Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 08:03 am GMT

PDB ID	:	6QW6
EMDB ID	:	EMD-4658
Title	:	Structure of the human U5.U4/U6 tri-snRNP at 2.9A resolution.
Authors	:	Charenton, C.; Wilkinson, M.E.; Nagai, K.
Deposited on	:	2019-03-05
Resolution	:	2.92 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

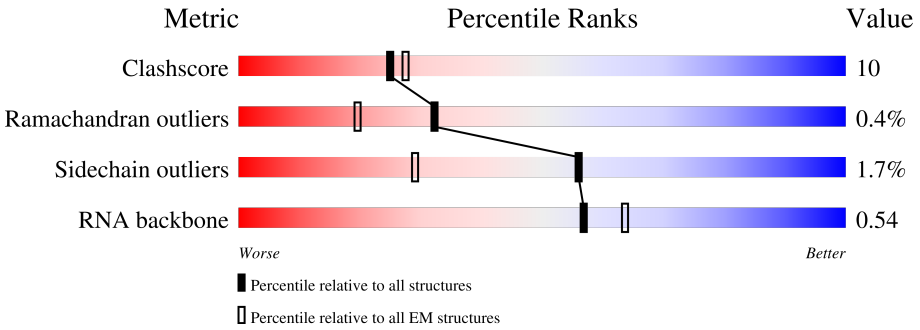
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.92 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	X	155	25% 18% 14% 68%
2	4	146	66% 42% 36% 8% 14%
3	41	119	67% 35% 29% • • 32%
3	51	119	67% 38% 26% • • 32%
4	42	118	75% 43% 35% 22%
4	52	118	83% 55% 27% • 17%
5	43	126	66% 46% 18% •• 34%

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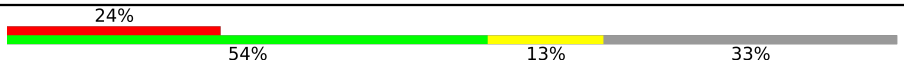
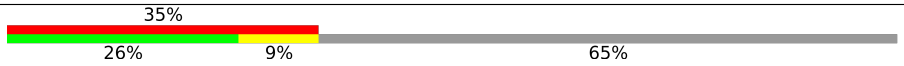
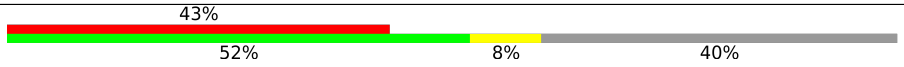
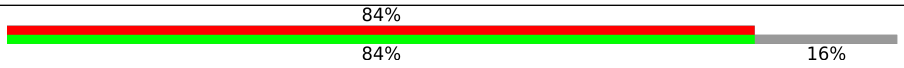
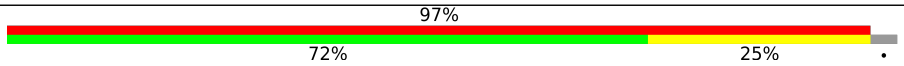
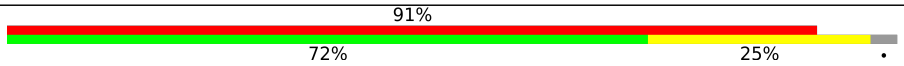
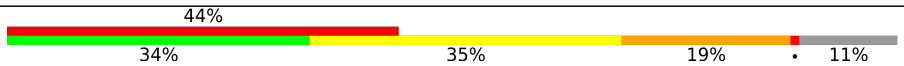
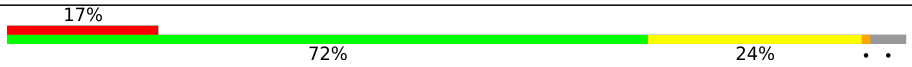
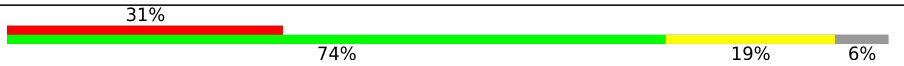
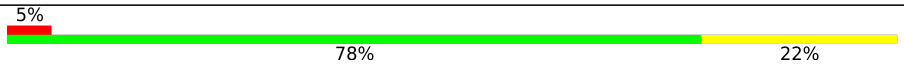
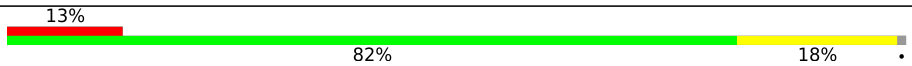
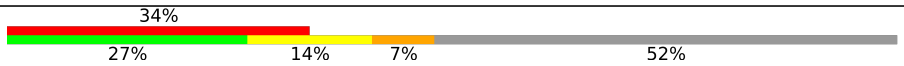
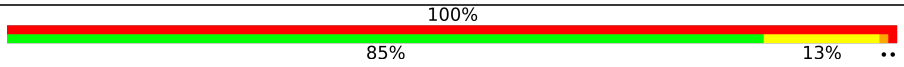
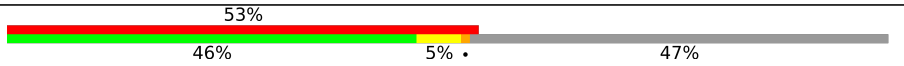
Mol	Chain	Length	Quality of chain
5	53	126	
6	4A	683	
7	4B	522	
8	4C	499	
9	4D	128	
10	4b	240	
10	5b	240	
11	4e	92	
11	5e	92	
12	4f	86	
12	5f	86	
13	4g	76	
13	5g	76	
14	5	117	
15	5A	2311	
16	5B	2136	
17	5C	853	
18	5D	142	
19	5J	941	
20	5O	357	
21	5X	820	
22	6	88	
23	62	95	
24	63	102	
25	64	139	

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Mol	Chain	Length	Quality of chain
26	65	91	84% 63% 18% 16%
27	66	80	90% 70% 18% 10%
28	67	103	75% 62% 12% 25%
29	68	96	99% 72% 21% 6%
30	R	480	19% 18% 78%
31	S	800	11% 12% 84%
32	U	555	6% 63% 19% 18%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 89236 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	49	Total	C	N	O	S	0	0
			394	247	74	69	4		

- Molecule 2 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	126	Total	C	N	O	P	0	0
			2690	1202	474	888	126		

- Molecule 3 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	41	81	Total	C	N	O	S	0	0
			641	408	112	118	3		
3	51	81	Total	C	N	O	S	0	0
			641	408	112	118	3		

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	42	92	Total	C	N	O	S	0	0
			737	463	138	131	5		
4	52	98	Total	C	N	O	S	0	0
			796	498	144	148	6		

- Molecule 5 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	43	83	Total	C	N	O	S	0	0
			652	409	115	122	6		
5	53	84	Total	C	N	O	S	0	0
			657	412	116	123	6		

- Molecule 6 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4A	239	Total	C	N	O	S	0	0
			1946	1237	360	342	7		

- Molecule 7 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	4B	359	Total	C	N	O	S	0	0
			2842	1793	509	521	19		

- Molecule 8 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	4C	301	Total	C	N	O	S	0	0
			2375	1486	418	456	15		

- Molecule 9 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	4D	123	Total	C	N	O	S	0	0
			955	604	170	176	5		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4b	82	Total	C	N	O	S	0	0
			669	423	122	117	7		
10	5b	73	Total	C	N	O	S	0	0
			594	376	108	103	7		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	4e	76	Total	C	N	O	S	0	0
			631	400	112	114	5		
11	5e	77	Total	C	N	O	S	0	0
			638	405	113	115	5		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	4f	72	Total	C	N	O	S	0	0
			562	364	93	100	5		
12	5f	73	Total	C	N	O	S	0	0
			567	367	94	101	5		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	4g	74	Total	C	N	O	S	0	0
			577	364	104	103	6		
13	5g	74	Total	C	N	O	S	0	0
			577	364	104	103	6		

- Molecule 14 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	5	104	Total	C	N	O	P	0	0
			2192	983	372	734	103		

- Molecule 15 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5A	2212	Total	C	N	O	S	0	0
			18366	11840	3193	3253	80		

- Molecule 16 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	5B	2001	Total	C	N	O	S	0	0
			16077	10235	2767	2991	84		

- Molecule 17 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5C	852	Total	C	N	O	S	0	0
			6727	4300	1127	1266	34		

- Molecule 18 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5D	141	Total	C	N	O	S	0	0
			1169	751	194	214	10		

- Molecule 19 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	5J	803	Total	C	N	O	S	0	0
			6316	3963	1155	1170	28		

- Molecule 20 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	5O	306	Total	C	N	O	S	0	0
			2394	1501	422	457	14		

- Molecule 21 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	5X	583	Total	C	N	O	S	7	0
			4780	3014	855	893	18		

- Molecule 22 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	6	42	Total	C	N	O	P	0	0
			897	401	161	293	42		

- Molecule 23 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	62	95	Total	C	N	O	S	0	0
			761	486	126	145	4		

- Molecule 24 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	63	85	Total	C	N	O	S	0	0
			699	440	120	136	3		

- Molecule 25 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	64	73	Total	C	N	O	S	0	0
			596	376	105	109	6		

- Molecule 26 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	65	76	Total	C	N	O	S	0	0
			587	373	96	114	4		

- Molecule 27 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	66	72	Total	C	N	O	S	0	0
			567	360	97	108	2		

- Molecule 28 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	67	77	Total	C	N	O	S	0	0
			604	383	102	116	3		

- Molecule 29 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	68	95	Total	C	N	O	S	0	0
			722	446	124	151	1		

- Molecule 30 is a protein called RNA-binding protein 42.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	R	106	Total	C	N	O	S	0	0
			874	553	160	157	4		

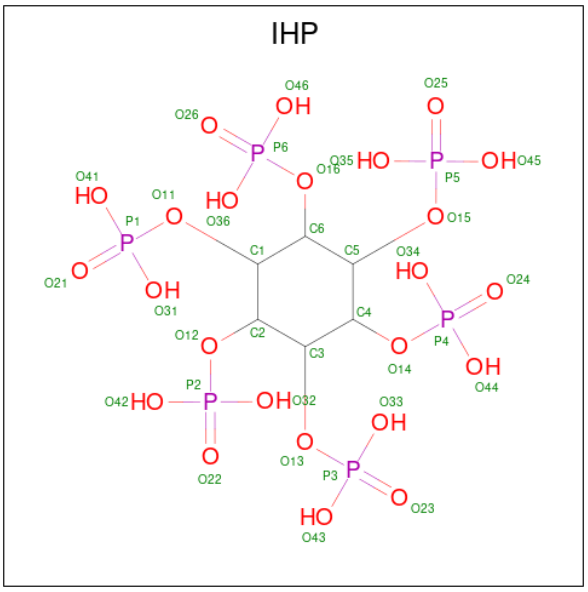
- Molecule 31 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	S	126	Total	C	N	O	S	0	0
			947	594	174	174	5		

- Molecule 32 is a protein called U4/U6.U5 tri-snRNP-associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	U	456	Total	C	N	O	S	0	0
			3750	2427	635	674	14		

- Molecule 33 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).

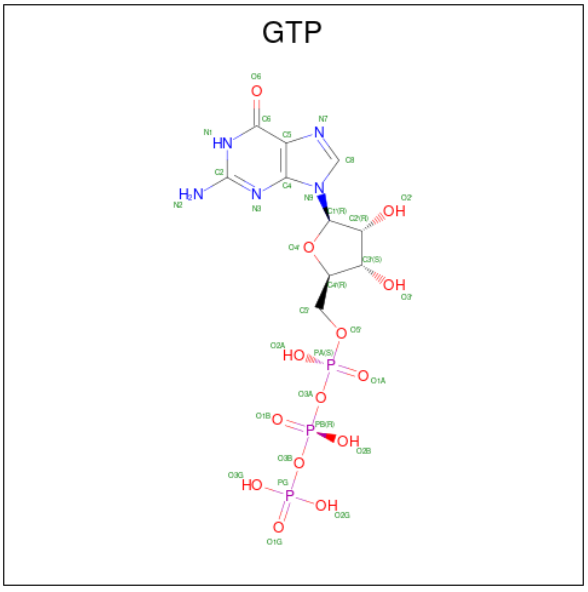


Mol	Chain	Residues	Atoms				AltConf
33	5A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
34	5C	1	Total	Mg	0
			1	1	

- Molecule 35 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
35	5C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

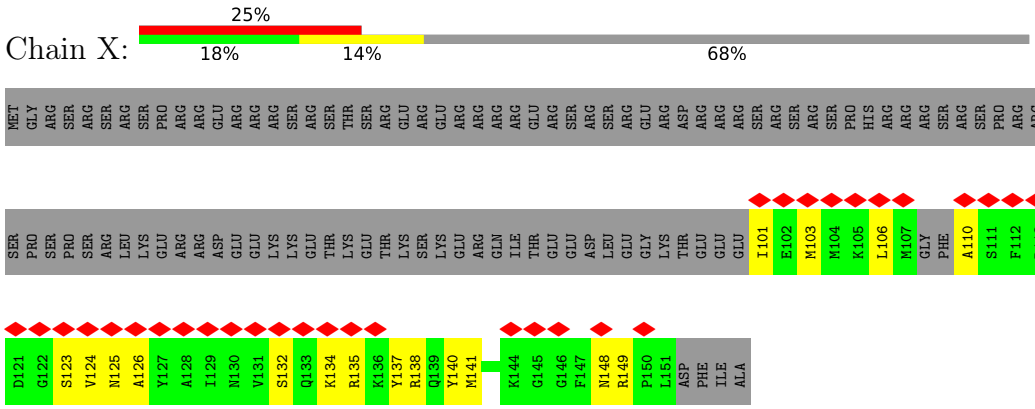
Mol	Chain	Residues	Atoms		AltConf
36	U	1	Total	Zn	0
			1	1	

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.

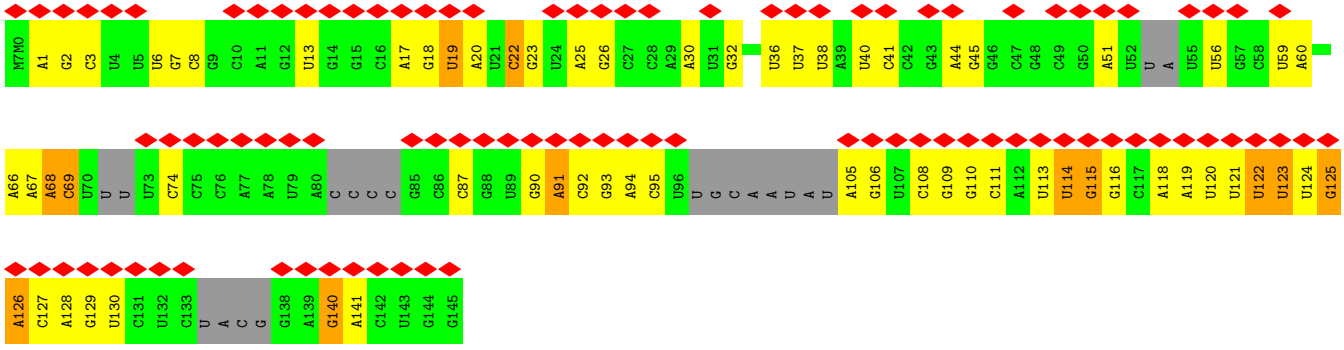
• Molecule 1: U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein

Chain X:



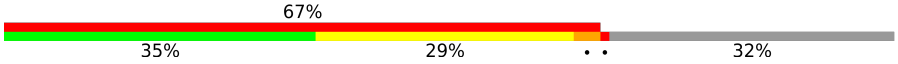
• Molecule 2: U4 snRNA

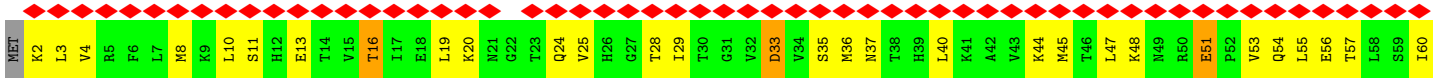
Chain 4:

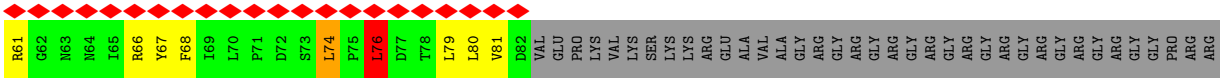


• Molecule 3: Small nuclear ribonucleoprotein Sm D1

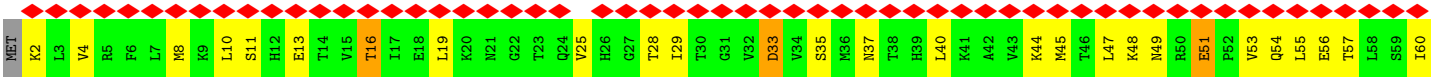
Chain 41:

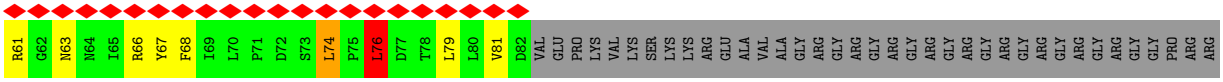




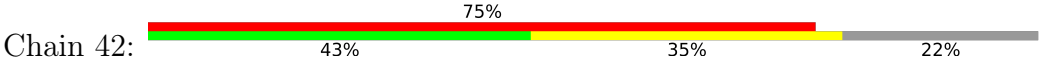


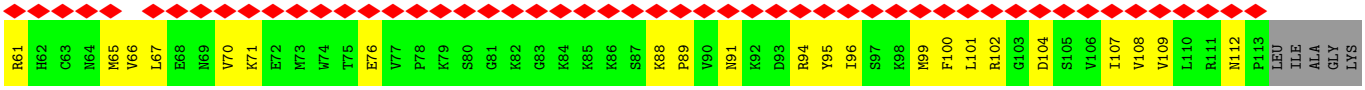
• Molecule 3: Small nuclear ribonucleoprotein Sm D1



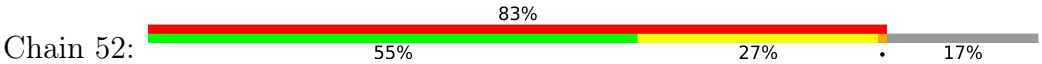


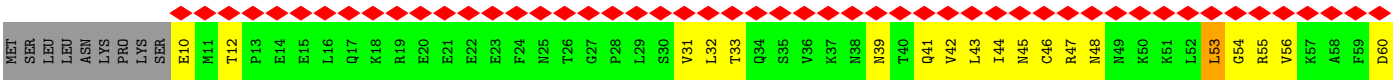
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

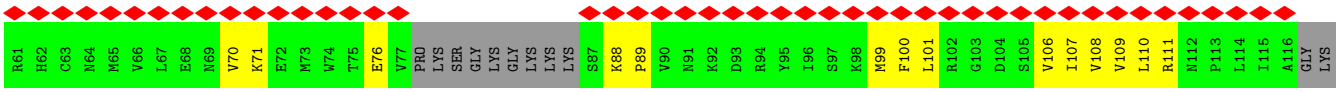




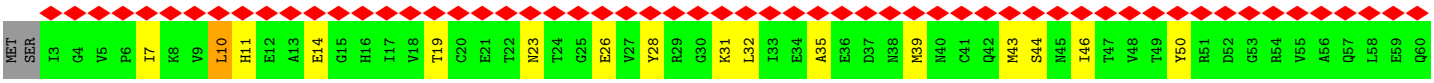
• Molecule 4: Small nuclear ribonucleoprotein Sm D2

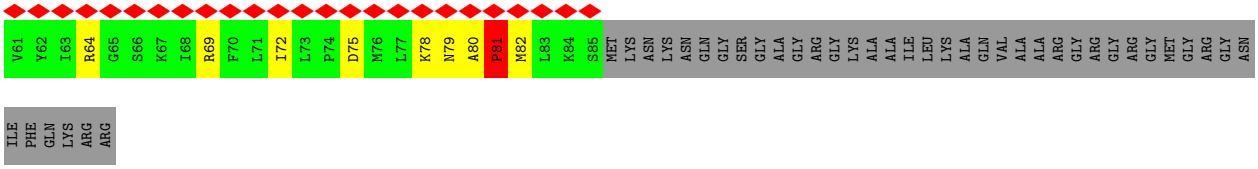






• Molecule 5: Small nuclear ribonucleoprotein Sm D3





• Molecule 5: Small nuclear ribonucleoprotein Sm D3

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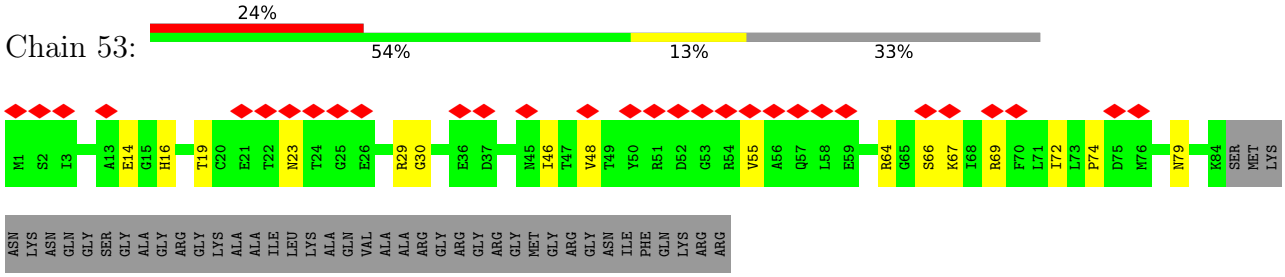
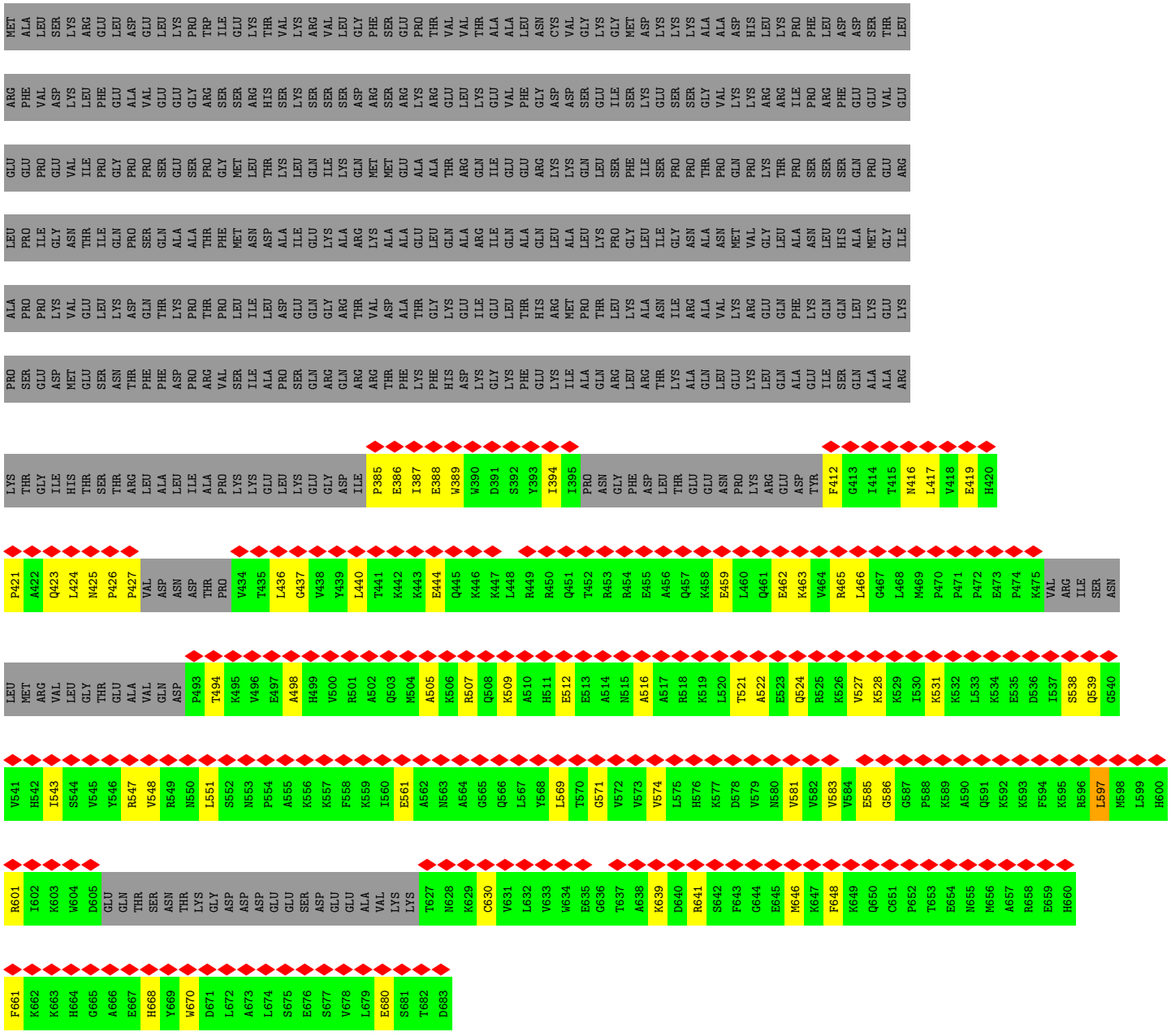


• Molecule 6: U4/U6 small nuclear ribonucleoprotein Prp3

Chain 4A:



• Molecule 7: U4/U6 small nuclear ribonucleoprotein Prp4

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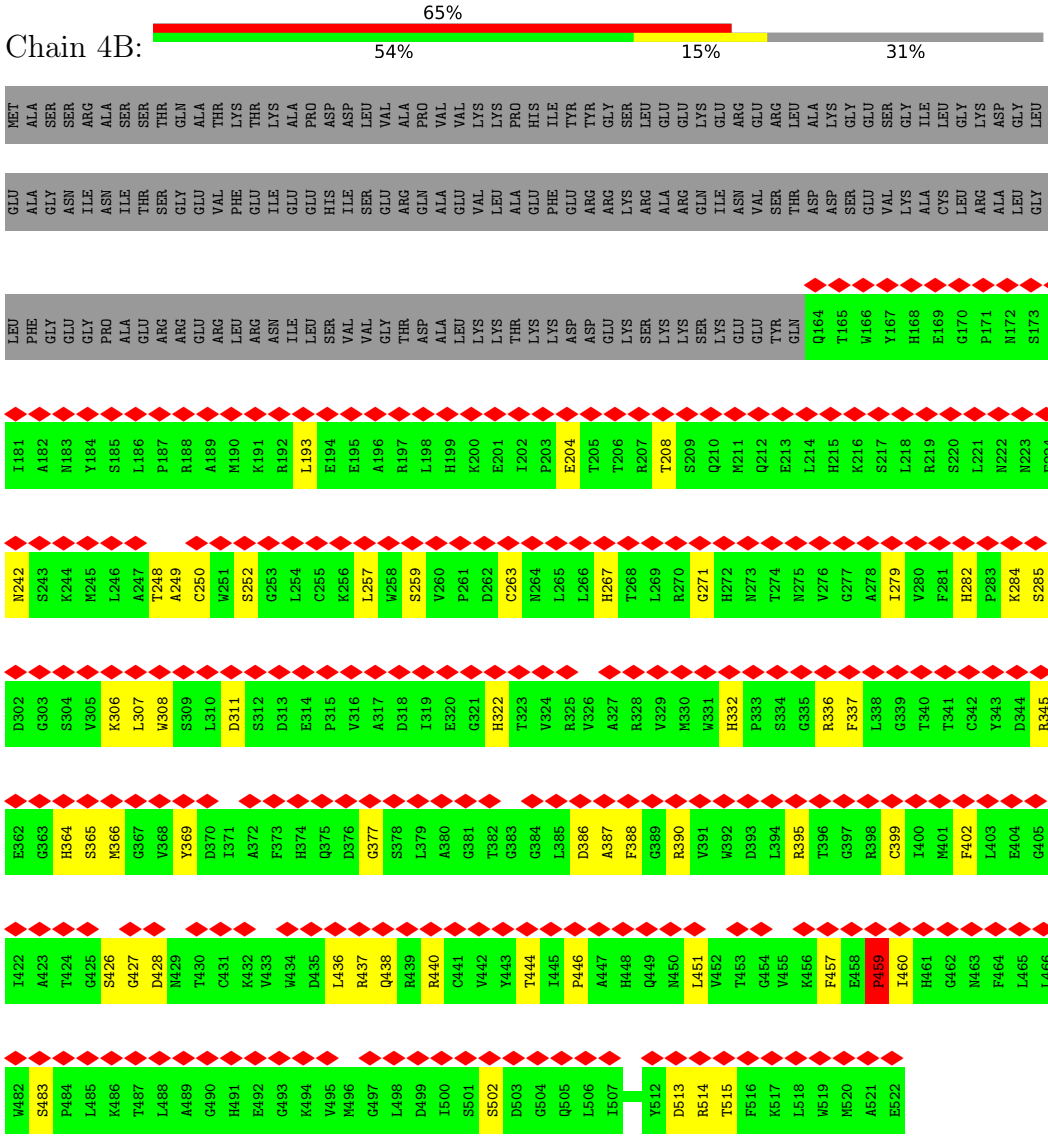

• Molecule 8: U4/U6 small nuclear ribonucleoprotein Prp31

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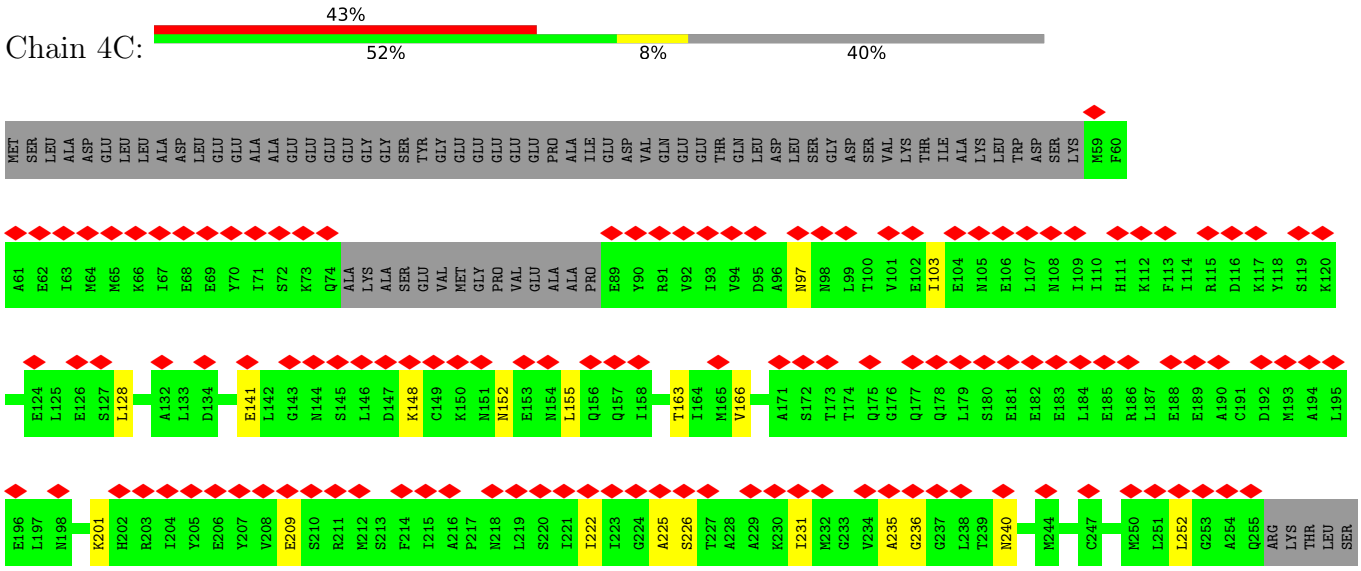
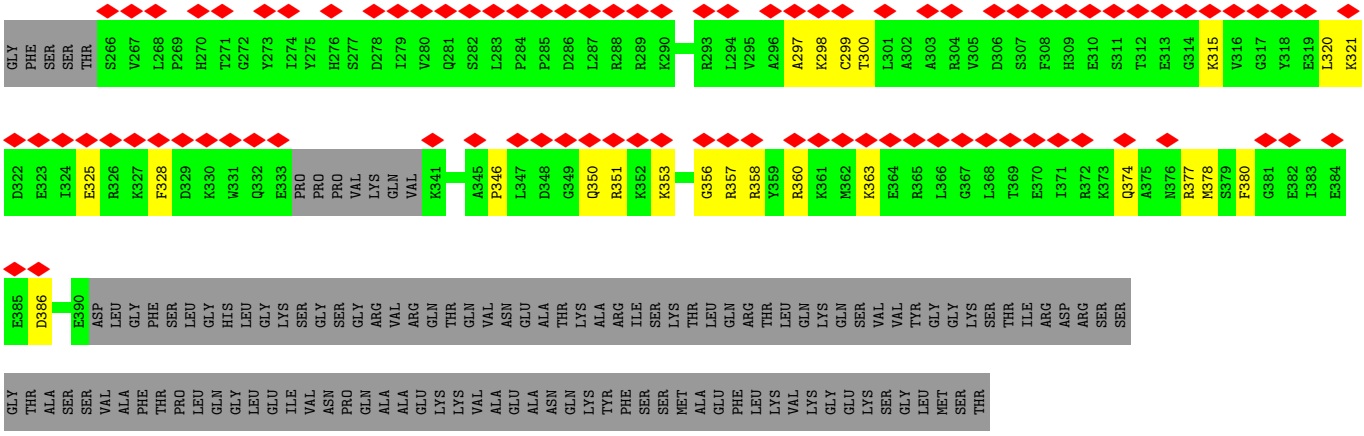
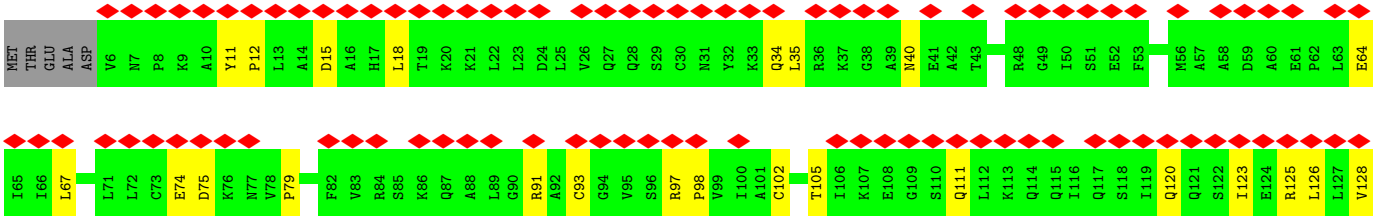




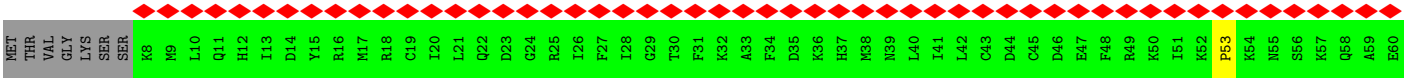
• Molecule 9: NHP2-like protein 1

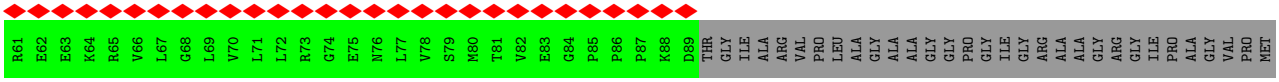
Chain 4D:

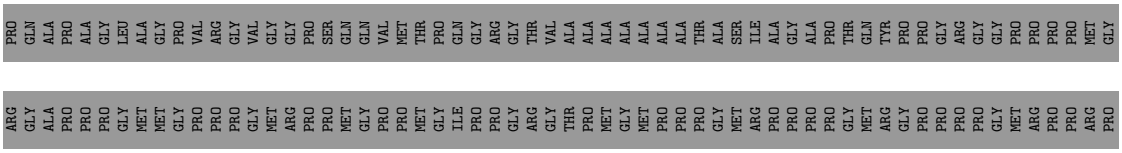


• Molecule 10: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain 4b:

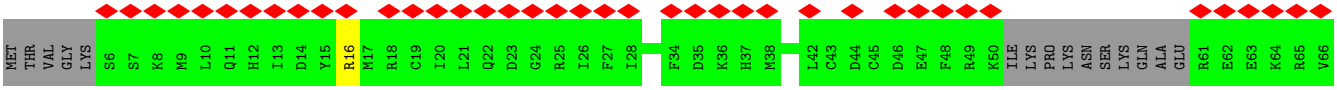


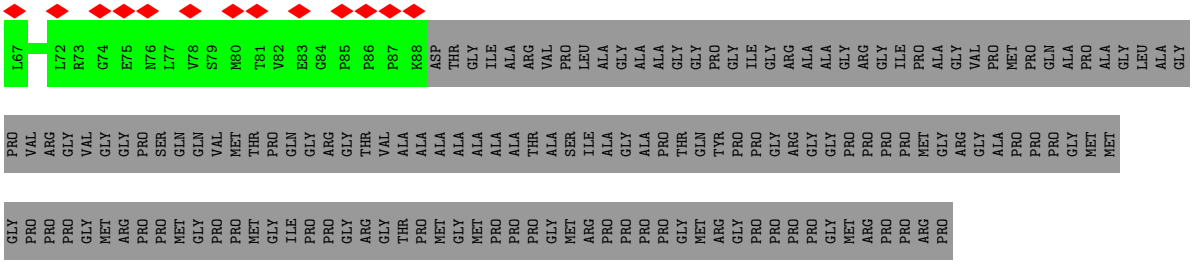




• Molecule 10: Small nuclear ribonucleoprotein-associated proteins B and B'

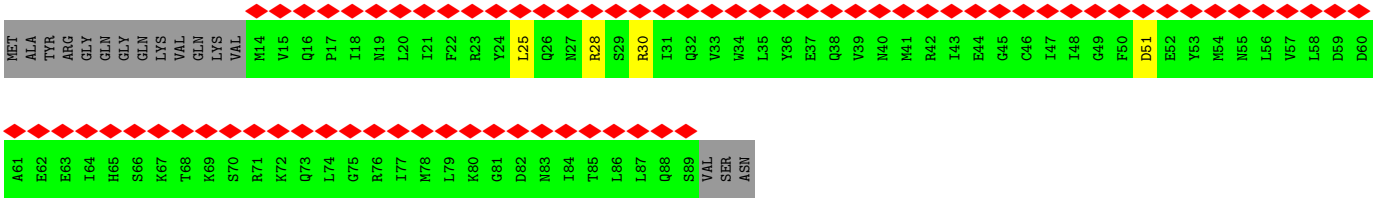
Chain 5b:





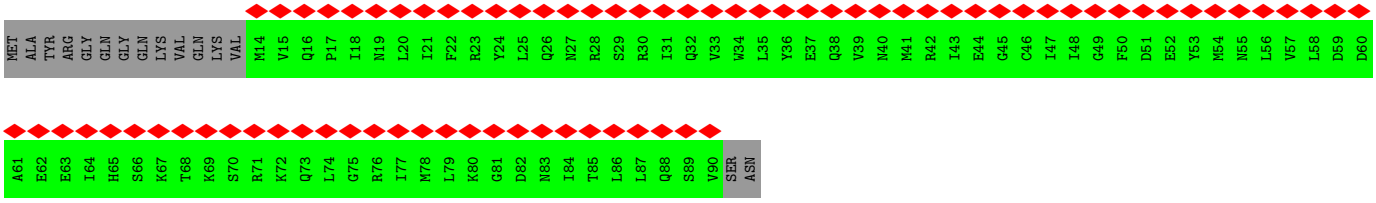
• Molecule 11: Small nuclear ribonucleoprotein E

Chain 4e:



• Molecule 11: Small nuclear ribonucleoprotein E

Chain 5e:



• Molecule 12: Small nuclear ribonucleoprotein F

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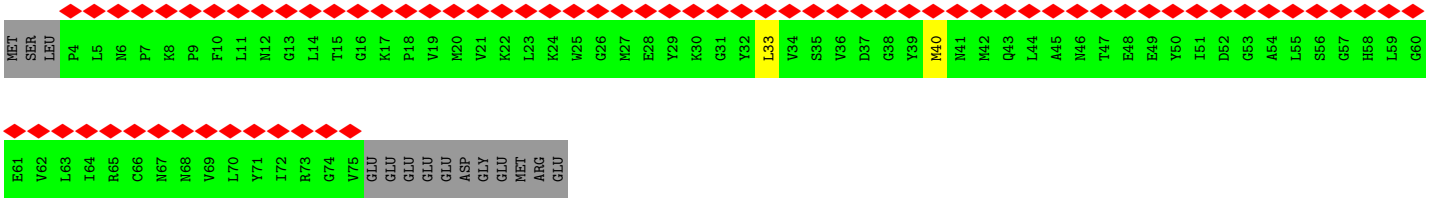
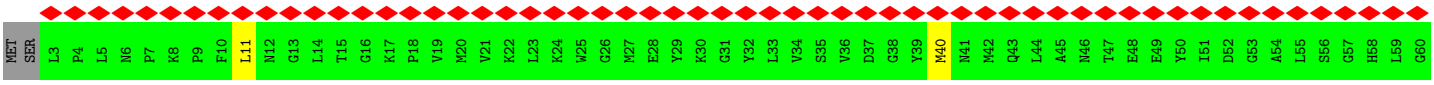
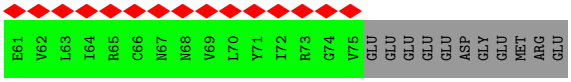


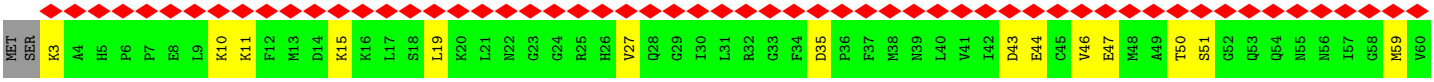
• Molecule 12: Small nuclear ribonucleoprotein F

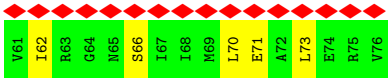
Chain 5f:



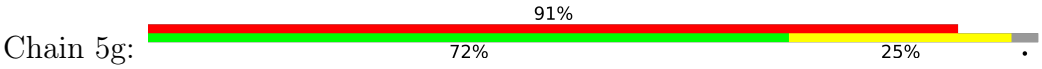


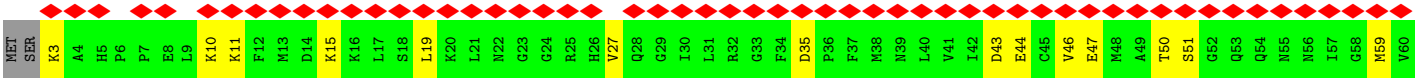
• Molecule 13: Small nuclear ribonucleoprotein G

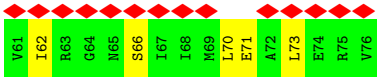




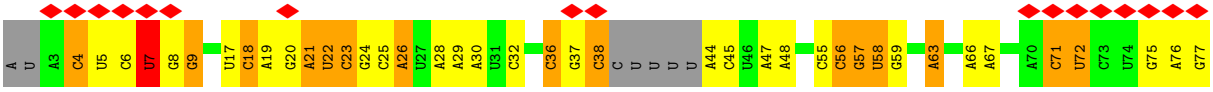
• Molecule 13: Small nuclear ribonucleoprotein G

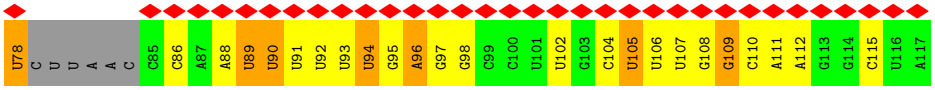




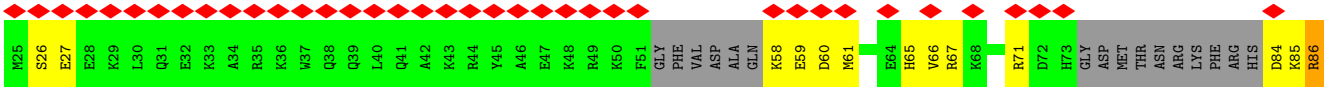


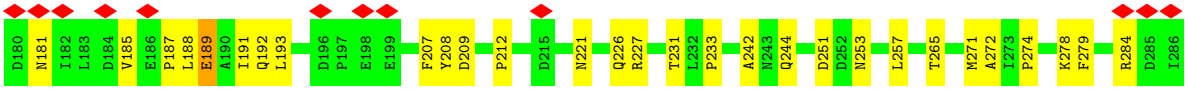
• Molecule 14: U5 snRNA

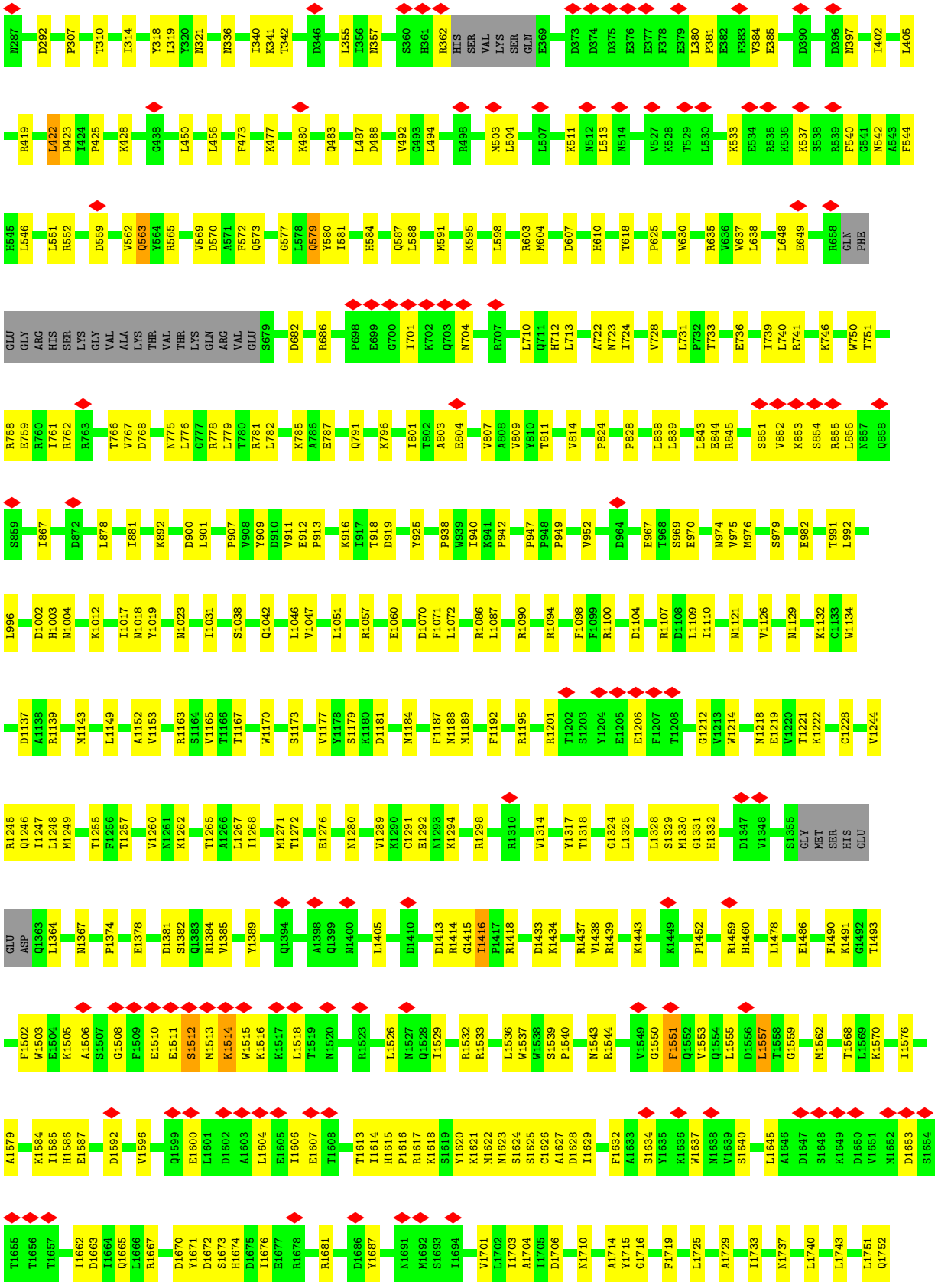




• Molecule 15: Pre-mRNA-processing-splicing factor 8



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B419 L422 D423 I424 P425 K428 G438 L450 L456 F473 K477 K480 Q483 L487 D488 V492 G493 L494 R498 M503 L504 L507 K511 N512 L513 N514 V527 K528 T529 L530 K533 E534 R535 K536 K537 S538 R539 F540 G541 N542 A543 F544
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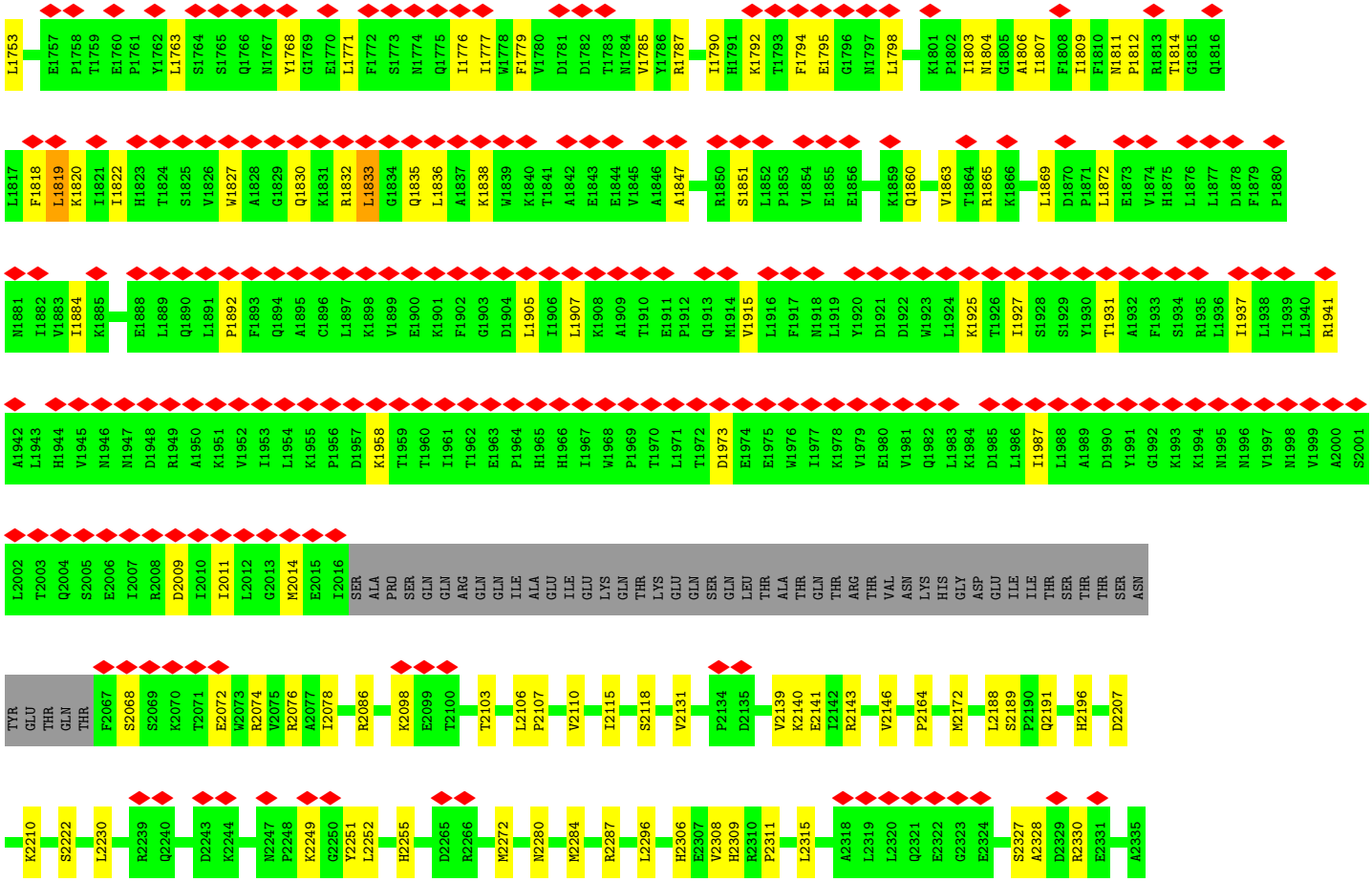
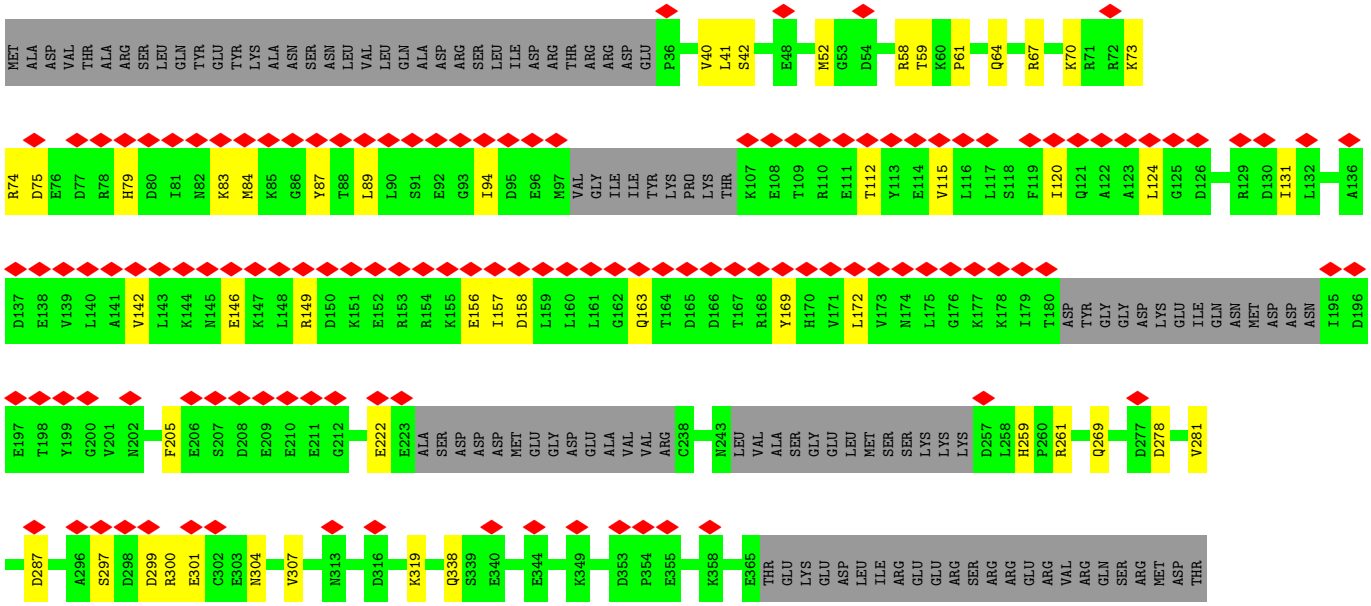


• Molecule 16: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain 5B:



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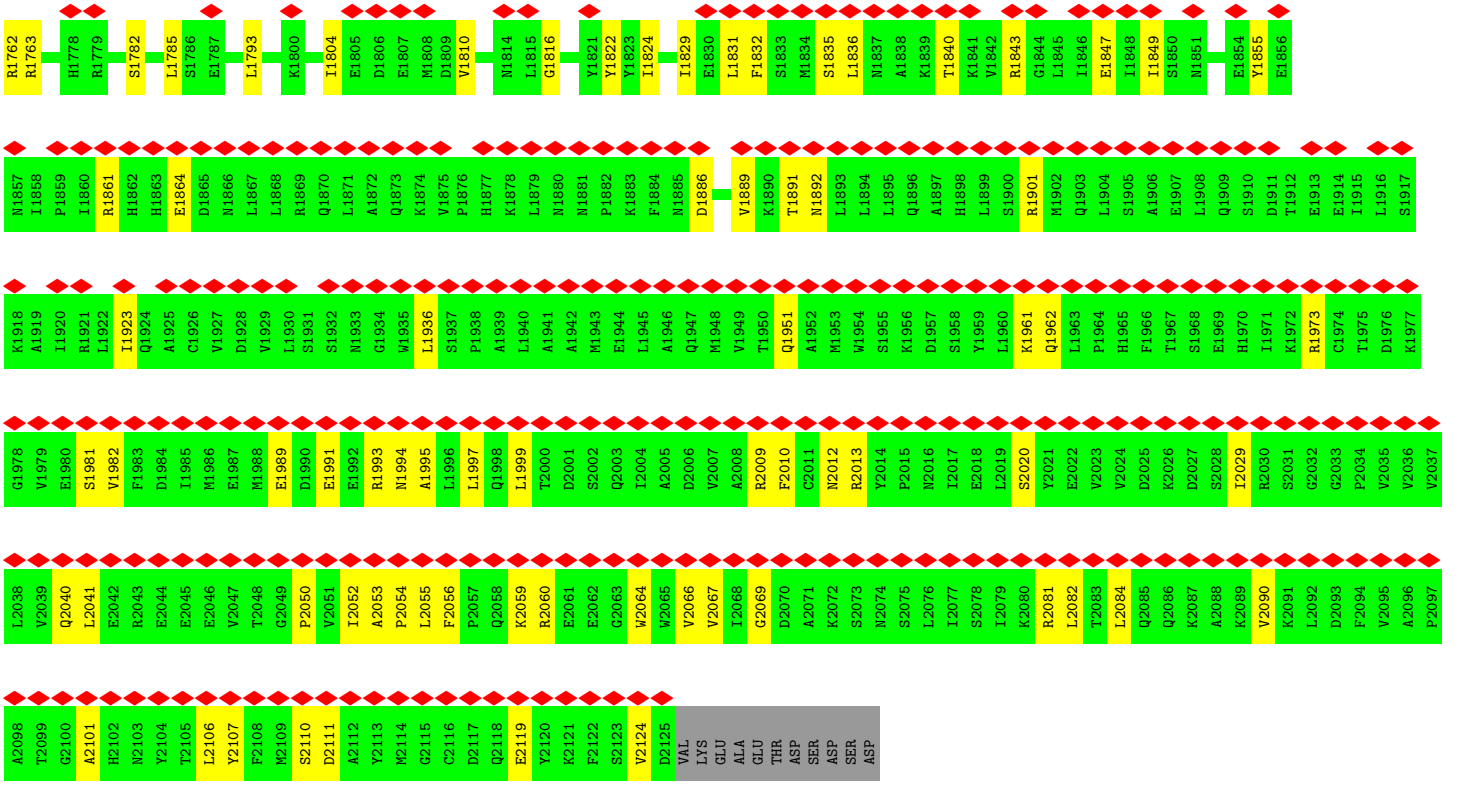
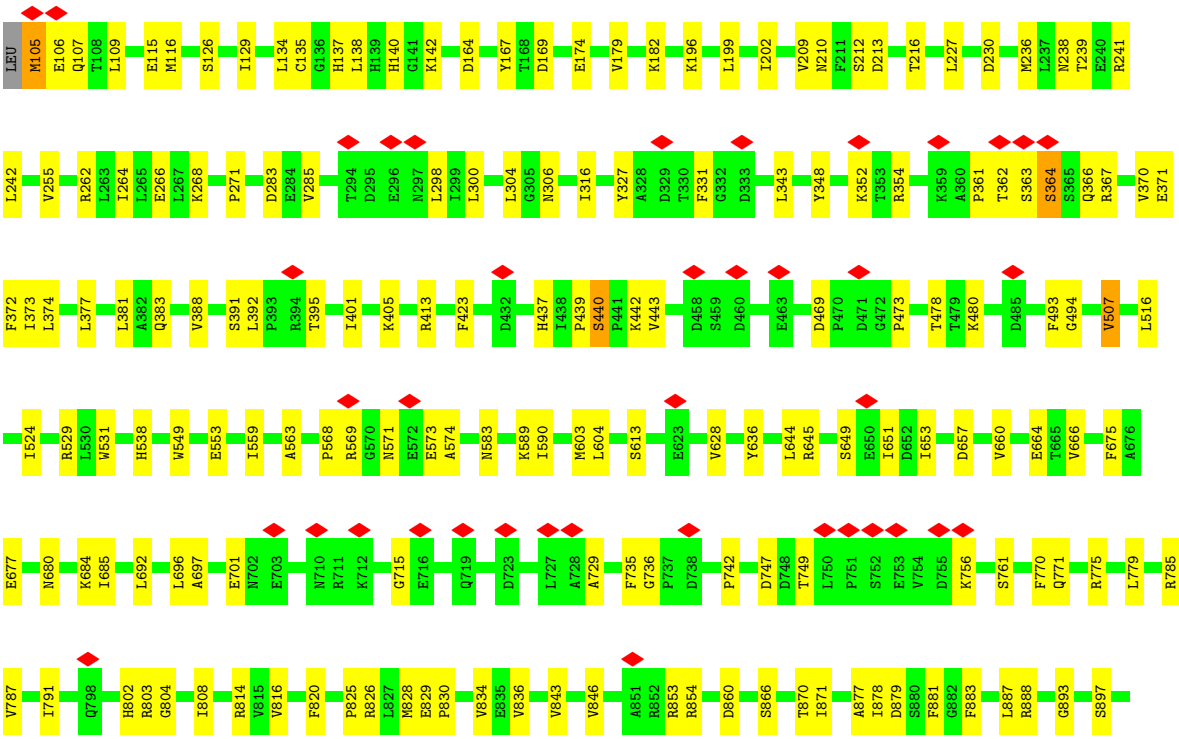
D1415 L1416 K1417 L1418 K1421 I1424 P1429 D1433 I1434 L1435 S1436 R1437 R1438 Q1441 R1442 K1443 N1444 N1447 I1448 N1449 D1454 E1455 V1456 E1462 N1463 V1469 I1470 R1473 I1481 E1482 R1483 I1487 L1490 S1491 S1492 D1499 L1504 T1509 F1514 H1515 P1516 N1517 V1518
R1519 P1520 V1521 T1535 R1538 L1539 K1544 K1556 K1557 R1566 K1567 Q1568 T1569 T1572 A1582 D1583 I1584 Q1585 R1586 Q1587 T1593 E1594 K1595 D1596 L1597 I1598 P1599 Y1600 L1601 E1602 K1603 L1604 S1605 D1606 S1607 L1614 N1615 G1616 V1617 H1621 E1622 G1623 L1624 S1625 P1626 M1627 E1628 R1629 R1630
Q1634 V1643 V1644 V1645 W1652 N1655 H1659 I1663 M1664 D1665 T1666 K1672 I1673 H1674 A1675 Y1676 A1691 L1695 D1698 E1699 G1700 R1701 I1704 D1712 E1720 P1723 D1729 H1735 F1736 N1737 A1738 K1743 E1746 Q1749 D1750 D1753 Y1754 L1755 T1756 Y1761

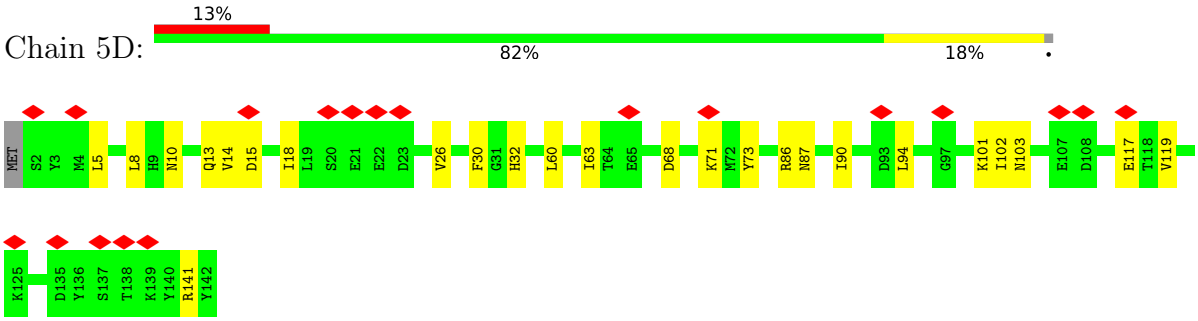


• Molecule 17: 116 kDa U5 small nuclear ribonucleoprotein component

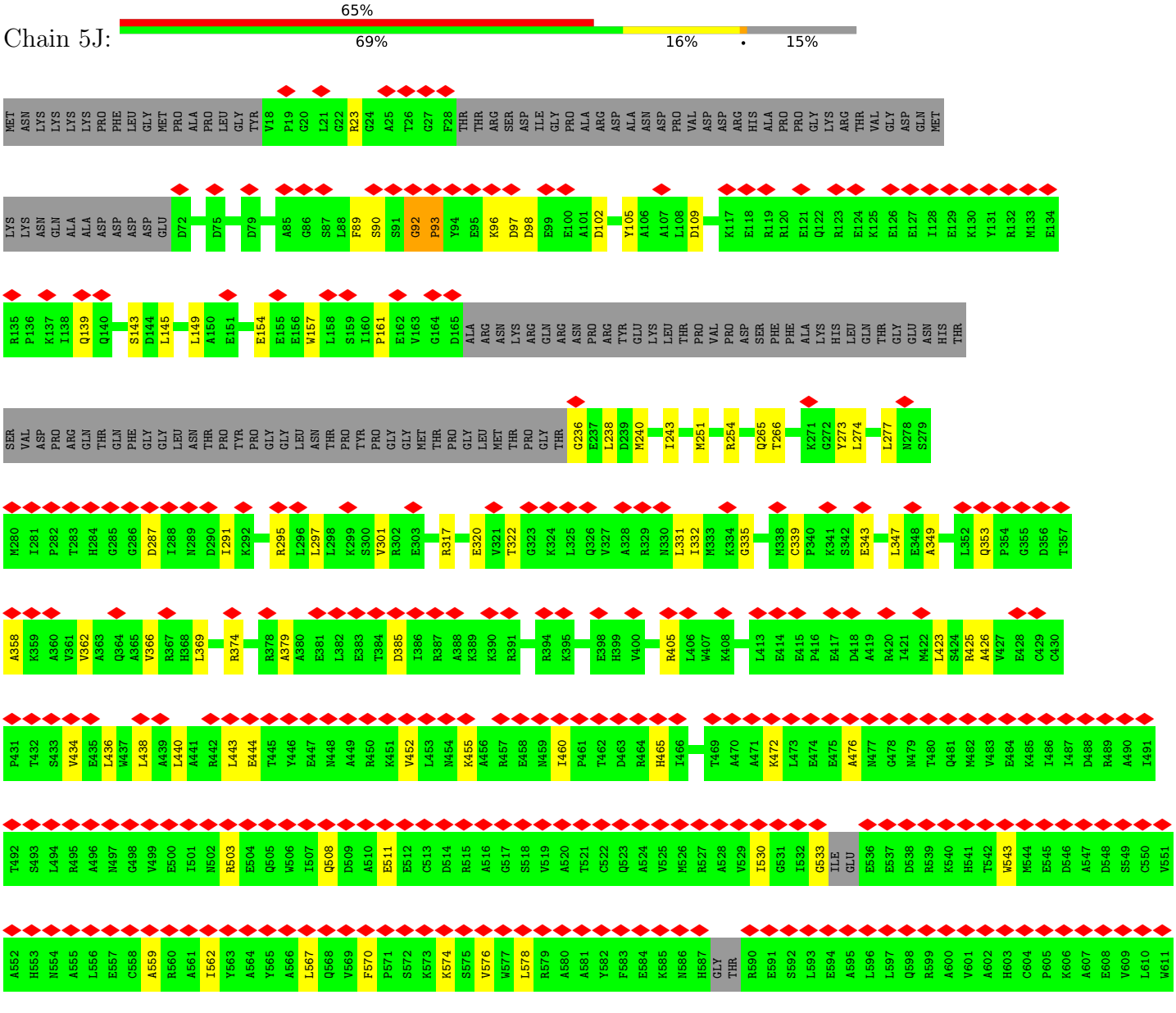
Chain 5C:

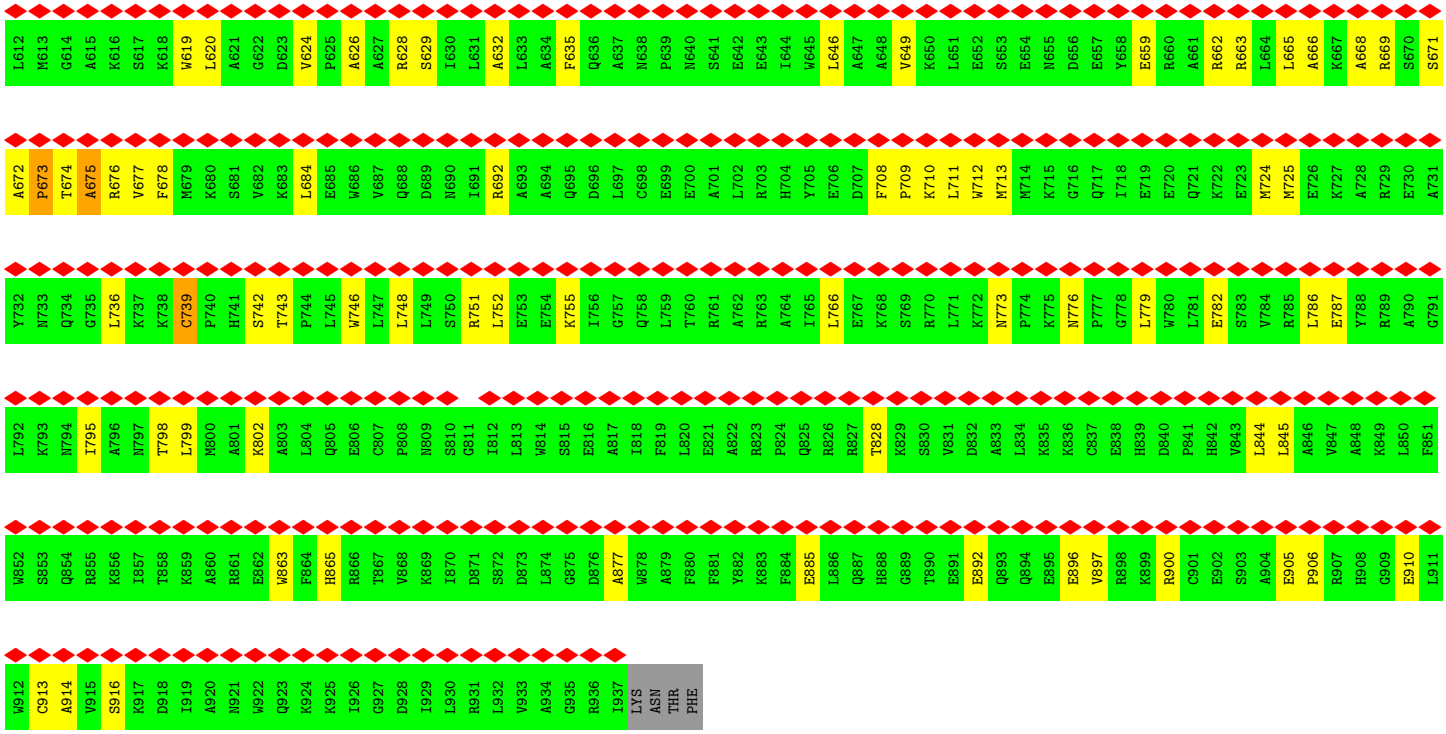


• Molecule 18: Thioredoxin-like protein 4A



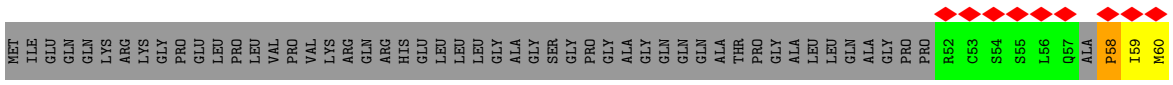
• Molecule 19: Pre-mRNA-processing factor 6

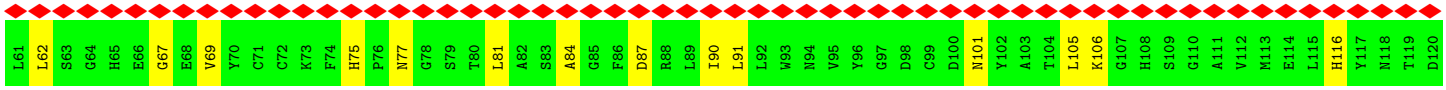


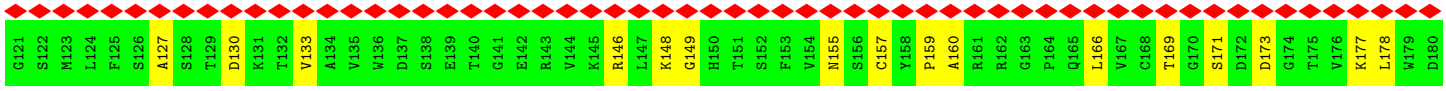


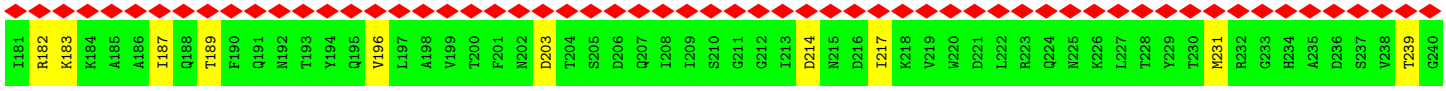
• Molecule 20: U5 small nuclear ribonucleoprotein 40 kDa protein

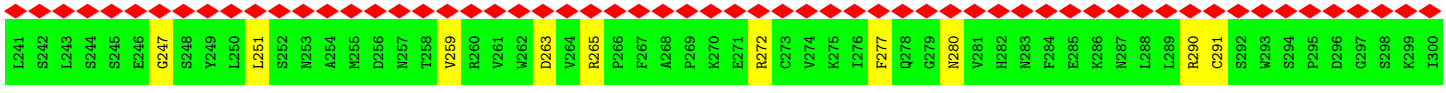
Chain 5O:

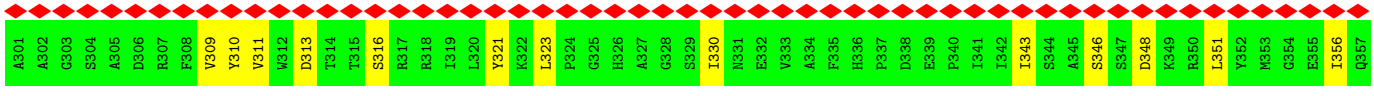






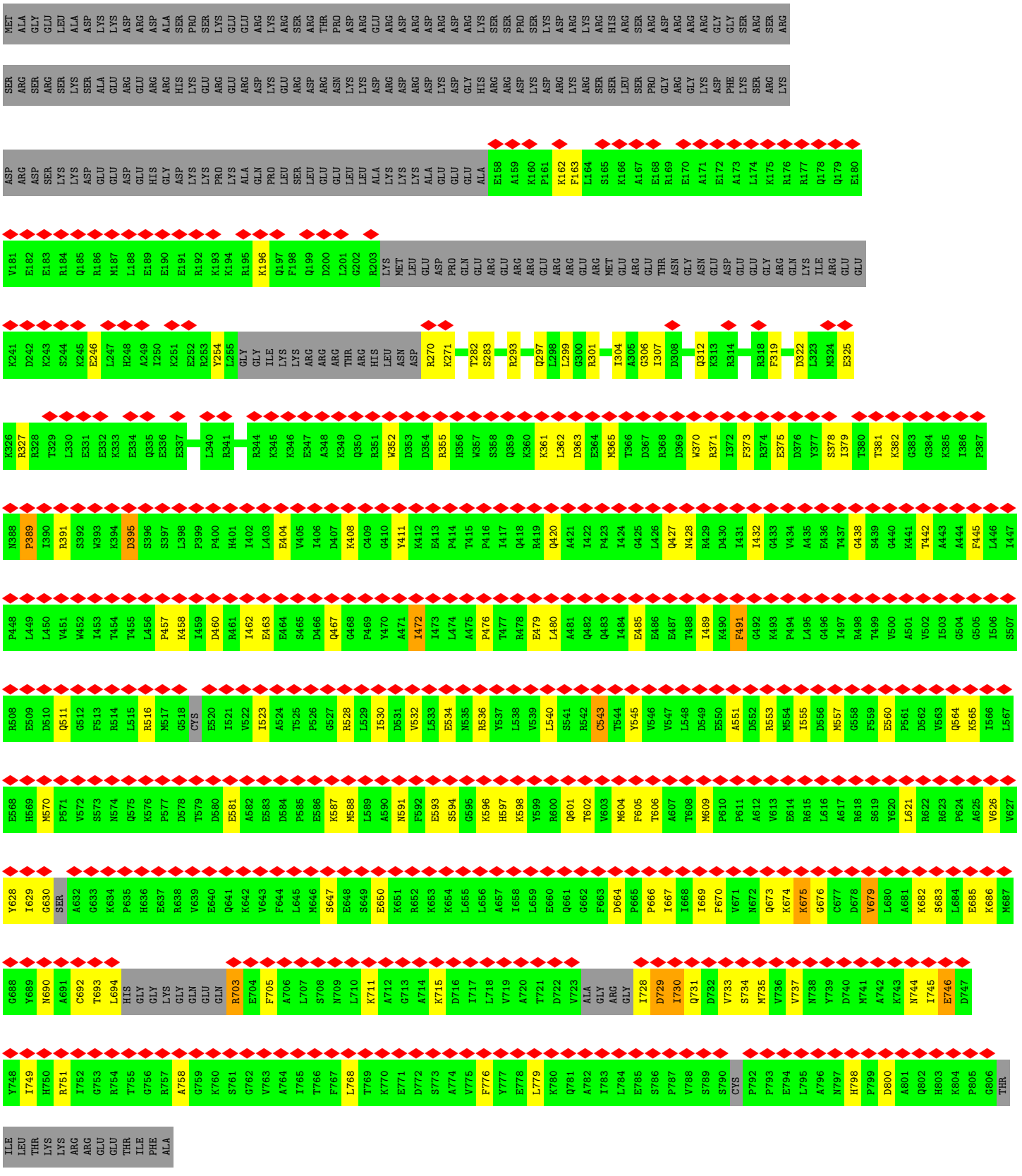






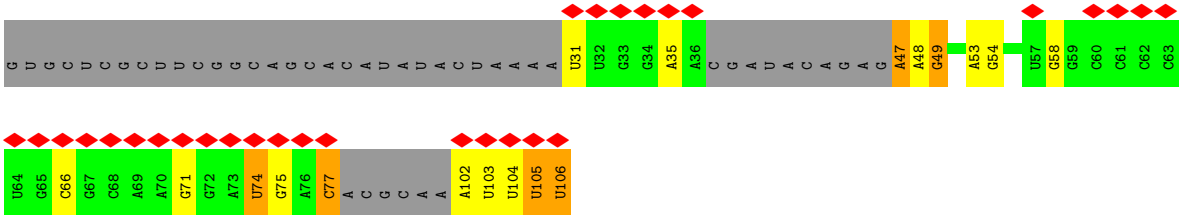
• Molecule 21: Probable ATP-dependent RNA helicase DDX23

Chain 5X:

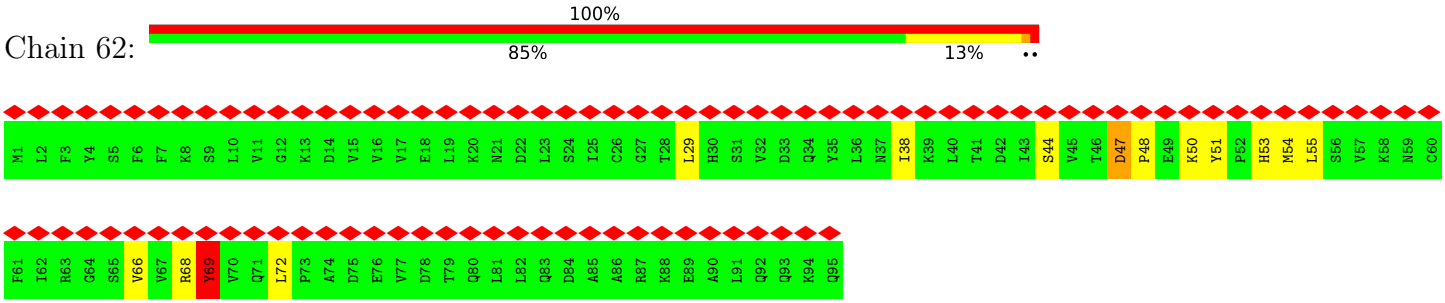


- Molecule 22: U6 snRNA

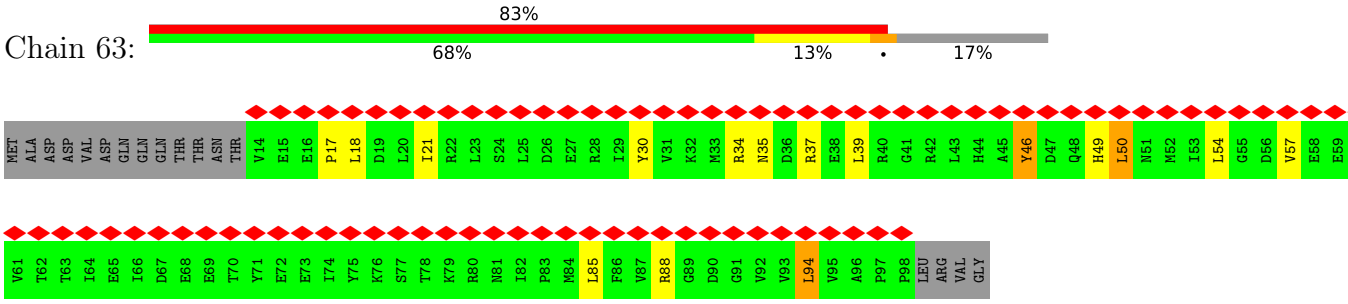
Chain 6:



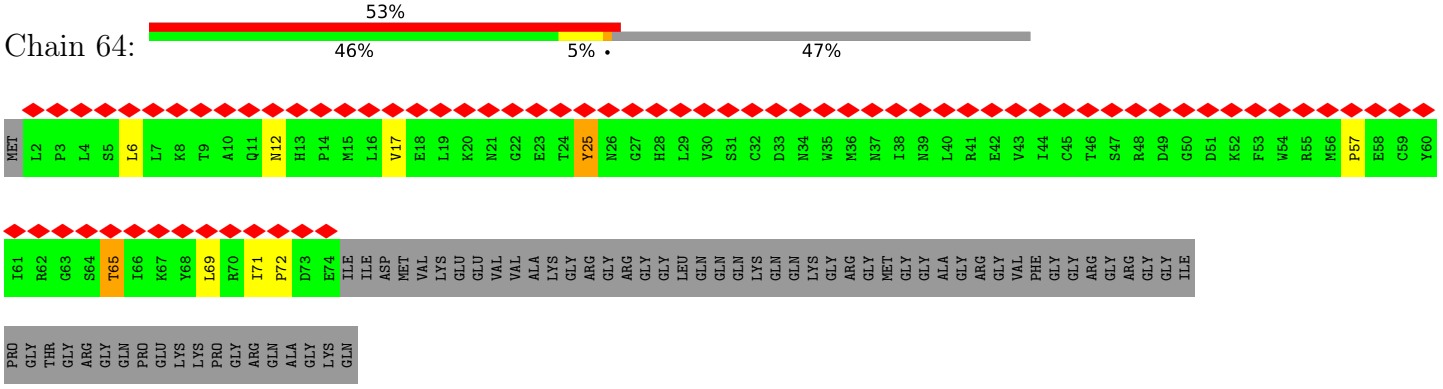
• Molecule 23: U6 snRNA-associated Sm-like protein LSm2



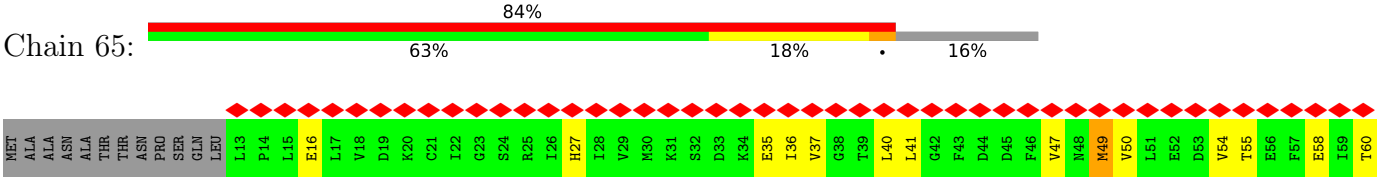
• Molecule 24: U6 snRNA-associated Sm-like protein LSm3

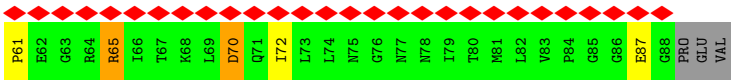


• Molecule 25: U6 snRNA-associated Sm-like protein LSm4



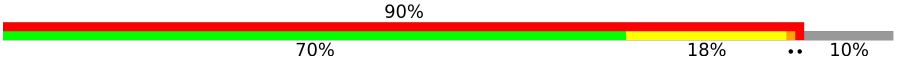
• Molecule 26: U6 snRNA-associated Sm-like protein LSm5

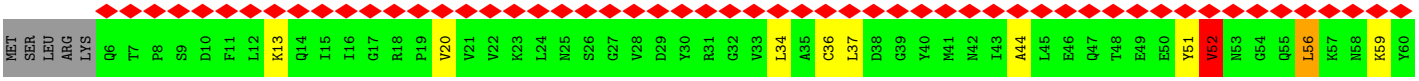


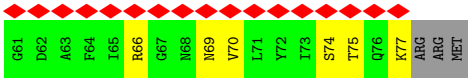


• Molecule 27: U6 snRNA-associated Sm-like protein LSm6

Chain 66:

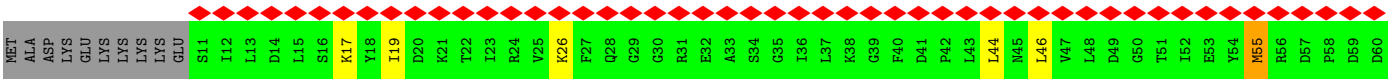


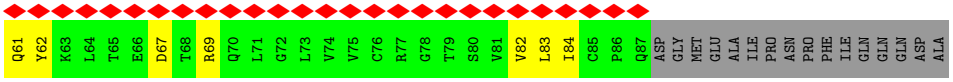




• Molecule 28: U6 snRNA-associated Sm-like protein LSm7

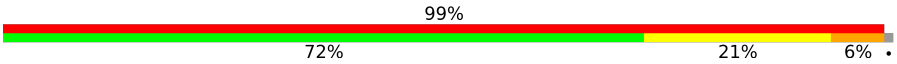
Chain 67:

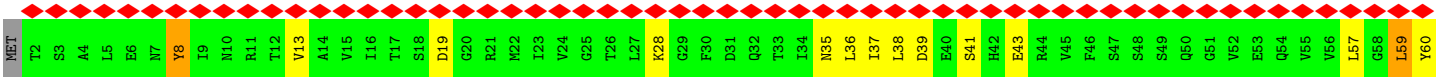


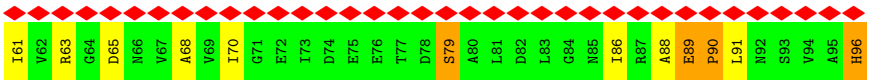


• Molecule 29: U6 snRNA-associated Sm-like protein LSm8

Chain 68:

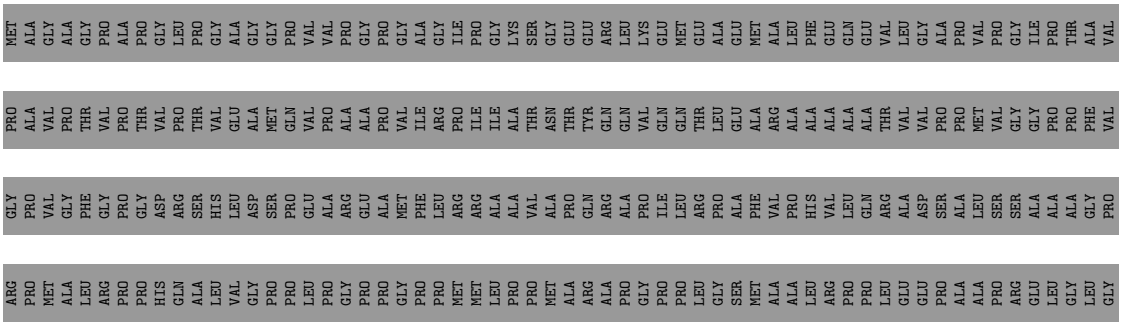


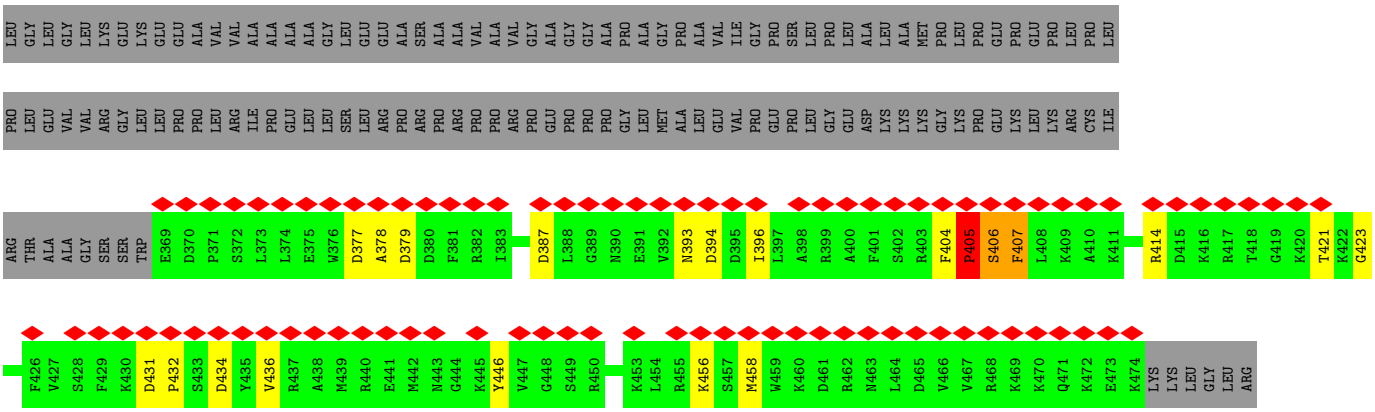




• Molecule 30: RNA-binding protein 42

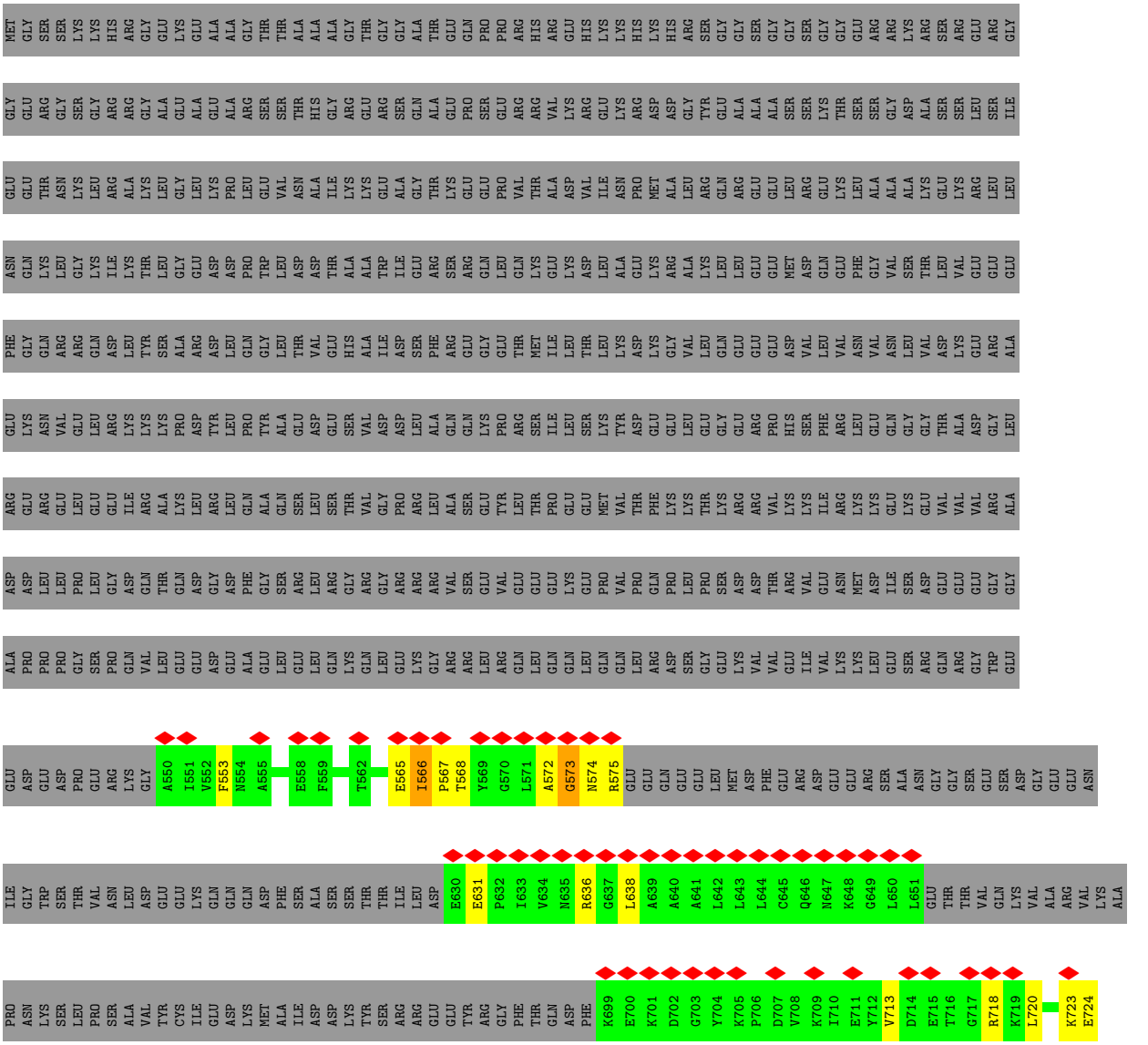
Chain R:

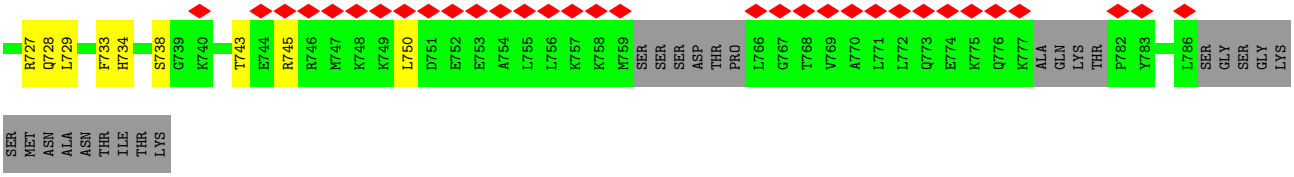




• Molecule 31: U4/U6.U5 tri-snRNP-associated protein 1

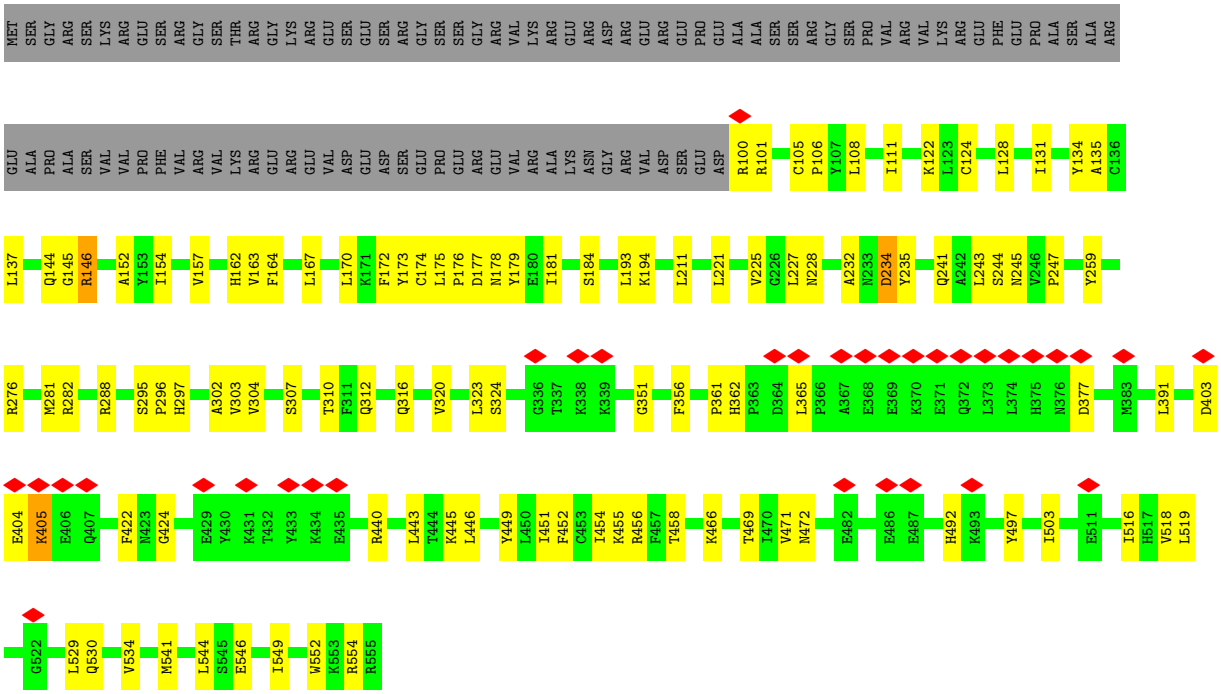
Chain S:





• Molecule 32: U4/U6.U5 tri-snRNP-associated protein 2

Chain U:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	585488	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.154	Depositor
Minimum map value	-0.079	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	429.24, 429.24, 429.24	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.022, 1.022, 1.022	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, ZN, IHP, MG, M7M

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	X	0.42	0/398	0.59	0/524
2	4	0.59	2/2966 (0.1%)	1.00	8/4606 (0.2%)
3	41	0.40	0/649	0.73	1/878 (0.1%)
3	51	0.40	0/649	0.73	1/878 (0.1%)
4	42	0.43	0/747	0.66	0/1000
4	52	0.40	0/805	0.74	1/1081 (0.1%)
5	43	0.40	0/660	0.73	2/889 (0.2%)
5	53	0.44	0/665	0.56	0/896
6	4A	0.42	0/1983	0.59	2/2657 (0.1%)
7	4B	0.48	0/2921	0.65	0/3966
8	4C	0.34	0/2406	0.56	0/3232
9	4D	0.52	1/967 (0.1%)	0.56	0/1305
10	4b	0.33	0/679	0.62	0/905
10	5b	0.38	0/602	0.57	0/801
11	4e	0.37	0/639	0.79	1/857 (0.1%)
11	5e	0.37	0/646	0.70	0/867
12	4f	0.42	0/574	0.74	1/775 (0.1%)
12	5f	0.41	0/579	0.78	0/783
13	4g	0.40	0/584	0.71	1/779 (0.1%)
13	5g	0.41	0/584	0.72	1/779 (0.1%)
14	5	0.63	0/2444	1.47	59/3798 (1.6%)
15	5A	0.48	1/18874 (0.0%)	0.59	8/25606 (0.0%)
16	5B	0.44	0/16393	0.59	3/22174 (0.0%)
17	5C	0.54	0/6879	0.61	3/9344 (0.0%)
18	5D	0.39	0/1198	0.57	1/1620 (0.1%)
19	5J	0.35	0/6430	0.61	6/8681 (0.1%)
20	5O	0.31	0/2448	0.58	0/3316
21	5X	0.51	1/4859 (0.0%)	0.61	0/6522
22	6	0.59	0/1001	1.21	8/1553 (0.5%)
23	62	0.79	0/773	1.21	5/1043 (0.5%)
24	63	0.80	0/709	1.21	3/959 (0.3%)
25	64	0.81	0/609	1.25	2/824 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
26	65	0.83	0/593	1.25	3/800 (0.4%)
27	66	0.83	1/575 (0.2%)	1.25	3/776 (0.4%)
28	67	0.81	1/611 (0.2%)	1.29	3/824 (0.4%)
29	68	0.80	0/728	1.30	6/987 (0.6%)
30	R	0.42	0/891	0.84	2/1188 (0.2%)
31	S	0.36	0/955	0.64	1/1271 (0.1%)
32	U	0.54	0/3846	0.64	1/5208 (0.0%)
All	All	0.49	7/91519 (0.0%)	0.73	136/124952 (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
2	4	0	1
4	52	0	3
6	4A	0	2
7	4B	0	3
8	4C	0	2
10	4b	0	1
11	4e	0	1
12	4f	0	1
12	5f	0	1
15	5A	0	2
16	5B	0	2
17	5C	0	2
19	5J	0	2
23	62	0	1
24	63	0	2
25	64	0	1
27	66	0	1
28	67	0	1
29	68	0	3
31	S	0	1
32	U	0	3
All	All	0	36

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	87	C	O3'-P	11.50	1.75	1.61

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5X	543	CYS	CB-SG	-6.88	1.70	1.82
9	4D	93	CYS	CB-SG	-6.33	1.71	1.82
28	67	61	GLN	C-O	-6.23	1.11	1.23
2	4	91	A	O3'-P	-5.42	1.54	1.61
15	5A	492	VAL	CB-CG1	-5.11	1.42	1.52
27	66	70	VAL	C-O	-5.07	1.13	1.23

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	5J	92	GLY	C-N-CD	-13.47	90.97	120.60
14	5	57	G	O4'-C1'-N9	12.56	118.25	108.20
14	5	58	U	O5'-P-OP2	-10.19	96.53	105.70
14	5	23	C	C2-N1-C1'	10.17	129.99	118.80
14	5	22	U	N1-C2-O2	10.14	129.90	122.80
14	5	22	U	C2-N1-C1'	9.93	129.62	117.70
14	5	115	C	C2-N1-C1'	9.69	129.46	118.80
14	5	58	U	C5-C6-N1	9.52	127.46	122.70
14	5	22	U	N3-C2-O2	-9.42	115.60	122.20
25	64	65	THR	CA-CB-CG2	-9.25	99.45	112.40
14	5	71	C	N1-C2-O2	9.02	124.31	118.90
14	5	23	C	N1-C2-O2	8.57	124.04	118.90
14	5	90	U	N1-C2-O2	8.56	128.79	122.80
28	67	69	ARG	NE-CZ-NH1	8.32	124.46	120.30
23	62	68	ARG	NE-CZ-NH1	8.31	124.46	120.30
24	63	37	ARG	NE-CZ-NH1	8.21	124.40	120.30
15	5A	1551	PHE	N-CA-C	-8.13	89.05	111.00
2	4	87	C	O3'-P-O5'	8.09	119.38	104.00
14	5	58	U	C2-N1-C1'	8.07	127.38	117.70
28	67	55	MET	CG-SD-CE	-8.06	87.31	100.20
29	68	8	TYR	CB-CG-CD1	8.04	125.82	121.00
14	5	71	C	C2-N1-C1'	8.03	127.63	118.80
14	5	110	C	C5-C6-N1	7.81	124.90	121.00
14	5	71	C	N3-C2-O2	-7.77	116.46	121.90
14	5	90	U	N3-C2-O2	-7.75	116.78	122.20
14	5	58	U	N1-C2-O2	7.74	128.22	122.80
14	5	23	C	N3-C2-O2	-7.64	116.55	121.90
14	5	110	C	C6-N1-C2	-7.57	117.27	120.30
14	5	90	U	C2-N1-C1'	7.54	126.74	117.70
19	5J	739	CYS	C-N-CD	-7.53	104.03	120.60
14	5	58	U	N3-C2-O2	-7.44	116.99	122.20
26	65	49	MET	CG-SD-CE	-7.41	88.34	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	5	58	U	C6-N1-C2	-7.39	116.57	121.00
14	5	71	C	C6-N1-C2	-7.38	117.35	120.30
22	6	31	U	N1-C2-O2	7.31	127.92	122.80
2	4	87	C	P-O3'-C3'	-7.31	110.93	119.70
30	R	405	PRO	N-CA-C	7.14	130.66	112.10
30	R	405	PRO	CA-N-CD	-7.10	101.56	111.50
18	5D	15	ASP	CB-CG-OD1	7.09	124.68	118.30
14	5	115	C	N1-C2-O2	7.04	123.12	118.90
14	5	23	C	C6-N1-C2	-6.95	117.52	120.30
14	5	23	C	C6-N1-C1'	-6.93	112.48	120.80
22	6	31	U	N3-C2-O2	-6.92	117.35	122.20
14	5	115	C	C6-N1-C1'	-6.91	112.51	120.80
14	5	22	U	C6-N1-C1'	-6.90	111.54	121.20
23	62	69	TYR	CB-CG-CD2	-6.89	116.86	121.00
12	4f	33	LEU	CA-CB-CG	6.84	131.04	115.30
15	5A	1557	LEU	CA-CB-CG	6.76	130.86	115.30
2	4	87	C	OP2-P-O3'	-6.67	90.52	105.20
14	5	115	C	C5-C6-N1	6.59	124.29	121.00
29	68	8	TYR	CB-CG-CD2	-6.57	117.06	121.00
23	62	47	ASP	CB-CA-C	6.57	123.54	110.40
32	U	377	ASP	CB-CG-OD2	6.56	124.21	118.30
14	5	105	U	N1-C2-O2	6.56	127.39	122.80
22	6	47	A	P-O3'-C3'	6.54	127.55	119.70
14	5	55	C	C6-N1-C2	-6.51	117.70	120.30
14	5	4	C	C2-N1-C1'	6.50	125.95	118.80
15	5A	1833	LEU	CA-CB-CG	6.47	130.19	115.30
14	5	57	G	P-O3'-C3'	6.46	127.45	119.70
14	5	105	U	N3-C2-O2	-6.45	117.68	122.20
15	5A	779	LEU	CB-CG-CD1	-6.42	100.09	111.00
14	5	110	C	N1-C2-O2	6.41	122.75	118.90
23	62	69	TYR	CB-CG-CD1	6.37	124.82	121.00
16	5B	821	LEU	CA-CB-CG	6.36	129.93	115.30
14	5	72	U	N1-C2-O2	6.34	127.24	122.80
29	68	63	ARG	NE-CZ-NH2	-6.32	117.14	120.30
14	5	55	C	N1-C2-O2	6.29	122.68	118.90
15	5A	1819	LEU	CA-CB-CG	6.26	129.70	115.30
14	5	96	A	N7-C8-N9	6.12	116.86	113.80
14	5	72	U	N3-C2-O2	-6.11	117.92	122.20
14	5	55	C	N3-C2-O2	-6.06	117.66	121.90
22	6	105	U	C5-C4-O4	6.04	129.53	125.90
29	68	79	SER	N-CA-CB	6.04	119.56	110.50
27	66	52	VAL	CA-CB-CG1	5.96	119.84	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	5	115	C	C6-N1-C2	-5.94	117.92	120.30
24	63	46	TYR	CB-CG-CD1	-5.93	117.44	121.00
14	5	71	C	C5-C6-N1	5.90	123.95	121.00
27	66	56	LEU	CB-CG-CD1	-5.90	100.97	111.00
19	5J	739	CYS	CA-CB-SG	5.88	124.58	114.00
5	43	10	LEU	CA-CB-CG	5.85	128.75	115.30
11	4e	25	LEU	CA-CB-CG	5.79	128.60	115.30
15	5A	638	LEU	CB-CG-CD1	-5.79	101.16	111.00
2	4	8	C	C6-N1-C2	-5.76	117.99	120.30
14	5	105	U	C2-N1-C1'	5.76	124.61	117.70
13	4g	19	LEU	CB-CG-CD2	-5.75	101.23	111.00
13	5g	19	LEU	CB-CG-CD2	-5.74	101.24	111.00
17	5C	298	LEU	CA-CB-CG	5.71	128.42	115.30
27	66	44	ALA	N-CA-CB	5.65	118.01	110.10
5	43	81	PRO	CA-N-CD	-5.61	103.65	111.50
14	5	96	A	C4-N9-C1'	5.61	136.39	126.30
19	5J	773	ASN	C-N-CD	-5.59	108.31	120.60
15	5A	1550	GLY	N-CA-C	5.57	127.03	113.10
14	5	32	C	C6-N1-C2	-5.55	118.08	120.30
25	64	25	TYR	CB-CG-CD2	-5.54	117.67	121.00
2	4	3	C	C6-N1-C2	-5.54	118.08	120.30
2	4	130	U	N3-C2-O2	-5.54	118.32	122.20
24	63	50	LEU	CB-CG-CD2	-5.52	101.62	111.00
16	5B	2084	LEU	CA-CB-CG	5.52	127.99	115.30
14	5	4	C	C5-C6-N1	5.50	123.75	121.00
14	5	7	U	N1-C2-O2	5.50	126.65	122.80
31	S	566	ILE	CG1-CB-CG2	-5.50	99.30	111.40
22	6	66	C	C6-N1-C2	-5.45	118.12	120.30
22	6	31	U	C2-N1-C1'	5.44	124.23	117.70
14	5	18	C	C5-C6-N1	5.39	123.70	121.00
14	5	22	U	O4'-C1'-N1	-5.39	103.89	108.20
14	5	56	C	N1-C2-O2	5.38	122.13	118.90
14	5	9	G	C4-N9-C1'	5.35	133.45	126.50
14	5	110	C	N3-C2-O2	-5.34	118.16	121.90
29	68	96	HIS	CB-CA-C	-5.34	99.73	110.40
15	5A	422	LEU	CA-CB-CG	5.30	127.48	115.30
3	51	76	LEU	CA-CB-CG	5.27	127.42	115.30
14	5	38	C	N1-C2-O2	5.26	122.06	118.90
17	5C	440	SER	C-N-CD	-5.26	109.03	120.60
26	65	70	ASP	CA-CB-CG	5.26	124.97	113.40
3	41	76	LEU	CA-CB-CG	5.24	127.35	115.30
14	5	7	U	C2-N1-C1'	5.20	123.94	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	5C	828	MET	C-N-CA	5.18	134.65	121.70
14	5	96	A	C8-N9-C4	-5.18	103.73	105.80
4	52	53	LEU	CA-CB-CG	5.18	127.21	115.30
22	6	77	C	N1-C2-O2	5.17	122.00	118.90
26	65	65	ARG	NE-CZ-NH2	5.16	122.88	120.30
6	4A	426	PRO	C-N-CD	5.13	139.17	128.40
29	68	88	ALA	C-N-CA	5.12	134.50	121.70
14	5	23	C	C5-C6-N1	5.11	123.56	121.00
22	6	105	U	C6-N1-C1'	5.11	128.35	121.20
6	4A	551	LEU	CA-CB-CG	5.11	127.04	115.30
2	4	3	C	C5-C6-N1	5.07	123.53	121.00
2	4	22	C	C6-N1-C2	-5.07	118.27	120.30
19	5J	739	CYS	C-N-CA	5.06	143.26	122.00
14	5	4	C	C6-N1-C2	-5.06	118.28	120.30
14	5	7	U	N3-C2-O2	-5.05	118.66	122.20
14	5	4	C	N1-C2-O2	5.02	121.91	118.90
28	67	69	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
19	5J	672	ALA	C-N-CD	5.01	138.92	128.40
16	5B	299	ASP	CB-CG-OD1	5.00	122.80	118.30
23	62	54	MET	CG-SD-CE	-5.00	92.20	100.20

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	4	90	G	Sidechain
6	4A	421	PRO	Peptide
6	4A	538	SER	Peptide
7	4B	420	TYR	Peptide
7	4B	459	PRO	Peptide
7	4B	470	TYR	Peptide
8	4C	350	GLN	Peptide
8	4C	386	ASP	Peptide
10	4b	53	PRO	Peptide
11	4e	51	ASP	Peptide
12	4f	40	MET	Peptide
4	52	46	CYS	Peptide
4	52	60	ASP	Peptide
4	52	88	LYS	Peptide
15	5A	1416	ILE	Peptide
15	5A	1792	LYS	Peptide
16	5B	1265	GLN	Peptide

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Mol	Chain	Res	Type	Group
16	5B	526	ASN	Peptide
17	5C	167	TYR	Peptide
17	5C	439	PRO	Peptide
19	5J	624	VAL	Peptide
19	5J	724	MET	Peptide
12	5f	40	MET	Peptide
23	62	69	TYR	Sidechain
24	63	30	TYR	Sidechain
24	63	46	TYR	Sidechain
25	64	25	TYR	Sidechain
27	66	51	TYR	Sidechain
28	67	62	TYR	Sidechain
29	68	60	TYR	Sidechain
29	68	8	TYR	Sidechain
29	68	89	GLU	Peptide
31	S	566	ILE	Peptide
32	U	243	LEU	Peptide
32	U	422	PHE	Peptide
32	U	530	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	394	0	406	53	0
2	4	2690	0	1369	56	0
3	41	641	0	681	18	0
3	51	641	0	681	14	0
4	42	737	0	780	40	0
4	52	796	0	821	20	0
5	43	652	0	670	20	0
5	53	657	0	675	11	0
6	4A	1946	0	2013	89	0
7	4B	2842	0	2746	87	0
8	4C	2375	0	2377	38	0
9	4D	955	0	1008	16	0
10	4b	669	0	697	0	0
10	5b	594	0	615	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	4e	631	0	648	0	0
11	5e	638	0	657	0	0
12	4f	562	0	574	0	0
12	5f	567	0	575	0	0
13	4g	577	0	603	0	0
13	5g	577	0	603	0	0
14	5	2192	0	1110	34	0
15	5A	18366	0	18268	456	0
16	5B	16077	0	16192	243	0
17	5C	6727	0	6735	126	0
18	5D	1169	0	1141	23	0
19	5J	6316	0	6229	114	0
20	5O	2394	0	2326	54	0
21	5X	4780	0	4850	147	0
22	6	897	0	454	32	0
23	62	761	0	777	5	0
24	63	699	0	702	11	0
25	64	596	0	591	7	0
26	65	587	0	605	12	0
27	66	567	0	571	18	0
28	67	604	0	623	7	0
29	68	722	0	712	20	0
30	R	874	0	883	56	0
31	S	947	0	933	36	0
32	U	3750	0	3767	78	0
33	5A	36	0	6	1	0
34	5C	1	0	0	0	0
35	5C	32	0	12	0	0
36	U	1	0	0	0	0
All	All	89236	0	86686	1645	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 10.

All (1645) 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)
6:4A:423:GLN:OE1	7:4B:365:SER:CA	1.64	1.43
6:4A:466:LEU:CD2	30:R:432:PRO:O	1.69	1.39
6:4A:465:ARG:HA	30:R:456:LYS:NZ	1.35	1.37
21:5X:362:LEU:HD11	21:5X:395:ASP:CG	1.42	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4A:524:GLN:OE1	27:66:13:LYS:NZ	1.63	1.31
1:X:135:ARG:NH2	15:5A:1592:ASP:OD1	1.60	1.31
21:5X:379:ILE:HG22	21:5X:629[B]:ILE:CD1	1.62	1.30
8:4C:357:ARG:NH1	22:6:58:G:O6	1.65	1.28
21:5X:362:LEU:HD23	21:5X:391:ARG:NE	1.50	1.26
21:5X:362:LEU:CD2	21:5X:391:ARG:NE	1.99	1.25
22:6:103:U:H1'	29:68:65:ASP:OD1	1.35	1.21
14:5:7:U:O5'	20:5O:148:LYS:NZ	1.75	1.20
7:4B:284:LYS:HE2	7:4B:288:SER:CB	1.73	1.19
6:4A:462:GLU:OE1	30:R:436:VAL:HG21	1.42	1.16
15:5A:192:GLN:HB3	15:5A:208:TYR:CD2	1.83	1.14
21:5X:362:LEU:HD21	21:5X:391:ARG:HE	1.03	1.13
14:5:7:U:O2'	20:5O:146:ARG:NH2	1.81	1.13
21:5X:362:LEU:CD2	21:5X:391:ARG:HE	1.59	1.13
6:4A:423:GLN:OE1	7:4B:365:SER:HA	1.43	1.12
6:4A:424:LEU:HD12	7:4B:402:PHE:CZ	1.83	1.12
6:4A:427:PRO:HB2	6:4A:639:LYS:HE3	1.27	1.12
7:4B:284:LYS:HE2	7:4B:288:SER:HB2	1.24	1.12
6:4A:423:GLN:OE1	7:4B:365:SER:CB	1.97	1.11
6:4A:466:LEU:HD22	30:R:432:PRO:HB2	1.23	1.11
2:4:17:A:N1	8:4C:357:ARG:NH1	1.99	1.09
19:5J:673:PRO:CB	19:5J:677:VAL:HG21	1.82	1.09
6:4A:423:GLN:OE1	7:4B:365:SER:N	1.86	1.09
22:6:103:U:C1'	29:68:65:ASP:OD1	2.00	1.08
15:5A:192:GLN:HB3	15:5A:208:TYR:CE2	1.88	1.08
15:5A:192:GLN:HG2	15:5A:208:TYR:CG	1.89	1.08
6:4A:466:LEU:HD22	30:R:432:PRO:O	1.49	1.07
7:4B:284:LYS:CE	7:4B:288:SER:CB	2.34	1.06
8:4C:357:ARG:HG3	8:4C:358:ARG:H	1.15	1.06
1:X:149:ARG:HH12	15:5A:1616:PRO:HG3	0.93	1.05
1:X:140:TYR:CE2	15:5A:1587:GLU:OE1	2.10	1.04
21:5X:362:LEU:CD1	21:5X:395:ASP:CG	2.25	1.04
6:4A:466:LEU:HD22	30:R:432:PRO:C	1.77	1.03
21:5X:379:ILE:HG22	21:5X:629[B]:ILE:HD12	1.05	1.03
19:5J:673:PRO:HB2	19:5J:677:VAL:HG21	1.35	1.02
19:5J:673:PRO:HB2	19:5J:677:VAL:CG2	1.88	1.02
14:5:45:C:O2	15:5A:603:ARG:NH2	1.92	1.02
6:4A:466:LEU:HD21	30:R:432:PRO:O	1.59	1.01
1:X:149:ARG:NH1	15:5A:1616:PRO:HG3	1.75	1.01
21:5X:362:LEU:HD11	21:5X:395:ASP:OD1	1.61	1.01
21:5X:362:LEU:HD21	21:5X:395:ASP:OD2	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4A:466:LEU:CD2	30:R:432:PRO:HB2	1.91	1.00
6:4A:466:LEU:HD22	30:R:432:PRO:CB	1.91	0.99
1:X:137:TYR:CE1	31:S:729:LEU:HD13	1.97	0.99
1:X:140:TYR:OH	15:5A:1587:GLU:OE1	1.78	0.99
30:R:406:SER:O	30:R:407:PHE:O	1.79	0.99
30:R:404:PHE:HZ	30:R:434:ASP:CA	1.74	0.98
15:5A:559:ASP:HA	15:5A:562:VAL:HG22	1.46	0.98
21:5X:379:ILE:CG2	21:5X:629[B]:ILE:HD12	1.94	0.96
6:4A:427:PRO:HB2	6:4A:639:LYS:CE	1.95	0.96
15:5A:169:PHE:CE1	15:5A:563:GLN:NE2	2.33	0.96
8:4C:357:ARG:HG3	8:4C:358:ARG:N	1.80	0.96
15:5A:110:TRP:O	15:5A:192:GLN:NE2	1.96	0.96
7:4B:284:LYS:CE	7:4B:288:SER:HB2	1.94	0.94
15:5A:1508:GLY:N	15:5A:1752:GLN:HE21	1.64	0.94
15:5A:1794:PHE:CD2	15:5A:1795:GLU:HG2	2.03	0.93
7:4B:284:LYS:O	7:4B:289:LEU:HB2	1.69	0.93
21:5X:362:LEU:CD1	21:5X:395:ASP:OD1	2.16	0.93
22:6:103:U:O3'	29:68:65:ASP:OD1	1.87	0.93
6:4A:423:GLN:OE1	7:4B:365:SER:HB3	1.65	0.93
1:X:137:TYR:CG	31:S:729:LEU:HD12	2.02	0.92
21:5X:445:PHE:CD2	21:5X:605:PHE:HE2	1.87	0.92
6:4A:465:ARG:HA	30:R:456:LYS:HZ1	0.96	0.92
6:4A:465:ARG:HA	30:R:456:LYS:HZ3	1.33	0.92
1:X:140:TYR:CZ	15:5A:1587:GLU:OE1	2.21	0.92
32:U:146:ARG:HH11	32:U:146:ARG:HG3	1.33	0.91
15:5A:1508:GLY:H	15:5A:1752:GLN:HE21	1.05	0.91
21:5X:379:ILE:HG22	21:5X:629[A]:ILE:HG13	1.53	0.91
6:4A:465:ARG:CA	30:R:456:LYS:NZ	2.30	0.91
32:U:403:ASP:OD1	32:U:405:LYS:NZ	2.03	0.91
30:R:404:PHE:HZ	30:R:434:ASP:HA	1.32	0.90
21:5X:379:ILE:CG2	21:5X:629[B]:ILE:CD1	2.49	0.90
21:5X:733[A]:VAL:HG12	21:5X:735:MET:H	1.35	0.90
15:5A:1510:GLU:O	15:5A:1513:MET:CE	2.19	0.90
4:52:76:GLU:O	4:52:89:PRO:HA	1.72	0.89
15:5A:85:LYS:NZ	19:5J:93:PRO:HG3	1.88	0.88
21:5X:362:LEU:HD11	21:5X:395:ASP:CB	2.04	0.88
1:X:125:ASN:OD1	4:42:61:ARG:HD3	1.71	0.88
6:4A:462:GLU:CD	30:R:436:VAL:HG21	1.93	0.87
1:X:137:TYR:CD1	31:S:729:LEU:CD1	2.57	0.87
7:4B:284:LYS:HE2	7:4B:288:SER:HB3	1.57	0.87
21:5X:362:LEU:HD23	21:5X:391:ARG:CZ	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5A:192:GLN:HG2	15:5A:208:TYR:CB	2.06	0.85
6:4A:465:ARG:CA	30:R:456:LYS:HZ1	1.87	0.85
21:5X:445:PHE:HD2	21:5X:605:PHE:CE2	1.94	0.84
1:X:140:TYR:HE2	15:5A:1587:GLU:OE1	1.59	0.84
15:5A:84:ASP:HB3	19:5J:97:ASP:OD1	1.78	0.84
15:5A:577:GLY:O	15:5A:581:ILE:HG13	1.78	0.83
15:5A:552:ARG:HG3	15:5A:552:ARG:HH21	1.41	0.83
1:X:137:TYR:CZ	31:S:729:LEU:HD13	2.15	0.82
30:R:404:PHE:CD2	30:R:405:PRO:CG	2.57	0.82
6:4A:462:GLU:OE1	30:R:436:VAL:CG2	2.25	0.81
15:5A:86:ARG:NE	15:5A:86:ARG:HA	1.92	0.81
5:43:78:LYS:HG3	5:43:79:ASN:OD1	1.80	0.81
15:5A:86:ARG:HH11	15:5A:89:LEU:CD1	1.93	0.81
15:5A:559:ASP:HA	15:5A:562:VAL:CG2	2.10	0.81
21:5X:472:ILE:HG13	21:5X:540:LEU:HD21	1.62	0.81
21:5X:362:LEU:CD2	21:5X:395:ASP:OD2	2.28	0.80
15:5A:192:GLN:CG	15:5A:208:TYR:CG	2.63	0.80
8:4C:356:GLY:CA	22:6:54:G:OP2	2.29	0.80
1:X:149:ARG:HH12	15:5A:1616:PRO:CG	1.87	0.79
8:4C:356:GLY:N	22:6:54:G:OP2	2.13	0.79
6:4A:462:GLU:OE2	30:R:436:VAL:HG11	1.81	0.79
31:S:573:GLY:O	31:S:575:ARG:HG2	1.82	0.79
15:5A:579:GLN:HA	15:5A:579:GLN:HE21	1.46	0.79
21:5X:675:LYS:O	21:5X:679:VAL:HG12	1.83	0.79
32:U:174:CYS:O	32:U:177:ASP:O	2.00	0.78
15:5A:86:ARG:HH11	15:5A:89:LEU:HD13	1.48	0.78
15:5A:86:ARG:HD3	19:5J:102:ASP:OD2	1.82	0.78
1:X:125:ASN:HA	4:42:61:ARG:CG	2.13	0.78
32:U:403:ASP:OD2	32:U:404:GLU:N	2.16	0.78
15:5A:85:LYS:HG2	15:5A:89:LEU:CD1	2.13	0.78
15:5A:60:ASP:OD1	15:5A:61:MET:N	2.17	0.78
19:5J:444:GLU:OE2	31:S:574:ASN:ND2	2.15	0.78
7:4B:284:LYS:HB3	7:4B:288:SER:HB2	1.64	0.77
32:U:146:ARG:HD2	32:U:146:ARG:O	1.84	0.77
21:5X:540:LEU:HD22	21:5X:570:MET:SD	2.24	0.77
15:5A:192:GLN:CB	15:5A:208:TYR:CD2	2.65	0.77
15:5A:1317:TYR:CE1	15:5A:1329:SER:HB2	2.20	0.77
15:5A:192:GLN:HG2	15:5A:208:TYR:HB3	1.67	0.77
21:5X:692:CYS:SG	21:5X:715:LYS:HG3	2.25	0.77
14:5:7:U:H4'	20:5O:148:LYS:HZ3	1.50	0.76
1:X:137:TYR:CE1	31:S:729:LEU:CD1	2.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5X:445:PHE:CD2	21:5X:605:PHE:CE2	2.70	0.76
30:R:406:SER:O	30:R:407:PHE:C	2.21	0.76
15:5A:59:GLU:N	15:5A:59:GLU:OE2	2.18	0.76
32:U:131:ILE:O	32:U:144:GLN:HG3	1.86	0.76
15:5A:58:LYS:HB3	15:5A:59:GLU:OE2	1.86	0.76
17:5C:107:GLN:HE21	17:5C:109:LEU:HD11	1.49	0.76
17:5C:937:THR:O	17:5C:941:LYS:HG2	1.86	0.75
21:5X:378:SER:OG	21:5X:630:GLY:HA2	1.85	0.75
2:4:114:U:H4'	2:4:115:G:OP1	1.87	0.75
6:4A:466:LEU:HB3	30:R:432:PRO:HB2	1.68	0.75
15:5A:579:GLN:HE21	15:5A:579:GLN:CA	1.99	0.75
6:4A:466:LEU:HD22	30:R:432:PRO:CA	2.17	0.75
2:4:74:C:H42	22:6:35:A:H61	1.35	0.74
15:5A:1811:ASN:CG	15:5A:1814:THR:HG22	2.07	0.74
19:5J:673:PRO:HB3	19:5J:677:VAL:HG21	1.67	0.74
30:R:404:PHE:CG	30:R:405:PRO:HD2	2.22	0.74
22:6:103:U:H1'	29:68:65:ASP:CG	2.08	0.74
15:5A:1623:ASN:OD1	15:5A:1624:SER:N	2.21	0.74
22:6:103:U:H3	29:68:35:ASN:HD21	1.33	0.74
7:4B:414:ASN:HD22	7:4B:457:PHE:H	1.35	0.73
15:5A:384:VAL:HG22	17:5C:331:PHE:CD2	2.23	0.73
21:5X:679:VAL:O	21:5X:682:LYS:HG2	1.89	0.73
21:5X:711:LYS:HA	21:5X:731:GLN:HE22	1.51	0.73
1:X:134:LYS:HE3	31:S:728:GLN:NE2	2.02	0.73
30:R:404:PHE:CD2	30:R:405:PRO:CD	2.71	0.73
21:5X:442:THR:HA	21:5X:445:PHE:CE2	2.23	0.73
8:4C:356:GLY:HA2	22:6:54:G:OP2	1.89	0.73
15:5A:580:TYR:CE2	15:5A:588:LEU:HD11	2.23	0.73
8:4C:357:ARG:HG3	8:4C:358:ARG:HG3	1.69	0.73
15:5A:559:ASP:CA	15:5A:562:VAL:HG22	2.18	0.73
8:4C:357:ARG:CG	8:4C:358:ARG:H	1.90	0.72
7:4B:284:LYS:CE	7:4B:288:SER:HB3	2.13	0.72
15:5A:384:VAL:HG22	17:5C:331:PHE:CG	2.25	0.72
15:5A:1508:GLY:N	15:5A:1752:GLN:NE2	2.37	0.72
6:4A:424:LEU:CD1	7:4B:402:PHE:CZ	2.68	0.72
21:5X:682:LYS:HG3	21:5X:683:SER:N	2.03	0.72
15:5A:1752:GLN:OE1	15:5A:1752:GLN:HA	1.89	0.72
6:4A:466:LEU:CB	30:R:432:PRO:HB2	2.19	0.71
15:5A:112:GLN:HB3	15:5A:187:PRO:HG3	1.71	0.71
18:5D:86:ARG:NH2	30:R:446:TYR:CG	2.57	0.71
21:5X:690:ASN:HB3	21:5X:715:LYS:HD3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5A:85:LYS:HZ1	19:5J:93:PRO:HG3	1.56	0.71
15:5A:1779:PHE:O	15:5A:1809:ILE:HA	1.91	0.71
15:5A:1510:GLU:O	15:5A:1513:MET:HE2	1.91	0.70
19:5J:674:THR:O	19:5J:676:ARG:N	2.24	0.70
21:5X:362:LEU:HD21	21:5X:391:ARG:NE	1.78	0.70
15:5A:1385:VAL:HG21	15:5A:1414:ARG:HD2	1.74	0.70
15:5A:86:ARG:NH1	15:5A:89:LEU:HD13	2.05	0.70
15:5A:1510:GLU:O	15:5A:1513:MET:HE3	1.92	0.70
21:5X:463:GLU:HG3	21:5X:467:GLN:OE1	1.92	0.70
5:53:48:VAL:O	5:53:55:VAL:HA	1.92	0.69
15:5A:1510:GLU:O	15:5A:1513:MET:HG2	1.91	0.69
18:5D:86:ARG:NH2	30:R:446:TYR:CB	2.56	0.69
22:6:103:U:O4'	29:68:65:ASP:OD2	2.11	0.69
17:5C:440:SER:HB3	17:5C:443:VAL:H	1.57	0.69
16:5B:2106:LEU:O	16:5B:2119:GLU:HA	1.91	0.69
19:5J:668:ALA:O	19:5J:673:PRO:HG3	1.92	0.69
15:5A:112:GLN:HB3	15:5A:187:PRO:CG	2.21	0.69
15:5A:580:TYR:HE2	15:5A:588:LEU:HD11	1.57	0.69
15:5A:1621:LYS:HE3	15:5A:1623:ASN:OD1	1.91	0.69
15:5A:251:ASP:HB3	15:5A:253:ASN:H	1.57	0.69
21:5X:666:PRO:O	21:5X:733[A]:VAL:HG13	1.92	0.69
7:4B:284:LYS:HE3	7:4B:288:SER:CB	2.21	0.69
19:5J:632:ALA:O	19:5J:635:PHE:HB2	1.94	0.69
21:5X:560:GLU:O	21:5X:564:GLN:HG3	1.92	0.69
1:X:124:VAL:O	4:42:61:ARG:HG2	1.94	0.68
15:5A:1622:MET:O	15:5A:1687:TYR:OH	2.11	0.68
6:4A:466:LEU:HD23	30:R:432:PRO:O	1.87	0.68
15:5A:384:VAL:O	17:5C:354:ARG:NH2	2.24	0.68
8:4C:357:ARG:NH1	22:6:58:G:C6	2.54	0.68
14:5:7:U:H4'	20:5O:148:LYS:NZ	2.08	0.68
15:5A:110:TRP:HB2	15:5A:192:GLN:HG3	1.76	0.68
19:5J:662:ARG:HG2	19:5J:684:LEU:HD21	1.73	0.68
7:4B:284:LYS:O	7:4B:289:LEU:CB	2.40	0.68
1:X:137:TYR:CD2	31:S:729:LEU:HD12	2.29	0.68
15:5A:2311:PRO:O	15:5A:2315:LEU:HB2	1.94	0.68
27:66:52:VAL:HB	27:66:56:LEU:HD11	1.75	0.68
21:5X:432:ILE:HG21	21:5X:609:MET:HE3	1.75	0.68
15:5A:494:LEU:HD21	15:5A:562:VAL:HG11	1.75	0.67
6:4A:466:LEU:CG	30:R:432:PRO:HB2	2.23	0.67
24:63:94:LEU:HD13	27:66:59:LYS:HZ3	1.59	0.67
15:5A:1179:SER:O	15:5A:1201:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:U:157:VAL:HG13	32:U:176:PRO:HB3	1.75	0.67
15:5A:86:ARG:CG	19:5J:98:ASP:HB3	2.25	0.67
21:5X:362:LEU:CG	21:5X:395:ASP:OD2	2.42	0.67
2:4:114:U:P	2:4:114:U:H6	2.18	0.67
15:5A:85:LYS:HZ3	19:5J:93:PRO:HG3	1.57	0.67
21:5X:728:ILE:HG23	21:5X:729:ASP:H	1.58	0.67
15:5A:86:ARG:HA	15:5A:86:ARG:HE	1.59	0.67
7:4B:294:VAL:CG2	7:4B:307:LEU:HB3	2.25	0.67
15:5A:65:HIS:HE1	15:5A:483:GLN:OE1	1.78	0.67
30:R:404:PHE:CD2	30:R:405:PRO:HD2	2.30	0.67
21:5X:379:ILE:HG22	21:5X:629[B]:ILE:HD13	1.70	0.66
1:X:138:ARG:HH12	15:5A:1614:ILE:HD12	1.60	0.66
18:5D:86:ARG:NH2	30:R:446:TYR:HB2	2.10	0.66
16:5B:756:SER:O	16:5B:760:GLU:HB2	1.95	0.66
18:5D:86:ARG:CZ	30:R:446:TYR:CG	2.79	0.66
21:5X:362:LEU:CD2	21:5X:391:ARG:CD	2.74	0.66
15:5A:701:ILE:HG22	15:5A:704:ASN:HD22	1.61	0.66
21:5X:378:SER:OG	21:5X:630:GLY:CA	2.43	0.66
8:4C:357:ARG:CG	8:4C:358:ARG:N	2.50	0.66
15:5A:318:TYR:O	17:5C:645:ARG:NH1	2.29	0.66
2:4:109:G:H2'	2:4:110:G:C8	2.30	0.66
6:4A:427:PRO:CB	6:4A:639:LYS:NZ	2.58	0.66
15:5A:85:LYS:HG2	15:5A:89:LEU:HD12	1.77	0.65
15:5A:231:THR:HG22	15:5A:233:PRO:HD2	1.78	0.65
21:5X:733[A]:VAL:HG12	21:5X:735:MET:N	2.10	0.65
6:4A:466:LEU:HB3	30:R:432:PRO:CB	2.25	0.65
1:X:137:TYR:CD1	31:S:729:LEU:HD12	2.30	0.65
6:4A:465:ARG:HA	30:R:456:LYS:CE	2.26	0.65
15:5A:1511:GLU:HB3	15:5A:1513:MET:HE2	1.78	0.65
6:4A:427:PRO:CB	6:4A:639:LYS:HE3	2.17	0.65
15:5A:1374:PRO:HG3	16:5B:52:MET:HB3	1.77	0.65
21:5X:540:LEU:HD23	21:5X:543:CYS:HB2	1.78	0.65
15:5A:761:ILE:HD12	15:5A:775:ASN:HD22	1.61	0.64
21:5X:362:LEU:HD23	21:5X:391:ARG:CD	2.27	0.64
8:4C:346:PRO:HG3	18:5D:117:GLU:HG2	1.80	0.64
16:5B:1360:ALA:HB2	16:5B:1490:LEU:HD11	1.78	0.64
15:5A:686:ARG:HE	15:5A:710:LEU:HD11	1.62	0.64
17:5C:363:SER:O	17:5C:364:SER:OG	2.10	0.64
16:5B:1456:VAL:HG22	16:5B:1491:SER:HB2	1.79	0.64
19:5J:89:PHE:O	19:5J:90:SER:HB3	1.97	0.64
19:5J:426:ALA:HB1	19:5J:436:LEU:HD13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R:421:THR:HG22	30:R:423:GLY:H	1.63	0.64
15:5A:1737:ASN:HD22	15:5A:1740:LEU:H	1.44	0.64
30:R:404:PHE:CZ	30:R:434:ASP:CA	2.60	0.64
6:4A:597:LEU:HA	6:4A:601:ARG:HB2	1.80	0.64
15:5A:853:LYS:HE3	15:5A:856:LEU:HD22	1.79	0.64
16:5B:498:ASN:HD22	16:5B:648:LEU:HB2	1.62	0.64
15:5A:552:ARG:HH21	15:5A:552:ARG:CG	2.12	0.63
32:U:174:CYS:O	32:U:178:ASN:HA	1.98	0.63
30:R:404:PHE:CZ	30:R:434:ASP:O	2.51	0.63
15:5A:58:LYS:N	15:5A:477:LYS:HE2	2.14	0.63
19:5J:649:VAL:HG11	19:5J:665:LEU:HG	1.80	0.63
7:4B:242:ASN:CB	7:4B:286:THR:HG21	2.29	0.63
17:5C:829:GLU:HG3	17:5C:907:VAL:HG22	1.81	0.63
15:5A:1038:SER:OG	15:5A:1438:VAL:HG12	1.99	0.63
15:5A:1806:ALA:HA	15:5A:1820:LYS:O	1.98	0.63
16:5B:1793:LEU:HD13	16:5B:1810:VAL:HG11	1.81	0.63
16:5B:984:LEU:HD11	16:5B:1102:ARG:HH21	1.64	0.62
19:5J:663:ARG:O	19:5J:666:ALA:HB3	1.98	0.62
4:52:42:VAL:O	4:52:53:LEU:HA	1.99	0.62
15:5A:1579:ALA:O	15:5A:1584:LYS:NZ	2.31	0.62
16:5B:1822:TYR:HB2	16:5B:1824:ILE:HD11	1.80	0.62
1:X:119:LYS:HD3	2:4:116:G:H5”	1.82	0.62
20:5O:259:VAL:HB	20:5O:277:PHE:HB2	1.81	0.62
32:U:124:CYS:HB2	32:U:144:GLN:HB2	1.80	0.62
5:43:19:THR:HB	5:43:72:ILE:HB	1.80	0.62
15:5A:65:HIS:ND1	15:5A:120:TYR:OH	2.29	0.62
15:5A:272:ALA:HB2	15:5A:278:LYS:HD3	1.81	0.62
15:5A:1777:ILE:HG12	15:5A:1860:GLN:HB3	1.80	0.62
32:U:146:ARG:HH11	32:U:146:ARG:CG	2.10	0.62
15:5A:191:ILE:HG23	15:5A:572:PHE:CZ	2.35	0.62
8:4C:209:GLU:HG2	8:4C:225:ALA:HB3	1.82	0.62
16:5B:969:LEU:HD21	16:5B:998:VAL:HG21	1.82	0.62
32:U:162:HIS:HD2	32:U:176:PRO:HD3	1.64	0.62
7:4B:249:ALA:HB2	7:4B:279:ILE:HG22	1.82	0.62
15:5A:192:GLN:HG2	15:5A:208:TYR:CD2	2.33	0.62
4:52:10:GLU:HG2	4:52:12:THR:H	1.64	0.61
15:5A:1794:PHE:HD2	15:5A:1795:GLU:HG2	1.62	0.61
26:65:72:ILE:HG22	27:66:74:SER:CB	2.30	0.61
15:5A:2207:ASP:HB3	15:5A:2210:LYS:HG2	1.81	0.61
6:4A:423:GLN:NE2	7:4B:364:HIS:O	2.34	0.61
16:5B:2067:VAL:HG13	16:5B:2107:TYR:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5X:362:LEU:CG	21:5X:395:ASP:CG	2.69	0.61
15:5A:150:MET:SD	15:5A:153:ARG:NH1	2.74	0.61
16:5B:421:HIS:NE2	16:5B:875:GLU:OE1	2.30	0.61
21:5X:379:ILE:HD12	21:5X:420:GLN:HB2	1.81	0.61
30:R:377:ASP:OD1	30:R:379:ASP:N	2.23	0.61
15:5A:1212:GLY:HA2	15:5A:1276:GLU:HB3	1.82	0.61
17:5C:137:HIS:O	17:5C:142:LYS:NZ	2.34	0.61
21:5X:536:ARG:HG3	21:5X:536:ARG:O	2.00	0.61
21:5X:667:ILE:HA	21:5X:733[A]:VAL:HG11	1.83	0.61
6:4A:465:ARG:CA	30:R:456:LYS:HZ3	2.05	0.61
14:5:36:C:O2	14:5:44:A:N6	2.33	0.61
3:51:66:ARG:HH12	4:52:47:ARG:HB2	1.65	0.61
22:6:103:U:C1’	29:68:65:ASP:CG	2.65	0.61
14:5:7:U:H4’	20:5O:146:ARG:HH12	1.65	0.61
16:5B:877:GLN:HG3	31:S:553:PHE:HB3	1.82	0.61
6:4A:423:GLN:HE22	7:4B:364:HIS:C	2.04	0.61
32:U:174:CYS:C	32:U:175:LEU:HD12	2.21	0.61
15:5A:257:LEU:HD22	15:5A:314:ILE:HG22	1.83	0.60
15:5A:1513:MET:O	15:5A:1514:LYS:C	2.39	0.60
16:5B:626:PRO:HG3	16:5B:893:MET:HA	1.81	0.60
20:5O:62:LEU:HB2	20:5O:351:LEU:HB2	1.82	0.60
15:5A:86:ARG:NH1	15:5A:89:LEU:CB	2.65	0.60
15:5A:1042:GLN:OE1	15:5A:1090:ARG:NH2	2.35	0.60
20:5O:91:LEU:HD22	20:5O:101:ASN:HD21	1.66	0.60
21:5X:768:LEU:HD11	21:5X:779:LEU:HD23	1.82	0.60
4:42:102:ARG:NE	4:42:104:ASP:OD1	2.33	0.60
15:5A:191:ILE:HG22	15:5A:191:ILE:O	2.01	0.60
19:5J:844:LEU:HD22	19:5J:863:TRP:HZ3	1.67	0.60
2:4:122:U:O2’	3:41:61:ARG:NH1	2.32	0.60
6:4A:427:PRO:CB	6:4A:639:LYS:CE	2.77	0.60
20:5O:177:LYS:HG2	20:5O:189:THR:HG22	1.82	0.60
15:5A:761:ILE:HD12	15:5A:775:ASN:ND2	2.16	0.60
15:5A:1626:CYS:SG	15:5A:1627:ALA:N	2.74	0.60
17:5C:846:VAL:HG22	17:5C:887:LEU:HD11	1.82	0.60
5:43:28:TYR:HB3	5:43:46:ILE:HD11	1.84	0.60
15:5A:192:GLN:CB	15:5A:208:TYR:CE2	2.75	0.60
19:5J:574:LYS:O	19:5J:578:LEU:HB2	2.01	0.60
1:X:116:LYS:HA	2:4:119:A:OP1	2.02	0.60
14:5:78:U:OP1	20:5O:182:ARG:O	2.20	0.60
1:X:125:ASN:HA	4:42:61:ARG:HG3	1.82	0.60
8:4C:357:ARG:HG3	8:4C:358:ARG:CG	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5A:976:MET:HG2	15:5A:1187:PHE:HB3	1.83	0.60
6:4A:524:GLN:CD	27:66:13:LYS:NZ	2.52	0.59
3:51:76:LEU:HA	3:51:79:LEU:HB2	1.84	0.59
15:5A:1790:ILE:HG22	15:5A:1798:LEU:HD11	1.84	0.59
16:5B:1861:ARG:H	16:5B:1864:GLU:HG3	1.66	0.59
32:U:146:ARG:HG3	32:U:146:ARG:NH1	2.11	0.59
1:X:124:VAL:HG13	2:4:118:A:N6	2.16	0.59
32:U:362:HIS:HB3	32:U:365:LEU:HD13	1.82	0.59
5:53:19:THR:HG23	5:53:72:ILE:HB	1.84	0.59
15:5A:1838:LYS:NZ	16:5B:205:PHE:O	2.34	0.59
17:5C:362:THR:HG22	17:5C:362:THR:O	2.03	0.59
19:5J:317:ARG:HA	19:5J:320:GLU:HG2	1.83	0.59
21:5X:601[B]:GLN:HG2	21:5X:602:THR:N	2.16	0.59
15:5A:1905:LEU:HD21	15:5A:1915:VAL:HG11	1.83	0.59
17:5C:388:VAL:HA	17:5C:392:LEU:HB2	1.84	0.59
5:53:14:GLU:HB2	17:5C:196:LYS:HE2	1.84	0.59
16:5B:1499:ASP:OD2	16:5B:1763:ARG:NH1	2.36	0.59
17:5C:137:HIS:HD2	17:5C:238:ASN:H	1.48	0.59
15:5A:761:ILE:CD1	15:5A:775:ASN:HD22	2.16	0.59
15:5A:853:LYS:O	15:5A:855:ARG:N	2.36	0.59
21:5X:540:LEU:CD2	21:5X:543:CYS:SG	2.91	0.59
22:6:102:A:O2'	22:6:103:U:OP2	2.16	0.59
22:6:103:U:C3'	29:68:65:ASP:OD1	2.51	0.59
32:U:455:LYS:HE2	32:U:458:THR:HG22	1.85	0.59
3:41:68:PHE:HB2	4:42:100:PHE:HB3	1.85	0.58
15:5A:1434:LYS:O	15:5A:1439:ARG:NH2	2.35	0.58
15:5A:1794:PHE:CE2	15:5A:1795:GLU:HG2	2.38	0.58
4:42:91:ASN:ND2	31:S:631:GLU:O	2.35	0.58
4:52:39:ASN:O	4:52:55:ARG:NH1	2.36	0.58
16:5B:971:LYS:HB2	16:5B:980:GLN:HB2	1.84	0.58
18:5D:30:PHE:HB3	18:5D:63:ILE:HD11	1.84	0.58
6:4A:423:GLN:OE1	7:4B:364:HIS:C	2.40	0.58
16:5B:1228:VAL:HG11	16:5B:1264:PRO:HD2	1.85	0.58
17:5C:343:LEU:HD13	17:5C:373:ILE:HD11	1.86	0.58
7:4B:242:ASN:HB3	7:4B:286:THR:HG21	1.84	0.58
15:5A:563:GLN:OE1	15:5A:563:GLN:HA	2.01	0.58
16:5B:120:ILE:O	16:5B:124:LEU:HB3	2.03	0.58
15:5A:341:LYS:O	21:5X:301:ARG:NH1	2.37	0.58
19:5J:766:LEU:HD11	19:5J:782:GLU:HG3	1.85	0.58
15:5A:85:LYS:HG2	15:5A:89:LEU:HD11	1.85	0.58
17:5C:478:THR:HA	17:5C:494:GLY:HA3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:52:107:ILE:HG22	4:52:108:VAL:HG13	1.86	0.58
15:5A:1537:TRP:CE3	15:5A:1751:LEU:HD13	2.39	0.58
19:5J:626:ALA:O	19:5J:629:SER:HB3	2.04	0.58
32:U:225:VAL:O	32:U:241:GLN:NE2	2.37	0.58
3:41:3:LEU:HD23	4:42:60:ASP:HB3	1.83	0.58
18:5D:101:LYS:HG3	18:5D:103:ASN:HB3	1.85	0.58
8:4C:97:ASN:ND2	8:4C:226:SER:O	2.37	0.58
1:X:137:TYR:CG	31:S:729:LEU:CD1	2.75	0.57
17:5C:182:LYS:HE2	17:5C:613:SER:HB3	1.84	0.57
22:6:106:U:O4	29:68:96:HIS:ND1	2.36	0.57
22:6:106:U:OP2	27:66:66:ARG:NH1	2.34	0.57
32:U:134:TYR:CZ	32:U:146:ARG:HB2	2.39	0.57
1:X:116:LYS:NZ	2:4:124:U:OP1	2.35	0.57
3:41:76:LEU:HA	3:41:79:LEU:HB2	1.85	0.57
6:4A:394:ILE:O	6:4A:412:PHE:N	2.36	0.57
15:5A:2164:PRO:HB3	15:5A:2296:LEU:HD11	1.84	0.57
19:5J:423:LEU:HD12	19:5J:443:LEU:HD12	1.86	0.57
16:5B:2101:ALA:HA	16:5B:2124:VAL:O	2.03	0.57
30:R:404:PHE:CZ	30:R:434:ASP:HA	2.24	0.57
15:5A:336:ASN:O	17:5C:262:ARG:NH2	2.37	0.57
4:42:30:SER:HA	4:42:33:THR:HG22	1.86	0.57
19:5J:503:ARG:HD3	19:5J:533:GLY:HA3	1.86	0.57
15:5A:853:LYS:HE3	15:5A:856:LEU:CD2	2.34	0.57
16:5B:1002:ASN:OD1	16:5B:1102:ARG:NH2	2.37	0.57
1:X:114:SER:HB2	2:4:120:U:OP2	2.05	0.57
8:4C:141:GLU:HG2	8:4C:155:LEU:HD13	1.86	0.57
15:5A:2284:MET:SD	15:5A:2287:ARG:NH1	2.78	0.57
16:5B:269:GLN:NE2	32:U:106:PRO:O	2.33	0.57
17:5C:559:ILE:HG21	17:5C:563:ALA:HB2	1.86	0.57
16:5B:2052:ILE:HG22	16:5B:2054:PRO:HD3	1.87	0.57
32:U:234:ASP:N	32:U:234:ASP:OD1	2.37	0.56
1:X:134:LYS:HE3	31:S:728:GLN:HE22	1.68	0.56
8:4C:377:ARG:O	15:5A:1505:LYS:NZ	2.38	0.56
16:5B:1060:ASN:OD1	16:5B:1064:GLN:NE2	2.35	0.56
16:5B:1663:ILE:HD12	16:5B:1704:ILE:HG12	1.87	0.56
16:5B:2066:VAL:HG21	16:5B:2090:VAL:HG11	1.87	0.56
21:5X:728:ILE:HG23	21:5X:729:ASP:N	2.20	0.56
3:41:25:VAL:HG22	3:41:45:MET:HG3	1.86	0.56
5:43:14:GLU:HA	5:43:32:LEU:HD22	1.86	0.56
15:5A:1042:GLN:HA	15:5A:1090:ARG:HH22	1.71	0.56
19:5J:455:LYS:HG2	31:S:572:ALA:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:5O:183:LYS:HG3	20:5O:187:ILE:HD11	1.87	0.56
32:U:307:SER:HB2	32:U:310:THR:HB	1.87	0.56
7:4B:294:VAL:HG23	7:4B:307:LEU:HB3	1.87	0.56
15:5A:1491:LYS:O	15:5A:1710:ASN:ND2	2.38	0.56
6:4A:424:LEU:HD12	7:4B:402:PHE:CE1	2.39	0.56
6:4A:462:GLU:OE2	30:R:436:VAL:HG21	2.05	0.56
8:4C:360:ARG:HH11	22:6:54:G:H5”	1.70	0.56
3:51:25:VAL:HG22	3:51:45:MET:HG3	1.86	0.56
15:5A:221:ASN:HD22	15:5A:226:GLN:HB2	1.69	0.56
15:5A:733:THR:HA	15:5A:736:GLU:HB3	1.87	0.56
15:5A:1381:ASP:O	15:5A:1385:VAL:HB	2.06	0.56
18:5D:86:ARG:NH2	30:R:446:TYR:CD1	2.72	0.56
32:U:259:TYR:OH	32:U:282:ARG:NH1	2.34	0.56
4:42:45:ASN:HB2	31:S:638:LEU:HD13	1.88	0.56
8:4C:235:ALA:HB2	8:4C:252:LEU:HD21	1.87	0.56
15:5A:1621:LYS:HE3	15:5A:1624:SER:OG	2.05	0.56
21:5X:370:TRP:CE3	21:5X:389:PRO:HD2	2.41	0.56
15:5A:1289:VAL:HG11	16:5B:42:SER:HA	1.88	0.56
16:5B:89:LEU:HD13	19:5J:366:VAL:HG21	1.88	0.56
17:5C:105:MET:N	17:5C:107:GLN:HE22	2.03	0.56
20:5O:311:VAL:HB	20:5O:321:TYR:HB2	1.88	0.56
21:5X:675:LYS:H	21:5X:675:LYS:HD2	1.71	0.56
32:U:404:GLU:O	32:U:405:LYS:HG3	2.04	0.56
4:52:53:LEU:HD11	4:52:71:LYS:HD3	1.86	0.56
15:5A:405:LEU:O	17:5C:413:ARG:NH2	2.38	0.56
15:5A:892:LYS:HD2	15:5A:912:GLU:HG3	1.87	0.56
15:5A:67:ARG:HD3	15:5A:179:ALA:HB2	1.88	0.56
15:5A:192:GLN:CG	15:5A:208:TYR:CD2	2.89	0.56
15:5A:852:VAL:O	15:5A:852:VAL:HG22	2.04	0.56
15:5A:2141:GLU:OE2	15:5A:2143:ARG:NH2	2.39	0.56
16:5B:1351:PRO:HG3	16:5B:1516:PRO:HA	1.88	0.56
16:5B:1130:ARG:HG2	16:5B:1140:VAL:HG11	1.88	0.56
18:5D:86:ARG:NE	30:R:446:TYR:CD2	2.74	0.56
1:X:141:MET:HB2	31:S:734:HIS:HA	1.88	0.55
17:5C:853:ARG:NH1	17:5C:879:ASP:O	2.36	0.55
14:5:7:U:C5’	20:5O:148:LYS:NZ	2.69	0.55
16:5B:722:LEU:HB3	16:5B:826:VAL:HG12	1.88	0.55
16:5B:1188:VAL:HG23	16:5B:1200:VAL:HG13	1.88	0.55
8:4C:374:GLN:H	8:4C:377:ARG:HD2	1.71	0.55
3:51:33:ASP:HB2	3:51:37:ASN:HB2	1.88	0.55
16:5B:278:ASP:HB3	16:5B:281:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:114:U:O2	2:4:114:U:H2'	2.06	0.55
3:41:33:ASP:HB2	3:41:37:ASN:HB2	1.88	0.55
6:4A:586:GLY:HA2	6:4A:641:ARG:HH21	1.71	0.55
15:5A:209:ASP:HB2	15:5A:212:PRO:HA	1.89	0.55
19:5J:725:MET:SD	19:5J:755:LYS:NZ	2.75	0.55
21:5X:458:LYS:O	21:5X:462:ILE:HG13	2.06	0.55
30:R:404:PHE:CZ	30:R:434:ASP:C	2.79	0.55
15:5A:1511:GLU:O	15:5A:1512:SER:HB3	2.07	0.55
16:5B:406:ARG:NH2	16:5B:974:LYS:O	2.40	0.55
16:5B:668:ASP:OD1	16:5B:671:LYS:NZ	2.39	0.55
16:5B:1063:LEU:HD11	16:5B:1118:ILE:HG12	1.88	0.55
16:5B:1729:ASP:OD1	16:5B:1729:ASP:N	2.39	0.55
6:4A:528:LYS:HA	6:4A:531:LYS:HG2	1.89	0.55
15:5A:188:LEU:O	15:5A:189:GLU:C	2.45	0.55
21:5X:381:THR:HG21	21:5X:420:GLN:HG2	1.87	0.55
32:U:162:HIS:HD2	32:U:176:PRO:CD	2.19	0.55
9:4D:18:LEU:HD21	9:4D:123:ILE:HG22	1.88	0.55
15:5A:844:GLU:OE2	15:5A:1459:ARG:NH1	2.40	0.55
15:5A:1559:GLY:HA3	15:5A:1622:MET:HE2	1.88	0.55
16:5B:1855:TYR:HB3	16:5B:1891:THR:HG21	1.88	0.55
2:4:17:A:C6	8:4C:357:ARG:NH1	2.75	0.55
15:5A:152:ARG:NH2	15:5A:618:THR:O	2.39	0.55
16:5B:531:ILE:HG13	16:5B:562:TYR:HB3	1.89	0.55
16:5B:1538:ARG:NH1	16:5B:1665:ASP:OD2	2.40	0.55
5:43:26:GLU:OE1	5:43:28:TYR:OH	2.25	0.55
15:5A:1265:THR:HG22	15:5A:1452:PRO:HG3	1.88	0.55
15:5A:1615:HIS:HE1	15:5A:1617:ARG:HE	1.53	0.55
16:5B:1108:THR:HG21	16:5B:1233:ILE:HD11	1.89	0.55
16:5B:1782:SER:OG	21:5X:162:LYS:O	2.25	0.55
17:5C:836:VAL:HG22	17:5C:897:SER:HB3	1.89	0.55
19:5J:295:ARG:HH21	19:5J:322:THR:HG23	1.71	0.55
19:5J:910:GLU:O	19:5J:914:ALA:HB2	2.06	0.55
32:U:403:ASP:OD2	32:U:404:GLU:HG3	2.07	0.55
15:5A:191:ILE:HG23	15:5A:572:PHE:CE2	2.42	0.55
15:5A:193:LEU:N	15:5A:208:TYR:OH	2.32	0.55
15:5A:911:VAL:HB	15:5A:916:LYS:HG3	1.89	0.55
16:5B:84:MET:HG2	16:5B:87:TYR:HB2	1.89	0.55
17:5C:804:GLY:H	17:5C:808:ILE:HD12	1.72	0.55
20:5O:81:LEU:HD21	20:5O:343:ILE:HD12	1.88	0.55
20:5O:309:VAL:HB	20:5O:323:LEU:HB2	1.88	0.55
21:5X:669:ILE:HG12	21:5X:737:VAL:CG1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4A:494:THR:O	6:4A:498:ALA:HB2	2.05	0.54
9:4D:64:GLU:HA	9:4D:67:LEU:HB2	1.90	0.54
4:52:41:GLN:HE21	4:52:53:LEU:HD13	1.72	0.54
32:U:227:LEU:HG	32:U:241:GLN:HE21	1.72	0.54
2:4:13:U:OP1	6:4A:507:ARG:NH2	2.38	0.54
4:42:49:ASN:HD21	31:S:636:ARG:H	1.55	0.54
15:5A:86:ARG:HB2	19:5J:98:ASP:HA	1.89	0.54
15:5A:1827:TRP:HA	15:5A:1830:GLN:HB2	1.89	0.54
15:5A:2068:SER:HB2	15:5A:2072:GLU:HB2	1.90	0.54
16:5B:463:PRO:HA	16:5B:480:THR:HA	1.90	0.54
16:5B:1617:VAL:HG22	16:5B:1643:VAL:HB	1.90	0.54
16:5B:1804:ILE:HG12	16:5B:1810:VAL:HG12	1.88	0.54
21:5X:604:MET:HE3	21:5X:621:LEU:HD11	1.89	0.54
4:42:39:ASN:O	4:42:55:ARG:NH1	2.39	0.54
6:4A:543:ILE:HG12	6:4A:585:GLU:HG3	1.89	0.54
16:5B:1041:LEU:HD22	16:5B:1052:ILE:HD13	1.90	0.54
20:5O:265:ARG:H	20:5O:272:ARG:HH12	1.54	0.54
20:5O:346:SER:OG	20:5O:348:ASP:OD1	2.24	0.54
21:5X:379:ILE:HG13	21:5X:379:ILE:O	2.06	0.54
21:5X:551:ALA:HB3	21:5X:606[A]:THR:CG2	2.37	0.54
15:5A:1795:GLU:OE1	15:5A:1795:GLU:HA	2.06	0.54
15:5A:1809:ILE:HB	15:5A:1818:PHE:HB2	1.89	0.54
16:5B:705:ASN:OD1	16:5B:829:LYS:NZ	2.39	0.54
21:5X:428:ASN:HD21	21:5X:598:LYS:NZ	2.05	0.54
15:5A:1604:LEU:HD11	15:5A:1725:LEU:HD22	1.90	0.54
16:5B:1093:ARG:NH1	16:5B:1273:ASP:O	2.38	0.54
14:5:7:U:HO2'	20:5O:146:ARG:HH22	1.42	0.54
15:5A:712:HIS:HE1	15:5A:728:VAL:HG11	1.73	0.54
16:5B:1139:VAL:HG23	16:5B:1167:MET:HG3	1.89	0.54
17:5C:366:GLN:HB2	17:5C:371:GLU:HG3	1.90	0.54
17:5C:524:ILE:HD12	17:5C:568:PRO:HB3	1.89	0.54
8:4C:353:LYS:O	22:6:53:A:N6	2.41	0.54
15:5A:86:ARG:HG3	19:5J:98:ASP:HB3	1.89	0.54
15:5A:271:MET:HB3	15:5A:310:THR:HG23	1.89	0.54
15:5A:900:ASP:O	15:5A:1246:GLN:NE2	2.41	0.54
15:5A:1163:ARG:HE	15:5A:1167:THR:HG23	1.73	0.54
19:5J:619:TRP:HD1	19:5J:620:LEU:HD23	1.72	0.54
20:5O:239:THR:O	20:5O:290:ARG:NH1	2.40	0.54
6:4A:388:GLU:HG3	7:4B:193:LEU:HD11	1.90	0.54
9:4D:97:ARG:HE	9:4D:98:PRO:HD2	1.71	0.54
15:5A:1537:TRP:HE3	15:5A:1751:LEU:HD13	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5A:2103:THR:HB	15:5A:2139:VAL:HG23	1.89	0.54
16:5B:660:ASP:OD1	16:5B:928:ARG:NH1	2.40	0.54
6:4A:440:LEU:HD23	6:4A:444:GLU:HB3	1.90	0.54
15:5A:357:ASN:ND2	17:5C:866:SER:O	2.41	0.54
15:5A:1038:SER:OG	15:5A:1438:VAL:CG1	2.56	0.54
16:5B:1195:ARG:NH1	16:5B:1292:PRO:O	2.39	0.54
18:5D:10:ASN:OD1	18:5D:13:GLN:NE2	2.41	0.54
7:4B:282:HIS:HD2	7:4B:284:LYS:H	1.54	0.54
15:5A:801:ILE:HD12	15:5A:1165:VAL:HG22	1.90	0.54
16:5B:2054:PRO:HG2	16:5B:2055:LEU:HD12	1.89	0.54
21:5X:540:LEU:HD13	21:5X:570:MET:SD	2.48	0.54
21:5X:728:ILE:HG12	21:5X:729:ASP:N	2.23	0.54
6:4A:385:PRO:HG2	7:4B:437:ARG:HH21	1.72	0.53
6:4A:425:ASN:O	7:4B:388:PHE:CZ	2.61	0.53
15:5A:1513:MET:O	15:5A:1515:TRP:N	2.41	0.53
24:63:54:LEU:HB3	24:63:57:VAL:CG1	2.38	0.53
15:5A:86:ARG:CD	19:5J:102:ASP:OD2	2.55	0.53
15:5A:1017:ILE:HD11	15:5A:1031:ILE:HG12	1.91	0.53
15:5A:1510:GLU:O	15:5A:1513:MET:CG	2.55	0.53
16:5B:1368:LEU:HD22	16:5B:1403:LYS:HE2	1.89	0.53
16:5B:1433:ASP:OD2	16:5B:1473:ARG:NH2	2.32	0.53
15:5A:996:LEU:HD13	15:5A:1047:VAL:HG21	1.89	0.53
17:5C:241:ARG:HB3	17:5C:583:ASN:HD21	1.73	0.53
30:R:393:ASN:HA	30:R:396:ILE:HB	1.88	0.53
15:5A:362:ARG:NH1	17:5C:283:ASP:OD2	2.41	0.53
15:5A:768:ASP:OD1	15:5A:768:ASP:N	2.41	0.53
17:5C:105:MET:N	17:5C:105:MET:SD	2.82	0.53
19:5J:362:VAL:HG11	19:5J:379:ALA:HB2	1.90	0.53
15:5A:1292:GLU:HG2	16:5B:40:VAL:HG21	1.91	0.53
17:5C:138:LEU:HD11	17:5C:179:VAL:HG22	1.91	0.53
17:5C:210:ASN:HB3	17:5C:636:TYR:HB2	1.91	0.53
21:5X:744:ASN:OD1	21:5X:746:GLU:HG2	2.09	0.53
15:5A:86:ARG:NH1	15:5A:89:LEU:HB2	2.24	0.53
16:5B:1849:ILE:HD13	16:5B:1923:ILE:HG12	1.90	0.53
6:4A:419:GLU:O	7:4B:361:GLN:NE2	2.42	0.53
14:5:91:U:O2'	3:51:61:ARG:NH1	2.42	0.53
15:5A:1771:LEU:HD22	15:5A:1812:PRO:HG3	1.91	0.53
16:5B:912:ASN:OD1	16:5B:912:ASN:N	2.40	0.53
16:5B:1991:GLU:O	16:5B:1995:ALA:N	2.41	0.53
27:66:66:ARG:HB2	27:66:69:ASN:HD22	1.74	0.53
14:5:7:U:HO2'	20:5O:146:ARG:NH2	2.04	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:52:44:ILE:HG23	4:52:106:VAL:HG23	1.90	0.53
16:5B:1756:THR:O	16:5B:1762:ARG:NH2	2.42	0.53
19:5J:662:ARG:HA	19:5J:684:LEU:HD11	1.91	0.53
8:4C:231:ILE:HB	8:4C:252:LEU:HD23	1.90	0.52
15:5A:1625:SER:OG	15:5A:1626:CYS:N	2.43	0.52
15:5A:1941:ARG:NE	15:5A:2011:ILE:O	2.38	0.52
16:5B:488:LEU:HD21	16:5B:501:LEU:HD13	1.92	0.52
20:5O:203:ASP:HB3	20:5O:247:GLY:HA3	1.92	0.52
29:68:36:LEU:HB3	29:68:38:LEU:CD1	2.39	0.52
1:X:123:SER:HB2	4:42:23:GLU:O	2.09	0.52
16:5B:1030:ARG:HH21	16:5B:1076:ALA:HB1	1.73	0.52
21:5X:322:ASP:HA	21:5X:325:GLU:HG2	1.91	0.52
7:4B:427:GLY:O	9:4D:125:ARG:NH2	2.38	0.52
8:4C:148:LYS:O	8:4C:152:ASN:ND2	2.35	0.52
8:4C:378:MET:HB3	15:5A:1503:TRP:HB2	1.92	0.52
16:5B:444:GLU:OE2	16:5B:446:HIS:NE2	2.39	0.52
16:5B:602:GLU:OE1	16:5B:606:THR:OG1	2.23	0.52
18:5D:87:ASN:OD1	19:5J:23:ARG:NH2	2.43	0.52
1:X:114:SER:HA	2:4:119:A:O2'	2.08	0.52
6:4A:571:GLY:HA3	6:4A:583:VAL:O	2.10	0.52
14:5:63:A:OP1	20:5O:106:LYS:HE2	2.09	0.52
15:5A:85:LYS:NZ	15:5A:85:LYS:CB	2.73	0.52
15:5A:1018:ASN:ND2	15:5A:1019:TYR:O	2.42	0.52
15:5A:1737:ASN:HB3	15:5A:1740:LEU:HB2	1.91	0.52
16:5B:691:GLY:HA3	16:5B:876:LEU:HD12	1.92	0.52
19:5J:708:PHE:HD2	19:5J:711:LEU:HD13	1.75	0.52
20:5O:67:GLY:N	20:5O:87:ASP:OD1	2.43	0.52
1:X:123:SER:CB	4:42:23:GLU:O	2.57	0.52
15:5A:838:LEU:HD13	15:5A:925:TYR:HA	1.92	0.52
15:5A:845:ARG:HD2	15:5A:1443:LYS:HE3	1.91	0.52
19:5J:332:ILE:HD12	19:5J:349:ALA:HA	1.90	0.52
4:52:32:LEU:HD22	4:52:56:VAL:HG11	1.90	0.52
15:5A:26:SER:OG	15:5A:27:GLU:N	2.42	0.52
16:5B:1598:ILE:HG13	16:5B:1599:PRO:HD3	1.91	0.52
17:5C:749:THR:OG1	17:5C:756:LYS:NZ	2.43	0.52
6:4A:427:PRO:HB2	6:4A:639:LYS:NZ	2.21	0.52
15:5A:570:ASP:HB3	15:5A:573:GLN:HG3	1.91	0.52
16:5B:720:GLN:NE2	16:5B:806:ILE:O	2.42	0.52
17:5C:169:ASP:HB3	17:5C:174:GLU:HB3	1.92	0.52
15:5A:824:PRO:HB2	19:5J:266:THR:HG22	1.92	0.52
15:5A:1212:GLY:HA3	15:5A:1280:ASN:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:5B:987:ILE:HG21	16:5B:1098:ILE:HG13	1.92	0.52
21:5X:365:MET:SD	21:5X:391:ARG:HD3	2.50	0.52
6:4A:444:GLU:OE2	9:4D:91:ARG:NH2	2.42	0.52
16:5B:419:GLY:O	16:5B:892:GLN:NE2	2.43	0.52
16:5B:1321:TYR:OH	16:5B:1361:GLU:OE1	2.22	0.52
16:5B:1829:ILE:HA	16:5B:1832:PHE:HB2	1.92	0.52
17:5C:660:VAL:HG22	17:5C:878:ILE:HD13	1.91	0.52
17:5C:761:SER:OG	17:5C:803:ARG:NH1	2.43	0.52
20:5O:160:ALA:HB3	20:5O:166:LEU:H	1.74	0.52
21:5X:371:ARG:O	21:5X:375:GLU:HB2	2.10	0.52
21:5X:540:LEU:HD23	21:5X:543:CYS:CB	2.39	0.52
2:4:114:U:P	2:4:114:U:C6	3.02	0.51
2:4:126:A:OP2	4:42:47:ARG:NH2	2.41	0.51
15:5A:397:ASN:N	15:5A:397:ASN:OD1	2.42	0.51
15:5A:1508:GLY:H	15:5A:1752:GLN:NE2	1.89	0.51
17:5C:779:LEU:O	17:5C:938:ARG:NH1	2.37	0.51
19:5J:628:ARG:O	19:5J:632:ALA:N	2.41	0.51
21:5X:361:LYS:O	21:5X:391:ARG:NH1	2.43	0.51
2:4:91:A:H2	2:4:110:G:H22	1.58	0.51
3:51:29:ILE:HA	3:51:40:LEU:HD23	1.93	0.51
17:5C:348:TYR:OH	17:5C:367:ARG:NH1	2.43	0.51
15:5A:221:ASN:HB2	15:5A:227:ARG:H	1.75	0.51
15:5A:97:HIS:ND1	15:5A:649:GLU:OE2	2.33	0.51
15:5A:321:ASN:O	17:5C:645:ARG:NH2	2.42	0.51
15:5A:1543:ASN:HD21	15:5A:1562:MET:HA	1.75	0.51
15:5A:1606:ILE:HG12	15:5A:1637:TRP:HZ2	1.75	0.51
17:5C:137:HIS:HA	17:5C:238:ASN:HB3	1.93	0.51
17:5C:383:GLN:HG3	17:5C:395:THR:HG21	1.93	0.51
21:5X:745:ILE:O	21:5X:749:ILE:HG12	2.10	0.51
28:67:26:LYS:HB2	28:67:83:LEU:HG	1.92	0.51
3:41:29:ILE:HA	3:41:40:LEU:HD23	1.93	0.51
9:4D:12:PRO:HB2	9:4D:126:LEU:HB3	1.92	0.51
15:5A:1057:ARG:NH1	15:5A:1060:GLU:OE1	2.44	0.51
15:5A:1413:ASP:OD2	16:5B:59:THR:OG1	2.27	0.51
16:5B:522:GLY:HA2	16:5B:525:ILE:HD11	1.93	0.51
16:5B:2060:ARG:NH2	16:5B:2111:ASP:O	2.44	0.51
15:5A:1002:ASP:OD2	15:5A:1004:ASN:ND2	2.39	0.51
15:5A:1927:ILE:HD12	15:5A:1931:THR:HG23	1.92	0.51
31:S:738:SER:HB2	31:S:743:THR:HG23	1.92	0.51
32:U:245:ASN:ND2	32:U:519:LEU:O	2.33	0.51
15:5A:139:VAL:HG11	15:5A:212:PRO:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5A:2188:LEU:O	15:5A:2251:TYR:OH	2.29	0.51
17:5C:300:LEU:HG	17:5C:306:ASN:HB3	1.92	0.51
32:U:323:LEU:HD21	32:U:451:ILE:HG21	1.93	0.51
4:42:53:LEU:O	4:42:70:VAL:HA	2.11	0.51
7:4B:332:HIS:NE2	7:4B:377:GLY:O	2.41	0.51
15:5A:1129:ASN:ND2	15:5A:1170:TRP:O	2.42	0.51
16:5B:1068:SER:HB2	16:5B:1070:LEU:HG	1.92	0.51
19:5J:154:GLU:HA	19:5J:157:TRP:HD1	1.75	0.51
19:5J:885:GLU:HG3	19:5J:897:VAL:HG11	1.93	0.51
20:5O:127:ALA:HB2	20:5O:157:CYS:HB3	1.91	0.51
15:5A:881:ILE:HG23	15:5A:918:THR:HG23	1.91	0.51
16:5B:131:ILE:HG12	16:5B:697:ALA:HB1	1.92	0.51
16:5B:259:HIS:HD2	16:5B:261:ARG:H	1.58	0.51
17:5C:304:LEU:O	17:5C:437:HIS:NE2	2.40	0.51
20:5O:263:ASP:OD1	20:5O:263:ASP:N	2.39	0.51
21:5X:479[B]:GLU:H	21:5X:479[B]:GLU:CD	2.12	0.51
7:4B:369:TYR:OH	9:4D:128:VAL:O	2.29	0.51
15:5A:488:ASP:OD2	15:5A:565:ARG:NH1	2.33	0.51
15:5A:913:PRO:HA	15:5A:916:LYS:HB2	1.93	0.51
15:5A:1184:ASN:OD1	15:5A:1195:ARG:NH1	2.39	0.51
15:5A:1586:HIS:NE2	15:5A:1628:ASP:OD2	2.44	0.51
17:5C:473:PRO:HB2	17:5C:571:ASN:HD21	1.76	0.51
21:5X:438:GLY:HA3	21:5X:758:ALA:CB	2.40	0.51
23:62:48:PRO:HG2	23:62:50:LYS:HB3	1.92	0.51
7:4B:332:HIS:HB2	7:4B:337:PHE:HB2	1.94	0.50
14:5:72:U:O2	17:5C:405:LYS:NZ	2.39	0.50
15:5A:419:ARG:NH1	15:5A:423:ASP:O	2.44	0.50
17:5C:571:ASN:HB3	17:5C:574:ALA:HB2	1.93	0.50
21:5X:485:GLU:HA	21:5X:523:ILE:HD13	1.93	0.50
22:6:74:U:H2'	22:6:75:G:H8	1.76	0.50
23:62:66:VAL:HG11	29:68:68:ALA:HA	1.93	0.50
6:4A:505:ALA:O	6:4A:509:LYS:HB2	2.11	0.50
15:5A:65:HIS:CE1	15:5A:483:GLN:OE1	2.62	0.50
15:5A:1510:GLU:N	15:5A:1510:GLU:OE1	2.44	0.50
16:5B:1901:ARG:HD2	16:5B:1961:LYS:HE3	1.92	0.50
18:5D:86:ARG:NE	30:R:446:TYR:CG	2.79	0.50
21:5X:352:TRP:O	21:5X:355:ARG:NE	2.38	0.50
21:5X:768:LEU:HD22	21:5X:776:PHE:CE1	2.46	0.50
25:64:65:THR:HG21	28:67:82:VAL:HG12	1.93	0.50
32:U:456:ARG:NH1	32:U:469:THR:O	2.37	0.50
5:43:19:THR:HA	5:43:28:TYR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5A:839:LEU:HD22	15:5A:878:LEU:HG	1.93	0.50
15:5A:1255:THR:HG22	15:5A:1257:THR:H	1.77	0.50
15:5A:1318:THR:HB	15:5A:1324:GLY:HA3	1.94	0.50
17:5C:137:HIS:HB2	17:5C:239:THR:HG23	1.92	0.50
21:5X:432:ILE:HG21	21:5X:609:MET:CE	2.41	0.50
21:5X:667:ILE:HA	21:5X:733[A]:VAL:CG1	2.40	0.50
1:X:132:SER:O	31:S:713:VAL:HG21	2.11	0.50
5:43:32:LEU:HD11	5:43:35:ALA:HB2	1.93	0.50
17:5C:950:SER:HB2	17:5C:956:PRO:HG2	1.94	0.50
2:4:59:U:H2'	2:4:60:A:H8	1.76	0.50
6:4A:423:GLN:CD	7:4B:365:SER:HA	2.25	0.50
4:52:54:GLY:HA3	4:52:70:VAL:HG12	1.92	0.50
15:5A:2074:ARG:O	15:5A:2078:ILE:HG13	2.11	0.50
19:5J:673:PRO:HB2	19:5J:677:VAL:HG23	1.83	0.50
23:62:69:TYR:HB3	24:63:85:LEU:HD11	1.92	0.50
32:U:145:GLY:O	32:U:152:ALA:HB3	2.10	0.50
7:4B:232:ARG:NH2	9:4D:74:GLU:OE1	2.44	0.50
16:5B:610:ARG:NH2	16:5B:645:ASP:O	2.44	0.50
16:5B:2013:ARG:HB3	16:5B:2052:ILE:HD11	1.93	0.50
17:5C:692:LEU:HD22	17:5C:696:LEU:HD23	1.92	0.50
21:5X:530:ILE:HD11	21:5X:565:LYS:HB3	1.93	0.50
15:5A:161:PHE:HB3	15:5A:625:PRO:HG2	1.92	0.50
15:5A:265:THR:HG22	15:5A:314:ILE:HG13	1.92	0.50
15:5A:759:GLU:OE2	15:5A:762:ARG:NH2	2.45	0.50
15:5A:1544:ARG:NH1	15:5A:1672:ASP:OD2	2.42	0.50
16:5B:617:ILE:HG22	16:5B:652:SER:HB2	1.93	0.50
16:5B:1156:LEU:HB2	16:5B:1161:ILE:HG13	1.93	0.50
19:5J:472:LYS:O	19:5J:476:ALA:HB2	2.12	0.50
25:64:71:ILE:HD11	29:68:59:LEU:HD22	1.93	0.50
1:X:140:TYR:CG	31:S:733:PHE:CE1	3.00	0.50
6:4A:569:LEU:HD23	6:4A:586:GLY:HA3	1.92	0.50
15:5A:221:ASN:N	15:5A:227:ARG:O	2.45	0.50
15:5A:292:ASP:OD1	15:5A:1139:ARG:NE	2.44	0.50
15:5A:843:LEU:HB3	15:5A:867:ILE:HG23	1.92	0.50
15:5A:851:SER:OG	15:5A:852:VAL:N	2.42	0.50
16:5B:1227:ASP:OD1	16:5B:1227:ASP:N	2.40	0.50
19:5J:438:LEU:HD11	19:5J:465:HIS:HB3	1.93	0.50
8:4C:236:GLY:O	8:4C:240:ASN:ND2	2.44	0.50
16:5B:1626:PRO:HA	16:5B:1629:ARG:HB2	1.94	0.50
21:5X:591:ASN:O	21:5X:594[B]:SER:HB3	2.12	0.50
32:U:232:ALA:HB1	32:U:316:GLN:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:123:U:OP1	3:41:61:ARG:NH2	2.38	0.49
3:41:24:GLN:HE22	4:42:94:ARG:HH12	1.59	0.49
6:4A:521:THR:OG1	6:4A:522:ALA:N	2.45	0.49
15:5A:504:LEU:HD11	15:5A:551:LEU:HD12	1.93	0.49
15:5A:1070:ASP:OD1	15:5A:1070:ASP:N	2.36	0.49
15:5A:1804:ASN:HD22	15:5A:1907:LEU:HA	1.77	0.49
17:5C:164:ASP:N	17:5C:164:ASP:OD1	2.45	0.49
17:5C:843:VAL:HG22	17:5C:871:ILE:HD11	1.94	0.49
25:64:71:ILE:HB	25:64:72:PRO:HD2	1.93	0.49
1:X:149:ARG:HG2	15:5A:1614:ILE:O	2.12	0.49
2:4:66:A:H5"	31:S:738:SER:HA	1.94	0.49
16:5B:1222:TRP:NE1	16:5B:1273:ASP:OD2	2.38	0.49
17:5C:666:VAL:HG22	17:5C:787:VAL:HG22	1.95	0.49
2:4:32:G:N7	9:4D:40:ASN:ND2	2.53	0.49
15:5A:1104:ASP:OD1	15:5A:1107:ARG:NH2	2.44	0.49
16:5B:1749:GLN:HE22	21:5X:163:PHE:H	1.59	0.49
1:X:138:ARG:HH12	15:5A:1614:ILE:CD1	2.26	0.49
5:43:23:ASN:OD1	5:43:69:ARG:NH2	2.45	0.49
15:5A:85:LYS:NZ	15:5A:85:LYS:HB2	2.28	0.49
15:5A:853:LYS:O	15:5A:853:LYS:HG3	2.12	0.49
15:5A:2131:VAL:HG13	15:5A:2172:MET:HG2	1.94	0.49
16:5B:604:THR:O	16:5B:607:GLN:NE2	2.43	0.49
17:5C:391:SER:O	17:5C:391:SER:OG	2.29	0.49
17:5C:401:ILE:HD11	17:5C:423:PHE:HB2	1.95	0.49
19:5J:89:PHE:O	19:5J:90:SER:CB	2.59	0.49
7:4B:294:VAL:HG21	7:4B:307:LEU:HB3	1.93	0.49
15:5A:559:ASP:C	15:5A:562:VAL:HG22	2.33	0.49
16:5B:79:HIS:O	16:5B:83:LYS:HB2	2.13	0.49
16:5B:517:MET:HG2	16:5B:538:ILE:HG21	1.94	0.49
19:5J:674:THR:C	19:5J:676:ARG:N	2.66	0.49
20:5O:69:VAL:HG11	20:5O:351:LEU:HD21	1.94	0.49
32:U:276:ARG:HD2	32:U:302:ALA:HB2	1.94	0.49
32:U:454:ILE:HD13	32:U:471:VAL:HG21	1.94	0.49
8:4C:356:GLY:HA2	22:6:54:G:P	2.53	0.49
15:5A:853:LYS:HG3	15:5A:856:LEU:CD2	2.42	0.49
16:5B:1666:THR:O	16:5B:1666:THR:OG1	2.30	0.49
17:5C:531:TRP:HB3	17:5C:538:HIS:HB3	1.94	0.49
20:5O:90:ILE:HB	20:5O:105:LEU:HB2	1.95	0.49
2:4:56:U:H4'	6:4A:465:ARG:HH22	1.77	0.49
5:53:23:ASN:O	5:53:69:ARG:NH2	2.46	0.49
15:5A:86:ARG:NH1	15:5A:89:LEU:CD1	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5A:1872:LEU:HB3	15:5A:1884:ILE:HD13	1.95	0.49
16:5B:491:ALA:O	16:5B:647:ARG:NH2	2.44	0.49
17:5C:105:MET:N	17:5C:107:GLN:NE2	2.60	0.49
19:5J:567:LEU:HD11	19:5J:576:VAL:HG12	1.95	0.49
19:5J:751:ARG:NH1	19:5J:782:GLU:OE2	2.45	0.49
20:5O:166:LEU:HD23	20:5O:178:LEU:HD11	1.94	0.49
21:5X:768:LEU:HD22	21:5X:776:PHE:HE1	1.77	0.49
22:6:105:U:C2	24:63:49:HIS:HB3	2.47	0.49
25:64:65:THR:HG21	28:67:82:VAL:CG1	2.43	0.49
16:5B:597:THR:OG1	16:5B:634:ARG:NH1	2.45	0.49
17:5C:126:SER:HA	17:5C:129:ILE:HD12	1.95	0.49
32:U:351:GLY:HA2	32:U:445:LYS:HD3	1.94	0.49
32:U:529:LEU:HG	32:U:534:VAL:HG22	1.93	0.49
2:4:109:G:H2'	2:4:110:G:H8	1.77	0.49
6:4A:427:PRO:HD3	7:4B:388:PHE:CZ	2.48	0.49
7:4B:290:ASP:OD1	7:4B:293:ASP:CB	2.61	0.49
7:4B:390:ARG:NH2	7:4B:399:CYS:SG	2.85	0.49
16:5B:1143:ILE:HG12	16:5B:1165:ILE:HD12	1.94	0.49
16:5B:1418:LEU:HD23	16:5B:1421:LYS:HD3	1.95	0.49
19:5J:530:ILE:O	19:5J:543:TRP:NE1	2.43	0.49
32:U:162:HIS:CD2	32:U:176:PRO:HD3	2.47	0.49
2:4:94:A:O2'	2:4:95:C:H5'	2.13	0.49
6:4A:668:HIS:HB2	7:4B:446:PRO:HD3	1.95	0.49
7:4B:284:LYS:O	7:4B:289:LEU:N	2.45	0.49
7:4B:290:ASP:OD1	7:4B:293:ASP:HB2	2.13	0.49
15:5A:712:HIS:NE2	19:5J:161:PRO:O	2.45	0.49
16:5B:537:LYS:N	16:5B:608:LEU:O	2.46	0.49
19:5J:347:LEU:HD11	19:5J:374:ARG:HB3	1.94	0.49
19:5J:646:LEU:HA	19:5J:649:VAL:HG22	1.95	0.49
24:63:50:LEU:HD22	27:66:66:ARG:CG	2.43	0.49
32:U:122:LYS:HE3	32:U:193:LEU:HD11	1.95	0.49
7:4B:322:HIS:CE1	7:4B:348:ARG:HD2	2.48	0.48
4:52:43:LEU:HB3	4:52:110:LEU:HD23	1.94	0.48
15:5A:279:PHE:HE2	15:5A:456:LEU:HG	1.78	0.48
15:5A:713:LEU:HD12	15:5A:739:ILE:HG12	1.94	0.48
15:5A:2086:ARG:NH1	15:5A:2222:SER:O	2.46	0.48
21:5X:304:ILE:O	21:5X:312:GLN:NE2	2.39	0.48
21:5X:485:GLU:O	21:5X:489:ILE:HG12	2.13	0.48
24:63:18:LEU:HA	24:63:21:ILE:HG22	1.95	0.48
6:4A:547:ARG:NH1	6:4A:680:GLU:OE1	2.46	0.48
17:5C:107:GLN:HG3	17:5C:109:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:5C:262:ARG:HA	17:5C:266:GLU:HG3	1.95	0.48
20:5O:116:HIS:HB3	20:5O:159:PRO:HD3	1.96	0.48
7:4B:366:MET:H	7:4B:386:ASP:HB3	1.76	0.48
15:5A:1776:ILE:HG13	15:5A:1811:ASN:HD21	1.78	0.48
16:5B:633:ALA:O	16:5B:637:ARG:HB2	2.13	0.48
16:5B:1186:LEU:HB3	16:5B:1202:LEU:HD11	1.96	0.48
17:5C:129:ILE:HG12	17:5C:199:LEU:HD23	1.95	0.48
19:5J:674:THR:C	19:5J:676:ARG:H	2.16	0.48
9:4D:111:GLN:HE22	22:6:71:G:H21	1.61	0.48
15:5A:96:PRO:HG3	15:5A:648:LEU:HB2	1.96	0.48
16:5B:928:ARG:NH2	16:5B:932:SER:OG	2.45	0.48
17:5C:105:MET:O	17:5C:106:GLU:HB2	2.13	0.48
32:U:356:PHE:HB2	32:U:440:ARG:HB2	1.96	0.48
1:X:148:ASN:HB3	15:5A:1613:THR:HB	1.94	0.48
7:4B:284:LYS:HE3	7:4B:288:SER:OG	2.12	0.48
7:4B:514:ARG:NH2	9:4D:75:ASP:OD2	2.47	0.48
5:53:79:ASN:ND2	17:5C:115:GLU:OE2	2.45	0.48
15:5A:162:LYS:N	21:5X:375:GLU:OE2	2.45	0.48
15:5A:274:PRO:HA	21:5X:282:THR:HG22	1.95	0.48
15:5A:1532:ARG:HG2	15:5A:1568:THR:HG23	1.95	0.48
16:5B:969:LEU:HD22	16:5B:985:GLY:HA2	1.95	0.48
16:5B:1836:LEU:HD22	16:5B:1840:THR:HG21	1.94	0.48
17:5C:644:LEU:O	17:5C:649:SER:OG	2.30	0.48
26:65:72:ILE:HG22	27:66:74:SER:HB2	1.95	0.48
27:66:52:VAL:CB	27:66:56:LEU:HD11	2.42	0.48
15:5A:104:GLU:HB2	15:5A:422:LEU:HD11	1.96	0.48
15:5A:109:PRO:HB2	15:5A:191:ILE:HD12	1.95	0.48
15:5A:974:ASN:OD1	15:5A:1100:ARG:NH1	2.42	0.48
15:5A:1892:PRO:HD2	15:5A:1937:ILE:HD11	1.96	0.48
17:5C:135:CYS:O	17:5C:227:LEU:HA	2.13	0.48
18:5D:8:LEU:HD13	18:5D:14:VAL:HA	1.96	0.48
19:5J:508:GLN:NE2	19:5J:511:GLU:OE1	2.46	0.48
19:5J:795:ILE:HA	19:5J:798:THR:HG22	1.94	0.48
15:5A:853:LYS:C	15:5A:855:ARG:H	2.17	0.48
15:5A:1244:VAL:HG11	15:5A:1291:CYS:HB3	1.95	0.48
16:5B:949:LEU:HG	16:5B:952:ARG:HB3	1.95	0.48
16:5B:1180:LEU:HD13	16:5B:1214:VAL:HG21	1.96	0.48
2:4:125:G:O6	3:41:66:ARG:NH2	2.44	0.48
14:5:7:U:C4'	20:5O:148:LYS:NZ	2.76	0.48
15:5A:559:ASP:O	15:5A:562:VAL:HG22	2.14	0.48
15:5A:1329:SER:O	15:5A:1367:ASN:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:5B:2064:TRP:O	16:5B:2081:ARG:HA	2.14	0.48
17:5C:603:MET:HB2	17:5C:651:ILE:HD11	1.95	0.48
4:42:54:GLY:HA3	4:42:70:VAL:HG12	1.96	0.48
6:4A:389:TRP:NE1	7:4B:436:LEU:O	2.37	0.48
9:4D:15:ASP:OD1	9:4D:15:ASP:N	2.47	0.48
3:51:68:PHE:HB2	4:52:100:PHE:HB3	1.96	0.48
16:5B:1332:GLN:NE2	16:5B:1355:GLY:O	2.43	0.48
16:5B:1361:GLU:OE2	16:5B:1393:TRP:NE1	2.41	0.48
16:5B:1981:SER:OG	16:5B:1982:VAL:N	2.47	0.48
17:5C:604:LEU:HD22	32:U:128:LEU:HD11	1.95	0.48
17:5C:826:ARG:NH1	17:5C:910:ASP:OD1	2.47	0.48
20:5O:251:LEU:HD23	20:5O:291:CYS:HB3	1.95	0.48
20:5O:263:ASP:O	20:5O:272:ARG:NH1	2.44	0.48
20:5O:330:ILE:HG12	20:5O:346:SER:HB3	1.96	0.48
14:5:78:U:P	20:5O:182:ARG:O	2.72	0.48
15:5A:1540:PRO:O	15:5A:1671:TYR:N	2.47	0.48
15:5A:2306:HIS:HD2	15:5A:2308:VAL:HG22	1.77	0.48
16:5B:74:ARG:NH2	16:5B:75:ASP:OD1	2.47	0.48
16:5B:428:CYS:HB3	31:S:553:PHE:HB2	1.96	0.48
16:5B:1378:TYR:OH	16:5B:1454:ASP:OD2	2.30	0.48
18:5D:73:TYR:OH	19:5J:23:ARG:NH1	2.47	0.48
20:5O:171:SER:OG	20:5O:173:ASP:OD1	2.32	0.48
21:5X:457:PRO:HG2	21:5X:460:ASP:OD2	2.14	0.48
21:5X:485:GLU:HA	21:5X:523:ILE:CD1	2.44	0.48
15:5A:274:PRO:HB3	21:5X:283:SER:HA	1.96	0.47
15:5A:425:PRO:HB2	15:5A:428:LYS:HB2	1.96	0.47
15:5A:1378:GLU:HB3	15:5A:1416:ILE:HD11	1.96	0.47
17:5C:645:ARG:NH2	17:5C:653:ILE:O	2.47	0.47
17:5C:680:ASN:ND2	17:5C:802:HIS:O	2.47	0.47
21:5X:551:ALA:HB3	21:5X:606[A]:THR:HG22	1.95	0.47
32:U:304:VAL:HG22	32:U:312:GLN:HA	1.96	0.47
2:4:108:C:H2'	2:4:109:G:C8	2.49	0.47
14:5:7:U:H3'	14:5:8:G:H8	1.78	0.47
16:5B:1265:GLN:HE21	16:5B:1287:ARG:HH12	1.61	0.47
16:5B:1699:GLU:OE2	16:5B:1701:ARG:NH2	2.46	0.47
19:5J:787:GLU:HG3	19:5J:799:LEU:HD12	1.96	0.47
21:5X:682:LYS:CG	21:5X:683:SER:N	2.74	0.47
25:64:6:LEU:HD23	29:68:37:ILE:HD12	1.96	0.47
15:5A:1214:TRP:NE1	15:5A:1276:GLU:OE1	2.42	0.47
16:5B:447:VAL:HB	16:5B:687:GLN:HG3	1.96	0.47
16:5B:756:SER:HA	16:5B:759:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:5C:836:VAL:O	17:5C:870:THR:HA	2.14	0.47
21:5X:540:LEU:CD2	21:5X:543:CYS:CB	2.92	0.47
22:6:103:U:C2'	29:68:65:ASP:OD1	2.61	0.47
2:4:68:A:N1	30:R:387:ASP:N	2.61	0.47
2:4:92:C:O2'	2:4:93:G:H5'	2.14	0.47
7:4B:438:GLN:OE1	7:4B:440:ARG:NH2	2.48	0.47
15:5A:2115:ILE:O	15:5A:2118:SER:OG	2.31	0.47
17:5C:135:CYS:HB2	17:5C:242:LEU:HD13	1.95	0.47
17:5C:916:ILE:HB	17:5C:931:ARG:HG2	1.96	0.47
32:U:424:GLY:O	32:U:440:ARG:NH2	2.42	0.47
4:42:41:GLN:O	4:42:112:ASN:ND2	2.48	0.47
4:52:32:LEU:HD11	4:52:109:VAL:HG11	1.95	0.47
15:5A:307:PRO:HG3	21:5X:246:GLU:HG3	1.96	0.47
15:5A:1219:GLU:O	15:5A:1222:LYS:NZ	2.44	0.47
16:5B:156:GLU:HG3	16:5B:157:ILE:HG12	1.97	0.47
16:5B:756:SER:O	16:5B:760:GLU:CB	2.63	0.47
16:5B:1298:PRO:HG3	16:5B:1515:HIS:HD2	1.78	0.47
20:5O:133:VAL:HG21	20:5O:169:THR:HG21	1.96	0.47
21:5X:540:LEU:HD23	21:5X:543:CYS:SG	2.54	0.47
15:5A:919:ASP:OD2	15:5A:1012:LYS:NZ	2.41	0.47
16:5B:1438:ARG:HB3	16:5B:1441:GLN:HE21	1.80	0.47
18:5D:73:TYR:O	18:5D:101:LYS:NZ	2.39	0.47
21:5X:530:ILE:HD11	21:5X:565:LYS:CG	2.44	0.47
21:5X:675:LYS:HG2	21:5X:676:GLY:N	2.30	0.47
32:U:135:ALA:HB2	32:U:167:LEU:HD21	1.96	0.47
32:U:172:PHE:HB2	32:U:181:ILE:HB	1.97	0.47
1:X:101:ILE:HG12	1:X:103:MET:HG2	1.95	0.47
2:4:140:G:H2'	2:4:141:A:H8	1.79	0.47
5:43:31:LYS:O	5:43:44:SER:N	2.47	0.47
7:4B:426:SER:OG	7:4B:428:ASP:OD1	2.23	0.47
14:5:7:U:P	20:5O:148:LYS:HZ2	2.34	0.47
15:5A:604:MET:O	15:5A:607:ASP:HB2	2.15	0.47
15:5A:828:PRO:O	19:5J:273:TYR:OH	2.22	0.47
15:5A:1267:LEU:O	15:5A:1271:MET:HB2	2.15	0.47
15:5A:1413:ASP:HB2	16:5B:58:ARG:HB3	1.97	0.47
15:5A:1640:SER:HA	15:5A:1653:ASP:H	1.79	0.47
15:5A:1787:ARG:HG3	15:5A:1803:ILE:HG13	1.96	0.47
17:5C:264:ILE:HD12	17:5C:381:LEU:HD22	1.96	0.47
17:5C:878:ILE:HD12	17:5C:881:PHE:HE2	1.79	0.47
18:5D:68:ASP:OD1	18:5D:68:ASP:N	2.48	0.47
4:52:31:VAL:HG13	4:52:111:ARG:HE	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5A:552:ARG:HG3	15:5A:552:ARG:NH2	2.20	0.47
15:5A:579:GLN:CA	15:5A:579:GLN:NE2	2.73	0.47
15:5A:1143:MET:HG3	15:5A:1181:ASP:HB3	1.97	0.47
15:5A:1260:VAL:HG21	15:5A:1325:LEU:HD13	1.97	0.47
19:5J:236:GLY:O	32:U:472:ASN:ND2	2.48	0.47
21:5X:362:LEU:HG	21:5X:395:ASP:OD2	2.14	0.47
21:5X:378:SER:O	21:5X:629[A]:ILE:HA	2.15	0.47
21:5X:673:GLN:HB3	21:5X:675:LYS:CD	2.45	0.47
2:4:110:G:O2'	2:4:111:C:H5'	2.13	0.47
7:4B:349:LEU:HB3	7:4B:359:LEU:HB3	1.96	0.47
15:5A:618:THR:HG21	21:5X:307:ILE:HG23	1.97	0.47
15:5A:1433:ASP:OD2	15:5A:1460:HIS:NE2	2.46	0.47
16:5B:61:PRO:HD2	16:5B:64:GLN:HE21	1.79	0.47
16:5B:297:SER:N	16:5B:301:GLU:OE2	2.47	0.47
16:5B:993:ILE:HD11	16:5B:998:VAL:HG13	1.96	0.47
17:5C:742:PRO:HG2	17:5C:785:ARG:HG3	1.97	0.47
19:5J:385:ASP:N	19:5J:385:ASP:OD1	2.48	0.47
14:5:89:U:O2'	5:53:64:ARG:NH2	2.48	0.47
5:53:16:HIS:HB3	5:53:74:PRO:HG2	1.97	0.47
15:5A:226:GLN:OE1	15:5A:227:ARG:NH1	2.48	0.47
16:5B:1737:ASN:HD21	16:5B:1816:GLY:HA2	1.78	0.47
16:5B:1831:LEU:O	16:5B:1835:SER:HB3	2.15	0.47
21:5X:798:HIS:HE1	21:5X:800:ASP:OD2	1.98	0.47
15:5A:947:PRO:HB2	15:5A:949:PRO:HD2	1.97	0.46
15:5A:1137:ASP:OD1	15:5A:1137:ASP:N	2.41	0.46
15:5A:1206:GLU:HG3	15:5A:2098:LYS:HA	1.96	0.46
15:5A:1551:PHE:O	15:5A:1553:VAL:HG23	2.14	0.46
16:5B:447:VAL:HG11	16:5B:884:ASN:HD21	1.79	0.46
16:5B:825:THR:HA	16:5B:866:GLU:O	2.15	0.46
17:5C:860:ASP:OD2	17:5C:860:ASP:N	2.48	0.46
32:U:466:LYS:NZ	32:U:546:GLU:OE1	2.44	0.46
4:42:43:LEU:HD13	4:42:53:LEU:HD12	1.97	0.46
3:51:19:LEU:HD21	3:51:60:ILE:HD13	1.98	0.46
15:5A:952:VAL:HG22	15:5A:1189:MET:HE3	1.96	0.46
15:5A:1701:VAL:HA	15:5A:1716:GLY:HA3	1.97	0.46
15:5A:2103:THR:O	15:5A:2140:LYS:N	2.46	0.46
16:5B:1277:SER:O	16:5B:1277:SER:OG	2.31	0.46
16:5B:2053:ALA:HB1	16:5B:2056:PHE:HB3	1.98	0.46
22:6:105:U:O2'	27:66:66:ARG:NH2	2.48	0.46
1:X:140:TYR:CD2	31:S:733:PHE:CE1	3.04	0.46
5:43:81:PRO:O	5:43:82:MET:SD	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5A:94:TYR:OH	19:5J:109:ASP:OD1	2.32	0.46
15:5A:1072:LEU:HD13	15:5A:1087:LEU:HD13	1.96	0.46
15:5A:1729:ALA:O	15:5A:1733:ILE:HB	2.14	0.46
16:5B:544:MET:HG3	16:5B:817:TRP:CE2	2.51	0.46
16:5B:1487:ILE:HG21	16:5B:1504:LEU:HD22	1.96	0.46
2:4:125:G:C2	3:41:20:LYS:HD3	2.51	0.46
7:4B:282:HIS:CD2	7:4B:284:LYS:H	2.32	0.46
7:4B:336:ARG:HE	7:4B:353:GLU:HB2	1.80	0.46
14:5:30:A:OP1	15:5A:595:LYS:NZ	2.44	0.46
15:5A:85:LYS:HB2	15:5A:85:LYS:HZ2	1.81	0.46
15:5A:976:MET:HE2	15:5A:1098:PHE:HD1	1.79	0.46
16:5B:1009:LEU:HD22	16:5B:1013:GLU:HG2	1.98	0.46
28:67:44:LEU:HD11	28:67:84:ILE:HD11	1.98	0.46
6:4A:427:PRO:CB	6:4A:639:LYS:HZ2	2.29	0.46
6:4A:427:PRO:HB3	6:4A:639:LYS:NZ	2.29	0.46
7:4B:513:ASP:OD1	19:5J:802:LYS:NZ	2.42	0.46
15:5A:71:ARG:NH1	15:5A:177:ASP:OD2	2.48	0.46
15:5A:340:ILE:HG23	15:5A:355:LEU:HD12	1.97	0.46
15:5A:1218:ASN:HB3	15:5A:1221:THR:HG22	1.98	0.46
15:5A:1600:GLU:HG2	15:5A:1725:LEU:HD13	1.98	0.46
19:5J:343:GLU:HG2	19:5J:369:LEU:HD13	1.97	0.46
21:5X:728:ILE:HG12	21:5X:729:ASP:H	1.80	0.46
32:U:175:LEU:CD1	32:U:175:LEU:N	2.79	0.46
14:5:109:G:O3'	3:51:49:ASN:ND2	2.48	0.46
17:5C:701:GLU:OE2	17:5C:785:ARG:NH1	2.43	0.46
19:5J:92:GLY:O	19:5J:93:PRO:HB3	2.16	0.46
1:X:126:ALA:HA	4:42:24:PHE:CD1	2.50	0.46
4:42:70:VAL:HG23	4:42:96:ILE:HB	1.98	0.46
9:4D:11:TYR:OH	9:4D:128:VAL:OXT	2.34	0.46
14:5:56:C:H4'	15:5A:100:LEU:HD21	1.97	0.46
15:5A:1248:LEU:HD11	15:5A:1294:LYS:HB3	1.97	0.46
15:5A:1512:SER:O	15:5A:1513:MET:HB2	2.15	0.46
15:5A:1526:LEU:HD13	15:5A:1529:ILE:HD12	1.97	0.46
15:5A:1832:ARG:HG3	15:5A:1836:LEU:HD13	1.98	0.46
17:5C:675:PHE:HA	17:5C:685:ILE:O	2.16	0.46
19:5J:659:GLU:O	19:5J:662:ARG:HB2	2.15	0.46
32:U:391:LEU:HD12	32:U:452:PHE:HE1	1.81	0.46
2:4:60:A:H3'	31:S:745:ARG:HH21	1.80	0.46
7:4B:271:GLY:O	7:4B:306:LYS:NZ	2.44	0.46
15:5A:1555:LEU:HD11	15:5A:1570:LYS:HG3	1.96	0.46
21:5X:693:THR:O	21:5X:694:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:U:497:TYR:CZ	32:U:554:ARG:HG3	2.51	0.46
32:U:503:ILE:HB	32:U:549:ILE:HB	1.98	0.46
15:5A:811:THR:HA	15:5A:814:VAL:HG22	1.98	0.46
15:5A:1381:ASP:HA	15:5A:1384:ARG:HG2	1.98	0.46
15:5A:1585:ILE:HD11	15:5A:1743:LEU:HB2	1.98	0.46
15:5A:1645:LEU:HB2	15:5A:1714:ALA:H	1.81	0.46
15:5A:1973:ASP:N	15:5A:1973:ASP:OD1	2.49	0.46
16:5B:1951:GLN:HG3	16:5B:1962:GLN:HG3	1.98	0.46
19:5J:97:ASP:OD2	19:5J:97:ASP:N	2.49	0.46
20:5O:130:ASP:OD1	20:5O:130:ASP:N	2.49	0.46
1:X:138:ARG:HH22	15:5A:1614:ILE:HD12	1.81	0.46
15:5A:552:ARG:CG	15:5A:552:ARG:NH2	2.73	0.46
15:5A:1600:GLU:HG3	15:5A:1604:LEU:HG	1.98	0.46
15:5A:1676:ILE:HD13	15:5A:1706:ASP:HB2	1.97	0.46
30:R:393:ASN:H	30:R:396:ILE:HD12	1.81	0.46
2:4:69:C:C4	30:R:458:MET:HG2	2.51	0.45
7:4B:427:GLY:HA2	7:4B:451:LEU:HB2	1.97	0.45
15:5A:166:PHE:CE1	15:5A:581:ILE:HD11	2.51	0.45
15:5A:1443:LYS:HD3	15:5A:1443:LYS:HA	1.78	0.45
16:5B:439:ARG:NH1	16:5B:442:TYR:OH	2.49	0.45
16:5B:462:LEU:HD12	16:5B:466:LYS:HB2	1.97	0.45
16:5B:1886:ASP:HB3	16:5B:1889:VAL:HG22	1.97	0.45
19:5J:425:ARG:HH12	31:S:568:THR:HG23	1.79	0.45
19:5J:665:LEU:HD12	19:5J:684:LEU:HD12	1.98	0.45
1:X:103:MET:HB2	1:X:110:ALA:HB2	1.99	0.45
8:4C:298:LYS:HD2	8:4C:320:LEU:HD22	1.98	0.45
15:5A:181:ASN:O	15:5A:185:VAL:HG21	2.16	0.45
15:5A:533:LYS:HD2	18:5D:71:LYS:HG3	1.97	0.45
19:5J:444:GLU:CD	31:S:574:ASN:ND2	2.70	0.45
30:R:394:ASP:OD1	30:R:394:ASP:N	2.49	0.45
32:U:320:VAL:O	32:U:324:SER:OG	2.30	0.45
4:42:33:THR:HA	4:42:36:VAL:HG12	1.96	0.45
6:4A:425:ASN:O	7:4B:388:PHE:HZ	2.00	0.45
7:4B:282:HIS:CD2	7:4B:289:LEU:HD12	2.52	0.45
7:4B:408:LYS:HB2	7:4B:428:ASP:HB3	1.98	0.45
15:5A:750:TRP:HH2	15:5A:781:ARG:HB2	1.81	0.45
15:5A:1987:ILE:HG21	15:5A:2011:ILE:HG13	1.98	0.45
16:5B:432:ASP:OD1	16:5B:432:ASP:N	2.49	0.45
30:R:414:ARG:HA	30:R:421:THR:HA	1.98	0.45
32:U:227:LEU:HD22	32:U:296:PRO:HB3	1.97	0.45
32:U:497:TYR:HB3	32:U:552:TRP:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:41:19:LEU:HD21	3:41:60:ILE:HD13	1.98	0.45
5:43:10:LEU:HD21	5:43:39:MET:HG2	1.99	0.45
15:5A:542:ASN:O	15:5A:546:LEU:HB2	2.16	0.45
15:5A:591:MET:HE2	15:5A:598:LEU:HD21	1.98	0.45
16:5B:1824:ILE:HD13	16:5B:1829:ILE:HD11	1.98	0.45
17:5C:109:LEU:HD13	17:5C:116:MET:HG3	1.98	0.45
17:5C:589:LYS:HG3	17:5C:628:VAL:HG13	1.98	0.45
17:5C:834:VAL:HG11	17:5C:883:PHE:HE2	1.81	0.45
20:5O:173:ASP:OD1	20:5O:173:ASP:N	2.50	0.45
21:5X:511:GLN:OE1	21:5X:528:ARG:NE	2.49	0.45
25:64:71:ILE:CG1	29:68:59:LEU:HB3	2.47	0.45
1:X:137:TYR:CD2	31:S:729:LEU:HA	2.52	0.45
15:5A:513:LEU:HD21	15:5A:537:LYS:HE2	1.97	0.45
15:5A:975:VAL:HG22	15:5A:1177:VAL:HG22	1.97	0.45
15:5A:1317:TYR:HE1	15:5A:1329:SER:HB2	1.74	0.45
15:5A:1847:ALA:O	15:5A:1851:SER:OG	2.28	0.45
16:5B:1535:THR:O	16:5B:1539:LEU:HB2	2.15	0.45
17:5C:677:GLU:O	17:5C:814:ARG:NH1	2.50	0.45
21:5X:378:SER:O	21:5X:629[B]:ILE:HA	2.16	0.45
26:65:58:GLU:HG3	26:65:65:ARG:HH21	1.82	0.45
4:42:32:LEU:HD21	4:42:109:VAL:HG11	1.99	0.45
15:5A:1389:TYR:OH	16:5B:222:GLU:OE2	2.35	0.45
15:5A:1604:LEU:HB3	15:5A:1719:PHE:HE1	1.81	0.45
16:5B:1066:PHE:CG	16:5B:1085:THR:HG21	2.52	0.45
20:5O:155:ASN:ND2	20:5O:196:VAL:O	2.48	0.45
21:5X:730:ILE:HD12	21:5X:731:GLN:O	2.16	0.45
27:66:34:LEU:HD21	27:66:37:LEU:HD23	1.99	0.45
31:S:723:LYS:HZ3	31:S:727:ARG:HH12	1.64	0.45
2:4:18:G:H4'	2:4:19:U:H5'	1.98	0.45
4:42:88:LYS:HD2	4:42:89:PRO:HD2	1.98	0.45
8:4C:103:ILE:HG21	8:4C:201:LYS:HB2	1.98	0.45
14:5:7:U:P	20:5O:148:LYS:NZ	2.86	0.45
15:5A:1267:LEU:HD11	15:5A:1330:MET:CG	2.47	0.45
16:5B:730:GLU:HA	16:5B:733:LYS:HB2	1.99	0.45
16:5B:2020:SER:HB2	16:5B:2040:GLN:HB2	1.99	0.45
20:5O:58:PRO:O	20:5O:60:MET:N	2.45	0.45
22:6:49:G:N2	30:R:387:ASP:HA	2.31	0.45
6:4A:423:GLN:NE2	7:4B:364:HIS:C	2.68	0.45
14:5:26:A:O3'	15:5A:635:ARG:NH2	2.50	0.45
15:5A:66:VAL:HG11	15:5A:487:LEU:HD11	1.99	0.45
15:5A:761:ILE:HG12	15:5A:767:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5A:1134:TRP:O	15:5A:1139:ARG:NH1	2.50	0.45
15:5A:2330:ARG:HH11	16:5B:1086:GLN:HE21	1.64	0.45
16:5B:414:LEU:HB2	16:5B:894:VAL:HG11	1.99	0.45
17:5C:644:LEU:HG	17:5C:653:ILE:HD13	1.99	0.45
19:5J:238:LEU:HD21	32:U:544:LEU:HD23	1.99	0.45
21:5X:545:TYR:CE1	21:5X:601[B]:GLN:OE1	2.69	0.45
31:S:565:GLU:HB3	31:S:567:PRO:HD2	1.99	0.45
4:42:71:LYS:HZ3	4:42:95:TYR:HB2	1.81	0.45
3:51:67:TYR:HB3	4:52:101:LEU:HD12	1.98	0.45
15:5A:598:LEU:HD11	15:5A:637:TRP:HZ3	1.81	0.45
15:5A:2189:SER:OG	15:5A:2191:GLN:OE1	2.34	0.45
24:63:50:LEU:HD22	27:66:66:ARG:HG2	1.98	0.45
1:X:119:LYS:HD3	2:4:116:G:C5’	2.47	0.45
8:4C:222:ILE:HA	8:4C:321:LYS:HD3	1.98	0.45
15:5A:121:HIS:NE2	19:5J:105:TYR:OH	2.50	0.45
15:5A:319:LEU:HD11	17:5C:590:ILE:HG21	1.99	0.45
15:5A:1110:ILE:HD11	15:5A:1149:LEU:HB2	1.98	0.45
15:5A:1703:ILE:HG12	15:5A:1714:ALA:HB2	1.99	0.45
16:5B:112:THR:HA	16:5B:115:VAL:HG12	1.98	0.45
16:5B:1568:GLN:NE2	16:5B:1572:THR:OG1	2.44	0.45
17:5C:374:LEU:HD23	17:5C:374:LEU:HA	1.82	0.45
18:5D:94:LEU:HD11	18:5D:102:ILE:HD13	1.98	0.45
21:5X:673:GLN:HB3	21:5X:675:LYS:HD2	1.98	0.45
21:5X:679:VAL:HG23	21:5X:682:LYS:HE2	1.99	0.45
22:6:103:U:O4’	29:68:65:ASP:CG	2.55	0.45
32:U:211:LEU:HD13	32:U:221:LEU:HG	1.99	0.45
2:4:114:U:C6	2:4:114:U:O5’	2.70	0.44
9:4D:79:PRO:HG2	9:4D:120:GLN:HG2	2.00	0.44
15:5A:853:LYS:C	15:5A:855:ARG:N	2.71	0.44
15:5A:1214:TRP:HB2	15:5A:1228:CYS:HB3	1.99	0.44
15:5A:1629:ILE:HB	15:5A:1662:ILE:HB	1.98	0.44
16:5B:540:TYR:HD1	16:5B:587:VAL:HG13	1.82	0.44
17:5C:529:ARG:H	17:5C:553:GLU:HB3	1.82	0.44
21:5X:730:ILE:O	21:5X:730:ILE:HG13	2.16	0.44
32:U:170:LEU:HD11	32:U:194:LYS:HD3	1.98	0.44
15:5A:340:ILE:HG22	21:5X:301:ARG:NH1	2.32	0.44
15:5A:1486:GLU:OE1	15:5A:1674:HIS:NE2	2.50	0.44
17:5C:213:ASP:O	17:5C:216:THR:OG1	2.29	0.44
17:5C:316:ILE:HD13	17:5C:377:LEU:HD11	1.98	0.44
21:5X:581[A]:GLU:CD	21:5X:587:LYS:HD3	2.38	0.44
26:65:70:ASP:HB3	27:66:75:THR:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:5:29:A:H2'	14:5:30:A:H8	1.82	0.44
15:5A:610:HIS:NE2	33:5A:2401:IHP:O31	2.39	0.44
15:5A:2107:PRO:HG2	15:5A:2110:VAL:HG22	1.98	0.44
16:5B:681:ARG:HG2	16:5B:682:PRO:HD2	1.99	0.44
16:5B:1569:THR:OG1	16:5B:1645:VAL:O	2.34	0.44
17:5C:366:GLN:HB3	17:5C:370:VAL:HB	1.99	0.44
18:5D:18:ILE:HA	18:5D:26:VAL:HG21	2.00	0.44
21:5X:297:GLN:HE22	21:5X:319:PHE:HB3	1.80	0.44
21:5X:362:LEU:CD2	21:5X:391:ARG:CZ	2.75	0.44
3:41:67:TYR:OH	4:42:94:ARG:NH2	2.49	0.44
15:5A:142:SER:HA	15:5A:242:ALA:HB2	1.98	0.44
15:5A:580:TYR:CD2	15:5A:588:LEU:HD11	2.52	0.44
15:5A:801:ILE:HD13	15:5A:992:LEU:HD22	2.00	0.44
15:5A:1121:ASN:HD21	32:U:297:HIS:HE1	1.65	0.44
16:5B:1659:HIS:HE1	16:5B:1701:ARG:HE	1.65	0.44
20:5O:155:ASN:O	20:5O:290:ARG:NH2	2.51	0.44
20:5O:217:ILE:HB	20:5O:231:MET:HB2	1.98	0.44
15:5A:86:ARG:HH11	15:5A:89:LEU:HD12	1.78	0.44
15:5A:384:VAL:HG12	15:5A:385:GLU:N	2.31	0.44
15:5A:746:LYS:O	15:5A:750:TRP:HB2	2.17	0.44
15:5A:1536:LEU:O	15:5A:1539:SER:OG	2.30	0.44
15:5A:1807:ILE:O	15:5A:1819:LEU:HA	2.17	0.44
21:5X:404:GLU:O	21:5X:408:LYS:HG2	2.17	0.44
21:5X:427:GLN:O	21:5X:588:MET:HB3	2.17	0.44
21:5X:670:PHE:CG	21:5X:751:ARG:HD3	2.52	0.44
22:6:53:A:H2'	22:6:54:G:C8	2.52	0.44
1:X:125:ASN:HA	4:42:61:ARG:CD	2.47	0.44
14:5:77:G:O3'	20:5O:182:ARG:O	2.35	0.44
4:52:48:ASN:OD1	4:52:48:ASN:N	2.42	0.44
15:5A:402:ILE:HG21	17:5C:268:LYS:HD3	2.00	0.44
15:5A:1502:PHE:O	15:5A:1753:LEU:HD12	2.18	0.44
16:5B:876:LEU:HD23	16:5B:880:LEU:HD23	2.00	0.44
17:5C:775:ARG:HH21	32:U:154:ILE:HD11	1.83	0.44
19:5J:725:MET:HG2	19:5J:752:LEU:HD11	1.99	0.44
32:U:449:TYR:HA	32:U:552:TRP:O	2.17	0.44
2:4:113:U:O3'	2:4:114:U:C6	2.71	0.44
15:5A:422:LEU:O	15:5A:635:ARG:NE	2.44	0.44
15:5A:1863:VAL:HG21	15:5A:1869:LEU:HB3	1.99	0.44
16:5B:1225:VAL:HG11	16:5B:1256:VAL:HG11	1.99	0.44
17:5C:469:ASP:OD1	17:5C:469:ASP:N	2.49	0.44
19:5J:710:LYS:HA	19:5J:713:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5X:530:ILE:O	21:5X:534:GLU:HG2	2.17	0.44
22:6:53:A:H2'	22:6:54:G:H8	1.83	0.44
26:65:27:HIS:HE2	26:65:35:GLU:CD	2.21	0.44
32:U:228:ASN:HB2	32:U:295:SER:HA	2.00	0.44
2:4:113:U:O3'	2:4:114:U:C5	2.71	0.44
4:42:56:VAL:HA	4:42:67:LEU:HD23	1.99	0.44
15:5A:380:LEU:HA	15:5A:381:PRO:HD3	1.72	0.44
15:5A:750:TRP:CE2	15:5A:778:ARG:HG2	2.53	0.44
16:5B:466:LYS:HB3	16:5B:466:LYS:HE3	1.84	0.44
16:5B:815:LEU:HD21	16:5B:821:LEU:HD11	1.99	0.44
16:5B:968:ASN:ND2	16:5B:999:GLN:OE1	2.51	0.44
17:5C:568:PRO:HB2	17:5C:569:ARG:HD2	1.99	0.44
19:5J:675:ALA:O	19:5J:678:PHE:HB2	2.17	0.44
19:5J:709:PRO:HA	19:5J:712:TRP:HD1	1.83	0.44
14:5:111:A:H2'	14:5:112:A:C8	2.52	0.44
15:5A:92:LEU:HD13	15:5A:503:MET:HG3	2.00	0.44
15:5A:723:ASN:OD1	15:5A:785:LYS:NZ	2.50	0.44
15:5A:2280:ASN:HB3	15:5A:2309:HIS:CG	2.52	0.44
16:5B:304:ASN:HA	16:5B:307:VAL:HG22	1.99	0.44
16:5B:690:VAL:HG11	16:5B:707:ILE:HG21	2.00	0.44
16:5B:1437:ARG:HG2	16:5B:1738:ALA:HB1	1.99	0.44
16:5B:1557:LYS:HD3	16:5B:1659:HIS:CD2	2.53	0.44
21:5X:530:ILE:CD1	21:5X:565:LYS:HB3	2.48	0.44
21:5X:683:SER:O	21:5X:686:LYS:HB2	2.18	0.44
7:4B:459:PRO:HG2	7:4B:502:SER:HA	2.00	0.43
8:4C:163:THR:HA	8:4C:166:VAL:HG12	1.99	0.43
15:5A:1267:LEU:HD23	15:5A:1328:LEU:HB2	2.00	0.43
15:5A:1838:LYS:HE3	15:5A:1865:ARG:HH22	1.83	0.43
16:5B:338:GLN:HA	32:U:184:SER:HB2	2.00	0.43
19:5J:845:LEU:HD13	19:5J:877:ALA:HA	1.98	0.43
19:5J:905:GLU:HA	19:5J:906:PRO:HD3	1.80	0.43
21:5X:428:ASN:HD21	21:5X:598:LYS:HZ2	1.66	0.43
22:6:105:U:O2	24:63:49:HIS:HB3	2.18	0.43
32:U:108:LEU:HD11	32:U:181:ILE:HG21	2.00	0.43
3:41:51:GLU:OE1	3:41:51:GLU:N	2.52	0.43
7:4B:336:ARG:HH21	7:4B:353:GLU:HB3	1.83	0.43
14:5:29:A:H2'	14:5:30:A:C8	2.53	0.43
15:5A:731:LEU:HD21	15:5A:739:ILE:HD12	2.00	0.43
15:5A:751:THR:HA	15:5A:782:LEU:HD11	2.00	0.43
15:5A:942:PRO:HB2	15:5A:1437:ARG:HD2	2.00	0.43
15:5A:970:GLU:HG3	15:5A:970:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:5B:1989:GLU:O	16:5B:1993:ARG:N	2.43	0.43
1:X:125:ASN:HA	4:42:61:ARG:HD3	2.01	0.43
2:4:93:G:H2'	2:4:94:A:H8	1.82	0.43
15:5A:292:ASP:OD2	15:5A:1132:LYS:NZ	2.39	0.43
15:5A:355:LEU:HD13	21:5X:299:LEU:HB3	2.00	0.43
15:5A:766:THR:O	18:5D:141:ARG:NH1	2.51	0.43
15:5A:991:THR:HB	19:5J:251:MET:HE2	2.00	0.43
15:5A:1516:LYS:HB3	15:5A:1518:LEU:HD22	1.99	0.43
16:5B:146:GLU:OE2	16:5B:149:ARG:NH1	2.51	0.43
16:5B:769:CYS:O	16:5B:775:LYS:NZ	2.49	0.43
17:5C:480:LYS:NZ	17:5C:613:SER:O	2.50	0.43
20:5O:149:GLY:O	20:5O:177:LYS:NZ	2.43	0.43
26:65:40:LEU:HD13	26:65:49:MET:HE3	1.99	0.43
32:U:105:CYS:HB3	32:U:108:LEU:HD13	1.99	0.43
5:43:78:LYS:CG	5:43:79:ASN:OD1	2.60	0.43
5:53:23:ASN:N	5:53:67:LYS:O	2.52	0.43
15:5A:143:GLN:NE2	15:5A:207:PHE:O	2.35	0.43
15:5A:682:ASP:N	15:5A:682:ASP:OD1	2.47	0.43
16:5B:694:GLU:O	16:5B:700:ARG:NH1	2.46	0.43
16:5B:1109:ASP:OD2	16:5B:1269:ARG:NH2	2.51	0.43
16:5B:1415:ASP:HB3	16:5B:1435:LEU:HD11	2.00	0.43
17:5C:770:PHE:HA	17:5C:816:VAL:HG21	2.00	0.43
19:5J:92:GLY:O	19:5J:93:PRO:CB	2.64	0.43
31:S:720:LEU:HG	31:S:724:GLU:HG3	2.00	0.43
32:U:144:GLN:HE21	32:U:144:GLN:HB3	1.67	0.43
32:U:516:ILE:HG12	32:U:518:VAL:HG13	2.01	0.43
2:4:22:C:H2'	2:4:23:G:H8	1.82	0.43
2:4:105:A:H2'	2:4:106:G:H8	1.83	0.43
4:42:41:GLN:HG2	4:42:55:ARG:HG2	2.00	0.43
7:4B:230:ASP:OD2	7:4B:252:SER:OG	2.35	0.43
7:4B:290:ASP:OD1	7:4B:293:ASP:CG	2.57	0.43
15:5A:511:LYS:HB2	15:5A:513:LEU:HG	1.99	0.43
16:5B:905:ILE:HD13	16:5B:970:VAL:HG21	2.00	0.43
16:5B:1004:LEU:HB3	16:5B:1017:VAL:HG22	2.01	0.43
16:5B:1313:ARG:HG2	16:5B:1340:TYR:HE1	1.84	0.43
16:5B:1469:VAL:HG21	16:5B:1735:HIS:CG	2.54	0.43
16:5B:1763:ARG:HA	16:5B:1763:ARG:HD2	1.71	0.43
16:5B:1847:GLU:HG2	16:5B:1892:ASN:HD21	1.83	0.43
16:5B:2050:PRO:HB3	16:5B:2059:LYS:HE2	1.99	0.43
21:5X:711:LYS:HA	21:5X:731:GLN:NE2	2.26	0.43
2:4:41:C:H5'	19:5J:828:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:124:U:H1'	4:42:104:ASP:HB3	2.01	0.43
3:41:36:MET:HE3	4:42:102:ARG:HH21	1.82	0.43
7:4B:259:SER:O	7:4B:263:CYS:N	2.51	0.43
8:4C:128:LEU:HD13	8:4C:166:VAL:HG13	1.99	0.43
15:5A:188:LEU:O	15:5A:189:GLU:O	2.37	0.43
15:5A:979:SER:O	15:5A:1094:ARG:HA	2.18	0.43
26:65:37:VAL:HG12	26:65:55:THR:HB	2.00	0.43
30:R:394:ASP:HB3	30:R:414:ARG:HH21	1.84	0.43
4:42:107:ILE:HG22	4:42:108:VAL:HG13	2.01	0.43
15:5A:450:LEU:HG	15:5A:607:ASP:HB3	2.01	0.43
15:5A:559:ASP:O	15:5A:562:VAL:CG2	2.67	0.43
15:5A:1544:ARG:HD3	15:5A:1671:TYR:HB3	2.00	0.43
16:5B:142:VAL:HG11	16:5B:157:ILE:HD11	2.01	0.43
16:5B:485:GLN:HB3	16:5B:515:MET:HE1	2.00	0.43
16:5B:834:TYR:OH	16:5B:1030:ARG:NH2	2.51	0.43
16:5B:1152:ARG:HH21	16:5B:1156:LEU:HD21	1.83	0.43
16:5B:1973:ARG:HB3	16:5B:1997:LEU:HD11	2.00	0.43
32:U:235:TYR:OH	32:U:312:GLN:O	2.34	0.43
6:4A:427:PRO:HB3	6:4A:639:LYS:HZ1	1.83	0.43
7:4B:257:LEU:HD22	7:4B:267:HIS:HE1	1.84	0.43
14:5:93:U:H4'	14:5:94:U:H5"	2.00	0.43
15:5A:569:VAL:HB	15:5A:573:GLN:HB2	2.00	0.43
15:5A:1536:LEU:HD21	15:5A:1576:ILE:HD11	2.01	0.43
15:5A:2106:LEU:HD12	15:5A:2107:PRO:HD2	2.01	0.43
16:5B:520:GLU:HG3	16:5B:611:LEU:HB2	2.00	0.43
16:5B:1379:ILE:HG21	16:5B:1470:ILE:HD11	1.99	0.43
17:5C:442:LYS:HB2	17:5C:442:LYS:HE3	1.83	0.43
17:5C:697:ALA:HB1	17:5C:742:PRO:HB3	2.01	0.43
20:5O:75:HIS:ND1	20:5O:77:ASN:OD1	2.52	0.43
26:65:70:ASP:HB2	27:66:77:LYS:HE3	2.00	0.43
32:U:307:SER:OG	32:U:310:THR:O	2.37	0.43
5:43:32:LEU:HA	5:43:43:MET:HA	2.00	0.43
7:4B:311:ASP:N	7:4B:311:ASP:OD1	2.50	0.43
15:5A:540:PHE:HB3	15:5A:544:PHE:HB3	2.00	0.43
15:5A:584:HIS:HB3	15:5A:587:GLN:HB2	2.00	0.43
15:5A:776:LEU:HD22	15:5A:900:ASP:HB2	2.00	0.43
16:5B:2009:ARG:HA	16:5B:2012:ASN:HB2	2.00	0.43
19:5J:434:VAL:HG12	19:5J:460:ILE:HD13	2.00	0.43
32:U:111:ILE:HG23	32:U:137:LEU:HB3	2.01	0.43
5:43:80:ALA:HA	5:43:81:PRO:HA	1.59	0.43
6:4A:459:GLU:HA	6:4A:462:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:53:19:THR:HB	5:53:29:ARG:HG3	2.01	0.43
16:5B:811:SER:OG	16:5B:812:THR:N	2.52	0.43
16:5B:1382:MET:HG3	16:5B:1652:TRP:CD2	2.54	0.43
16:5B:1491:SER:OG	16:5B:1492:SER:N	2.52	0.43
16:5B:1514:PHE:HB3	16:5B:1518:VAL:HG11	2.00	0.43
16:5B:1962:GLN:HG2	16:5B:2010:PHE:HZ	1.84	0.43
25:64:17:VAL:HG22	25:64:69:LEU:CD2	2.49	0.43
6:4A:427:PRO:HD2	7:4B:387:ALA:HB3	2.01	0.42
7:4B:230:ASP:HB3	7:4B:232:ARG:H	1.84	0.42
8:4C:297:ALA:O	8:4C:300:THR:HB	2.18	0.42
14:5:92:U:OP1	3:51:63:ASN:ND2	2.52	0.42
15:5A:1332:HIS:CE1	15:5A:1364:LEU:HD22	2.54	0.42
16:5B:814:THR:O	16:5B:818:GLY:N	2.50	0.42
16:5B:2110:SER:OG	16:5B:2111:ASP:N	2.52	0.42
17:5C:134:LEU:HG	17:5C:202:ILE:HG23	2.01	0.42
20:5O:214:ASP:N	20:5O:214:ASP:OD1	2.46	0.42
5:53:64:ARG:NE	5:53:66:SER:OG	2.49	0.42
15:5A:2009:ASP:HB2	15:5A:2014:MET:HB3	2.01	0.42
16:5B:319:LYS:HB2	16:5B:319:LYS:HE3	1.79	0.42
16:5B:755:GLY:O	16:5B:758:SER:N	2.44	0.42
16:5B:1062:LEU:HD22	16:5B:1081:MET:HB2	2.01	0.42
19:5J:287:ASP:O	19:5J:291:ILE:N	2.47	0.42
24:63:17:PRO:HA	27:66:36:CYS:SG	2.59	0.42
26:65:60:THR:HB	26:65:61:PRO:HD3	2.01	0.42
2:4:128:A:H1'	31:S:636:ARG:HH12	1.84	0.42
4:42:58:ALA:O	4:42:65:MET:HA	2.19	0.42
5:43:75:ASP:HB2	5:43:78:LYS:HD2	2.00	0.42
6:4A:561:GLU:HB2	6:4A:648:PHE:HE1	1.85	0.42
7:4B:257:LEU:HD21	7:4B:296:LEU:HD11	2.00	0.42
15:5A:59:GLU:N	15:5A:59:GLU:CD	2.73	0.42
15:5A:758:ARG:NH2	15:5A:901:LEU:O	2.52	0.42
16:5B:429:GLN:N	16:5B:886:GLN:OE1	2.45	0.42
27:66:20:VAL:HG12	27:66:75:THR:HA	2.01	0.42
2:4:127:C:H2'	2:4:128:A:C8	2.55	0.42
5:53:30:GLY:HA3	5:53:46:ILE:HD13	2.01	0.42
15:5A:1268:ILE:O	15:5A:1272:THR:OG1	2.30	0.42
15:5A:1811:ASN:CG	15:5A:1814:THR:CG2	2.85	0.42
16:5B:1566:ARG:HG2	16:5B:1621:HIS:HB2	2.02	0.42
17:5C:507:VAL:HA	17:5C:568:PRO:HD3	2.01	0.42
17:5C:516:LEU:HD21	17:5C:573:GLU:HG3	2.00	0.42
21:5X:378:SER:O	21:5X:630:GLY:N	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5X:703:ARG:HE	21:5X:703:ARG:HB2	1.43	0.42
22:6:105:U:C6	24:63:88:ARG:NH2	2.86	0.42
2:4:6:U:H2'	2:4:7:G:C8	2.55	0.42
6:4A:661:PHE:CD2	6:4A:670:TRP:HB2	2.55	0.42
15:5A:796:LYS:HG3	19:5J:240:MET:HB3	2.01	0.42
15:5A:912:GLU:HA	15:5A:913:PRO:HD3	1.91	0.42
15:5A:1382:SER:HA	15:5A:1415:GLY:HA2	2.00	0.42
18:5D:5:LEU:HD23	18:5D:60:LEU:HD21	2.01	0.42
19:5J:559:ALA:HA	19:5J:562:ILE:HG22	2.01	0.42
19:5J:739:CYS:HG	19:5J:742:SER:HG	1.61	0.42
29:68:36:LEU:HD11	29:68:70:ILE:HD11	2.00	0.42
2:4:108:C:H2'	2:4:109:G:H8	1.85	0.42
6:4A:436:LEU:HD12	6:4A:437:GLY:N	2.35	0.42
15:5A:193:LEU:N	15:5A:208:TYR:CZ	2.87	0.42
15:5A:1667:ARG:NH1	15:5A:1673:SER:O	2.52	0.42
16:5B:1192:PRO:HG3	16:5B:1289:LEU:HD11	2.00	0.42
17:5C:370:VAL:HA	17:5C:374:LEU:HB2	2.02	0.42
17:5C:939:ARG:NH1	17:5C:945:GLU:OE2	2.53	0.42
19:5J:736:LEU:HD22	19:5J:746:TRP:CE2	2.55	0.42
26:65:36:ILE:HG23	26:65:54:VAL:CG1	2.50	0.42
30:R:377:ASP:OD1	30:R:378:ALA:N	2.52	0.42
32:U:164:PHE:O	32:U:173:TYR:N	2.43	0.42
2:4:59:U:H2'	2:4:60:A:C8	2.54	0.42
4:42:76:GLU:O	4:42:89:PRO:HA	2.20	0.42
6:4A:386:GLU:HG3	6:4A:387:ILE:H	1.85	0.42
6:4A:524:GLN:HA	6:4A:527:VAL:HG12	2.00	0.42
3:51:51:GLU:OE1	3:51:51:GLU:N	2.52	0.42
15:5A:87:VAL:HG12	15:5A:121:HIS:CE1	2.55	0.42
15:5A:853:LYS:HG3	15:5A:856:LEU:HD23	2.02	0.42
15:5A:2252:LEU:H	15:5A:2255:HIS:CD2	2.37	0.42
16:5B:443:GLU:OE1	16:5B:873:HIS:NE2	2.42	0.42
21:5X:411:TYR:CZ	21:5X:491:PHE:HE2	2.37	0.42
1:X:119:LYS:HB2	2:4:116:G:H4'	2.01	0.42
6:4A:494:THR:O	6:4A:498:ALA:CB	2.68	0.42
15:5A:274:PRO:HB2	21:5X:293:ARG:HH22	1.85	0.42
15:5A:852:VAL:O	15:5A:852:VAL:HG13	2.20	0.42
16:5B:1761:TYR:HD2	16:5B:1785:LEU:HD11	1.84	0.42
16:5B:1936:LEU:HD13	16:5B:2069:GLY:HA3	2.02	0.42
17:5C:677:GLU:HG3	17:5C:684:LYS:HB2	2.00	0.42
2:4:120:U:O2'	5:43:64:ARG:NH2	2.53	0.42
2:4:128:A:H2'	2:4:129:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4A:425:ASN:O	7:4B:388:PHE:CE1	2.73	0.42
7:4B:228:ILE:HD13	7:4B:515:THR:HG22	2.02	0.42
7:4B:234:ILE:HG21	7:4B:248:THR:HB	2.01	0.42
7:4B:296:LEU:HB2	7:4B:308:TRP:HB2	2.00	0.42
4:52:32:LEU:HA	4:52:32:LEU:HD23	1.82	0.42
15:5A:86:ARG:HG2	19:5J:98:ASP:HB3	1.99	0.42
15:5A:2196:HIS:HD2	15:5A:2230:LEU:HD22	1.83	0.42
16:5B:1225:VAL:HG22	16:5B:1268:ILE:HG12	2.01	0.42
17:5C:701:GLU:OE1	17:5C:785:ARG:NH2	2.41	0.42
17:5C:747:ASP:HA	17:5C:791:ILE:HB	2.02	0.42
17:5C:830:PRO:HG2	17:5C:877:ALA:HB3	2.02	0.42
19:5J:274:LEU:HD23	19:5J:277:LEU:HD12	2.01	0.42
21:5X:379:ILE:HA	21:5X:628:TYR:O	2.19	0.42
32:U:404:GLU:O	32:U:405:LYS:CB	2.68	0.42
6:4A:548:VAL:HG22	6:4A:630:CYS:HB2	2.01	0.42
7:4B:289:LEU:HD23	7:4B:289:LEU:HA	1.86	0.42
15:5A:736:GLU:O	15:5A:740:LEU:HG	2.19	0.42
15:5A:940:ILE:HD11	15:5A:1046:LEU:HB2	2.01	0.42
15:5A:1416:ILE:HA	15:5A:1416:ILE:HD13	1.81	0.42
15:5A:1833:LEU:HD22	15:5A:1835:GLN:HG2	2.01	0.42
18:5D:90:ILE:HG21	18:5D:119:VAL:HG13	2.02	0.42
19:5J:776:ASN:HD21	19:5J:779:LEU:HG	1.84	0.42
32:U:146:ARG:CG	32:U:146:ARG:NH1	2.72	0.42
5:43:26:GLU:HG2	5:43:50:TYR:HA	2.02	0.41
7:4B:284:LYS:HE2	7:4B:284:LYS:HB3	1.82	0.41
4:52:45:ASN:HB3	4:52:108:VAL:HG22	2.02	0.41
15:5A:804:GLU:HA	15:5A:807:VAL:HG22	2.01	0.41
15:5A:1557:LEU:HA	15:5A:1620:TYR:CZ	2.55	0.41
15:5A:1607:GLU:HB2	15:5A:1634:SER:HB3	2.01	0.41
15:5A:2327:SER:OG	15:5A:2328:ALA:N	2.52	0.41
16:5B:70:LYS:HA	16:5B:73:LYS:HE2	2.01	0.41
16:5B:1301:LEU:HD23	16:5B:1301:LEU:HA	1.85	0.41
16:5B:2029:ILE:HG21	16:5B:2124:VAL:HG12	2.02	0.41
17:5C:779:LEU:HD11	17:5C:825:PRO:HB2	2.02	0.41
17:5C:888:ARG:O	17:5C:893:GLY:N	2.47	0.41
32:U:175:LEU:HD12	32:U:175:LEU:N	2.35	0.41
32:U:446:LEU:H	32:U:492:HIS:CE1	2.38	0.41
3:41:16:THR:HA	3:41:25:VAL:O	2.20	0.41
7:4B:349:LEU:HD23	7:4B:358:ILE:HD11	2.01	0.41
9:4D:34:GLN:O	9:4D:105:THR:OG1	2.31	0.41
15:5A:169:PHE:CD1	15:5A:563:GLN:NE2	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5A:1405:LEU:HD11	16:5B:67:ARG:HH11	1.84	0.41
15:5A:1490:PHE:O	15:5A:1493:THR:OG1	2.30	0.41
15:5A:1596:VAL:HG11	15:5A:1729:ALA:HB2	2.02	0.41
15:5A:1681:ARG:HG3	15:5A:1715:TYR:CZ	2.55	0.41
15:5A:1763:LEU:HD11	15:5A:1768:TYR:HA	2.02	0.41
16:5B:94:ILE:HD11	16:5B:840:ARG:HB2	2.01	0.41
16:5B:492:ALA:HA	16:5B:647:ARG:HH22	1.85	0.41
16:5B:557:LYS:HD2	16:5B:557:LYS:HA	1.85	0.41
17:5C:271:PRO:HB2	17:5C:370:VAL:HG13	2.03	0.41
4:42:52:LEU:HD12	4:42:101:LEU:HD22	2.02	0.41
5:43:7:ILE:HA	5:43:10:LEU:HG	2.00	0.41
7:4B:478:THR:HG22	7:4B:483:SER:H	1.84	0.41
3:51:16:THR:HA	3:51:25:VAL:O	2.20	0.41
15:5A:244:GLN:O	21:5X:306:GLY:N	2.45	0.41
15:5A:1003:HIS:HE1	19:5J:265:GLN:HB3	1.85	0.41
15:5A:1332:HIS:HB3	16:5B:41:LEU:HB2	2.01	0.41
16:5B:436:ARG:NE	16:5B:443:GLU:OE2	2.43	0.41
16:5B:789:MET:O	16:5B:794:ARG:NH1	2.53	0.41
16:5B:823:ALA:O	16:5B:857:GLY:N	2.44	0.41
16:5B:973:ASP:N	16:5B:973:ASP:OD1	2.50	0.41
16:5B:2064:TRP:HB2	16:5B:2082:LEU:HB3	2.02	0.41
17:5C:352:LYS:HE3	17:5C:352:LYS:HB2	1.87	0.41
17:5C:657:ASP:OD2	21:5X:254:TYR:OH	2.28	0.41
17:5C:692:LEU:HD23	17:5C:692:LEU:HA	1.87	0.41
18:5D:32:HIS:CE1	18:5D:63:ILE:HB	2.55	0.41
28:67:55:MET:HB2	28:67:67:ASP:OD2	2.20	0.41
32:U:247:PRO:HD2	32:U:449:TYR:CE2	2.55	0.41
1:X:149:ARG:NH2	15:5A:1614:ILE:O	2.53	0.41
7:4B:234:ILE:HA	7:4B:250:CYS:HA	2.02	0.41
15:5A:480:LYS:HB3	15:5A:480:LYS:HE2	1.89	0.41
15:5A:938:PRO:HB2	15:5A:1071:PHE:HA	2.02	0.41
15:5A:967:GLU:OE2	15:5A:969:SER:OG	2.32	0.41
15:5A:1331:GLY:HA3	16:5B:40:VAL:HG12	2.03	0.41
16:5B:831:THR:HA	16:5B:844:LEU:HD12	2.02	0.41
16:5B:1225:VAL:HG21	16:5B:1254:PHE:CE1	2.56	0.41
16:5B:1973:ARG:HA	16:5B:1973:ARG:HD2	1.72	0.41
17:5C:715:GLY:HA2	17:5C:729:ALA:HB1	2.02	0.41
17:5C:749:THR:O	17:5C:756:LYS:NZ	2.41	0.41
19:5J:692:ARG:HD2	19:5J:692:ARG:HA	1.80	0.41
21:5X:382:LYS:HB2	21:5X:626:VAL:HB	2.02	0.41
21:5X:647:SER:OG	21:5X:650:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5X:703:ARG:N	21:5X:705:PHE:HD2	2.19	0.41
23:62:29:LEU:CD1	23:62:38:ILE:HG23	2.51	0.41
1:X:125:ASN:HA	4:42:61:ARG:HG2	1.99	0.41
3:41:13:GLU:HG2	3:41:74:LEU:HD11	2.02	0.41
14:5:17:U:H2'	14:5:18:C:C6	2.56	0.41
15:5A:101:LYS:HG3	15:5A:473:PHE:CE1	2.55	0.41
15:5A:787:GLU:OE2	15:5A:791:GLN:NE2	2.44	0.41
15:5A:803:ALA:HB1	19:5J:254:ARG:HD3	2.01	0.41
15:5A:1314:VAL:HA	15:5A:1478:LEU:HD22	2.03	0.41
16:5B:513:ALA:HB2	16:5B:651:LEU:HD11	2.02	0.41
16:5B:1028:THR:O	16:5B:1030:ARG:NH1	2.53	0.41
19:5J:865:HIS:HD2	19:5J:900:ARG:HH22	1.67	0.41
21:5X:363:ASP:OD1	21:5X:363:ASP:N	2.51	0.41
31:S:718:ARG:HH12	31:S:750:LEU:HD13	1.85	0.41
7:4B:285:SER:O	7:4B:289:LEU:O	2.39	0.41
9:4D:35:LEU:HD11	9:4D:102:CYS:HB3	2.03	0.41
15:5A:1245:ARG:O	15:5A:1249:MET:HB2	2.21	0.41
15:5A:1260:VAL:HG11	15:5A:1325:LEU:HB3	2.03	0.41
15:5A:1433:ASP:HB3	15:5A:1460:HIS:CE1	2.56	0.41
16:5B:688:THR:HB	16:5B:868:ILE:HG13	2.02	0.41
16:5B:1062:LEU:HD23	16:5B:1062:LEU:HA	1.91	0.41
17:5C:327:TYR:OH	17:5C:372:PHE:O	2.30	0.41
29:68:37:ILE:CD1	29:68:61:ILE:HG12	2.51	0.41
1:X:120:VAL:H	1:X:120:VAL:HG22	1.63	0.41
2:4:17:A:H61	8:4C:357:ARG:CZ	2.34	0.41
2:4:113:U:O2'	2:4:114:U:P	2.79	0.41
6:4A:512:GLU:O	6:4A:516:ALA:HB2	2.20	0.41
15:5A:87:VAL:HG12	15:5A:121:HIS:HE1	1.85	0.41
15:5A:357:ASN:OD1	21:5X:327:ARG:NH2	2.53	0.41
15:5A:1072:LEU:HD22	15:5A:1087:LEU:HD22	2.01	0.41
15:5A:1109:LEU:HG	15:5A:1152:ALA:HB1	2.03	0.41
15:5A:1618:LYS:NZ	15:5A:1663:ASP:OD1	2.37	0.41
15:5A:2072:GLU:HG3	15:5A:2076:ARG:HD3	2.03	0.41
16:5B:158:ASP:O	16:5B:163:GLN:N	2.40	0.41
16:5B:1185:GLU:HG3	16:5B:1207:ASP:HB2	2.03	0.41
16:5B:1454:ASP:HA	16:5B:1490:LEU:HB2	2.03	0.41
16:5B:1519:ARG:NH2	16:5B:1691:ALA:O	2.54	0.41
16:5B:1585:GLN:H	16:5B:1585:GLN:HG2	1.66	0.41
16:5B:1755:LEU:HD12	16:5B:1755:LEU:HA	1.90	0.41
16:5B:1994:ASN:HB3	16:5B:1999:LEU:HD13	2.02	0.41
17:5C:664:GLU:HB3	17:5C:820:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5J:139:GLN:O	19:5J:143:SER:OG	2.28	0.41
19:5J:331:LEU:HD12	19:5J:331:LEU:HA	1.94	0.41
20:5O:280:ASN:HA	20:5O:310:TYR:HE2	1.86	0.41
1:X:137:TYR:CZ	31:S:729:LEU:CD1	2.95	0.41
6:4A:463:LYS:HD3	6:4A:463:LYS:HA	1.87	0.41
7:4B:345:ARG:HH11	7:4B:365:SER:HA	1.86	0.41
15:5A:975:VAL:HG11	15:5A:1153:VAL:HG21	2.02	0.41
15:5A:982:GLU:N	15:5A:1167:THR:O	2.53	0.41
15:5A:1086:ARG:HB2	15:5A:1098:PHE:HD2	1.85	0.41
15:5A:1415:GLY:O	15:5A:1418:ARG:NH1	2.42	0.41
15:5A:1785:VAL:HG13	15:5A:1822:ILE:HD13	2.02	0.41
17:5C:829:GLU:OE2	17:5C:854:ARG:NH2	2.46	0.41
19:5J:423:LEU:HD23	19:5J:423:LEU:HA	1.92	0.41
28:67:44:LEU:HD21	28:67:84:ILE:HD11	2.03	0.41
2:4:128:A:H1'	31:S:636:ARG:HH22	1.85	0.41
5:43:7:ILE:O	5:43:11:HIS:ND1	2.47	0.41
5:43:10:LEU:HD13	5:43:35:ALA:HB1	2.03	0.41
8:4C:325:GLU:HA	8:4C:328:PHE:HB2	2.03	0.41
8:4C:357:ARG:CG	8:4C:358:ARG:HG3	2.45	0.41
8:4C:357:ARG:O	8:4C:360:ARG:HG2	2.21	0.41
8:4C:380:PHE:H	15:5A:1502:PHE:HA	1.85	0.41
14:5:76:A:H2'	14:5:77:G:H8	1.85	0.41
15:5A:126:ILE:HD12	15:5A:128:PHE:CE1	2.56	0.41
15:5A:907:PRO:HB2	15:5A:909:TYR:CE1	2.56	0.41
15:5A:1023:ASN:OD1	15:5A:1023:ASN:N	2.52	0.41
16:5B:572:ASP:OD1	16:5B:1274:ARG:NH2	2.53	0.41
16:5B:1194:THR:HG22	16:5B:1723:PRO:HG3	2.03	0.41
16:5B:1196:SER:O	16:5B:1258:VAL:N	2.43	0.41
16:5B:1233:ILE:HG21	16:5B:1236:HIS:HB3	2.02	0.41
16:5B:1831:LEU:O	16:5B:1835:SER:CB	2.69	0.41
17:5C:209:VAL:O	17:5C:212:SER:OG	2.32	0.41
17:5C:236:MET:N	17:5C:239:THR:OG1	2.49	0.41
19:5J:335:GLY:O	19:5J:339:CYS:N	2.44	0.41
19:5J:665:LEU:O	19:5J:669:ARG:N	2.50	0.41
19:5J:673:PRO:O	19:5J:673:PRO:HD2	2.21	0.41
21:5X:373:PHE:CZ	21:5X:391:ARG:HA	2.56	0.41
22:6:105:U:C5	24:63:88:ARG:NH2	2.89	0.41
26:65:41:LEU:HD12	26:65:50:VAL:HG12	2.01	0.41
28:67:44:LEU:HD12	28:67:46:LEU:HD21	2.01	0.41
32:U:177:ASP:OD2	32:U:179:TYR:CE1	2.74	0.41
7:4B:228:ILE:HG21	19:5J:795:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5A:976:MET:HE2	15:5A:976:MET:HB2	1.90	0.41
15:5A:1872:LEU:HD23	15:5A:1872:LEU:HA	1.85	0.41
16:5B:120:ILE:O	16:5B:124:LEU:CB	2.66	0.41
16:5B:698:ILE:HG13	16:5B:702:GLN:HE21	1.86	0.41
17:5C:736:GLY:O	17:5C:771:GLN:HG2	2.21	0.41
19:5J:243:ILE:HD11	32:U:541:MET:HG2	2.03	0.41
19:5J:297:LEU:O	19:5J:301:VAL:HG23	2.21	0.41
21:5X:553:ARG:HD3	21:5X:557:MET:HE1	2.03	0.41
29:68:28:LYS:HB2	29:68:39:ASP:OD2	2.20	0.41
32:U:111:ILE:HD11	32:U:163:VAL:HG21	2.01	0.41
32:U:303:VAL:O	32:U:307:SER:OG	2.31	0.41
32:U:443:LEU:HD13	32:U:446:LEU:HD21	2.02	0.41
6:4A:417:LEU:HD23	6:4A:417:LEU:HA	1.95	0.40
15:5A:1544:ARG:HB3	15:5A:1670:ASP:HB2	2.04	0.40
15:5A:2146:VAL:HG13	15:5A:2272:MET:HB2	2.04	0.40
16:5B:259:HIS:CD2	16:5B:261:ARG:H	2.37	0.40
16:5B:708:VAL:HG21	16:5B:829:LYS:HZ2	1.86	0.40
17:5C:140:HIS:CD2	17:5C:230:ASP:HB2	2.56	0.40
17:5C:255:VAL:HG21	17:5C:285:VAL:HG11	2.03	0.40
19:5J:766:LEU:HD12	19:5J:786:LEU:HD13	2.04	0.40
20:5O:313:ASP:HB3	20:5O:316:SER:HB3	2.03	0.40
21:5X:476:PRO:HD2	21:5X:480:LEU:HD23	2.03	0.40
21:5X:669:ILE:HG12	21:5X:737:VAL:HG13	2.02	0.40
1:X:106:LEU:HD23	1:X:106:LEU:HA	1.91	0.40
1:X:138:ARG:NH1	15:5A:1614:ILE:HD12	2.30	0.40
14:5:19:A:N3	14:5:21:A:N6	2.70	0.40
15:5A:67:ARG:O	15:5A:71:ARG:HB2	2.21	0.40
15:5A:456:LEU:HD23	15:5A:456:LEU:HA	1.87	0.40
15:5A:546:LEU:HD12	15:5A:546:LEU:HA	1.89	0.40
15:5A:809:VAL:HG22	15:5A:1051:LEU:HD11	2.03	0.40
15:5A:1188:ASN:ND2	15:5A:1192:PHE:O	2.53	0.40
16:5B:538:ILE:HB	16:5B:585:ILE:HD13	2.03	0.40
16:5B:1405:VAL:HG22	16:5B:1424:ILE:HD12	2.03	0.40
16:5B:2041:LEU:HD13	16:5B:2041:LEU:HA	1.93	0.40
19:5J:713:MET:HG2	19:5J:748:LEU:HD22	2.03	0.40
19:5J:892:GLU:O	19:5J:896:GLU:HG3	2.21	0.40
2:4:127:C:H2'	2:4:128:A:H8	1.87	0.40
6:4A:466:LEU:CB	30:R:432:PRO:CB	2.93	0.40
7:4B:204:GLU:OE2	7:4B:208:THR:OG1	2.35	0.40
7:4B:359:LEU:HD21	7:4B:361:GLN:HB2	2.03	0.40
14:5:45:C:N4	21:5X:271:LYS:O	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:52:70:VAL:HG21	4:52:99:MET:SD	2.62	0.40
15:5A:1247:ILE:HG12	15:5A:1262:LYS:HB3	2.03	0.40
15:5A:1607:GLU:N	15:5A:1632:PHE:O	2.48	0.40
16:5B:169:TYR:HA	16:5B:172:LEU:HG	2.02	0.40
19:5J:96:LYS:HE3	19:5J:96:LYS:HB2	1.89	0.40
20:5O:84:ALA:HB2	20:5O:90:ILE:HG23	2.03	0.40
20:5O:127:ALA:HA	20:5O:133:VAL:HG22	2.03	0.40
6:4A:436:LEU:HD12	6:4A:437:GLY:H	1.85	0.40
6:4A:574:VAL:HG22	6:4A:581:VAL:HB	2.04	0.40
3:51:13:GLU:HG2	3:51:74:LEU:HD11	2.02	0.40
15:5A:722:ALA:HB3	15:5A:724:ILE:HG12	2.03	0.40
15:5A:1129:ASN:ND2	15:5A:1173:SER:O	2.53	0.40
15:5A:1506:ALA:HA	15:5A:1533:ARG:HH12	1.87	0.40
16:5B:1535:THR:HG21	16:5B:1676:TYR:CE1	2.57	0.40
17:5C:361:PRO:O	17:5C:362:THR:HB	2.21	0.40
19:5J:353:GLN:HB2	19:5J:358:ALA:HB2	2.02	0.40
21:5X:196:LYS:HE2	21:5X:196:LYS:HB3	1.93	0.40
21:5X:555:ILE:HD13	21:5X:555:ILE:HA	1.89	0.40
26:65:72:ILE:HG22	27:66:74:SER:HB3	2.03	0.40
29:68:41:SER:HB3	29:68:57:LEU:HD11	2.03	0.40
32:U:244:SER:HA	32:U:281:MET:HE1	2.04	0.40
3:41:80:LEU:HD21	4:42:66:VAL:HG11	2.02	0.40
4:42:70:VAL:HG21	4:42:99:MET:SD	2.62	0.40
6:4A:416:ASN:N	6:4A:416:ASN:OD1	2.54	0.40
7:4B:228:ILE:HD12	19:5J:795:ILE:HG21	2.04	0.40
15:5A:109:PRO:HD3	15:5A:630:TRP:CZ2	2.56	0.40
15:5A:1665:GLN:O	15:5A:1704:ALA:HA	2.22	0.40
16:5B:531:ILE:HG21	16:5B:564:ILE:HD11	2.03	0.40
16:5B:1084:VAL:O	16:5B:1088:ALA:HB2	2.21	0.40
16:5B:1429:PRO:O	16:5B:1433:ASP:HB2	2.22	0.40
17:5C:493:PHE:CZ	17:5C:549:TRP:HB3	2.56	0.40
17:5C:649:SER:HB2	17:5C:651:ILE:HG12	2.03	0.40
19:5J:145:LEU:O	19:5J:149:LEU:HB2	2.22	0.40
19:5J:440:LEU:HD22	19:5J:452:VAL:HG21	2.02	0.40
19:5J:913:CYS:HA	19:5J:916:SER:HB2	2.03	0.40
20:5O:321:TYR:CZ	20:5O:356:ILE:HG13	2.56	0.40
21:5X:596:LYS:HD2	21:5X:597:HIS:CE1	2.57	0.40
21:5X:733[A]:VAL:CG1	21:5X:734:SER:N	2.84	0.40
23:62:50:LYS:HE2	23:62:51:TYR:CZ	2.57	0.40
31:S:723:LYS:HZ3	31:S:727:ARG:HH22	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	45/155 (29%)	39 (87%)	6 (13%)	0	100	100
3	41	79/119 (66%)	75 (95%)	4 (5%)	0	100	100
3	51	79/119 (66%)	75 (95%)	4 (5%)	0	100	100
4	42	90/118 (76%)	84 (93%)	6 (7%)	0	100	100
4	52	94/118 (80%)	87 (93%)	7 (7%)	0	100	100
5	43	81/126 (64%)	79 (98%)	1 (1%)	1 (1%)	11	33
5	53	82/126 (65%)	77 (94%)	5 (6%)	0	100	100
6	4A	229/683 (34%)	210 (92%)	18 (8%)	1 (0%)	30	59
7	4B	357/522 (68%)	330 (92%)	25 (7%)	2 (1%)	22	51
8	4C	293/499 (59%)	275 (94%)	18 (6%)	0	100	100
9	4D	121/128 (94%)	119 (98%)	2 (2%)	0	100	100
10	4b	80/240 (33%)	71 (89%)	9 (11%)	0	100	100
10	5b	69/240 (29%)	67 (97%)	2 (3%)	0	100	100
11	4e	74/92 (80%)	71 (96%)	3 (4%)	0	100	100
11	5e	75/92 (82%)	72 (96%)	3 (4%)	0	100	100
12	4f	70/86 (81%)	69 (99%)	1 (1%)	0	100	100
12	5f	71/86 (83%)	64 (90%)	7 (10%)	0	100	100
13	4g	72/76 (95%)	66 (92%)	6 (8%)	0	100	100
13	5g	72/76 (95%)	66 (92%)	6 (8%)	0	100	100
15	5A	2198/2311 (95%)	2089 (95%)	105 (5%)	4 (0%)	44	72
16	5B	1989/2136 (93%)	1885 (95%)	103 (5%)	1 (0%)	48	76
17	5C	850/853 (100%)	817 (96%)	31 (4%)	2 (0%)	44	72
18	5D	139/142 (98%)	133 (96%)	6 (4%)	0	100	100
19	5J	793/941 (84%)	746 (94%)	43 (5%)	4 (0%)	25	55
20	5O	304/357 (85%)	283 (93%)	19 (6%)	2 (1%)	19	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
21	5X	574/820 (70%)	561 (98%)	13 (2%)	0	100 100
23	62	93/95 (98%)	84 (90%)	6 (6%)	3 (3%)	3 12
24	63	83/102 (81%)	79 (95%)	3 (4%)	1 (1%)	11 33
25	64	71/139 (51%)	66 (93%)	3 (4%)	2 (3%)	4 15
26	65	74/91 (81%)	70 (95%)	2 (3%)	2 (3%)	4 15
27	66	70/80 (88%)	69 (99%)	0	1 (1%)	9 30
28	67	75/103 (73%)	72 (96%)	2 (3%)	1 (1%)	10 31
29	68	93/96 (97%)	81 (87%)	6 (6%)	6 (6%)	1 3
30	R	104/480 (22%)	90 (86%)	11 (11%)	3 (3%)	3 14
31	S	116/800 (14%)	105 (90%)	10 (9%)	1 (1%)	14 41
32	U	454/555 (82%)	425 (94%)	27 (6%)	2 (0%)	30 59
All	All	10213/13802 (74%)	9651 (94%)	523 (5%)	39 (0%)	32 59

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	5C	364	SER
19	5J	93	PRO
19	5J	675	ALA
20	5O	59	ILE
23	62	47	ASP
23	62	53	HIS
29	68	89	GLU
30	R	405	PRO
30	R	406	SER
30	R	407	PHE
32	U	405	LYS
7	4B	460	ILE
15	5A	854	SER
19	5J	673	PRO
26	65	87	GLU
27	66	52	VAL
29	68	86	ILE
29	68	90	PRO
31	S	573	GLY
15	5A	189	GLU
15	5A	1512	SER
15	5A	1514	LYS

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Mol	Chain	Res	Type
29	68	79	SER
5	43	81	PRO
20	5O	58	PRO
23	62	55	LEU
24	63	35	ASN
25	64	12	ASN
29	68	43	GLU
6	4A	539	GLN
19	5J	671	SER
25	64	57	PRO
29	68	59	LEU
16	5B	756	SER
17	5C	943	LEU
28	67	19	ILE
7	4B	459	PRO
32	U	361	PRO
26	65	47	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	X	42/144 (29%)	42 (100%)	0	100 100
3	41	76/101 (75%)	55 (72%)	21 (28%)	0 1
3	51	76/101 (75%)	55 (72%)	21 (28%)	0 1
4	42	86/110 (78%)	86 (100%)	0	100 100
4	52	93/110 (84%)	92 (99%)	1 (1%)	70 89
5	43	73/101 (72%)	73 (100%)	0	100 100
5	53	73/101 (72%)	73 (100%)	0	100 100
6	4A	210/599 (35%)	208 (99%)	2 (1%)	73 90
7	4B	306/442 (69%)	303 (99%)	3 (1%)	73 90
8	4C	255/424 (60%)	251 (98%)	4 (2%)	58 83
9	4D	107/111 (96%)	107 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	4b	75/177 (42%)	75 (100%)	0	100 100
10	5b	67/177 (38%)	66 (98%)	1 (2%)	60 84
11	4e	71/84 (84%)	69 (97%)	2 (3%)	38 71
11	5e	72/84 (86%)	72 (100%)	0	100 100
12	4f	61/74 (82%)	61 (100%)	0	100 100
12	5f	61/74 (82%)	60 (98%)	1 (2%)	58 83
13	4g	64/66 (97%)	46 (72%)	18 (28%)	0 1
13	5g	64/66 (97%)	46 (72%)	18 (28%)	0 1
15	5A	2002/2090 (96%)	1990 (99%)	12 (1%)	84 94
16	5B	1779/1908 (93%)	1766 (99%)	13 (1%)	81 93
17	5C	754/755 (100%)	750 (100%)	4 (0%)	86 95
18	5D	129/130 (99%)	129 (100%)	0	100 100
19	5J	636/792 (80%)	633 (100%)	3 (0%)	86 95
20	5O	263/300 (88%)	263 (100%)	0	100 100
21	5X	517/721 (72%)	501 (97%)	16 (3%)	35 68
23	62	88/88 (100%)	86 (98%)	2 (2%)	45 75
24	63	79/94 (84%)	76 (96%)	3 (4%)	28 61
25	64	68/111 (61%)	68 (100%)	0	100 100
26	65	68/80 (85%)	67 (98%)	1 (2%)	60 84
27	66	62/70 (89%)	62 (100%)	0	100 100
28	67	69/91 (76%)	68 (99%)	1 (1%)	62 85
29	68	81/82 (99%)	77 (95%)	4 (5%)	21 51
30	R	94/369 (26%)	92 (98%)	2 (2%)	48 77
31	S	91/681 (13%)	91 (100%)	0	100 100
32	U	418/503 (83%)	413 (99%)	5 (1%)	67 87
All	All	9130/12011 (76%)	8972 (98%)	158 (2%)	56 82

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	41	2	LYS
3	41	4	VAL
3	41	8	MET

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Mol	Chain	Res	Type
3	41	10	LEU
3	41	11	SER
3	41	16	THR
3	41	28	THR
3	41	33	ASP
3	41	35	SER
3	41	44	LYS
3	41	47	LEU
3	41	48	LYS
3	41	51	GLU
3	41	53	VAL
3	41	54	GLN
3	41	55	LEU
3	41	56	GLU
3	41	57	THR
3	41	74	LEU
3	41	76	LEU
3	41	81	VAL
6	4A	597	LEU
6	4A	646	MET
7	4B	395	ARG
7	4B	407	LEU
7	4B	444	THR
8	4C	299	CYS
8	4C	315	LYS
8	4C	351	ARG
8	4C	363	LYS
11	4e	28	ARG
11	4e	30	ARG
13	4g	3	LYS
13	4g	10	LYS
13	4g	11	LYS
13	4g	15	LYS
13	4g	27	VAL
13	4g	35	ASP
13	4g	43	ASP
13	4g	44	GLU
13	4g	46	VAL
13	4g	47	GLU
13	4g	50	THR
13	4g	51	SER
13	4g	59	MET

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Mol	Chain	Res	Type
13	4g	62	ILE
13	4g	66	SER
13	4g	70	LEU
13	4g	71	GLU
13	4g	73	LEU
3	51	2	LYS
3	51	4	VAL
3	51	8	MET
3	51	10	LEU
3	51	11	SER
3	51	16	THR
3	51	28	THR
3	51	33	ASP
3	51	35	SER
3	51	44	LYS
3	51	47	LEU
3	51	48	LYS
3	51	51	GLU
3	51	53	VAL
3	51	54	GLN
3	51	55	LEU
3	51	56	GLU
3	51	57	THR
3	51	74	LEU
3	51	76	LEU
3	51	81	VAL
4	52	33	THR
15	5A	86	ARG
15	5A	165	ARG
15	5A	284	ARG
15	5A	342	THR
15	5A	563	GLN
15	5A	579	GLN
15	5A	741	ARG
15	5A	1126	VAL
15	5A	1298	ARG
15	5A	1925	LYS
15	5A	1958	LYS
15	5A	2249	LYS
16	5B	287	ASP
16	5B	300	ARG
16	5B	406	ARG

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Mol	Chain	Res	Type
16	5B	681	ARG
16	5B	753	ARG
16	5B	992	TYR
16	5B	998	VAL
16	5B	1030	ARG
16	5B	1152	ARG
16	5B	1228	VAL
16	5B	1518	VAL
16	5B	1521	VAL
16	5B	1843	ARG
17	5C	105	MET
17	5C	507	VAL
17	5C	735	PHE
17	5C	919	ARG
19	5J	405	ARG
19	5J	570	PHE
19	5J	743	THR
21	5X	270	ARG
21	5X	389	PRO
21	5X	395	ASP
21	5X	472	ILE
21	5X	491	PHE
21	5X	516	ARG
21	5X	532	VAL
21	5X	664	ASP
21	5X	674	LYS
21	5X	675	LYS
21	5X	679	VAL
21	5X	685	GLU
21	5X	703	ARG
21	5X	729	ASP
21	5X	730	ILE
21	5X	746	GLU
10	5b	16	ARG
12	5f	11	LEU
13	5g	3	LYS
13	5g	10	LYS
13	5g	11	LYS
13	5g	15	LYS
13	5g	27	VAL
13	5g	35	ASP
13	5g	43	ASP

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Mol	Chain	Res	Type
13	5g	44	GLU
13	5g	46	VAL
13	5g	47	GLU
13	5g	50	THR
13	5g	51	SER
13	5g	59	MET
13	5g	62	ILE
13	5g	66	SER
13	5g	70	LEU
13	5g	71	GLU
13	5g	73	LEU
23	62	44	SER
23	62	72	LEU
24	63	34	ARG
24	63	39	LEU
24	63	94	LEU
26	65	16	GLU
28	67	17	LYS
29	68	13	VAL
29	68	19	ASP
29	68	90	PRO
29	68	91	LEU
30	R	405	PRO
30	R	431	ASP
32	U	100	ARG
32	U	101	ARG
32	U	146	ARG
32	U	234	ASP
32	U	288	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
3	41	24	GLN
4	42	49	ASN
4	42	69	ASN
4	42	112	ASN
6	4A	425	ASN
7	4B	282	HIS
7	4B	414	ASN
8	4C	389	GLN
9	4D	111	GLN

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Mol	Chain	Res	Type
12	4f	6	ASN
13	4g	26	HIS
13	4g	55	ASN
3	51	63	ASN
3	51	64	ASN
4	52	41	GLN
5	53	42	GLN
15	5A	221	ASN
15	5A	325	HIS
15	5A	434	HIS
15	5A	448	GLN
15	5A	579	GLN
15	5A	654	ASN
15	5A	704	ASN
15	5A	775	ASN
15	5A	875	HIS
15	5A	1003	HIS
15	5A	1014	ASN
15	5A	1159	ASN
15	5A	1172	ASN
15	5A	1332	HIS
15	5A	1345	GLN
15	5A	1487	HIS
15	5A	1543	ASN
15	5A	1737	ASN
15	5A	1752	GLN
15	5A	1830	GLN
15	5A	1875	HIS
15	5A	2166	HIS
15	5A	2203	ASN
15	5A	2260	GLN
15	5A	2276	GLN
15	5A	2306	HIS
16	5B	259	HIS
16	5B	304	ASN
16	5B	313	ASN
16	5B	485	GLN
16	5B	498	ASN
16	5B	524	HIS
16	5B	638	ASN
16	5B	702	GLN
16	5B	785	HIS

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Mol	Chain	Res	Type
16	5B	884	ASN
16	5B	885	GLN
16	5B	968	ASN
16	5B	999	GLN
16	5B	1003	GLN
16	5B	1086	GLN
16	5B	1209	GLN
16	5B	1247	GLN
16	5B	1265	GLN
16	5B	1423	ASN
16	5B	1441	GLN
16	5B	1659	HIS
16	5B	1674	HIS
16	5B	1769	ASN
16	5B	1885	ASN
16	5B	1994	ASN
17	5C	107	GLN
17	5C	137	HIS
17	5C	154	HIS
17	5C	571	ASN
17	5C	583	ASN
17	5C	702	ASN
17	5C	719	GLN
17	5C	743	ASN
17	5C	771	GLN
17	5C	903	HIS
17	5C	905	GLN
18	5D	7	HIS
18	5D	32	HIS
19	5J	140	GLN
19	5J	308	HIS
19	5J	353	GLN
19	5J	587	HIS
19	5J	733	ASN
19	5J	741	HIS
19	5J	865	HIS
20	5O	101	ASN
20	5O	165	GLN
20	5O	225	ASN
21	5X	297	GLN
21	5X	359	GLN
21	5X	420	GLN

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Mol	Chain	Res	Type
21	5X	428	ASN
21	5X	535	ASN
21	5X	597	HIS
21	5X	731	GLN
10	5b	22	GLN
11	5e	32	GLN
11	5e	38	GLN
11	5e	88	GLN
12	5f	6	ASN
12	5f	68	ASN
13	5g	26	HIS
13	5g	55	ASN
23	62	53	HIS
23	62	71	GLN
27	66	69	ASN
30	R	393	ASN
30	R	471	GLN
31	S	728	GLN
32	U	144	GLN
32	U	158	GLN
32	U	162	HIS
32	U	204	ASN
32	U	233	ASN
32	U	241	GLN
32	U	297	HIS
32	U	412	GLN
32	U	530	GLN
32	U	540	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	5	101/117 (86%)	42 (41%)	4 (3%)
2	4	119/146 (81%)	24 (20%)	3 (2%)
22	6	40/88 (45%)	5 (12%)	2 (5%)
All	All	260/351 (74%)	71 (27%)	9 (3%)

All (71) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	4	2	G

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Mol	Chain	Res	Type
2	4	19	U
2	4	20	A
2	4	25	A
2	4	26	G
2	4	30	A
2	4	36	U
2	4	37	U
2	4	38	U
2	4	40	U
2	4	44	A
2	4	45	G
2	4	51	A
2	4	67	A
2	4	68	A
2	4	69	C
2	4	114	U
2	4	115	G
2	4	121	U
2	4	122	U
2	4	123	U
2	4	125	G
2	4	126	A
2	4	140	G
14	5	4	C
14	5	5	U
14	5	6	C
14	5	7	U
14	5	9	G
14	5	20	G
14	5	21	A
14	5	22	U
14	5	23	C
14	5	24	G
14	5	25	C
14	5	26	A
14	5	28	A
14	5	36	C
14	5	37	G
14	5	38	C
14	5	47	A
14	5	48	A
14	5	57	G

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Mol	Chain	Res	Type
14	5	58	U
14	5	59	G
14	5	63	A
14	5	66	A
14	5	67	A
14	5	71	C
14	5	75	G
14	5	78	U
14	5	86	C
14	5	88	A
14	5	89	U
14	5	90	U
14	5	94	U
14	5	95	G
14	5	97	G
14	5	98	G
14	5	102	U
14	5	104	C
14	5	105	U
14	5	106	U
14	5	107	U
14	5	108	G
14	5	109	G
22	6	48	A
22	6	49	G
22	6	74	U
22	6	77	C
22	6	106	U

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	4	1	A
2	4	68	A
2	4	114	U
14	5	57	G
14	5	58	U
14	5	96	A
14	5	105	U
22	6	47	A
22	6	104	U

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
35	GTP	5C	2602	34	26,34,34	1.36	3 (11%)	32,54,54	1.61	7 (21%)
33	IHP	5A	2401	-	36,36,36	0.71	0	54,60,60	0.58	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
35	GTP	5C	2602	34	-	4/18/38/38	0/3/3/3
33	IHP	5A	2401	-	-	8/30/54/54	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	5C	2602	GTP	C5-C6	-4.48	1.38	1.47
35	5C	2602	GTP	C5-C4	-2.14	1.37	1.43
35	5C	2602	GTP	O4'-C4'	-2.11	1.40	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	5C	2602	GTP	PB-O3B-PG	-3.55	120.63	132.83
35	5C	2602	GTP	C5-C6-N1	3.50	120.12	113.95
35	5C	2602	GTP	C8-N7-C5	3.07	108.83	102.99
35	5C	2602	GTP	C2-N1-C6	-3.00	119.57	125.10
35	5C	2602	GTP	PA-O3A-PB	-2.50	124.25	132.83
35	5C	2602	GTP	O6-C6-C5	-2.35	119.79	124.37
35	5C	2602	GTP	C3'-C2'-C1'	2.23	104.34	100.98

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	5A	2401	IHP	C1-O11-P1-O41
33	5A	2401	IHP	C3-O13-P3-O23
35	5C	2602	GTP	O4'-C4'-C5'-O5'
35	5C	2602	GTP	PB-O3A-PA-O2A
35	5C	2602	GTP	C3'-C4'-C5'-O5'
33	5A	2401	IHP	C5-O15-P5-O25
33	5A	2401	IHP	C6-O16-P6-O26
33	5A	2401	IHP	C4-O14-P4-O34
33	5A	2401	IHP	C5-O15-P5-O35
33	5A	2401	IHP	C5-O15-P5-O45
33	5A	2401	IHP	C6-O16-P6-O46
35	5C	2602	GTP	C5'-O5'-PA-O1A

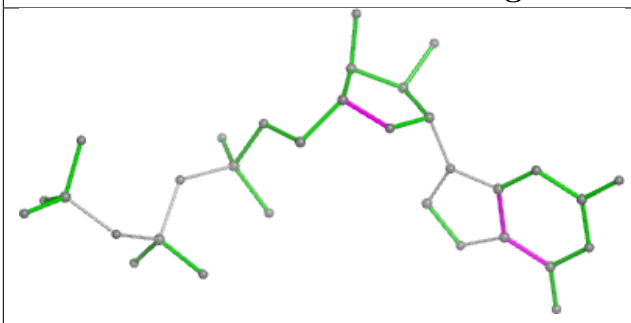
There are no ring outliers.

1 monomer is involved in 1 short contact:

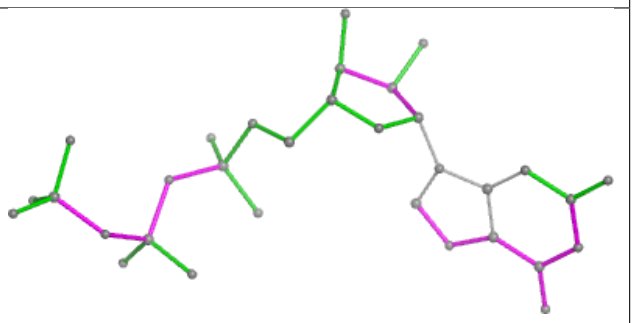
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	5A	2401	IHP	1	0

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.

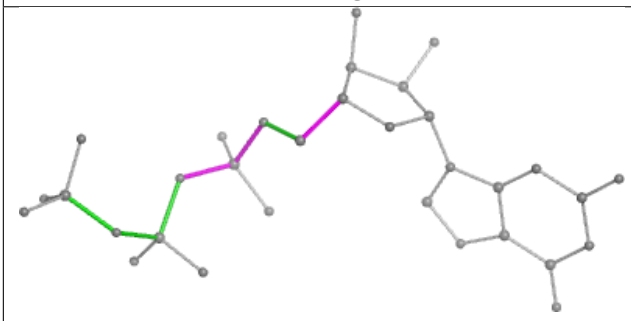
Ligand GTP 5C 2602



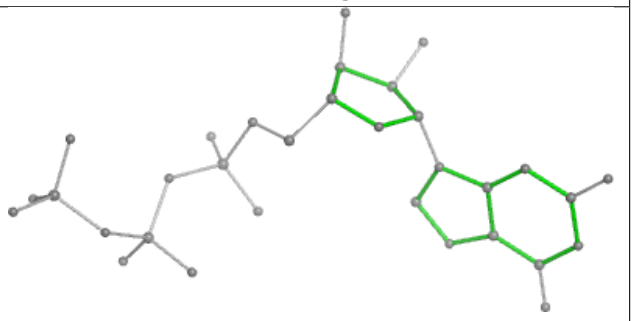
Bond lengths



Bond angles

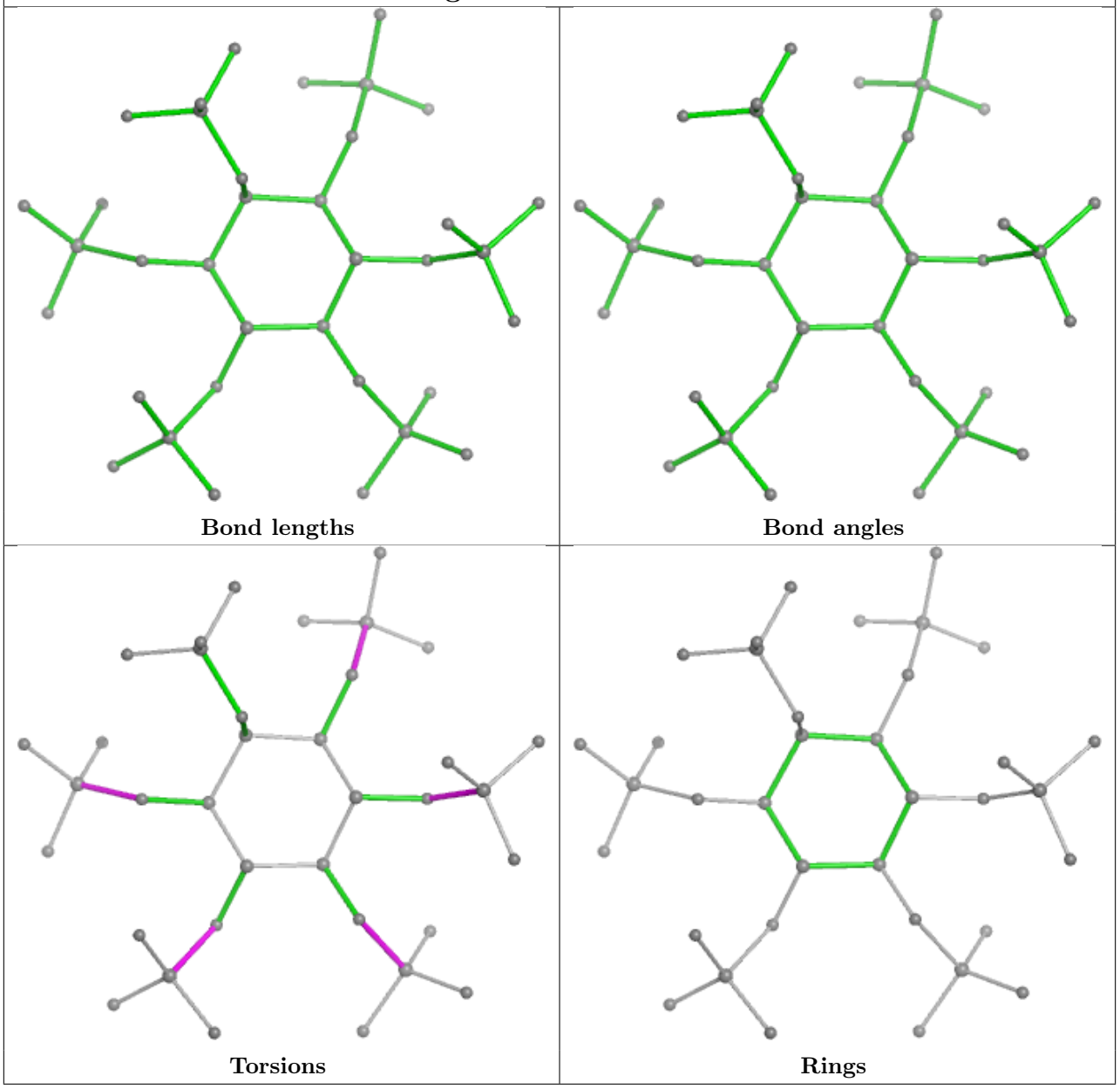


Torsions



Rings

Ligand IHP 5A 2401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	51:A	O3’	52:U	P	3.66

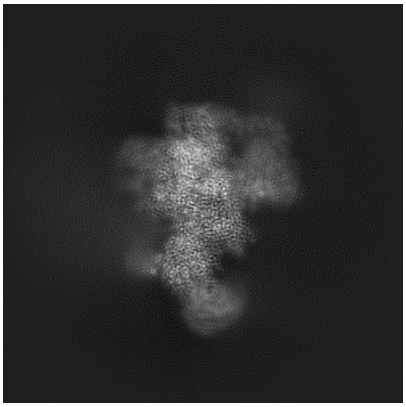
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4658. These allow visual inspection of the internal detail of the map and identification of artifacts.

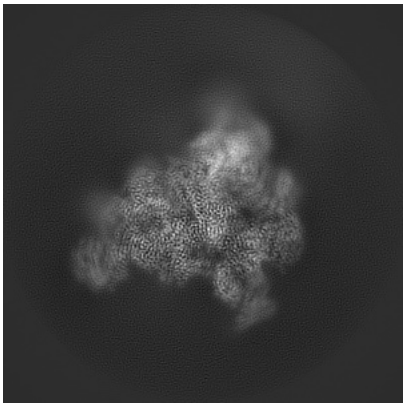
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map



X



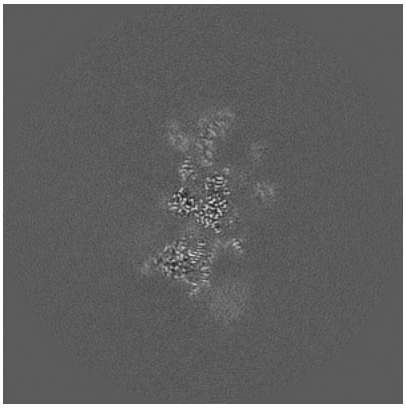
Y

Z

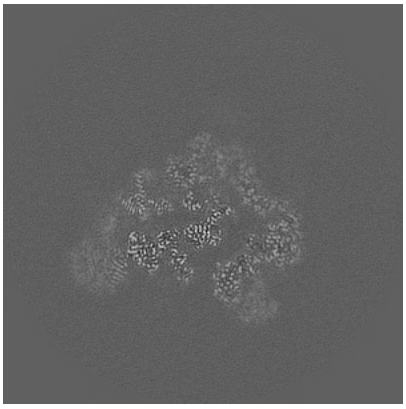
The images above show the map projected in three orthogonal directions.

6.2 Central slices

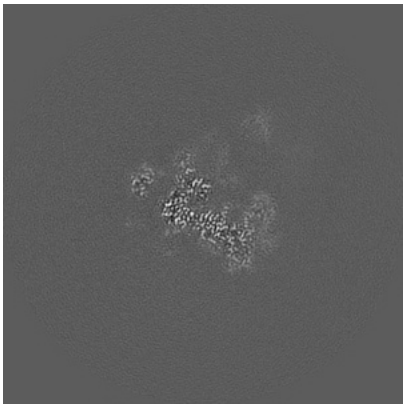
6.2.1 Primary map



X Index: 210



Y Index: 210

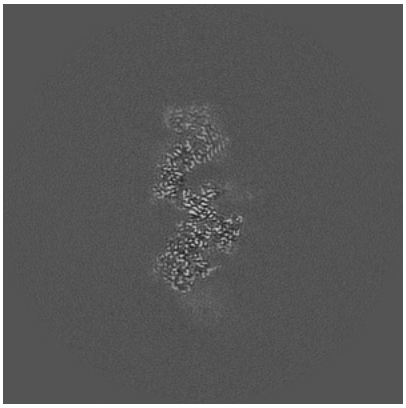


Z Index: 210

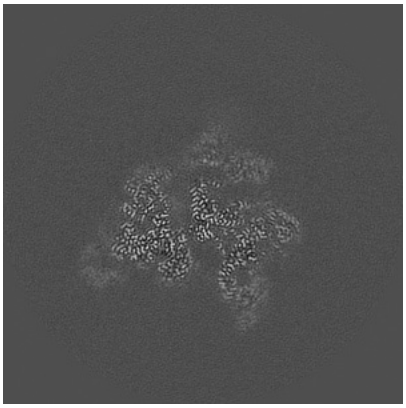
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

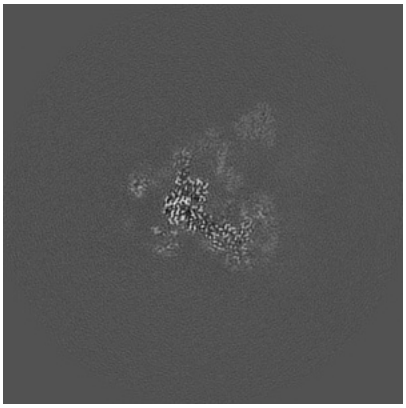
6.3.1 Primary map



X Index: 175



Y Index: 193

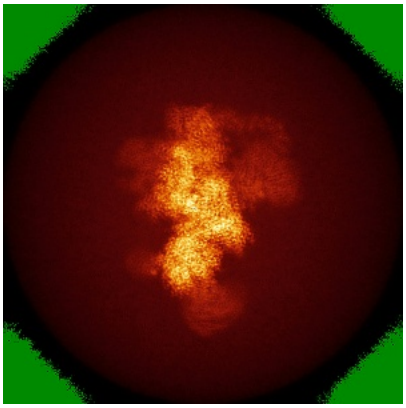


Z Index: 215

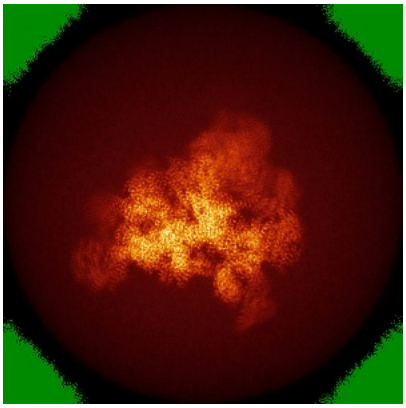
The images above show the largest variance slices of the map in three orthogonal directions.

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

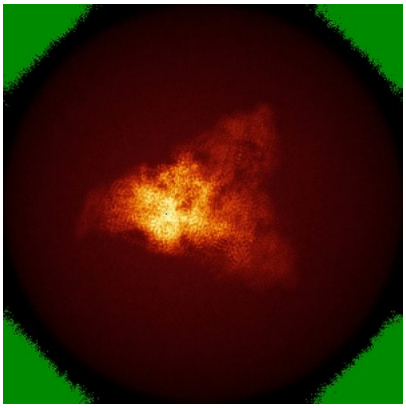
6.4.1 Primary map



X



Y

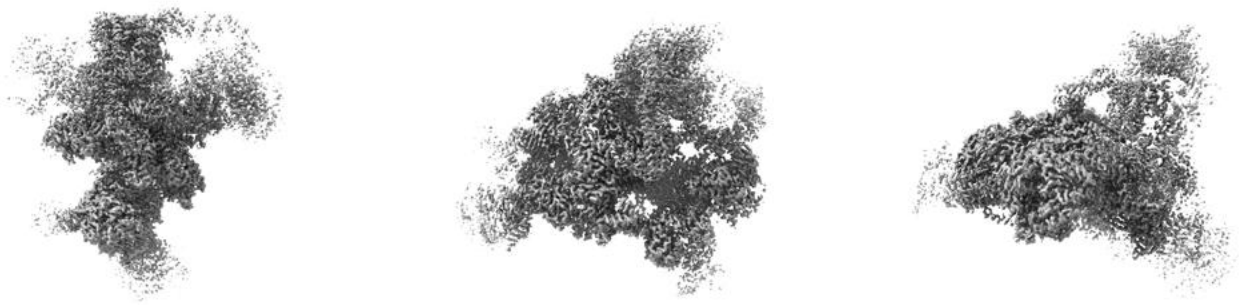


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

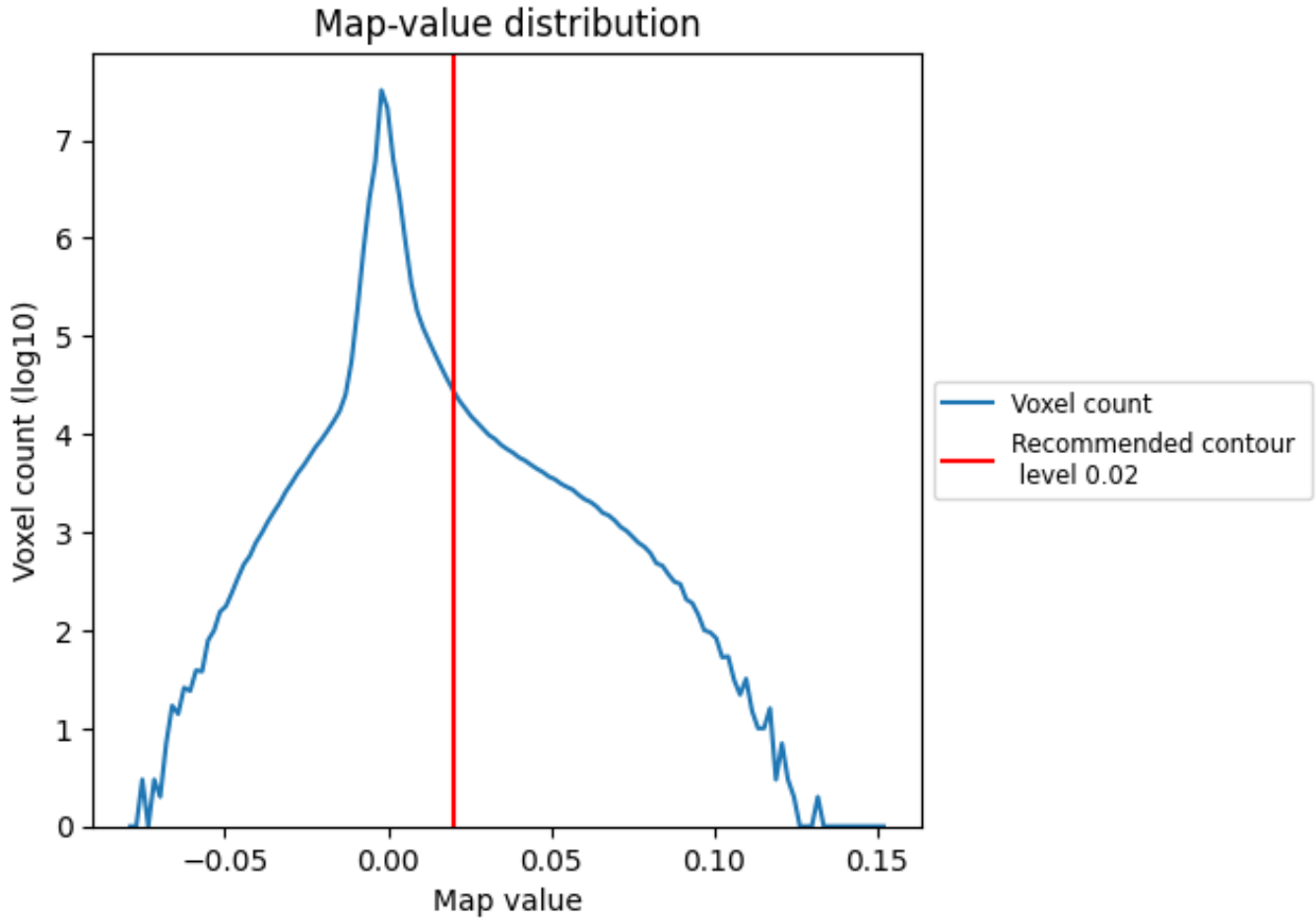
6.6 Mask visualisation (i)

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

7 Map analysis

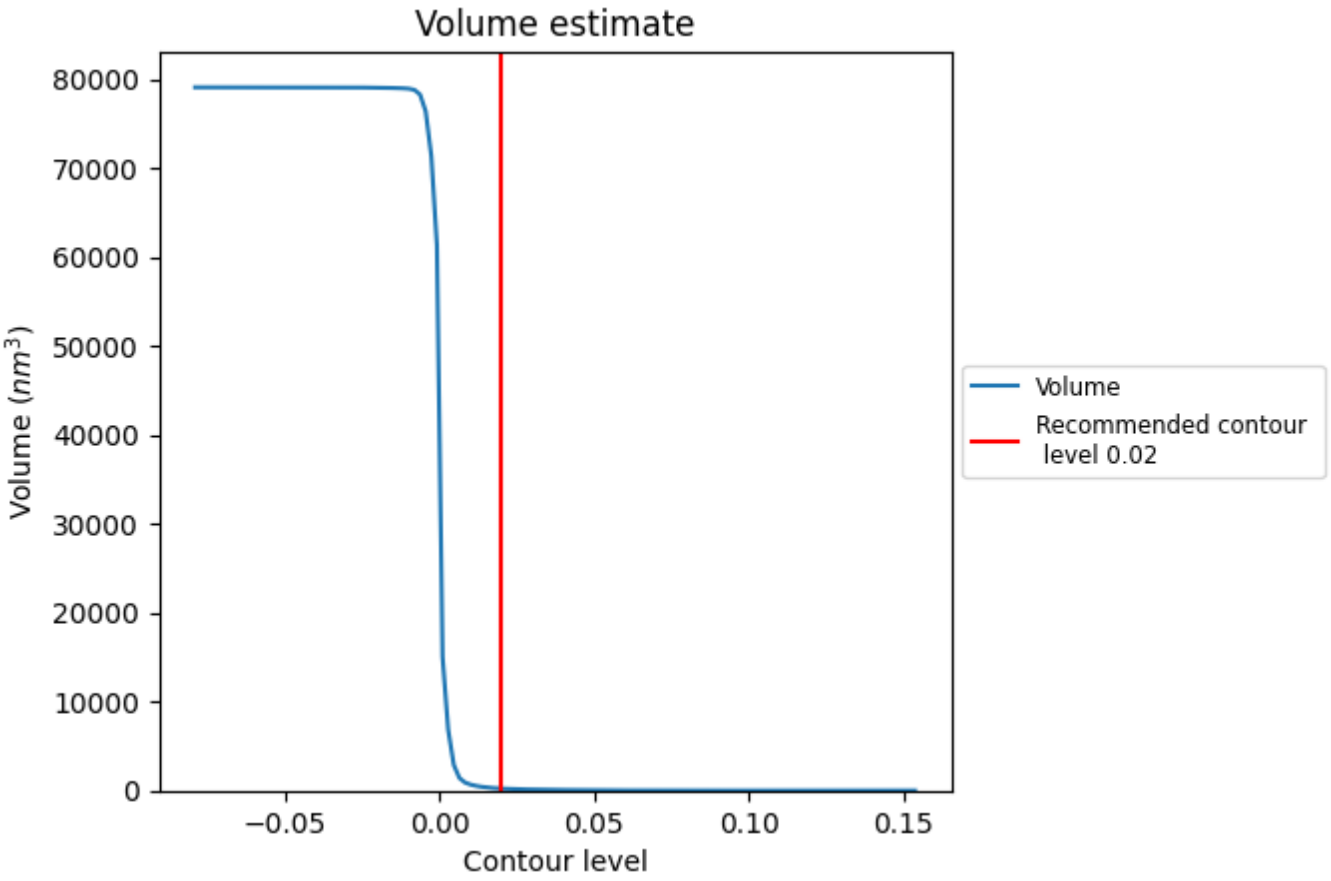
This section contains the results of statistical analysis of the map.

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.

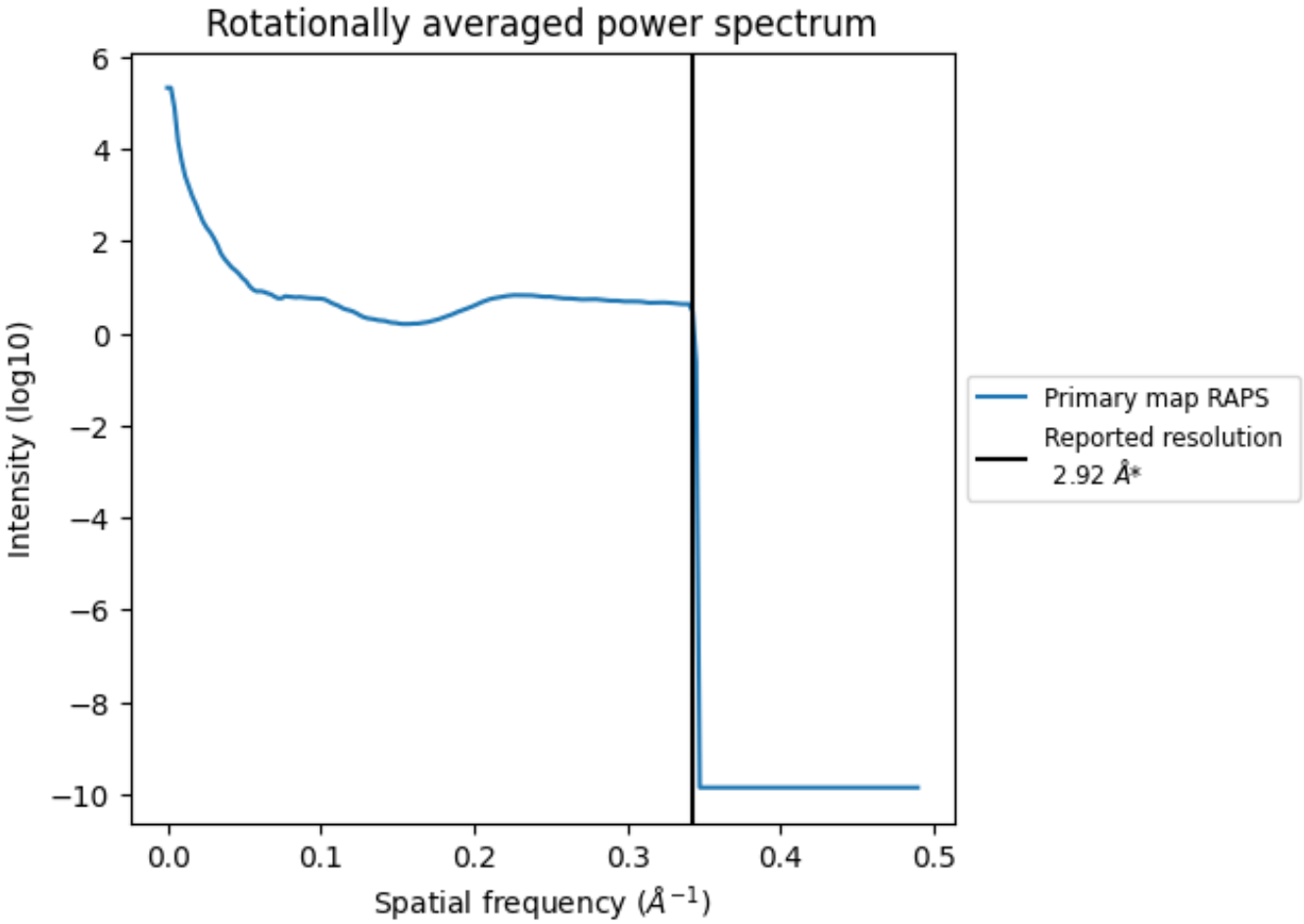
7.2 Volume estimate



The volume at the recommended contour level is 224 nm^3; this corresponds to an approximate mass of 203 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)

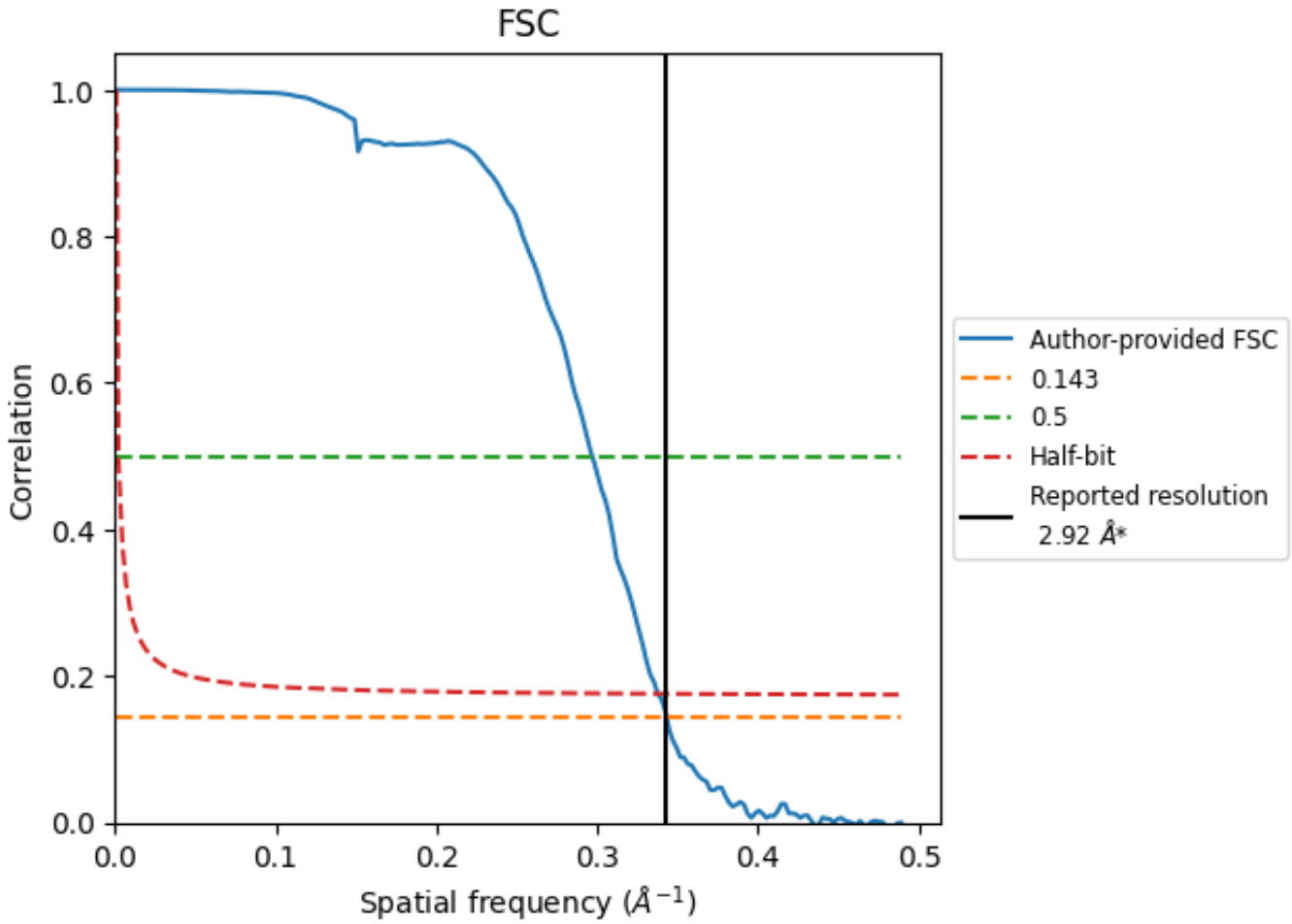


*Reported resolution corresponds to spatial frequency of 0.342 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.342 Å^{-1}

8.2 Resolution estimates (i)

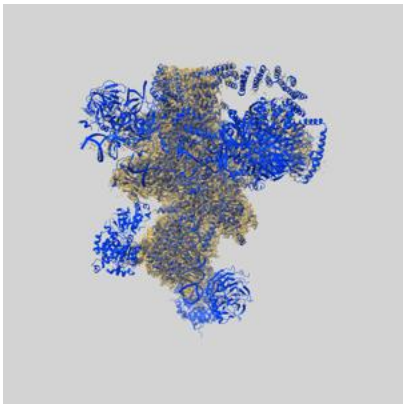
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.91	3.37	2.96
Unmasked-calculated*	-	-	-

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

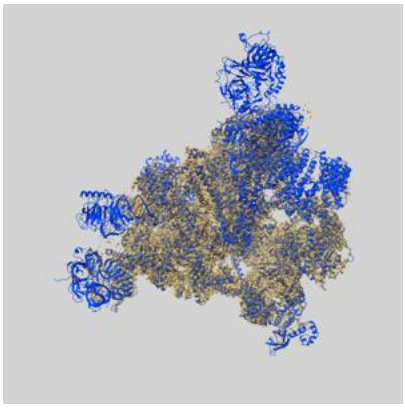
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4658 and PDB model 6QW6. Per-residue inclusion information can be found in section 3 on page 12.

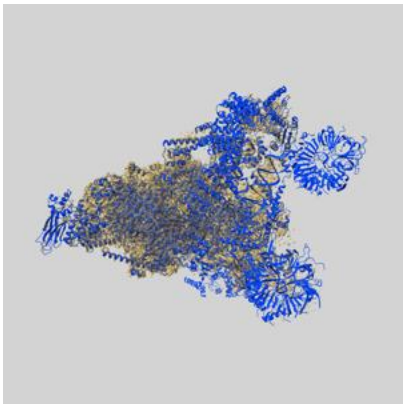
9.1 Map-model overlay



X



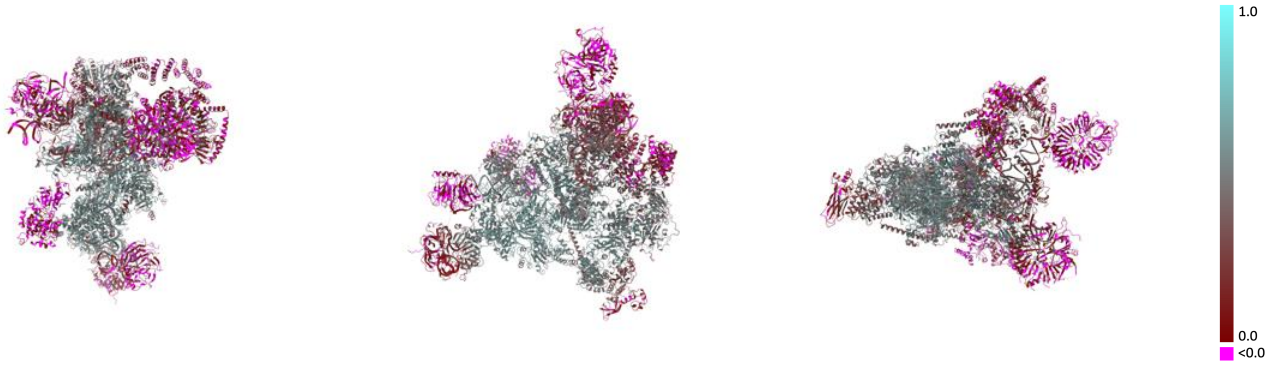
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

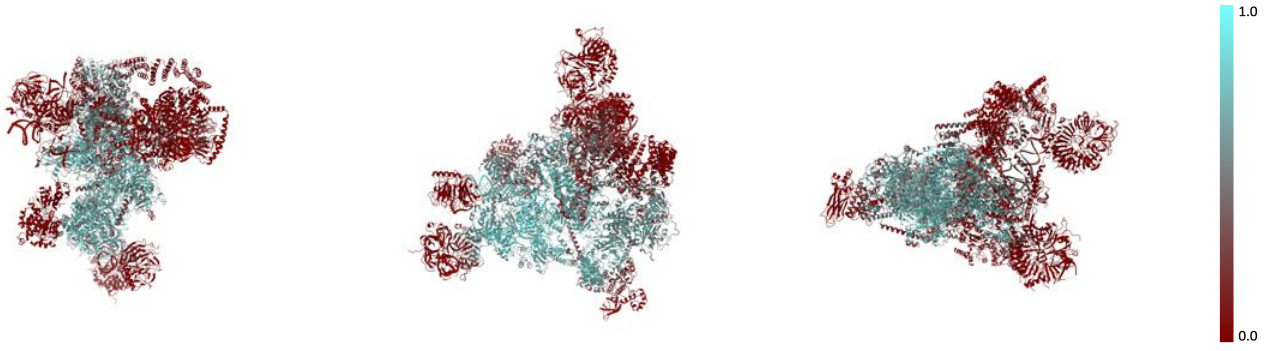
9.2 Q-score mapped to coordinate model



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.

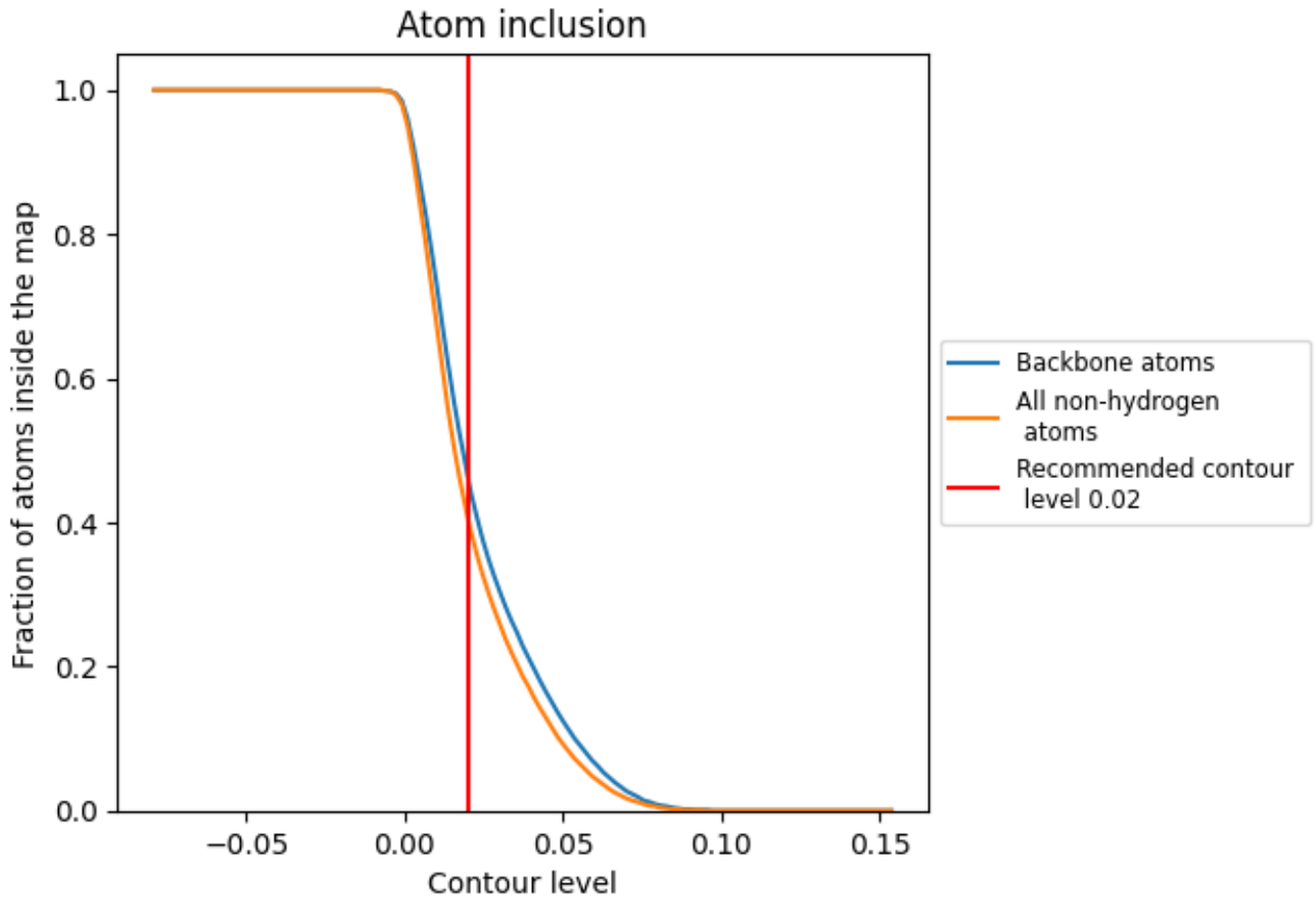
9.3 Atom inclusion mapped to coordinate model



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 46% of all backbone atoms, 41% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4060	0.3610
4	0.2320	0.2550
41	0.0520	0.2330
42	0.0900	0.2500
43	0.0020	0.0300
4A	0.0600	0.1910
4B	0.1020	0.2120
4C	0.2800	0.3870
4D	0.2780	0.3720
4b	0.0080	0.0660
4e	0.0080	0.0820
4f	0.0180	0.1280
4g	0.0040	0.0420
5	0.4430	0.3520
51	0.0550	0.1760
52	0.0080	0.0870
53	0.4490	0.4470
5A	0.6810	0.5270
5B	0.5210	0.4470
5C	0.7880	0.5720
5D	0.6190	0.5350
5J	0.2070	0.2710
5O	0.0010	0.0130
5X	0.1340	0.1550
5b	0.2300	0.3470
5e	0.0390	0.1770
5f	0.0110	0.1030
5g	0.1620	0.3090
6	0.2830	0.2890
62	0.0000	-0.0120
63	0.0000	0.0270
64	0.0000	0.0150
65	0.0000	-0.0050
66	0.0000	-0.0030
67	0.0000	0.0120

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Chain	Atom inclusion	Q-score
68	0.0000	-0.0090
R	0.1810	0.2600
S	0.2870	0.3640
U	0.7740	0.5650
X	0.2270	0.2650