	5		

- Molecule 40 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	5K	175	Total	C	N	O	S	0	0
			1403	896	256	241	10		

- Molecule 41 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	RC	175	Total	C	N	O	S	0	0
			1410	903	252	245	10		

- Molecule 42 is a protein called rRNA biogenesis protein RRP5.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	RD	265	Total 1314	C 784	N 265	O 265	0	0

- Molecule 43 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	RE	1079	Total 8716	C 5666	N 1437	O 1589	S 24	0	0

- Molecule 44 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	RF	174	Total 1404	C 905	N 230	O 261	S 8	0	0

- Molecule 45 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	RG	216	Total 1701	C 1079	N 296	O 315	S 11	0	0
45	RH	230	Total 1799	C 1142	N 313	O 333	S 11	0	0

- Molecule 46 is a protein called Ribosome biogenesis protein UTP30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	RI	252	Total 2045	C 1309	N 362	O 366	S 8	0	0

- Molecule 47 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	RJ	732	Total 5953	C 3829	N 1057	O 1041	S 26	0	0

- Molecule 48 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	RK	360	Total 2781	C 1781	N 473	O 516	S 11	0	0

- Molecule 49 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	RN	607	Total	C	N	O	S	0	0
			4529	2861	820	837	11		

- Molecule 50 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	RO	525	Total	C	N	O	S	0	0
			3766	2412	646	696	12		

- Molecule 51 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	RQ	194	Total	C	N	O	S	0	0
			1436	892	270	272	2		

- Molecule 52 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	RS	251	Total	C	N	O	S	0	0
			2051	1340	349	359	3		

- Molecule 53 is a protein called Pno1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	RT	171	Total	C	N	O	S	0	0
			1357	864	249	240	4		

- Molecule 54 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	RW	63	Total	C	N	O	0	0
			381	234	69	78		

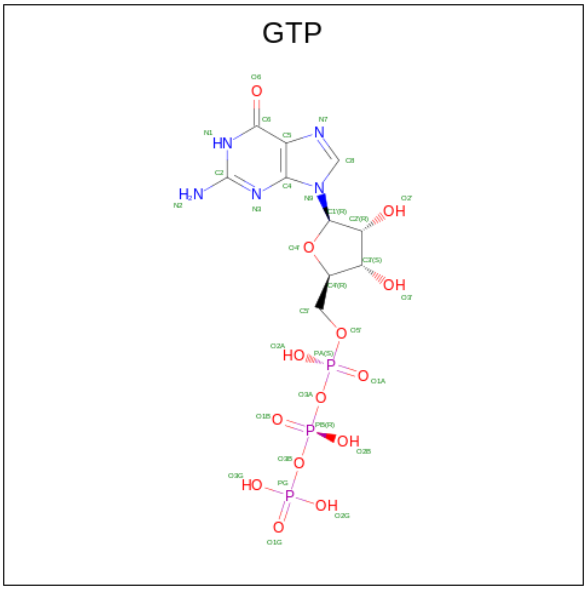
- Molecule 55 is a protein called Unassigned peptides 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	X1	61	Total	C	N	O	0	0
			305	183	61	61		

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
56	5K	1	Total Zn 1 1	0

- Molecule 57 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

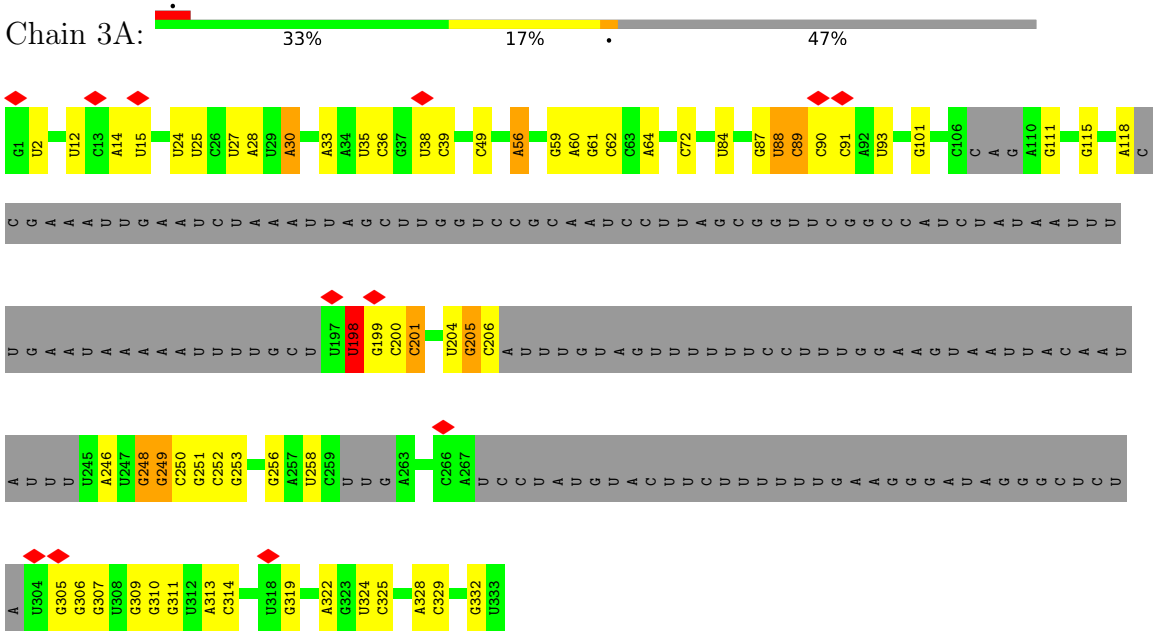
Mol	Chain	Residues	Atoms	AltConf
58	RJ	1	Total Mg 1 1	0

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.

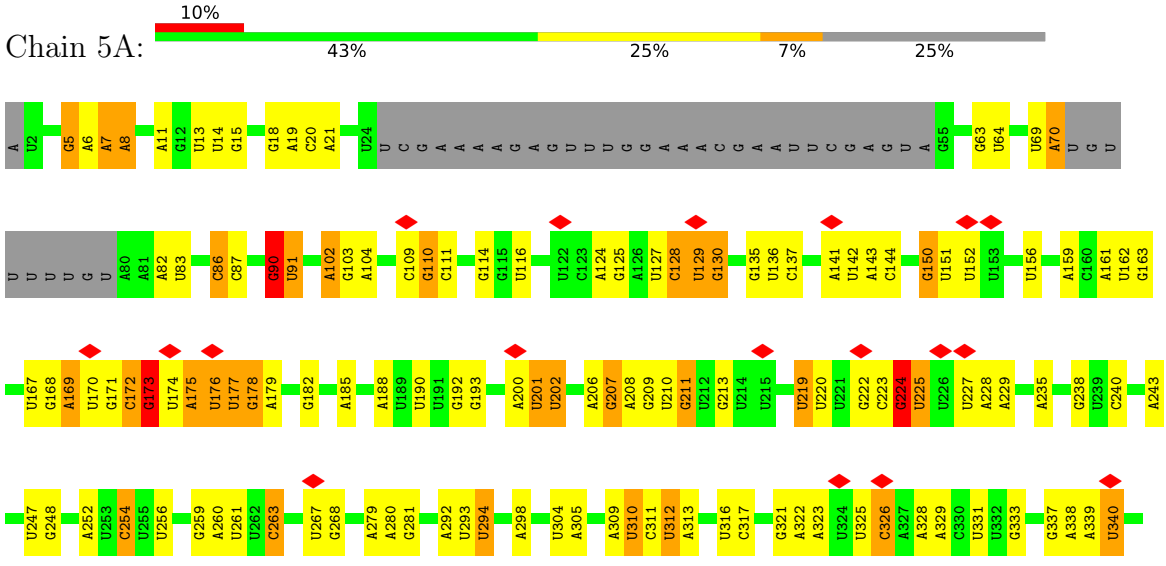
- Molecule 1: U3 snoRNA

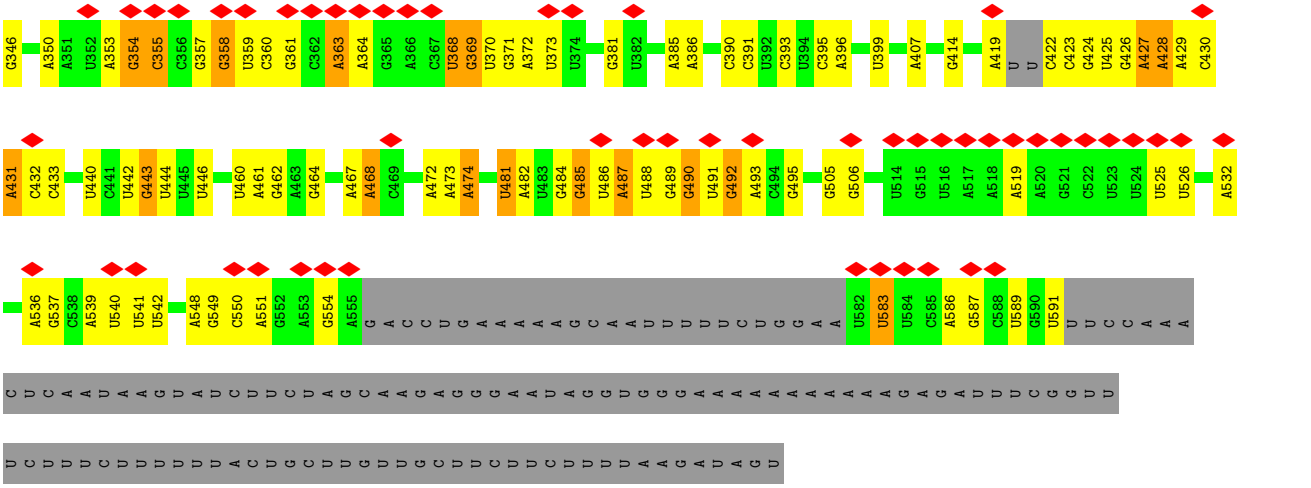
Chain 3A:



- Molecule 2: 5' ETS

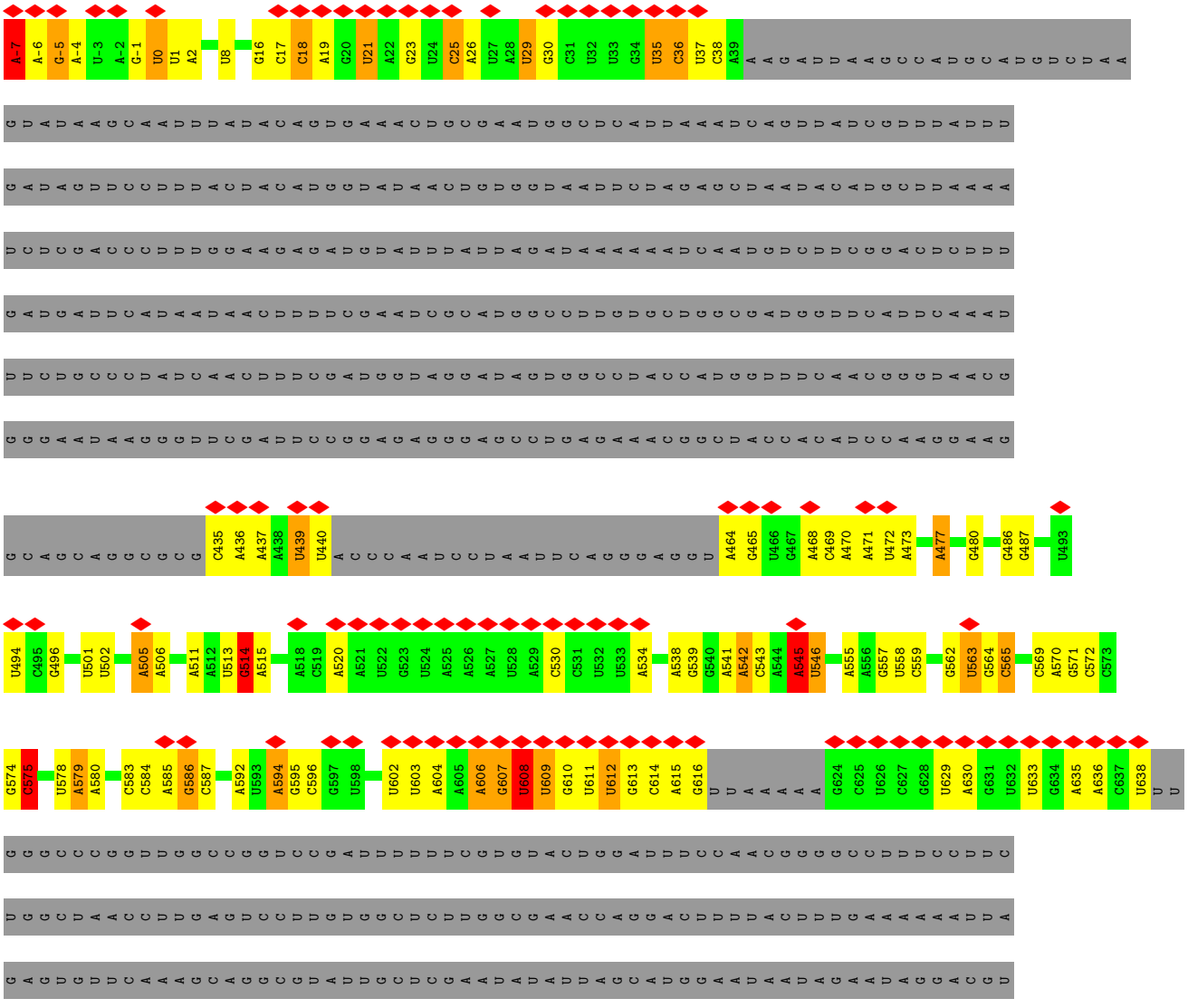
Chain 5A:

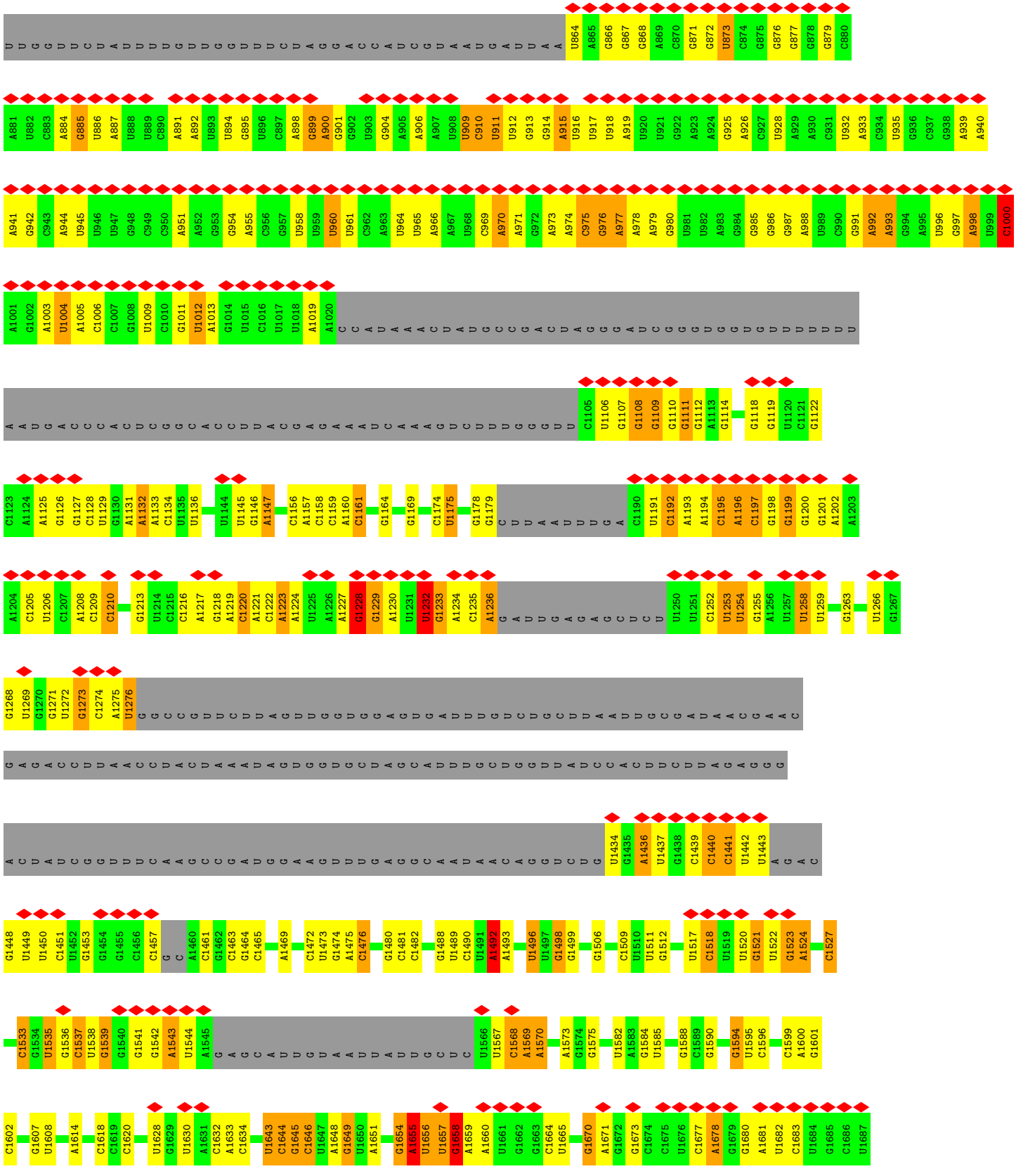


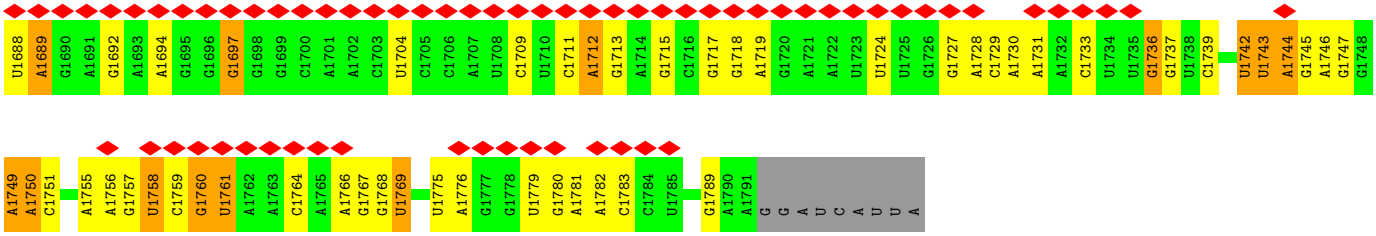


• Molecule 3: 18S rRNA

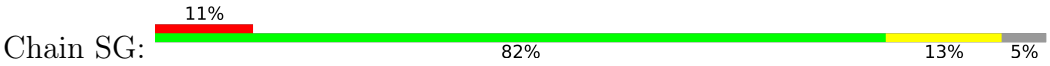
Chain SA:

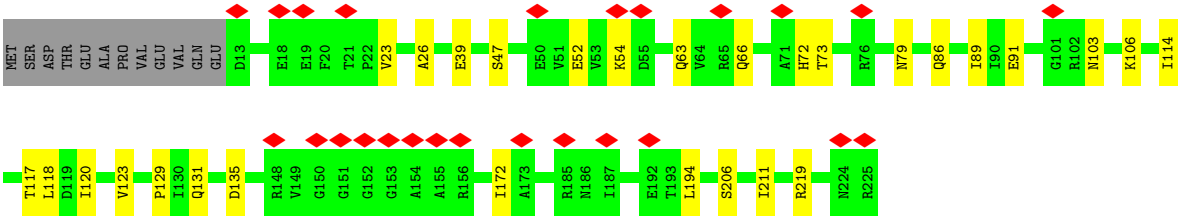




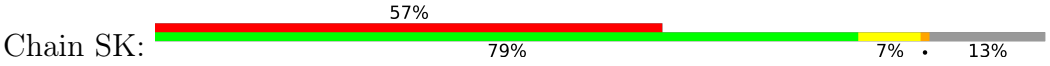


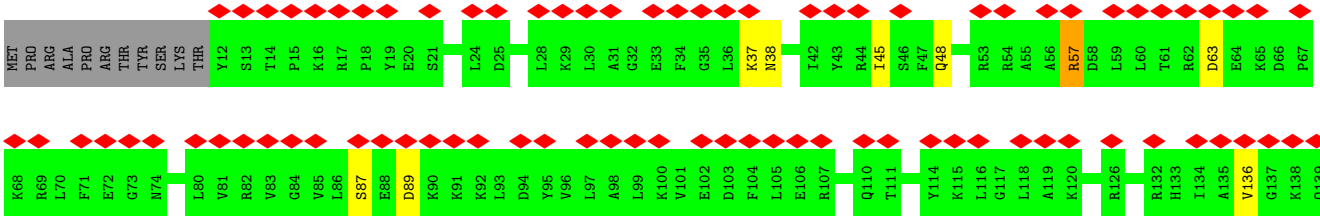
• Molecule 4: 40S ribosomal protein S5



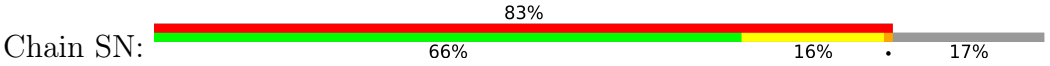


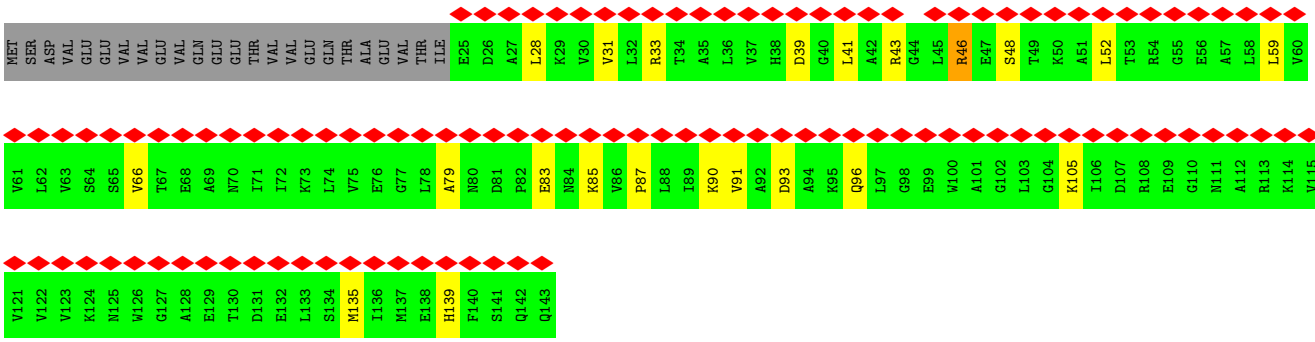
• Molecule 5: 40S ribosomal protein S9-A





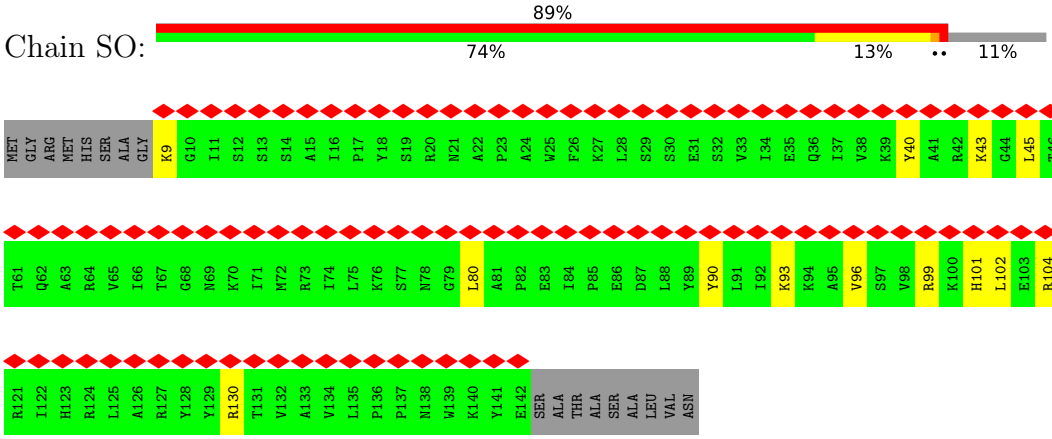
• Molecule 6: 40S ribosomal protein S12





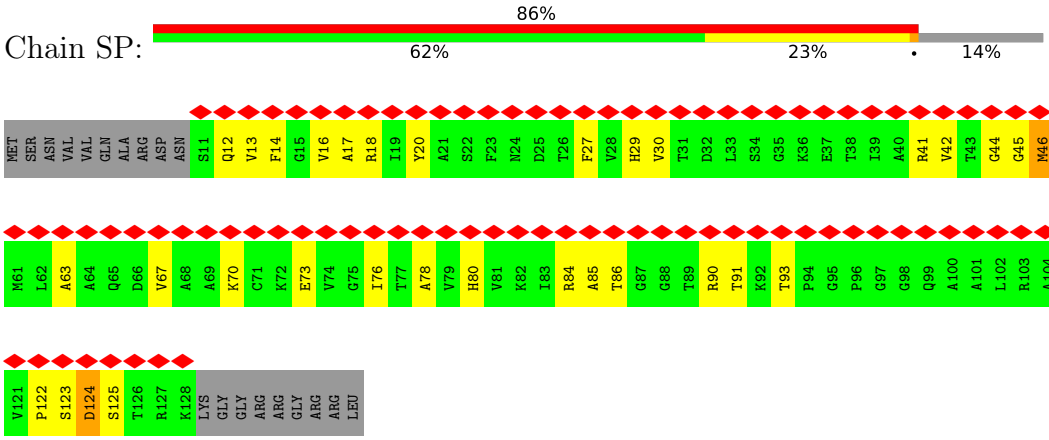
• Molecule 7: 40S ribosomal protein S13

Chain SO:



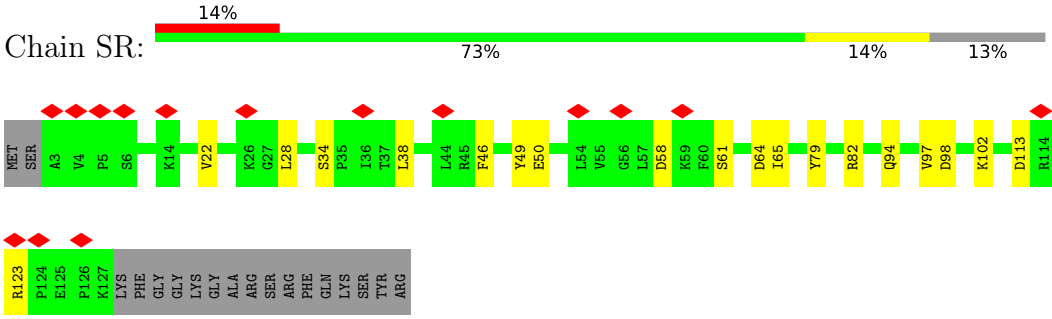
• Molecule 8: 40S ribosomal protein S14-A

Chain SP:



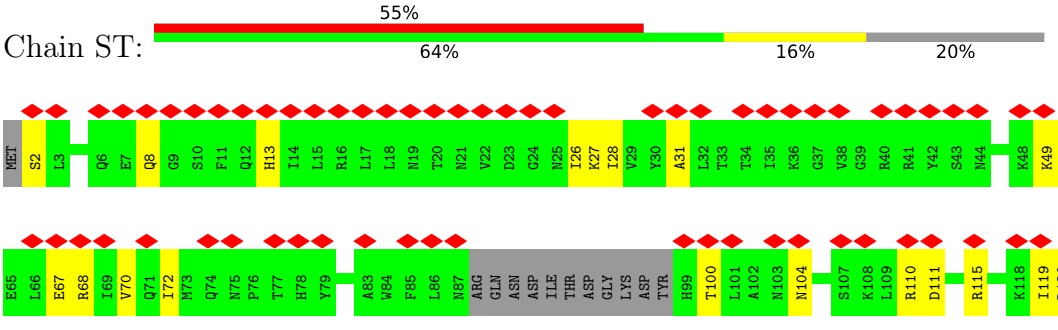
• Molecule 9: 40S ribosomal protein S16-A

Chain SR:



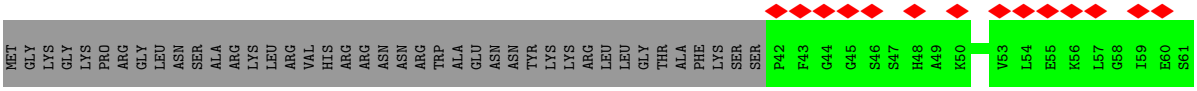
• Molecule 10: 40S ribosomal protein S18-A

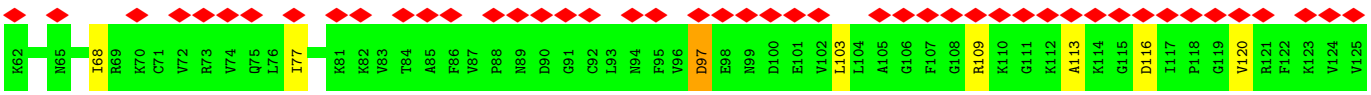
Chain ST:

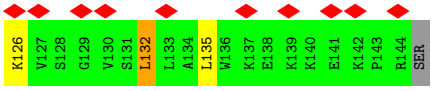


• Molecule 11: 40S ribosomal protein S23-A

Chain SY:

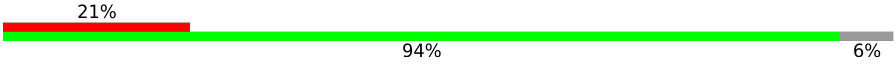


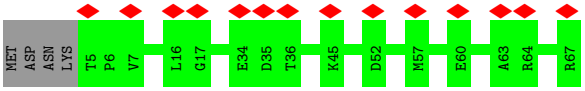




• Molecule 12: 40S ribosomal protein S28-A

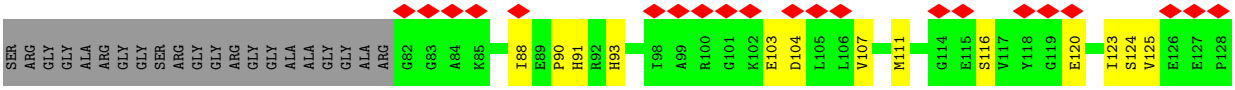
Chain Sd:

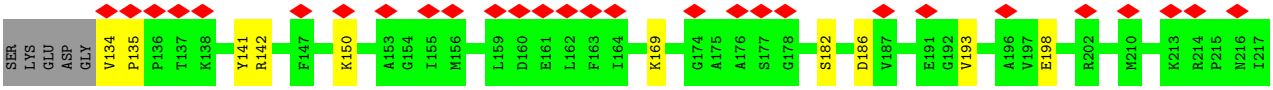


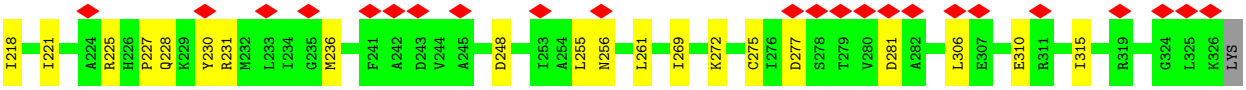


• Molecule 13: rRNA 2'-O-methyltransferase fibrillarin

Chain 3B:

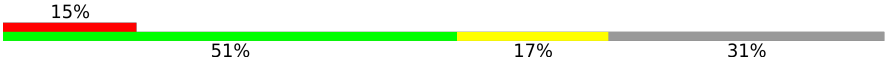


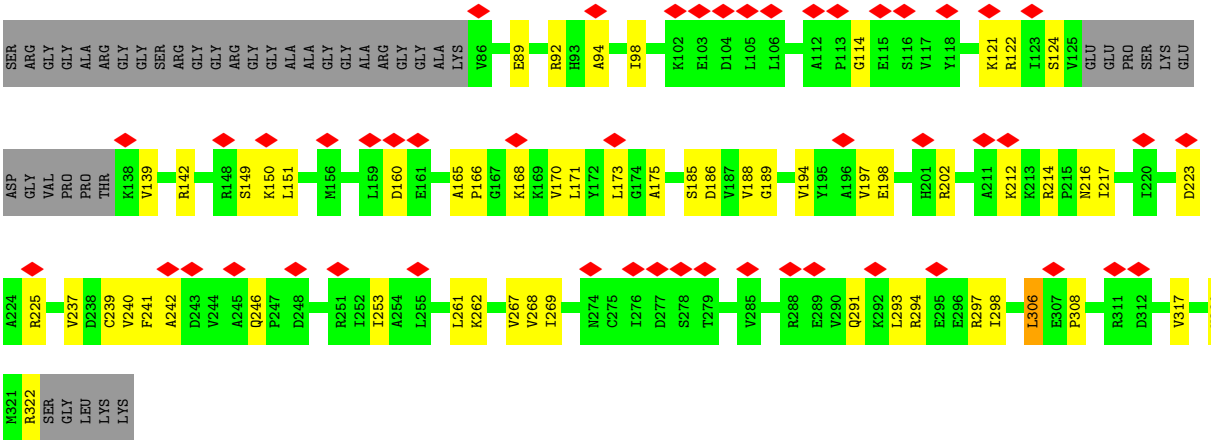




• Molecule 13: rRNA 2'-O-methyltransferase fibrillarin

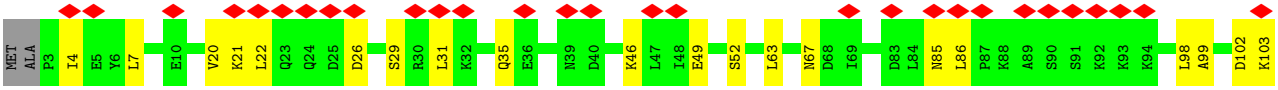
Chain 3C:

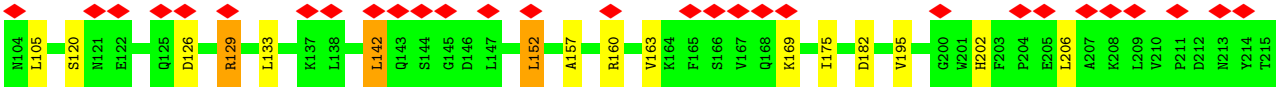


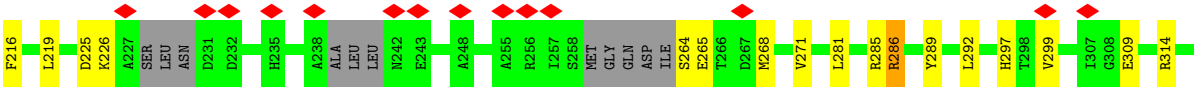


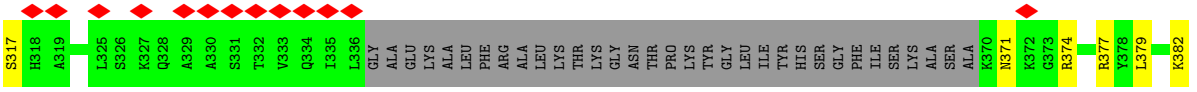
• Molecule 14: Nucleolar protein 56

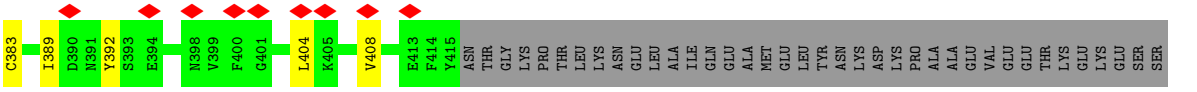
Chain 3D:

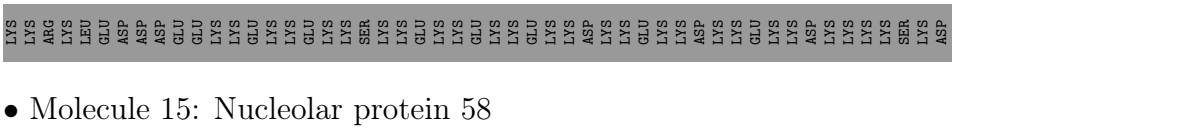


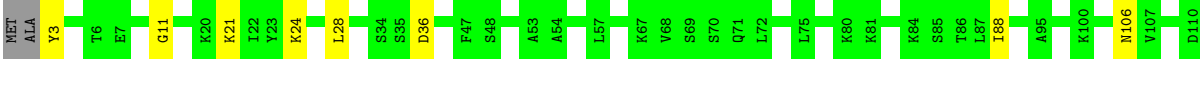






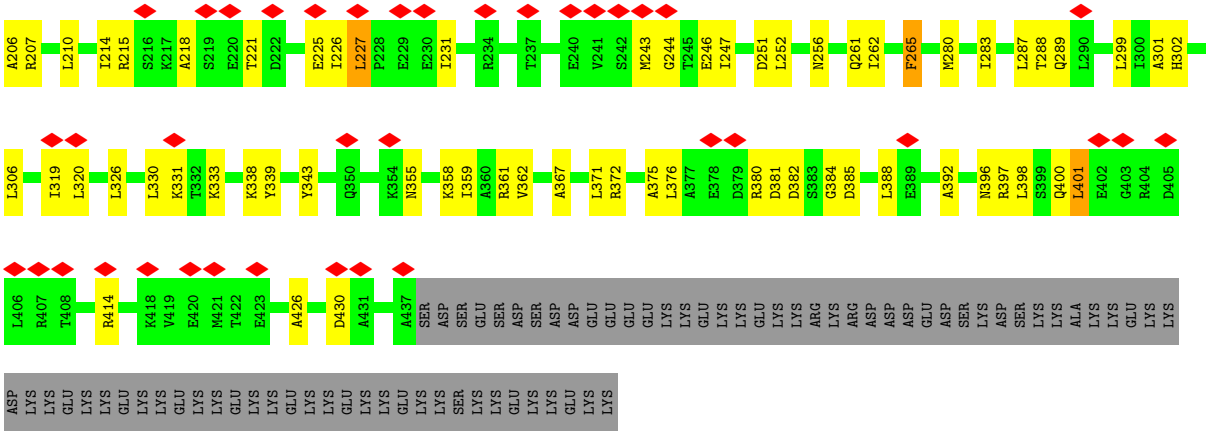






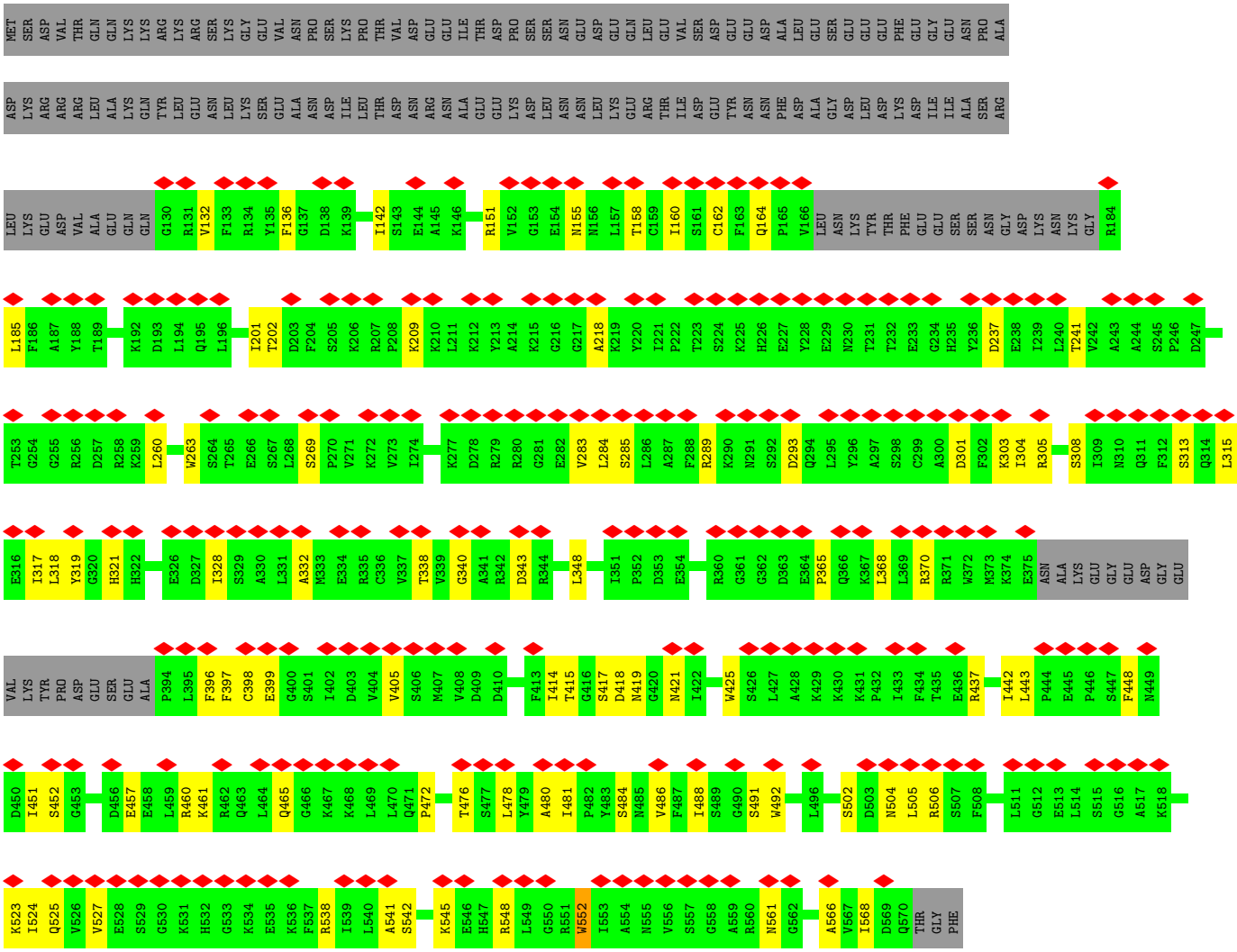
• Molecule 15: Nucleolar protein 58

Chain 3E:



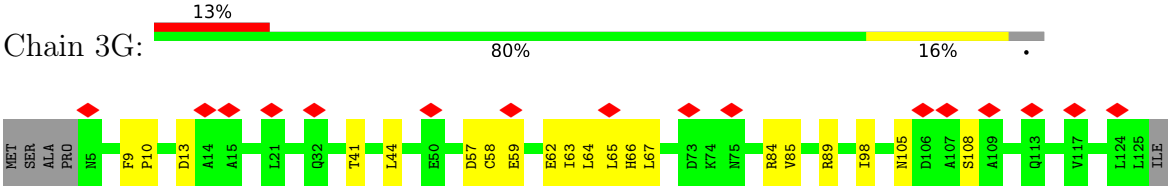
• Molecule 16: Ribosomal RNA-processing protein 9

Chain 3F:



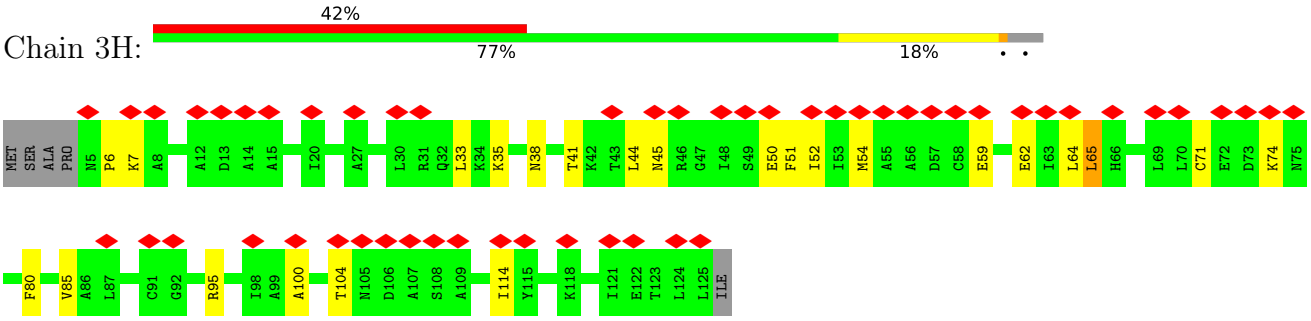
• Molecule 17: 13 kDa ribonucleoprotein-associated protein

Chain 3G:



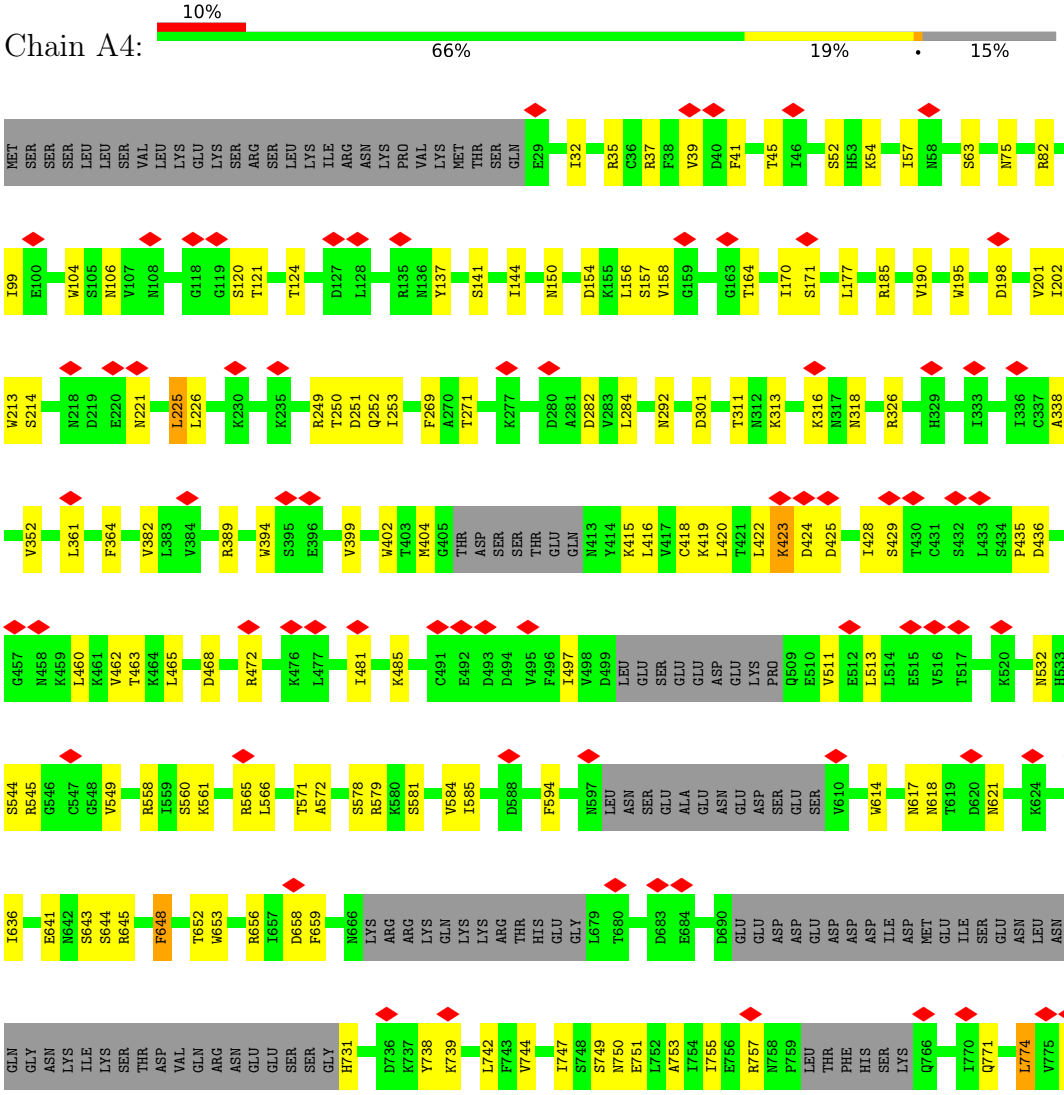
• Molecule 17: 13 kDa ribonucleoprotein-associated protein

Chain 3H:



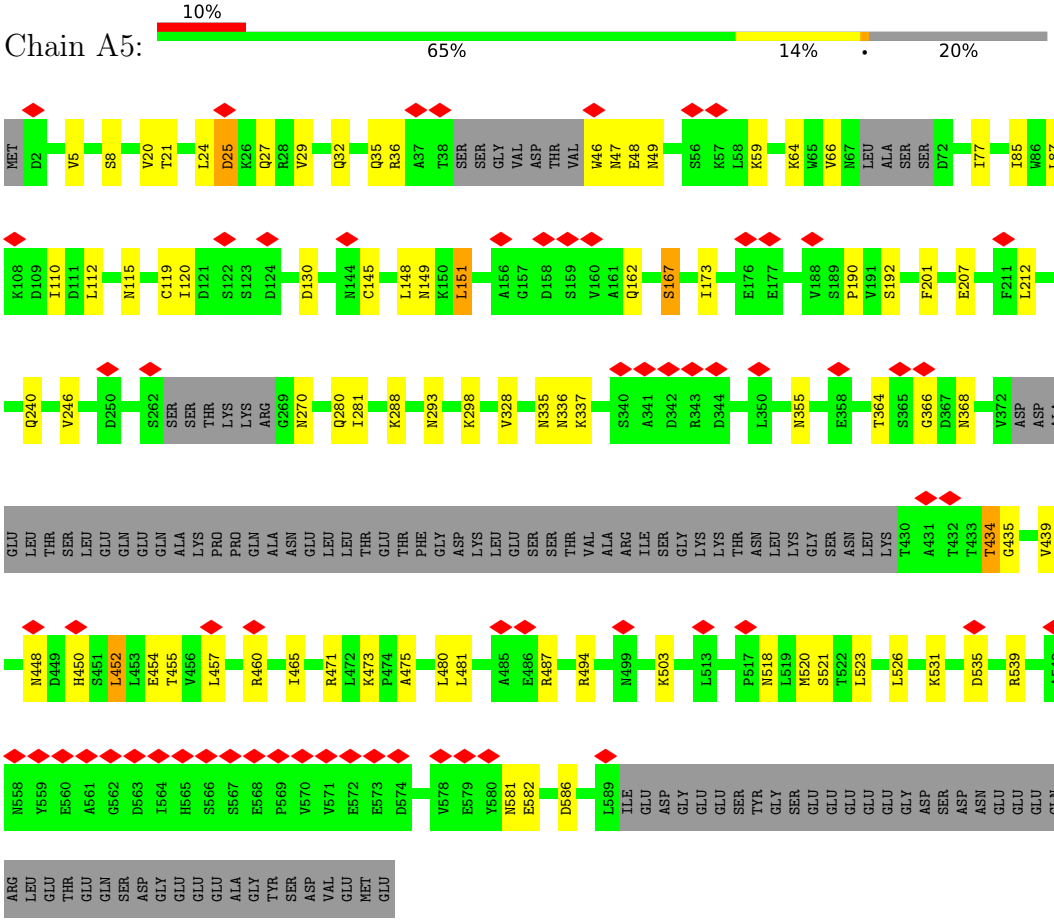
• Molecule 18: U3 small nucleolar RNA-associated protein 4

Chain A4:



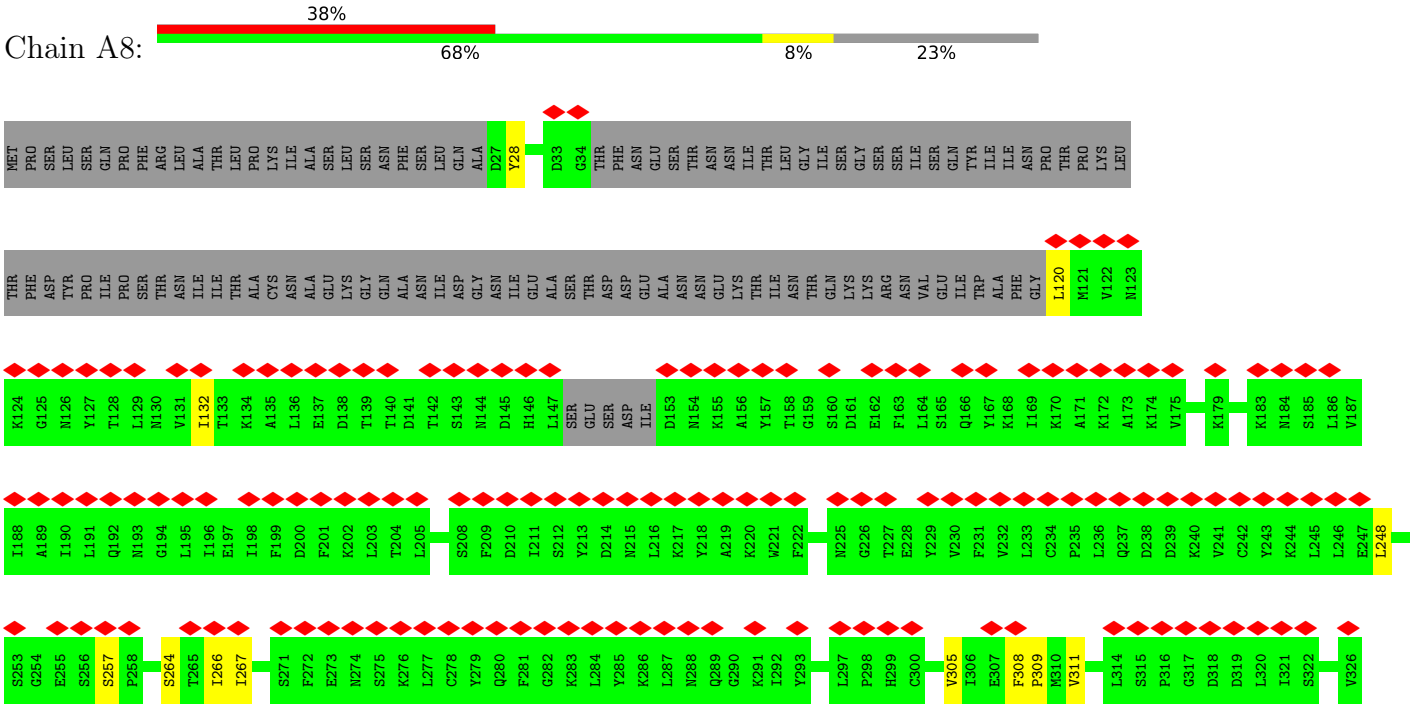
• Molecule 19: U3 small nucleolar RNA-associated protein 5

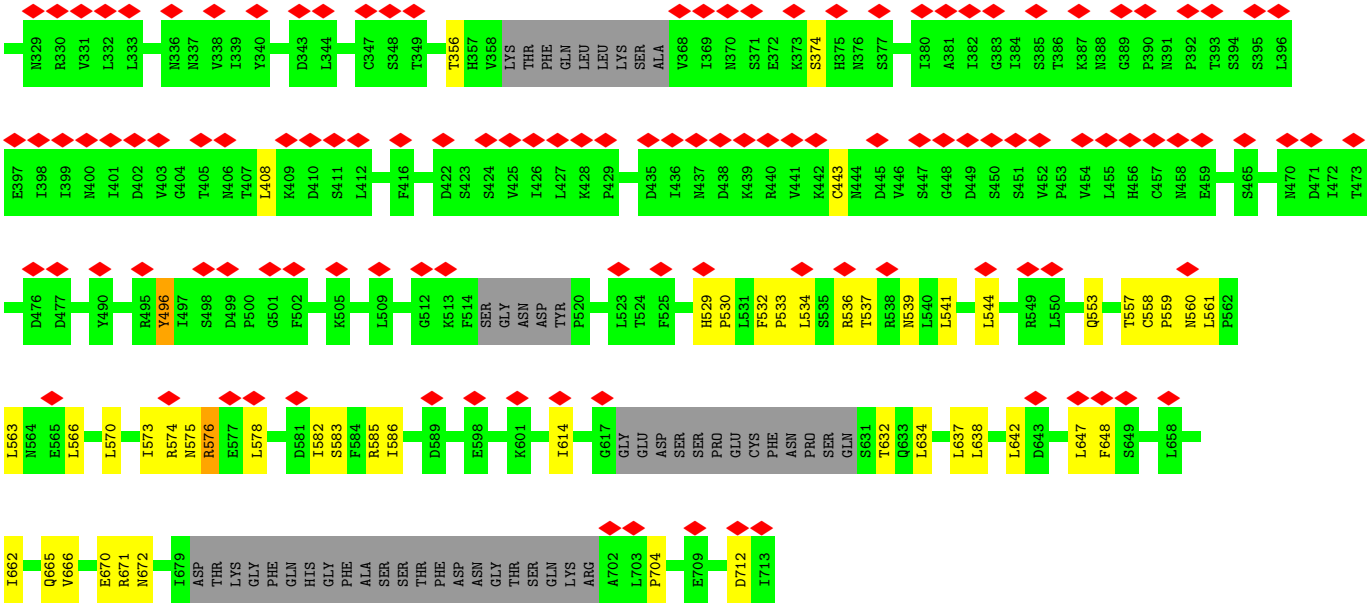
Chain A5:



• Molecule 20: U3 small nucleolar RNA-associated protein 8

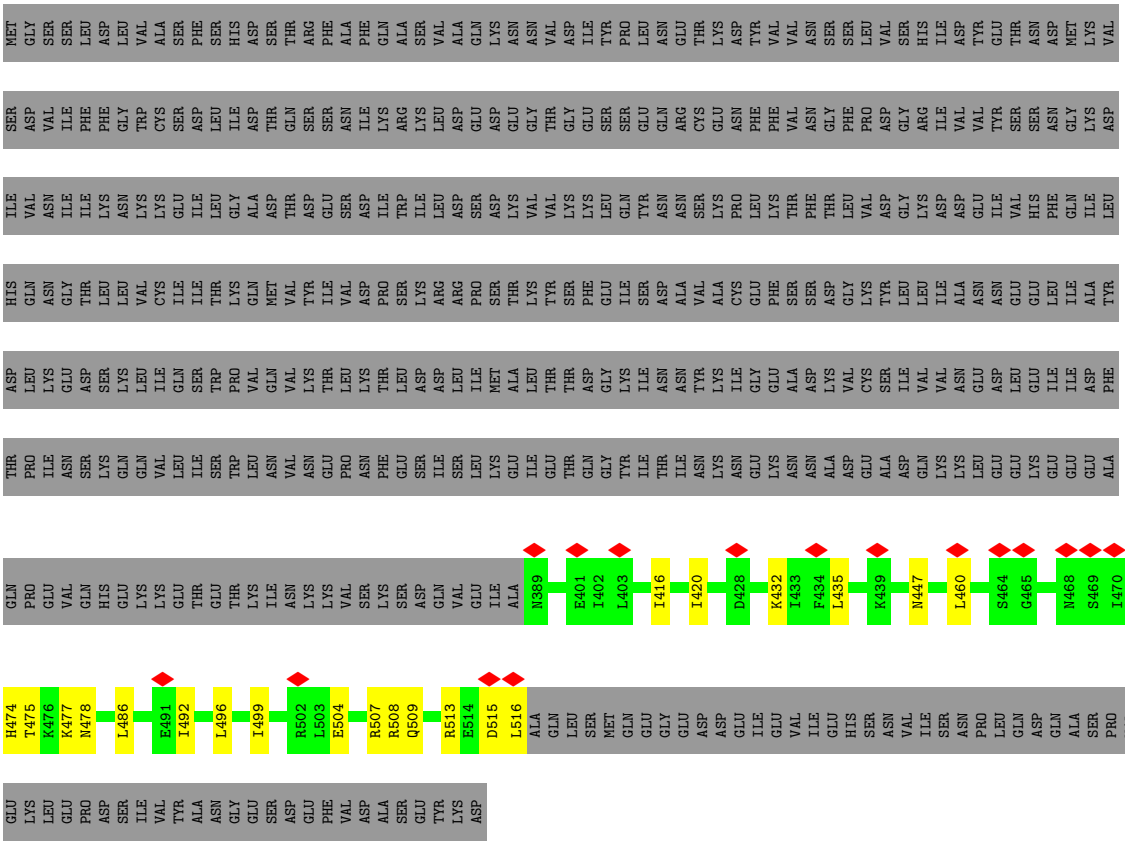
Chain A8:





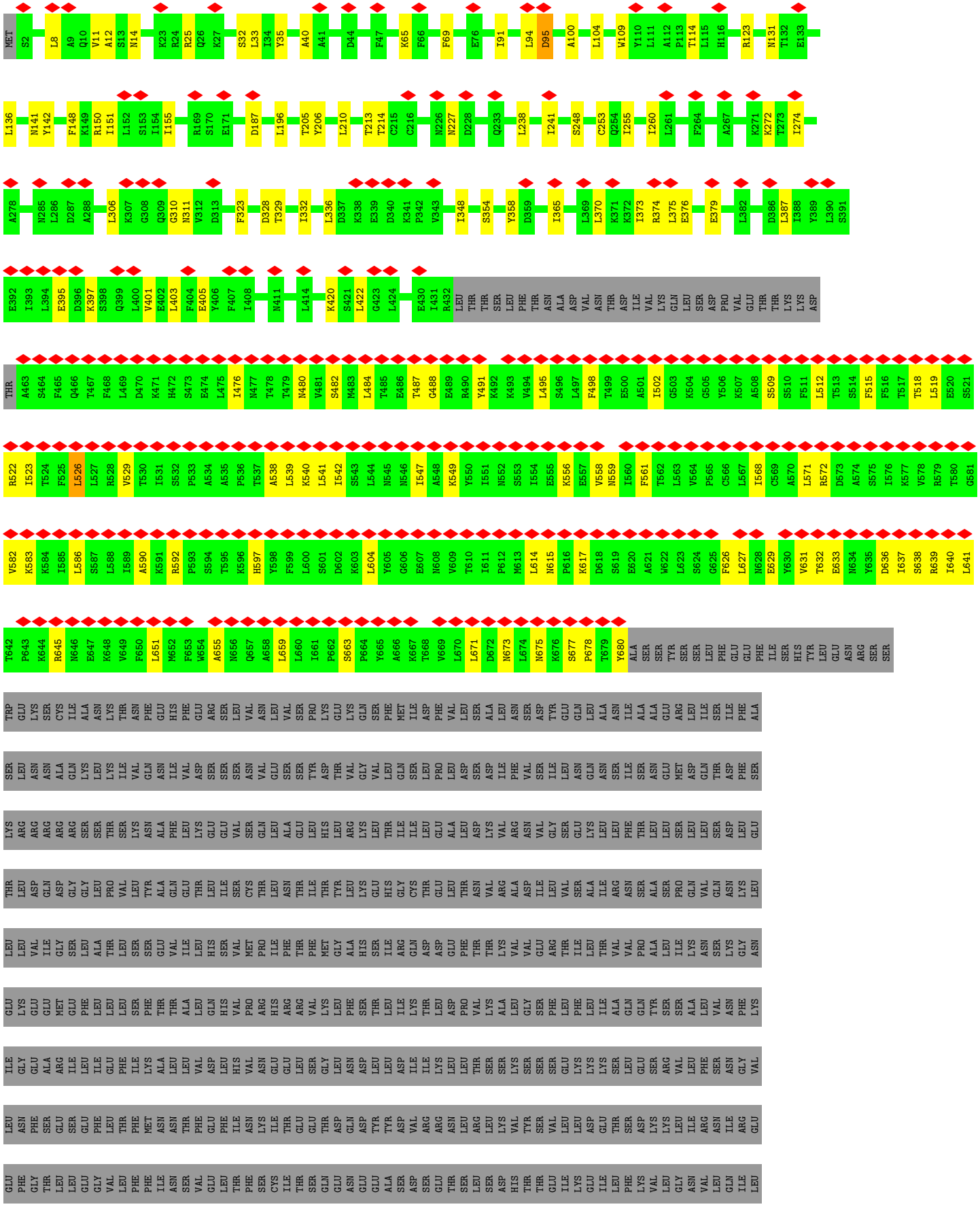
• Molecule 21: U3 small nucleolar RNA-associated protein 9

Chain A9:



• Molecule 22: U3 small nucleolar RNA-associated protein 10

Chain AE: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L136 N141 Y142 F148 K149 R150 I151 L152 S153 I154 T155 R169 S170 E171 D187 L196 T205 Y206 L210 T213 T214 C215 C216 N226 N227 D228 Q233 L238 I241 S248 C253 Q254 I255 I260 L261 F264 A267 K271 K272 T273 I274
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E392 I393 L394 E395 D396 K397 S398 Q399 L400 V401 E402 L403 F404 E405 Y406 F407 I408 N411 L414 K420 S421 L422 G423 L424 E430 I431 R432 LEU THR THR SER LEU PHE THR ASN ALA ASP VAL ASN THR ASP ILE VAL LYS GLN LEU SER ASP PRO VAL GLU THR THR LYS LYS ASP
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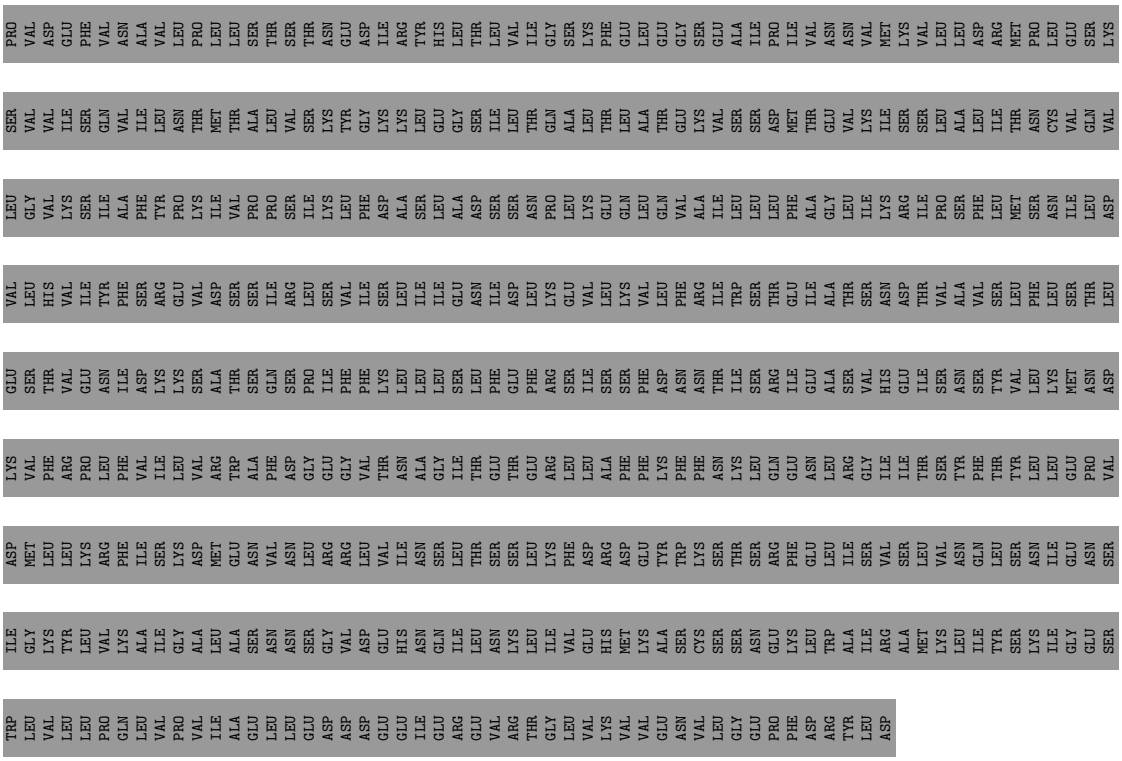
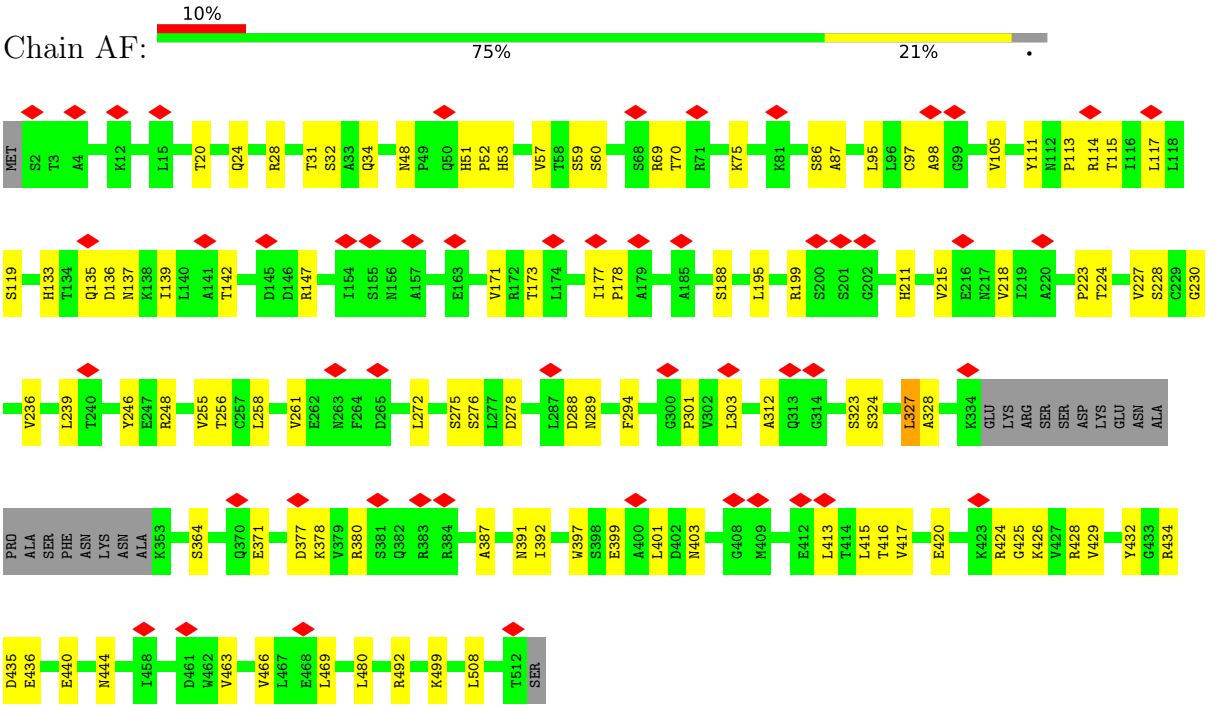


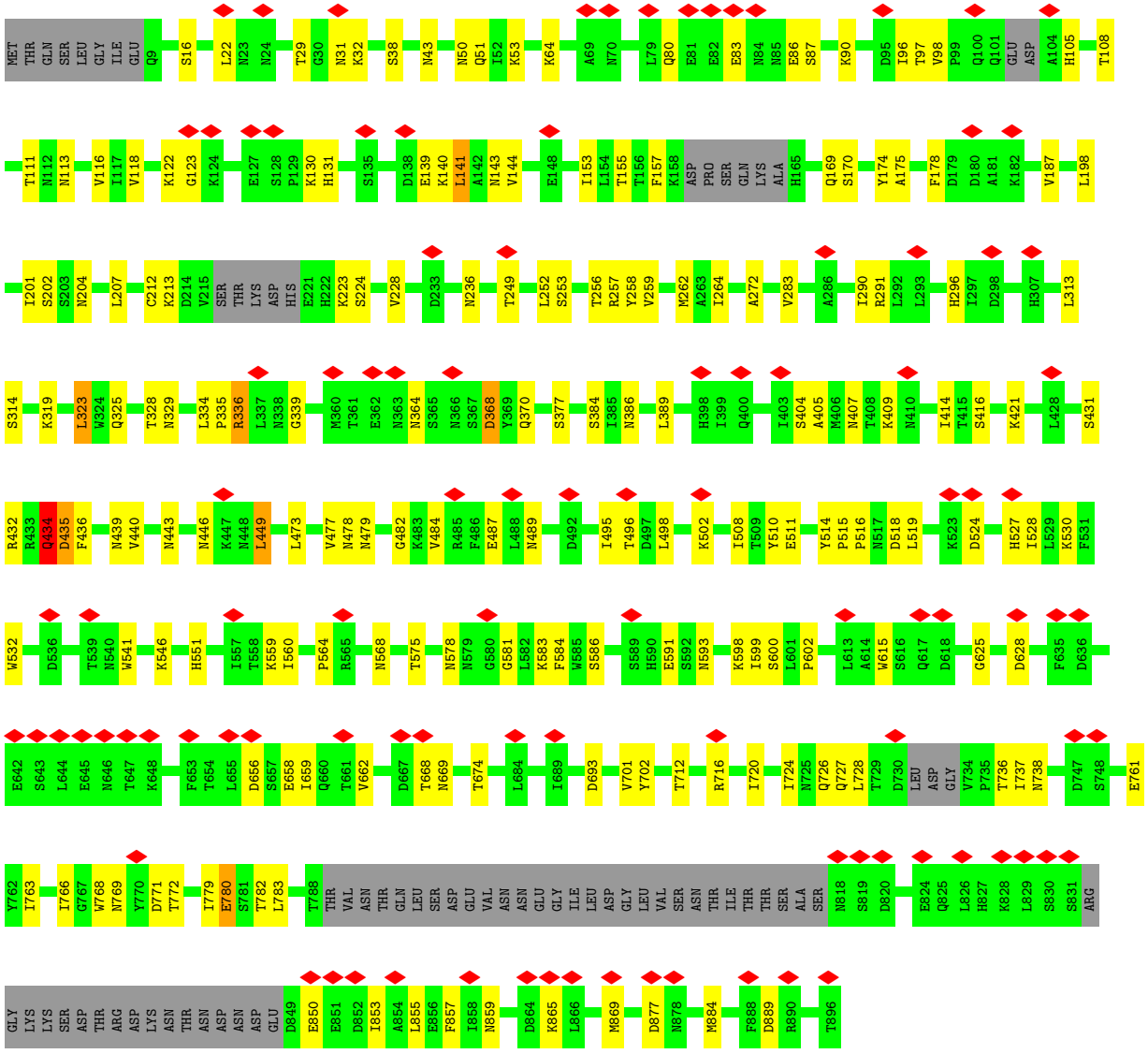
• Molecule 23: U3 small nucleolar RNA-associated protein 15

Chain AF:



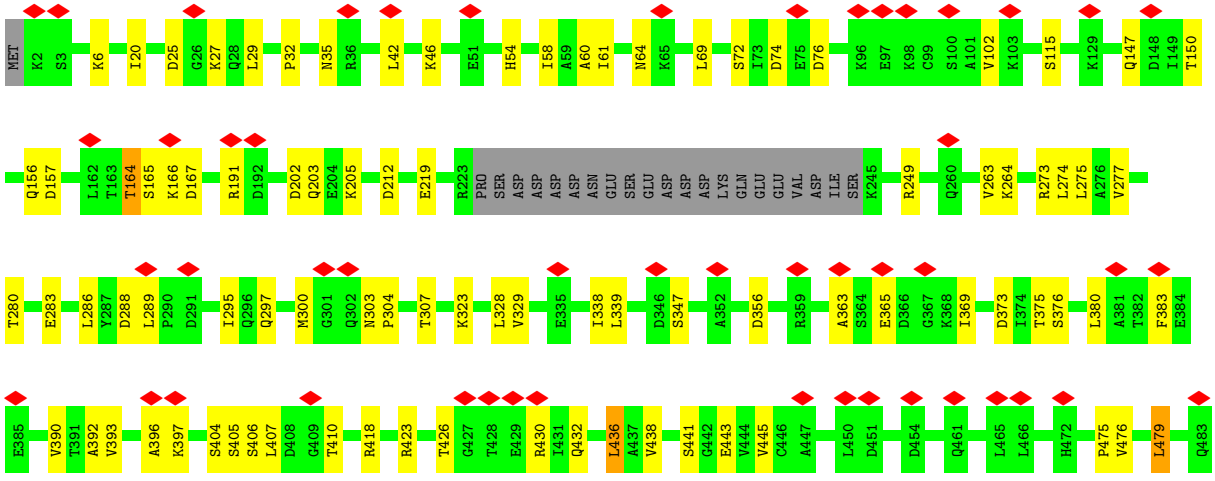
• Molecule 24: NET1-associated nuclear protein 1

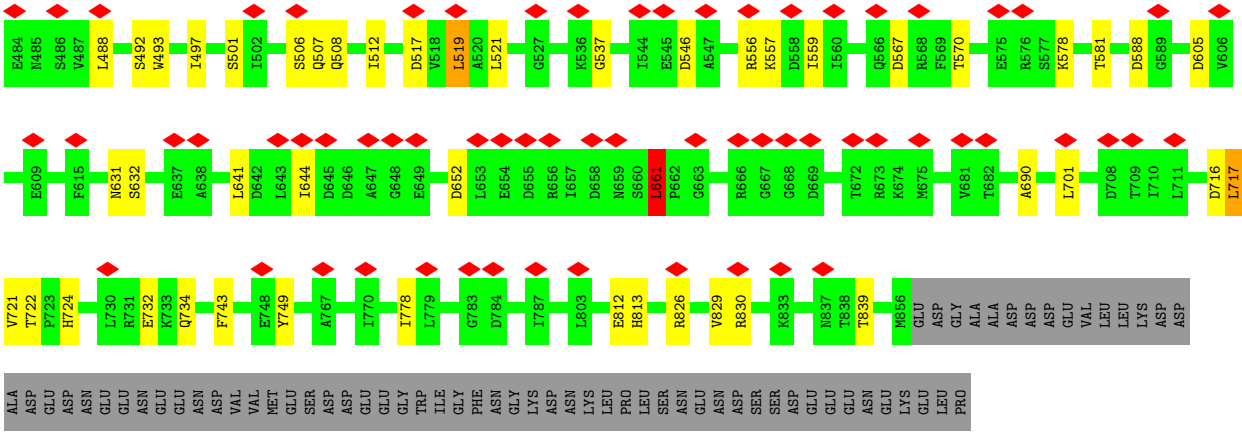
Chain AG:



• Molecule 25: Periodic tryptophan protein 2

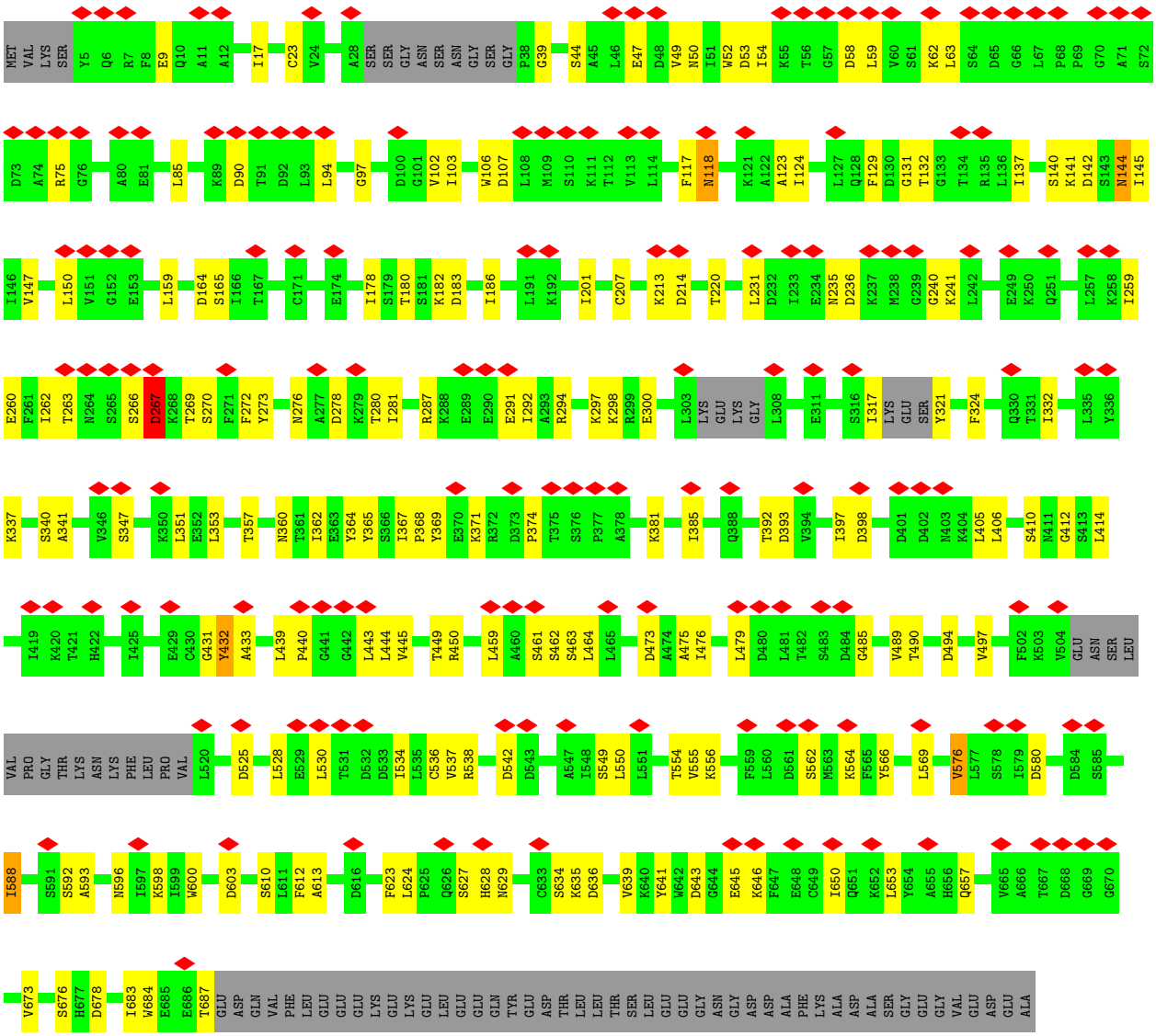
Chain B1:

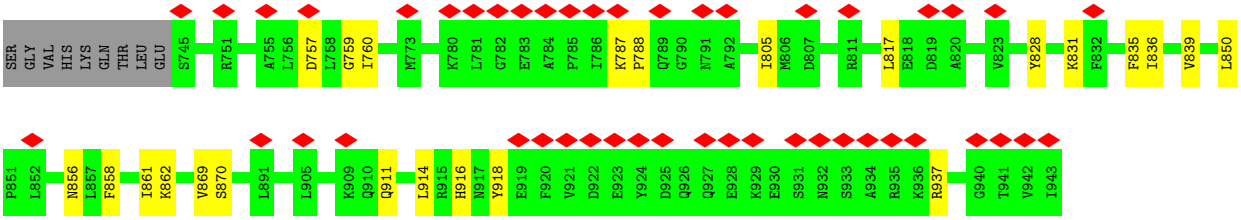




• Molecule 26: U3 small nucleolar RNA-associated protein 12

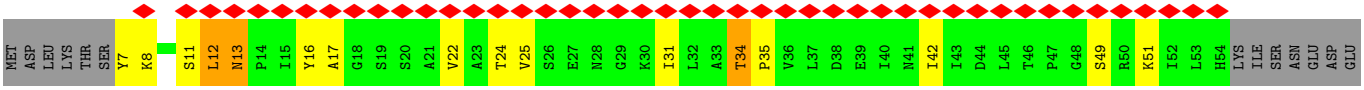
Chain B2:

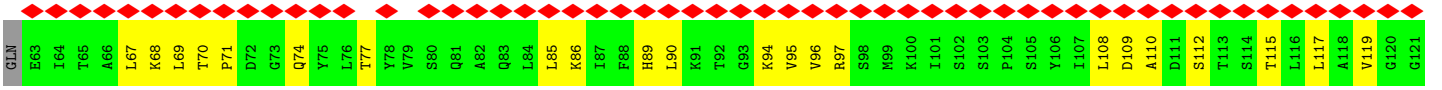


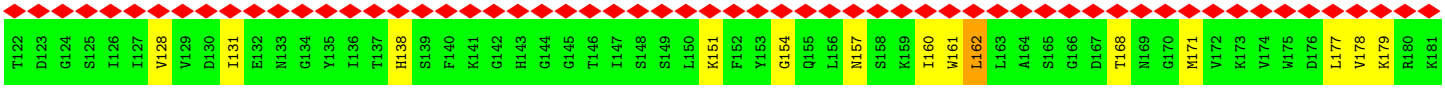


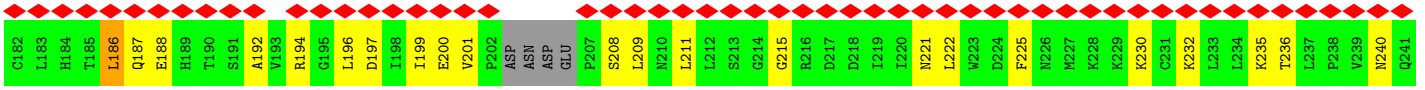
• Molecule 27: U3 small nucleolar RNA-associated protein 13

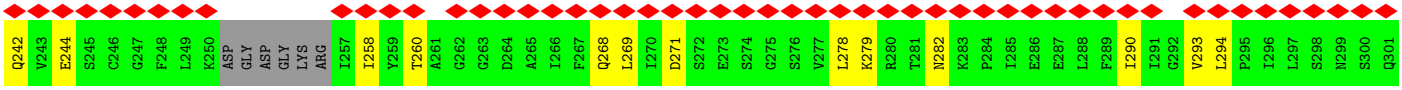
Chain B3:

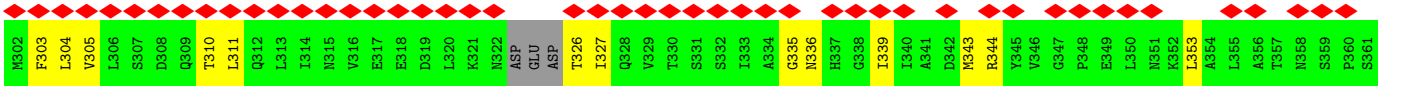


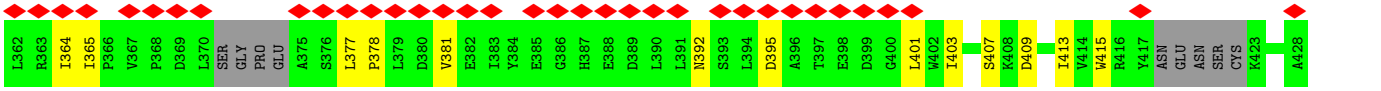


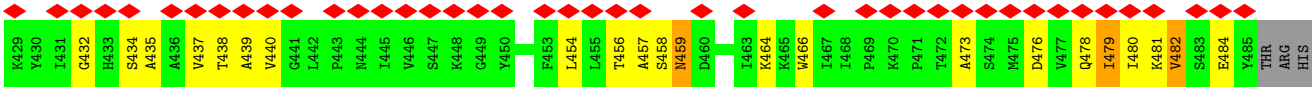


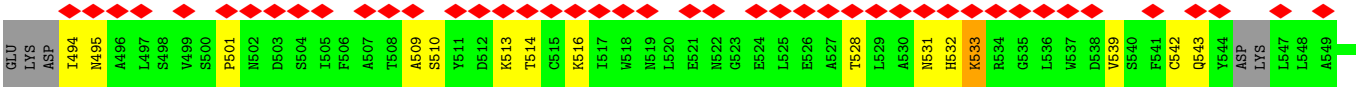


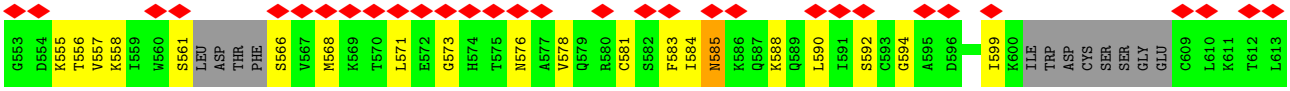


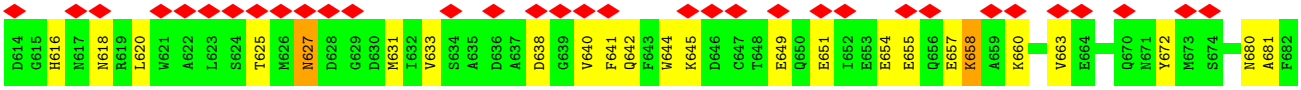


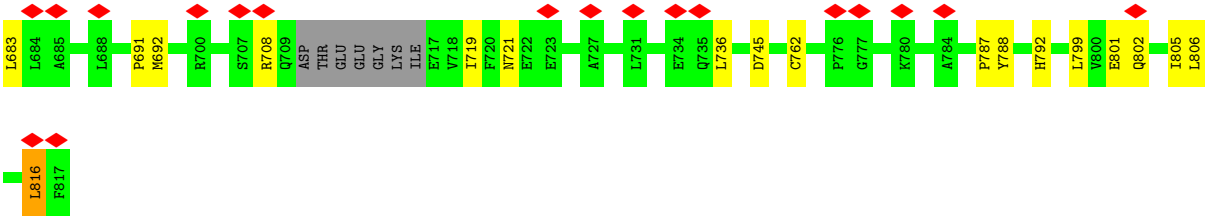






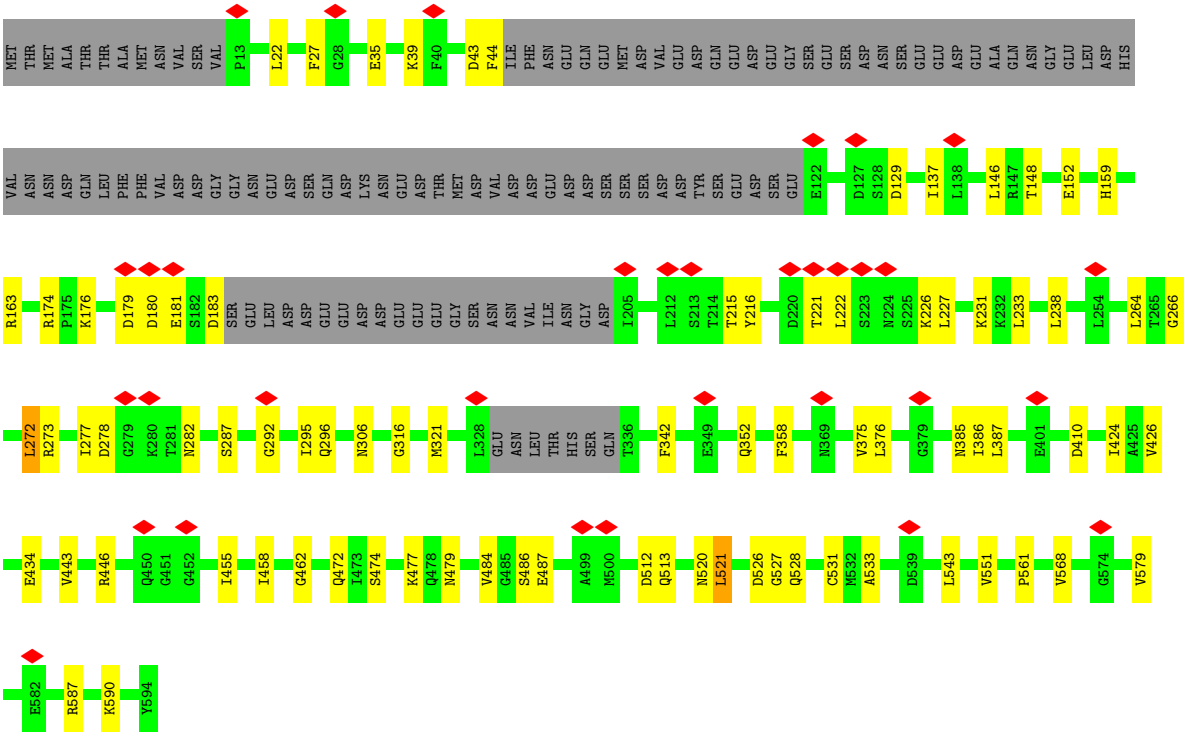






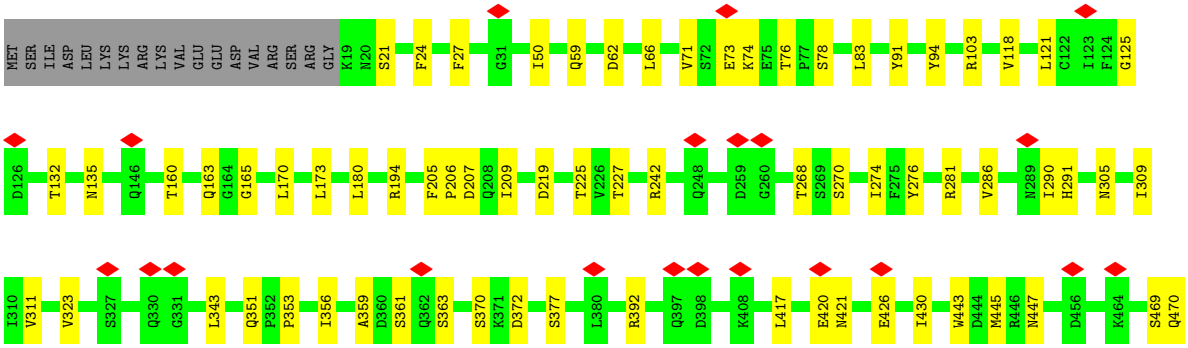
• Molecule 28: U3 small nucleolar RNA-associated protein 18

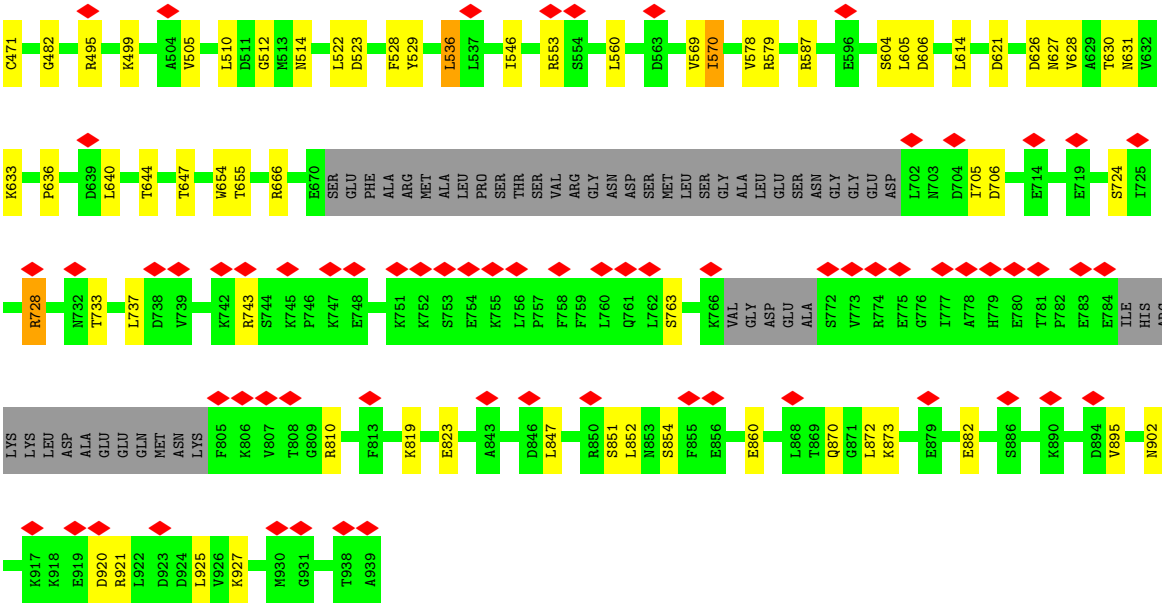
Chain B8:



• Molecule 29: U3 small nucleolar RNA-associated protein 21

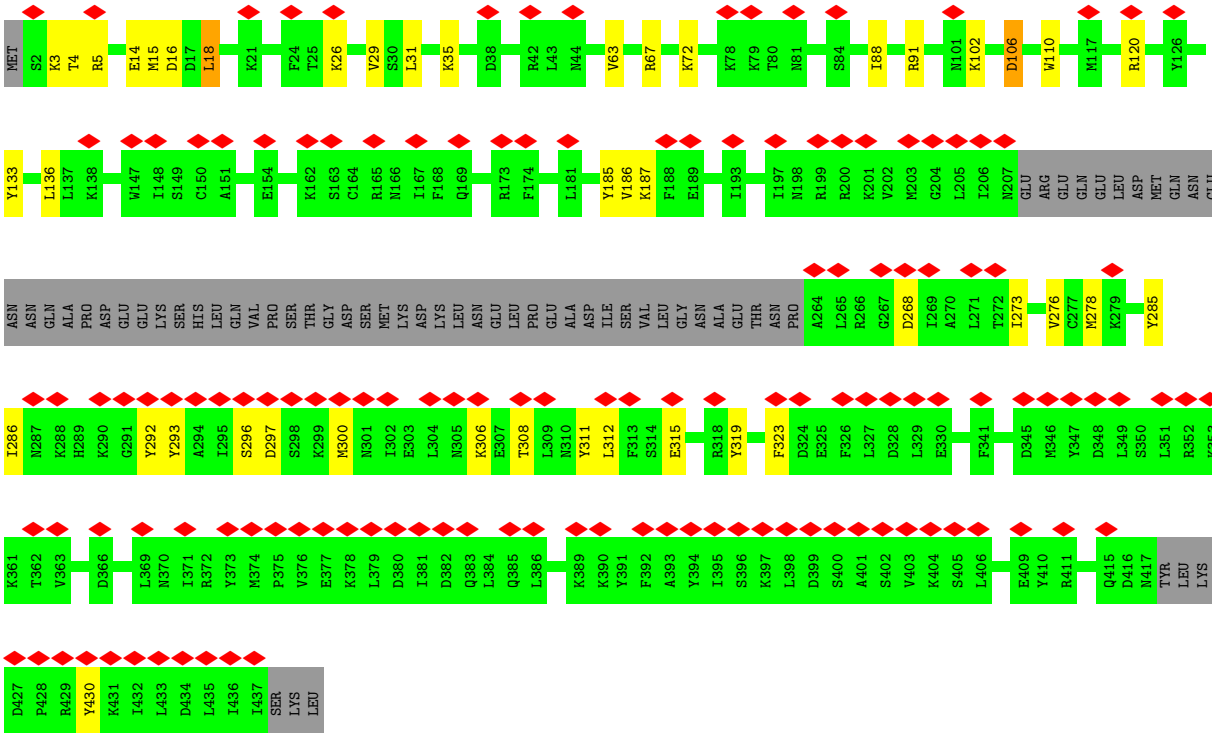
Chain BE:





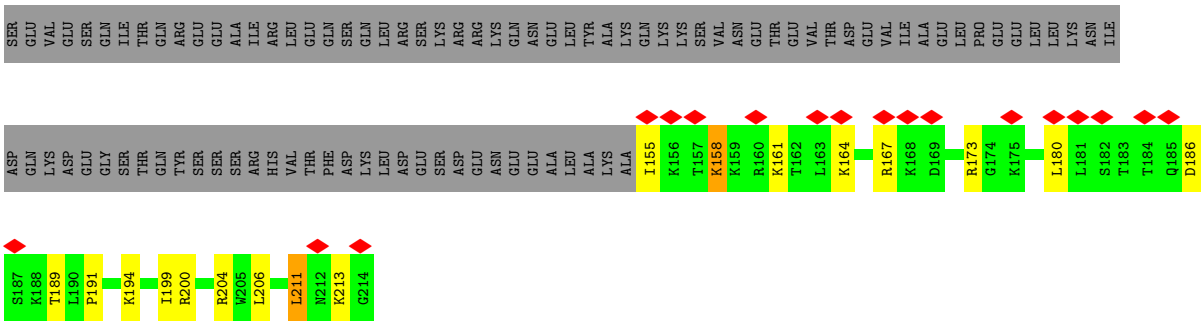
• Molecule 30: U3 small nucleolar RNA-associated protein 6

Chain B6:



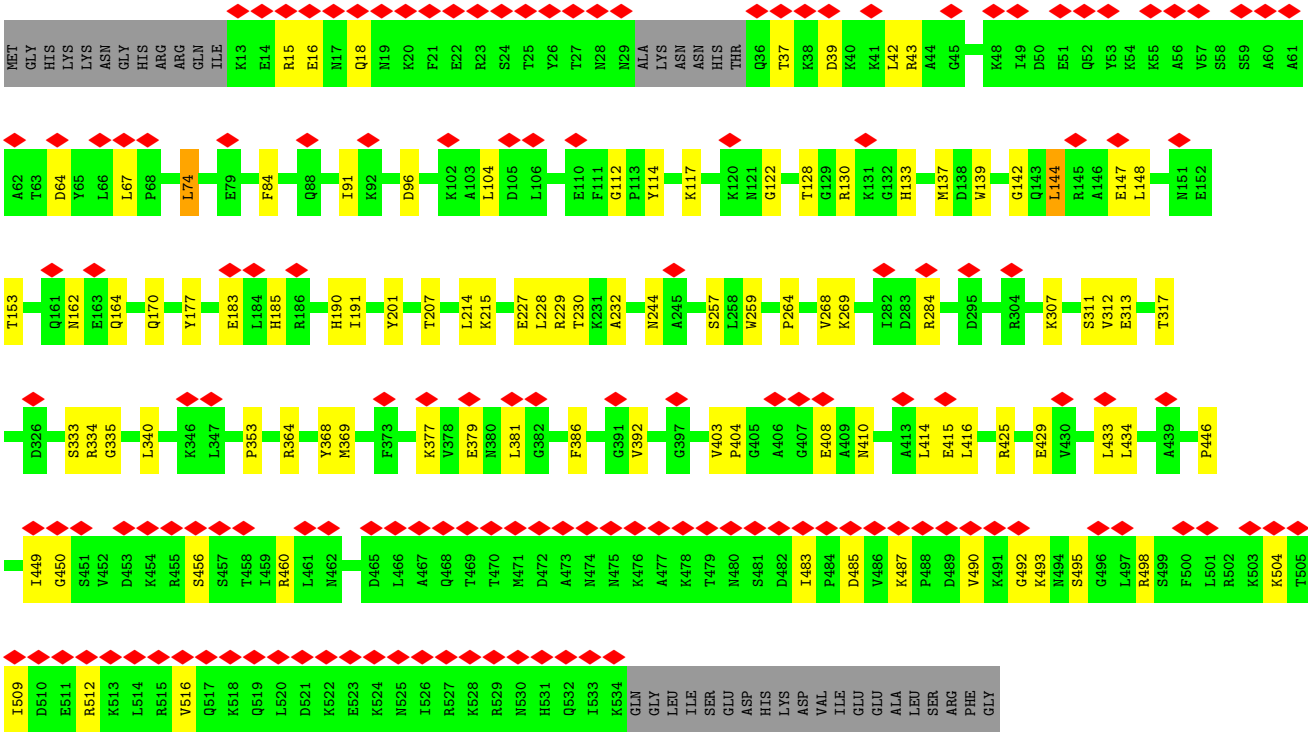
• Molecule 31: Bud site selection protein 21

Chain 5B:



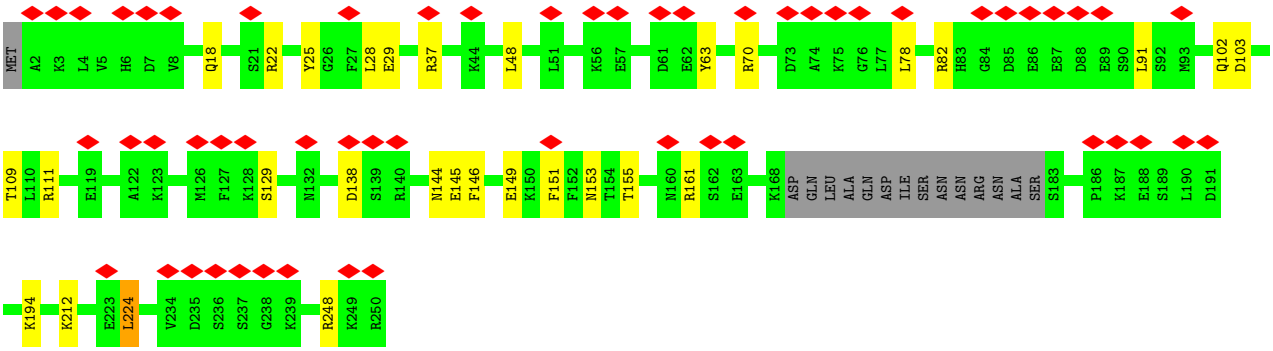
• Molecule 32: U3 small nucleolar RNA-associated protein 7

Chain 5C:



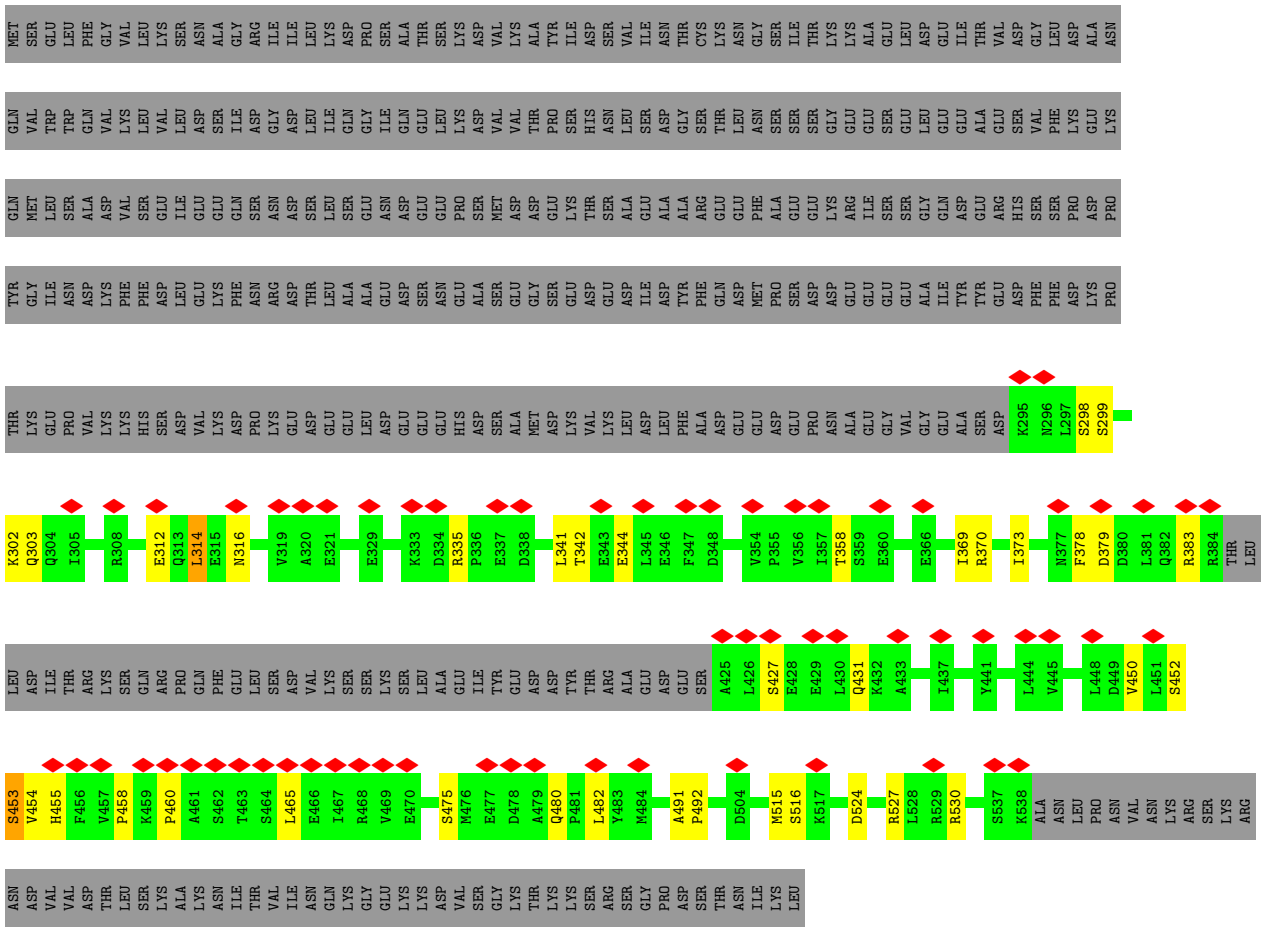
• Molecule 33: U3 small nucleolar RNA-associated protein 11

Chain 5D:



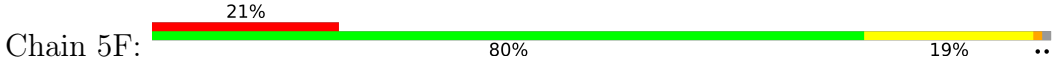
• Molecule 34: U3 small nucleolar RNA-associated protein MPP10

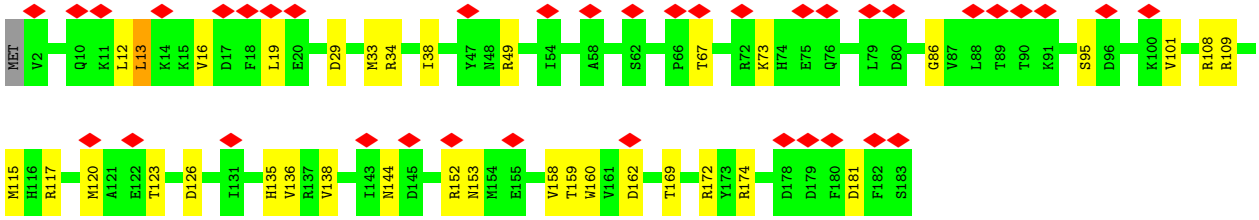
Chain 5E:



• Molecule 35: U3 small nucleolar ribonucleoprotein protein IMP3

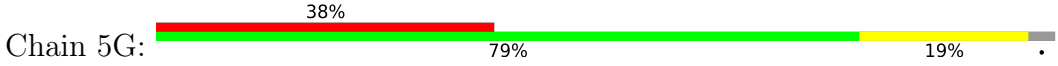
Chain 5F:

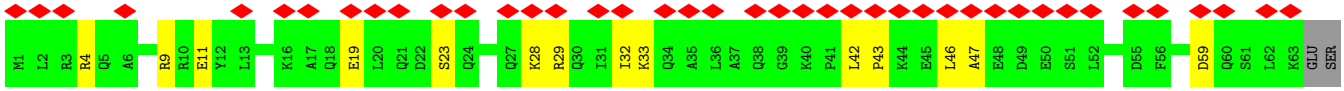


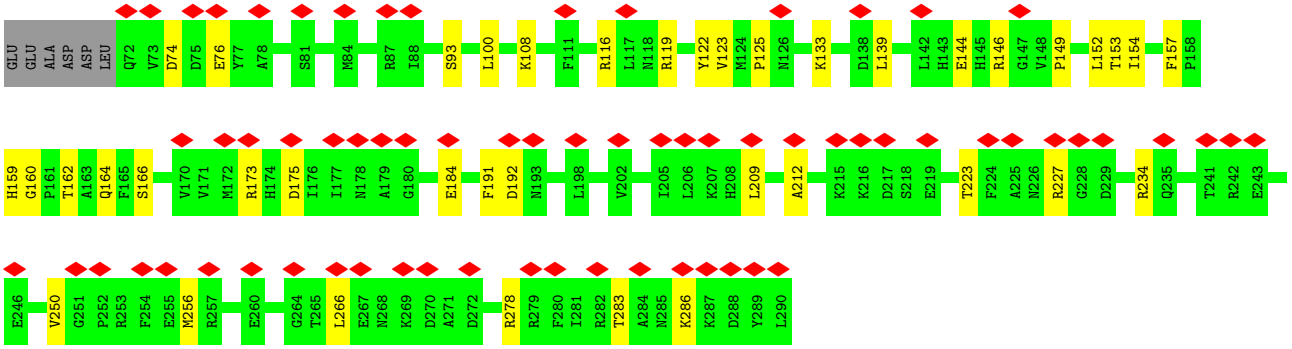


• Molecule 36: U3 small nucleolar ribonucleoprotein protein IMP4

Chain 5G:

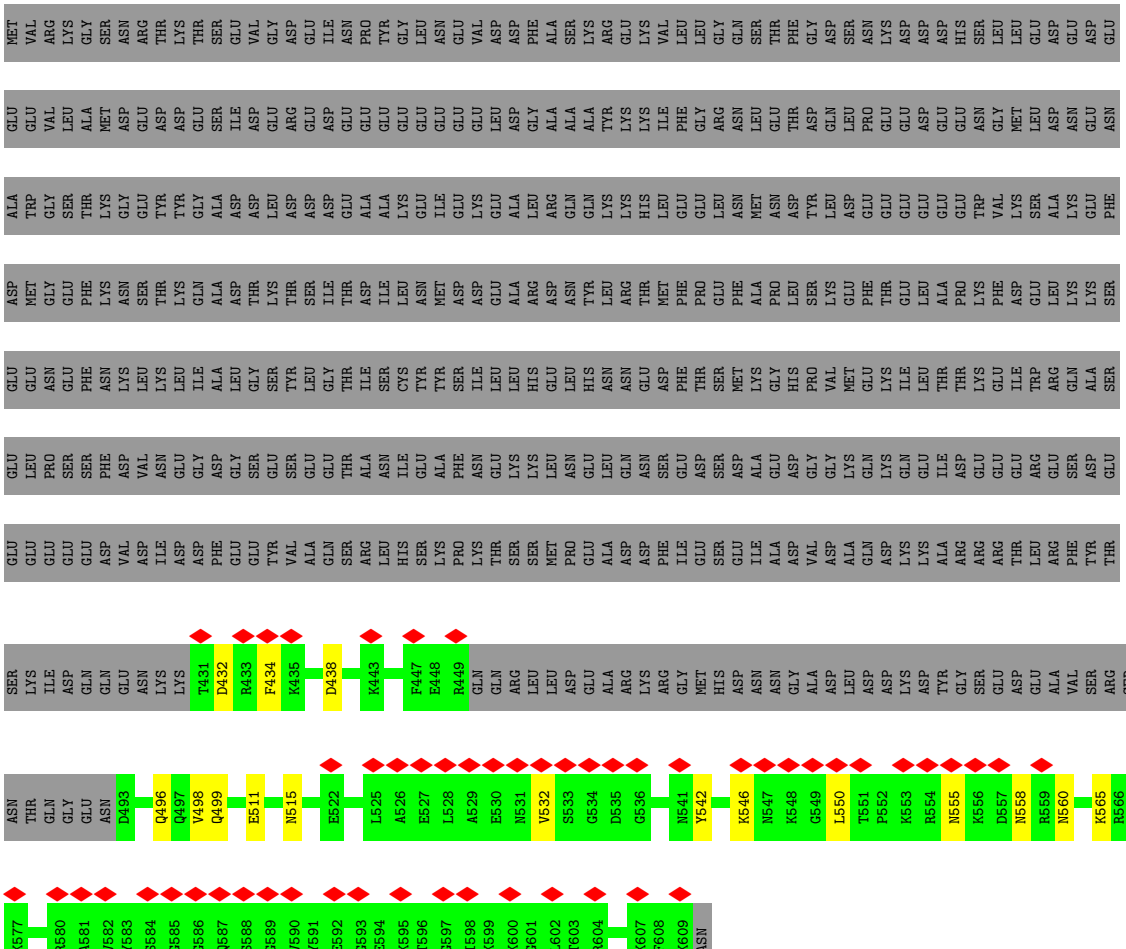






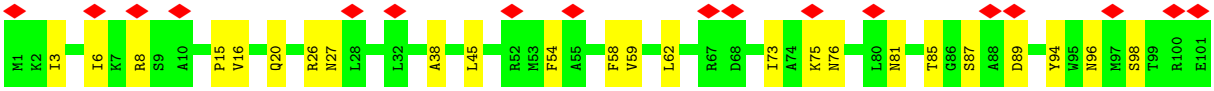
• Molecule 37: Something about silencing protein 10

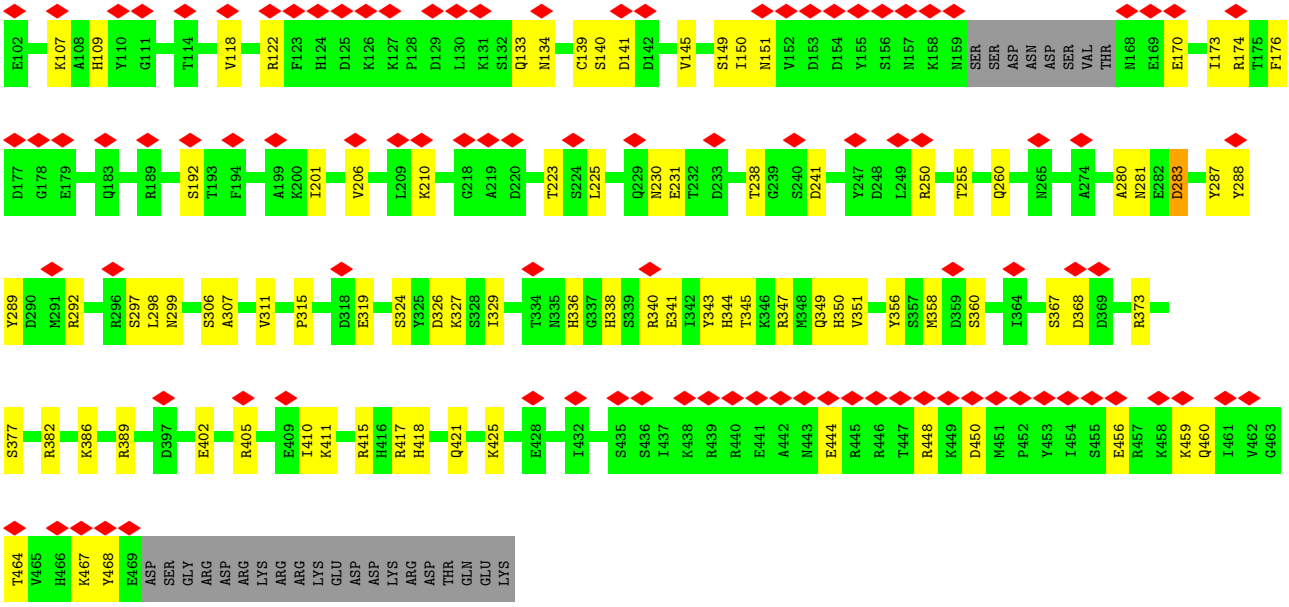
Chain 5H:



• Molecule 38: Protein SOF1

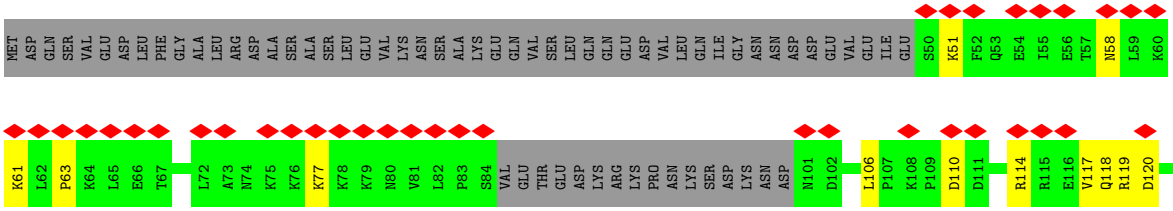
Chain 5I:





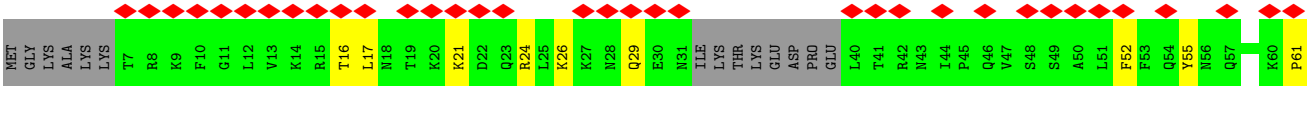
• Molecule 39: rRNA-processing protein FCF2

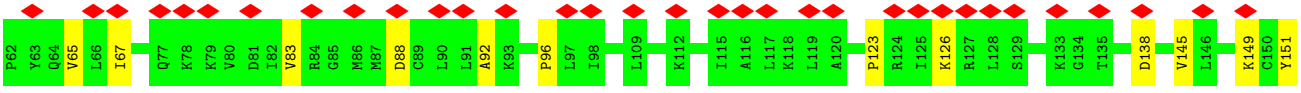
Chain 5J:

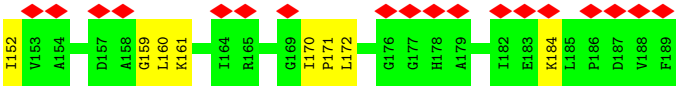


• Molecule 40: rRNA-processing protein FCF1

Chain 5K:

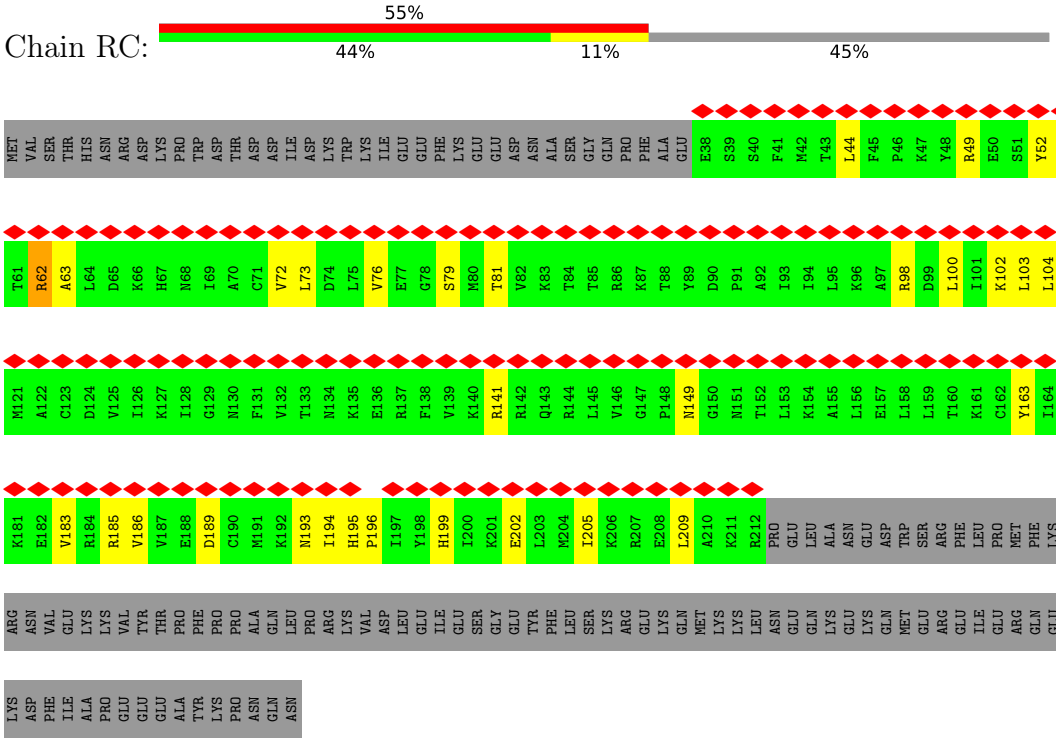






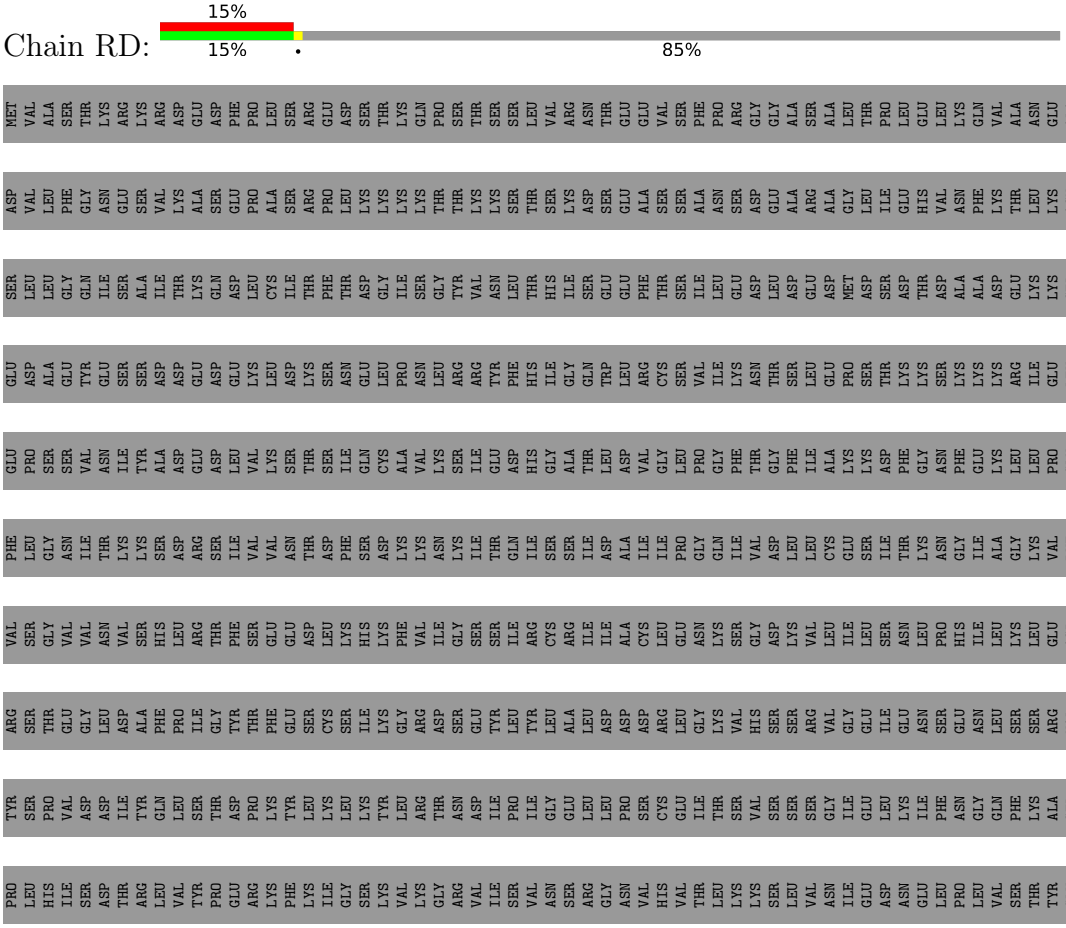
• Molecule 41: KRR1 small subunit processome component

Chain RC:



• Molecule 42: rRNA biogenesis protein RRP5

Chain RD:



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

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

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

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

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

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

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

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

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

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

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

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A1501 L1502 K1503 T1504 I1505 N1506 F1507 R1508 E1509 E1510 A1511 E1512 K1513 L1514 N1515 I1516 W1517 I1518 A1519 M1520 L1521 N1522 L1523 E1524 N1525 T1526 F1527 G1528 T1529 E1530 E1531 T1532 L1533 E1534 E1535 V1536 F1537 S1538 R1539 A1540 C1541 Q1542 Y1543 M1544 D1545 S1546 Y1547 T1548 I1549 H1550 T1551 K1552 L1553 L1554 G1555 I1556 Y1557 E1558 I1559 S1560

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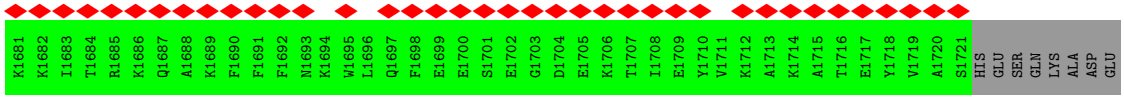
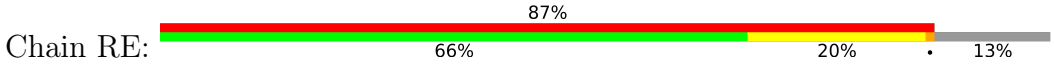
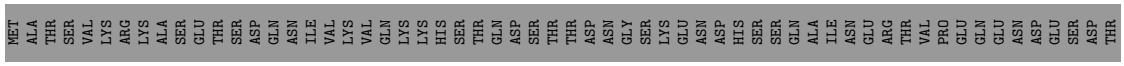
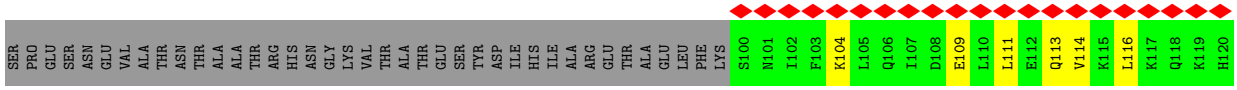
V1621 R1622 K1623 F1624 A1625 Q1626 L1627 E1628 F1629 A1630 K1631 G1632 D1633 P1634 E1635 R1636 G1637 R1638 S1639 L1640 F1641 E1642 G1643 L1644 V1645 A1646 D1647 A1648 P1649 K1650 R1651 I1652 D1653 L1654 W1655 N1656 V1657 Y1658 V1659 D1660 Q1661 E1662 V1663 K1664 A1665 K1666 D1667 K1668 K1669 K1670 V1671 E1672 D1673 L1674 F1675 E1676 R1677 I1678 I1679 T1680

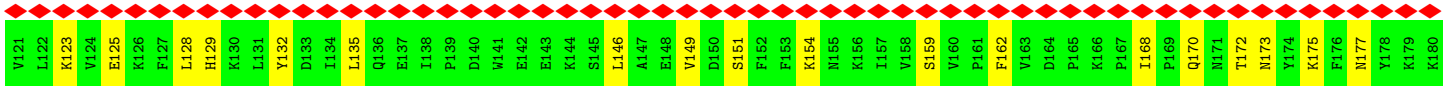


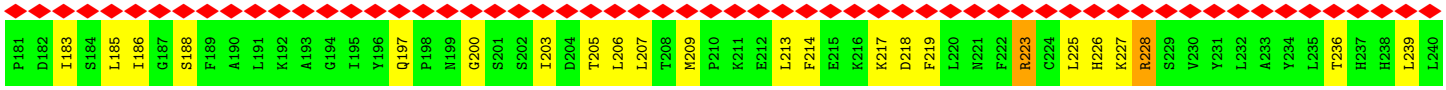
• Molecule 43: U3 small nucleolar RNA-associated protein 22

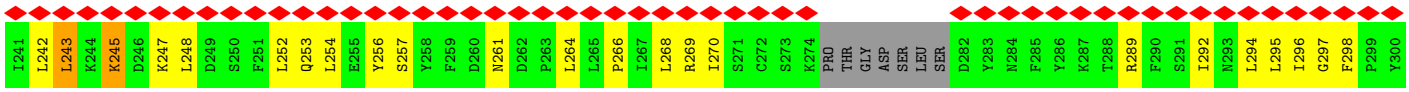


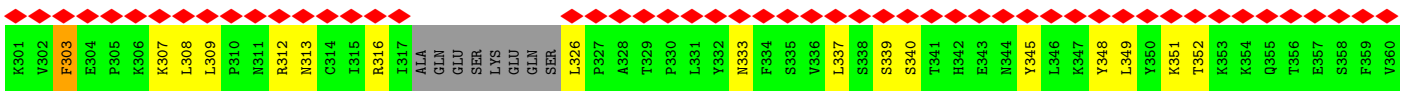


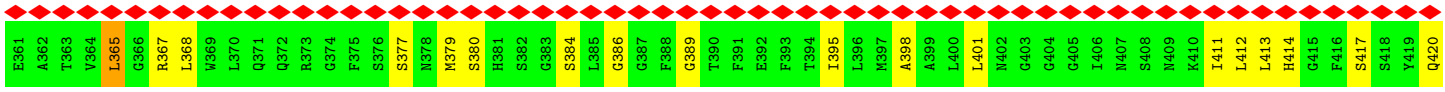


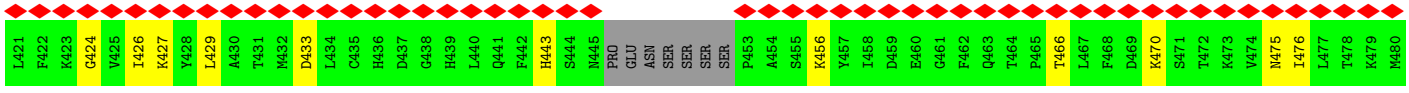


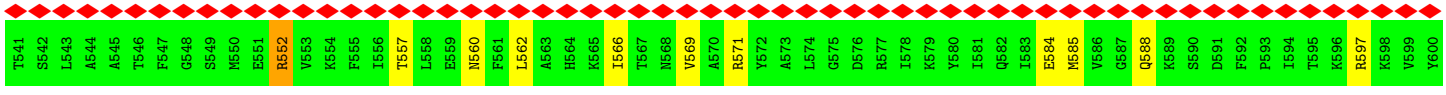


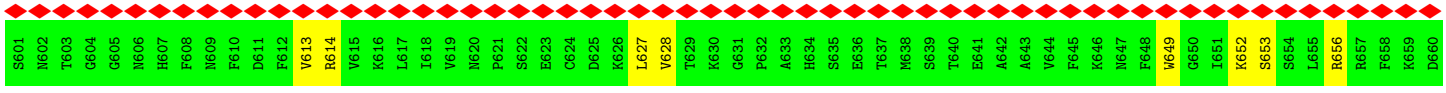


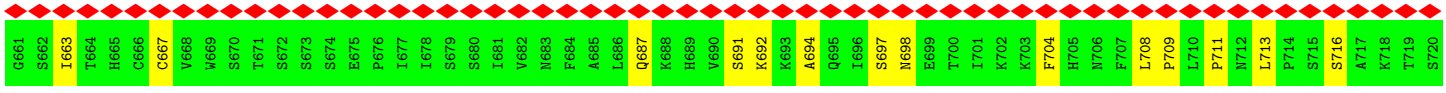


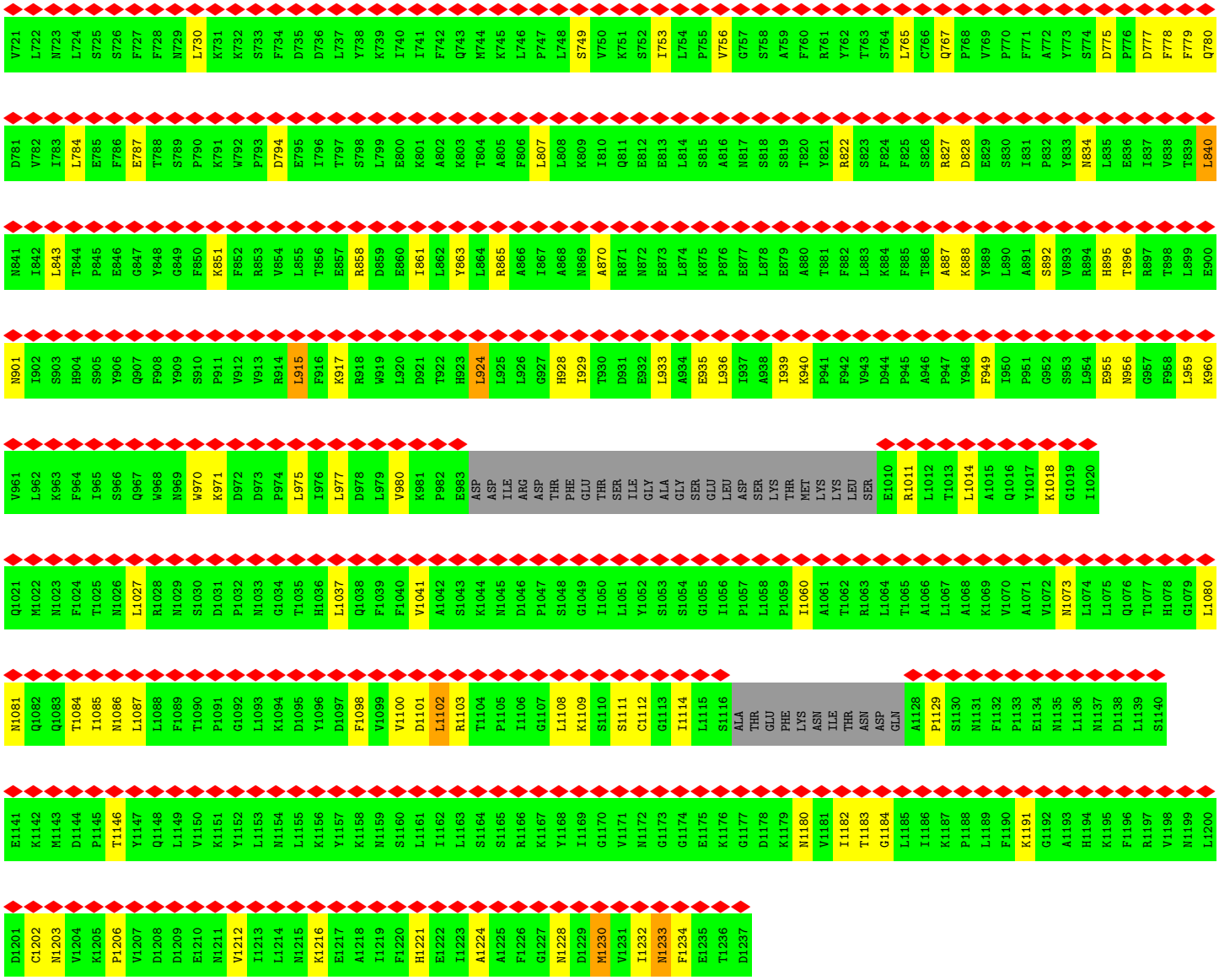






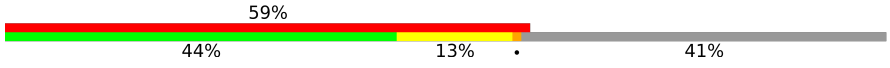


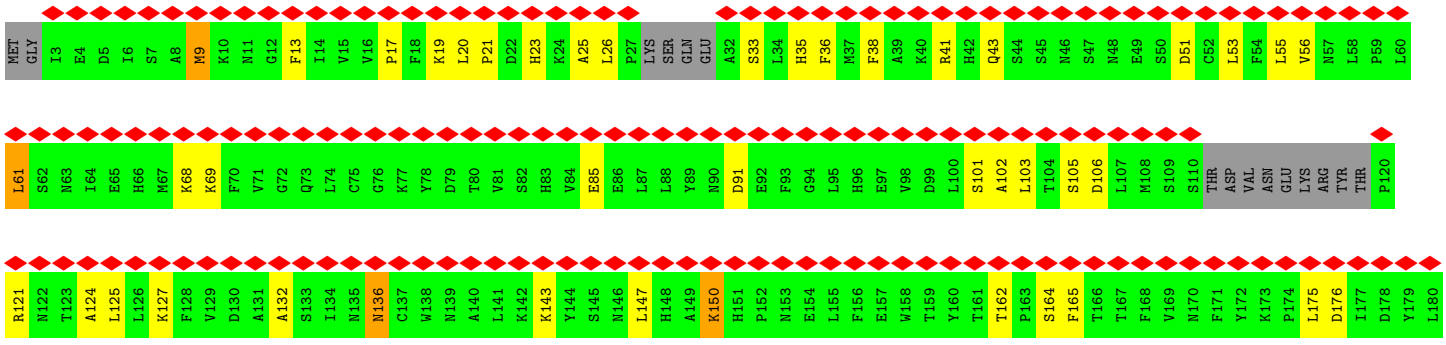


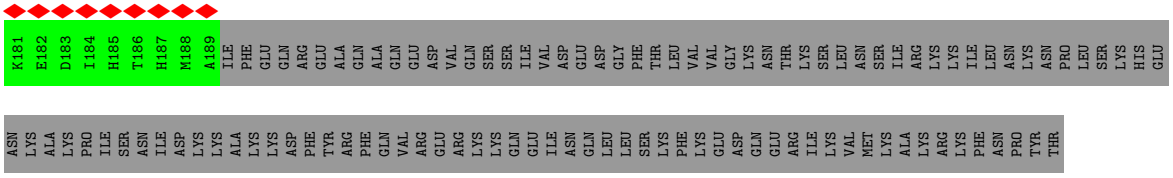


• Molecule 44: Ribosomal RNA-processing protein 7

Chain RF:

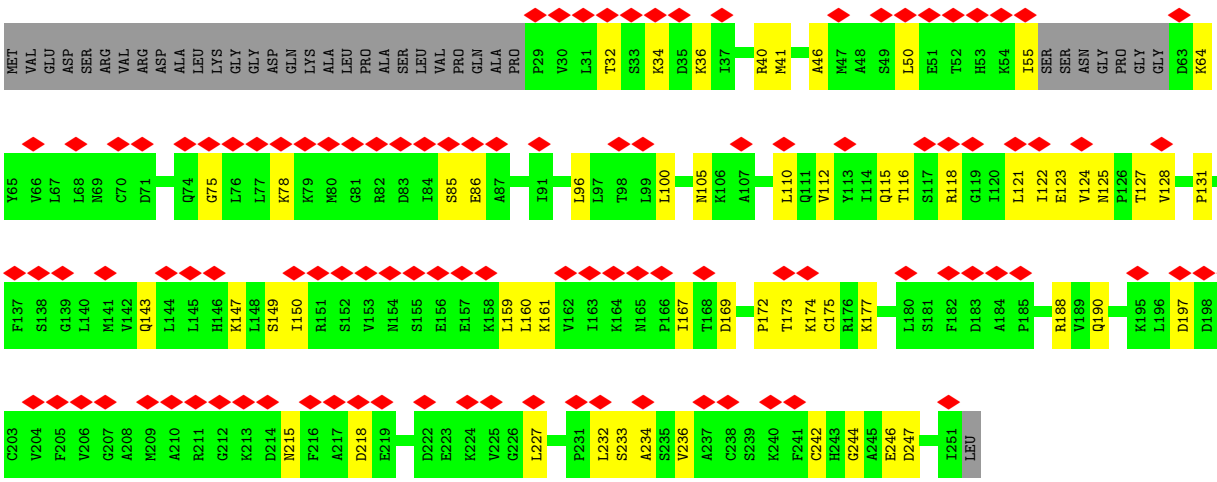






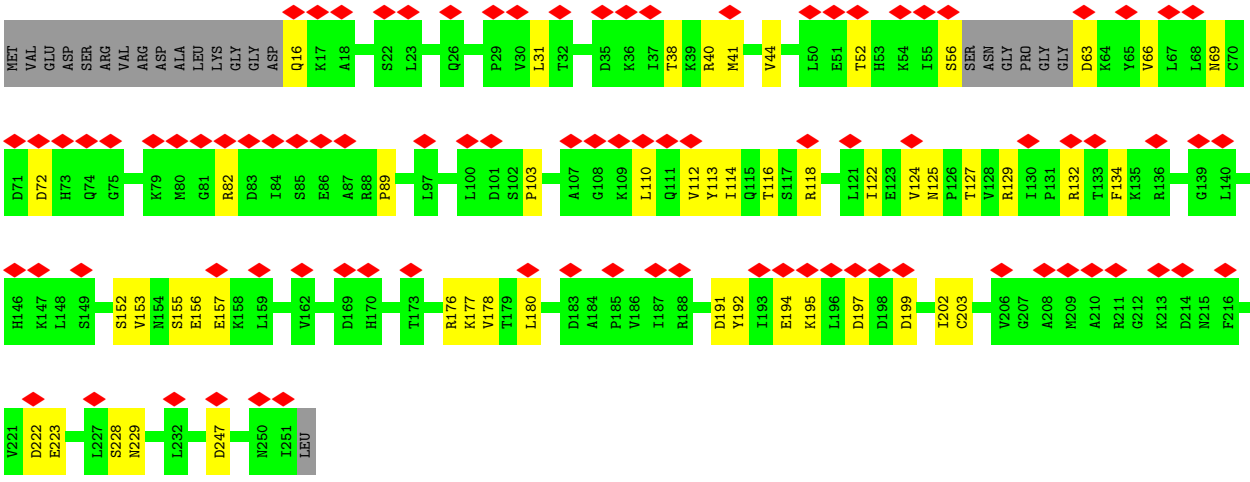
• Molecule 45: Ribosomal RNA small subunit methyltransferase NEP1

Chain RG:



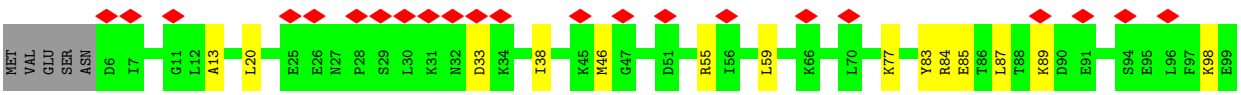
• Molecule 45: Ribosomal RNA small subunit methyltransferase NEP1

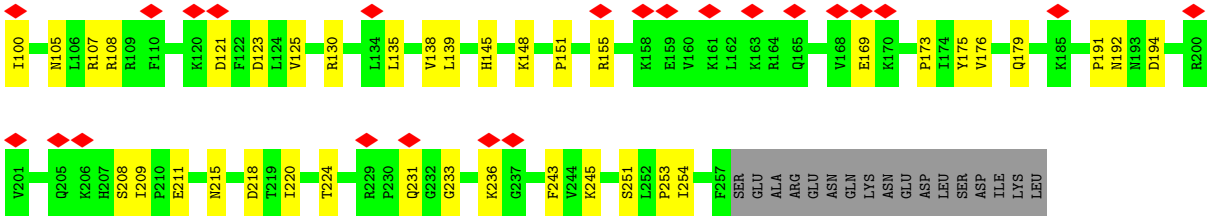
Chain RH:



• Molecule 46: Ribosome biogenesis protein UTP30

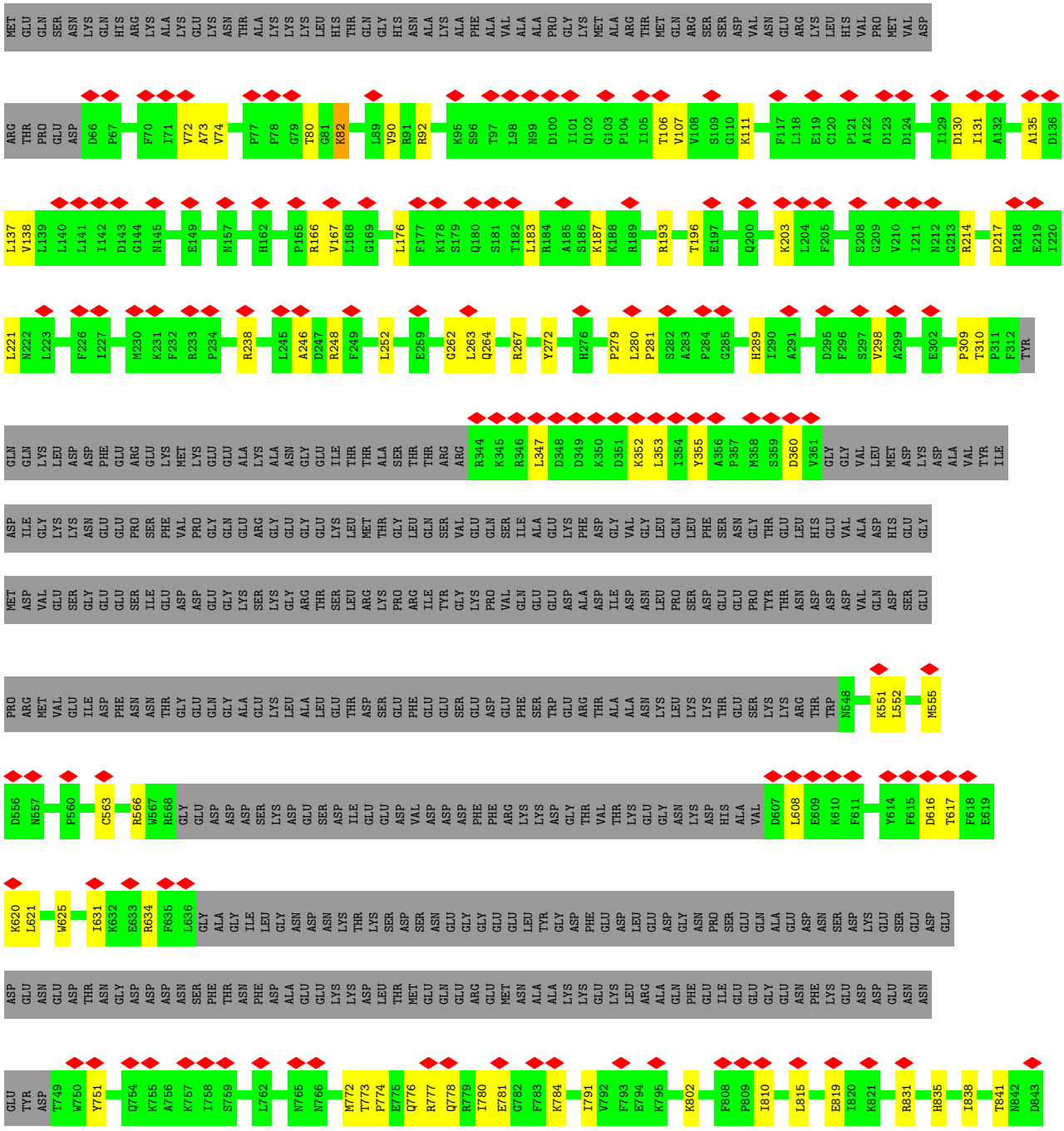
Chain RI:

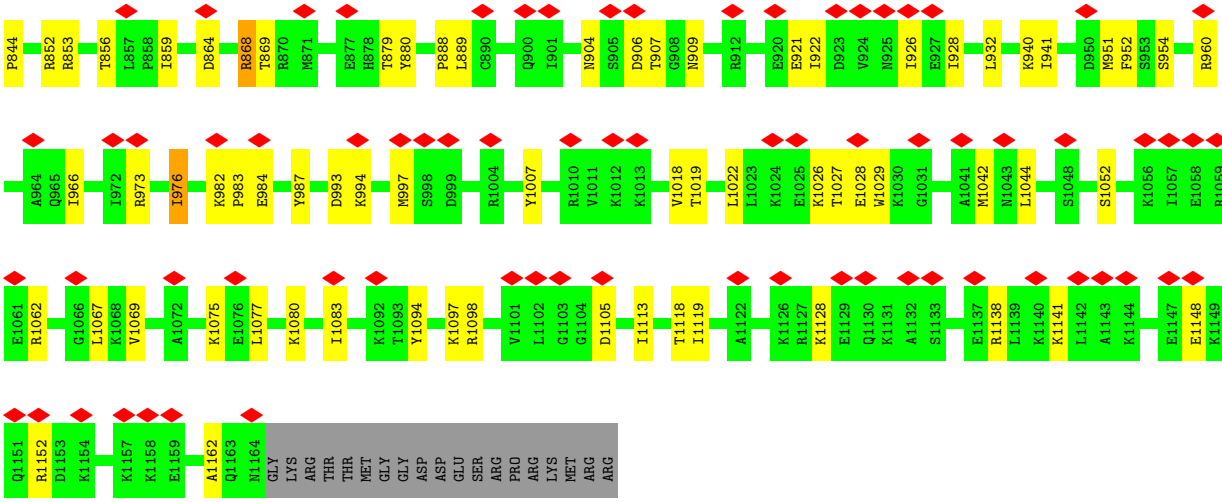




• Molecule 47: Ribosome biogenesis protein BMS1

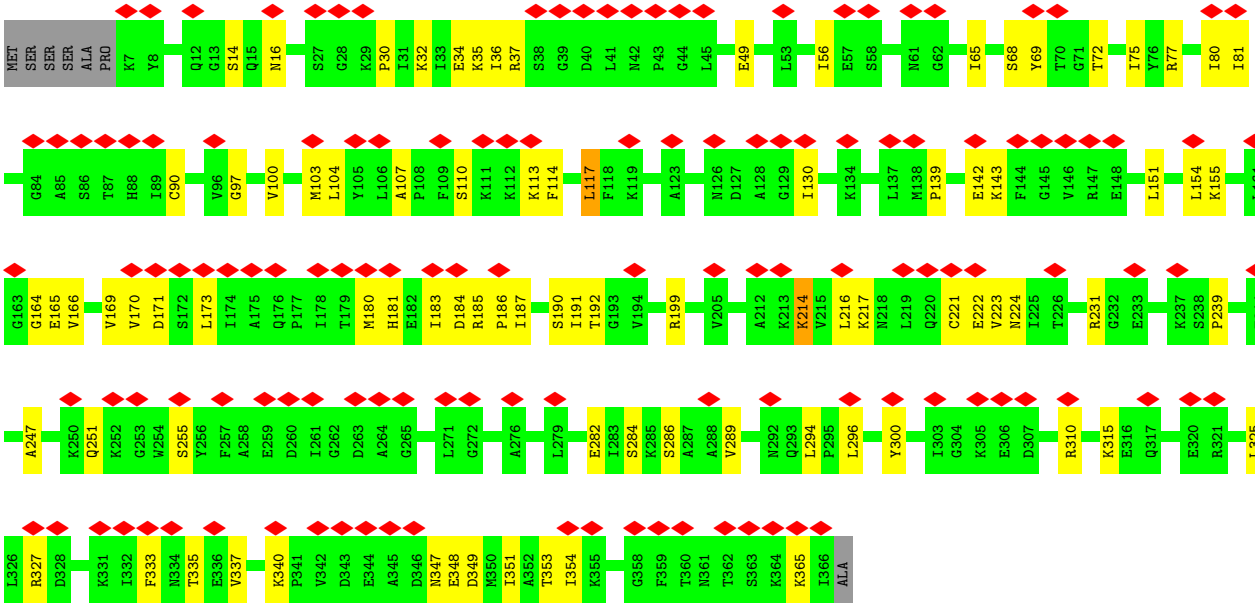
Chain RJ:





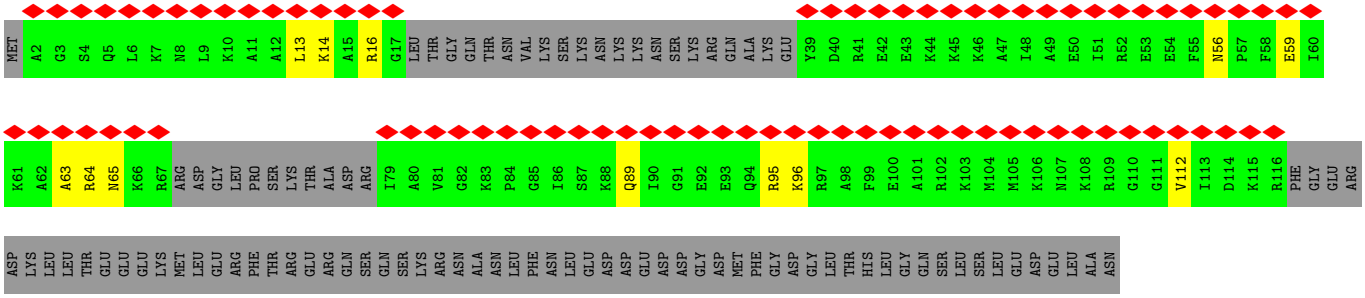
• Molecule 48: RNA 3'-terminal phosphate cyclase-like protein

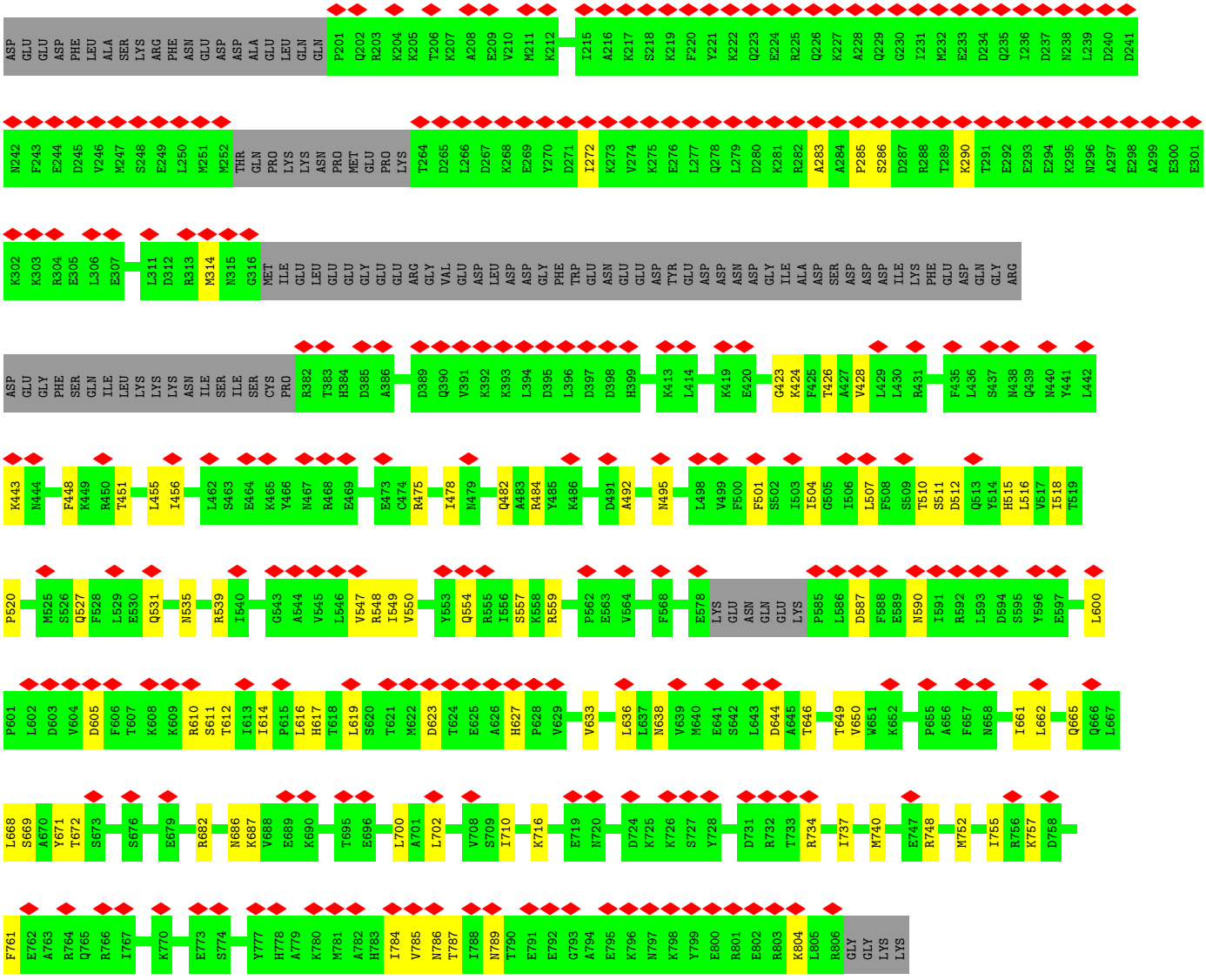
Chain RK:



• Molecule 49: Nucleolar complex protein 14

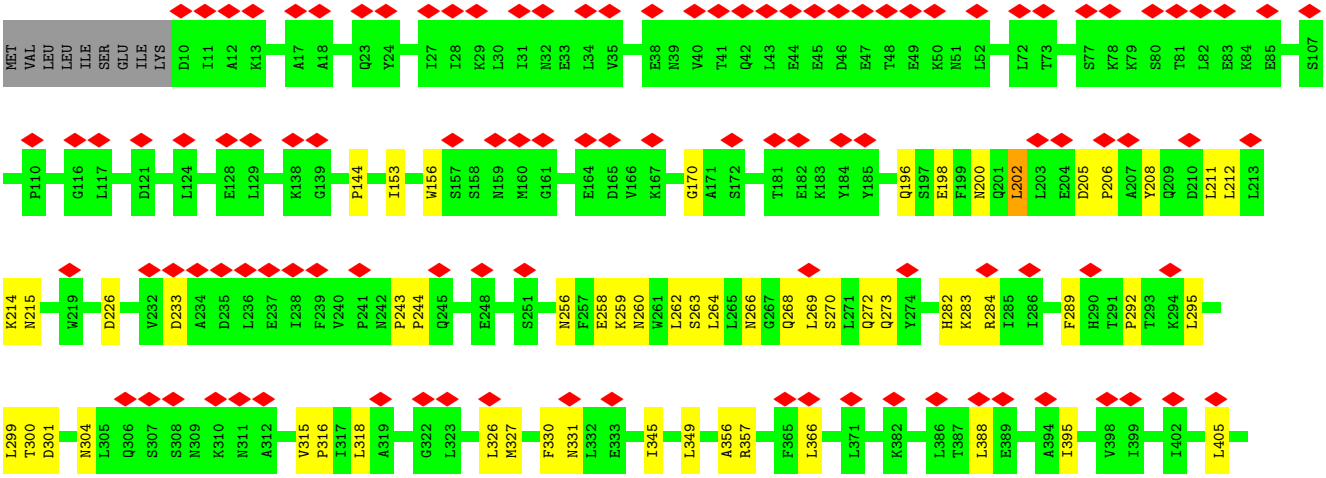
Chain RN:

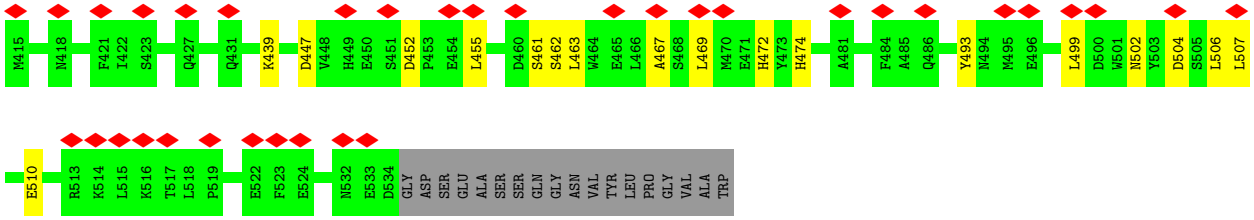




• Molecule 50: Nucleolar complex protein 4

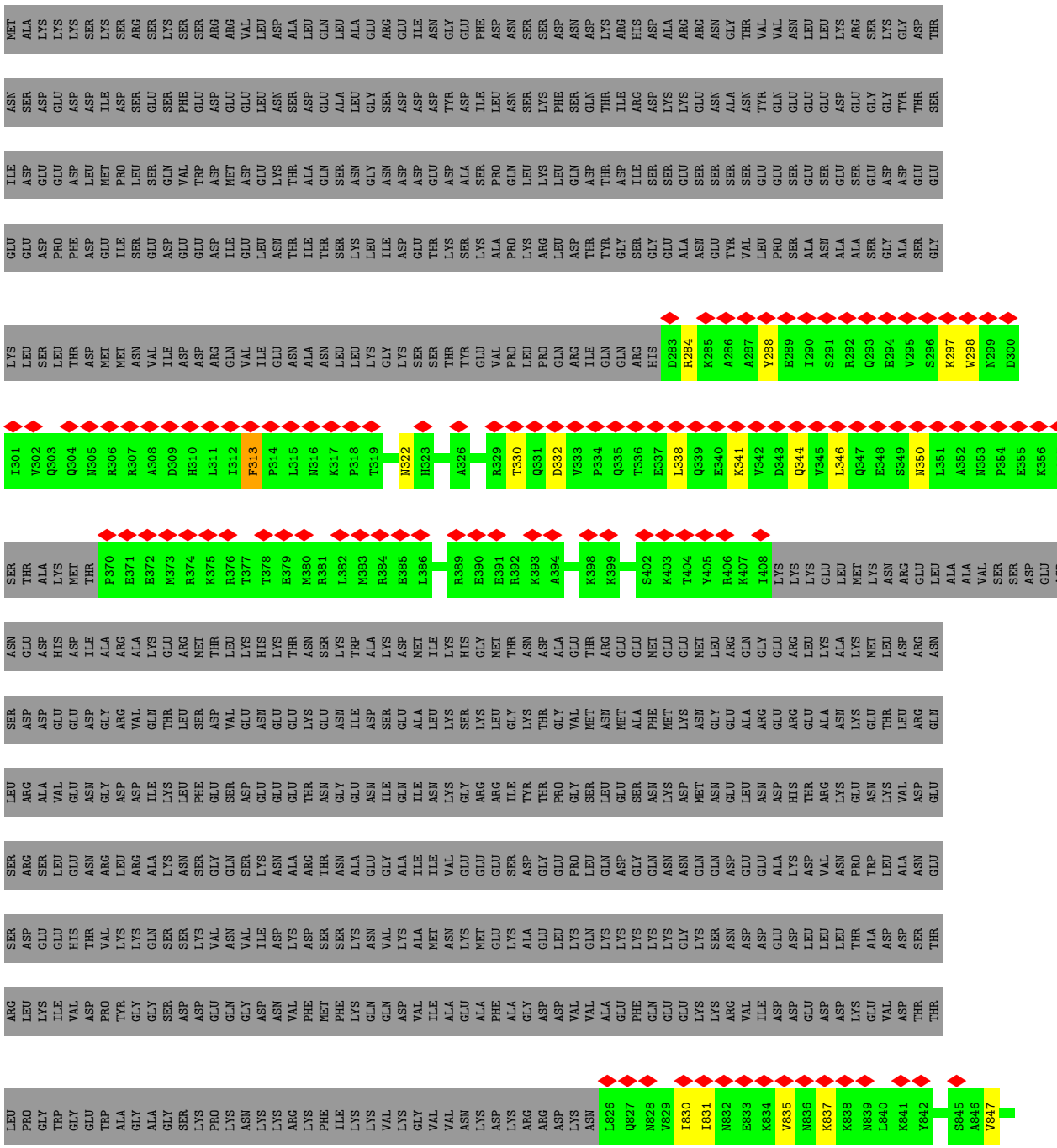
Chain RO:

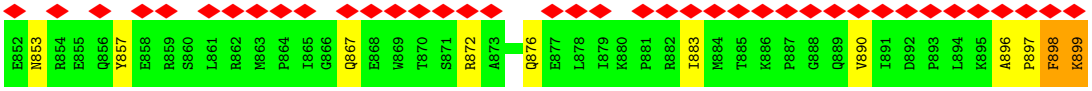




• Molecule 51: U3 small nucleolar RNA-associated protein 14

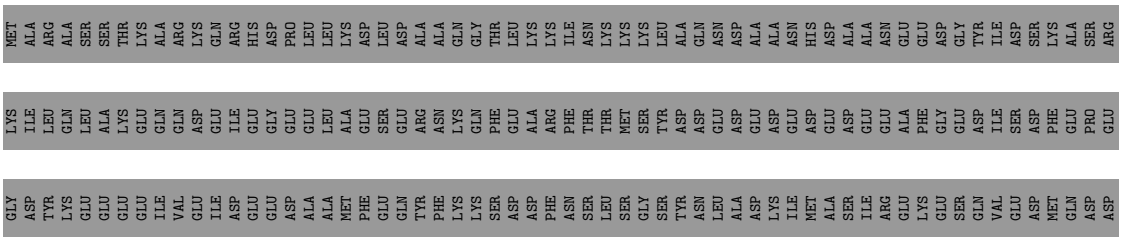
Chain RQ:

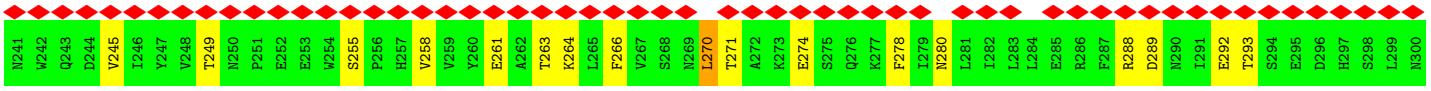


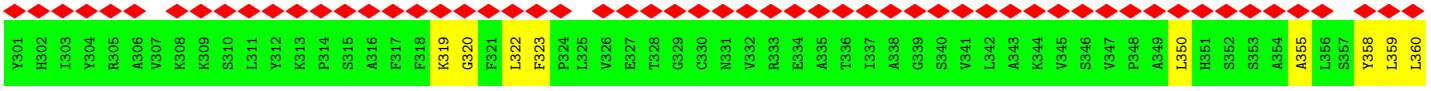


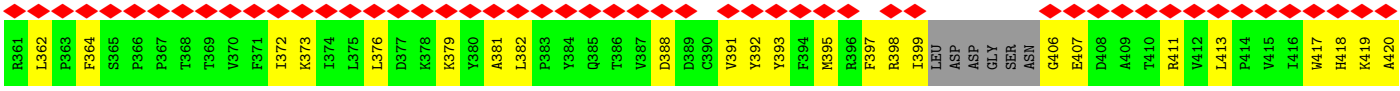
• Molecule 52: Essential nuclear protein 1

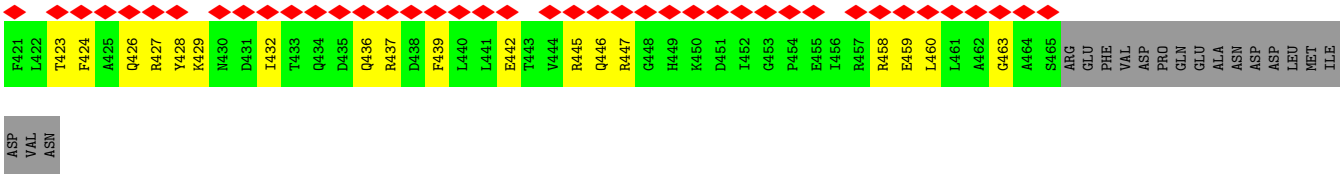
Chain RS:





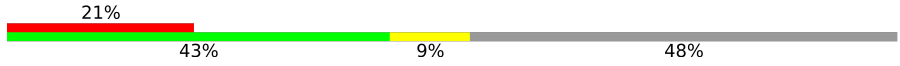


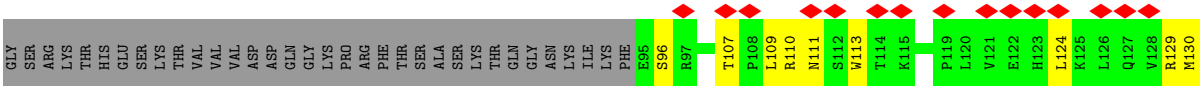


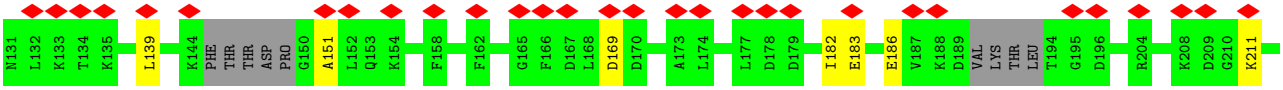


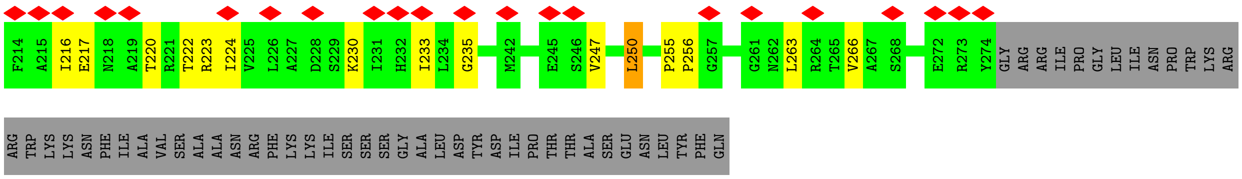
• Molecule 53: Pno1

Chain RT:

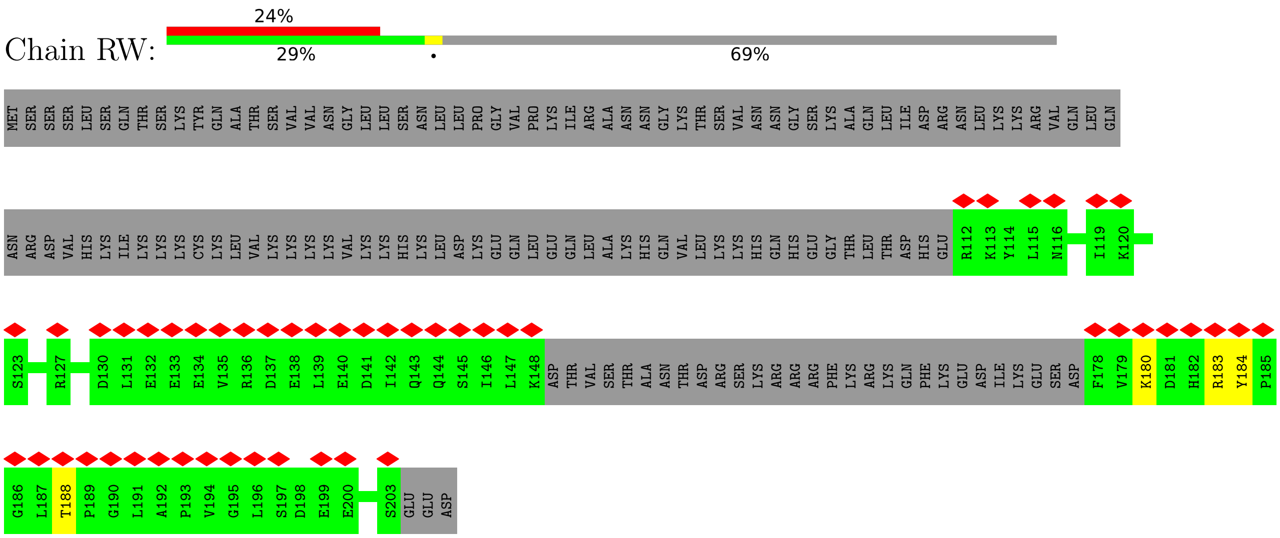




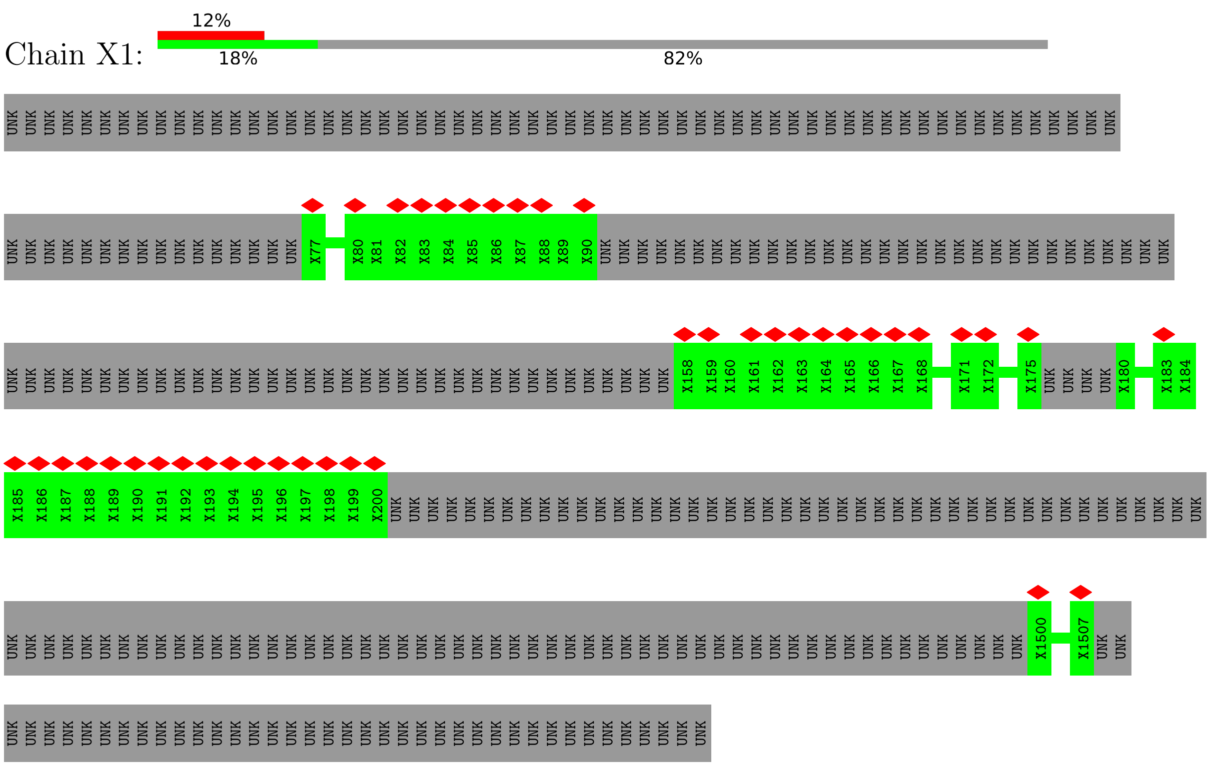




- Molecule 54: Regulator of rDNA transcription protein 14



- Molecule 55: Unassigned peptides 1



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40111	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	531.19995, 531.19995, 531.19995	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3279998, 1.3279998, 1.3279998	Depositor

5 Model quality

5.1 Standard geometry

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

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	3A	0.92	0/4141	1.17	24/6433 (0.4%)
2	5A	0.84	0/12485	1.11	50/19449 (0.3%)
3	SA	0.71	0/20532	1.15	138/31980 (0.4%)
4	SG	0.53	0/1690	0.64	0/2285
5	SK	0.47	0/1410	0.60	0/1888
6	SN	0.32	0/873	0.73	1/1185 (0.1%)
7	SO	0.35	0/1109	0.66	1/1495 (0.1%)
8	SP	0.36	0/879	0.75	1/1186 (0.1%)
9	SR	0.58	0/990	0.73	1/1335 (0.1%)
10	ST	0.38	0/980	0.63	0/1319
11	SY	0.54	0/798	0.67	1/1065 (0.1%)
12	Sd	0.54	0/499	0.66	0/670
13	3B	0.59	0/1901	0.66	1/2567 (0.0%)
13	3C	0.44	0/1796	0.62	1/2424 (0.0%)
14	3D	0.44	0/2891	0.63	3/3895 (0.1%)
15	3E	0.41	0/3059	0.62	3/4153 (0.1%)
16	3F	0.43	0/3317	0.64	2/4469 (0.0%)
17	3G	0.52	0/928	0.76	1/1262 (0.1%)
17	3H	0.47	0/928	0.69	2/1262 (0.2%)
18	A4	0.47	0/5321	0.66	5/7207 (0.1%)
19	A5	0.48	0/4044	0.68	5/5493 (0.1%)
20	A8	0.30	0/3328	0.61	0/4565
21	A9	0.31	0/951	0.58	1/1287 (0.1%)
22	AE	0.45	0/5274	0.64	6/7142 (0.1%)
23	AF	0.53	0/3993	0.67	4/5413 (0.1%)
24	AG	0.47	0/6699	0.65	3/9077 (0.0%)
25	B1	0.64	0/6780	0.68	7/9175 (0.1%)
26	B2	0.43	0/6853	0.67	3/9256 (0.0%)
27	B3	0.34	0/5977	0.73	7/8087 (0.1%)
28	B8	0.58	0/3848	0.66	4/5218 (0.1%)
29	BE	0.57	0/6948	0.66	7/9391 (0.1%)
30	B6	0.45	0/2849	0.58	1/3853 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	5B	0.34	0/499	0.62	0/659
32	5C	0.59	0/4166	0.68	5/5624 (0.1%)
33	5D	0.50	0/1998	0.66	3/2644 (0.1%)
34	5E	0.48	0/1665	0.64	1/2233 (0.0%)
35	5F	0.67	0/1559	0.73	2/2097 (0.1%)
36	5G	0.57	0/2337	0.66	1/3148 (0.0%)
37	5H	0.45	0/1074	0.56	0/1422
38	5I	0.61	0/3844	0.67	2/5174 (0.0%)
39	5J	0.42	0/1302	0.54	0/1728
40	5K	0.56	0/1426	0.67	1/1917 (0.1%)
41	RC	0.36	0/1432	0.64	0/1926
42	RD	0.27	0/1313	0.41	0/1830
43	RE	0.32	0/8924	0.67	9/12070 (0.1%)
44	RF	0.32	0/1441	0.69	2/1951 (0.1%)
45	RG	0.39	0/1727	0.68	2/2329 (0.1%)
45	RH	0.42	0/1828	0.61	0/2470
46	RI	0.46	0/2080	0.65	0/2797
47	RJ	0.51	0/6085	0.61	1/8186 (0.0%)
48	RK	0.44	0/2832	0.65	3/3825 (0.1%)
49	RN	0.36	0/4591	0.58	1/6187 (0.0%)
50	RO	0.38	0/3849	0.62	5/5261 (0.1%)
51	RQ	0.48	0/1459	0.58	0/1981
52	RS	0.33	0/2104	0.67	1/2854 (0.0%)
53	RT	0.42	0/1379	0.63	1/1853 (0.1%)
54	RW	0.34	0/385	0.50	0/529
All	All	0.55	0/185370	0.79	323/258181 (0.1%)

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
7	SO	0	1
10	ST	0	1
14	3D	0	3
15	3E	0	1
16	3F	0	1
17	3G	0	2
17	3H	0	1
18	A4	0	2
19	A5	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
20	A8	0	4
24	AG	0	2
25	B1	0	3
26	B2	0	9
27	B3	0	7
29	BE	0	1
33	5D	0	1
34	5E	0	1
35	5F	0	1
36	5G	0	1
38	5I	0	2
43	RE	0	2
47	RJ	0	2
48	RK	0	1
49	RN	0	1
50	RO	0	1
51	RQ	0	1
All	All	0	53

There are no bond length outliers.

All (323) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SA	1174	C	N1-C2-O2	10.37	125.12	118.90
35	5F	13	LEU	CA-CB-CG	10.29	138.97	115.30
19	A5	25	ASP	CB-CG-OD1	9.52	126.86	118.30
17	3G	67	LEU	CA-CB-CG	9.35	136.81	115.30
3	SA	1000	C	N1-C2-O2	9.32	124.49	118.90
3	SA	1274	C	C6-N1-C2	-9.19	116.62	120.30
2	5A	312	U	P-O3'-C3'	8.95	130.44	119.70
3	SA	1451	C	N3-C2-O2	-8.91	115.67	121.90
3	SA	1274	C	C2-N1-C1'	8.75	128.43	118.80
2	5A	310	U	N3-C2-O2	-8.69	116.12	122.20
3	SA	1174	C	N3-C2-O2	-8.69	115.82	121.90
1	3A	200	C	C2-N1-C1'	8.64	128.31	118.80
3	SA	1254	U	N1-C2-O2	8.59	128.81	122.80
3	SA	1000	C	C2-N1-C1'	8.54	128.19	118.80
22	AE	95	ASP	CB-CG-OD1	8.46	125.92	118.30
1	3A	89	C	C2-N1-C1'	8.38	128.02	118.80
3	SA	1451	C	C6-N1-C2	-8.35	116.96	120.30
3	SA	1274	C	C5-C6-N1	8.34	125.17	121.00
3	SA	1174	C	C2-N1-C1'	8.28	127.91	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SA	607	G	N3-C4-C5	-8.23	124.48	128.60
2	5A	355	C	C2-N1-C1'	8.18	127.80	118.80
1	3A	200	C	N1-C2-O2	8.17	123.81	118.90
3	SA	607	G	C2-N3-C4	8.14	115.97	111.90
13	3B	306	LEU	CA-CB-CG	8.05	133.82	115.30
3	SA	864	U	C2-N1-C1'	7.97	127.27	117.70
3	SA	1254	U	N3-C2-O2	-7.97	116.62	122.20
28	B8	521	LEU	CA-CB-CG	7.92	133.50	115.30
3	SA	1000	C	N3-C2-O2	-7.90	116.37	121.90
3	SA	864	U	N1-C2-O2	7.90	128.33	122.80
2	5A	399	U	C5-C6-N1	7.87	126.63	122.70
1	3A	89	C	C6-N1-C2	-7.83	117.17	120.30
3	SA	607	G	C4-N9-C1'	7.80	136.64	126.50
3	SA	1274	C	N1-C2-O2	7.79	123.58	118.90
2	5A	340	U	C5-C6-N1	7.74	126.57	122.70
1	3A	89	C	N1-C2-O2	7.71	123.52	118.90
1	3A	201	C	N1-C2-O2	7.70	123.52	118.90
1	3A	89	C	C5-C6-N1	7.58	124.79	121.00
3	SA	864	U	N3-C2-O2	-7.57	116.90	122.20
3	SA	1254	U	C2-N1-C1'	7.54	126.75	117.70
3	SA	1518	C	N1-C2-O2	7.53	123.42	118.90
2	5A	91	U	C5-C6-N1	7.52	126.46	122.70
43	RE	915	LEU	CA-CB-CG	7.51	132.57	115.30
18	A4	225	LEU	CA-CB-CG	7.47	132.48	115.30
29	BE	536	LEU	CA-CB-CG	7.36	132.23	115.30
52	RS	270	LEU	CA-CB-CG	7.35	132.22	115.30
2	5A	310	U	N1-C2-O2	7.34	127.94	122.80
3	SA	1258	U	C2-N1-C1'	7.33	126.50	117.70
3	SA	1228	G	N3-C4-C5	-7.32	124.94	128.60
3	SA	1760	G	C4-N9-C1'	7.24	135.92	126.50
53	RT	250	LEU	CA-CB-CG	7.24	131.95	115.30
43	RE	924	LEU	CA-CB-CG	7.23	131.94	115.30
2	5A	90	G	O4'-C1'-N9	7.20	113.96	108.20
3	SA	579	A	P-O3'-C3'	7.18	128.32	119.70
3	SA	1658	G	C4-N9-C1'	7.15	135.80	126.50
23	AF	469	LEU	CA-CB-CG	7.14	131.72	115.30
49	RN	662	LEU	CA-CB-CG	7.12	131.68	115.30
19	A5	24	LEU	CA-CB-CG	7.10	131.63	115.30
3	SA	1451	C	N1-C2-O2	7.10	123.16	118.90
2	5A	312	U	C5-C6-N1	-7.06	119.17	122.70
2	5A	173	G	P-O3'-C3'	7.04	128.15	119.70
32	5C	144	LEU	CA-CB-CG	7.04	131.49	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	3D	292	LEU	CA-CB-CG	7.00	131.41	115.30
17	3H	65	LEU	CB-CG-CD1	-6.95	99.19	111.00
3	SA	1518	C	C2-N1-C1'	6.94	126.43	118.80
1	3A	248	G	O4'-C1'-N9	6.91	113.73	108.20
3	SA	1760	G	N3-C4-N9	6.90	130.14	126.00
8	SP	124	ASP	CB-CG-OD1	6.86	124.47	118.30
3	SA	1258	U	N1-C2-O2	6.85	127.60	122.80
3	SA	1760	G	N3-C4-C5	-6.83	125.18	128.60
2	5A	312	U	OP1-P-O3'	6.80	120.17	105.20
34	5E	314	LEU	CA-CB-CG	6.78	130.90	115.30
11	SY	132	LEU	CA-CB-CG	6.75	130.84	115.30
3	SA	545	A	O4'-C1'-N9	6.73	113.58	108.20
3	SA	1527	C	N1-C2-O2	6.73	122.94	118.90
2	5A	219	U	C5-C6-N1	6.72	126.06	122.70
3	SA	607	G	N3-C4-N9	6.70	130.02	126.00
26	B2	757	ASP	CB-CG-OD1	6.70	124.33	118.30
2	5A	355	C	N1-C2-O2	6.69	122.91	118.90
2	5A	399	U	C2-N1-C1'	6.69	125.73	117.70
1	3A	72	C	C6-N1-C2	-6.69	117.62	120.30
2	5A	219	U	C2-N1-C1'	6.66	125.70	117.70
3	SA	1746	A	C4'-C3'-O3'	6.66	126.33	113.00
3	SA	1658	G	C8-N9-C1'	-6.66	118.35	127.00
2	5A	358	G	P-O3'-C3'	6.63	127.66	119.70
3	SA	1518	C	N3-C2-O2	-6.62	117.27	121.90
3	SA	1496	U	N3-C2-O2	-6.61	117.57	122.20
3	SA	1258	U	N3-C2-O2	-6.61	117.58	122.20
3	SA	1174	C	C6-N1-C2	-6.60	117.66	120.30
30	B6	18	LEU	CA-CB-CG	6.60	130.48	115.30
14	3D	142	LEU	CA-CB-CG	6.59	130.46	115.30
3	SA	608	U	C2-N1-C1'	6.57	125.59	117.70
3	SA	1476	C	C2-N1-C1'	6.56	126.02	118.80
3	SA	1274	C	N3-C2-O2	-6.55	117.31	121.90
3	SA	1228	G	C2-N3-C4	6.53	115.16	111.90
17	3H	65	LEU	CA-CB-CG	6.51	130.28	115.30
23	AF	327	LEU	CA-CB-CG	6.50	130.25	115.30
47	RJ	252	LEU	CA-CB-CG	6.50	130.25	115.30
38	5I	368	ASP	CB-CG-OD1	6.49	124.14	118.30
25	B1	717	LEU	CA-CB-CG	6.48	130.19	115.30
3	SA	1175	U	N3-C2-O2	-6.47	117.67	122.20
3	SA	1535	U	N3-C2-O2	-6.47	117.67	122.20
3	SA	1440	C	C6-N1-C2	-6.44	117.72	120.30
1	3A	250	C	N1-C2-O2	6.43	122.76	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A5	452	LEU	CA-CB-CG	6.42	130.07	115.30
3	SA	1496	U	N1-C2-O2	6.42	127.29	122.80
3	SA	1232	U	N1-C2-O2	6.41	127.29	122.80
3	SA	1175	U	N1-C2-O2	6.39	127.27	122.80
1	3A	200	C	C6-N1-C1'	-6.38	113.15	120.80
3	SA	1594	G	P-O3'-C3'	6.31	127.28	119.70
23	AF	95	LEU	CA-CB-CG	6.30	129.80	115.30
27	B3	401	LEU	CA-CB-CG	6.30	129.78	115.30
3	SA	38	C	N1-C2-O2	6.29	122.67	118.90
2	5A	443	G	O4'-C1'-N9	6.28	113.23	108.20
36	5G	152	LEU	CA-CB-CG	6.24	129.65	115.30
3	SA	1440	C	C5-C6-N1	6.23	124.11	121.00
19	A5	457	LEU	CA-CB-CG	6.23	129.62	115.30
3	SA	1769	U	N1-C2-O2	6.19	127.13	122.80
3	SA	1000	C	C6-N1-C2	-6.19	117.83	120.30
44	RF	61	LEU	CA-CB-CG	6.17	129.50	115.30
2	5A	219	U	N1-C2-O2	6.16	127.11	122.80
2	5A	312	U	C2-N1-C1'	-6.16	110.31	117.70
3	SA	1527	C	C2-N1-C1'	6.16	125.58	118.80
1	3A	198	U	P-O3'-C3'	6.15	127.08	119.70
3	SA	1228	G	C4-N9-C1'	6.15	134.49	126.50
3	SA	915	A	C4'-C3'-O3'	6.14	125.29	113.00
3	SA	514	G	N7-C8-N9	6.12	116.16	113.10
3	SA	607	G	C8-N9-C1'	-6.12	119.05	127.00
3	SA	1760	G	C8-N9-C1'	-6.10	119.07	127.00
50	RO	269	LEU	CA-CB-CG	6.09	129.32	115.30
2	5A	173	G	OP1-P-O3'	6.09	118.59	105.20
3	SA	1441	C	N3-C2-O2	-6.09	117.64	121.90
2	5A	225	U	N3-C2-O2	-6.07	117.95	122.20
3	SA	1259	U	C5-C6-N1	6.06	125.73	122.70
3	SA	1620	C	N1-C2-O2	6.05	122.53	118.90
1	3A	200	C	C5-C6-N1	6.05	124.02	121.00
2	5A	422	C	C6-N1-C2	-6.03	117.89	120.30
7	SO	80	LEU	CA-CB-CG	6.03	129.17	115.30
48	RK	117	LEU	CA-CB-CG	6.03	129.16	115.30
2	5A	492	G	P-O3'-C3'	6.02	126.92	119.70
3	SA	1439	C	N3-C2-O2	-6.01	117.69	121.90
3	SA	1664	C	N1-C2-O2	6.01	122.50	118.90
25	B1	521	LEU	CA-CB-CG	6.00	129.10	115.30
3	SA	608	U	N1-C2-O2	5.99	126.99	122.80
2	5A	202	U	C2-N1-C1'	5.99	124.89	117.70
3	SA	1228	G	N3-C4-N9	5.99	129.59	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SA	873	U	N1-C2-O2	5.98	126.99	122.80
43	RE	499	LEU	CA-CB-CG	5.98	129.06	115.30
3	SA	965	U	C2-N1-C1'	5.97	124.86	117.70
3	SA	1476	C	C5-C6-N1	5.97	123.98	121.00
3	SA	-7	A	P-O3'-C3'	5.96	126.86	119.70
3	SA	1476	C	C6-N1-C2	-5.95	117.92	120.30
3	SA	575	C	N1-C2-O2	5.95	122.47	118.90
3	SA	1769	U	N3-C2-O2	-5.94	118.04	122.20
2	5A	225	U	C2-N1-C1'	5.93	124.82	117.70
27	B3	745	ASP	CB-CG-OD1	5.93	123.64	118.30
43	RE	959	LEU	CA-CB-CG	5.93	128.94	115.30
3	SA	1658	G	N3-C4-N9	5.92	129.55	126.00
2	5A	172	C	P-O3'-C3'	5.91	126.80	119.70
3	SA	1232	U	C2-N1-C1'	5.91	124.79	117.70
25	B1	479	LEU	CA-CB-CG	5.90	128.86	115.30
3	SA	1232	U	N3-C2-O2	-5.90	118.07	122.20
1	3A	72	C	C5-C6-N1	5.89	123.95	121.00
3	SA	0	U	P-O3'-C3'	5.89	126.77	119.70
33	5D	28	LEU	CA-CB-CG	5.89	128.84	115.30
45	RG	96	LEU	CA-CB-CG	5.85	128.76	115.30
3	SA	562	G	O4'-C1'-N9	5.85	112.88	108.20
3	SA	542	A	P-O3'-C3'	5.84	126.71	119.70
3	SA	1216	C	N3-C2-O2	-5.84	117.81	121.90
25	B1	69	LEU	CA-CB-CG	5.84	128.73	115.30
3	SA	1254	U	C5-C6-N1	5.83	125.61	122.70
3	SA	1733	C	C6-N1-C2	-5.82	117.97	120.30
2	5A	263	C	C6-N1-C2	-5.79	117.98	120.30
29	BE	522	LEU	CA-CB-CG	5.78	128.60	115.30
32	5C	74	LEU	CA-CB-CG	5.77	128.57	115.30
3	SA	1199	G	N3-C4-N9	5.76	129.46	126.00
29	BE	872	LEU	CA-CB-CG	5.75	128.53	115.30
3	SA	612	U	C2-N1-C1'	5.75	124.59	117.70
2	5A	355	C	C6-N1-C2	-5.73	118.01	120.30
3	SA	633	U	N3-C2-O2	-5.73	118.19	122.20
23	AF	195	LEU	CA-CB-CG	5.72	128.45	115.30
29	BE	121	LEU	CA-CB-CG	5.71	128.44	115.30
3	SA	1000	C	C6-N1-C1'	-5.69	113.97	120.80
22	AE	604	LEU	CA-CB-CG	5.69	128.39	115.30
3	SA	911	U	N1-C1'-C2'	-5.69	105.74	112.00
38	5I	62	LEU	CA-CB-CG	5.68	128.36	115.30
3	SA	1521	G	P-O3'-C3'	5.67	126.51	119.70
3	SA	569	C	C6-N1-C2	-5.67	118.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SA	1448	G	C5-C6-O6	5.66	132.00	128.60
28	B8	387	LEU	CA-CB-CG	5.66	128.31	115.30
27	B3	736	LEU	CA-CB-CG	5.64	128.28	115.30
18	A4	422	LEU	CA-CB-CG	5.64	128.28	115.30
1	3A	201	C	N3-C2-O2	-5.64	117.95	121.90
24	AG	449	LEU	CA-CB-CG	5.63	128.25	115.30
43	RE	365	LEU	CA-CB-CG	5.63	128.25	115.30
3	SA	1174	C	C5-C6-N1	5.62	123.81	121.00
25	B1	716	ASP	CB-CG-OD1	5.62	123.36	118.30
3	SA	38	C	C6-N1-C2	-5.61	118.06	120.30
3	SA	873	U	C2-N1-C1'	5.60	124.42	117.70
2	5A	225	U	N1-C2-O2	5.60	126.72	122.80
3	SA	1655	A	N9-C1'-C2'	-5.58	105.86	112.00
18	A4	534	LEU	CA-CB-CG	5.57	128.11	115.30
2	5A	169	A	P-O3'-C3'	5.57	126.38	119.70
3	SA	1518	C	C6-N1-C2	-5.57	118.07	120.30
3	SA	1585	U	N1-C2-O2	5.56	126.69	122.80
21	A9	516	LEU	CA-CB-CG	5.56	128.09	115.30
33	5D	224	LEU	CB-CG-CD2	-5.56	101.55	111.00
2	5A	355	C	C6-N1-C1'	-5.54	114.15	120.80
6	SN	39	ASP	CB-CG-OD1	5.54	123.29	118.30
29	BE	417	LEU	CA-CB-CG	5.54	128.03	115.30
32	5C	414	LEU	CA-CB-CG	5.53	128.02	115.30
2	5A	326	C	N1-C2-O2	5.53	122.22	118.90
3	SA	1441	C	N1-C2-O2	5.52	122.21	118.90
45	RG	50	LEU	CA-CB-CG	5.52	127.99	115.30
2	5A	90	G	C8-N9-C1'	5.51	134.17	127.00
3	SA	1783	C	C6-N1-C2	-5.50	118.10	120.30
28	B8	272	LEU	CA-CB-CG	5.50	127.94	115.30
22	AE	526	LEU	CA-CB-CG	5.50	127.94	115.30
2	5A	360	C	C2-N1-C1'	5.49	124.84	118.80
3	SA	1585	U	N3-C2-O2	-5.48	118.36	122.20
40	5K	17	LEU	CA-CB-CG	5.48	127.90	115.30
43	RE	977	LEU	CA-CB-CG	5.48	127.89	115.30
3	SA	608	U	N3-C2-O2	-5.47	118.37	122.20
22	AE	370	LEU	CA-CB-CG	5.46	127.86	115.30
29	BE	614	LEU	CA-CB-CG	5.46	127.86	115.30
32	5C	416	LEU	CA-CB-CG	5.45	127.84	115.30
1	3A	89	C	N3-C2-O2	-5.45	118.08	121.90
3	SA	38	C	C2-N1-C1'	5.45	124.79	118.80
13	3C	306	LEU	CA-CB-CG	5.45	127.83	115.30
2	5A	252	A	C4-N9-C1'	5.44	136.09	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B3	196	LEU	CA-CB-CG	5.43	127.79	115.30
3	SA	1147	A	C4'-C3'-O3'	5.43	123.85	113.00
48	RK	296	LEU	CA-CB-CG	5.42	127.77	115.30
3	SA	1161	C	C5-C6-N1	5.41	123.70	121.00
24	AG	323	LEU	CA-CB-CG	5.41	127.73	115.30
3	SA	977	A	O4'-C1'-N9	5.40	112.52	108.20
22	AE	547	ILE	CG1-CB-CG2	-5.39	99.54	111.40
3	SA	1496	U	C2-N1-C1'	5.39	124.17	117.70
3	SA	1174	C	C6-N1-C1'	-5.39	114.33	120.80
1	3A	248	G	P-O3'-C3'	5.38	126.16	119.70
3	SA	38	C	N3-C2-O2	-5.38	118.13	121.90
24	AG	889	ASP	CB-CG-OD1	5.38	123.14	118.30
2	5A	312	U	O4'-C1'-N1	5.37	112.50	108.20
3	SA	1448	G	N1-C6-O6	-5.36	116.68	119.90
16	3F	315	LEU	CA-CB-CG	5.36	127.64	115.30
14	3D	152	LEU	CA-CB-CG	5.36	127.63	115.30
3	SA	873	U	N3-C2-O2	-5.36	118.45	122.20
3	SA	514	G	C8-N9-C4	-5.35	104.26	106.40
3	SA	1439	C	N1-C2-O2	5.35	122.11	118.90
3	SA	607	G	C8-N9-C4	-5.35	104.26	106.40
2	5A	90	G	C4-N9-C1'	-5.33	119.57	126.50
15	3E	401	LEU	CA-CB-CG	5.33	127.56	115.30
2	5A	252	A	C2-N3-C4	5.32	113.26	110.60
3	SA	1760	G	C2-N3-C4	5.32	114.56	111.90
3	SA	25	C	C2-N1-C1'	5.31	124.64	118.80
3	SA	530	C	N1-C2-O2	5.31	122.08	118.90
32	5C	148	LEU	CA-CB-CG	5.28	127.44	115.30
3	SA	1269	U	N3-C2-O2	-5.26	118.52	122.20
3	SA	1646	C	N1-C2-O2	5.26	122.06	118.90
16	3F	348	LEU	CA-CB-CG	5.25	127.38	115.30
50	RO	388	LEU	CA-CB-CG	5.25	127.36	115.30
29	BE	536	LEU	CB-CG-CD2	-5.24	102.09	111.00
3	SA	-7	A	OP1-P-O3'	5.23	116.71	105.20
3	SA	8	U	N3-C2-O2	-5.23	118.54	122.20
15	3E	227	LEU	CA-CB-CG	5.23	127.32	115.30
1	3A	39	C	C6-N1-C2	-5.22	118.21	120.30
2	5A	111	C	C2-N1-C1'	5.21	124.54	118.80
22	AE	94	LEU	CA-CB-CG	5.21	127.28	115.30
19	A5	151	LEU	CA-CB-CG	5.21	127.28	115.30
15	3E	141	LEU	CA-CB-CG	5.20	127.25	115.30
3	SA	1783	C	C5-C6-N1	5.19	123.60	121.00
35	5F	67	THR	C-N-CA	-5.19	108.72	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	3A	39	C	C2-N1-C1'	5.19	124.51	118.80
3	SA	1269	U	N1-C2-O2	5.19	126.43	122.80
26	B2	267	ASP	C-N-CA	5.18	134.65	121.70
28	B8	521	LEU	CB-CG-CD1	-5.17	102.21	111.00
27	B3	186	LEU	CA-CB-CG	5.17	127.19	115.30
1	3A	205	G	P-O3'-C3'	5.15	125.88	119.70
2	5A	111	C	C6-N1-C2	-5.15	118.24	120.30
2	5A	390	C	C5-C6-N1	5.15	123.57	121.00
3	SA	1222	C	C5-C6-N1	5.14	123.57	121.00
50	RO	211	LEU	CA-CB-CG	5.14	127.13	115.30
3	SA	1656	U	N1-C1'-C2'	-5.14	106.35	112.00
3	SA	612	U	N1-C2-O2	5.13	126.39	122.80
43	RE	1102	LEU	CA-CB-CG	5.13	127.10	115.30
2	5A	317	C	C6-N1-C2	-5.13	118.25	120.30
2	5A	224	G	P-O3'-C3'	5.12	125.85	119.70
48	RK	325	LEU	CA-CB-CG	5.12	127.09	115.30
1	3A	249	G	O5'-P-OP1	-5.12	101.09	105.70
2	5A	137	C	N1-C2-O2	5.12	121.97	118.90
2	5A	238	G	C8-N9-C4	-5.10	104.36	106.40
3	SA	1535	U	C6-N1-C2	-5.10	117.94	121.00
27	B3	162	LEU	CA-CB-CG	5.10	127.03	115.30
3	SA	1492	A	C4-N9-C1'	5.09	135.47	126.30
3	SA	864	U	C6-N1-C1'	-5.09	114.08	121.20
44	RF	125	LEU	CA-CB-CG	5.08	127.00	115.30
1	3A	200	C	C6-N1-C2	-5.08	118.27	120.30
18	A4	465	LEU	CA-CB-CG	5.08	126.99	115.30
2	5A	355	C	C5-C6-N1	5.08	123.54	121.00
3	SA	1658	G	N3-C4-C5	-5.08	126.06	128.60
1	3A	89	C	C6-N1-C1'	-5.08	114.71	120.80
2	5A	310	U	C6-N1-C2	-5.07	117.96	121.00
1	3A	198	U	OP1-P-O3'	5.06	116.33	105.20
27	B3	571	LEU	CA-CB-CG	5.06	126.94	115.30
50	RO	264	LEU	CA-CB-CG	5.05	126.92	115.30
3	SA	35	U	N1-C2-O2	5.05	126.34	122.80
43	RE	840	LEU	CA-CB-CG	5.05	126.92	115.30
26	B2	231	LEU	CA-CB-CG	5.05	126.91	115.30
3	SA	1147	A	C1'-C2'-O2'	-5.04	95.48	110.60
9	SR	123	ARG	C-N-CD	-5.04	109.51	120.60
2	5A	202	U	C5-C6-N1	5.04	125.22	122.70
3	SA	35	U	C5-C6-N1	5.04	125.22	122.70
18	A4	435	PRO	C-N-CA	5.04	134.29	121.70
25	B1	701	LEU	CA-CB-CG	5.04	126.88	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	5D	91	LEU	CA-CB-CG	5.03	126.87	115.30
3	SA	546	U	C5-C6-N1	5.02	125.21	122.70
3	SA	915	A	N9-C1'-C2'	-5.02	106.48	112.00
2	5A	363	A	P-O3'-C3'	5.02	125.72	119.70
3	SA	1729	C	N1-C2-O2	5.02	121.91	118.90
3	SA	885	G	C8-N9-C4	-5.01	104.39	106.40
2	5A	422	C	C5-C6-N1	5.01	123.51	121.00
25	B1	436	LEU	CA-CB-CG	5.01	126.83	115.30
50	RO	202	LEU	CA-CB-CG	5.01	126.83	115.30
43	RE	264	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (53) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	3D	142	LEU	Peptide
14	3D	202	HIS	Peptide
14	3D	286	ARG	Peptide
15	3E	331	LYS	Peptide
16	3F	237	ASP	Peptide
17	3G	59	GLU	Peptide
17	3G	9	PHE	Peptide
17	3H	59	GLU	Peptide
33	5D	138	ASP	Peptide
34	5E	453	SER	Peptide
35	5F	101	VAL	Peptide
36	5G	74	ASP	Peptide
38	5I	230	ASN	Peptide
38	5I	283	ASP	Peptide
18	A4	54	LYS	Peptide
18	A4	774	LEU	Peptide
19	A5	167	SER	Peptide
20	A8	257	SER	Peptide
20	A8	266	ILE	Peptide
20	A8	496	TYR	Peptide
20	A8	529	HIS	Peptide
24	AG	178	PHE	Peptide
24	AG	780	GLU	Peptide
25	B1	288	ASP	Peptide
25	B1	661	LEU	Peptide
25	B1	690	ALA	Peptide
26	B2	131	GLY	Peptide

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Mol	Chain	Res	Type	Group
26	B2	213	LYS	Peptide
26	B2	266	SER	Peptide
26	B2	267	ASP	Peptide
26	B2	278	ASP	Peptide
26	B2	44	SER	Peptide
26	B2	613	ALA	Peptide
26	B2	916	HIS	Peptide
26	B2	918	TYR	Peptide
27	B3	235	LYS	Peptide
27	B3	34	THR	Peptide
27	B3	473	ALA	Peptide
27	B3	585	ASN	Peptide
27	B3	594	GLY	Peptide
27	B3	627	ASN	Peptide
27	B3	90	LEU	Peptide
29	BE	94	TYR	Peptide
43	RE	116	LEU	Peptide
43	RE	173	ASN	Peptide
47	RJ	1026	LYS	Peptide
47	RJ	868	ARG	Peptide
48	RK	333	PHE	Peptide
49	RN	286	SER	Peptide
50	RO	144	PRO	Peptide
51	RQ	313	PHE	Peptide
7	SO	58	HIS	Peptide
10	ST	13	HIS	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	3A	3711	0	1882	19	0
2	5A	11163	0	5611	80	0
3	SA	18356	0	9246	200	0
4	SG	1669	0	1724	18	0
5	SK	1388	0	1467	12	0
6	SN	865	0	874	15	0
7	SO	1087	0	1152	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	SP	868	0	894	26	0
9	SR	973	0	1029	13	0
10	ST	964	0	991	17	0
11	SY	786	0	843	7	0
12	Sd	497	0	535	0	0
13	3B	1865	0	1910	29	0
13	3C	1763	0	1805	35	0
14	3D	2848	0	2815	42	0
15	3E	3028	0	2813	60	0
16	3F	3248	0	3274	56	0
17	3G	916	0	964	11	0
17	3H	916	0	964	23	0
18	A4	5226	0	5199	94	0
19	A5	3976	0	3919	57	0
20	A8	3307	0	2316	40	0
21	A9	939	0	898	17	0
22	AE	5181	0	5373	84	0
23	AF	3911	0	3906	71	0
24	AG	6570	0	6473	125	0
25	B1	6635	0	6525	93	0
26	B2	6723	0	6698	131	0
27	B3	5882	0	5964	143	0
28	B8	3764	0	3757	58	0
29	BE	6810	0	6787	89	0
30	B6	2800	0	2517	30	0
31	5B	495	0	561	14	0
32	5C	4084	0	4092	73	0
33	5D	1972	0	2054	25	0
34	5E	1647	0	1678	31	0
35	5F	1530	0	1572	26	0
36	5G	2296	0	2325	38	0
37	5H	1065	0	1097	16	0
38	5I	3765	0	3714	71	0
39	5J	1280	0	1331	20	0
40	5K	1403	0	1484	19	0
41	RC	1410	0	1503	40	0
42	RD	1314	0	610	21	0
43	RE	8716	0	8828	159	0
44	RF	1404	0	1364	25	0
45	RG	1701	0	1767	39	0
45	RH	1799	0	1872	33	0
46	RI	2045	0	2162	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	RJ	5953	0	6152	95	0
48	RK	2781	0	2878	52	0
49	RN	4529	0	4262	65	0
50	RO	3766	0	3269	48	0
51	RQ	1436	0	1280	28	0
52	RS	2051	0	2096	54	0
53	RT	1357	0	1426	17	0
54	RW	381	0	255	4	0
55	X1	305	0	73	0	0
56	5K	1	0	0	0	0
57	RJ	32	0	12	1	0
58	RJ	1	0	0	0	0
All	All	179154	0	160842	2432	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 7.

All (2432) 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)
42:RD:1487:GLN:O	43:RE:411:ILE:HG23	1.40	1.18
27:B3:12:LEU:HD23	27:B3:377:LEU:HB2	1.23	1.17
8:SP:42:VAL:HG12	8:SP:67:VAL:HG23	1.31	1.12
8:SP:42:VAL:CG1	8:SP:67:VAL:HG23	1.82	1.09
27:B3:12:LEU:CB	27:B3:377:LEU:HD12	1.84	1.07
41:RC:112:GLN:NE2	41:RC:163:TYR:CD2	2.25	1.04
41:RC:112:GLN:NE2	41:RC:163:TYR:HD2	1.54	1.04
27:B3:494:ILE:N	27:B3:510:SER:HG	1.58	1.02
49:RN:527:GLN:O	49:RN:531:GLN:HB2	1.60	1.01
26:B2:17:ILE:HG22	26:B2:52:TRP:CZ2	1.94	1.01
20:A8:264:SER:O	20:A8:267:ILE:HA	1.61	1.01
51:RQ:298:TRP:NE1	51:RQ:899:LYS:HG3	1.76	1.00
3:SA:1697:G:O5'	43:RE:326:LEU:HD11	1.62	1.00
3:SA:36:C:H42	3:SA:472:U:H3	1.00	1.00
25:B1:54:HIS:HE2	25:B1:72:SER:HG	1.13	0.95
3:SA:925:G:C5'	42:RD:1611:ALA:HB1	1.96	0.95
3:SA:1697:G:OP1	43:RE:326:LEU:HD12	1.66	0.95
41:RC:112:GLN:HG2	41:RC:163:TYR:CE2	2.00	0.95
27:B3:12:LEU:HD21	27:B3:378:PRO:HD2	1.45	0.94
27:B3:12:LEU:HB2	27:B3:377:LEU:HD12	1.46	0.94
8:SP:42:VAL:HG12	8:SP:67:VAL:CG2	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1665:U:H3	3:SA:1736:G:H1	1.17	0.93
7:SO:104:ARG:HG3	42:RD:1542:GLN:HA	1.50	0.93
3:SA:1658:G:N2	3:SA:1743:U:H1'	1.86	0.91
3:SA:36:C:N4	3:SA:472:U:H3	1.70	0.90
41:RC:112:GLN:CD	41:RC:163:TYR:CD2	2.46	0.89
7:SO:106:ARG:HG2	7:SO:106:ARG:HH21	1.34	0.88
27:B3:12:LEU:HB3	27:B3:377:LEU:HD12	1.55	0.88
38:5I:231:GLU:OE2	51:RQ:899:LYS:HD3	1.74	0.87
27:B3:12:LEU:HB3	27:B3:377:LEU:CD1	2.05	0.87
3:SA:925:G:H5'	42:RD:1611:ALA:CB	2.07	0.85
52:RS:424:PHE:O	52:RS:428:TYR:HB2	1.78	0.84
42:RD:1489:SER:CB	43:RE:427:LYS:HD3	2.07	0.84
42:RD:1459:GLU:CB	43:RE:413:LEU:HD22	2.08	0.84
16:3F:415:THR:HG1	16:3F:425:TRP:HE1	1.25	0.83
50:RO:502:ASN:O	50:RO:506:LEU:HB2	1.77	0.83
43:RE:656:ARG:O	43:RE:663:ILE:HA	1.79	0.83
27:B3:816:LEU:HD12	27:B3:816:LEU:O	1.78	0.82
27:B3:12:LEU:HD23	27:B3:377:LEU:CB	2.07	0.82
27:B3:12:LEU:H	27:B3:12:LEU:HD12	1.43	0.82
17:3H:44:LEU:HD22	17:3H:52:ILE:CD1	2.10	0.81
43:RE:1224:ALA:O	43:RE:1228:ASN:HB3	1.81	0.81
51:RQ:346:LEU:O	51:RQ:350:ASN:HA	1.80	0.81
22:AE:151:ILE:O	22:AE:155:ILE:HB	1.81	0.81
51:RQ:298:TRP:HE1	51:RQ:899:LYS:HG3	1.44	0.81
3:SA:1697:G:P	43:RE:326:LEU:CD1	2.69	0.80
3:SA:925:G:H5'	42:RD:1611:ALA:HB1	1.62	0.79
30:B6:319:TYR:O	30:B6:323:PHE:HB2	1.81	0.79
3:SA:1697:G:P	43:RE:326:LEU:HD11	2.24	0.77
23:AF:224:THR:O	23:AF:239:LEU:HB2	1.83	0.77
41:RC:49:ARG:HH21	41:RC:52:TYR:HD2	1.32	0.77
42:RD:1488:LEU:HA	43:RE:411:ILE:O	1.84	0.76
3:SA:1658:G:C2	3:SA:1743:U:C2	2.75	0.75
41:RC:112:GLN:HG2	41:RC:163:TYR:CD2	2.21	0.75
3:SA:1697:G:H1	3:SA:1704:U:H3	1.34	0.75
18:A4:614:TRP:O	18:A4:618:ASN:HB2	1.87	0.74
39:5J:114:ARG:O	39:5J:118:GLN:HB3	1.88	0.74
42:RD:1487:GLN:O	43:RE:411:ILE:CG2	2.28	0.74
27:B3:12:LEU:CD2	27:B3:378:PRO:HD2	2.17	0.73
8:SP:42:VAL:HG11	8:SP:67:VAL:HG23	1.68	0.73
27:B3:12:LEU:CB	27:B3:377:LEU:CD1	2.63	0.72
27:B3:11:SER:HB3	27:B3:642:GLN:HG3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:505:A:H61	3:SA:586:G:H8	1.38	0.72
15:3E:397:ARG:HH21	15:3E:400:GLN:HE21	1.38	0.71
43:RE:1098:PHE:HB2	43:RE:1184:GLY:H	1.53	0.71
24:AG:435:ASP:HB2	24:AG:702:TYR:CD1	2.26	0.71
3:SA:1673:G:H1	3:SA:1728:A:N6	1.88	0.70
3:SA:1658:G:C5	3:SA:1743:U:C4	2.79	0.70
41:RC:112:GLN:CG	41:RC:163:TYR:CD2	2.75	0.70
46:RI:77:LYS:HD2	46:RI:130:ARG:HH11	1.57	0.69
3:SA:925:G:H5"	42:RD:1611:ALA:HB1	1.74	0.69
4:SG:206:SER:H	4:SG:211:ILE:HD11	1.55	0.69
3:SA:942:G:O5'	3:SA:977:A:H5'	1.91	0.69
2:5A:135:G:H4'	19:A5:494:ARG:HD3	1.74	0.69
3:SA:1697:G:P	43:RE:326:LEU:HD12	2.33	0.69
25:B1:58:ILE:HA	25:B1:74:ASP:HA	1.74	0.69
2:5A:316:U:H5'	32:5C:364:ARG:HH22	1.57	0.69
48:RK:192:THR:HA	48:RK:224:ASN:O	1.92	0.68
51:RQ:297:LYS:HB2	51:RQ:899:LYS:HB3	1.76	0.68
23:AF:86:SER:O	23:AF:98:ALA:HA	1.93	0.68
3:SA:1658:G:C6	3:SA:1743:U:C4	2.82	0.68
3:SA:1673:G:H1	3:SA:1728:A:H61	1.40	0.68
27:B3:533:LYS:HE2	27:B3:533:LYS:O	1.94	0.68
27:B3:533:LYS:HE2	27:B3:533:LYS:C	2.13	0.68
16:3F:443:LEU:HD21	16:3F:492:TRP:HE1	1.59	0.68
38:5I:345:THR:HG22	38:5I:347:ARG:H	1.58	0.68
26:B2:17:ILE:HG22	26:B2:52:TRP:CH2	2.28	0.67
27:B3:513:LYS:HD3	27:B3:513:LYS:N	2.09	0.67
29:BE:209:ILE:HG22	29:BE:225:THR:HG22	1.76	0.67
43:RE:377:SER:HB2	43:RE:389:GLY:HA3	1.76	0.67
23:AF:211:HIS:HD1	23:AF:228:SER:HG	1.41	0.67
43:RE:345:TYR:O	43:RE:349:LEU:HB2	1.95	0.67
16:3F:185:LEU:H	16:3F:202:THR:HB	1.59	0.67
26:B2:536:CYS:HB3	26:B2:549:SER:HB3	1.77	0.67
27:B3:531:ASN:ND2	27:B3:568:MET:SD	2.67	0.67
27:B3:719:ILE:HD11	27:B3:762:CYS:HB3	1.76	0.67
3:SA:868:G:H1	3:SA:960:U:H3	1.41	0.67
3:SA:1658:G:O6	3:SA:1742:U:C4	2.48	0.67
25:B1:20:ILE:H	25:B1:307:THR:HG21	1.58	0.66
28:B8:513:GLN:HG3	28:B8:551:VAL:HG21	1.76	0.66
13:3B:103:GLU:HG3	39:5J:134:ARG:HH12	1.60	0.66
18:A4:645:ARG:HD2	18:A4:656:ARG:HD3	1.77	0.66
3:SA:885:G:N2	8:SP:124:ASP:OD1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:5G:123:VAL:HG12	36:5G:125:PRO:HD2	1.78	0.66
23:AF:52:PRO:HG2	23:AF:312:ALA:HA	1.77	0.66
24:AG:435:ASP:HB3	24:AG:701:VAL:O	1.96	0.66
11:SY:103:LEU:HB3	11:SY:126:LYS:HB2	1.76	0.66
24:AG:16:SER:HB2	24:AG:783:LEU:HB2	1.77	0.66
3:SA:1751:C:H5"	26:B2:142:ASP:HA	1.76	0.66
29:BE:209:ILE:HA	29:BE:225:THR:HA	1.77	0.65
47:RJ:248:ARG:HB3	47:RJ:272:TYR:HB2	1.78	0.65
43:RE:529:VAL:HB	43:RE:613:VAL:HB	1.79	0.65
18:A4:497:ILE:HD11	18:A4:511:VAL:HG23	1.78	0.65
8:SP:14:PHE:HA	8:SP:78:ALA:O	1.96	0.65
29:BE:847:LEU:HD11	53:RT:266:VAL:HG23	1.78	0.65
43:RE:822:ARG:HB2	43:RE:843:LEU:HB2	1.76	0.65
53:RT:222:THR:HG22	53:RT:235:GLY:HA3	1.79	0.65
1:3A:84:U:OP2	15:3E:361:ARG:NH2	2.30	0.65
20:A8:576:ARG:HG2	20:A8:578:LEU:H	1.61	0.65
32:5C:257:SER:HG	32:5C:259:TRP:HE1	1.41	0.65
5:SK:57:ARG:HE	40:5K:88:ASP:HB3	1.60	0.64
26:B2:262:ILE:O	26:B2:270:SER:HA	1.97	0.64
3:SA:976:G:C2	3:SA:978:A:C5	2.84	0.64
25:B1:438:VAL:HG12	25:B1:445:VAL:HG23	1.79	0.64
32:5C:170:GLN:NE2	32:5C:177:TYR:OH	2.30	0.64
43:RE:1108:LEU:O	43:RE:1112:CYS:HB2	1.97	0.64
47:RJ:263:LEU:HD23	47:RJ:267:ARG:HH22	1.63	0.64
34:5E:299:SER:HA	34:5E:302:LYS:HE2	1.80	0.64
50:RO:472:HIS:HD2	50:RO:474:HIS:H	1.46	0.64
41:RC:49:ARG:NH1	41:RC:104:LEU:O	2.30	0.64
50:RO:318:LEU:HA	50:RO:357:ARG:HH12	1.62	0.64
29:BE:631:ASN:HB2	29:BE:644:THR:HB	1.80	0.64
2:5A:487:A:H62	51:RQ:876:GLN:HE22	1.45	0.64
26:B2:439:LEU:HB2	26:B2:444:LEU:HB3	1.79	0.64
27:B3:788:TYR:O	27:B3:792:HIS:ND1	2.31	0.64
45:RG:122:ILE:HA	45:RG:161:LYS:O	1.97	0.64
19:A5:145:CYS:HB2	19:A5:148:LEU:HD21	1.80	0.64
27:B3:278:LEU:HD12	27:B3:279:LYS:HG2	1.78	0.64
3:SA:879:G:O2'	7:SO:105:ASN:HB2	1.98	0.64
3:SA:1658:G:C5	3:SA:1743:U:N3	2.65	0.64
8:SP:122:PRO:HB2	8:SP:125:SER:HB3	1.80	0.63
11:SY:97:ASP:OD1	11:SY:97:ASP:N	2.31	0.63
26:B2:201:ILE:HG13	27:B3:663:VAL:HG11	1.80	0.63
35:5F:33:MET:HB2	35:5F:38:ILE:HB	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:895:G:H1	3:SA:917:U:H3	1.46	0.63
3:SA:993:A:H62	3:SA:1011:G:H21	1.46	0.63
27:B3:11:SER:HB2	27:B3:641:PHE:O	1.98	0.63
28:B8:521:LEU:HA	28:B8:531:CYS:O	1.98	0.63
2:5A:173:G:N7	2:5A:175:A:N6	2.46	0.63
36:5G:32:ILE:HG22	36:5G:42:LEU:HD11	1.80	0.63
44:RF:68:LYS:HD2	44:RF:85:GLU:HA	1.81	0.63
47:RJ:831:ARG:NH2	47:RJ:835:HIS:O	2.30	0.63
2:5A:357:G:N7	32:5C:493:LYS:NZ	2.45	0.63
16:3F:538:ARG:HA	16:3F:566:ALA:O	1.97	0.63
9:SR:94:GLN:HB2	9:SR:102:LYS:HG3	1.80	0.63
32:5C:386:PHE:O	38:5I:8:ARG:NH2	2.31	0.63
44:RF:38:PHE:HB2	44:RF:56:VAL:HB	1.80	0.63
45:RH:129:ARG:HH11	45:RH:132:ARG:HD3	1.63	0.63
17:3H:44:LEU:HD22	17:3H:52:ILE:HD11	1.80	0.63
45:RH:192:TYR:HA	45:RH:195:LYS:HD2	1.81	0.63
27:B3:7:TYR:HB3	27:B3:644:TRP:HB3	1.80	0.63
43:RE:779:PHE:HB3	43:RE:851:LYS:HG3	1.80	0.63
27:B3:108:LEU:HG	27:B3:119:VAL:HG12	1.81	0.63
47:RJ:932:LEU:HD22	47:RJ:1007:TYR:HB2	1.80	0.63
3:SA:1658:G:C6	3:SA:1743:U:C5	2.87	0.63
27:B3:651:GLU:HA	27:B3:651:GLU:OE1	1.99	0.63
30:B6:285:TYR:HD2	30:B6:308:THR:HG22	1.63	0.63
15:3E:384:GLY:O	15:3E:388:LEU:HB2	1.99	0.62
8:SP:16:VAL:HA	8:SP:80:HIS:O	1.99	0.62
20:A8:553:GLN:NE2	20:A8:557:THR:OG1	2.32	0.62
48:RK:221:CYS:SG	48:RK:222:GLU:N	2.71	0.62
33:5D:29:GLU:OE2	33:5D:37:ARG:NH1	2.31	0.62
20:A8:530:PRO:HG2	20:A8:553:GLN:HE22	1.64	0.62
3:SA:1220:C:H2'	3:SA:1221:A:H8	1.64	0.62
22:AE:638:SER:HA	22:AE:641:LEU:HD12	1.80	0.62
27:B3:8:LYS:HG2	27:B3:645:LYS:HB2	1.81	0.62
41:RC:189:ASP:HB3	41:RC:194:ILE:HD11	1.81	0.62
21:A9:432:LYS:HB3	21:A9:435:LEU:HB3	1.81	0.62
50:RO:300:THR:O	50:RO:304:ASN:ND2	2.32	0.62
52:RS:379:LYS:HD2	52:RS:427:ARG:HE	1.64	0.62
49:RN:482:GLN:HG2	50:RO:507:LEU:HD11	1.80	0.62
18:A4:399:VAL:HG22	18:A4:420:LEU:HB2	1.80	0.62
43:RE:268:LEU:HB2	43:RE:294:LEU:HB2	1.82	0.62
49:RN:95:ARG:HH12	49:RN:757:LYS:HG3	1.64	0.62
29:BE:733:THR:O	29:BE:737:LEU:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1538:U:H2'	3:SA:1569:A:H61	1.65	0.62
19:A5:120:ILE:HB	19:A5:151:LEU:HD23	1.82	0.62
52:RS:214:TYR:HB3	52:RS:249:THR:HG22	1.80	0.62
3:SA:925:G:H5'	42:RD:1611:ALA:HB2	1.80	0.61
17:3H:50:GLU:HG3	17:3H:104:THR:HG22	1.82	0.61
25:B1:303:ASN:ND2	25:B1:323:LYS:HD3	2.15	0.61
27:B3:655:GLU:OE1	27:B3:655:GLU:HA	2.00	0.61
3:SA:1498:G:HO2'	46:RI:251:SER:HG	1.48	0.61
23:AF:428:ARG:NH2	24:AG:518:ASP:O	2.34	0.61
27:B3:633:VAL:HB	27:B3:644:TRP:HB2	1.81	0.61
29:BE:471:CYS:SG	29:BE:514:ASN:ND2	2.74	0.61
48:RK:155:LYS:HG2	48:RK:165:GLU:HG2	1.82	0.61
3:SA:477:A:H5'	37:5H:560:ASN:HD22	1.64	0.61
27:B3:692:MET:SD	34:5E:515:MET:HG2	2.40	0.61
28:B8:424:ILE:HG12	28:B8:434:GLU:HG2	1.83	0.61
41:RC:103:LEU:HB3	41:RC:108:VAL:CG2	2.30	0.61
52:RS:423:THR:HA	52:RS:426:GLN:HG2	1.81	0.61
3:SA:1512:G:H5"	46:RI:148:LYS:HD2	1.83	0.61
7:SO:109:LYS:H	7:SO:109:LYS:HD2	1.65	0.61
23:AF:440:GLU:O	23:AF:444:ASN:HB2	2.00	0.61
45:RG:36:LYS:HB3	45:RG:172:PRO:HA	1.82	0.61
19:A5:162:GLN:HA	19:A5:173:ILE:O	2.01	0.61
24:AG:335:PRO:HB2	24:AG:336:ARG:HD3	1.82	0.61
44:RF:101:SER:O	44:RF:105:SER:HB2	2.00	0.61
53:RT:224:ILE:HG12	53:RT:233:ILE:HG12	1.83	0.61
23:AF:51:HIS:O	23:AF:53:HIS:ND1	2.30	0.61
24:AG:769:ASN:ND2	24:AG:771:ASP:OD1	2.33	0.61
27:B3:221:ASN:OD1	27:B3:232:LYS:NZ	2.33	0.61
26:B2:861:ILE:HD13	27:B3:806:LEU:HD23	1.81	0.61
27:B3:294:LEU:HB2	27:B3:303:PHE:HB2	1.82	0.61
49:RN:511:SER:HA	49:RN:557:SER:HB2	1.82	0.61
3:SA:435:C:H42	47:RJ:166:ARG:HH12	1.47	0.60
3:SA:1658:G:N3	3:SA:1743:U:C2	2.69	0.60
49:RN:548:ARG:NH1	49:RN:638:ASN:OD1	2.33	0.60
13:3B:142:ARG:NH1	13:3B:186:ASP:OD2	2.34	0.60
13:3C:186:ASP:OD1	13:3C:214:ARG:NH1	2.33	0.60
16:3F:328:ILE:HG13	16:3F:338:THR:HG22	1.82	0.60
30:B6:286:ILE:HG22	30:B6:308:THR:HG21	1.83	0.60
43:RE:1111:SER:HA	43:RE:1129:PRO:HG3	1.83	0.60
19:A5:481:LEU:HD21	19:A5:526:LEU:HD22	1.83	0.60
45:RH:156:GLU:HG2	45:RH:157:GLU:HG2	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:5I:260:GLN:NE2	38:5I:289:TYR:OH	2.35	0.60
49:RN:649:THR:HG23	49:RN:650:VAL:HG23	1.82	0.60
50:RO:452:ASP:HB3	50:RO:455:LEU:HB2	1.84	0.60
27:B3:244:GLU:HG2	27:B3:293:VAL:H	1.66	0.60
34:5E:480:GLN:HG2	34:5E:482:LEU:H	1.66	0.60
45:RG:147:LYS:HD3	45:RG:150:ILE:HG22	1.83	0.60
50:RO:461:SER:OG	50:RO:462:SER:N	2.33	0.60
3:SA:1658:G:C4	3:SA:1743:U:C2	2.89	0.60
3:SA:1658:G:C4	3:SA:1743:U:N3	2.70	0.60
3:SA:606:A:N3	3:SA:607:G:N1	2.50	0.60
7:SO:106:ARG:HG2	7:SO:106:ARG:NH2	2.14	0.60
26:B2:54:ILE:HD13	26:B2:364:TYR:HD2	1.66	0.60
3:SA:941:A:N3	3:SA:976:G:O3'	2.35	0.60
27:B3:658:LYS:HB2	27:B3:658:LYS:NZ	2.15	0.60
18:A4:429:SER:HB3	18:A4:444:ARG:HA	1.83	0.60
23:AF:301:PRO:HG2	23:AF:323:SER:HB3	1.84	0.60
33:5D:22:ARG:NH1	47:RJ:997:MET:O	2.35	0.60
37:5H:434:PHE:HA	45:RH:129:ARG:HH12	1.67	0.60
14:3D:382:LYS:HD2	14:3D:404:LEU:HD22	1.83	0.59
24:AG:90:LYS:HG2	24:AG:144:VAL:HG22	1.84	0.59
43:RE:711:PRO:HG3	43:RE:767:GLN:HE21	1.67	0.59
14:3D:29:SER:O	14:3D:35:GLN:NE2	2.34	0.59
23:AF:248:ARG:NH1	23:AF:289:ASN:O	2.35	0.59
32:5C:96:ASP:OD1	32:5C:96:ASP:N	2.35	0.59
48:RK:14:SER:HB2	48:RK:36:ILE:HG23	1.83	0.59
4:SG:131:GLN:NE2	4:SG:135:ASP:OD1	2.35	0.59
23:AF:133:HIS:HD2	23:AF:135:GLN:H	1.50	0.59
43:RE:128:LEU:HD21	43:RE:185:LEU:HD21	1.85	0.59
3:SA:1643:U:OP2	34:5E:530:ARG:NH1	2.36	0.59
15:3E:210:LEU:HD23	15:3E:256:ASN:HD22	1.68	0.59
25:B1:497:ILE:HG23	25:B1:512:ILE:HB	1.84	0.59
27:B3:392:ASN:ND2	27:B3:435:ALA:O	2.34	0.59
45:RG:125:ASN:ND2	45:RG:127:THR:OG1	2.36	0.59
43:RE:495:THR:HA	43:RE:498:MET:HG2	1.84	0.59
49:RN:614:ILE:HG22	49:RN:616:LEU:HB2	1.85	0.59
43:RE:1100:VAL:HB	43:RE:1182:ILE:HB	1.83	0.59
49:RN:535:ASN:OD1	49:RN:539:ARG:NH1	2.36	0.59
3:SA:991:G:N1	3:SA:1012:U:OP2	2.36	0.59
14:3D:286:ARG:HA	14:3D:289:TYR:HB3	1.85	0.59
20:A8:533:PRO:HA	20:A8:559:PRO:HG2	1.85	0.59
24:AG:568:ASN:ND2	24:AG:586:SER:OG	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SP:17:ALA:HA	8:SP:30:VAL:HG22	1.85	0.59
24:AG:153:ILE:HG22	24:AG:174:TYR:HB2	1.85	0.59
30:B6:15:MET:HA	30:B6:18:LEU:HB3	1.85	0.58
43:RE:949:PHE:O	43:RE:960:LYS:NZ	2.36	0.58
53:RT:110:ARG:NH2	53:RT:130:MET:SD	2.76	0.58
3:SA:915:A:H2'	3:SA:916:U:H6	1.68	0.58
3:SA:1692:G:OP2	3:SA:1694:A:N6	2.37	0.58
2:5A:425:U:H3	2:5A:431:A:H61	1.51	0.58
13:3C:114:GLY:O	13:3C:122:ARG:NH1	2.35	0.58
1:3A:30:A:N6	38:5I:341:GLU:OE2	2.36	0.58
3:SA:563:U:H4'	36:5G:278:ARG:HG3	1.85	0.58
13:3B:236:MET:HG3	14:3D:133:LEU:HA	1.85	0.58
27:B3:25:VAL:HG23	27:B3:31:ILE:HG22	1.85	0.58
27:B3:211:LEU:O	27:B3:222:LEU:HA	2.02	0.58
27:B3:556:THR:HA	27:B3:573:GLY:HA2	1.85	0.58
32:5C:190:HIS:HB3	32:5C:207:THR:HG21	1.84	0.58
7:SO:106:ARG:HH21	7:SO:106:ARG:CG	2.09	0.58
25:B1:501:SER:HB2	25:B1:508:GLN:HB2	1.84	0.58
38:5I:411:LYS:O	38:5I:415:ARG:HB2	2.02	0.58
45:RH:44:VAL:HA	45:RH:113:TYR:O	2.03	0.58
50:RO:202:LEU:HD22	50:RO:212:LEU:HD22	1.86	0.58
2:5A:177:U:O2'	2:5A:178:G:N7	2.35	0.58
15:3E:11:GLY:HA2	15:3E:143:LEU:HD22	1.86	0.58
43:RE:219:PHE:CZ	43:RE:303:PHE:CD2	2.91	0.58
18:A4:565:ARG:HD3	22:AE:633:GLU:HB2	1.86	0.58
22:AE:248:SER:OG	22:AE:253:CYS:SG	2.62	0.58
33:5D:37:ARG:NH2	47:RJ:994:LYS:O	2.36	0.58
27:B3:616:HIS:NE2	27:B3:642:GLN:OE1	2.37	0.58
24:AG:435:ASP:CB	24:AG:702:TYR:HA	2.34	0.58
27:B3:510:SER:O	27:B3:514:THR:OG1	2.22	0.58
29:BE:482:GLY:HA2	29:BE:505:VAL:HG23	1.86	0.58
22:AE:671:LEU:O	22:AE:675:ASN:HB3	2.04	0.58
24:AG:118:VAL:HB	24:AG:130:LYS:HB2	1.85	0.58
43:RE:443:HIS:HB3	43:RE:470:LYS:HE2	1.86	0.58
18:A4:269:PHE:O	28:B8:446:ARG:NH2	2.36	0.57
25:B1:432:GLN:HE22	34:5E:455:HIS:HA	1.69	0.57
26:B2:97:GLY:HA3	26:B2:124:ILE:HD11	1.84	0.57
28:B8:227:LEU:HB2	28:B8:528:GLN:HE22	1.67	0.57
50:RO:270:SER:H	50:RO:273:GLN:HE21	1.50	0.57
24:AG:86:GLU:OE1	24:AG:113:ASN:ND2	2.36	0.57
27:B3:509:ALA:HB3	27:B3:539:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:5E:369:ILE:HG12	36:5G:223:THR:HG21	1.86	0.57
37:5H:532:VAL:HA	47:RJ:909:ASN:HD21	1.69	0.57
38:5I:87:SER:OG	38:5I:89:ASP:OD1	2.22	0.57
48:RK:114:PHE:HB2	48:RK:170:VAL:HG22	1.86	0.57
1:3A:251:G:H2'	16:3F:155:ASN:HD21	1.67	0.57
16:3F:241:THR:HG21	16:3F:285:SER:HA	1.86	0.57
24:AG:157:PHE:HB2	24:AG:170:SER:HB3	1.86	0.57
26:B2:861:ILE:CD1	27:B3:806:LEU:HD23	2.34	0.57
27:B3:12:LEU:CD2	27:B3:377:LEU:HB2	2.14	0.57
28:B8:221:THR:OG1	28:B8:222:LEU:N	2.38	0.57
31:5B:194:LYS:HD2	31:5B:199:ILE:HG13	1.86	0.57
32:5C:185:HIS:NE2	35:5F:19:LEU:O	2.36	0.57
47:RJ:773:THR:HA	47:RJ:777:ARG:HH11	1.69	0.57
3:SA:1196:A:N3	45:RG:136:ARG:NH2	2.52	0.57
26:B2:259:ILE:HA	26:B2:273:TYR:O	2.03	0.57
27:B3:16:TYR:O	27:B3:336:ASN:ND2	2.36	0.57
15:3E:339:TYR:HB3	15:3E:343:TYR:HB2	1.85	0.57
16:3F:293:ASP:N	16:3F:293:ASP:OD1	2.37	0.57
17:3H:44:LEU:HD13	17:3H:52:ILE:HD11	1.86	0.57
23:AF:303:LEU:HD13	23:AF:323:SER:HB2	1.86	0.57
29:BE:359:ALA:O	29:BE:421:ASN:ND2	2.38	0.57
32:5C:317:THR:HG23	32:5C:334:ARG:HB3	1.86	0.57
33:5D:111:ARG:HH11	33:5D:212:LYS:HD2	1.69	0.57
3:SA:942:G:H4'	3:SA:977:A:OP1	2.03	0.57
13:3C:267:VAL:HG21	13:3C:298:ILE:HD12	1.87	0.57
19:A5:434:THR:HG23	50:RO:266:ASN:HD21	1.69	0.57
23:AF:24:GLN:O	23:AF:28:ARG:HB3	2.05	0.57
24:AG:144:VAL:HG12	24:AG:153:ILE:HG13	1.86	0.57
28:B8:146:LEU:O	28:B8:163:ARG:NH1	2.37	0.57
34:5E:312:GLU:O	34:5E:316:ASN:ND2	2.38	0.57
43:RE:827:ARG:HB2	44:RF:175:LEU:HD11	1.87	0.57
3:SA:915:A:H2'	3:SA:916:U:C6	2.39	0.57
3:SA:1697:G:O5'	43:RE:326:LEU:CD1	2.45	0.57
11:SY:109:ARG:NH2	11:SY:120:VAL:O	2.37	0.57
25:B1:264:LYS:HD3	25:B1:280:THR:HG22	1.87	0.57
28:B8:129:ASP:OD1	29:BE:194:ARG:NH2	2.36	0.57
29:BE:666:ARG:NH1	29:BE:706:ASP:OD2	2.38	0.57
43:RE:242:LEU:HG	43:RE:245:LYS:HE3	1.87	0.57
43:RE:652:LYS:HG2	43:RE:667:CYS:HB2	1.87	0.57
52:RS:209:LYS:HE3	52:RS:212:LYS:HG3	1.87	0.57
13:3C:142:ARG:NH1	13:3C:186:ASP:OD2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3D:264:SER:OG	14:3D:265:GLU:N	2.37	0.57
26:B2:365:TYR:HA	26:B2:381:LYS:HA	1.85	0.57
26:B2:450:ARG:O	26:B2:475:ALA:HA	2.04	0.57
41:RC:141:ARG:NH2	41:RC:193:ASN:OD1	2.38	0.57
47:RJ:1042:MET:HG3	47:RJ:1044:LEU:HD13	1.86	0.57
3:SA:559:C:OP1	47:RJ:868:ARG:NH2	2.37	0.57
20:A8:536:ARG:NH1	20:A8:537:THR:OG1	2.38	0.57
25:B1:405:SER:HB3	25:B1:436:LEU:HD23	1.85	0.57
27:B3:581:CYS:HA	27:B3:590:LEU:O	2.04	0.57
45:RH:31:LEU:HD13	45:RH:40:ARG:HE	1.68	0.57
53:RT:217:GLU:HG2	53:RT:223:ARG:HA	1.86	0.57
3:SA:940:A:N1	3:SA:975:C:O2’	2.36	0.57
3:SA:1197:C:OP1	45:RG:136:ARG:NH1	2.38	0.57
3:SA:1657:U:H5”	26:B2:450:ARG:HH21	1.69	0.57
16:3F:442:ILE:HA	16:3F:472:PRO:HA	1.86	0.57
19:A5:148:LEU:HD23	19:A5:167:SER:HB3	1.86	0.57
22:AE:559:ASN:HA	22:AE:592:ARG:HD3	1.85	0.57
26:B2:432:TYR:HB3	26:B2:450:ARG:HB3	1.87	0.57
2:5A:481:U:O2’	30:B6:102:LYS:NZ	2.37	0.56
16:3F:545:LYS:HG2	16:3F:561:ASN:HD21	1.70	0.56
20:A8:614:ILE:HD12	20:A8:634:LEU:HD13	1.86	0.56
25:B1:479:LEU:HD12	25:B1:488:LEU:HD11	1.87	0.56
37:5H:438:ASP:OD1	37:5H:438:ASP:N	2.38	0.56
37:5H:498:VAL:HG21	46:RI:253:PRO:HD3	1.86	0.56
50:RO:170:GLY:O	50:RO:272:GLN:NE2	2.32	0.56
3:SA:1654:G:H2’	3:SA:1655:A:H8	1.71	0.56
24:AG:473:LEU:HB2	24:AG:495:ILE:HD11	1.87	0.56
24:AG:510:TYR:HH	24:AG:527:HIS:HD1	1.51	0.56
26:B2:180:THR:OG1	26:B2:207:CYS:SG	2.62	0.56
32:5C:493:LYS:O	32:5C:498:ARG:NH1	2.38	0.56
38:5I:15:PRO:HB3	38:5I:20:GLN:HE21	1.70	0.56
38:5I:81:ASN:ND2	38:5I:96:ASN:OD1	2.38	0.56
40:5K:26:LYS:HD3	40:5K:29:GLN:HG3	1.87	0.56
2:5A:323:A:N6	25:B1:212:ASP:OD2	2.37	0.56
11:SY:132:LEU:HA	11:SY:135:LEU:HB2	1.87	0.56
16:3F:142:ILE:HA	16:3F:568:ILE:HD11	1.87	0.56
16:3F:417:SER:OG	16:3F:418:ASP:N	2.37	0.56
18:A4:37:ARG:NH1	20:A8:704:PRO:O	2.38	0.56
19:A5:212:LEU:HD11	19:A5:246:VAL:HG11	1.87	0.56
20:A8:539:ASN:ND2	20:A8:560:ASN:O	2.38	0.56
21:A9:473:LYS:O	21:A9:477:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AF:147:ARG:NH2	45:RH:16:GLN:O	2.39	0.56
25:B1:373:ASP:HB2	25:B1:380:LEU:HD21	1.86	0.56
38:5I:45:LEU:HD13	38:5I:410:ILE:HG22	1.86	0.56
43:RE:466:THR:HG22	43:RE:475:ASN:HD21	1.70	0.56
3:SA:1749:A:H8	3:SA:1749:A:OP2	1.88	0.56
18:A4:32:ILE:O	18:A4:751:GLU:HA	2.06	0.56
43:RE:486:GLN:HE22	43:RE:571:ARG:HH22	1.52	0.56
43:RE:828:ASP:OD2	43:RE:888:LYS:NZ	2.36	0.56
45:RG:41:MET:HG3	45:RG:202:ILE:HG23	1.87	0.56
2:5A:484:G:OP2	30:B6:3:LYS:NZ	2.39	0.56
10:ST:27:LYS:HA	10:ST:57:ARG:HA	1.88	0.56
15:3E:414:ARG:NH1	22:AE:187:ASP:OD2	2.36	0.56
25:B1:329:VAL:HG12	25:B1:339:LEU:HG	1.87	0.56
2:5A:173:G:N2	2:5A:224:G:O2'	2.38	0.56
18:A4:301:ASP:O	18:A4:771:GLN:NE2	2.38	0.56
2:5A:5:G:N2	2:5A:8:A:OP2	2.39	0.56
14:3D:389:ILE:HA	17:3H:62:GLU:HB2	1.87	0.56
26:B2:463:SER:OG	26:B2:464:LEU:N	2.39	0.56
26:B2:598:LYS:NZ	26:B2:610:SER:OG	2.38	0.56
46:RI:33:ASP:N	46:RI:33:ASP:OD1	2.37	0.56
49:RN:478:ILE:HD13	49:RN:520:PRO:HB2	1.88	0.56
49:RN:512:ASP:OD1	49:RN:512:ASP:N	2.38	0.56
3:SA:925:G:H4'	42:RD:1611:ALA:HA	1.87	0.56
19:A5:435:GLY:HA3	50:RO:262:LEU:HD11	1.88	0.56
32:5C:284:ARG:NH1	32:5C:408:GLU:OE1	2.39	0.56
40:5K:123:PRO:O	40:5K:126:LYS:NZ	2.39	0.56
43:RE:1232:ILE:HD12	43:RE:1233:ASN:HB2	1.87	0.56
2:5A:329:A:OP1	32:5C:229:ARG:NH2	2.36	0.56
3:SA:439:U:H4'	3:SA:465:G:H22	1.69	0.56
13:3C:225:ARG:NH2	13:3C:246:GLN:OE1	2.38	0.56
22:AE:272:LYS:NZ	22:AE:310:GLY:O	2.39	0.56
24:AG:435:ASP:HB3	24:AG:702:TYR:HA	1.88	0.56
26:B2:347:SER:O	26:B2:371:LYS:NZ	2.39	0.56
32:5C:257:SER:OG	32:5C:259:TRP:NE1	2.36	0.56
38:5I:340:ARG:NH2	38:5I:377:SER:O	2.39	0.56
43:RE:708:LEU:HG	43:RE:915:LEU:HD23	1.88	0.56
3:SA:958:U:O2'	7:SO:55:ARG:NH1	2.39	0.56
13:3C:189:GLY:O	13:3C:216:ASN:ND2	2.39	0.56
19:A5:364:THR:OG1	19:A5:368:ASN:ND2	2.38	0.56
19:A5:471:ARG:NH2	50:RO:301:ASP:OD2	2.39	0.56
26:B2:145:ILE:HG23	26:B2:159:LEU:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B3:128:VAL:HB	27:B3:138:HIS:HB2	1.87	0.56
32:5C:433:LEU:HG	35:5F:13:LEU:HD11	1.88	0.56
36:5G:108:LYS:HD2	36:5G:116:ARG:HB2	1.87	0.56
36:5G:144:GLU:HA	36:5G:149:PRO:HA	1.88	0.56
22:AE:95:ASP:HB2	22:AE:131:ASN:HD21	1.71	0.55
26:B2:461:SER:OG	26:B2:462:SER:N	2.38	0.55
26:B2:858:PHE:O	26:B2:862:LYS:HB2	2.06	0.55
27:B3:12:LEU:HB3	27:B3:377:LEU:HD13	1.85	0.55
27:B3:501:PRO:HG3	27:B3:543:GLN:HG3	1.86	0.55
35:5F:29:ASP:N	35:5F:29:ASP:OD1	2.38	0.55
38:5I:73:ILE:HG12	38:5I:85:THR:HG22	1.88	0.55
43:RE:777:ASP:O	43:RE:780:GLN:NE2	2.39	0.55
48:RK:154:LEU:HB2	48:RK:165:GLU:HG3	1.88	0.55
53:RT:109:LEU:O	53:RT:113:TRP:HB2	2.06	0.55
26:B2:124:ILE:HA	26:B2:140:SER:HA	1.89	0.55
28:B8:181:GLU:HB3	29:BE:281:ARG:HH12	1.71	0.55
32:5C:162:ASN:HB3	32:5C:164:GLN:H	1.71	0.55
47:RJ:279:PRO:HB3	47:RJ:784:LYS:HA	1.88	0.55
3:SA:1655:A:H2'	3:SA:1656:U:C6	2.41	0.55
10:ST:8:GLN:NE2	23:AF:324:SER:O	2.39	0.55
38:5I:329:ILE:HG12	38:5I:343:TYR:HB2	1.89	0.55
39:5J:129:ALA:HB1	47:RJ:1119:ILE:HG22	1.89	0.55
48:RK:34:GLU:HG3	48:RK:35:LYS:HG2	1.88	0.55
48:RK:139:PRO:HA	48:RK:142:GLU:HB2	1.89	0.55
48:RK:171:ASP:N	48:RK:171:ASP:OD1	2.39	0.55
3:SA:1232:U:O4	3:SA:1234:A:N6	2.39	0.55
13:3B:225:ARG:NH1	13:3B:248:ASP:OD2	2.38	0.55
13:3C:320:TYR:OH	13:3C:322:ARG:NH2	2.39	0.55
17:3H:41:THR:O	17:3H:45:ASN:ND2	2.39	0.55
18:A4:57:ILE:HD13	18:A4:340:GLN:HG2	1.89	0.55
19:A5:5:VAL:HA	19:A5:21:THR:HG22	1.89	0.55
24:AG:262:MET:HA	24:AG:272:ALA:O	2.07	0.55
38:5I:26:ARG:NH1	51:RQ:867:GLN:O	2.40	0.55
41:RC:52:TYR:HE1	41:RC:56:ILE:HG21	1.70	0.55
47:RJ:608:LEU:HB2	48:RK:16:ASN:HD22	1.72	0.55
3:SA:1490:C:OP1	47:RJ:1062:ARG:NH2	2.38	0.55
3:SA:1542:G:O6	3:SA:1568:C:N4	2.36	0.55
8:SP:86:THR:OG1	8:SP:90:ARG:NH2	2.36	0.55
16:3F:289:ARG:NH2	16:3F:332:ALA:O	2.39	0.55
16:3F:552:TRP:HB3	17:3H:85:VAL:HG13	1.88	0.55
27:B3:513:LYS:HG3	27:B3:532:HIS:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B6:278:MET:HA	30:B6:312:LEU:HD11	1.89	0.55
37:5H:432:ASP:O	45:RH:129:ARG:NH2	2.39	0.55
43:RE:526:CYS:O	43:RE:698:ASN:ND2	2.40	0.55
49:RN:682:ARG:O	49:RN:686:ASN:ND2	2.40	0.55
51:RQ:896:ALA:HB1	51:RQ:897:PRO:HD2	1.89	0.55
53:RT:169:ASP:OD1	53:RT:169:ASP:N	2.39	0.55
17:3G:57:ASP:O	17:3G:84:ARG:NH1	2.40	0.55
24:AG:583:LYS:HE2	24:AG:599:ILE:HD13	1.88	0.55
27:B3:516:LYS:HA	27:B3:528:THR:HG22	1.89	0.55
28:B8:561:PRO:O	28:B8:587:ARG:NH1	2.39	0.55
38:5I:173:ILE:HG13	38:5I:174:ARG:HG2	1.87	0.55
47:RJ:130:ASP:OD2	47:RJ:853:ARG:NH2	2.40	0.55
48:RK:155:LYS:HG3	48:RK:164:GLY:HA2	1.89	0.55
13:3C:160:ASP:OD1	13:3C:160:ASP:N	2.37	0.55
19:A5:454:GLU:OE2	19:A5:487:ARG:NH1	2.39	0.55
23:AF:420:GLU:O	23:AF:424:ARG:HB3	2.07	0.55
24:AG:51:GLN:HE21	24:AG:53:LYS:HD3	1.72	0.55
26:B2:142:ASP:OD2	26:B2:144:ASN:ND2	2.39	0.55
43:RE:209:MET:SD	43:RE:227:LYS:NZ	2.70	0.55
43:RE:980:VAL:HG21	43:RE:1011:ARG:HG2	1.88	0.55
47:RJ:360:ASP:OD1	47:RJ:360:ASP:N	2.35	0.55
47:RJ:921:GLU:HB2	48:RK:365:LYS:HG3	1.88	0.55
48:RK:37:ARG:NH2	48:RK:49:GLU:OE2	2.36	0.55
19:A5:531:LYS:O	19:A5:535:ASP:HB2	2.07	0.55
20:A8:443:CYS:HA	24:AG:728:LEU:HD22	1.87	0.55
25:B1:418:ARG:HH22	34:5E:491:ALA:HA	1.72	0.55
26:B2:267:ASP:OD1	26:B2:267:ASP:N	2.36	0.55
28:B8:526:ASP:OD1	28:B8:526:ASP:N	2.38	0.55
34:5E:299:SER:O	34:5E:303:GLN:NE2	2.40	0.55
3:SA:1750:A:H2'	3:SA:1751:C:C6	2.42	0.55
3:SA:1758:U:O4	26:B2:937:ARG:NH2	2.40	0.55
22:AE:558:VAL:O	22:AE:592:ARG:NH1	2.40	0.55
27:B3:258:ILE:HD12	27:B3:271:ASP:HA	1.88	0.55
28:B8:176:LYS:O	28:B8:180:ASP:CB	2.55	0.55
34:5E:344:GLU:HA	47:RJ:960:ARG:HH21	1.71	0.55
6:SN:90:LYS:HE3	6:SN:91:VAL:HG12	1.88	0.55
18:A4:534:LEU:HA	18:A4:542:VAL:O	2.07	0.55
22:AE:196:LEU:HD11	22:AE:213:THR:HG21	1.88	0.55
24:AG:510:TYR:OH	24:AG:527:HIS:ND1	2.35	0.55
25:B1:430:ARG:HD2	34:5E:460:PRO:HA	1.89	0.55
35:5F:162:ASP:OD1	35:5F:162:ASP:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:RJ:289:HIS:HB2	47:RJ:815:LEU:HD21	1.89	0.55
47:RJ:551:LYS:O	47:RJ:555:MET:HB2	2.07	0.55
49:RN:290:LYS:O	52:RS:458:ARG:NH1	2.40	0.55
50:RO:156:TRP:O	50:RO:215:ASN:ND2	2.40	0.55
52:RS:445:ARG:NH1	52:RS:445:ARG:O	2.40	0.55
2:5A:354:G:N1	32:5C:485:ASP:O	2.38	0.54
9:SR:22:VAL:HG22	9:SR:65:ILE:HG23	1.89	0.54
14:3D:21:LYS:HE2	14:3D:49:GLU:HB2	1.88	0.54
14:3D:63:LEU:O	14:3D:67:ASN:ND2	2.40	0.54
22:AE:12:ALA:HB2	32:5C:142:GLY:HA3	1.89	0.54
22:AE:636:ASP:OD1	22:AE:639:ARG:NH1	2.40	0.54
26:B2:592:SER:OG	26:B2:593:ALA:N	2.40	0.54
27:B3:721:ASN:OD1	27:B3:721:ASN:N	2.39	0.54
30:B6:187:LYS:HE3	39:5J:63:PRO:HB2	1.90	0.54
38:5I:402:GLU:O	38:5I:405:ARG:NH2	2.40	0.54
41:RC:103:LEU:HB3	41:RC:108:VAL:HG21	1.89	0.54
48:RK:347:ASN:ND2	48:RK:349:ASP:OD2	2.40	0.54
50:RO:345:ILE:HA	50:RO:349:LEU:HD13	1.89	0.54
2:5A:243:A:H4'	33:5D:224:LEU:HD21	1.89	0.54
16:3F:398:CYS:O	16:3F:419:ASN:ND2	2.40	0.54
22:AE:519:LEU:HD23	22:AE:523:ILE:HD13	1.88	0.54
25:B1:356:ASP:HB2	25:B1:826:ARG:HG3	1.88	0.54
25:B1:375:THR:OG1	25:B1:376:SER:N	2.41	0.54
26:B2:787:LYS:NZ	26:B2:788:PRO:O	2.38	0.54
27:B3:353:LEU:HD23	27:B3:365:ILE:HD11	1.88	0.54
35:5F:115:MET:HG3	35:5F:120:MET:HB3	1.89	0.54
45:RH:114:ILE:HG12	45:RH:122:ILE:HB	1.89	0.54
4:SG:26:ALA:HB3	9:SR:28:LEU:HB3	1.89	0.54
15:3E:280:MET:HG3	15:3E:288:THR:HG22	1.89	0.54
24:AG:850:GLU:HA	24:AG:853:ILE:HD12	1.89	0.54
25:B1:202:ASP:N	25:B1:202:ASP:OD1	2.40	0.54
25:B1:396:ALA:HB2	25:B1:438:VAL:HG21	1.90	0.54
25:B1:641:LEU:HD23	25:B1:644:ILE:HD12	1.89	0.54
27:B3:592:SER:HB3	27:B3:620:LEU:HD22	1.88	0.54
37:5H:565:LYS:HA	37:5H:568:LYS:HG2	1.89	0.54
43:RE:1014:LEU:HG	43:RE:1018:LYS:HE3	1.90	0.54
51:RQ:898:PHE:N	51:RQ:898:PHE:CD1	2.73	0.54
17:3G:13:ASP:OD1	17:3G:13:ASP:N	2.39	0.54
18:A4:641:GLU:OE2	18:A4:645:ARG:NH1	2.40	0.54
38:5I:133:GLN:NE2	38:5I:151:ASN:OD1	2.40	0.54
43:RE:218:ASP:HA	43:RE:223:ARG:HH22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:RE:929:ILE:HG13	43:RE:933:LEU:HD23	1.90	0.54
14:3D:379:LEU:O	14:3D:383:CYS:HB2	2.07	0.54
18:A4:252:GLN:NE2	18:A4:318:ASN:OD1	2.40	0.54
26:B2:287:ARG:NH1	26:B2:324:PHE:O	2.41	0.54
27:B3:12:LEU:HD12	27:B3:12:LEU:N	2.17	0.54
27:B3:434:SER:H	27:B3:458:SER:HB2	1.73	0.54
29:BE:626:ASP:N	29:BE:626:ASP:OD1	2.35	0.54
38:5I:349:GLN:O	38:5I:367:SER:OG	2.24	0.54
43:RE:687:GLN:NE2	43:RE:694:ALA:O	2.41	0.54
47:RJ:1018:VAL:O	47:RJ:1029:TRP:NE1	2.41	0.54
3:SA:511:A:OP2	5:SK:176:ASN:ND2	2.40	0.54
16:3F:414:ILE:HD11	16:3F:480:ALA:HB2	1.90	0.54
19:A5:20:VAL:HG22	19:A5:29:VAL:HG22	1.89	0.54
22:AE:274:ILE:HD11	28:B8:215:THR:HG21	1.90	0.54
23:AF:387:ALA:O	23:AF:391:ASN:ND2	2.40	0.54
27:B3:17:ALA:HB3	27:B3:35:PRO:HA	1.90	0.54
42:RD:1488:LEU:CA	43:RE:411:ILE:O	2.55	0.54
47:RJ:966:ILE:HD13	47:RJ:976:ILE:HG22	1.88	0.54
9:SR:34:SER:HB2	9:SR:38:LEU:HD12	1.90	0.54
16:3F:481:ILE:HD12	16:3F:486:VAL:HG13	1.90	0.54
20:A8:666:VAL:HG22	21:A9:496:LEU:HB3	1.90	0.54
22:AE:205:THR:HB	22:AE:210:LEU:HD21	1.89	0.54
23:AF:75:LYS:HD3	23:AF:113:PRO:HD3	1.89	0.54
24:AG:727:GLN:OE1	24:AG:738:ASN:ND2	2.40	0.54
26:B2:317:ILE:O	26:B2:321:TYR:N	2.41	0.54
27:B3:279:LYS:NZ	27:B3:326:THR:OG1	2.39	0.54
28:B8:486:SER:OG	28:B8:487:GLU:N	2.41	0.54
32:5C:449:ILE:HD11	38:5I:38:ALA:HA	1.89	0.54
1:3A:258:U:O4	14:3D:377:ARG:NH2	2.41	0.54
3:SA:918:U:O3'	8:SP:18:ARG:NH1	2.41	0.54
13:3C:268:VAL:HG22	13:3C:317:VAL:HG12	1.89	0.54
14:3D:392:TYR:HB3	17:3H:65:LEU:HD22	1.90	0.54
23:AF:215:VAL:HA	23:AF:230:GLY:HA3	1.90	0.54
24:AG:368:ASP:OD1	24:AG:368:ASP:N	2.38	0.54
27:B3:494:ILE:N	27:B3:510:SER:OG	2.33	0.54
47:RJ:73:ALA:HB1	47:RJ:131:ILE:HD12	1.90	0.54
47:RJ:1027:THR:HG23	47:RJ:1028:GLU:HG2	1.89	0.54
2:5A:354:G:N2	32:5C:495:SER:O	2.41	0.54
3:SA:494:U:OP1	47:RJ:1138:ARG:NH2	2.32	0.54
3:SA:1108:G:O2'	3:SA:1109:G:N7	2.37	0.54
18:A4:578:SER:HG	18:A4:643:SER:HG	1.52	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B8:176:LYS:O	28:B8:180:ASP:HB3	2.07	0.54
37:5H:511:GLU:O	37:5H:515:ASN:ND2	2.40	0.54
49:RN:515:HIS:HB3	49:RN:518:ILE:HG22	1.90	0.54
52:RS:319:LYS:HA	52:RS:323:PHE:HB2	1.89	0.54
2:5A:338:A:O2'	2:5A:340:U:O4	2.20	0.54
13:3B:124:SER:HB3	39:5J:153:ILE:HD11	1.90	0.54
15:3E:380:ARG:NH1	15:3E:382:ASP:OD1	2.40	0.54
24:AG:157:PHE:O	24:AG:169:GLN:NE2	2.40	0.54
26:B2:260:GLU:O	26:B2:272:PHE:HA	2.08	0.54
29:BE:73:GLU:OE2	29:BE:74:LYS:NZ	2.40	0.54
29:BE:160:THR:OG1	29:BE:163:GLN:NE2	2.41	0.54
3:SA:1159:C:N4	36:5G:184:GLU:OE2	2.38	0.53
3:SA:1175:U:OP1	49:RN:748:ARG:NH1	2.41	0.53
3:SA:1697:G:C5'	43:RE:326:LEU:HD11	2.38	0.53
13:3B:90:PRO:HD3	39:5J:106:LEU:HD12	1.90	0.53
16:3F:162:CYS:SG	16:3F:525:GLN:NE2	2.79	0.53
17:3H:38:ASN:HA	17:3H:41:THR:HG22	1.91	0.53
18:A4:271:THR:HG21	28:B8:443:VAL:HG21	1.91	0.53
20:A8:573:ILE:HG22	20:A8:575:ASN:H	1.72	0.53
22:AE:651:LEU:HD21	22:AE:680:TYR:HB2	1.90	0.53
24:AG:724:ILE:HD11	24:AG:763:ILE:HG22	1.90	0.53
43:RE:524:ASP:OD1	43:RE:956:ASN:ND2	2.39	0.53
43:RE:1202:CYS:SG	43:RE:1203:ASN:N	2.81	0.53
45:RG:36:LYS:NZ	45:RG:169:ASP:O	2.40	0.53
47:RJ:954:SER:HA	47:RJ:984:GLU:HG3	1.89	0.53
49:RN:605:ASP:OD1	49:RN:610:ARG:NH1	2.41	0.53
3:SA:1539:G:N1	3:SA:1569:A:OP2	2.41	0.53
6:SN:105:LYS:HA	52:RS:350:LEU:HD22	1.91	0.53
16:3F:399:GLU:OE2	16:3F:417:SER:OG	2.26	0.53
25:B1:661:LEU:HD11	34:5E:450:VAL:HG12	1.90	0.53
26:B2:412:GLY:HA2	26:B2:431:GLY:H	1.73	0.53
26:B2:525:ASP:OD1	26:B2:525:ASP:N	2.40	0.53
28:B8:352:GLN:HE21	28:B8:385:ASN:HD22	1.54	0.53
29:BE:604:SER:OG	29:BE:606:ASP:OD1	2.25	0.53
40:5K:145:VAL:HG23	40:5K:151:TYR:HB2	1.89	0.53
43:RE:207:LEU:O	43:RE:297:GLY:N	2.39	0.53
45:RH:125:ASN:ND2	45:RH:127:THR:OG1	2.42	0.53
4:SG:73:THR:OG1	4:SG:91:GLU:OE1	2.27	0.53
17:3H:45:ASN:HA	17:3H:74:LYS:HE2	1.90	0.53
18:A4:311:THR:HG22	18:A4:313:LYS:H	1.74	0.53
23:AF:173:THR:HG21	23:AF:218:VAL:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BE:430:ILE:HB	29:BE:443:TRP:HB2	1.89	0.53
36:5G:93:SER:O	36:5G:119:ARG:NH2	2.41	0.53
2:5A:175:A:N6	2:5A:177:U:O2	2.40	0.53
3:SA:867:G:H1	3:SA:961:U:H3	1.56	0.53
3:SA:976:G:C6	3:SA:978:A:H2'	2.44	0.53
7:SO:99:ARG:NH2	7:SO:119:GLU:OE2	2.40	0.53
18:A4:641:GLU:HB3	18:A4:749:SER:HB3	1.90	0.53
24:AG:291:ARG:HD2	24:AG:329:ASN:HD21	1.73	0.53
27:B3:151:LYS:NZ	27:B3:197:ASP:OD1	2.38	0.53
48:RK:289:VAL:HG21	48:RK:294:LEU:HD13	1.90	0.53
14:3D:157:ALA:O	30:B6:293:TYR:OH	2.26	0.53
14:3D:392:TYR:HB2	17:3H:62:GLU:HB3	1.90	0.53
19:A5:46:TRP:HD1	19:A5:48:GLU:HG3	1.74	0.53
25:B1:283:GLU:OE2	25:B1:297:GLN:NE2	2.42	0.53
27:B3:168:THR:HA	27:B3:192:ALA:HA	1.91	0.53
27:B3:625:THR:HG22	27:B3:633:VAL:HG13	1.90	0.53
45:RG:169:ASP:N	45:RG:169:ASP:OD1	2.40	0.53
46:RI:83:TYR:OH	46:RI:169:GLU:OE1	2.27	0.53
49:RN:96:LYS:HD2	49:RN:761:PHE:HZ	1.73	0.53
3:SA:513:U:H2'	3:SA:514:G:C8	2.44	0.53
22:AE:40:ALA:HB1	22:AE:123:ARG:HH12	1.73	0.53
24:AG:213:LYS:HA	24:AG:223:LYS:HA	1.91	0.53
38:5I:192:SER:HB2	38:5I:206:VAL:HG22	1.89	0.53
46:RI:83:TYR:O	46:RI:87:LEU:HB2	2.08	0.53
3:SA:629:U:H2'	3:SA:630:A:H8	1.74	0.53
26:B2:869:VAL:O	27:B3:816:LEU:HD22	2.09	0.53
35:5F:108:ARG:O	35:5F:117:ARG:NH1	2.42	0.53
3:SA:1658:G:O6	3:SA:1742:U:O4	2.26	0.53
24:AG:404:SER:OG	24:AG:405:ALA:N	2.40	0.53
32:5C:312:VAL:HG21	32:5C:353:PRO:HG2	1.90	0.53
36:5G:153:THR:HG23	36:5G:164:GLN:HG2	1.91	0.53
43:RE:162:PHE:HZ	43:RE:597:ARG:HH11	1.57	0.53
46:RI:231:GLN:NE2	54:RW:188:THR:O	2.42	0.53
14:3D:102:ASP:HB3	14:3D:105:LEU:HB3	1.91	0.53
21:A9:513:ARG:HH21	21:A9:515:ASP:HA	1.72	0.53
23:AF:87:ALA:HA	23:AF:97:CYS:O	2.08	0.53
27:B3:96:VAL:HG12	27:B3:97:ARG:HG3	1.90	0.53
32:5C:369:MET:HE1	32:5C:404:PRO:HD2	1.91	0.53
32:5C:483:ILE:HG23	32:5C:516:VAL:HG22	1.90	0.53
43:RE:1101:ASP:OD2	43:RE:1103:ARG:NH1	2.42	0.53
45:RG:121:LEU:HD21	45:RG:167:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1671:A:N6	3:SA:1730:A:O2'	2.42	0.53
13:3B:230:TYR:OH	13:3B:256:ASN:OD1	2.25	0.53
24:AG:283:VAL:HG12	24:AG:290:ILE:HG22	1.91	0.53
25:B1:567:ASP:HB3	35:5F:144:ASN:HD21	1.74	0.53
27:B3:403:ILE:HB	27:B3:415:TRP:HB2	1.91	0.53
43:RE:257:SER:O	43:RE:266:PRO:HA	2.09	0.53
45:RG:188:ARG:NH2	45:RH:247:ASP:OD2	2.41	0.53
51:RQ:298:TRP:HE1	51:RQ:899:LYS:CG	2.19	0.53
1:3A:198:U:O4	16:3F:151:ARG:NE	2.38	0.52
2:5A:254:C:H2'	54:RW:183:ARG:HH21	1.74	0.52
3:SA:1136:U:O2'	26:B2:596:ASN:ND2	2.43	0.52
3:SA:1209:C:N3	3:SA:1210:C:N4	2.56	0.52
13:3B:281:ASP:OD1	13:3B:281:ASP:N	2.41	0.52
18:A4:35:ARG:HH11	18:A4:738:TYR:HD1	1.57	0.52
20:A8:558:CYS:O	20:A8:585:ARG:NH2	2.42	0.52
22:AE:626:PHE:HB3	22:AE:629:GLU:HB2	1.90	0.52
25:B1:812:GLU:HG3	25:B1:813:HIS:HD2	1.74	0.52
27:B3:616:HIS:HD2	27:B3:640:VAL:HG23	1.74	0.52
43:RE:254:LEU:HD11	43:RE:268:LEU:HD12	1.91	0.52
45:RH:116:THR:HG22	45:RH:118:ARG:H	1.73	0.52
50:RO:233:ASP:N	50:RO:233:ASP:OD1	2.42	0.52
15:3E:289:GLN:HE21	15:3E:388:LEU:HD13	1.74	0.52
27:B3:16:TYR:HD1	27:B3:34:THR:H	1.58	0.52
43:RE:128:LEU:HD11	43:RE:185:LEU:HD11	1.91	0.52
43:RE:1206:PRO:HB3	43:RE:1212:VAL:HG12	1.90	0.52
52:RS:437:ARG:NH2	52:RS:459:GLU:O	2.42	0.52
2:5A:135:G:O3'	19:A5:494:ARG:NH1	2.42	0.52
8:SP:42:VAL:HG11	8:SP:63:ALA:O	2.09	0.52
18:A4:39:VAL:H	18:A4:755:ILE:HD11	1.75	0.52
22:AE:556:LYS:O	22:AE:592:ARG:NH2	2.43	0.52
22:AE:571:LEU:HD11	22:AE:582:VAL:HG11	1.91	0.52
29:BE:578:VAL:O	29:BE:579:ARG:NH1	2.42	0.52
36:5G:43:PRO:HG2	36:5G:46:LEU:HB2	1.91	0.52
47:RJ:90:VAL:HG23	47:RJ:107:VAL:HG11	1.92	0.52
47:RJ:135:ALA:O	47:RJ:238:ARG:NH2	2.42	0.52
49:RN:587:ASP:OD1	49:RN:587:ASP:N	2.42	0.52
22:AE:502:ILE:HG23	22:AE:542:ILE:HG13	1.90	0.52
35:5F:123:THR:HG23	35:5F:126:ASP:H	1.73	0.52
46:RI:135:LEU:HD22	46:RI:139:LEU:HD13	1.91	0.52
47:RJ:982:LYS:HG3	47:RJ:983:PRO:HD3	1.92	0.52
2:5A:176:U:O2'	2:5A:178:G:OP2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3B:228:GLN:O	13:3B:231:ARG:NH2	2.43	0.52
18:A4:420:LEU:HD23	19:A5:581:ASN:HA	1.91	0.52
28:B8:216:TYR:OH	29:BE:276:TYR:OH	2.27	0.52
29:BE:470:GLN:NE2	29:BE:512:GLY:O	2.42	0.52
43:RE:1221:HIS:NE2	44:RF:21:PRO:O	2.42	0.52
47:RJ:844:PRO:HA	47:RJ:856:THR:O	2.08	0.52
48:RK:97:GLY:HA2	48:RK:100:VAL:HG12	1.92	0.52
3:SA:1533:C:OP1	10:ST:27:LYS:NZ	2.41	0.52
7:SO:102:LEU:C	7:SO:104:ARG:H	2.13	0.52
13:3C:297:ARG:HD3	13:3C:322:ARG:HA	1.92	0.52
15:3E:251:ASP:OD1	15:3E:251:ASP:N	2.43	0.52
18:A4:658:ASP:OD2	18:A4:731:HIS:N	2.42	0.52
19:A5:481:LEU:HD22	19:A5:523:LEU:HD22	1.92	0.52
20:A8:566:LEU:HG	20:A8:582:ILE:HD11	1.92	0.52
23:AF:364:SER:O	23:AF:364:SER:OG	2.26	0.52
26:B2:398:ASP:HB2	26:B2:406:LEU:HB3	1.92	0.52
27:B3:282:ASN:HD21	27:B3:327:ILE:HD11	1.75	0.52
42:RD:1489:SER:CB	43:RE:427:LYS:CD	2.83	0.52
43:RE:197:GLN:HB2	43:RE:200:GLY:H	1.73	0.52
43:RE:713:LEU:HB2	43:RE:716:SER:HB3	1.90	0.52
43:RE:834:ASN:ND2	43:RE:863:TYR:OH	2.42	0.52
43:RE:1109:LYS:HD3	43:RE:1114:ILE:HB	1.92	0.52
44:RF:101:SER:O	44:RF:105:SER:CB	2.58	0.52
44:RF:176:ASP:N	44:RF:176:ASP:OD1	2.41	0.52
3:SA:594:A:OP1	5:SK:38:ASN:ND2	2.43	0.52
21:A9:504:GLU:OE2	21:A9:507:ARG:NH1	2.43	0.52
24:AG:319:LYS:HD2	24:AG:339:GLY:H	1.74	0.52
26:B2:53:ASP:OD2	26:B2:58:ASP:OD1	2.27	0.52
26:B2:281:ILE:HB	26:B2:332:ILE:HG23	1.91	0.52
26:B2:554:THR:OG1	26:B2:556:LYS:NZ	2.39	0.52
29:BE:268:THR:HG22	29:BE:270:SER:H	1.75	0.52
29:BE:605:LEU:HD23	29:BE:628:VAL:HG11	1.92	0.52
29:BE:819:LYS:NZ	29:BE:823:GLU:OE2	2.40	0.52
38:5I:75:LYS:NZ	38:5I:356:TYR:O	2.34	0.52
38:5I:319:GLU:OE2	38:5I:356:TYR:OH	2.27	0.52
38:5I:324:SER:OG	38:5I:326:ASP:OD1	2.23	0.52
43:RE:270:ILE:HB	43:RE:292:ILE:HG13	1.92	0.52
46:RI:155:ARG:O	46:RI:179:GLN:NE2	2.42	0.52
1:3A:256:G:OP1	14:3D:382:LYS:NZ	2.37	0.52
3:SA:1004:U:OP2	3:SA:1006:C:N4	2.43	0.52
13:3B:277:ASP:N	13:3B:277:ASP:OD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3D:169:LYS:HA	14:3D:299:VAL:HG22	1.91	0.52
39:5J:58:ASN:HA	39:5J:61:LYS:HG2	1.92	0.52
47:RJ:246:ALA:HB3	47:RJ:810:ILE:HB	1.91	0.52
47:RJ:616:ASP:HB2	47:RJ:621:LEU:HG	1.90	0.52
52:RS:397:PHE:HD1	52:RS:407:GLU:HG2	1.75	0.52
3:SA:1436:A:H1'	52:RS:419:LYS:HD2	1.90	0.52
4:SG:120:ILE:HA	4:SG:123:VAL:HG12	1.92	0.52
15:3E:426:ALA:HB2	29:BE:305:ASN:HD21	1.75	0.52
19:A5:503:LYS:HD3	21:A9:508:ARG:HH22	1.75	0.52
23:AF:256:THR:N	23:AF:275:SER:O	2.39	0.52
24:AG:64:LYS:NZ	24:AG:123:GLY:O	2.39	0.52
25:B1:506:SER:OG	25:B1:507:GLN:N	2.43	0.52
26:B2:54:ILE:CD1	26:B2:364:TYR:CD2	2.93	0.52
26:B2:861:ILE:HD13	27:B3:806:LEU:CD2	2.40	0.52
29:BE:59:GLN:HG2	29:BE:71:VAL:HG22	1.91	0.52
41:RC:103:LEU:O	41:RC:108:VAL:HG22	2.10	0.52
43:RE:307:LYS:HE3	43:RE:312:ARG:HD3	1.92	0.52
48:RK:30:PRO:HB3	48:RK:77:ARG:HG3	1.90	0.52
2:5A:294:U:OP1	25:B1:631:ASN:ND2	2.43	0.52
10:ST:28:ILE:HD13	10:ST:61:LEU:HD11	1.92	0.52
15:3E:359:ILE:HA	15:3E:362:VAL:HG12	1.92	0.52
24:AG:431:SER:OG	24:AG:432:ARG:N	2.43	0.52
32:5C:495:SER:O	32:5C:495:SER:OG	2.29	0.52
51:RQ:298:TRP:NE1	51:RQ:899:LYS:CG	2.62	0.52
51:RQ:298:TRP:CD1	51:RQ:899:LYS:HG3	2.44	0.52
52:RS:360:LEU:HD21	52:RS:393:TYR:HB2	1.92	0.52
3:SA:1533:C:OP2	23:AF:114:ARG:NH2	2.43	0.51
13:3B:120:GLU:OE2	13:3B:142:ARG:NE	2.41	0.51
18:A4:63:SER:HA	18:A4:82:ARG:HH12	1.75	0.51
18:A4:402:TRP:HB3	18:A4:416:LEU:HA	1.91	0.51
20:A8:28:TYR:HA	20:A8:356:THR:HA	1.92	0.51
24:AG:407:ASN:ND2	24:AG:416:SER:OG	2.44	0.51
25:B1:722:THR:HG22	25:B1:724:HIS:H	1.75	0.51
32:5C:130:ARG:NH2	32:5C:379:GLU:OE2	2.42	0.51
43:RE:756:VAL:HA	43:RE:896:THR:HG21	1.91	0.51
47:RJ:193:ARG:NH2	47:RJ:196:THR:OG1	2.43	0.51
47:RJ:864:ASP:OD1	47:RJ:864:ASP:N	2.43	0.51
8:SP:20:TYR:HB3	8:SP:27:PHE:HB2	1.93	0.51
14:3D:126:ASP:HA	14:3D:129:ARG:HG2	1.93	0.51
20:A8:563:LEU:HA	20:A8:566:LEU:HB2	1.92	0.51
20:A8:672:ASN:HB2	21:A9:486:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B2:634:SER:OG	26:B2:635:LYS:N	2.41	0.51
27:B3:787:PRO:HB2	34:5E:492:PRO:HG3	1.92	0.51
32:5C:410:ASN:O	38:5I:27:ASN:ND2	2.43	0.51
36:5G:139:LEU:HD23	36:5G:266:LEU:HD12	1.92	0.51
44:RF:9:MET:HB2	44:RF:13:PHE:HB2	1.92	0.51
45:RG:105:ASN:HD21	45:RG:110:LEU:HD22	1.75	0.51
48:RK:315:LYS:HB2	48:RK:348:GLU:HB3	1.92	0.51
50:RO:258:GLU:HG3	50:RO:289:PHE:HD1	1.74	0.51
3:SA:1670:G:N2	3:SA:1731:A:OP2	2.42	0.51
18:A4:420:LEU:HD11	18:A4:462:VAL:HG21	1.92	0.51
23:AF:59:SER:OG	23:AF:60:SER:N	2.43	0.51
29:BE:854:SER:HB2	29:BE:895:VAL:HG21	1.92	0.51
34:5E:373:ILE:HG13	34:5E:378:PHE:HZ	1.76	0.51
42:RD:1537:PHE:HA	42:RD:1540:ALA:HB3	1.92	0.51
50:RO:356:ALA:HA	50:RO:499:LEU:HD22	1.91	0.51
52:RS:229:LEU:HD11	52:RS:233:PHE:HD2	1.74	0.51
2:5A:426:G:C2	2:5A:428:A:H5"	2.46	0.51
8:SP:42:VAL:O	8:SP:42:VAL:HG13	2.10	0.51
10:ST:67:GLU:HA	10:ST:70:VAL:HG12	1.91	0.51
15:3E:3:TYR:N	15:3E:21:LYS:O	2.43	0.51
24:AG:736:THR:HG23	24:AG:738:ASN:H	1.74	0.51
25:B1:588:ASP:OD1	25:B1:588:ASP:N	2.43	0.51
29:BE:370:SER:OG	29:BE:372:ASP:OD1	2.20	0.51
47:RJ:72:VAL:HG22	47:RJ:137:LEU:HB3	1.91	0.51
50:RO:200:ASN:ND2	50:RO:256:ASN:O	2.43	0.51
1:3A:93:U:OP2	15:3E:302:HIS:ND1	2.42	0.51
6:SN:48:SER:O	6:SN:52:LEU:HB2	2.10	0.51
10:ST:120:ARG:NH2	34:5E:341:LEU:O	2.44	0.51
13:3C:94:ALA:HB3	13:3C:166:PRO:HG3	1.92	0.51
19:A5:439:VAL:HG11	50:RO:300:THR:HG21	1.92	0.51
26:B2:362:ILE:HG12	26:B2:385:ILE:HB	1.91	0.51
27:B3:658:LYS:NZ	27:B3:658:LYS:CB	2.74	0.51
38:5I:122:ARG:HB2	38:5I:192:SER:HB3	1.93	0.51
38:5I:327:LYS:HG2	38:5I:350:HIS:H	1.76	0.51
41:RC:52:TYR:CE1	41:RC:56:ILE:HG12	2.45	0.51
43:RE:379:MET:O	43:RE:384:SER:OG	2.29	0.51
43:RE:584:GLU:HG3	43:RE:614:ARG:HB2	1.93	0.51
45:RG:150:ILE:HD11	45:RG:160:LEU:HD23	1.92	0.51
49:RN:661:ILE:HG22	49:RN:665:GLN:HG3	1.92	0.51
50:RO:214:LYS:O	50:RO:268:GLN:NE2	2.43	0.51
2:5A:7:A:N7	24:AG:578:ASN:ND2	2.55	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5A:293:U:H3	25:B1:632:SER:HB3	1.75	0.51
2:5A:473:A:H5"	32:5C:164:GLN:HE22	1.76	0.51
3:SA:-5:G:N1	32:5C:39:ASP:OD1	2.36	0.51
3:SA:29:U:H2'	3:SA:30:G:H8	1.74	0.51
16:3F:136:PHE:HE1	16:3F:484:SER:HB2	1.74	0.51
22:AE:558:VAL:HG13	22:AE:615:ASN:HA	1.93	0.51
22:AE:586:LEU:O	22:AE:590:ALA:CB	2.58	0.51
23:AF:258:LEU:HD22	23:AF:272:LEU:HD21	1.93	0.51
24:AG:877:ASP:N	24:AG:877:ASP:OD1	2.43	0.51
25:B1:273:ARG:NH1	29:BE:763:SER:O	2.43	0.51
26:B2:759:GLY:HA3	26:B2:805:ILE:HD11	1.91	0.51
30:B6:296:SER:HB3	30:B6:300:MET:HB2	1.91	0.51
1:3A:319:G:OP1	13:3C:122:ARG:NH2	2.44	0.51
14:3D:26:ASP:OD1	38:5I:98:SER:OG	2.29	0.51
18:A4:481:ILE:HB	18:A4:485:LYS:HB2	1.91	0.51
21:A9:471:LYS:HZ3	21:A9:474:HIS:H	1.59	0.51
23:AF:399:GLU:O	23:AF:403:ASN:ND2	2.42	0.51
24:AG:434:GLN:OE1	24:AG:434:GLN:N	2.44	0.51
25:B1:329:VAL:HG13	25:B1:338:ILE:HB	1.92	0.51
26:B2:562:SER:HB2	26:B2:564:LYS:HB2	1.93	0.51
28:B8:512:ASP:O	33:5D:248:ARG:NH1	2.42	0.51
38:5I:54:PHE:O	38:5I:382:ARG:NH2	2.44	0.51
43:RE:858:ARG:HD2	43:RE:861:ILE:HD11	1.93	0.51
46:RI:107:ARG:HB3	46:RI:138:VAL:HG13	1.93	0.51
47:RJ:776:GLN:NE2	47:RJ:781:GLU:OE2	2.40	0.51
52:RS:263:THR:HA	52:RS:266:PHE:HB2	1.93	0.51
13:3B:111:MET:HB2	13:3B:186:ASP:HB3	1.92	0.51
15:3E:355:ASN:HB2	15:3E:401:LEU:HD13	1.93	0.51
16:3F:284:LEU:O	16:3F:548:ARG:NH2	2.38	0.51
17:3H:44:LEU:HD22	17:3H:52:ILE:HD12	1.90	0.51
24:AG:325:GLN:NE2	24:AG:328:THR:OG1	2.41	0.51
27:B3:110:ALA:HB2	27:B3:117:LEU:HD12	1.92	0.51
38:5I:329:ILE:HG22	38:5I:351:VAL:HG11	1.93	0.51
1:3A:59:G:H5'	25:B1:570:THR:HG23	1.92	0.51
2:5A:427:A:H2'	2:5A:428:A:H4'	1.93	0.51
3:SA:630:A:C5	3:SA:970:A:N7	2.79	0.51
3:SA:976:G:N2	3:SA:978:A:C6	2.79	0.51
28:B8:321:MET:HE1	28:B8:375:VAL:HG21	1.93	0.51
32:5C:74:LEU:HD23	32:5C:404:PRO:HG2	1.93	0.51
32:5C:434:LEU:HD11	35:5F:12:LEU:HD23	1.93	0.51
43:RE:111:LEU:HA	43:RE:114:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:RI:173:PRO:HA	46:RI:176:VAL:HG12	1.93	0.51
3:SA:910:C:H2'	3:SA:911:U:H6	1.76	0.51
3:SA:978:A:H5"	3:SA:979:A:H5'	1.92	0.51
3:SA:1194:A:OP2	3:SA:1195:C:N4	2.40	0.51
13:3B:91:HIS:HD2	13:3B:93:HIS:H	1.57	0.51
13:3B:142:ARG:NH2	13:3B:182:SER:OG	2.44	0.51
24:AG:855:LEU:HD23	28:B8:477:LYS:HE3	1.93	0.51
25:B1:392:ALA:O	25:B1:404:SER:HA	2.10	0.51
27:B3:654:GLU:OE1	27:B3:654:GLU:HA	2.10	0.51
32:5C:91:ILE:HG23	38:5I:3:ILE:HD11	1.92	0.51
39:5J:120:ASP:HB2	39:5J:173:ILE:HD12	1.92	0.51
47:RJ:776:GLN:HA	47:RJ:780:ILE:HG22	1.93	0.51
3:SA:886:U:H2'	3:SA:887:A:H8	1.75	0.50
13:3C:223:ASP:OD2	13:3C:225:ARG:NH1	2.44	0.50
20:A8:570:LEU:HD21	20:A8:637:LEU:HD21	1.91	0.50
24:AG:668:THR:OG1	24:AG:669:ASN:OD1	2.29	0.50
25:B1:732:GLU:HG2	25:B1:734:GLN:HE22	1.76	0.50
27:B3:658:LYS:HB2	27:B3:658:LYS:HZ3	1.75	0.50
45:RH:178:VAL:HG12	45:RH:223:GLU:HB2	1.93	0.50
46:RI:84:ARG:NH1	46:RI:100:ILE:O	2.42	0.50
48:RK:214:LYS:O	48:RK:217:LYS:NZ	2.40	0.50
3:SA:1499:G:N2	46:RI:194:ASP:OD2	2.44	0.50
4:SG:118:LEU:HG	4:SG:129:PRO:HB2	1.92	0.50
6:SN:93:ASP:HB3	6:SN:96:GLN:HG3	1.93	0.50
13:3C:171:LEU:HD23	13:3C:240:VAL:HG12	1.92	0.50
26:B2:627:SER:OG	26:B2:628:HIS:N	2.45	0.50
29:BE:135:ASN:ND2	29:BE:165:GLY:O	2.42	0.50
35:5F:86:GLY:HA3	35:5F:109:ARG:HD2	1.93	0.50
43:RE:765:LEU:HD21	43:RE:917:LYS:HB2	1.92	0.50
48:RK:183:ILE:HG22	48:RK:351:ILE:HD13	1.93	0.50
53:RT:107:THR:O	53:RT:111:ASN:ND2	2.44	0.50
3:SA:1192:C:H1'	45:RG:131:PRO:HA	1.92	0.50
18:A4:382:VAL:HG11	18:A4:755:ILE:HG21	1.92	0.50
20:A8:248:LEU:HA	20:A8:264:SER:HA	1.92	0.50
20:A8:712:ASP:OD1	20:A8:712:ASP:N	2.39	0.50
22:AE:522:ARG:HH12	22:AE:561:PHE:HB2	1.76	0.50
27:B3:186:LEU:HD11	27:B3:230:LYS:HD3	1.93	0.50
27:B3:407:SER:OG	27:B3:409:ASP:OD1	2.26	0.50
34:5E:298:SER:OG	34:5E:299:SER:N	2.43	0.50
43:RE:401:LEU:HD11	43:RE:414:HIS:HB3	1.93	0.50
44:RF:105:SER:OG	44:RF:106:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SP:12:GLN:HE21	8:SP:78:ALA:HB2	1.76	0.50
23:AF:401:LEU:HB3	23:AF:434:ARG:HH22	1.77	0.50
24:AG:249:THR:HG22	24:AG:256:THR:HB	1.93	0.50
29:BE:810:ARG:NH2	53:RT:183:GLU:OE2	2.45	0.50
43:RE:219:PHE:CE2	43:RE:303:PHE:CD2	2.99	0.50
45:RG:150:ILE:HG12	45:RG:160:LEU:HB2	1.94	0.50
48:RK:65:ILE:HB	49:RN:112:VAL:HG12	1.93	0.50
52:RS:439:PHE:HA	52:RS:442:GLU:HG3	1.94	0.50
10:ST:49:LYS:HG3	10:ST:72:ILE:HD13	1.94	0.50
20:A8:671:ARG:NH1	21:A9:447:ASN:O	2.45	0.50
27:B3:618:ASN:ND2	27:B3:638:ASP:OD2	2.41	0.50
37:5H:496:GLN:HA	37:5H:499:GLN:HE21	1.75	0.50
41:RC:72:VAL:HG22	41:RC:81:THR:HG22	1.94	0.50
43:RE:186:ILE:HD11	43:RE:206:LEU:HB2	1.93	0.50
43:RE:214:PHE:HE2	43:RE:218:ASP:HB3	1.75	0.50
43:RE:426:ILE:HA	43:RE:429:LEU:HG	1.93	0.50
46:RI:211:GLU:O	46:RI:215:ASN:ND2	2.44	0.50
47:RJ:634:ARG:HD2	48:RK:185:ARG:HH21	1.77	0.50
2:5A:505:G:H2'	2:5A:506:G:C8	2.47	0.50
3:SA:1134:C:H1'	26:B2:610:SER:HB2	1.94	0.50
19:A5:115:ASN:ND2	19:A5:130:ASP:OD1	2.45	0.50
19:A5:192:SER:HB3	19:A5:207:GLU:HG3	1.93	0.50
24:AG:207:LEU:HG	24:AG:264:ILE:HD12	1.93	0.50
26:B2:90:ASP:N	26:B2:90:ASP:OD1	2.39	0.50
27:B3:115:THR:HA	27:B3:131:ILE:HG22	1.92	0.50
29:BE:587:ARG:HB3	29:BE:605:LEU:HD12	1.92	0.50
32:5C:37:THR:O	32:5C:43:ARG:NH2	2.45	0.50
38:5I:76:ASN:HA	38:5I:118:VAL:HG21	1.93	0.50
43:RE:253:GLN:NE2	43:RE:254:LEU:O	2.44	0.50
48:RK:114:PHE:O	48:RK:169:VAL:HA	2.12	0.50
15:3E:385:ASP:OD1	15:3E:385:ASP:N	2.42	0.50
19:A5:8:SER:OG	19:A5:293:ASN:ND2	2.43	0.50
23:AF:224:THR:O	23:AF:239:LEU:CB	2.57	0.50
24:AG:370:GLN:NE2	24:AG:384:SER:OG	2.44	0.50
26:B2:828:TYR:HA	26:B2:831:LYS:HG2	1.93	0.50
27:B3:42:ILE:HG22	27:B3:49:SER:HA	1.94	0.50
30:B6:297:ASP:OD1	30:B6:297:ASP:N	2.44	0.50
36:5G:153:THR:HG21	36:5G:266:LEU:HD21	1.93	0.50
41:RC:52:TYR:HE1	41:RC:56:ILE:CG2	2.25	0.50
41:RC:205:ILE:O	41:RC:209:LEU:HB2	2.12	0.50
45:RH:41:MET:HG3	45:RH:202:ILE:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:RJ:1069:VAL:HG11	47:RJ:1083:ILE:HD13	1.93	0.50
53:RT:216:ILE:O	53:RT:220:THR:OG1	2.28	0.50
15:3E:430:ASP:HA	29:BE:125:GLY:HA2	1.93	0.50
18:A4:415:LYS:NZ	18:A4:416:LEU:O	2.45	0.50
23:AF:378:LYS:NZ	28:B8:292:GLY:O	2.44	0.50
29:BE:225:THR:OG1	29:BE:227:THR:O	2.29	0.50
35:5F:174:ARG:NH2	47:RJ:1077:LEU:O	2.44	0.50
41:RC:195:HIS:HD2	41:RC:196:PRO:HD2	1.77	0.50
43:RE:887:ALA:O	43:RE:892:SER:OG	2.28	0.50
45:RH:41:MET:O	45:RH:110:LEU:HA	2.11	0.50
45:RH:228:SER:OG	45:RH:229:ASN:N	2.44	0.50
52:RS:322:LEU:HD21	52:RS:359:LEU:HD11	1.92	0.50
2:5A:20:C:H2'	2:5A:21:A:H8	1.77	0.50
3:SA:1588:G:H1	3:SA:1608:U:H3	1.60	0.50
18:A4:566:LEU:HD11	18:A4:584:VAL:HG21	1.94	0.50
19:A5:355:ASN:OD1	24:AG:479:ASN:ND2	2.44	0.50
20:A8:541:LEU:HA	20:A8:544:LEU:HD13	1.93	0.50
24:AG:80:GLN:NE2	24:AG:83:GLU:OE1	2.44	0.50
24:AG:139:GLU:HB3	24:AG:155:THR:HB	1.94	0.50
27:B3:160:ILE:HD13	27:B3:209:LEU:HD21	1.93	0.50
27:B3:484:GLU:O	42:RD:1642:GLU:CB	2.59	0.50
31:5B:173:ARG:HE	33:5D:146:PHE:HA	1.76	0.50
43:RE:753:ILE:HD13	43:RE:784:LEU:HB3	1.94	0.50
46:RI:233:GLY:O	46:RI:236:LYS:NZ	2.41	0.50
47:RJ:262:GLY:O	47:RJ:264:GLN:NE2	2.44	0.50
2:5A:484:G:O6	51:RQ:872:ARG:NH1	2.45	0.49
18:A4:156:LEU:HD22	18:A4:170:ILE:HD11	1.93	0.49
22:AE:306:LEU:HD22	22:AE:311:ASN:HA	1.94	0.49
23:AF:133:HIS:HB2	23:AF:139:ILE:HG13	1.94	0.49
24:AG:628:ASP:H	24:AG:658:GLU:HA	1.77	0.49
24:AG:736:THR:OG1	24:AG:737:ILE:N	2.45	0.49
25:B1:839:THR:HG22	29:BE:882:GLU:HG3	1.94	0.49
26:B2:817:LEU:HD11	26:B2:856:ASN:HD21	1.77	0.49
28:B8:410:ASP:OD1	28:B8:479:ASN:ND2	2.45	0.49
33:5D:149:GLU:HB3	33:5D:153:ASN:HA	1.94	0.49
41:RC:199:HIS:HA	41:RC:202:GLU:HG2	1.93	0.49
43:RE:162:PHE:HE2	43:RE:597:ARG:HB2	1.77	0.49
47:RJ:852:ARG:HD2	47:RJ:888:PRO:HG3	1.94	0.49
47:RJ:1094:TYR:HA	47:RJ:1097:LYS:HG2	1.94	0.49
3:SA:976:G:N2	3:SA:978:A:C5	2.81	0.49
22:AE:637:ILE:HA	22:AE:640:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B3:437:VAL:N	27:B3:457:ALA:O	2.44	0.49
28:B8:520:ASN:HB2	28:B8:533:ALA:HB3	1.94	0.49
13:3C:170:VAL:HG23	13:3C:194:VAL:HG13	1.93	0.49
16:3F:343:ASP:OD1	16:3F:343:ASP:N	2.46	0.49
18:A4:418:CYS:SG	18:A4:419:LYS:N	2.85	0.49
20:A8:533:PRO:HG2	24:AG:656:ASP:HA	1.94	0.49
22:AE:558:VAL:HG22	22:AE:615:ASN:HD22	1.76	0.49
23:AF:48:ASN:ND2	23:AF:111:TYR:OH	2.45	0.49
24:AG:584:PHE:HB3	24:AG:598:LYS:HB2	1.94	0.49
25:B1:406:SER:OG	25:B1:407:LEU:N	2.46	0.49
26:B2:102:VAL:HA	26:B2:118:ASN:HA	1.94	0.49
27:B3:672:TYR:HB3	27:B3:681:ALA:HB2	1.95	0.49
32:5C:183:GLU:HB3	40:5K:16:THR:HG22	1.94	0.49
36:5G:192:ASP:OD2	36:5G:227:ARG:NH2	2.37	0.49
43:RE:1081:ASN:H	43:RE:1084:THR:HB	1.77	0.49
45:RG:46:ALA:HA	45:RG:115:GLN:HG3	1.93	0.49
45:RH:38:THR:O	45:RH:40:ARG:NH1	2.45	0.49
47:RJ:138:VAL:HB	47:RJ:167:VAL:HG22	1.93	0.49
49:RN:623:ASP:O	49:RN:627:HIS:HB3	2.13	0.49
50:RO:327:MET:O	50:RO:331:ASN:HA	2.11	0.49
51:RQ:853:ASN:OD1	51:RQ:853:ASN:N	2.45	0.49
53:RT:182:ILE:HA	53:RT:233:ILE:O	2.12	0.49
2:5A:293:U:H2'	25:B1:631:ASN:HA	1.93	0.49
6:SN:28:LEU:HA	6:SN:31:VAL:HG12	1.94	0.49
17:3H:7:LYS:HB3	17:3H:65:LEU:HD11	1.95	0.49
17:3H:54:MET:O	17:3H:80:PHE:HA	2.12	0.49
18:A4:452:HIS:HB3	18:A4:463:THR:HG23	1.94	0.49
22:AE:387:LEU:HD21	22:AE:403:LEU:HD13	1.93	0.49
32:5C:84:PHE:HA	32:5C:369:MET:HA	1.95	0.49
44:RF:143:LYS:HD2	44:RF:147:LEU:HD23	1.94	0.49
46:RI:38:ILE:HA	46:RI:243:PHE:O	2.12	0.49
48:RK:180:MET:O	48:RK:181:HIS:ND1	2.45	0.49
53:RT:96:SER:HA	53:RT:139:LEU:O	2.12	0.49
2:5A:323:A:OP1	25:B1:191:ARG:NH2	2.46	0.49
3:SA:1665:U:O4	3:SA:1736:G:O6	2.29	0.49
6:SN:33:ARG:HH12	49:RN:272:ILE:HA	1.76	0.49
10:ST:111:ASP:OD1	10:ST:115:ARG:NH1	2.46	0.49
17:3H:52:ILE:HG22	17:3H:54:MET:SD	2.52	0.49
17:3H:54:MET:HB3	17:3H:64:LEU:HD13	1.93	0.49
18:A4:150:ASN:ND2	18:A4:198:ASP:OD1	2.37	0.49
26:B2:476:ILE:HD11	26:B2:490:THR:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B3:13:ASN:N	27:B3:13:ASN:ND2	2.60	0.49
29:BE:118:VAL:HA	29:BE:132:THR:HA	1.94	0.49
32:5C:456:SER:O	32:5C:456:SER:OG	2.28	0.49
45:RH:112:VAL:O	45:RH:124:VAL:HB	2.12	0.49
47:RJ:106:THR:HG23	47:RJ:355:TYR:HB3	1.94	0.49
48:RK:107:ALA:HB1	48:RK:170:VAL:HG21	1.94	0.49
1:3A:88:U:OP2	15:3E:338:LYS:NZ	2.41	0.49
13:3B:116:SER:OG	13:3B:120:GLU:OE1	2.28	0.49
15:3E:24:LYS:O	15:3E:28:LEU:CB	2.60	0.49
18:A4:389:ARG:HE	18:A4:404:MET:HB2	1.78	0.49
24:AG:116:VAL:O	24:AG:131:HIS:HA	2.13	0.49
25:B1:286:LEU:HD12	25:B1:295:ILE:HB	1.94	0.49
26:B2:291:GLU:HA	26:B2:294:ARG:HG2	1.94	0.49
26:B2:624:LEU:HD12	26:B2:629:ASN:HB2	1.93	0.49
31:5B:186:ASP:HA	31:5B:189:THR:HG22	1.94	0.49
43:RE:1080:LEU:HD22	43:RE:1085:ILE:HD11	1.93	0.49
47:RJ:777:ARG:O	47:RJ:778:GLN:NE2	2.46	0.49
2:5A:485:G:H4'	2:5A:486:U:H5'	1.94	0.49
3:SA:1718:G:H2'	3:SA:1719:A:H8	1.77	0.49
17:3G:105:ASN:HB3	17:3G:108:SER:HB2	1.94	0.49
18:A4:207:ASP:OD2	18:A4:209:ARG:NH1	2.37	0.49
26:B2:392:THR:HG21	26:B2:410:SER:HB3	1.93	0.49
26:B2:397:ILE:HD11	26:B2:405:LEU:HD21	1.94	0.49
29:BE:274:ILE:HG23	29:BE:286:VAL:HG22	1.94	0.49
29:BE:469:SER:HB3	29:BE:510:LEU:HD23	1.95	0.49
33:5D:111:ARG:HE	33:5D:212:LYS:HB2	1.77	0.49
38:5I:421:GLN:HG3	38:5I:425:LYS:HD2	1.95	0.49
46:RI:85:GLU:OE2	46:RI:89:LYS:NZ	2.43	0.49
47:RJ:309:PRO:HD2	47:RJ:353:LEU:HD22	1.95	0.49
49:RN:752:MET:HA	49:RN:755:ILE:HG12	1.93	0.49
52:RS:388:ASP:HA	52:RS:391:VAL:HG22	1.93	0.49
13:3B:269:ILE:O	13:3B:315:ILE:HA	2.13	0.49
16:3F:365:PRO:HB3	16:3F:397:PHE:HA	1.93	0.49
20:A8:305:VAL:HA	20:A8:311:VAL:HA	1.95	0.49
22:AE:482:SER:HB2	22:AE:484:LEU:HG	1.94	0.49
24:AG:31:ASN:HD21	24:AG:201:ILE:HB	1.78	0.49
24:AG:96:ILE:HG12	24:AG:108:THR:HG21	1.95	0.49
28:B8:233:LEU:HD11	28:B8:543:LEU:HD12	1.95	0.49
29:BE:173:LEU:HD13	29:BE:219:ASP:HA	1.95	0.49
29:BE:528:PHE:HZ	29:BE:570:ILE:HD11	1.78	0.49
38:5I:315:PRO:HG2	38:5I:360:SER:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RC:112:GLN:CG	41:RC:163:TYR:CE2	2.83	0.49
43:RE:146:LEU:HA	43:RE:149:VAL:HG22	1.93	0.49
46:RI:125:VAL:O	46:RI:151:PRO:HA	2.12	0.49
46:RI:155:ARG:NH1	46:RI:175:TYR:OH	2.46	0.49
47:RJ:176:LEU:HD12	47:RJ:183:LEU:HA	1.94	0.49
3:SA:992:A:OP2	3:SA:1011:G:N1	2.38	0.49
3:SA:1133:A:OP1	48:RK:231:ARG:NE	2.42	0.49
18:A4:424:ASP:N	18:A4:424:ASP:OD1	2.45	0.49
20:A8:561:LEU:HD13	20:A8:566:LEU:HD11	1.95	0.49
23:AF:428:ARG:HH21	24:AG:518:ASP:HB3	1.76	0.49
26:B2:440:PRO:HG3	26:B2:485:GLY:HA3	1.94	0.49
28:B8:462:GLY:HA2	28:B8:527:GLY:HA3	1.95	0.49
29:BE:902:ASN:HB3	29:BE:905:ILE:HG22	1.95	0.49
32:5C:340:LEU:O	32:5C:368:TYR:N	2.43	0.49
32:5C:508:VAL:HG12	41:RC:72:VAL:HB	1.95	0.49
38:5I:140:SER:OG	38:5I:141:ASP:N	2.44	0.49
40:5K:65:VAL:HG22	40:5K:152:ILE:HB	1.94	0.49
43:RE:132:TYR:HB2	43:RE:183:ILE:HG21	1.94	0.49
43:RE:936:LEU:HA	43:RE:939:ILE:HG22	1.94	0.49
45:RG:197:ASP:OD1	45:RG:197:ASP:N	2.45	0.49
46:RI:13:ALA:HA	46:RI:254:ILE:HG12	1.95	0.49
49:RN:600:LEU:HD21	49:RN:636:LEU:HD13	1.94	0.49
19:A5:149:ASN:HD21	19:A5:190:PRO:HB3	1.77	0.49
26:B2:549:SER:OG	26:B2:576:VAL:O	2.29	0.49
27:B3:194:ARG:HG3	27:B3:244:GLU:H	1.78	0.49
30:B6:63:VAL:HG13	30:B6:88:ILE:HD11	1.94	0.49
32:5C:492:GLY:HA2	32:5C:495:SER:HB2	1.94	0.49
40:5K:149:LYS:HD3	40:5K:170:ILE:HD11	1.95	0.49
43:RE:749:SER:OG	43:RE:787:GLU:OE2	2.22	0.49
43:RE:1102:LEU:HD12	43:RE:1230:MET:HB3	1.95	0.49
47:RJ:634:ARG:NH2	48:RK:186:PRO:O	2.42	0.49
49:RN:646:THR:HA	49:RN:649:THR:HG22	1.95	0.49
3:SA:919:A:H5'	8:SP:18:ARG:HH12	1.77	0.48
4:SG:219:ARG:NH2	45:RH:222:ASP:OD2	2.45	0.48
14:3D:297:HIS:NE2	14:3D:309:GLU:OE2	2.46	0.48
15:3E:164:ILE:HG12	15:3E:301:ALA:HA	1.93	0.48
16:3F:305:ARG:HG2	16:3F:317:ILE:HD13	1.94	0.48
23:AF:75:LYS:HD2	23:AF:111:TYR:HA	1.95	0.48
26:B2:643:ASP:HB3	26:B2:650:ILE:HD11	1.95	0.48
27:B3:454:LEU:HB3	27:B3:466:TRP:HB2	1.95	0.48
28:B8:148:THR:OG1	28:B8:152:GLU:OE2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:RE:151:SER:HA	43:RE:154:LYS:HB2	1.94	0.48
45:RG:190:GLN:HE22	45:RG:247:ASP:HB2	1.78	0.48
47:RJ:951:MET:SD	47:RJ:987:TYR:OH	2.63	0.48
49:RN:786:ASN:HA	49:RN:789:ASN:HB2	1.95	0.48
3:SA:1645:G:H2'	3:SA:1646:C:H6	1.78	0.48
17:3H:51:PHE:HE1	17:3H:114:ILE:HG23	1.78	0.48
18:A4:338:ALA:HB1	18:A4:361:LEU:HD11	1.95	0.48
25:B1:150:THR:OG1	25:B1:164:THR:OG1	2.31	0.48
26:B2:263:THR:HA	26:B2:269:THR:O	2.14	0.48
27:B3:305:VAL:HG12	27:B3:311:LEU:HG	1.95	0.48
28:B8:43:ASP:N	28:B8:43:ASP:OD1	2.40	0.48
28:B8:266:GLY:HA3	28:B8:295:ILE:HD11	1.95	0.48
29:BE:630:THR:N	29:BE:644:THR:O	2.44	0.48
38:5I:145:VAL:HB	38:5I:176:PHE:HB2	1.94	0.48
38:5I:260:GLN:NE2	38:5I:460:GLN:OE1	2.47	0.48
40:5K:67:ILE:HD11	40:5K:96:PRO:HB2	1.95	0.48
41:RC:52:TYR:CE1	41:RC:56:ILE:HG21	2.47	0.48
43:RE:125:GLU:OE2	43:RE:129:HIS:NE2	2.45	0.48
1:3A:64:A:OP2	29:BE:392:ARG:NH2	2.45	0.48
7:SO:49:GLN:HA	7:SO:52:VAL:HG12	1.94	0.48
19:A5:280:GLN:HB2	19:A5:288:LYS:HE2	1.95	0.48
23:AF:246:TYR:OH	23:AF:289:ASN:ND2	2.44	0.48
28:B8:458:ILE:HG13	28:B8:484:VAL:HG22	1.95	0.48
38:5I:283:ASP:OD2	38:5I:287:TYR:OH	2.30	0.48
41:RC:183:VAL:HA	41:RC:186:VAL:HG12	1.93	0.48
43:RE:1027:LEU:HD11	43:RE:1037:LEU:HB3	1.95	0.48
45:RH:69:ASN:HD22	45:RH:72:ASP:HB3	1.77	0.48
3:SA:1465:C:N3	36:5G:146:ARG:NH1	2.58	0.48
14:3D:225:ASP:OD1	14:3D:226:LYS:N	2.46	0.48
16:3F:421:ASN:HD22	16:3F:437:ARG:HA	1.78	0.48
22:AE:8:LEU:HD12	32:5C:144:LEU:HD23	1.96	0.48
25:B1:717:LEU:HD12	29:BE:578:VAL:HB	1.94	0.48
27:B3:290:ILE:HG12	27:B3:304:LEU:HD22	1.95	0.48
28:B8:183:ASP:OD1	29:BE:281:ARG:NH2	2.45	0.48
43:RE:704:PHE:CE2	43:RE:955:GLU:HB2	2.49	0.48
48:RK:103:MET:O	48:RK:107:ALA:HB2	2.13	0.48
3:SA:884:A:H2'	3:SA:885:G:C8	2.48	0.48
3:SA:925:G:C5'	42:RD:1611:ALA:CB	2.70	0.48
9:SR:58:ASP:OD1	9:SR:58:ASP:N	2.43	0.48
14:3D:160:ARG:NH2	15:3E:243:MET:O	2.43	0.48
16:3F:523:LYS:O	16:3F:541:ALA:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A4:579:ARG:NH2	18:A4:644:SER:OG	2.47	0.48
24:AG:771:ASP:OD1	24:AG:771:ASP:N	2.46	0.48
26:B2:118:ASN:OD1	26:B2:118:ASN:N	2.46	0.48
26:B2:214:ASP:OD1	26:B2:214:ASP:N	2.45	0.48
30:B6:16:ASP:OD2	32:5C:15:ARG:NH2	2.46	0.48
31:5B:155:ILE:HD12	31:5B:158:LYS:HE3	1.95	0.48
32:5C:112:GLY:HA3	32:5C:130:ARG:HB3	1.94	0.48
43:RE:395:ILE:HD11	43:RE:476:ILE:HG21	1.95	0.48
43:RE:975:LEU:HD12	43:RE:1041:VAL:HG23	1.95	0.48
47:RJ:298:VAL:HG23	47:RJ:791:ILE:HG23	1.94	0.48
49:RN:734:ARG:HA	49:RN:737:ILE:HG12	1.95	0.48
3:SA:954:G:H2'	3:SA:955:A:C8	2.49	0.48
3:SA:976:G:N3	3:SA:978:A:C5	2.82	0.48
3:SA:1658:G:C2	3:SA:1743:U:N1	2.81	0.48
7:SO:101:HIS:HA	7:SO:104:ARG:HH21	1.78	0.48
13:3C:170:VAL:HG12	13:3C:239:CYS:HB3	1.96	0.48
15:3E:214:ILE:HD11	15:3E:252:LEU:HD22	1.94	0.48
16:3F:448:PHE:HA	16:3F:451:ILE:HG22	1.95	0.48
22:AE:395:GLU:OE2	22:AE:397:LYS:NZ	2.44	0.48
23:AF:276:SER:OG	23:AF:278:ASP:OD1	2.30	0.48
26:B2:183:ASP:OD1	26:B2:183:ASP:N	2.42	0.48
29:BE:529:TYR:HA	29:BE:536:LEU:HA	1.95	0.48
46:RI:98:LYS:NZ	46:RI:121:ASP:OD1	2.38	0.48
51:RQ:322:ASN:N	51:RQ:322:ASN:OD1	2.46	0.48
3:SA:464:A:H2'	3:SA:465:G:H8	1.79	0.48
5:SK:136:VAL:HG12	5:SK:156:ILE:HG12	1.96	0.48
22:AE:329:THR:HG21	22:AE:365:ILE:HG21	1.95	0.48
24:AG:105:HIS:HB2	24:AG:122:LYS:HG3	1.95	0.48
24:AG:855:LEU:O	24:AG:859:ASN:HB2	2.13	0.48
25:B1:441:SER:O	25:B1:443:GLU:N	2.43	0.48
27:B3:557:VAL:HG22	27:B3:578:VAL:HG11	1.95	0.48
28:B8:183:ASP:HB2	29:BE:242:ARG:HA	1.96	0.48
43:RE:412:LEU:HD21	43:RE:424:GLY:HA3	1.96	0.48
45:RG:173:THR:OG1	45:RG:174:LYS:N	2.47	0.48
50:RO:153:ILE:HD13	50:RO:202:LEU:HD21	1.94	0.48
22:AE:336:LEU:HD22	22:AE:373:ILE:HG21	1.96	0.48
26:B2:414:LEU:HD11	26:B2:445:VAL:HG11	1.94	0.48
30:B6:273:ILE:HA	30:B6:276:VAL:HG22	1.95	0.48
30:B6:426:ASP:O	30:B6:430:TYR:N	2.47	0.48
43:RE:507:PHE:HA	43:RE:510:ILE:HG12	1.95	0.48
47:RJ:1105:ASP:N	47:RJ:1105:ASP:OD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:RO:447:ASP:OD1	50:RO:447:ASP:N	2.46	0.48
19:A5:335:ASN:O	19:A5:337:LYS:NZ	2.47	0.48
24:AG:249:THR:O	24:AG:257:ARG:NH1	2.41	0.48
43:RE:308:LEU:HG	43:RE:337:LEU:HD21	1.96	0.48
45:RG:232:LEU:HD21	45:RH:103:PRO:HG3	1.96	0.48
48:RK:130:ILE:HG23	48:RK:151:LEU:HD23	1.95	0.48
9:SR:120:ASP:OD1	9:SR:120:ASP:N	2.40	0.48
15:3E:207:ARG:HH11	15:3E:226:ILE:HG12	1.78	0.48
18:A4:171:SER:O	18:A4:171:SER:OG	2.32	0.48
18:A4:560:SER:OG	18:A4:561:LYS:N	2.47	0.48
18:A4:747:ILE:HD11	18:A4:753:ALA:HB2	1.96	0.48
20:A8:496:TYR:OH	24:AG:693:ASP:OD1	2.28	0.48
22:AE:376:GLU:H	22:AE:379:GLU:HG3	1.79	0.48
24:AG:141:LEU:HD11	24:AG:153:ILE:HD11	1.96	0.48
24:AG:498:LEU:HA	24:AG:508:ILE:O	2.14	0.48
25:B1:205:LYS:HG2	25:B1:219:GLU:HG2	1.96	0.48
32:5C:133:HIS:HE1	32:5C:147:GLU:HG3	1.79	0.48
43:RE:316:ARG:HH22	43:RE:552:ARG:HD3	1.78	0.48
43:RE:417:SER:OG	43:RE:420:GLN:OE1	2.32	0.48
3:SA:1645:G:H2'	3:SA:1646:C:C6	2.49	0.47
15:3E:225:GLU:HG2	15:3E:226:ILE:HG13	1.96	0.47
19:A5:460:ARG:HA	19:A5:465:ILE:HD11	1.96	0.47
24:AG:440:VAL:HG11	24:AG:449:LEU:HD12	1.95	0.47
26:B2:9:GLU:O	26:B2:684:TRP:HA	2.14	0.47
26:B2:54:ILE:CD1	26:B2:364:TYR:HD2	2.27	0.47
27:B3:22:VAL:HG22	27:B3:67:LEU:HD11	1.96	0.47
32:5C:137:MET:HA	32:5C:144:LEU:HA	1.96	0.47
35:5F:152:ARG:NH1	36:5G:11:GLU:OE2	2.46	0.47
23:AF:135:GLN:HE22	23:AF:178:PRO:HA	1.79	0.47
25:B1:150:THR:N	25:B1:164:THR:O	2.45	0.47
26:B2:479:LEU:HA	26:B2:489:VAL:O	2.14	0.47
43:RE:219:PHE:CZ	43:RE:303:PHE:CE2	3.02	0.47
3:SA:1658:G:N1	3:SA:1742:U:N3	2.62	0.47
4:SG:52:GLU:OE2	4:SG:54:LYS:NZ	2.48	0.47
5:SK:87:SER:OG	5:SK:89:ASP:OD1	2.32	0.47
18:A4:157:SER:OG	18:A4:195:TRP:NE1	2.47	0.47
22:AE:484:LEU:HD13	22:AE:663:SER:HB3	1.95	0.47
23:AF:420:GLU:O	23:AF:424:ARG:CB	2.61	0.47
23:AF:435:ASP:OD1	23:AF:435:ASP:N	2.45	0.47
26:B2:676:SER:OG	26:B2:678:ASP:OD1	2.22	0.47
29:BE:363:SER:O	29:BE:363:SER:OG	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:RH:153:VAL:HA	49:RN:716:LYS:HB2	1.96	0.47
46:RI:105:ASN:HA	46:RI:108:ARG:HB3	1.96	0.47
47:RJ:80:THR:O	57:RJ:1201:GTP:O2B	2.31	0.47
48:RK:282:GLU:O	48:RK:286:SER:HB3	2.14	0.47
2:5A:201:U:H2'	2:5A:202:U:H6	1.78	0.47
3:SA:1179:G:H3'	10:ST:127:HIS:HB2	1.96	0.47
3:SA:1511:U:H2'	3:SA:1512:G:C8	2.49	0.47
3:SA:1760:G:H5'	3:SA:1761:U:H5'	1.96	0.47
15:3E:355:ASN:HA	15:3E:358:LYS:HB2	1.97	0.47
18:A4:534:LEU:HB3	18:A4:543:ILE:HG22	1.95	0.47
18:A4:744:VAL:HA	18:A4:753:ALA:O	2.14	0.47
19:A5:25:ASP:OD2	28:B8:590:LYS:NZ	2.37	0.47
24:AG:581:GLY:HA2	24:AG:602:PRO:HD2	1.97	0.47
25:B1:537:GLY:HA3	25:B1:556:ARG:HB3	1.96	0.47
27:B3:432:GLY:O	27:B3:464:LYS:NZ	2.41	0.47
40:5K:152:ILE:HG12	40:5K:171:PRO:HG2	1.95	0.47
41:RC:195:HIS:CD2	41:RC:196:PRO:HD2	2.50	0.47
43:RE:940:LYS:HG3	43:RE:975:LEU:HD21	1.96	0.47
47:RJ:631:ILE:HG13	47:RJ:634:ARG:HB2	1.97	0.47
50:RO:507:LEU:HA	50:RO:510:GLU:HB3	1.95	0.47
51:RQ:341:LYS:HA	51:RQ:344:GLN:HE21	1.79	0.47
51:RQ:835:VAL:HG13	51:RQ:837:LYS:HG3	1.96	0.47
2:5A:116:U:H3	2:5A:130:G:H1	1.61	0.47
3:SA:941:A:C2	3:SA:976:G:O3'	2.67	0.47
18:A4:284:LEU:HD21	31:5B:206:LEU:HD21	1.95	0.47
18:A4:511:VAL:HA	18:A4:558:ARG:HB3	1.96	0.47
22:AE:141:ASN:ND2	22:AE:206:TYR:OH	2.46	0.47
26:B2:530:LEU:HD13	26:B2:550:LEU:HD11	1.94	0.47
30:B6:14:GLU:OE2	30:B6:91:ARG:NH2	2.38	0.47
32:5C:450:GLY:O	51:RQ:857:TYR:OH	2.21	0.47
34:5E:452:SER:O	34:5E:452:SER:OG	2.29	0.47
43:RE:168:ILE:O	43:RE:172:THR:OG1	2.28	0.47
43:RE:177:ASN:HB2	43:RE:213:LEU:HB2	1.96	0.47
47:RJ:92:ARG:HH21	47:RJ:221:LEU:HG	1.79	0.47
50:RO:198:GLU:O	50:RO:202:LEU:HB2	2.13	0.47
13:3C:173:LEU:HA	13:3C:197:VAL:HG13	1.97	0.47
26:B2:235:ASN:ND2	26:B2:240:GLY:O	2.40	0.47
44:RF:55:LEU:HB3	44:RF:124:ALA:HB3	1.96	0.47
47:RJ:111:LYS:O	47:RJ:310:THR:OG1	2.32	0.47
47:RJ:879:THR:OG1	47:RJ:880:TYR:N	2.48	0.47
3:SA:1512:G:O6	46:RI:145:HIS:NE2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1677:C:H2'	3:SA:1678:A:C8	2.50	0.47
3:SA:1677:C:H2'	3:SA:1678:A:H8	1.80	0.47
15:3E:262:ILE:HA	15:3E:265:PHE:HB2	1.96	0.47
18:A4:97:ARG:NE	31:5B:191:PRO:O	2.39	0.47
19:A5:473:LYS:HE3	19:A5:475:ALA:HB3	1.96	0.47
23:AF:31:THR:OG1	23:AF:32:SER:N	2.46	0.47
25:B1:165:SER:OG	25:B1:166:LYS:N	2.48	0.47
26:B2:137:ILE:HG22	26:B2:147:VAL:HG22	1.97	0.47
28:B8:238:LEU:HD11	28:B8:590:LYS:HB2	1.97	0.47
28:B8:568:VAL:HG23	28:B8:579:VAL:HG22	1.96	0.47
29:BE:207:ASP:N	29:BE:207:ASP:OD1	2.47	0.47
32:5C:333:SER:HB3	32:5C:381:LEU:HD11	1.95	0.47
33:5D:25:TYR:HD1	39:5J:213:ARG:HE	1.62	0.47
37:5H:434:PHE:H	45:RH:129:ARG:HH22	1.63	0.47
38:5I:201:ILE:HD12	38:5I:225:LEU:HD21	1.97	0.47
43:RE:123:LYS:HE2	43:RE:123:LYS:HB3	1.77	0.47
52:RS:379:LYS:HA	52:RS:379:LYS:HD3	1.73	0.47
2:5A:207:G:H2'	2:5A:208:A:H8	1.79	0.47
8:SP:16:VAL:O	8:SP:30:VAL:HA	2.14	0.47
10:ST:2:SER:O	10:ST:2:SER:OG	2.32	0.47
22:AE:136:LEU:HD21	22:AE:155:ILE:HG12	1.97	0.47
24:AG:22:LEU:HD12	24:AG:32:LYS:HB2	1.97	0.47
24:AG:175:ALA:O	24:AG:187:VAL:HA	2.15	0.47
25:B1:156:GLN:HB2	25:B1:203:GLN:HE21	1.79	0.47
26:B2:23:CYS:HG	26:B2:340:SER:HG	1.61	0.47
26:B2:201:ILE:HD12	27:B3:660:LYS:HA	1.97	0.47
29:BE:430:ILE:HD11	29:BE:445:MET:HB2	1.97	0.47
49:RN:451:THR:O	49:RN:455:LEU:HB2	2.15	0.47
52:RS:258:VAL:HA	52:RS:261:GLU:HG2	1.97	0.47
15:3E:176:GLU:HA	15:3E:179:THR:HG22	1.97	0.47
26:B2:367:ILE:HD12	26:B2:368:PRO:HD2	1.97	0.47
26:B2:393:ASP:OD1	26:B2:393:ASP:N	2.46	0.47
26:B2:588:ILE:HG12	26:B2:600:TRP:HB2	1.97	0.47
34:5E:383:ARG:NH2	36:5G:212:ALA:O	2.48	0.47
47:RJ:347:LEU:O	47:RJ:352:LYS:NZ	2.48	0.47
50:RO:504:ASP:OD1	50:RO:504:ASP:N	2.48	0.47
2:5A:69:U:O4	2:5A:70:A:N6	2.48	0.47
3:SA:545:A:OP2	37:5H:542:TYR:OH	2.33	0.47
3:SA:1228:G:H22	6:SN:119:SER:HB2	1.79	0.47
9:SR:50:GLU:OE2	9:SR:82:ARG:NH2	2.47	0.47
25:B1:29:LEU:HD22	25:B1:42:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B1:32:PRO:HG3	25:B1:61:ILE:HG13	1.97	0.47
25:B1:115:SER:O	25:B1:115:SER:OG	2.33	0.47
29:BE:170:LEU:HG	29:BE:180:LEU:HD21	1.97	0.47
35:5F:153:ASN:HB3	36:5G:4:ARG:HH22	1.80	0.47
36:5G:173:ARG:HH21	36:5G:250:VAL:HG23	1.80	0.47
47:RJ:819:GLU:O	47:RJ:852:ARG:NH2	2.47	0.47
2:5A:90:G:O2'	2:5A:91:U:O4'	2.25	0.46
2:5A:414:G:N1	2:5A:442:U:O2	2.48	0.46
2:5A:485:G:H2'	14:3D:22:LEU:HD21	1.97	0.46
9:SR:113:ASP:N	9:SR:113:ASP:OD1	2.48	0.46
19:A5:366:GLY:O	24:AG:583:LYS:NZ	2.48	0.46
24:AG:446:ASN:OD1	24:AG:446:ASN:N	2.46	0.46
24:AG:530:LYS:HG2	24:AG:546:LYS:HB3	1.97	0.46
26:B2:123:ALA:HB3	26:B2:141:LYS:CD	2.45	0.46
43:RE:242:LEU:HA	43:RE:245:LYS:HG3	1.97	0.46
49:RN:510:THR:HB	49:RN:518:ILE:HD13	1.96	0.46
2:5A:446:U:H5'	47:RJ:1118:THR:HB	1.96	0.46
8:SP:91:THR:HG22	8:SP:93:THR:HG22	1.98	0.46
15:3E:191:HIS:HD2	15:3E:246:GLU:HA	1.80	0.46
22:AE:509:SER:HA	22:AE:512:LEU:HD12	1.98	0.46
24:AG:43:ASN:OD1	24:AG:43:ASN:N	2.48	0.46
24:AG:443:ASN:ND2	24:AG:446:ASN:OD1	2.48	0.46
26:B2:63:LEU:HD21	26:B2:106:TRP:CD2	2.50	0.46
31:5B:173:ARG:NH2	33:5D:144:ASN:O	2.48	0.46
43:RE:203:ILE:HG22	43:RE:292:ILE:HA	1.97	0.46
44:RF:43:GLN:HG2	44:RF:51:ASP:HA	1.97	0.46
2:5A:116:U:O2	2:5A:130:G:N2	2.43	0.46
2:5A:396:A:H62	36:5G:11:GLU:HG2	1.81	0.46
5:SK:37:LYS:HB3	5:SK:37:LYS:HE2	1.76	0.46
7:SO:93:LYS:HA	7:SO:96:VAL:HG12	1.97	0.46
18:A4:214:SER:OG	18:A4:221:ASN:O	2.28	0.46
18:A4:418:CYS:HB2	18:A4:460:LEU:HB2	1.97	0.46
22:AE:374:ARG:NH1	22:AE:375:LEU:O	2.48	0.46
24:AG:204:ASN:OD1	24:AG:204:ASN:N	2.47	0.46
24:AG:435:ASP:HB2	24:AG:702:TYR:HD1	1.75	0.46
39:5J:110:ASP:OD1	39:5J:110:ASP:N	2.36	0.46
43:RE:269:ARG:HA	43:RE:292:ILE:O	2.15	0.46
48:RK:282:GLU:O	48:RK:286:SER:CB	2.64	0.46
49:RN:56:ASN:HD21	49:RN:59:GLU:HG3	1.81	0.46
2:5A:18:G:H2'	2:5A:19:A:C8	2.50	0.46
2:5A:128:C:H5"	2:5A:129:U:H4'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5A:188:A:H61	2:5A:209:G:H1	1.63	0.46
3:SA:1673:G:N1	3:SA:1728:A:N6	2.50	0.46
18:A4:326:ARG:NH2	18:A4:364:PHE:O	2.49	0.46
18:A4:742:LEU:HD12	18:A4:757:ARG:HG3	1.96	0.46
23:AF:436:GLU:HG2	23:AF:480:LEU:HD23	1.98	0.46
30:B6:185:TYR:HE2	51:RQ:338:LEU:HD21	1.81	0.46
38:5I:280:ALA:HB2	38:5I:311:VAL:HB	1.97	0.46
45:RH:152:SER:OG	45:RH:155:SER:N	2.49	0.46
48:RK:104:LEU:O	48:RK:300:TYR:OH	2.33	0.46
50:RO:202:LEU:HD23	50:RO:208:TYR:HB3	1.98	0.46
2:5A:86:C:N4	24:AG:482:GLY:O	2.45	0.46
3:SA:925:G:H4'	42:RD:1611:ALA:CA	2.46	0.46
13:3C:194:VAL:HB	13:3C:217:ILE:HD13	1.97	0.46
13:3C:308:PRO:HG3	33:5D:129:SER:HA	1.96	0.46
16:3F:417:SER:HB3	16:3F:421:ASN:HB2	1.97	0.46
17:3G:57:ASP:HB3	17:3G:84:ARG:HG2	1.97	0.46
22:AE:568:ILE:HD11	22:AE:673:ASN:HD21	1.80	0.46
28:B8:472:GLN:NE2	28:B8:474:SER:OG	2.49	0.46
43:RE:1108:LEU:O	43:RE:1112:CYS:CB	2.61	0.46
46:RI:20:LEU:HD11	46:RI:245:LYS:HA	1.97	0.46
46:RI:55:ARG:HD2	46:RI:191:PRO:HD3	1.98	0.46
47:RJ:853:ARG:HE	47:RJ:853:ARG:HB2	1.61	0.46
48:RK:199:ARG:HB2	48:RK:239:PRO:HA	1.97	0.46
48:RK:337:VAL:HG23	48:RK:354:ILE:HG12	1.98	0.46
52:RS:270:LEU:HB3	52:RS:278:PHE:HZ	1.80	0.46
52:RS:271:THR:OG1	52:RS:274:GLU:OE1	2.31	0.46
1:3A:306:G:H2'	1:3A:307:G:H8	1.80	0.46
3:SA:1160:A:H2'	3:SA:1161:C:H6	1.80	0.46
3:SA:1276:U:H3	3:SA:1434:U:H3	1.64	0.46
14:3D:175:ILE:HD12	14:3D:317:SER:HA	1.98	0.46
19:A5:66:VAL:HG12	19:A5:112:LEU:HD21	1.97	0.46
19:A5:85:ILE:HB	19:A5:99:PHE:HB2	1.98	0.46
24:AG:212:CYS:HB2	24:AG:224:SER:HB3	1.98	0.46
26:B2:341:ALA:HB1	26:B2:353:LEU:HD11	1.96	0.46
28:B8:278:ASP:N	28:B8:278:ASP:OD1	2.46	0.46
43:RE:223:ARG:HA	43:RE:226:HIS:HB2	1.97	0.46
43:RE:1224:ALA:O	43:RE:1228:ASN:CB	2.60	0.46
45:RG:55:ILE:O	45:RG:64:LYS:HB2	2.16	0.46
50:RO:462:SER:OG	50:RO:463:LEU:N	2.48	0.46
52:RS:392:TYR:HA	52:RS:395:MET:HB2	1.96	0.46
1:3A:56:A:O2'	33:5D:63:TYR:OH	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A8:647:LEU:HG	21:A9:509:GLN:HE22	1.79	0.46
26:B2:542:ASP:N	26:B2:542:ASP:OD1	2.45	0.46
28:B8:512:ASP:OD1	28:B8:512:ASP:N	2.48	0.46
29:BE:323:VAL:HB	29:BE:343:LEU:HD22	1.98	0.46
29:BE:351:GLN:HG3	29:BE:372:ASP:HB3	1.97	0.46
43:RE:228:ARG:HG3	43:RE:296:ILE:HG12	1.98	0.46
44:RF:17:PRO:HA	44:RF:35:HIS:O	2.15	0.46
46:RI:59:LEU:HD22	46:RI:215:ASN:HB2	1.97	0.46
49:RN:547:VAL:HA	49:RN:550:VAL:HG12	1.97	0.46
50:RO:366:LEU:HD13	50:RO:405:LEU:HD11	1.96	0.46
52:RS:413:LEU:O	52:RS:418:HIS:NE2	2.49	0.46
1:3A:36:C:O2'	38:5I:389:ARG:NH1	2.48	0.46
3:SA:1111:G:C8	47:RJ:1162:ALA:HA	2.51	0.46
3:SA:1273:G:H1	3:SA:1437:U:H2'	1.80	0.46
18:A4:164:THR:HG22	18:A4:185:ARG:HG2	1.98	0.46
22:AE:583:LYS:HE2	22:AE:627:LEU:HA	1.98	0.46
25:B1:557:LYS:NZ	29:BE:426:GLU:OE1	2.44	0.46
27:B3:440:VAL:HG12	27:B3:456:THR:HA	1.97	0.46
29:BE:420:GLU:HG2	29:BE:470:GLN:HA	1.97	0.46
31:5B:211:LEU:HD13	31:5B:213:LYS:HE3	1.96	0.46
41:RC:44:LEU:HA	41:RC:79:SER:HA	1.97	0.46
49:RN:554:GLN:HE21	49:RN:559:ARG:H	1.63	0.46
52:RS:359:LEU:HB2	52:RS:372:ILE:HD11	1.97	0.46
2:5A:426:G:H21	2:5A:428:A:H8	1.64	0.46
2:5A:486:U:H4'	2:5A:487:A:H5"	1.98	0.46
14:3D:371:ASN:OD1	14:3D:374:ARG:NH1	2.48	0.46
15:3E:381:ASP:OD1	15:3E:381:ASP:N	2.49	0.46
25:B1:280:THR:HA	25:B1:304:PRO:HB3	1.98	0.46
28:B8:306:ASN:OD1	28:B8:306:ASN:N	2.43	0.46
32:5C:335:GLY:HA2	32:5C:377:LYS:HG3	1.98	0.46
38:5I:255:THR:HG22	51:RQ:288:TYR:HD1	1.81	0.46
43:RE:243:LEU:HD13	43:RE:248:LEU:HG	1.96	0.46
45:RG:112:VAL:HB	45:RG:124:VAL:HG22	1.97	0.46
3:SA:1542:G:H2'	3:SA:1543:A:C4	2.51	0.46
19:A5:452:LEU:HA	19:A5:455:THR:HG22	1.98	0.46
20:A8:374:SER:HA	20:A8:408:LEU:HA	1.97	0.46
23:AF:69:ARG:HG3	23:AF:70:THR:HG23	1.97	0.46
26:B2:220:THR:HG22	26:B2:259:ILE:HD11	1.96	0.46
26:B2:360:ASN:OD1	26:B2:360:ASN:N	2.47	0.46
27:B3:85:LEU:HD23	27:B3:95:VAL:HG11	1.98	0.46
27:B3:584:ILE:HD11	27:B3:599:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:5G:76:GLU:HG2	36:5G:160:GLY:HA2	1.98	0.46
38:5I:288:TYR:O	38:5I:298:LEU:N	2.42	0.46
40:5K:83:VAL:HG12	40:5K:96:PRO:HG3	1.98	0.46
41:RC:112:GLN:NE2	41:RC:163:TYR:CE2	2.80	0.46
43:RE:188:SER:HB2	43:RE:367:ARG:HH12	1.81	0.46
50:RO:395:ILE:HG23	50:RO:469:LEU:HD21	1.98	0.46
52:RS:280:ASN:ND2	52:RS:320:GLY:O	2.46	0.46
8:SP:44:GLY:O	8:SP:46:MET:N	2.50	0.45
8:SP:85:ALA:H	8:SP:119:THR:HB	1.81	0.45
11:SY:113:ALA:HB3	11:SY:116:ASP:HB2	1.96	0.45
14:3D:195:VAL:HG12	14:3D:216:PHE:HE2	1.81	0.45
14:3D:379:LEU:HD13	14:3D:408:VAL:HG21	1.98	0.45
18:A4:545:ARG:HG3	18:A4:549:VAL:HB	1.98	0.45
22:AE:495:LEU:HA	22:AE:498:PHE:HB2	1.97	0.45
24:AG:726:GLN:NE2	24:AG:736:THR:O	2.42	0.45
29:BE:640:LEU:HD23	29:BE:655:THR:HG22	1.98	0.45
35:5F:95:SER:OG	36:5G:59:ASP:OD2	2.32	0.45
38:5I:94:TYR:OH	38:5I:134:ASN:ND2	2.41	0.45
38:5I:281:ASN:ND2	38:5I:283:ASP:OD1	2.49	0.45
43:RE:205:THR:HG22	43:RE:295:LEU:HD23	1.97	0.45
45:RG:143:GLN:HE22	45:RG:149:SER:HA	1.81	0.45
2:5A:192:G:H21	33:5D:155:THR:HG21	1.81	0.45
3:SA:891:A:H2'	3:SA:892:A:H8	1.82	0.45
3:SA:910:C:H2'	3:SA:911:U:C6	2.50	0.45
3:SA:976:G:C2	3:SA:978:A:C4	3.03	0.45
3:SA:993:A:H62	3:SA:1011:G:N2	2.14	0.45
3:SA:1228:G:N2	6:SN:118:ALA:O	2.49	0.45
4:SG:39:GLU:OE2	4:SG:47:SER:OG	2.33	0.45
15:3E:392:ALA:O	15:3E:396:ASN:ND2	2.49	0.45
18:A4:444:ARG:HG3	18:A4:446:SER:H	1.81	0.45
19:A5:539:ARG:NH1	24:AG:524:ASP:OD2	2.49	0.45
26:B2:760:ILE:HD11	26:B2:835:PHE:HB2	1.98	0.45
27:B3:561:SER:O	27:B3:566:SER:N	2.49	0.45
30:B6:186:VAL:HG12	30:B6:273:ILE:HG13	1.98	0.45
31:5B:200:ARG:O	31:5B:204:ARG:HB3	2.15	0.45
33:5D:48:LEU:HG	47:RJ:1067:LEU:HD11	1.99	0.45
38:5I:306:SER:HB3	38:5I:326:ASP:H	1.82	0.45
43:RE:557:THR:HG23	43:RE:560:ASN:H	1.81	0.45
45:RG:227:LEU:HA	45:RG:227:LEU:HD23	1.79	0.45
49:RN:495:ASN:HD22	49:RN:617:HIS:HB2	1.80	0.45
2:5A:102:A:H61	23:AF:415:LEU:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:1463:C:H4'	49:RN:63:ALA:HB1	1.98	0.45
13:3B:261:LEU:O	14:3D:129:ARG:NH1	2.49	0.45
23:AF:171:VAL:HG22	23:AF:188:SER:HB3	1.99	0.45
24:AG:253:SER:O	24:AG:256:THR:OG1	2.33	0.45
29:BE:851:SER:O	29:BE:851:SER:OG	2.31	0.45
43:RE:298:PHE:HB2	43:RE:340:SER:HA	1.98	0.45
44:RF:132:ALA:O	44:RF:136:ASN:HB2	2.16	0.45
49:RN:423:GLY:O	49:RN:426:THR:OG1	2.31	0.45
50:RO:259:LYS:HB3	50:RO:259:LYS:HE2	1.72	0.45
2:5A:550:C:H2'	2:5A:551:A:C8	2.52	0.45
17:3G:58:CYS:HB3	17:3G:98:ILE:HD12	1.99	0.45
18:A4:124:THR:HG21	31:5B:191:PRO:HG3	1.97	0.45
18:A4:652:THR:HG23	18:A4:653:TRP:HD1	1.81	0.45
19:A5:518:ASN:HB2	19:A5:521:SER:HB3	1.98	0.45
22:AE:11:VAL:HA	22:AE:14:ASN:HD22	1.80	0.45
22:AE:583:LYS:HD3	22:AE:631:VAL:HG21	1.99	0.45
24:AG:143:ASN:N	24:AG:143:ASN:OD1	2.47	0.45
26:B2:54:ILE:HD13	26:B2:364:TYR:CD2	2.48	0.45
26:B2:580:ASP:OD2	26:B2:623:PHE:N	2.40	0.45
32:5C:39:ASP:HB3	32:5C:42:LEU:HB3	1.97	0.45
36:5G:19:GLU:O	36:5G:23:SER:HB2	2.17	0.45
43:RE:427:LYS:HA	43:RE:496:LEU:HD21	1.98	0.45
47:RJ:772:MET:HG3	47:RJ:774:PRO:HD2	1.98	0.45
49:RN:13:LEU:HD22	49:RN:16:ARG:HE	1.82	0.45
52:RS:289:ASP:O	52:RS:293:THR:OG1	2.26	0.45
1:3A:12:U:H3	3:SA:1112:G:H1	1.65	0.45
26:B2:566:TYR:OH	26:B2:603:ASP:O	2.33	0.45
26:B2:641:TYR:O	26:B2:650:ILE:N	2.49	0.45
27:B3:24:THR:HG21	27:B3:70:THR:H	1.82	0.45
32:5C:15:ARG:HB2	32:5C:18:GLN:HG3	1.98	0.45
32:5C:104:LEU:HD21	32:5C:139:TRP:HB2	1.99	0.45
38:5I:210:LYS:HA	38:5I:210:LYS:HD3	1.69	0.45
43:RE:217:LYS:O	43:RE:223:ARG:NH1	2.50	0.45
43:RE:348:TYR:HA	43:RE:351:LYS:HD3	1.98	0.45
49:RN:600:LEU:HD22	49:RN:633:VAL:HG22	1.98	0.45
52:RS:271:THR:H	52:RS:274:GLU:HB2	1.82	0.45
7:SO:106:ARG:CD	42:RD:1544:MET:HA	2.47	0.45
16:3F:164:GLN:HE21	16:3F:527:VAL:HG13	1.82	0.45
16:3F:452:SER:HB3	16:3F:460:ARG:HG2	1.99	0.45
18:A4:137:TYR:HB2	18:A4:177:LEU:HD12	1.99	0.45
22:AE:255:ILE:HD11	24:AG:884:MET:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AF:227:VAL:HG22	23:AF:236:VAL:HG12	1.99	0.45
27:B3:542:CYS:HB3	27:B3:583:PHE:HB2	1.99	0.45
29:BE:76:THR:OG1	29:BE:78:SER:O	2.29	0.45
43:RE:352:THR:HG21	43:RE:398:ALA:HB1	1.98	0.45
45:RH:191:ASP:HA	45:RH:194:GLU:HG2	1.98	0.45
2:5A:110:G:N2	2:5A:136:U:O2	2.49	0.45
3:SA:608:U:O2'	3:SA:609:U:O4'	2.34	0.45
3:SA:977:A:H2'	3:SA:978:A:C8	2.52	0.45
3:SA:1509:C:O2'	46:RI:192:ASN:ND2	2.50	0.45
18:A4:636:ILE:HG23	18:A4:648:PHE:HD2	1.82	0.45
20:A8:662:ILE:HA	20:A8:665:GLN:HB2	1.98	0.45
22:AE:348:ILE:HD13	22:AE:348:ILE:HA	1.87	0.45
24:AG:761:GLU:HG3	24:AG:779:ILE:HG22	1.99	0.45
25:B1:64:ASN:N	25:B1:64:ASN:OD1	2.49	0.45
26:B2:103:ILE:HB	26:B2:117:PHE:HB2	1.99	0.45
26:B2:337:LYS:O	26:B2:357:THR:OG1	2.25	0.45
26:B2:870:SER:HA	27:B3:816:LEU:CD2	2.46	0.45
27:B3:162:LEU:HD21	27:B3:225:PHE:HE2	1.82	0.45
27:B3:801:GLU:HB3	29:BE:927:LYS:CD	2.47	0.45
32:5C:509:ILE:HG22	41:RC:76:VAL:HG21	1.99	0.45
43:RE:209:MET:HG2	43:RE:213:LEU:HD21	1.98	0.45
45:RH:56:SER:HA	45:RH:63:ASP:HB2	1.99	0.45
49:RN:804:LYS:HD3	49:RN:804:LYS:HA	1.75	0.45
52:RS:399:ILE:O	52:RS:406:GLY:N	2.50	0.45
3:SA:1223:A:H2'	3:SA:1224:A:C8	2.52	0.45
3:SA:1537:C:N4	45:RH:155:SER:O	2.37	0.45
8:SP:84:ARG:HG3	8:SP:119:THR:HA	1.99	0.45
24:AG:38:SER:OG	24:AG:43:ASN:O	2.35	0.45
27:B3:112:SER:OG	27:B3:154:GLY:O	2.30	0.45
27:B3:799:LEU:HD12	27:B3:802:GLN:HE21	1.81	0.45
28:B8:264:LEU:HD11	28:B8:272:LEU:HD12	1.97	0.45
29:BE:377:SER:O	29:BE:377:SER:OG	2.35	0.45
41:RC:62:ARG:HH21	41:RC:63:ALA:HB2	1.82	0.45
2:5A:554:G:H1	2:5A:583:U:H3	1.64	0.45
3:SA:1634:C:O2	25:B1:397:LYS:NZ	2.50	0.45
3:SA:1775:U:H2'	3:SA:1776:A:C8	2.51	0.45
7:SO:109:LYS:HD2	7:SO:109:LYS:N	2.30	0.45
18:A4:249:ARG:HB2	18:A4:292:ASN:HD22	1.81	0.45
19:A5:520:MET:H	19:A5:520:MET:HG3	1.60	0.45
26:B2:107:ASP:OD1	26:B2:107:ASP:N	2.46	0.45
29:BE:546:ILE:HG21	29:BE:560:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:5E:358:THR:HB	49:RN:89:GLN:HB3	1.98	0.45
41:RC:98:ARG:HD2	41:RC:102:LYS:HE3	1.98	0.45
43:RE:1101:ASP:HB3	43:RE:1233:ASN:HB3	1.99	0.45
48:RK:187:ILE:HB	48:RK:251:GLN:HE22	1.82	0.45
52:RS:235:VAL:HG12	52:RS:238:SER:HB3	1.98	0.45
52:RS:429:LYS:HD2	52:RS:437:ARG:HH22	1.82	0.45
3:SA:592:A:O2'	3:SA:596:C:OP1	2.35	0.45
4:SG:117:THR:HG21	4:SG:194:LEU:HD23	1.98	0.45
13:3B:218:ILE:HD11	14:3D:152:LEU:HD22	1.98	0.45
13:3C:253:ILE:HD11	13:3C:293:LEU:HD21	1.99	0.45
14:3D:120:SER:O	14:3D:120:SER:OG	2.33	0.45
16:3F:209:LYS:HA	16:3F:209:LYS:HD2	1.82	0.45
17:3H:33:LEU:HD23	17:3H:35:LYS:HE3	1.98	0.45
20:A8:583:SER:HB2	20:A8:637:LEU:HD22	1.97	0.45
22:AE:65:LYS:HB3	22:AE:104:LEU:HD11	1.99	0.45
23:AF:117:LEU:HD12	23:AF:117:LEU:HA	1.79	0.45
24:AG:600:SER:O	24:AG:600:SER:OG	2.33	0.45
26:B2:49:VAL:HG22	26:B2:63:LEU:HD22	1.98	0.45
27:B3:188:GLU:OE2	27:B3:232:LYS:NZ	2.44	0.45
28:B8:358:PHE:HA	28:B8:376:LEU:O	2.17	0.45
29:BE:921:ARG:O	29:BE:925:LEU:HB2	2.17	0.45
32:5C:460:ARG:HB3	51:RQ:847:VAL:HB	1.99	0.45
38:5I:8:ARG:HD3	38:5I:8:ARG:HA	1.80	0.45
38:5I:297:SER:OG	38:5I:299:ASN:O	2.33	0.45
20:A8:574:ARG:H	20:A8:576:ARG:NH1	2.16	0.44
23:AF:51:HIS:O	23:AF:53:HIS:N	2.49	0.44
23:AF:371:GLU:OE2	28:B8:273:ARG:NH2	2.50	0.44
25:B1:369:ILE:HD11	25:B1:390:VAL:HG11	1.99	0.44
25:B1:475:PRO:HD2	25:B1:493:TRP:HB2	1.99	0.44
29:BE:920:ASP:OD1	29:BE:920:ASP:N	2.48	0.44
32:5C:433:LEU:HD21	35:5F:16:VAL:HG11	1.99	0.44
45:RH:199:ASP:OD1	45:RH:199:ASP:N	2.49	0.44
47:RJ:889:LEU:HD22	47:RJ:922:ILE:HB	2.00	0.44
47:RJ:1148:GLU:OE2	47:RJ:1152:ARG:NH1	2.49	0.44
52:RS:373:LYS:HG3	52:RS:420:ALA:HA	1.99	0.44
2:5A:228:A:H2'	2:5A:229:A:C8	2.52	0.44
4:SG:63:GLN:HE22	4:SG:66:GLN:HB3	1.82	0.44
8:SP:29:HIS:HD2	8:SP:41:ARG:HB2	1.82	0.44
13:3B:88:ILE:HD11	13:3B:123:ILE:HG21	1.98	0.44
14:3D:281:LEU:HD23	15:3E:261:GLN:HE21	1.82	0.44
20:A8:648:PHE:HD1	21:A9:509:GLN:HE21	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AG:364:ASN:OD1	24:AG:364:ASN:N	2.42	0.44
26:B2:292:ILE:HG23	26:B2:324:PHE:HE2	1.83	0.44
27:B3:627:ASN:HB2	27:B3:631:MET:HB2	1.99	0.44
32:5C:214:LEU:HD23	32:5C:228:LEU:HD12	1.99	0.44
35:5F:169:THR:HA	35:5F:172:ARG:HG2	1.99	0.44
44:RF:23:HIS:CD2	44:RF:25:ALA:H	2.35	0.44
50:RO:196:GLN:OE1	50:RO:260:ASN:ND2	2.37	0.44
6:SN:41:LEU:HB3	6:SN:43:ARG:HG3	1.99	0.44
13:3C:175:ALA:N	13:3C:198:GLU:OE2	2.48	0.44
22:AE:109:TRP:HA	22:AE:114:THR:HG21	2.00	0.44
26:B2:443:LEU:HG	26:B2:459:LEU:HD13	1.99	0.44
27:B3:74:GLN:HA	27:B3:89:HIS:HB3	2.00	0.44
27:B3:392:ASN:H	27:B3:407:SER:HA	1.82	0.44
27:B3:691:PRO:HD2	34:5E:516:SER:HB2	1.97	0.44
32:5C:122:GLY:O	32:5C:139:TRP:NE1	2.34	0.44
37:5H:555:ASN:HB3	37:5H:558:ASN:HB2	1.98	0.44
43:RE:1098:PHE:HE1	43:RE:1216:LYS:HE2	1.82	0.44
50:RO:282:HIS:CD2	50:RO:283:LYS:HG2	2.52	0.44
2:5A:485:G:OP2	14:3D:46:LYS:NZ	2.39	0.44
10:ST:50:ALA:O	10:ST:68:ARG:NH1	2.50	0.44
13:3C:92:ARG:HH12	33:5D:151:PHE:HB2	1.81	0.44
13:3C:261:LEU:O	15:3E:118:ARG:NH2	2.35	0.44
15:3E:372:ARG:HG3	17:3G:63:ILE:HA	2.00	0.44
18:A4:579:ARG:HH12	18:A4:659:PHE:HD1	1.65	0.44
19:A5:582:GLU:O	19:A5:586:ASP:N	2.50	0.44
24:AG:559:LYS:HE2	24:AG:559:LYS:HB2	1.79	0.44
24:AG:768:TRP:HE1	24:AG:772:THR:HA	1.83	0.44
32:5C:269:LYS:HB2	51:RQ:830:ILE:HG23	1.98	0.44
32:5C:311:SER:OG	32:5C:313:GLU:OE2	2.33	0.44
34:5E:524:ASP:OD2	34:5E:527:ARG:NH2	2.42	0.44
36:5G:166:SER:O	36:5G:256:MET:HA	2.17	0.44
43:RE:775:ASP:HB3	43:RE:778:PHE:HB2	1.98	0.44
44:RF:162:THR:HG22	44:RF:165:PHE:H	1.82	0.44
45:RG:242:CYS:O	45:RG:246:GLU:HG3	2.18	0.44
47:RJ:617:THR:HG23	47:RJ:620:LYS:HE2	1.99	0.44
49:RN:737:ILE:HA	49:RN:740:MET:HG2	2.00	0.44
2:5A:247:U:OP1	33:5D:82:ARG:NH1	2.50	0.44
4:SG:86:GLN:HE22	25:B1:546:ASP:HB3	1.83	0.44
8:SP:13:VAL:HG13	8:SP:76:ILE:HA	1.98	0.44
14:3D:31:LEU:HD21	38:5I:59:VAL:HG13	1.99	0.44
18:A4:75:ASN:HB3	18:A4:92:GLU:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A4:201:VAL:HG13	18:A4:213:TRP:HB2	1.99	0.44
19:A5:87:LEU:O	19:A5:96:THR:N	2.50	0.44
22:AE:488:GLY:HA2	22:AE:491:TYR:HB3	1.98	0.44
24:AG:712:THR:HG23	24:AG:720:ILE:HD13	1.99	0.44
25:B1:25:ASP:O	25:B1:27:LYS:N	2.49	0.44
25:B1:157:ASP:N	25:B1:157:ASP:OD1	2.50	0.44
25:B1:356:ASP:OD1	25:B1:356:ASP:N	2.50	0.44
29:BE:356:ILE:HG22	29:BE:633:LYS:HG3	2.00	0.44
32:5C:162:ASN:ND2	32:5C:429:GLU:OE1	2.51	0.44
41:RC:52:TYR:CD1	41:RC:52:TYR:O	2.70	0.44
43:RE:159:SER:HB2	43:RE:256:TYR:HE2	1.82	0.44
47:RJ:187:LYS:HB2	47:RJ:187:LYS:HE3	1.75	0.44
47:RJ:841:THR:HB	47:RJ:859:ILE:HA	2.00	0.44
49:RN:443:LYS:HG3	49:RN:448:PHE:HE2	1.81	0.44
2:5A:207:G:H2'	2:5A:208:A:C8	2.52	0.44
3:SA:1169:G:N1	3:SA:1575:G:OP2	2.44	0.44
16:3F:405:VAL:HG12	16:3F:415:THR:HG22	2.00	0.44
18:A4:120:SER:OG	18:A4:121:THR:N	2.50	0.44
22:AE:100:ALA:HB1	28:B8:44:PHE:HZ	1.82	0.44
24:AG:202:SER:OG	24:AG:204:ASN:OD1	2.30	0.44
24:AG:510:TYR:HE1	24:AG:527:HIS:HB3	1.83	0.44
25:B1:476:VAL:HA	25:B1:492:SER:HB3	1.98	0.44
35:5F:34:ARG:NH2	40:5K:16:THR:OG1	2.50	0.44
11:SY:77:ILE:HG22	47:RJ:751:TYR:HB2	1.99	0.44
16:3F:502:SER:OG	16:3F:504:ASN:OD1	2.32	0.44
18:A4:212:ILE:O	18:A4:226:LEU:N	2.50	0.44
18:A4:468:ASP:OD2	18:A4:472:ARG:NH1	2.44	0.44
18:A4:571:THR:HG21	18:A4:632:ASN:HB3	2.00	0.44
24:AG:140:LYS:HA	24:AG:140:LYS:HD3	1.78	0.44
24:AG:484:VAL:O	24:AG:487:GLU:N	2.51	0.44
24:AG:516:PRO:HG2	24:AG:519:LEU:HD21	2.00	0.44
24:AG:532:TRP:HB3	24:AG:541:TRP:HB3	1.99	0.44
26:B2:129:PHE:HE1	26:B2:150:LEU:HD11	1.82	0.44
27:B3:269:LEU:HB2	27:B3:279:LYS:HB2	1.99	0.44
28:B8:277:ILE:HA	28:B8:282:ASN:HD22	1.83	0.44
31:5B:164:LYS:HE3	31:5B:164:LYS:HB3	1.76	0.44
33:5D:194:LYS:HA	33:5D:194:LYS:HD3	1.83	0.44
36:5G:139:LEU:HB2	36:5G:157:PHE:CE2	2.53	0.44
45:RG:135:LYS:HD3	45:RG:135:LYS:HA	1.87	0.44
49:RN:65:ASN:N	49:RN:65:ASN:OD1	2.50	0.44
2:5A:20:C:H2'	2:5A:21:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3B:169:LYS:HA	13:3B:193:VAL:O	2.18	0.44
14:3D:206:LEU:HD11	14:3D:219:LEU:HD11	2.00	0.44
15:3E:36:ASP:O	15:3E:123:TYR:OH	2.34	0.44
18:A4:45:THR:HB	18:A4:352:VAL:HA	1.99	0.44
23:AF:20:THR:HA	23:AF:24:GLN:HE21	1.83	0.44
27:B3:304:LEU:O	27:B3:311:LEU:HA	2.18	0.44
34:5E:379:ASP:HB2	36:5G:191:PHE:HD2	1.83	0.44
38:5I:241:ASP:OD1	38:5I:241:ASP:N	2.39	0.44
42:RD:1524:GLU:HA	42:RD:1528:GLY:HA3	2.00	0.44
48:RK:143:LYS:HE3	48:RK:143:LYS:HB2	1.75	0.44
3:SA:1234:A:O2'	3:SA:1236:A:N6	2.50	0.44
7:SO:109:LYS:H	7:SO:109:LYS:CD	2.29	0.44
13:3B:125:VAL:HG12	39:5J:150:GLY:HA3	2.00	0.44
15:3E:227:LEU:HG	15:3E:231:ILE:HB	2.00	0.44
18:A4:144:ILE:HD12	18:A4:158:VAL:HB	2.00	0.44
22:AE:422:LEU:HD12	22:AE:422:LEU:HA	1.87	0.44
25:B1:743:PHE:HZ	25:B1:778:ILE:HD13	1.83	0.44
38:5I:139:CYS:HB3	38:5I:145:VAL:HG22	1.99	0.44
3:SA:1697:G:OP1	43:RE:326:LEU:CD1	2.48	0.43
9:SR:64:ASP:OD1	9:SR:64:ASP:N	2.50	0.43
17:3H:52:ILE:HD12	17:3H:71:CYS:SG	2.58	0.43
17:3H:95:ARG:HA	17:3H:95:ARG:HD2	1.88	0.43
18:A4:572:ALA:HB3	18:A4:585:ILE:HD11	2.00	0.43
22:AE:538:ALA:HA	22:AE:541:LEU:HB2	2.00	0.43
27:B3:476:ASP:N	27:B3:476:ASP:OD1	2.50	0.43
28:B8:27:PHE:HB3	30:B6:31:LEU:HD23	1.98	0.43
32:5C:228:LEU:HD22	32:5C:264:PRO:HA	1.99	0.43
35:5F:115:MET:HE1	35:5F:136:VAL:HG11	1.99	0.43
40:5K:161:LYS:HG2	40:5K:172:LEU:HD21	1.99	0.43
46:RI:123:ASP:OD1	46:RI:123:ASP:N	2.49	0.43
50:RO:315:VAL:HG23	50:RO:316:PRO:HD3	1.98	0.43
52:RS:359:LEU:HD23	52:RS:362:LEU:HD12	2.00	0.43
3:SA:1132:A:O3'	48:RK:231:ARG:NH1	2.43	0.43
18:A4:750:ASN:N	18:A4:750:ASN:OD1	2.50	0.43
22:AE:238:LEU:HA	22:AE:241:ILE:HG22	1.99	0.43
26:B2:645:GLU:HG2	26:B2:646:LYS:HG3	1.99	0.43
27:B3:161:TRP:HB3	27:B3:177:LEU:HG	1.99	0.43
27:B3:464:LYS:HA	27:B3:482:VAL:HG21	2.00	0.43
29:BE:852:LEU:HD22	29:BE:860:GLU:HG2	2.00	0.43
38:5I:444:GLU:OE2	38:5I:448:ARG:NH2	2.37	0.43
45:RH:89:PRO:HG2	45:RH:134:PHE:HZ	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:RJ:904:ASN:HA	47:RJ:907:THR:HB	2.00	0.43
49:RN:590:ASN:OD1	49:RN:590:ASN:N	2.50	0.43
52:RS:221:LEU:HD22	52:RS:258:VAL:HG11	2.00	0.43
2:5A:467:A:N1	2:5A:468:A:N6	2.66	0.43
3:SA:886:U:H1'	8:SP:123:SER:HB3	2.00	0.43
3:SA:1599:C:H2'	3:SA:1600:A:C8	2.53	0.43
3:SA:1643:U:H2'	3:SA:1644:C:C6	2.52	0.43
3:SA:1658:G:C2	3:SA:1743:U:H1'	2.50	0.43
5:SK:38:ASN:HA	37:5H:565:LYS:HE2	1.99	0.43
13:3C:121:LYS:HA	13:3C:121:LYS:HD3	1.78	0.43
20:A8:638:LEU:HD21	20:A8:662:ILE:HD11	1.99	0.43
22:AE:348:ILE:HG21	22:AE:373:ILE:HD11	2.00	0.43
24:AG:296:HIS:NE2	24:AG:314:SER:OG	2.37	0.43
25:B1:35:ASN:HA	25:B1:58:ILE:HG23	1.99	0.43
26:B2:59:LEU:HD21	26:B2:62:LYS:HE2	1.99	0.43
27:B3:199:ILE:O	27:B3:209:LEU:HA	2.19	0.43
32:5C:64:ASP:HA	32:5C:67:LEU:HG	1.99	0.43
35:5F:138:VAL:HG12	35:5F:158:VAL:HG22	2.00	0.43
38:5I:358:MET:HB3	51:RQ:890:VAL:HG23	2.00	0.43
40:5K:52:PHE:HB3	40:5K:55:TYR:HB3	2.01	0.43
40:5K:171:PRO:HA	40:5K:184:LYS:HB2	2.01	0.43
43:RE:380:SER:OG	43:RE:386:GLY:O	2.36	0.43
43:RE:970:TRP:HB2	43:RE:971:LYS:HD2	2.00	0.43
47:RJ:625:TRP:HZ2	48:RK:284:SER:HB3	1.83	0.43
49:RN:314:MET:HA	49:RN:512:ASP:HA	1.99	0.43
3:SA:18:C:O2'	3:SA:21:U:O4'	2.37	0.43
10:ST:110:ARG:NH1	49:RN:740:MET:HB2	2.33	0.43
11:SY:68:ILE:HD12	49:RN:785:VAL:HG23	2.00	0.43
13:3B:221:ILE:HD13	14:3D:163:VAL:HB	2.00	0.43
15:3E:191:HIS:HB2	15:3E:247:ILE:HG23	1.99	0.43
15:3E:330:LEU:HD13	33:5D:109:THR:HG21	2.00	0.43
17:3G:62:GLU:HA	17:3G:65:LEU:HG	2.00	0.43
18:A4:214:SER:HB3	18:A4:226:LEU:HD13	1.99	0.43
19:A5:240:GLN:HE22	19:A5:298:LYS:HB3	1.83	0.43
22:AE:655:ALA:O	22:AE:659:LEU:HB2	2.18	0.43
23:AF:115:THR:O	23:AF:115:THR:OG1	2.35	0.43
23:AF:413:LEU:HA	23:AF:416:THR:HG22	2.00	0.43
24:AG:228:VAL:HG23	24:AG:236:ASN:HB3	2.00	0.43
25:B1:369:ILE:HB	25:B1:383:PHE:HB2	1.99	0.43
26:B2:596:ASN:HB3	26:B2:612:PHE:HA	1.99	0.43
27:B3:532:HIS:CE1	27:B3:558:LYS:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BE:569:VAL:HB	29:BE:579:ARG:HB2	2.01	0.43
30:B6:72:LYS:HD2	30:B6:72:LYS:HA	1.78	0.43
32:5C:508:VAL:HG12	41:RC:72:VAL:CB	2.48	0.43
36:5G:119:ARG:NH1	36:5G:122:TYR:O	2.52	0.43
51:RQ:284:ARG:HE	51:RQ:284:ARG:HB3	1.51	0.43
3:SA:871:G:H2'	3:SA:872:G:C8	2.53	0.43
3:SA:904:G:OP2	41:RC:185:ARG:NH2	2.52	0.43
4:SG:89:ILE:HD11	4:SG:172:ILE:HD11	2.00	0.43
13:3C:185:SER:HB3	13:3C:217:ILE:HD11	2.00	0.43
16:3F:415:THR:OG1	16:3F:425:TRP:NE1	2.39	0.43
19:A5:336:ASN:OD1	19:A5:336:ASN:N	2.49	0.43
22:AE:586:LEU:O	22:AE:590:ALA:HB2	2.18	0.43
23:AF:288:ASP:OD1	23:AF:288:ASP:N	2.48	0.43
23:AF:377:ASP:OD1	23:AF:377:ASP:N	2.51	0.43
24:AG:50:ASN:HD21	24:AG:782:THR:HG22	1.84	0.43
24:AG:780:GLU:O	24:AG:782:THR:N	2.49	0.43
25:B1:829:VAL:HG23	25:B1:830:ARG:HG2	2.01	0.43
27:B3:200:GLU:HB3	27:B3:209:LEU:HD23	2.01	0.43
27:B3:260:THR:HA	27:B3:268:GLN:O	2.18	0.43
27:B3:440:VAL:HB	27:B3:454:LEU:HD11	2.01	0.43
28:B8:376:LEU:HG	28:B8:386:ILE:HG12	1.99	0.43
36:5G:283:THR:HG22	36:5G:286:LYS:HB2	2.00	0.43
38:5I:133:GLN:HA	38:5I:150:ILE:O	2.18	0.43
46:RI:208:SER:OG	46:RI:209:ILE:N	2.52	0.43
47:RJ:280:LEU:HD12	47:RJ:281:PRO:HD2	2.01	0.43
48:RK:36:ILE:HB	48:RK:72:THR:HA	2.01	0.43
49:RN:616:LEU:HB3	49:RN:619:LEU:HD13	2.01	0.43
2:5A:192:G:H2'	2:5A:193:G:C8	2.53	0.43
2:5A:489:G:O6	30:B6:120:ARG:NH1	2.51	0.43
3:SA:513:U:H2'	3:SA:514:G:H8	1.82	0.43
3:SA:1655:A:H2'	3:SA:1656:U:H6	1.83	0.43
5:SK:155:HIS:NE2	16:3F:321:HIS:O	2.50	0.43
10:ST:119:ILE:HD13	34:5E:342:THR:HG22	2.00	0.43
16:3F:414:ILE:HG13	16:3F:478:LEU:HD21	2.00	0.43
18:A4:106:ASN:OD1	18:A4:106:ASN:N	2.51	0.43
23:AF:24:GLN:HB2	23:AF:294:PHE:HD1	1.83	0.43
28:B8:35:GLU:O	28:B8:39:LYS:HB2	2.18	0.43
32:5C:512:ARG:O	32:5C:516:VAL:HG23	2.18	0.43
36:5G:100:LEU:HD13	36:5G:144:GLU:HB3	2.01	0.43
43:RE:313:ASN:HD22	43:RE:326:LEU:HA	1.84	0.43
53:RT:186:GLU:HG3	53:RT:230:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:545:A:O2'	3:SA:546:U:O4'	2.22	0.43
4:SG:72:HIS:O	9:SR:79:TYR:OH	2.37	0.43
4:SG:103:ASN:HA	4:SG:106:LYS:HD2	2.01	0.43
5:SK:154:LYS:HE2	5:SK:154:LYS:HB3	1.88	0.43
15:3E:372:ARG:O	15:3E:376:LEU:HB2	2.18	0.43
16:3F:201:ILE:HG12	16:3F:538:ARG:HD3	2.00	0.43
19:A5:281:ILE:HG12	19:A5:328:VAL:HB	2.01	0.43
22:AE:210:LEU:HD13	22:AE:210:LEU:HA	1.90	0.43
24:AG:414:ILE:HA	24:AG:414:ILE:HD12	1.80	0.43
26:B2:657:GLN:HE21	26:B2:657:GLN:HB3	1.64	0.43
27:B3:11:SER:CB	27:B3:641:PHE:O	2.64	0.43
27:B3:438:THR:OG1	27:B3:439:ALA:N	2.50	0.43
38:5I:306:SER:OG	38:5I:307:ALA:N	2.50	0.43
43:RE:895:HIS:NE2	43:RE:935:GLU:OE1	2.39	0.43
48:RK:68:SER:OG	48:RK:69:TYR:N	2.52	0.43
50:RO:472:HIS:CD2	50:RO:474:HIS:H	2.31	0.43
14:3D:52:SER:HB2	14:3D:85:ASN:HD21	1.84	0.43
15:3E:206:ALA:HB2	15:3E:262:ILE:HD11	2.00	0.43
16:3F:303:LYS:HB3	16:3F:317:ILE:HD11	2.01	0.43
19:A5:270:ASN:OD1	19:A5:270:ASN:N	2.49	0.43
20:A8:583:SER:HA	20:A8:586:ILE:HG22	2.00	0.43
25:B1:493:TRP:HA	25:B1:517:ASP:HB2	2.01	0.43
26:B2:473:ASP:N	26:B2:494:ASP:OD2	2.47	0.43
43:RE:649:TRP:HB2	43:RE:653:SER:HB2	2.01	0.43
45:RG:75:GLY:HA2	45:RG:78:LYS:HE3	2.01	0.43
50:RO:292:PRO:HG2	50:RO:330:PHE:HE2	1.82	0.43
3:SA:1012:U:H2'	3:SA:1013:A:C8	2.53	0.43
6:SN:79:ALA:HA	6:SN:85:LYS:HD2	2.01	0.43
18:A4:532:ASN:N	18:A4:544:SER:O	2.50	0.43
26:B2:178:ILE:HD11	26:B2:186:ILE:HD11	2.01	0.43
29:BE:24:PHE:HB3	29:BE:654:TRP:HB3	2.01	0.43
29:BE:50:ILE:HD13	29:BE:311:VAL:HG11	2.01	0.43
29:BE:499:LYS:HE2	29:BE:499:LYS:HB3	1.85	0.43
32:5C:268:VAL:HG13	51:RQ:831:ILE:HG12	2.00	0.43
33:5D:102:GLN:HE21	47:RJ:1098:ARG:NH1	2.17	0.43
36:5G:28:LYS:HB2	36:5G:46:LEU:HD11	2.00	0.43
36:5G:29:ARG:HD2	36:5G:59:ASP:HB3	2.01	0.43
38:5I:6:ILE:HG21	38:5I:8:ARG:HH21	1.84	0.43
38:5I:344:HIS:NE2	38:5I:418:HIS:O	2.51	0.43
49:RN:475:ARG:HH22	49:RN:516:LEU:HB3	1.84	0.43
50:RO:260:ASN:HA	50:RO:263:SER:HG	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RS:437:ARG:HH21	52:RS:463:GLY:HA3	1.84	0.43
3:SA:866:G:OP1	7:SO:9:LYS:NZ	2.50	0.43
3:SA:909:U:H2'	3:SA:910:C:C6	2.54	0.43
3:SA:985:G:H2'	3:SA:986:G:C8	2.54	0.43
7:SO:40:TYR:HA	7:SO:43:LYS:HG2	2.00	0.43
13:3B:198:GLU:O	13:3B:221:ILE:HA	2.18	0.43
16:3F:160:ILE:HG12	16:3F:542:SER:HB2	2.00	0.43
18:A4:566:LEU:HA	18:A4:566:LEU:HD23	1.83	0.43
18:A4:617:ASN:O	18:A4:621:ASN:HB2	2.19	0.43
19:A5:110:ILE:HG22	19:A5:119:CYS:HB2	2.00	0.43
19:A5:448:ASN:OD1	19:A5:450:HIS:NE2	2.52	0.43
23:AF:463:VAL:HA	23:AF:466:VAL:HG12	2.01	0.43
24:AG:87:SER:O	24:AG:111:THR:OG1	2.32	0.43
24:AG:857:PHE:HE2	28:B8:226:LYS:HB3	1.84	0.43
25:B1:25:ASP:OD1	25:B1:25:ASP:N	2.50	0.43
26:B2:861:ILE:HD11	27:B3:805:ILE:CD1	2.48	0.43
27:B3:160:ILE:HG22	27:B3:162:LEU:HB2	1.99	0.43
27:B3:225:PHE:HD1	27:B3:230:LYS:HD2	1.84	0.43
28:B8:426:VAL:HG11	28:B8:455:ILE:HG21	2.01	0.43
29:BE:627:ASN:ND2	29:BE:647:THR:OG1	2.52	0.43
33:5D:145:GLU:OE1	33:5D:146:PHE:N	2.52	0.43
40:5K:61:PRO:HB3	40:5K:92:ALA:HB1	2.01	0.43
44:RF:61:LEU:HD11	44:RF:164:SER:HA	2.00	0.43
49:RN:484:ARG:HB3	49:RN:492:ALA:HB1	2.01	0.43
49:RN:669:SER:HA	49:RN:672:THR:HG22	2.01	0.43
52:RS:266:PHE:O	52:RS:270:LEU:HB3	2.18	0.43
52:RS:398:ARG:H	52:RS:406:GLY:HA3	1.83	0.43
3:SA:899:G:H2'	3:SA:900:A:C8	2.54	0.42
3:SA:941:A:H2	3:SA:976:G:H4'	1.84	0.42
3:SA:960:U:H5'	7:SO:55:ARG:HD3	2.01	0.42
13:3C:185:SER:HA	13:3C:188:VAL:HG12	2.01	0.42
15:3E:319:ILE:HD12	15:3E:326:LEU:HD22	2.01	0.42
17:3G:64:LEU:O	17:3G:66:HIS:N	2.43	0.42
18:A4:313:LYS:HA	18:A4:316:LYS:HG2	2.01	0.42
23:AF:177:ILE:HA	23:AF:178:PRO:HD3	1.84	0.42
24:AG:252:LEU:HD23	24:AG:256:THR:HG21	2.00	0.42
25:B1:661:LEU:H	25:B1:661:LEU:HG	1.62	0.42
25:B1:749:TYR:HE2	29:BE:705:ILE:HG13	1.84	0.42
26:B2:276:ASN:ND2	26:B2:280:THR:O	2.47	0.42
32:5C:230:THR:HG22	32:5C:232:ALA:H	1.83	0.42
37:5H:496:GLN:HA	37:5H:499:GLN:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:5H:550:LEU:HD23	37:5H:550:LEU:HA	1.88	0.42
45:RG:190:GLN:NE2	45:RG:244:GLY:HA2	2.34	0.42
47:RJ:831:ARG:HD3	47:RJ:838:ILE:HD12	2.01	0.42
47:RJ:1019:THR:HB	47:RJ:1022:LEU:HD12	2.01	0.42
48:RK:56:ILE:HD13	48:RK:56:ILE:HA	1.89	0.42
48:RK:80:ILE:HD13	48:RK:80:ILE:HA	1.90	0.42
52:RS:264:LYS:HB2	52:RS:264:LYS:HE3	1.81	0.42
52:RS:382:LEU:HD11	52:RS:428:TYR:CG	2.55	0.42
3:SA:1656:U:H1'	3:SA:1744:A:H61	1.84	0.42
21:A9:475:THR:HA	21:A9:478:ASN:HB2	1.99	0.42
25:B1:76:ASP:N	25:B1:76:ASP:OD1	2.51	0.42
26:B2:351:LEU:HB2	26:B2:367:ILE:HG23	2.01	0.42
26:B2:432:TYR:CD1	26:B2:450:ARG:HB2	2.53	0.42
27:B3:77:THR:HG22	27:B3:86:LYS:HB3	2.01	0.42
27:B3:466:TRP:HZ3	27:B3:478:GLN:HA	1.82	0.42
29:BE:27:PHE:HB2	29:BE:655:THR:HG23	2.00	0.42
32:5C:487:LYS:HD3	32:5C:490:VAL:HG11	2.00	0.42
34:5E:335:ARG:HH22	47:RJ:952:PHE:HA	1.84	0.42
39:5J:134:ARG:HD2	39:5J:134:ARG:HA	1.83	0.42
47:RJ:1075:LYS:HE3	47:RJ:1075:LYS:HB2	1.84	0.42
52:RS:210:VAL:HG23	52:RS:212:LYS:HG2	2.00	0.42
3:SA:555:A:N6	3:SA:571:G:O2'	2.50	0.42
3:SA:1233:G:H1	3:SA:1253:U:H2'	1.83	0.42
5:SK:45:ILE:HD12	5:SK:48:GLN:HE21	1.84	0.42
10:ST:120:ARG:NH1	34:5E:344:GLU:OE2	2.50	0.42
14:3D:4:ILE:HG23	14:3D:20:VAL:HG21	2.01	0.42
22:AE:354:SER:O	22:AE:358:TYR:HB2	2.20	0.42
24:AG:313:LEU:HD23	24:AG:323:LEU:HB3	2.01	0.42
26:B2:39:GLY:O	26:B2:54:ILE:HG13	2.20	0.42
26:B2:673:VAL:HG23	26:B2:683:ILE:HD13	2.01	0.42
29:BE:470:GLN:HB3	29:BE:553:ARG:NH1	2.34	0.42
30:B6:5:ARG:HD2	30:B6:5:ARG:HA	1.80	0.42
30:B6:35:LYS:HE3	30:B6:35:LYS:HB3	1.88	0.42
34:5E:370:ARG:HA	34:5E:373:ILE:HG22	2.01	0.42
41:RC:52:TYR:CD1	41:RC:52:TYR:C	2.87	0.42
41:RC:100:LEU:HD22	41:RC:117:LEU:HD21	2.02	0.42
42:RD:1535:GLU:O	42:RD:1539:ARG:N	2.45	0.42
47:RJ:940:LYS:HE2	47:RJ:940:LYS:HB2	1.73	0.42
48:RK:81:ILE:HG22	48:RK:110:SER:HB3	2.01	0.42
52:RS:373:LYS:HE2	52:RS:373:LYS:HB3	1.84	0.42
13:3B:272:LYS:HD3	13:3B:275:CYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3C:149:SER:OG	13:3C:150:LYS:N	2.53	0.42
15:3E:218:ALA:HA	15:3E:221:THR:HG22	2.00	0.42
18:A4:774:LEU:HD12	18:A4:774:LEU:HA	1.83	0.42
20:A8:120:LEU:HA	20:A8:132:ILE:HA	2.01	0.42
22:AE:476:ILE:HG23	22:AE:515:PHE:HE2	1.84	0.42
24:AG:551:HIS:HA	24:AG:583:LYS:HE3	2.00	0.42
24:AG:865:LYS:HE2	24:AG:865:LYS:HB3	1.81	0.42
25:B1:60:ALA:HB1	25:B1:102:VAL:HG12	2.02	0.42
25:B1:275:LEU:HD22	25:B1:289:LEU:HD13	2.02	0.42
26:B2:297:LYS:HA	26:B2:300:GLU:HB2	2.02	0.42
26:B2:369:TYR:HA	26:B2:374:PRO:HA	2.01	0.42
26:B2:636:ASP:N	26:B2:636:ASP:OD1	2.52	0.42
26:B2:836:ILE:HA	26:B2:839:VAL:HG12	2.00	0.42
27:B3:479:ILE:HB	27:B3:480:ILE:HG23	2.02	0.42
29:BE:606:ASP:OD1	29:BE:606:ASP:N	2.41	0.42
36:5G:133:LYS:HE3	36:5G:133:LYS:HB3	1.85	0.42
47:RJ:203:LYS:HD2	47:RJ:203:LYS:HA	1.78	0.42
47:RJ:217:ASP:O	47:RJ:221:LEU:HB2	2.20	0.42
49:RN:501:PHE:HB3	49:RN:549:ILE:HG21	2.02	0.42
49:RN:700:LEU:HD21	50:RO:467:ALA:HB2	2.00	0.42
2:5A:298:A:OP2	29:BE:103:ARG:NH2	2.45	0.42
3:SA:-7:A:N7	38:5I:292:ARG:NH1	2.68	0.42
3:SA:954:G:H2'	3:SA:955:A:H8	1.84	0.42
3:SA:1000:C:H41	3:SA:1003:A:H2'	1.83	0.42
3:SA:1229:G:O6	6:SN:46:ARG:NH1	2.52	0.42
10:ST:100:THR:O	10:ST:104:ASN:ND2	2.53	0.42
13:3C:124:SER:HA	13:3C:139:VAL:O	2.19	0.42
14:3D:182:ASP:OD1	14:3D:314:ARG:NH2	2.39	0.42
19:A5:441:LEU:HD11	19:A5:480:LEU:HD13	2.02	0.42
22:AE:323:PHE:CZ	22:AE:332:ILE:HD11	2.54	0.42
22:AE:487:THR:HG22	22:AE:488:GLY:H	1.85	0.42
25:B1:157:ASP:OD1	25:B1:203:GLN:NE2	2.38	0.42
26:B2:497:VAL:HG12	26:B2:528:LEU:HB3	2.01	0.42
27:B3:215:GLY:N	27:B3:242:GLN:OE1	2.52	0.42
27:B3:555:LYS:HG2	27:B3:576:ASN:HA	2.00	0.42
34:5E:453:SER:O	34:5E:455:HIS:ND1	2.52	0.42
36:5G:28:LYS:HB2	36:5G:46:LEU:HD21	2.01	0.42
45:RH:176:ARG:NH2	45:RH:192:TYR:OH	2.52	0.42
52:RS:382:LEU:HD21	52:RS:428:TYR:CZ	2.53	0.42
1:3A:62:C:O2'	29:BE:447:ASN:O	2.35	0.42
2:5A:192:G:H2'	2:5A:193:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5A:460:U:OP1	40:5K:21:LYS:NZ	2.42	0.42
3:SA:630:A:C6	3:SA:970:A:N7	2.87	0.42
5:SK:63:ASP:OD1	5:SK:63:ASP:N	2.46	0.42
5:SK:163:PRO:HB3	5:SK:169:PRO:HA	2.01	0.42
10:ST:27:LYS:O	10:ST:31:ALA:HB2	2.19	0.42
13:3C:291:GLN:HA	13:3C:294:ARG:HG2	2.01	0.42
15:3E:117:TYR:HA	15:3E:120:ILE:HG12	2.01	0.42
15:3E:160:ASP:HB3	15:3E:283:ILE:HG21	2.01	0.42
17:3G:44:LEU:HD23	17:3G:44:LEU:HA	1.87	0.42
18:A4:513:LEU:HD12	18:A4:513:LEU:HA	1.89	0.42
22:AE:539:LEU:HD12	22:AE:540:LYS:HG3	2.01	0.42
23:AF:424:ARG:HA	24:AG:477:VAL:HG11	2.01	0.42
26:B2:534:ILE:HD11	26:B2:537:VAL:HG12	2.01	0.42
27:B3:680:ASN:HA	27:B3:683:LEU:HG	2.02	0.42
29:BE:724:SER:O	29:BE:728:ARG:NH2	2.39	0.42
32:5C:215:LYS:HG2	32:5C:227:GLU:HG2	2.00	0.42
36:5G:154:ILE:O	36:5G:162:THR:HA	2.20	0.42
43:RE:135:LEU:HD21	43:RE:207:LEU:HD21	2.01	0.42
43:RE:566:ILE:HA	43:RE:569:VAL:HG22	2.00	0.42
43:RE:627:LEU:HD12	43:RE:628:VAL:HG23	2.01	0.42
45:RG:128:VAL:HG22	45:RG:159:LEU:HD22	2.01	0.42
47:RJ:773:THR:HG23	47:RJ:777:ARG:HD3	2.02	0.42
48:RK:190:SER:OG	48:RK:191:ILE:N	2.51	0.42
48:RK:310:ARG:HB3	48:RK:353:THR:HG22	2.02	0.42
50:RO:208:TYR:O	50:RO:212:LEU:HB2	2.19	0.42
50:RO:243:PRO:HA	50:RO:244:PRO:HD3	1.81	0.42
50:RO:395:ILE:HD12	50:RO:469:LEU:HD11	2.02	0.42
52:RS:364:PHE:HE1	52:RS:417:TRP:HE1	1.67	0.42
52:RS:437:ARG:HD2	52:RS:460:LEU:HG	2.02	0.42
53:RT:124:LEU:HG	53:RT:151:ALA:HB1	2.02	0.42
3:SA:976:G:N3	3:SA:978:A:N7	2.67	0.42
19:A5:27:GLN:HG3	19:A5:59:LYS:HA	2.02	0.42
19:A5:233:LYS:HD3	19:A5:233:LYS:HA	1.82	0.42
22:AE:25:ARG:HH21	38:5I:16:VAL:HG22	1.83	0.42
22:AE:549:LYS:HD3	22:AE:549:LYS:HA	1.91	0.42
24:AG:31:ASN:OD1	24:AG:31:ASN:N	2.52	0.42
24:AG:478:ASN:OD1	24:AG:478:ASN:N	2.51	0.42
26:B2:861:ILE:HD11	27:B3:805:ILE:HD13	2.01	0.42
29:BE:353:PRO:HA	29:BE:370:SER:HA	2.01	0.42
32:5C:117:LYS:HD2	32:5C:117:LYS:HA	1.85	0.42
33:5D:78:LEU:HD12	33:5D:78:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:RE:433:ASP:OD1	43:RE:489:LYS:NZ	2.41	0.42
50:RO:153:ILE:HD12	50:RO:153:ILE:HA	1.91	0.42
3:SA:1492:A:N6	47:RJ:941:ILE:O	2.46	0.42
4:SG:23:VAL:HG23	9:SR:61:SER:HB3	2.00	0.42
4:SG:114:ILE:HA	4:SG:117:THR:HG22	2.02	0.42
6:SN:59:LEU:HB2	6:SN:87:PRO:HG2	2.02	0.42
15:3E:132:SER:OG	15:3E:134:ASN:OD1	2.34	0.42
15:3E:172:ASP:O	15:3E:176:GLU:HG2	2.20	0.42
16:3F:368:LEU:HB3	16:3F:396:PHE:HE2	1.83	0.42
19:A5:49:ASN:OD1	19:A5:49:ASN:N	2.49	0.42
19:A5:224:CYS:SG	19:A5:225:VAL:N	2.93	0.42
26:B2:236:ASP:OD1	26:B2:236:ASP:N	2.46	0.42
27:B3:201:VAL:O	27:B3:208:SER:HB3	2.20	0.42
36:5G:43:PRO:O	36:5G:47:ALA:HB2	2.20	0.42
36:5G:175:ASP:O	49:RN:64:ARG:NH2	2.53	0.42
38:5I:456:GLU:HA	38:5I:459:LYS:HE2	2.01	0.42
38:5I:464:THR:HG21	38:5I:468:TYR:HE1	1.85	0.42
43:RE:1206:PRO:HD2	44:RF:36:PHE:HD2	1.85	0.42
44:RF:20:LEU:HB2	44:RF:33:SER:HB2	2.01	0.42
44:RF:147:LEU:HA	44:RF:150:LYS:HD3	2.01	0.42
1:3A:49:C:H42	2:5A:467:A:H61	1.67	0.42
1:3A:118:A:C5	16:3F:218:ALA:HB2	2.55	0.42
9:SR:97:VAL:HG12	9:SR:98:ASP:H	1.83	0.42
16:3F:303:LYS:HE3	16:3F:319:TYR:HE2	1.85	0.42
18:A4:213:TRP:HA	18:A4:225:LEU:HA	2.02	0.42
22:AE:420:LYS:HB2	22:AE:420:LYS:HE2	1.91	0.42
38:5I:149:SER:OG	38:5I:170:GLU:O	2.29	0.42
52:RS:255:SER:HB3	52:RS:258:VAL:HG22	2.01	0.42
53:RT:263:LEU:HA	53:RT:266:VAL:HG12	2.02	0.42
3:SA:941:A:C2	3:SA:976:G:H4'	2.54	0.42
15:3E:333:LYS:HD3	33:5D:103:ASP:HB3	2.02	0.42
16:3F:301:ASP:OD1	16:3F:301:ASP:N	2.51	0.42
23:AF:119:SER:O	23:AF:119:SER:OG	2.36	0.42
24:AG:502:LYS:HD2	24:AG:564:PRO:HA	2.02	0.42
24:AG:659:ILE:HG22	24:AG:674:THR:HB	2.01	0.42
25:B1:147:GLN:HB2	25:B1:167:ASP:H	1.85	0.42
26:B2:141:LYS:O	26:B2:165:SER:HA	2.20	0.42
27:B3:178:VAL:HG13	27:B3:179:LYS:HG2	2.02	0.42
39:5J:207:LYS:HE2	39:5J:207:LYS:HB3	1.88	0.42
43:RE:1100:VAL:HG22	43:RE:1234:PHE:HD1	1.85	0.42
45:RH:180:LEU:HD23	45:RH:180:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RS:355:ALA:HA	52:RS:358:TYR:CE2	2.55	0.42
52:RS:432:ILE:HG23	52:RS:436:GLN:HB2	2.00	0.42
2:5A:368:U:HO2'	2:5A:369:G:H8	1.66	0.41
3:SA:565:C:N4	47:RJ:993:ASP:HB3	2.35	0.41
6:SN:90:LYS:HD2	6:SN:90:LYS:HA	1.80	0.41
13:3B:150:LYS:NZ	13:3B:310:GLU:OE2	2.44	0.41
13:3C:242:ALA:HB3	13:3C:269:ILE:HA	2.01	0.41
16:3F:260:LEU:HD21	16:3F:283:VAL:HG11	2.02	0.41
16:3F:421:ASN:ND2	16:3F:437:ARG:HA	2.34	0.41
18:A4:98:SER:OG	18:A4:99:ILE:N	2.53	0.41
18:A4:154:ASP:OD1	18:A4:154:ASP:N	2.49	0.41
23:AF:492:ARG:HA	23:AF:492:ARG:HD3	1.80	0.41
25:B1:410:THR:HG22	25:B1:426:THR:HG22	2.01	0.41
25:B1:605:ASP:OD1	25:B1:605:ASP:N	2.40	0.41
25:B1:721:VAL:O	29:BE:579:ARG:NH2	2.53	0.41
48:RK:216:LEU:HB3	48:RK:223:VAL:HG21	2.01	0.41
49:RN:700:LEU:HD23	49:RN:702:LEU:HG	2.01	0.41
52:RS:373:LYS:HA	52:RS:376:LEU:HG	2.02	0.41
2:5A:150:G:C6	23:AF:380:ARG:HG3	2.54	0.41
2:5A:532:A:O2'	51:RQ:332:ASP:OD2	2.37	0.41
3:SA:1156:C:H2'	3:SA:1157:A:C8	2.54	0.41
9:SR:46:PHE:HA	9:SR:49:TYR:HB2	2.02	0.41
13:3C:212:LYS:HA	13:3C:212:LYS:HD3	1.89	0.41
14:3D:206:LEU:HB3	14:3D:216:PHE:HE1	1.84	0.41
18:A4:423:LYS:NZ	31:5B:167:ARG:HH11	2.19	0.41
19:A5:32:GLN:HE22	19:A5:47:ASN:HB3	1.85	0.41
22:AE:559:ASN:HB2	22:AE:614:LEU:HD12	2.02	0.41
24:AG:258:TYR:CD1	24:AG:414:ILE:HD11	2.55	0.41
25:B1:274:LEU:HD11	25:B1:286:LEU:HD13	2.02	0.41
26:B2:405:LEU:HD11	26:B2:673:VAL:HG21	2.02	0.41
26:B2:555:VAL:HG22	26:B2:569:LEU:HB2	2.02	0.41
27:B3:531:ASN:O	27:B3:558:LYS:NZ	2.53	0.41
41:RC:53:LEU:O	41:RC:57:TRP:HB2	2.20	0.41
43:RE:296:ILE:HD11	43:RE:339:SER:HB2	2.02	0.41
44:RF:102:ALA:HA	44:RF:105:SER:HB3	2.03	0.41
45:RG:177:LYS:HE2	45:RG:177:LYS:HB3	1.68	0.41
49:RN:616:LEU:HD13	49:RN:619:LEU:HD22	2.01	0.41
13:3B:107:VAL:HG13	13:3B:141:TYR:HB3	2.01	0.41
16:3F:158:THR:HG23	16:3F:548:ARG:HB2	2.02	0.41
16:3F:476:THR:HG22	16:3F:491:SER:HA	2.02	0.41
18:A4:313:LYS:HA	18:A4:316:LYS:HZ3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AE:148:PHE:HA	22:AE:151:ILE:HG12	2.01	0.41
23:AF:105:VAL:HG21	23:AF:142:THR:HG21	2.01	0.41
23:AF:255:VAL:HA	23:AF:276:SER:HA	2.02	0.41
24:AG:386:ASN:HD21	24:AG:389:LEU:HD11	1.86	0.41
25:B1:6:LYS:HD3	25:B1:6:LYS:HA	1.91	0.41
25:B1:46:LYS:HE2	25:B1:46:LYS:HB3	1.87	0.41
29:BE:361:SER:HA	29:BE:636:PRO:HB2	2.02	0.41
29:BE:495:ARG:HD3	29:BE:495:ARG:HA	1.84	0.41
32:5C:244:ASN:HB3	32:5C:446:PRO:HG3	2.02	0.41
34:5E:427:SER:O	34:5E:431:GLN:HB2	2.19	0.41
38:5I:223:THR:HG1	38:5I:238:THR:HG1	1.69	0.41
39:5J:106:LEU:O	39:5J:146:ARG:NH1	2.44	0.41
41:RC:180:LEU:HA	41:RC:183:VAL:HG12	2.01	0.41
45:RG:215:ASN:HB2	45:RG:218:ASP:HB2	2.01	0.41
46:RI:215:ASN:HA	46:RI:218:ASP:HB2	2.03	0.41
2:5A:490:G:H1'	2:5A:495:G:H5'	2.01	0.41
3:SA:939:A:H2'	3:SA:940:A:C8	2.56	0.41
3:SA:1658:G:N1	3:SA:1743:U:C6	2.88	0.41
16:3F:321:HIS:CE1	16:3F:340:GLY:H	2.39	0.41
24:AG:511:GLU:HG2	24:AG:528:ILE:HB	2.00	0.41
24:AG:625:GLY:HA3	24:AG:662:VAL:HG11	2.02	0.41
25:B1:275:LEU:HB2	25:B1:289:LEU:HD22	2.02	0.41
25:B1:300:MET:HG2	25:B1:328:LEU:HD22	2.01	0.41
25:B1:363:ALA:HB2	25:B1:393:VAL:HG13	2.02	0.41
25:B1:501:SER:O	25:B1:506:SER:OG	2.37	0.41
26:B2:433:ALA:HA	26:B2:449:THR:HA	2.03	0.41
26:B2:538:ARG:HD3	26:B2:580:ASP:HA	2.02	0.41
28:B8:296:GLN:HB3	28:B8:316:GLY:HA2	2.03	0.41
29:BE:21:SER:OG	29:BE:621:ASP:OD2	2.29	0.41
30:B6:106:ASP:OD1	30:B6:106:ASP:N	2.38	0.41
35:5F:135:HIS:HB3	35:5F:160:TRP:CD1	2.55	0.41
36:5G:42:LEU:HD12	36:5G:43:PRO:HD2	2.02	0.41
38:5I:58:PHE:HE1	38:5I:373:ARG:HB3	1.85	0.41
38:5I:336:HIS:CE1	38:5I:338:HIS:HB2	2.55	0.41
41:RC:52:TYR:CE1	41:RC:56:ILE:CG2	3.01	0.41
46:RI:192:ASN:N	46:RI:192:ASN:OD1	2.53	0.41
47:RJ:802:LYS:HB2	47:RJ:802:LYS:HE3	1.92	0.41
47:RJ:1080:LYS:HA	47:RJ:1080:LYS:HD2	1.80	0.41
54:RW:180:LYS:HB2	54:RW:180:LYS:HE2	1.82	0.41
3:SA:1489:U:N3	39:5J:202:ARG:O	2.53	0.41
13:3C:89:GLU:HG2	13:3C:98:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3C:151:LEU:HD13	13:3C:241:PHE:HE1	1.86	0.41
14:3D:268:MET:HA	14:3D:271:VAL:HG12	2.02	0.41
16:3F:457:GLU:HG3	16:3F:461:LYS:HE2	2.02	0.41
18:A4:389:ARG:HG2	18:A4:747:ILE:HG21	2.02	0.41
18:A4:428:ILE:HD12	18:A4:444:ARG:HH21	1.85	0.41
20:A8:632:THR:HG22	21:A9:492:ILE:HD13	2.01	0.41
21:A9:416:ILE:O	21:A9:420:ILE:CB	2.69	0.41
22:AE:35:TYR:O	22:AE:150:ARG:NH1	2.53	0.41
22:AE:91:ILE:HD13	22:AE:91:ILE:HA	1.90	0.41
22:AE:480:ASN:HA	22:AE:518:THR:HG21	2.02	0.41
22:AE:526:LEU:HA	22:AE:529:VAL:HG12	2.02	0.41
23:AF:34:GLN:O	23:AF:328:ALA:HA	2.21	0.41
23:AF:392:ILE:HD11	23:AF:417:VAL:HG23	2.03	0.41
24:AG:97:THR:OG1	24:AG:98:VAL:N	2.54	0.41
26:B2:50:ASN:HB3	26:B2:62:LYS:HG3	2.02	0.41
26:B2:241:LYS:HB2	26:B2:241:LYS:HE3	1.89	0.41
27:B3:68:LYS:HE3	27:B3:68:LYS:HB3	1.81	0.41
29:BE:62:ASP:O	29:BE:66:LEU:N	2.48	0.41
30:B6:268:ASP:N	30:B6:268:ASP:OD1	2.53	0.41
30:B6:311:TYR:O	30:B6:315:GLU:HG2	2.21	0.41
36:5G:33:LYS:HB2	36:5G:33:LYS:HE3	1.79	0.41
38:5I:141:ASP:N	38:5I:141:ASP:OD1	2.49	0.41
39:5J:117:VAL:HG11	39:5J:149:ILE:HG13	2.02	0.41
41:RC:62:ARG:NH2	41:RC:63:ALA:HB2	2.35	0.41
43:RE:254:LEU:HD21	43:RE:268:LEU:HB3	2.02	0.41
43:RE:924:LEU:HD11	43:RE:1183:THR:HG22	2.01	0.41
43:RE:928:HIS:HB2	43:RE:1060:ILE:HG21	2.03	0.41
44:RF:91:ASP:O	44:RF:121:ARG:NH2	2.54	0.41
45:RG:175:CYS:SG	45:RG:201:SER:OG	2.67	0.41
49:RN:456:ILE:HA	49:RN:456:ILE:HD13	1.79	0.41
49:RN:611:SER:OG	49:RN:612:THR:N	2.52	0.41
49:RN:644:ASP:OD1	49:RN:687:LYS:NZ	2.51	0.41
49:RN:710:ILE:HD13	49:RN:710:ILE:HA	1.91	0.41
51:RQ:313:PHE:HE2	51:RQ:883:ILE:HD12	1.84	0.41
2:5A:474:A:OP2	32:5C:425:ARG:NH2	2.37	0.41
3:SA:1523:G:H1'	3:SA:1524:A:H5'	2.02	0.41
7:SO:106:ARG:NH2	7:SO:106:ARG:CG	2.72	0.41
16:3F:304:ILE:HB	16:3F:318:LEU:HG	2.03	0.41
18:A4:141:SER:O	18:A4:141:SER:OG	2.34	0.41
19:A5:64:LYS:HB3	19:A5:77:ILE:HG13	2.02	0.41
22:AE:32:SER:OG	22:AE:33:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AE:33:LEU:HD11	22:AE:151:ILE:HG22	2.03	0.41
22:AE:109:TRP:HB2	22:AE:142:TYR:CZ	2.56	0.41
25:B1:347:SER:HB2	25:B1:365:GLU:HB3	2.03	0.41
25:B1:559:ILE:HG21	25:B1:578:LYS:HA	2.03	0.41
27:B3:310:THR:HA	27:B3:335:GLY:HA2	2.02	0.41
27:B3:459:ASN:HA	27:B3:494:ILE:HD11	2.03	0.41
27:B3:495:ASN:N	27:B3:510:SER:OG	2.49	0.41
27:B3:801:GLU:HB3	29:BE:927:LYS:HD2	2.01	0.41
28:B8:159:HIS:O	28:B8:163:ARG:HG2	2.21	0.41
30:B6:306:LYS:HE3	30:B6:306:LYS:HB2	1.77	0.41
40:5K:138:ASP:OD1	40:5K:160:LEU:HD22	2.20	0.41
43:RE:508:SER:HA	43:RE:512:LEU:HB2	2.03	0.41
44:RF:23:HIS:HD2	44:RF:26:LEU:HG	1.85	0.41
49:RN:784:ILE:HA	49:RN:787:THR:HG22	2.03	0.41
2:5A:248:G:OP1	33:5D:82:ARG:NH2	2.53	0.41
2:5A:485:G:N2	38:5I:386:LYS:O	2.41	0.41
3:SA:575:C:O2	47:RJ:1052:SER:OG	2.28	0.41
3:SA:899:G:H2'	3:SA:900:A:H8	1.85	0.41
10:ST:26:ILE:HG13	10:ST:31:ALA:HB2	2.03	0.41
15:3E:192:PHE:CD2	15:3E:195:LEU:HB2	2.56	0.41
15:3E:283:ILE:HD13	15:3E:283:ILE:HA	1.88	0.41
16:3F:308:SER:OG	16:3F:313:SER:OG	2.36	0.41
21:A9:475:THR:HA	21:A9:478:ASN:HD22	1.86	0.41
22:AE:214:THR:HG23	22:AE:260:ILE:HG13	2.03	0.41
22:AE:241:ILE:HD12	22:AE:241:ILE:HA	1.93	0.41
22:AE:572:ARG:NH2	22:AE:632:THR:O	2.40	0.41
25:B1:423:ARG:HD3	25:B1:423:ARG:HA	1.88	0.41
25:B1:652:ASP:N	25:B1:652:ASP:OD1	2.52	0.41
28:B8:137:ILE:HD13	28:B8:137:ILE:HA	1.86	0.41
36:5G:9:ARG:HD3	36:5G:159:HIS:CD2	2.56	0.41
37:5H:542:TYR:CZ	37:5H:546:LYS:HG3	2.56	0.41
39:5J:51:LYS:HE2	39:5J:51:LYS:HB2	1.95	0.41
43:RE:109:GLU:OE2	43:RE:113:GLN:NE2	2.47	0.41
43:RE:219:PHE:HZ	43:RE:303:PHE:CD2	2.35	0.41
43:RE:219:PHE:HZ	43:RE:303:PHE:CE2	2.37	0.41
43:RE:498:MET:O	43:RE:506:GLN:NE2	2.42	0.41
45:RG:34:LYS:HD3	45:RG:34:LYS:HA	1.84	0.41
45:RG:116:THR:HG22	45:RG:118:ARG:H	1.86	0.41
45:RG:232:LEU:HB3	45:RG:236:VAL:HG13	2.03	0.41
47:RJ:926:ILE:HG12	47:RJ:928:ILE:HG23	2.01	0.41
48:RK:32:LYS:HG2	48:RK:75:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:RN:283:ALA:HA	52:RS:381:ALA:HB1	2.03	0.41
50:RO:226:ASP:OD1	50:RO:284:ARG:NE	2.54	0.41
2:5A:333:G:H5'	35:5F:49:ARG:HE	1.86	0.41
3:SA:976:G:N2	3:SA:978:A:C4	2.89	0.41
3:SA:1538:U:H1'	3:SA:1570:A:H61	1.84	0.41
8:SP:46:MET:O	8:SP:46:MET:SD	2.79	0.41
8:SP:70:LYS:HA	8:SP:73:GLU:HG2	2.02	0.41
13:3B:104:ASP:OD1	13:3B:104:ASP:N	2.38	0.41
14:3D:157:ALA:HB2	30:B6:292:TYR:CZ	2.56	0.41
16:3F:465:GLN:HG2	17:3H:6:PRO:HG3	2.02	0.41
18:A4:39:VAL:HG12	18:A4:41:PHE:H	1.85	0.41
18:A4:425:ASP:OD2	18:A4:444:ARG:NH2	2.53	0.41
19:A5:551:ILE:HA	19:A5:554:PHE:CE2	2.56	0.41
24:AG:514:TYR:HA	24:AG:515:PRO:HD3	1.94	0.41
27:B3:339:ILE:HG22	27:B3:638:ASP:HB2	2.03	0.41
28:B8:278:ASP:H	28:B8:282:ASN:HD22	1.67	0.41
43:RE:312:ARG:HH21	43:RE:333:ASN:HB3	1.86	0.41
45:RG:233:SER:OG	45:RG:234:ALA:N	2.54	0.41
47:RJ:193:ARG:HA	47:RJ:193:ARG:HD2	1.88	0.41
47:RJ:906:ASP:OD1	47:RJ:906:ASP:N	2.45	0.41
2:5A:211:G:OP1	31:5B:161:LYS:NZ	2.54	0.41
2:5A:329:A:O2'	2:5A:331:U:OP2	2.39	0.41
3:SA:976:G:N1	3:SA:978:A:H2'	2.36	0.41
3:SA:1689:A:H2	3:SA:1712:A:H62	1.67	0.41
4:SG:79:ASN:N	4:SG:79:ASN:OD1	2.54	0.41
6:SN:83:GLU:HG3	6:SN:85:LYS:HB2	2.03	0.41
6:SN:135:MET:HG3	6:SN:139:HIS:CE1	2.56	0.41
14:3D:7:LEU:HD12	14:3D:99:ALA:HB3	2.02	0.41
15:3E:201:ASP:HB3	15:3E:204:ALA:HB3	2.03	0.41
15:3E:359:ILE:HD13	15:3E:398:LEU:HD13	2.03	0.41
16:3F:132:VAL:HG21	16:3F:505:LEU:HD21	2.02	0.41
16:3F:488:ILE:HG22	16:3F:524:ILE:HD13	2.02	0.41
17:3G:85:VAL:O	17:3G:89:ARG:HG2	2.21	0.41
18:A4:394:TRP:HB3	18:A4:399:VAL:HG12	2.03	0.41
18:A4:581:SER:HA	18:A4:594:PHE:O	2.21	0.41
18:A4:652:THR:O	18:A4:652:THR:OG1	2.34	0.41
21:A9:460:LEU:HD23	21:A9:460:LEU:HA	1.96	0.41
22:AE:227:ASN:OD1	22:AE:227:ASN:N	2.53	0.41
22:AE:328:ASP:N	22:AE:328:ASP:OD1	2.49	0.41
24:AG:591:GLU:O	24:AG:593:ASN:N	2.54	0.41
24:AG:712:THR:HG22	24:AG:766:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B2:17:ILE:CG2	26:B2:52:TRP:CH2	3.01	0.41
26:B2:294:ARG:O	26:B2:298:LYS:NZ	2.44	0.41
26:B2:911:GLN:HA	26:B2:914:LEU:HG	2.03	0.41
29:BE:870:GLN:HA	29:BE:873:LYS:HE3	2.03	0.41
32:5C:307:LYS:HA	32:5C:307:LYS:HD3	1.89	0.41
33:5D:70:ARG:HD3	33:5D:78:LEU:HD11	2.02	0.41
34:5E:465:LEU:HD12	34:5E:465:LEU:HA	1.96	0.41
43:RE:205:THR:HG21	43:RE:294:LEU:HA	2.03	0.41
43:RE:528:ASP:OD1	43:RE:697:SER:N	2.47	0.41
43:RE:794:ASP:OD1	43:RE:865:ARG:NH2	2.45	0.41
43:RE:870:ALA:HA	44:RF:103:LEU:HD21	2.03	0.41
43:RE:1146:THR:HG21	43:RE:1180:ASN:HD22	1.86	0.41
45:RG:40:ARG:O	45:RG:201:SER:HA	2.20	0.41
47:RJ:74:VAL:HG11	47:RJ:82:LYS:HA	2.03	0.41
48:RK:117:LEU:HA	48:RK:166:VAL:O	2.21	0.41
49:RN:504:ILE:HA	49:RN:507:LEU:HG	2.03	0.41
49:RN:668:LEU:HD23	49:RN:671:TYR:HD2	1.86	0.41
52:RS:238:SER:O	52:RS:238:SER:OG	2.33	0.41
52:RS:288:ARG:O	52:RS:292:GLU:HG2	2.21	0.41
52:RS:407:GLU:HB2	52:RS:411:ARG:HD2	2.03	0.41
1:3A:253:G:OP2	17:3H:95:ARG:NH1	2.54	0.41
2:5A:18:G:H2'	2:5A:19:A:H8	1.85	0.41
2:5A:210:U:H2'	2:5A:211:G:C8	2.55	0.41
2:5A:254:C:OP2	54:RW:184:TYR:OH	2.31	0.41
3:SA:909:U:H2'	3:SA:910:C:H6	1.86	0.41
3:SA:1648:A:H2'	3:SA:1649:G:C8	2.55	0.41
7:SO:45:LEU:HD21	7:SO:53:LEU:HD12	2.03	0.41
13:3C:202:ARG:HA	13:3C:202:ARG:HD2	1.96	0.41
15:3E:299:LEU:HD22	15:3E:320:LEU:HD23	2.03	0.41
15:3E:367:ALA:O	15:3E:371:LEU:HB3	2.21	0.41
17:3G:41:THR:HG21	17:3G:66:HIS:CE1	2.55	0.41
20:A8:539:ASN:OD1	20:A8:539:ASN:N	2.46	0.41
20:A8:670:GLU:OE2	23:AF:499:LYS:NZ	2.45	0.41
22:AE:597:HIS:HB3	22:AE:615:ASN:HB3	2.03	0.41
23:AF:397:TRP:CZ3	23:AF:425:GLY:HA3	2.56	0.41
23:AF:426:LYS:HB3	23:AF:429:VAL:HB	2.03	0.41
24:AG:334:LEU:HA	24:AG:335:PRO:HD3	1.85	0.41
24:AG:439:ASN:ND2	24:AG:496:THR:O	2.54	0.41
26:B2:164:ASP:HB3	26:B2:182:LYS:HB3	2.02	0.41
28:B8:278:ASP:H	28:B8:282:ASN:ND2	2.18	0.41
29:BE:743:ARG:HB2	34:5E:475:SER:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BE:927:LYS:HD3	29:BE:927:LYS:HA	1.92	0.41
35:5F:181:ASP:OD1	35:5F:181:ASP:N	2.42	0.41
43:RE:236:THR:HA	43:RE:239:LEU:HB2	2.03	0.41
43:RE:807:LEU:HB3	43:RE:840:LEU:HD23	2.02	0.41
44:RF:41:ARG:HA	44:RF:53:LEU:HA	2.02	0.41
45:RH:177:LYS:HG2	45:RH:203:CYS:HB3	2.02	0.41
2:5A:423:C:H2'	2:5A:424:G:H8	1.86	0.40
7:SO:90:TYR:HA	7:SO:93:LYS:HG2	2.02	0.40
18:A4:52:SER:HA	18:A4:104:TRP:CG	2.56	0.40
18:A4:250:THR:OG1	18:A4:251:ASP:N	2.53	0.40
22:AE:69:PHE:HE2	22:AE:104:LEU:HD13	1.85	0.40
23:AF:136:ASP:OD1	23:AF:137:ASN:N	2.54	0.40
24:AG:29:THR:HB	24:AG:198:LEU:HD11	2.03	0.40
24:AG:409:LYS:HG2	24:AG:489:ASN:HA	2.03	0.40
25:B1:519:LEU:HD13	25:B1:581:THR:HG22	2.04	0.40
26:B2:687:THR:OG1	26:B2:687:THR:O	2.38	0.40
29:BE:205:PHE:HA	29:BE:206:PRO:HD3	1.91	0.40
39:5J:77:LYS:HA	39:5J:77:LYS:HD2	1.84	0.40
43:RE:168:ILE:HD12	43:RE:170:GLN:HE21	1.86	0.40
43:RE:248:LEU:HD12	43:RE:252:LEU:HD12	2.02	0.40
43:RE:708:LEU:HA	43:RE:709:PRO:HD3	1.94	0.40
46:RI:46:MET:H	46:RI:46:MET:HG2	1.65	0.40
46:RI:105:ASN:N	46:RI:105:ASN:OD1	2.48	0.40
48:RK:184:ASP:OD1	48:RK:185:ARG:N	2.53	0.40
49:RN:424:LYS:O	49:RN:428:VAL:HG23	2.20	0.40
53:RT:255:PRO:HA	53:RT:256:PRO:HD3	1.99	0.40
3:SA:16:G:H4'	40:5K:159:GLY:HA2	2.03	0.40
3:SA:973:A:H2'	3:SA:974:A:C8	2.56	0.40
7:SO:102:LEU:C	7:SO:104:ARG:N	2.73	0.40
13:3B:134:VAL:HA	13:3B:135:PRO:HD3	1.89	0.40
15:3E:88:ILE:HA	15:3E:106:ASN:O	2.22	0.40
15:3E:163:ILE:HD13	15:3E:163:ILE:HA	1.86	0.40
24:AG:560:ILE:HG22	24:AG:575:THR:HG22	2.03	0.40
25:B1:263:VAL:HG13	25:B1:277:VAL:HG13	2.03	0.40
25:B1:430:ARG:HH21	34:5E:458:PRO:HB2	1.85	0.40
27:B3:344:ARG:HE	27:B3:395:ASP:HA	1.86	0.40
28:B8:231:LYS:HA	28:B8:231:LYS:HD2	1.91	0.40
29:BE:290:ILE:HG23	29:BE:291:HIS:CD2	2.56	0.40
30:B6:26:LYS:HA	30:B6:29:VAL:HG12	2.03	0.40
31:5B:180:LEU:HD13	31:5B:180:LEU:HA	1.94	0.40
32:5C:340:LEU:HD22	32:5C:403:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:5F:73:LYS:HE2	35:5F:73:LYS:HB3	1.88	0.40
39:5J:195:GLN:O	39:5J:199:THR:HG22	2.22	0.40
43:RE:261:ASN:OD1	43:RE:588:GLN:NE2	2.54	0.40
45:RG:123:GLU:HB2	45:RG:161:LYS:HB2	2.03	0.40
47:RJ:563:CYS:SG	48:RK:327:ARG:NH2	2.95	0.40
50:RO:326:LEU:HD12	50:RO:326:LEU:HA	1.90	0.40
52:RS:245:VAL:O	52:RS:249:THR:HG23	2.22	0.40
3:SA:997:G:H2'	3:SA:998:A:C8	2.56	0.40
15:3E:287:LEU:HD12	15:3E:287:LEU:HA	1.90	0.40
18:A4:202:ILE:HD13	18:A4:253:ILE:HG12	2.03	0.40
22:AE:677:SER:HA	22:AE:678:PRO:HD3	1.98	0.40
23:AF:371:GLU:HG3	28:B8:287:SER:OG	2.21	0.40
28:B8:174:ARG:NE	28:B8:179:ASP:OD2	2.44	0.40
29:BE:83:LEU:HA	29:BE:91:TYR:O	2.21	0.40
32:5C:504:LYS:HD3	32:5C:504:LYS:HA	1.82	0.40
39:5J:119:ARG:HD3	47:RJ:1113:ILE:HG13	2.02	0.40
41:RC:57:TRP:CD2	41:RC:73:LEU:HD22	2.56	0.40
43:RE:225:LEU:HA	43:RE:228:ARG:HB3	2.03	0.40
45:RG:85:SER:OG	45:RG:86:GLU:OE1	2.39	0.40
46:RI:220:ILE:O	46:RI:224:THR:HG22	2.21	0.40
52:RS:446:GLN:HG2	52:RS:447:ARG:HE	1.86	0.40
3:SA:1480:G:H2'	3:SA:1481:C:O4'	2.22	0.40
7:SO:101:HIS:HA	7:SO:104:ARG:NH2	2.37	0.40
15:3E:169:LEU:HD23	15:3E:169:LEU:HA	1.92	0.40
15:3E:215:ARG:NH1	15:3E:244:GLY:O	2.54	0.40
15:3E:388:LEU:HD12	15:3E:388:LEU:HA	1.89	0.40
19:A5:444:ALA:HB2	19:A5:452:LEU:HD12	2.03	0.40
20:A8:532:PHE:HD1	20:A8:534:LEU:H	1.69	0.40
20:A8:642:LEU:HD12	21:A9:499:ILE:HG23	2.04	0.40
22:AE:401:VAL:O	22:AE:405:GLU:HG2	2.22	0.40
23:AF:57:VAL:HG21	23:AF:327:LEU:HD11	2.04	0.40
23:AF:178:PRO:HD2	23:AF:223:PRO:HA	2.02	0.40
23:AF:420:GLU:OE1	23:AF:424:ARG:NH1	2.37	0.40
26:B2:85:LEU:HD12	26:B2:94:LEU:HD11	2.04	0.40
26:B2:639:VAL:HG22	26:B2:653:LEU:HB2	2.03	0.40
27:B3:364:ILE:O	27:B3:381:VAL:HA	2.21	0.40
29:BE:523:ASP:OD1	29:BE:523:ASP:N	2.38	0.40
32:5C:114:TYR:HA	32:5C:128:THR:O	2.22	0.40
38:5I:467:LYS:H	38:5I:467:LYS:HG2	1.69	0.40
43:RE:492:ALA:HA	43:RE:495:THR:HG22	2.03	0.40
46:RI:85:GLU:O	46:RI:89:LYS:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:RK:113:LYS:HG2	48:RK:173:LEU:HD11	2.03	0.40
50:RO:439:LYS:HE2	50:RO:439:LYS:HB3	1.83	0.40
53:RT:247:VAL:HA	53:RT:250:LEU:HD23	2.04	0.40
3:SA:514:G:H2'	3:SA:515:A:H8	1.87	0.40
3:SA:1463:C:H2'	3:SA:1464:G:O4'	2.22	0.40
13:3B:227:PRO:HG2	13:3B:255:LEU:HB3	2.02	0.40
13:3C:165:ALA:HB3	13:3C:168:LYS:HD3	2.04	0.40
14:3D:86:LEU:HD21	14:3D:98:LEU:HD13	2.03	0.40
15:3E:306:LEU:HG	15:3E:375:ALA:HB2	2.04	0.40
16:3F:263:TRP:HA	16:3F:269:SER:O	2.22	0.40
17:3H:33:LEU:HD11	17:3H:100:ALA:HB1	2.03	0.40
19:A5:35:GLN:OE1	19:A5:36:ARG:N	2.55	0.40
19:A5:201:PHE:CZ	19:A5:223:LYS:HD2	2.56	0.40
24:AG:377:SER:HB2	28:B8:342:PHE:HE1	1.85	0.40
24:AG:869:MET:N	24:AG:869:MET:SD	2.95	0.40
25:B1:567:ASP:HB3	35:5F:144:ASN:ND2	2.36	0.40
26:B2:850:LEU:HD23	26:B2:850:LEU:HA	1.90	0.40
27:B3:69:LEU:HD13	27:B3:109:ASP:HA	2.02	0.40
27:B3:171:MET:HB3	27:B3:187:GLN:NE2	2.37	0.40
30:B6:110:TRP:CD2	30:B6:136:LEU:HD13	2.56	0.40
32:5C:191:ILE:HD13	32:5C:191:ILE:HA	1.87	0.40
32:5C:201:TYR:OH	32:5C:415:GLU:OE1	2.29	0.40
35:5F:19:LEU:HD11	40:5K:24:ARG:HB3	2.04	0.40
38:5I:107:LYS:NZ	38:5I:109:HIS:O	2.45	0.40
38:5I:231:GLU:HG2	51:RQ:298:TRP:HE1	1.86	0.40
38:5I:450:ASP:OD1	38:5I:450:ASP:N	2.55	0.40
43:RE:691:SER:OG	43:RE:692:LYS:N	2.54	0.40
45:RH:52:THR:HA	45:RH:66:VAL:O	2.22	0.40
47:RJ:552:LEU:HD23	47:RJ:552:LEU:HA	1.92	0.40
48:RK:247:ALA:O	48:RK:255:SER:HA	2.22	0.40
49:RN:14:LYS:HA	49:RN:14:LYS:HD2	1.84	0.40
50:RO:205:ASP:HA	50:RO:206:PRO:HD3	1.90	0.40
50:RO:295:LEU:O	50:RO:299:LEU:HG	2.22	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	
4	SG	211/225 (94%)	195 (92%)	16 (8%)	0	100	100
5	SK	169/197 (86%)	163 (96%)	6 (4%)	0	100	100
6	SN	117/143 (82%)	89 (76%)	28 (24%)	0	100	100
7	SO	132/151 (87%)	121 (92%)	10 (8%)	1 (1%)	19	60
8	SP	116/137 (85%)	100 (86%)	15 (13%)	1 (1%)	17	56
9	SR	123/143 (86%)	112 (91%)	11 (9%)	0	100	100
10	ST	113/146 (77%)	103 (91%)	10 (9%)	0	100	100
11	SY	101/145 (70%)	90 (89%)	11 (11%)	0	100	100
12	Sd	61/67 (91%)	57 (93%)	4 (7%)	0	100	100
13	3B	236/327 (72%)	222 (94%)	14 (6%)	0	100	100
13	3C	221/327 (68%)	207 (94%)	14 (6%)	0	100	100
14	3D	359/504 (71%)	346 (96%)	13 (4%)	0	100	100
15	3E	427/511 (84%)	387 (91%)	40 (9%)	0	100	100
16	3F	400/573 (70%)	362 (90%)	37 (9%)	1 (0%)	41	76
17	3G	119/126 (94%)	107 (90%)	11 (9%)	1 (1%)	19	60
17	3H	119/126 (94%)	111 (93%)	8 (7%)	0	100	100
18	A4	648/776 (84%)	591 (91%)	57 (9%)	0	100	100
19	A5	504/643 (78%)	465 (92%)	39 (8%)	0	100	100
20	A8	534/713 (75%)	398 (74%)	134 (25%)	2 (0%)	34	72
21	A9	126/575 (22%)	115 (91%)	11 (9%)	0	100	100
22	AE	645/1769 (36%)	595 (92%)	50 (8%)	0	100	100
23	AF	489/513 (95%)	442 (90%)	47 (10%)	0	100	100
24	AG	812/896 (91%)	732 (90%)	79 (10%)	1 (0%)	51	85
25	B1	830/923 (90%)	767 (92%)	63 (8%)	0	100	100
26	B2	839/943 (89%)	748 (89%)	89 (11%)	2 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
27	B3	728/817 (89%)	595 (82%)	131 (18%)	2 (0%)	41 76
28	B8	469/594 (79%)	438 (93%)	31 (7%)	0	100 100
29	BE	857/939 (91%)	803 (94%)	54 (6%)	0	100 100
30	B6	368/440 (84%)	341 (93%)	27 (7%)	0	100 100
31	5B	58/214 (27%)	55 (95%)	3 (5%)	0	100 100
32	5C	512/554 (92%)	474 (93%)	37 (7%)	1 (0%)	47 81
33	5D	231/250 (92%)	205 (89%)	26 (11%)	0	100 100
34	5E	200/593 (34%)	183 (92%)	16 (8%)	1 (0%)	29 68
35	5F	180/183 (98%)	172 (96%)	8 (4%)	0	100 100
36	5G	278/290 (96%)	256 (92%)	22 (8%)	0	100 100
37	5H	132/610 (22%)	123 (93%)	9 (7%)	0	100 100
38	5I	457/489 (94%)	421 (92%)	36 (8%)	0	100 100
39	5J	147/217 (68%)	136 (92%)	11 (8%)	0	100 100
40	5K	171/189 (90%)	166 (97%)	5 (3%)	0	100 100
41	RC	173/316 (55%)	169 (98%)	4 (2%)	0	100 100
42	RD	263/1729 (15%)	254 (97%)	9 (3%)	0	100 100
43	RE	1067/1237 (86%)	998 (94%)	69 (6%)	0	100 100
44	RF	168/297 (57%)	145 (86%)	23 (14%)	0	100 100
45	RG	212/252 (84%)	182 (86%)	30 (14%)	0	100 100
45	RH	226/252 (90%)	219 (97%)	7 (3%)	0	100 100
46	RI	250/274 (91%)	233 (93%)	17 (7%)	0	100 100
47	RJ	722/1183 (61%)	670 (93%)	51 (7%)	1 (0%)	51 85
48	RK	358/367 (98%)	341 (95%)	17 (5%)	0	100 100
49	RN	593/810 (73%)	545 (92%)	47 (8%)	1 (0%)	47 81
50	RO	523/552 (95%)	455 (87%)	68 (13%)	0	100 100
51	RQ	188/899 (21%)	177 (94%)	11 (6%)	0	100 100
52	RS	247/483 (51%)	225 (91%)	22 (9%)	0	100 100
53	RT	165/326 (51%)	150 (91%)	15 (9%)	0	100 100
54	RW	59/206 (29%)	54 (92%)	5 (8%)	0	100 100
All	All	18453/27161 (68%)	16810 (91%)	1628 (9%)	15 (0%)	54 85

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	5E	454	VAL
7	SO	106	ARG
8	SP	45	GLY
47	RJ	82	LYS
20	A8	309	PRO
24	AG	434	GLN
26	B2	132	THR
27	B3	236	THR
49	RN	285	PRO
16	3F	552	TRP
20	A8	308	PHE
26	B2	118	ASN
27	B3	71	PRO
32	5C	16	GLU
17	3G	10	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	
4	SG	180/191 (94%)	180 (100%)	0	100	100
5	SK	147/166 (89%)	146 (99%)	1 (1%)	84	90
6	SN	88/119 (74%)	86 (98%)	2 (2%)	50	70
7	SO	117/128 (91%)	114 (97%)	3 (3%)	46	67
8	SP	90/105 (86%)	89 (99%)	1 (1%)	73	85
9	SR	105/119 (88%)	105 (100%)	0	100	100
10	ST	105/129 (81%)	104 (99%)	1 (1%)	76	86
11	SY	85/120 (71%)	84 (99%)	1 (1%)	71	84
12	Sd	56/60 (93%)	56 (100%)	0	100	100
13	3B	201/240 (84%)	201 (100%)	0	100	100
13	3C	190/240 (79%)	187 (98%)	3 (2%)	62	79
14	3D	296/435 (68%)	293 (99%)	3 (1%)	76	86
15	3E	262/433 (60%)	261 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	3F	354/503 (70%)	352 (99%)	2 (1%)	86 92
17	3G	100/104 (96%)	100 (100%)	0	100 100
17	3H	100/104 (96%)	100 (100%)	0	100 100
18	A4	591/713 (83%)	584 (99%)	7 (1%)	71 84
19	A5	433/574 (75%)	432 (100%)	1 (0%)	93 96
20	A8	174/657 (26%)	173 (99%)	1 (1%)	86 92
21	A9	89/533 (17%)	89 (100%)	0	100 100
22	AE	589/1633 (36%)	587 (100%)	2 (0%)	92 95
23	AF	437/454 (96%)	433 (99%)	4 (1%)	78 87
24	AG	750/826 (91%)	740 (99%)	10 (1%)	69 82
25	B1	730/812 (90%)	726 (100%)	4 (0%)	88 93
26	B2	736/832 (88%)	730 (99%)	6 (1%)	81 89
27	B3	660/719 (92%)	640 (97%)	20 (3%)	41 63
28	B8	421/529 (80%)	420 (100%)	1 (0%)	93 96
29	BE	757/819 (92%)	754 (100%)	3 (0%)	91 94
30	B6	251/414 (61%)	247 (98%)	4 (2%)	62 79
31	5B	57/196 (29%)	55 (96%)	2 (4%)	36 60
32	5C	448/480 (93%)	445 (99%)	3 (1%)	84 90
33	5D	221/234 (94%)	219 (99%)	2 (1%)	78 87
34	5E	185/535 (35%)	184 (100%)	1 (0%)	88 93
35	5F	171/172 (99%)	170 (99%)	1 (1%)	86 92
36	5G	251/258 (97%)	249 (99%)	2 (1%)	81 89
37	5H	107/538 (20%)	107 (100%)	0	100 100
38	5I	416/443 (94%)	414 (100%)	2 (0%)	88 93
39	5J	140/200 (70%)	140 (100%)	0	100 100
40	5K	157/169 (93%)	157 (100%)	0	100 100
41	RC	158/289 (55%)	156 (99%)	2 (1%)	69 82
43	RE	984/1125 (88%)	960 (98%)	24 (2%)	49 69
44	RF	159/274 (58%)	153 (96%)	6 (4%)	33 58
45	RG	195/222 (88%)	193 (99%)	2 (1%)	76 86
45	RH	206/222 (93%)	204 (99%)	2 (1%)	76 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	RI	235/256 (92%)	235 (100%)	0	100 100
47	RJ	648/1039 (62%)	641 (99%)	7 (1%)	73 85
48	RK	307/312 (98%)	303 (99%)	4 (1%)	69 82
49	RN	422/732 (58%)	422 (100%)	0	100 100
50	RO	329/506 (65%)	328 (100%)	1 (0%)	92 95
51	RQ	132/808 (16%)	129 (98%)	3 (2%)	50 70
52	RS	225/424 (53%)	225 (100%)	0	100 100
53	RT	148/282 (52%)	146 (99%)	2 (1%)	67 81
54	RW	22/192 (12%)	22 (100%)	0	100 100
All	All	15417/22619 (68%)	15270 (99%)	147 (1%)	77 86

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	SK	57	ARG
6	SN	46	ARG
6	SN	66	VAL
7	SO	106	ARG
7	SO	109	LYS
7	SO	130	ARG
8	SP	46	MET
10	ST	126	ARG
11	SY	97	ASP
13	3C	237	VAL
13	3C	262	LYS
13	3C	306	LEU
14	3D	103	LYS
14	3D	129	ARG
14	3D	285	ARG
15	3E	265	PHE
16	3F	370	ARG
16	3F	506	ARG
18	A4	190	VAL
18	A4	282	ASP
18	A4	423	LYS
18	A4	436	ASP
18	A4	648	PHE
18	A4	739	LYS
18	A4	776	PHE

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Mol	Chain	Res	Type
19	A5	434	THR
20	A8	576	ARG
22	AE	617	LYS
22	AE	645	ARG
23	AF	199	ARG
23	AF	261	VAL
23	AF	432	TYR
23	AF	508	LEU
24	AG	141	LEU
24	AG	259	VAL
24	AG	336	ARG
24	AG	368	ASP
24	AG	421	LYS
24	AG	434	GLN
24	AG	435	ASP
24	AG	436	PHE
24	AG	615	TRP
24	AG	716	ARG
25	B1	164	THR
25	B1	249	ARG
25	B1	519	LEU
25	B1	661	LEU
26	B2	47	GLU
26	B2	75	ARG
26	B2	144	ASN
26	B2	432	TYR
26	B2	576	VAL
26	B2	588	ILE
27	B3	12	LEU
27	B3	13	ASN
27	B3	51	LYS
27	B3	94	LYS
27	B3	157	ASN
27	B3	240	ASN
27	B3	343	MET
27	B3	413	ILE
27	B3	459	ASN
27	B3	479	ILE
27	B3	481	LYS
27	B3	482	VAL
27	B3	533	LYS
27	B3	585	ASN

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Mol	Chain	Res	Type
27	B3	588	LYS
27	B3	649	GLU
27	B3	657	GLU
27	B3	658	LYS
27	B3	708	ARG
27	B3	816	LEU
28	B8	22	LEU
29	BE	309	ILE
29	BE	570	ILE
29	BE	728	ARG
30	B6	4	THR
30	B6	67	ARG
30	B6	106	ASP
30	B6	133	TYR
31	5B	158	LYS
31	5B	211	LEU
32	5C	153	THR
32	5C	392	VAL
32	5C	507	ASN
33	5D	18	GLN
33	5D	161	ARG
34	5E	314	LEU
35	5F	159	THR
36	5G	209	LEU
36	5G	234	ARG
38	5I	250	ARG
38	5I	417	ARG
41	RC	62	ARG
41	RC	149	ASN
43	RE	104	LYS
43	RE	175	LYS
43	RE	223	ARG
43	RE	228	ARG
43	RE	243	LEU
43	RE	245	LYS
43	RE	247	LYS
43	RE	289	ARG
43	RE	303	PHE
43	RE	309	LEU
43	RE	365	LEU
43	RE	368	LEU
43	RE	456	LYS

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Mol	Chain	Res	Type
43	RE	552	ARG
43	RE	562	LEU
43	RE	585	MET
43	RE	730	LEU
43	RE	901	ASN
43	RE	1073	ASN
43	RE	1086	ASN
43	RE	1087	LEU
43	RE	1191	LYS
43	RE	1230	MET
43	RE	1233	ASN
44	RF	9	MET
44	RF	19	LYS
44	RF	69	LYS
44	RF	127	LYS
44	RF	136	ASN
44	RF	150	LYS
45	RG	32	THR
45	RG	100	LEU
45	RH	82	ARG
45	RH	197	ASP
47	RJ	214	ARG
47	RJ	566	ARG
47	RJ	869	THR
47	RJ	973	ARG
47	RJ	976	ILE
47	RJ	1128	LYS
47	RJ	1141	LYS
48	RK	90	CYS
48	RK	214	LYS
48	RK	335	THR
48	RK	340	LYS
50	RO	493	TYR
51	RQ	330	THR
51	RQ	898	PHE
51	RQ	899	LYS
53	RT	129	ARG
53	RT	211	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (263) such sidechains are listed below:

Mol	Chain	Res	Type
4	SG	63	GLN
4	SG	104	ASN
4	SG	169	ASN
4	SG	186	ASN
7	SO	105	ASN
8	SP	12	GLN
8	SP	80	HIS
9	SR	32	ASN
9	SR	74	HIS
10	ST	103	ASN
10	ST	104	ASN
13	3B	91	HIS
13	3B	183	HIS
13	3B	258	HIS
14	3D	39	ASN
14	3D	85	ASN
14	3D	168	GLN
14	3D	213	ASN
15	3E	191	HIS
15	3E	256	ASN
15	3E	286	ASN
15	3E	289	GLN
15	3E	400	GLN
16	3F	155	ASN
16	3F	235	HIS
16	3F	525	GLN
16	3F	561	ASN
17	3G	19	GLN
17	3G	29	ASN
17	3G	38	ASN
17	3H	5	ASN
17	3H	18	GLN
17	3H	45	ASN
18	A4	179	HIS
18	A4	274	GLN
18	A4	279	HIS
18	A4	292	ASN
18	A4	317	ASN
18	A4	426	GLN
18	A4	438	GLN
18	A4	452	HIS
18	A4	529	ASN
18	A4	589	ASN

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Mol	Chain	Res	Type
19	A5	32	GLN
19	A5	67	ASN
19	A5	115	ASN
19	A5	293	ASN
19	A5	302	ASN
19	A5	316	ASN
19	A5	324	ASN
19	A5	333	ASN
19	A5	443	GLN
20	A8	553	GLN
20	A8	609	ASN
20	A8	636	GLN
21	A9	478	ASN
21	A9	509	GLN
22	AE	14	ASN
22	AE	141	ASN
22	AE	166	ASN
22	AE	219	ASN
22	AE	224	ASN
22	AE	258	HIS
22	AE	477	ASN
22	AE	480	ASN
22	AE	545	ASN
22	AE	673	ASN
23	AF	48	ASN
23	AF	64	GLN
23	AF	125	HIS
23	AF	133	HIS
23	AF	156	ASN
23	AF	289	ASN
23	AF	481	GLN
24	AG	50	ASN
24	AG	105	HIS
24	AG	190	GLN
24	AG	266	ASN
24	AG	269	GLN
24	AG	325	GLN
24	AG	332	GLN
24	AG	370	GLN
24	AG	375	ASN
24	AG	393	ASN
24	AG	407	ASN

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Mol	Chain	Res	Type
24	AG	410	ASN
24	AG	453	HIS
24	AG	467	GLN
24	AG	489	ASN
24	AG	568	ASN
24	AG	579	ASN
24	AG	669	ASN
24	AG	706	HIS
24	AG	881	ASN
25	B1	92	HIS
25	B1	142	HIS
25	B1	190	HIS
25	B1	201	HIS
25	B1	297	GLN
25	B1	303	ASN
25	B1	349	ASN
25	B1	386	HIS
25	B1	432	GLN
25	B1	452	ASN
25	B1	456	HIS
25	B1	483	GLN
25	B1	549	GLN
25	B1	552	ASN
25	B1	650	ASN
25	B1	795	ASN
25	B1	813	HIS
25	B1	837	ASN
25	B1	842	ASN
26	B2	172	GLN
26	B2	390	GLN
26	B2	455	GLN
26	B2	524	HIS
26	B2	596	ASN
26	B2	628	HIS
26	B2	629	ASN
26	B2	657	GLN
26	B2	770	ASN
26	B2	791	ASN
26	B2	856	ASN
26	B2	879	GLN
26	B2	916	HIS
27	B3	13	ASN

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Mol	Chain	Res	Type
27	B3	143	HIS
27	B3	157	ASN
27	B3	187	GLN
27	B3	240	ASN
27	B3	282	ASN
27	B3	433	HIS
27	B3	459	ASN
27	B3	585	ASN
27	B3	767	HIS
27	B3	802	GLN
28	B8	162	ASN
28	B8	167	GLN
28	B8	224	ASN
28	B8	282	ASN
28	B8	311	ASN
28	B8	352	GLN
28	B8	472	GLN
28	B8	492	ASN
28	B8	528	GLN
28	B8	592	ASN
29	BE	163	GLN
29	BE	289	ASN
29	BE	481	ASN
29	BE	501	HIS
29	BE	514	ASN
29	BE	627	ASN
29	BE	708	ASN
29	BE	877	ASN
29	BE	911	ASN
29	BE	916	HIS
30	B6	90	GLN
30	B6	115	ASN
30	B6	166	ASN
30	B6	287	ASN
31	5B	207	ASN
32	5C	101	ASN
32	5C	124	HIS
32	5C	133	HIS
32	5C	151	ASN
32	5C	164	GLN
32	5C	170	GLN
32	5C	371	HIS

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Mol	Chain	Res	Type
32	5C	394	HIS
32	5C	525	ASN
33	5D	18	GLN
33	5D	42	HIS
33	5D	144	ASN
33	5D	153	ASN
34	5E	303	GLN
34	5E	316	ASN
35	5F	125	GLN
35	5F	135	HIS
35	5F	144	ASN
36	5G	143	HIS
36	5G	156	HIS
36	5G	159	HIS
36	5G	193	ASN
37	5H	499	GLN
37	5H	513	HIS
37	5H	515	ASN
37	5H	560	ASN
38	5I	20	GLN
38	5I	46	ASN
38	5I	109	HIS
38	5I	134	ASN
38	5I	242	ASN
38	5I	260	GLN
38	5I	336	HIS
38	5I	371	ASN
38	5I	406	HIS
38	5I	460	GLN
39	5J	135	HIS
39	5J	184	ASN
39	5J	195	GLN
40	5K	43	ASN
41	RC	149	ASN
41	RC	195	HIS
43	RE	120	HIS
43	RE	170	GLN
43	RE	634	HIS
43	RE	767	GLN
43	RE	811	GLN
43	RE	834	ASN
43	RE	841	ASN

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Mol	Chain	Res	Type
43	RE	901	ASN
43	RE	928	HIS
43	RE	1073	ASN
43	RE	1086	ASN
43	RE	1194	HIS
43	RE	1233	ASN
44	RF	23	HIS
44	RF	66	HIS
44	RF	136	ASN
44	RF	148	HIS
44	RF	187	HIS
45	RG	105	ASN
45	RG	125	ASN
45	RH	69	ASN
45	RH	125	ASN
45	RH	250	ASN
46	RI	52	ASN
46	RI	186	ASN
46	RI	215	ASN
46	RI	221	ASN
47	RJ	157	ASN
47	RJ	254	HIS
47	RJ	276	HIS
47	RJ	289	HIS
47	RJ	778	GLN
47	RJ	909	ASN
48	RK	16	ASN
48	RK	334	ASN
49	RN	8	ASN
49	RN	56	ASN
49	RN	482	GLN
49	RN	703	GLN
49	RN	771	ASN
49	RN	797	ASN
50	RO	266	ASN
50	RO	268	GLN
50	RO	273	GLN
50	RO	290	HIS
50	RO	304	ASN
50	RO	306	GLN
50	RO	343	GLN
50	RO	472	HIS

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Mol	Chain	Res	Type
50	RO	474	HIS
51	RQ	303	GLN
51	RQ	310	HIS
51	RQ	344	GLN
51	RQ	839	ASN
51	RQ	867	GLN
51	RQ	876	GLN
53	RT	127	GLN
53	RT	218	ASN
53	RT	232	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3A	169/333 (50%)	44 (26%)	2 (1%)
2	5A	518/700 (74%)	161 (31%)	11 (2%)
3	SA	848/1808 (46%)	299 (35%)	20 (2%)
All	All	1535/2841 (54%)	504 (32%)	33 (2%)

All (504) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3A	2	U
1	3A	14	A
1	3A	15	U
1	3A	24	U
1	3A	25	U
1	3A	27	U
1	3A	28	A
1	3A	30	A
1	3A	33	A
1	3A	35	U
1	3A	38	U
1	3A	56	A
1	3A	60	A
1	3A	61	G
1	3A	87	G
1	3A	88	U
1	3A	89	C
1	3A	90	C
1	3A	91	C

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Mol	Chain	Res	Type
1	3A	101	G
1	3A	111	G
1	3A	115	G
1	3A	198	U
1	3A	199	G
1	3A	201	C
1	3A	204	U
1	3A	205	G
1	3A	206	C
1	3A	246	A
1	3A	248	G
1	3A	249	G
1	3A	252	C
1	3A	305	G
1	3A	309	G
1	3A	310	G
1	3A	311	G
1	3A	313	A
1	3A	314	C
1	3A	322	A
1	3A	324	U
1	3A	325	C
1	3A	328	A
1	3A	329	C
1	3A	332	G
2	5A	5	G
2	5A	6	A
2	5A	7	A
2	5A	8	A
2	5A	11	A
2	5A	13	U
2	5A	14	U
2	5A	15	G
2	5A	63	G
2	5A	64	U
2	5A	70	A
2	5A	82	A
2	5A	83	U
2	5A	86	C
2	5A	87	C
2	5A	90	G
2	5A	102	A

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Mol	Chain	Res	Type
2	5A	103	G
2	5A	104	A
2	5A	109	C
2	5A	110	G
2	5A	114	G
2	5A	124	A
2	5A	125	G
2	5A	127	U
2	5A	128	C
2	5A	129	U
2	5A	130	G
2	5A	141	A
2	5A	142	U
2	5A	143	A
2	5A	144	C
2	5A	150	G
2	5A	151	U
2	5A	152	U
2	5A	156	U
2	5A	159	A
2	5A	161	A
2	5A	162	U
2	5A	163	G
2	5A	167	U
2	5A	168	G
2	5A	169	A
2	5A	170	U
2	5A	171	G
2	5A	172	C
2	5A	173	G
2	5A	174	U
2	5A	175	A
2	5A	176	U
2	5A	177	U
2	5A	178	G
2	5A	179	A
2	5A	182	G
2	5A	185	A
2	5A	190	U
2	5A	200	A
2	5A	201	U
2	5A	206	A

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Mol	Chain	Res	Type
2	5A	207	G
2	5A	211	G
2	5A	213	G
2	5A	219	U
2	5A	220	U
2	5A	222	G
2	5A	223	C
2	5A	224	G
2	5A	225	U
2	5A	227	U
2	5A	235	A
2	5A	240	C
2	5A	254	C
2	5A	256	U
2	5A	259	G
2	5A	260	A
2	5A	261	U
2	5A	263	C
2	5A	267	U
2	5A	268	G
2	5A	279	A
2	5A	280	A
2	5A	281	G
2	5A	292	A
2	5A	294	U
2	5A	304	U
2	5A	305	A
2	5A	309	A
2	5A	310	U
2	5A	311	C
2	5A	312	U
2	5A	313	A
2	5A	321	G
2	5A	322	A
2	5A	325	U
2	5A	326	C
2	5A	328	A
2	5A	337	G
2	5A	339	A
2	5A	346	G
2	5A	350	A
2	5A	353	A

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Mol	Chain	Res	Type
2	5A	354	G
2	5A	355	C
2	5A	359	U
2	5A	361	G
2	5A	363	A
2	5A	364	A
2	5A	368	U
2	5A	369	G
2	5A	370	U
2	5A	371	G
2	5A	372	A
2	5A	373	U
2	5A	381	G
2	5A	385	A
2	5A	386	A
2	5A	391	C
2	5A	393	C
2	5A	395	C
2	5A	407	A
2	5A	419	A
2	5A	427	A
2	5A	428	A
2	5A	429	A
2	5A	430	C
2	5A	431	A
2	5A	432	C
2	5A	433	C
2	5A	440	U
2	5A	443	G
2	5A	444	U
2	5A	461	A
2	5A	462	G
2	5A	464	G
2	5A	468	A
2	5A	472	A
2	5A	474	A
2	5A	481	U
2	5A	482	A
2	5A	485	G
2	5A	487	A
2	5A	488	U
2	5A	490	G

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Mol	Chain	Res	Type
2	5A	491	U
2	5A	493	A
2	5A	519	A
2	5A	525	U
2	5A	526	U
2	5A	536	A
2	5A	537	G
2	5A	539	A
2	5A	540	U
2	5A	541	U
2	5A	542	U
2	5A	548	A
2	5A	549	G
2	5A	583	U
2	5A	586	A
2	5A	587	G
2	5A	589	U
2	5A	591	U
3	SA	-6	A
3	SA	-5	G
3	SA	-4	A
3	SA	-1	G
3	SA	0	U
3	SA	1	U
3	SA	2	A
3	SA	17	C
3	SA	18	C
3	SA	19	A
3	SA	21	U
3	SA	23	G
3	SA	25	C
3	SA	26	A
3	SA	29	U
3	SA	35	U
3	SA	36	C
3	SA	37	U
3	SA	436	A
3	SA	437	A
3	SA	439	U
3	SA	440	U
3	SA	468	A
3	SA	469	C

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Mol	Chain	Res	Type
3	SA	470	A
3	SA	471	A
3	SA	473	A
3	SA	477	A
3	SA	480	G
3	SA	486	G
3	SA	487	G
3	SA	496	G
3	SA	501	U
3	SA	502	U
3	SA	505	A
3	SA	506	A
3	SA	514	G
3	SA	520	A
3	SA	534	A
3	SA	538	A
3	SA	539	G
3	SA	541	A
3	SA	542	A
3	SA	543	C
3	SA	545	A
3	SA	557	G
3	SA	558	U
3	SA	563	U
3	SA	564	G
3	SA	565	C
3	SA	570	A
3	SA	572	C
3	SA	574	G
3	SA	575	C
3	SA	578	U
3	SA	579	A
3	SA	580	A
3	SA	583	C
3	SA	584	C
3	SA	585	A
3	SA	586	G
3	SA	587	C
3	SA	594	A
3	SA	595	G
3	SA	602	U
3	SA	603	U

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Mol	Chain	Res	Type
3	SA	604	A
3	SA	606	A
3	SA	608	U
3	SA	609	U
3	SA	610	G
3	SA	611	U
3	SA	612	U
3	SA	613	G
3	SA	614	C
3	SA	615	A
3	SA	616	G
3	SA	635	A
3	SA	636	A
3	SA	638	U
3	SA	873	U
3	SA	876	G
3	SA	877	G
3	SA	894	U
3	SA	898	A
3	SA	900	A
3	SA	901	G
3	SA	906	A
3	SA	909	U
3	SA	910	C
3	SA	912	U
3	SA	913	G
3	SA	914	G
3	SA	926	A
3	SA	928	U
3	SA	932	U
3	SA	933	A
3	SA	935	U
3	SA	944	A
3	SA	945	U
3	SA	951	A
3	SA	960	U
3	SA	964	U
3	SA	966	A
3	SA	969	C
3	SA	970	A
3	SA	971	A
3	SA	975	C

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Mol	Chain	Res	Type
3	SA	976	G
3	SA	980	G
3	SA	987	G
3	SA	988	A
3	SA	992	A
3	SA	993	A
3	SA	996	U
3	SA	998	A
3	SA	1000	C
3	SA	1004	U
3	SA	1005	A
3	SA	1009	U
3	SA	1012	U
3	SA	1019	A
3	SA	1106	U
3	SA	1107	G
3	SA	1108	G
3	SA	1109	G
3	SA	1110	G
3	SA	1111	G
3	SA	1114	G
3	SA	1118	G
3	SA	1119	G
3	SA	1122	G
3	SA	1125	A
3	SA	1126	G
3	SA	1127	G
3	SA	1128	C
3	SA	1129	U
3	SA	1131	A
3	SA	1132	A
3	SA	1145	U
3	SA	1146	G
3	SA	1147	A
3	SA	1158	C
3	SA	1164	G
3	SA	1178	G
3	SA	1191	U
3	SA	1192	C
3	SA	1193	A
3	SA	1195	C
3	SA	1196	A

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Mol	Chain	Res	Type
3	SA	1197	C
3	SA	1198	G
3	SA	1199	G
3	SA	1200	G
3	SA	1201	G
3	SA	1202	A
3	SA	1205	C
3	SA	1206	U
3	SA	1208	A
3	SA	1210	C
3	SA	1213	G
3	SA	1217	A
3	SA	1218	G
3	SA	1219	A
3	SA	1220	C
3	SA	1223	A
3	SA	1227	A
3	SA	1228	G
3	SA	1229	G
3	SA	1230	A
3	SA	1232	U
3	SA	1233	G
3	SA	1235	C
3	SA	1236	A
3	SA	1252	C
3	SA	1253	U
3	SA	1254	U
3	SA	1255	G
3	SA	1258	U
3	SA	1263	G
3	SA	1266	U
3	SA	1268	G
3	SA	1271	G
3	SA	1272	U
3	SA	1273	G
3	SA	1275	A
3	SA	1276	U
3	SA	1436	A
3	SA	1440	C
3	SA	1441	C
3	SA	1442	U
3	SA	1443	U

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Mol	Chain	Res	Type
3	SA	1449	U
3	SA	1450	U
3	SA	1453	G
3	SA	1457	C
3	SA	1461	C
3	SA	1469	A
3	SA	1472	C
3	SA	1473	U
3	SA	1474	G
3	SA	1475	A
3	SA	1476	C
3	SA	1482	C
3	SA	1488	G
3	SA	1492	A
3	SA	1493	A
3	SA	1496	U
3	SA	1498	G
3	SA	1506	G
3	SA	1517	U
3	SA	1518	C
3	SA	1520	U
3	SA	1521	G
3	SA	1522	U
3	SA	1523	G
3	SA	1524	A
3	SA	1527	C
3	SA	1533	C
3	SA	1535	U
3	SA	1536	G
3	SA	1537	C
3	SA	1539	G
3	SA	1541	G
3	SA	1543	A
3	SA	1544	U
3	SA	1567	U
3	SA	1568	C
3	SA	1569	A
3	SA	1570	A
3	SA	1573	A
3	SA	1582	U
3	SA	1584	G
3	SA	1590	G

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Mol	Chain	Res	Type
3	SA	1594	G
3	SA	1595	U
3	SA	1596	C
3	SA	1601	G
3	SA	1602	C
3	SA	1607	G
3	SA	1614	A
3	SA	1618	C
3	SA	1628	U
3	SA	1630	U
3	SA	1633	A
3	SA	1643	U
3	SA	1644	C
3	SA	1645	G
3	SA	1649	G
3	SA	1651	A
3	SA	1654	G
3	SA	1655	A
3	SA	1657	U
3	SA	1658	G
3	SA	1659	A
3	SA	1660	A
3	SA	1670	G
3	SA	1678	A
3	SA	1680	G
3	SA	1681	A
3	SA	1682	U
3	SA	1683	C
3	SA	1688	U
3	SA	1689	A
3	SA	1697	G
3	SA	1709	C
3	SA	1711	C
3	SA	1712	A
3	SA	1713	G
3	SA	1715	G
3	SA	1717	G
3	SA	1724	U
3	SA	1727	G
3	SA	1736	G
3	SA	1737	G
3	SA	1739	C

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Mol	Chain	Res	Type
3	SA	1742	U
3	SA	1743	U
3	SA	1744	A
3	SA	1745	G
3	SA	1747	G
3	SA	1749	A
3	SA	1750	A
3	SA	1755	A
3	SA	1756	A
3	SA	1757	G
3	SA	1758	U
3	SA	1759	C
3	SA	1761	U
3	SA	1764	C
3	SA	1766	A
3	SA	1767	G
3	SA	1768	G
3	SA	1769	U
3	SA	1779	U
3	SA	1780	G
3	SA	1781	A
3	SA	1782	A
3	SA	1789	G

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3A	198	U
1	3A	248	G
2	5A	169	A
2	5A	172	C
2	5A	173	G
2	5A	224	G
2	5A	312	U
2	5A	358	G
2	5A	363	A
2	5A	368	U
2	5A	487	A
2	5A	492	G
2	5A	536	A
3	SA	-7	A
3	SA	0	U

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Mol	Chain	Res	Type
3	SA	538	A
3	SA	542	A
3	SA	579	A
3	SA	602	U
3	SA	899	G
3	SA	909	U
3	SA	913	G
3	SA	970	A
3	SA	971	A
3	SA	1146	G
3	SA	1197	C
3	SA	1521	G
3	SA	1594	G
3	SA	1632	C
3	SA	1654	G
3	SA	1743	U
3	SA	1744	A
3	SA	1749	A

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
57	GTP	RJ	1201	58	26,34,34	0.94	2 (7%)	32,54,54	0.92	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
57	GTP	RJ	1201	58	-	3/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	RJ	1201	GTP	C5-C6	-2.46	1.42	1.47
57	RJ	1201	GTP	C8-N7	-2.02	1.31	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	RJ	1201	GTP	O4'-C4'-C5'-O5'
57	RJ	1201	GTP	C3'-C4'-C5'-O5'
57	RJ	1201	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

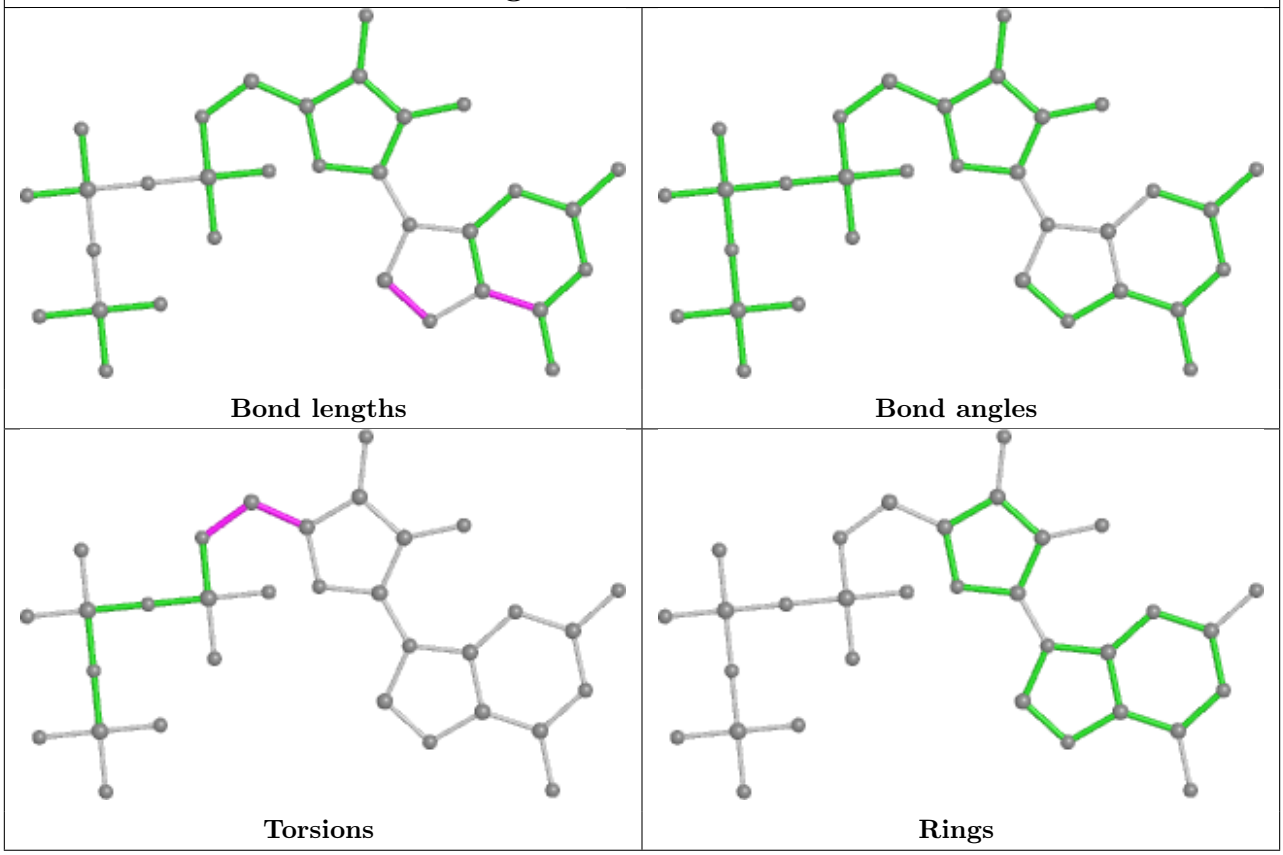
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	RJ	1201	GTP	1	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 RJ 1201



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.

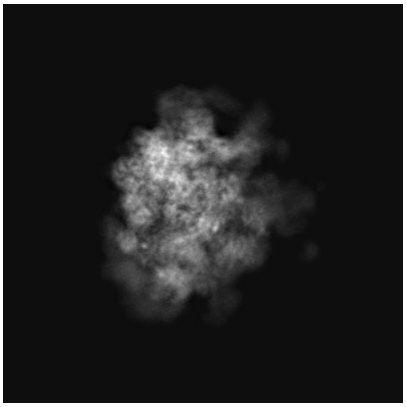
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30584. These allow visual inspection of the internal detail of the map and identification of artifacts.

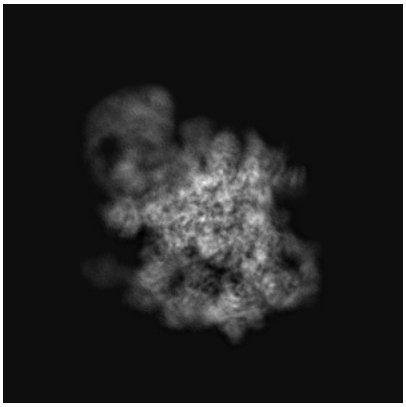
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

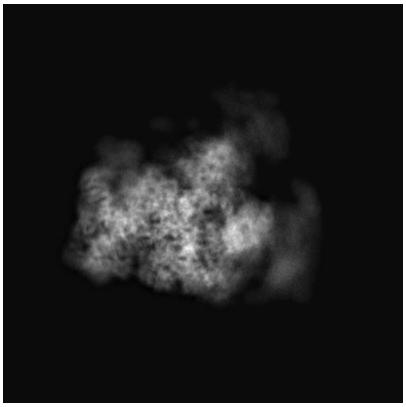
6.1.1 Primary map



X



Y

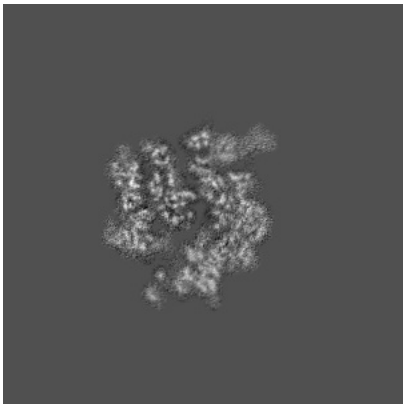


Z

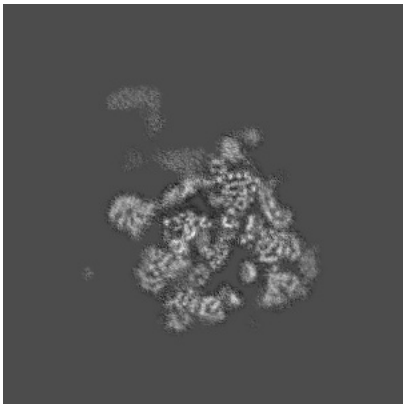
The images above show the map projected in three orthogonal directions.

6.2 Central slices

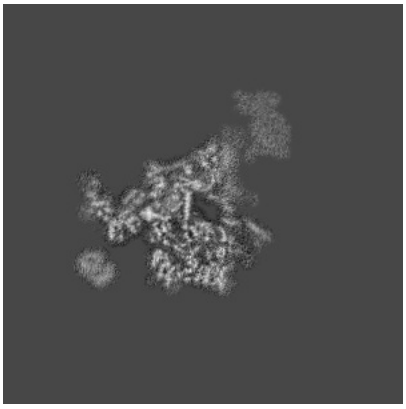
6.2.1 Primary map



X Index: 200



Y Index: 200

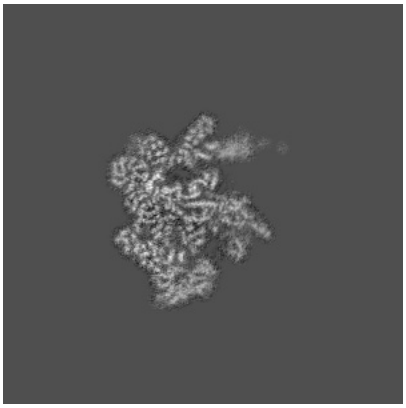


Z Index: 200

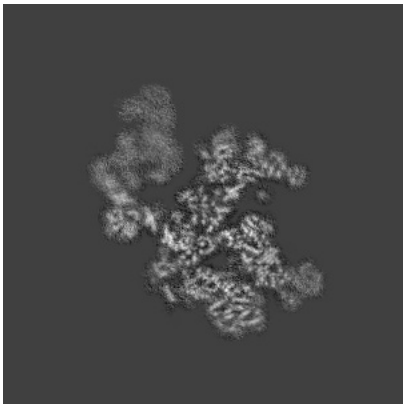
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

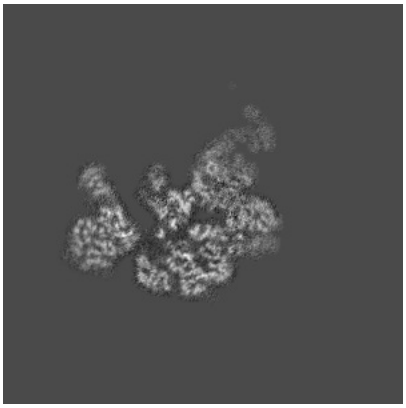
6.3.1 Primary map



X Index: 184



Y Index: 177



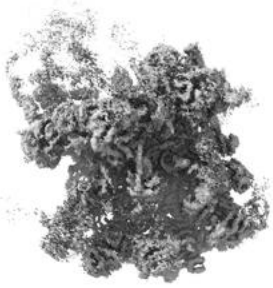
Z Index: 222

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

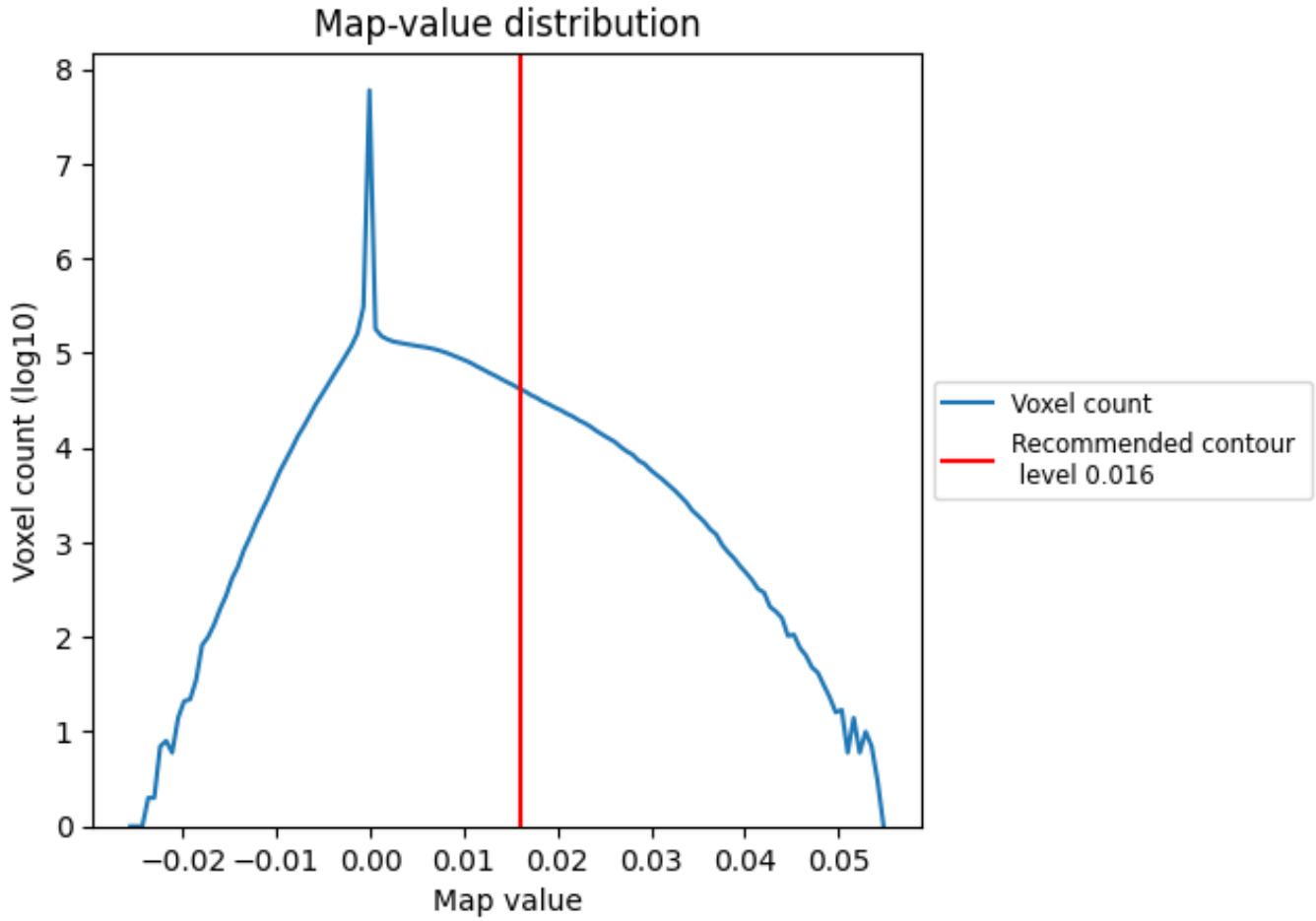
6.5 Mask visualisation (i)

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

7 Map analysis

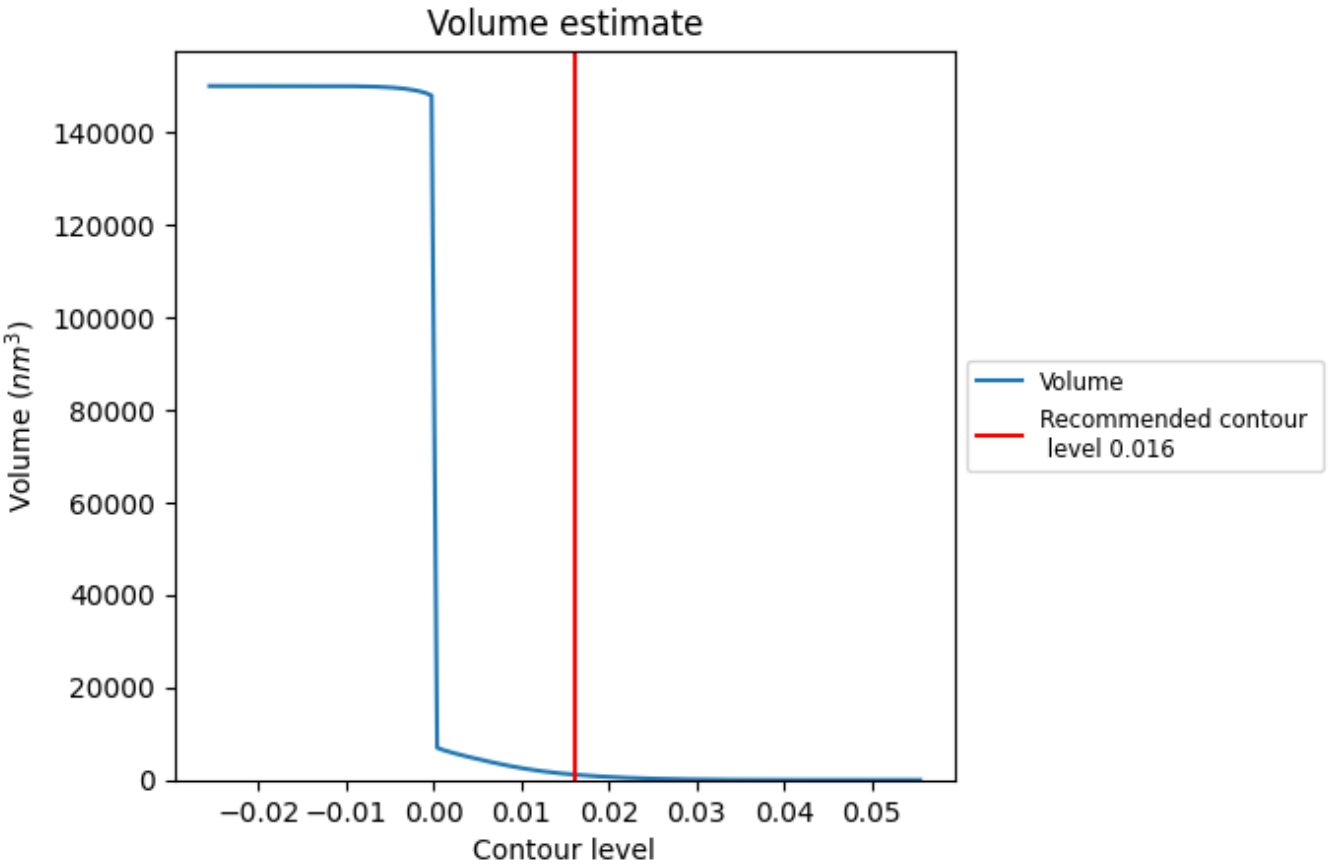
This section contains the results of statistical analysis of the map.

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.

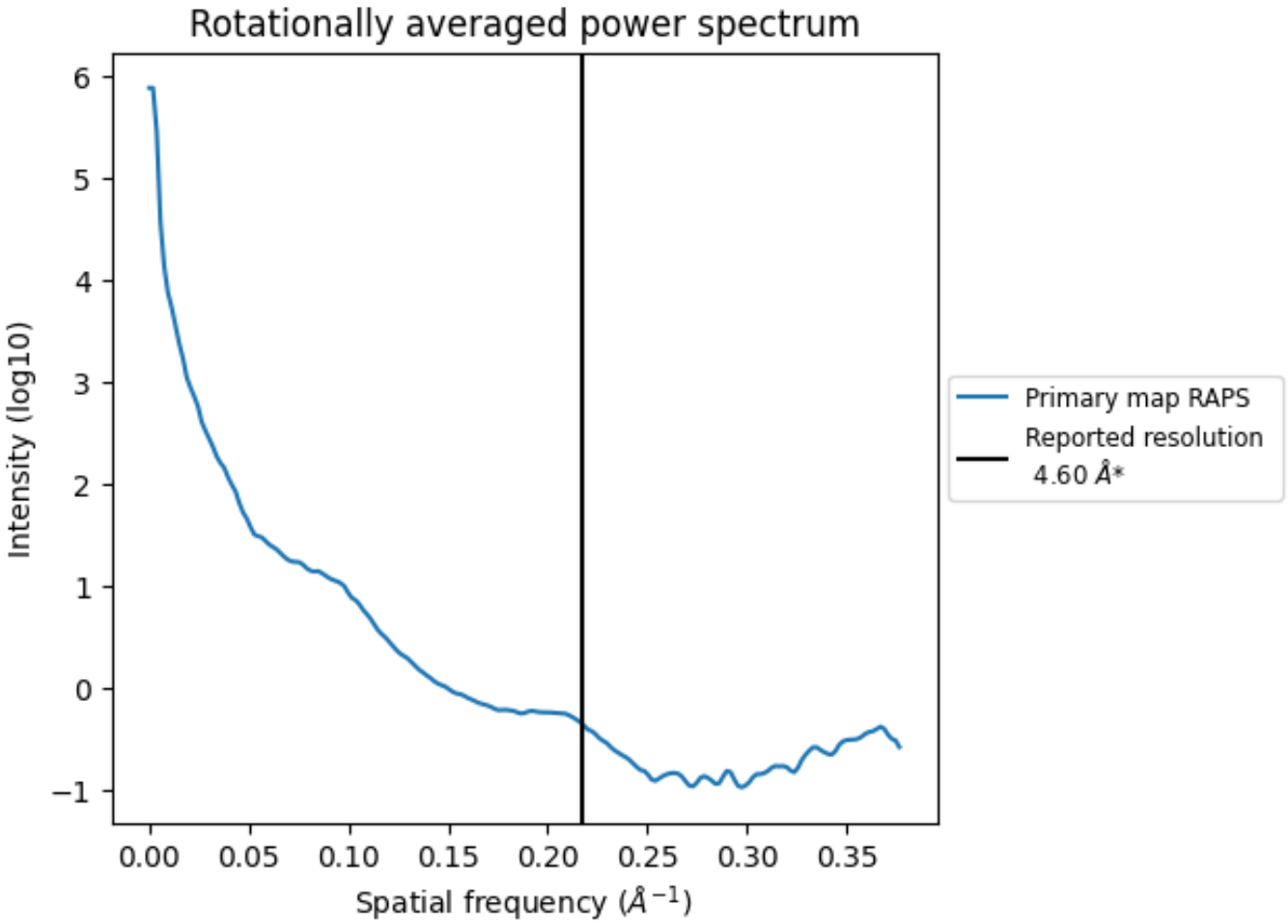
7.2 Volume estimate



The volume at the recommended contour level is 1155 nm^3; this corresponds to an approximate mass of 1044 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 0.217 Å^{-1}

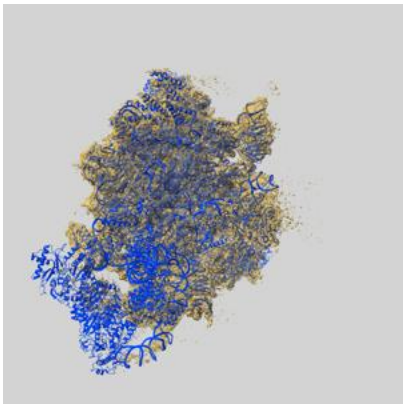
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

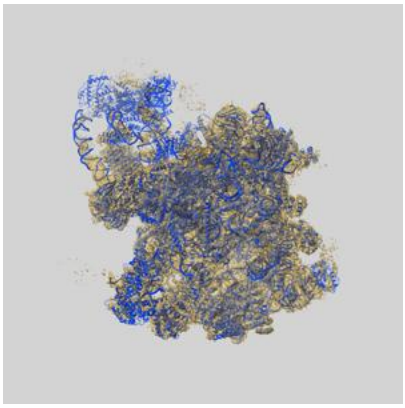
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30584 and PDB model 7D5S. Per-residue inclusion information can be found in section 3 on page 15.

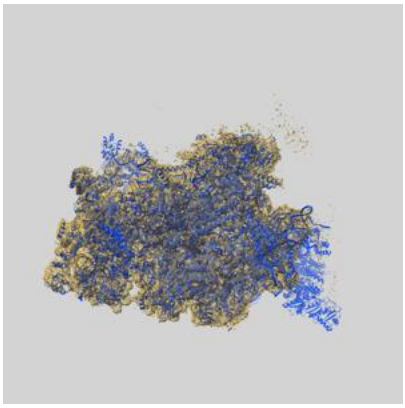
9.1 Map-model overlay



X



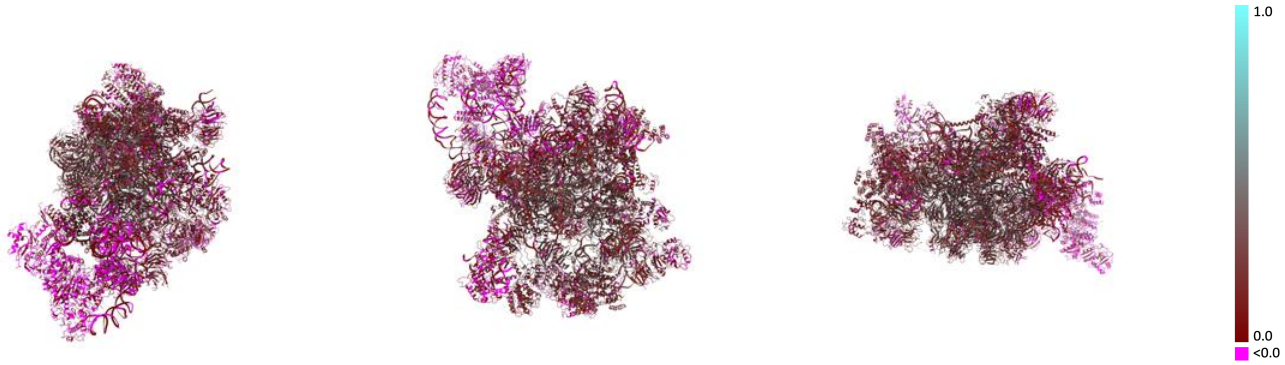
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 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.

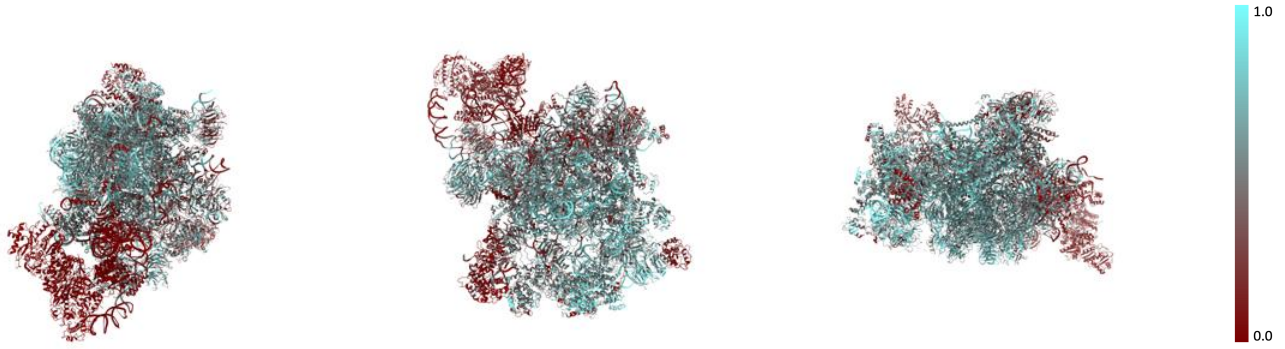
9.2 Q-score mapped to coordinate model (i)



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.

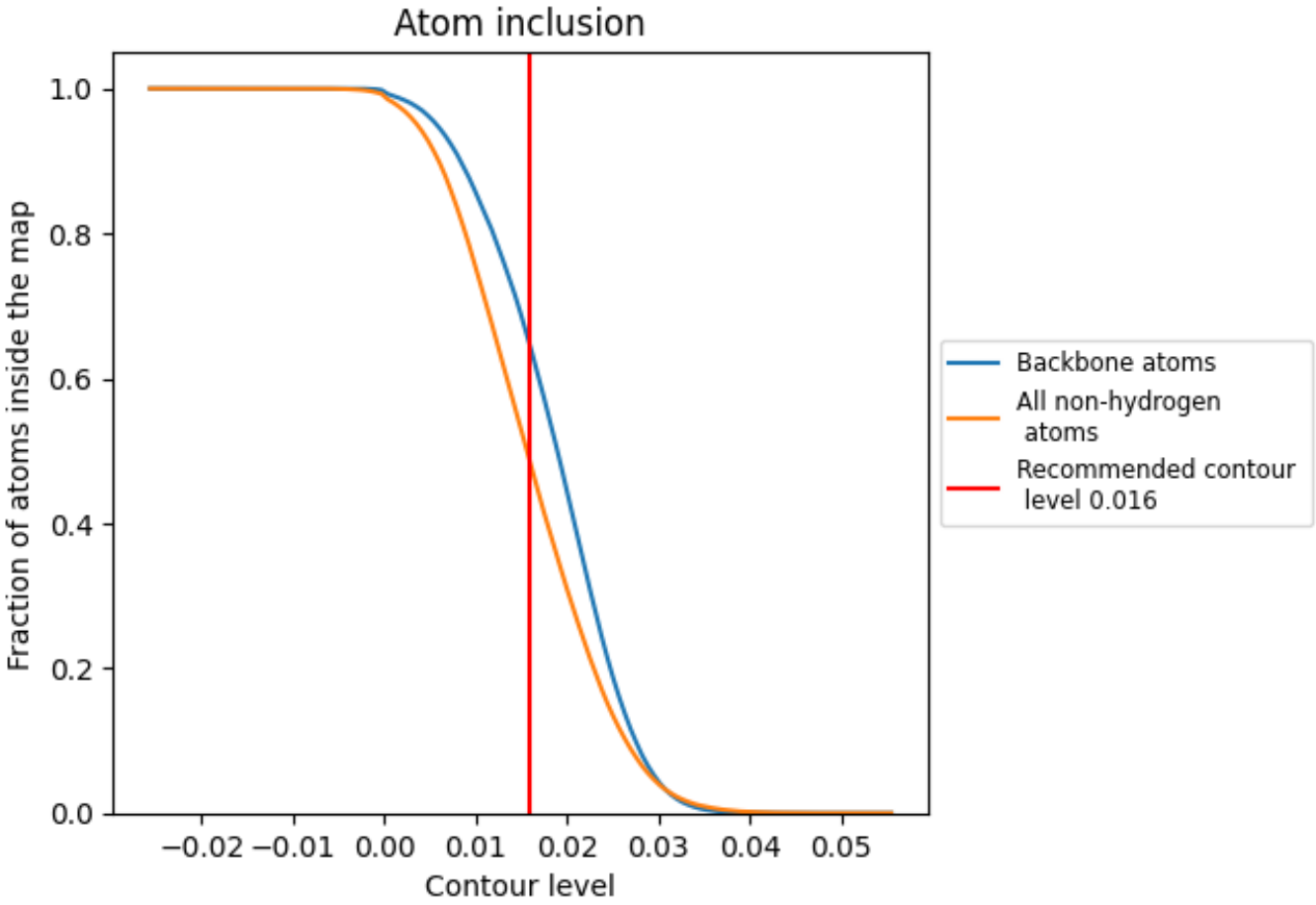
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 48% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4821	0.1810
3A	0.7747	0.2400
3B	0.5187	0.2300
3C	0.5634	0.2000
3D	0.5417	0.1850
3E	0.5949	0.2150
3F	0.3598	0.1270
3G	0.6173	0.2850
3H	0.4436	0.2030
5A	0.7377	0.2250
5B	0.5021	0.1960
5C	0.5186	0.2300
5D	0.5618	0.2480
5E	0.4919	0.2040
5F	0.5777	0.2600
5G	0.4709	0.2230
5H	0.4359	0.1930
5I	0.5635	0.1830
5J	0.3767	0.1950
5K	0.4330	0.1940
A4	0.6488	0.2330
A5	0.6404	0.2520
A8	0.4595	0.1310
A9	0.6134	0.2000
AE	0.3960	0.1900
AF	0.6418	0.2690
AG	0.6369	0.2400
B1	0.6166	0.2730
B2	0.5789	0.1620
B3	0.2622	0.0760
B6	0.4860	0.1650
B8	0.6632	0.2900
BE	0.6515	0.2670
RC	0.0181	0.0130
RD	0.0381	0.0320

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Chain	Atom inclusion	Q-score
RE	0.0027	0.0090
RF	0.0000	-0.0220
RG	0.3784	0.1680
RH	0.4416	0.2090
RI	0.5756	0.2190
RJ	0.5173	0.1940
RK	0.4682	0.1600
RN	0.3658	0.1580
RO	0.5489	0.1940
RQ	0.2303	0.1500
RS	0.1147	0.0550
RT	0.4887	0.1240
RW	0.2090	0.1480
SA	0.4455	0.1350
SG	0.5978	0.2850
SK	0.3333	0.1550
SN	0.0094	0.0370
SO	0.0057	-0.0100
SP	0.0106	0.0160
SR	0.5681	0.3000
ST	0.2812	0.1720
SY	0.2994	0.1390
Sd	0.5744	0.2920
X1	0.3115	0.1720