Full wwPDB EM Validation Report (i)

Jul 10, 2026 – 07:29 AM JST

PDB ID	:	9XAH / pdb_00009xah
EMDB ID	:	EMD-66687
Title	:	Cryo-EM structure of the 90S pre-ribosome (Enp1-Rrp12 Mut) from Chaetomium thermophilum, state B1*
Authors	:	Lau, B.; Li, Y.; Zhu, J.; Fischer, P.; Hong, X.; Yuan, R.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on	:	2025-10-22
Resolution	:	3.10 Å(reported)
Based on initial model	:	6RXU

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 (i) 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 (i)) were used in the production of this report:

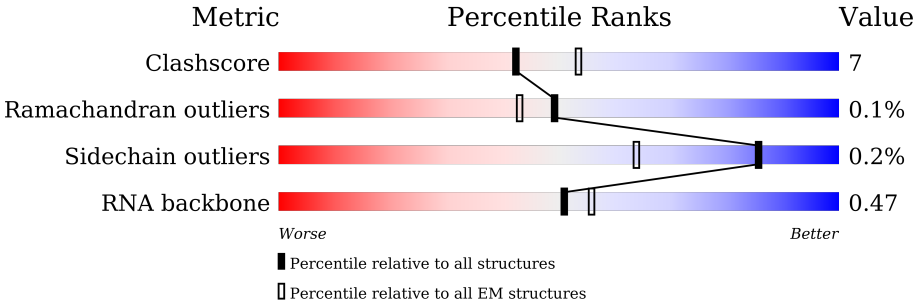
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

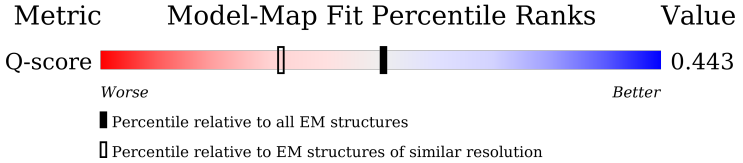
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	UA	904	82% 11% 7%
2	UB	907	53% 10% 38%

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Mol	Chain	Length	Quality of chain
3	UC	648	19% 33% 5% 62%
4	UD	884	67% 21% 12%
5	UF	414	70% 9% 20%
6	UG	558	76% 10% 14%
7	UJ	1802	11% 70% 22% 8%
8	UK	270	70% 10% 20%
9	UL	962	65% 16% 18%
10	UM	912	74% 18% 8%
11	UN	633	24% 72%
12	UO	557	77% 13% 10%
13	UQ	960	66% 16% 18%
14	UR	618	62% 10% 28%
15	UU	1049	71% 15% 13%
16	UX	193	83% 16%
17	UZ	391	52% 8% 40%
18	CA	313	67% 10% 23%
18	CB	313	59% 17% 24%
19	CC	523	61% 13% 26%
20	CD	582	63% 13% 23%
21	CE	127	87% 9% 5%
21	CF	127	83% 11% 6%
22	CG	630	53% 13% 34%
23	CH	411	77% 18% 5%
24	CI	1163	62% 10% 28%
25	CJ	183	81% 16%

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Mol	Chain	Length	Quality of chain
26	CK	297	90% 10%
27	CL	720	12% 38% 7% 56%
28	CM	446	84% 15%
29	CN	252	71% 18% 10%
29	CO	252	63% 21% 15%
30	CP	322	60% 13% 28%
31	CQ	259	61% 8% 31%
32	CR	1073	60% 18% 21%
32	CS	1073	6% 55% 22% 22%
33	CT	203	58% 6% 35%
34	Ca	255	70% 18% 12%
35	Cb	264	66% 22% 12%
36	Cc	212	79% 11% 9%
37	Cd	239	71% 23% 5%
38	Ce	203	61% 17% 22%
39	Cf	202	67% 19% 14%
40	Cg	190	67% 17% 16%
41	Ch	151	5% 34% 9% 56%
42	Ci	150	67% 10% 23%
43	Cj	143	74% 14% 12%
44	Ck	161	64% 17% 19%
45	Cm	130	81% 16%
46	Cn	145	60% 6% 34%
47	Co	136	46% 21% 32%
48	Cp	68	79% 10% 10%

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Mol	Chain	Length	Quality of chain
49	CU	311	50% 6% 43%
50	C1	2344	44% 20% 33%
51	C2	274	59% 20% 5% 16%
52	CW	668	49% 9% 43%
53	UT	2612	58% 20% 22%
54	UH	930	20% 74% 11% 14%
55	UE	410	35% 8% 57%
55	UI	410	25% 6% 69%
56	US	549	67% 15% 18%
57	Cl	156	44% 7% 49%
58	CX	480	44% 43% 12% 44%
59	CY	381	36% 56% 13% 31%
60	CZ	609	38% 36% 10% 54%
61	UP	364	12% 85%

2 Entry composition (i)

There are 65 unique types of molecules in this entry. The entry contains 228132 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 Periodic tryptophan protein 2-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
1	UA	839	6411	4118	1136	1132	1	24	0	0

- Molecule 2 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	UB	566	4506	2845	858	790	13	0	0

- Molecule 3 is a protein called Sas10 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	UC	248	1970	1238	362	363	7	0	0

- Molecule 4 is a protein called UTP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	UD	777	6108	3872	1099	1113	24	0	0

- Molecule 5 is a protein called U3 snoRNP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	UF	331	2599	1678	504	403	14	0	0

- Molecule 6 is a protein called U three protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	UG	479	3765	2391	700	662	12	0	0

- Molecule 7 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	UJ	1654	12725	8149	2177	2347	52	0	0

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	UK	217	1695	1066	351	273	5	0	0

- Molecule 9 is a protein called Small-subunit processome Utp12 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	UL	785	6175	3940	1088	1130	17	0	0

- Molecule 10 is a protein called U3 small nucleolar RNA-associated protein 13 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	UM	843	6545	4139	1151	1241	14	0	0

- Molecule 11 is a protein called UTP14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	UN	177	1401	892	263	239	7	0	0

- Molecule 12 is a protein called U3 small nucleolar RNA-associated protein 15 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	UO	503	3811	2417	698	683	13	0	0

- Molecule 13 is a protein called UTP17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	UQ	789	6008	3831	1037	1119	21	0	0

- Molecule 14 is a protein called UTP18.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
14	UR	447	3495	2209	656	619	1	10	0	0

- Molecule 15 is a protein called Putative U3 snoRNP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	UU	908	6778	4361	1243	1148	26	0	0

- Molecule 16 is a protein called UTP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	UX	190	1480	938	286	246	10	0	0

- Molecule 17 is a protein called Ribosome biogenesis protein C8F11.04.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	UZ	235	1815	1184	330	298	3	0	0

- Molecule 18 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	CA	242	1778	1149	327	293	9	0	0
18	CB	237	1816	1154	318	335	9	0	0

- Molecule 19 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	CC	387	2866	1836	527	492	11	0	0

- Molecule 20 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	CD	446	3355	2150	594	600	11	0	0

- Molecule 21 is a protein called H/ACA ribonucleoprotein complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	CE	121	879	557	165	154	3	0	0
21	CF	120	864	550	161	150	3	0	0

- Molecule 22 is a protein called Ribosomal RNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	CG	416	3245	2065	587	580	13	0	0

- Molecule 23 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	CH	389	2888	1827	526	525	10	0	0

- Molecule 24 is a protein called Bms1-type G domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	CI	841	6666	4277	1246	1113	30	0	0

- Molecule 25 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	CJ	179	1434	918	283	226	7	0	0

- Molecule 26 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	CK	297	2329	1476	445	400	8	0	0

- Molecule 27 is a protein called mpp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	CL	320	2466	1550	460	450	6	0	0

- Molecule 28 is a protein called DDB1- and CUL4-associated factor 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	CM	445	3501	2195	672	619	15	0	0

- Molecule 29 is a protein called Nucleolar essential protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	CN	226	1762	1119	306	327	10	0	0
29	CO	215	1683	1067	293	313	10	0	0

- Molecule 30 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	CP	233	1893	1209	340	335	9	0	0

- Molecule 31 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	CQ	180	1413	898	257	251	7	0	0

- Molecule 32 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	CR	846	6677	4278	1137	1233	29	0	0
32	CS	836	6591	4217	1118	1228	28	0	0

- Molecule 33 is a protein called Fcf2 pre-rRNA processing C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	CT	131	1035	656	197	178	4	0	0

- Molecule 34 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Ca	225	1821	1160	341	315	5	0	0

- Molecule 35 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Cb	232	1851	1179	340	325	7	0	0

- Molecule 36 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Cc	192	1464	926	278	253	7	0	0

- Molecule 37 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Cd	226	1819	1138	363	313	5	0	0

- Molecule 38 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	Ce	159	1279	810	237	232	0	0

- Molecule 39 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Cf	174	1398	872	283	242	1	0	0

- Molecule 40 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Cg	159	1248	804	258	184	2	0	0

- Molecule 41 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	Ch	66	546	355	101	90	0	0

- Molecule 42 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Ci	115	808	506	156	141	5	0	0

- Molecule 43 is a protein called 40S ribosomal protein S16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Cj	126	943	613	177	151	2	0	0

- Molecule 44 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Ck	131	1082	695	210	172	5	0	0

- Molecule 45 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Cm	126	985	632	184	164	5	0	0

- Molecule 46 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Cn	96	702	456	134	110	2	0	0

- Molecule 47 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Co	92	741	474	139	126	2	0	0

- Molecule 48 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Cp	61	458	286	97	74	1	0	0

- Molecule 49 is a protein called Faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	CU	176	1337	822	265	244	6	0	0

- Molecule 50 is a RNA chain called 35s rna.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	C1	1574	33584	14984	6018	11008	1574	0	0

- Molecule 51 is a RNA chain called u3 rna.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
51	C2	229	4869	2172	851	1617	229	0	0

- Molecule 52 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	CW	383	2932	1862	531	525	14	0	0

- Molecule 53 is a protein called UTP20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	UT	2027	15998	10300	2811	2819	68	0	0

- Molecule 54 is a protein called UTP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	UH	799	6198	3903	1105	1171	19	0	0

- Molecule 55 is a protein called Small-subunit processome Utp12 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	UE	178	1362	851	251	254	6	0	0
55	UI	128	996	622	187	181	6	0	0

- Molecule 56 is a protein called CCAAT-binding factor domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	US	451	3672	2389	608	660	15	0	0

- Molecule 57 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	Cl	80	633	400	115	117	1	0	0

- Molecule 58 is a protein called Bystin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	CX	267	2130	1384	374	362	10	0	0

- Molecule 59 is a protein called U3 small nucleolar ribonucleoprotein protein lcp5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	CY	264	2095	1296	388	406	5	0	0

- Molecule 60 is a protein called Protein BFR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	CZ	283	2270	1398	426	439	7	0	0

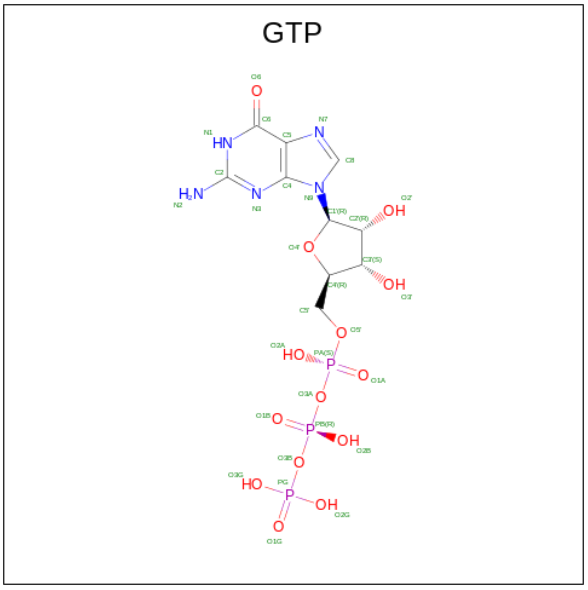
- Molecule 61 is a protein called UTP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
61	UP	54	422	264	88	70	0	0

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
62	UX	1	1	1	0

- Molecule 63 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

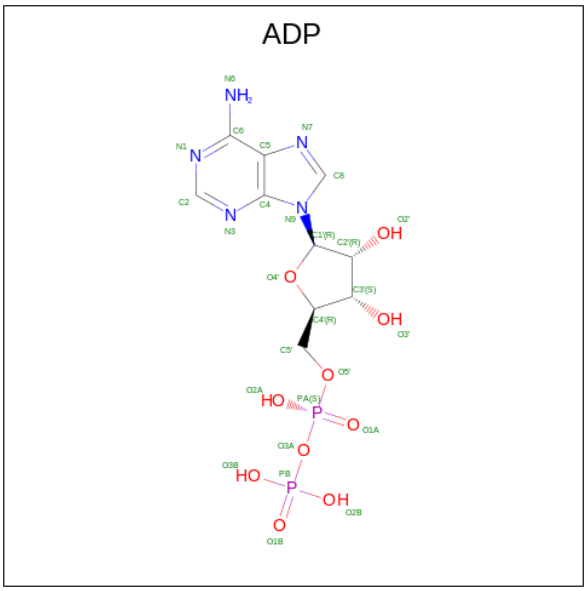


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
63	CI	1	32	10	5	14	3	0

- Molecule 64 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
64	CI	1	1	1	0

- Molecule 65 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



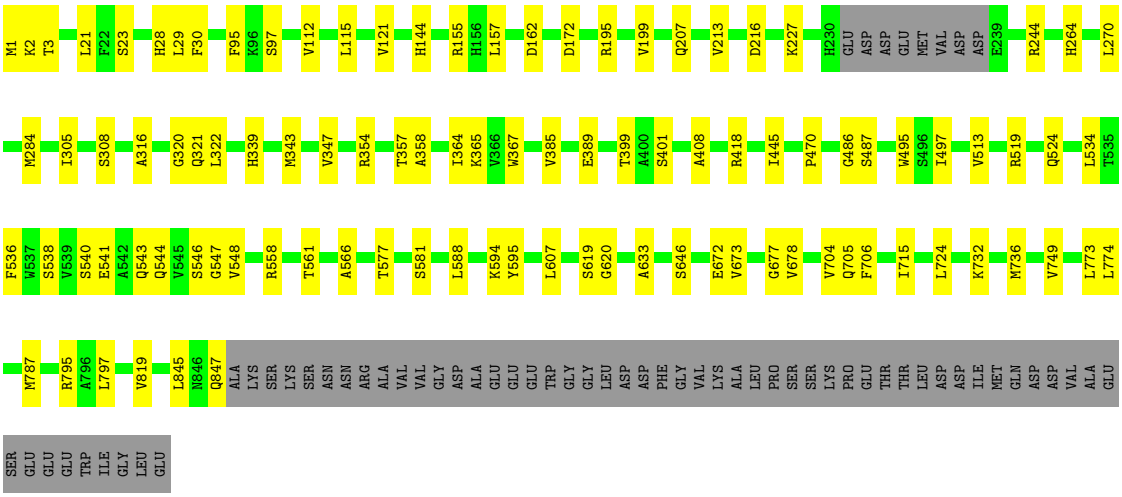
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
65	CS	1	27	10	5	10	2	0

3 Residue-property plots (i)

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

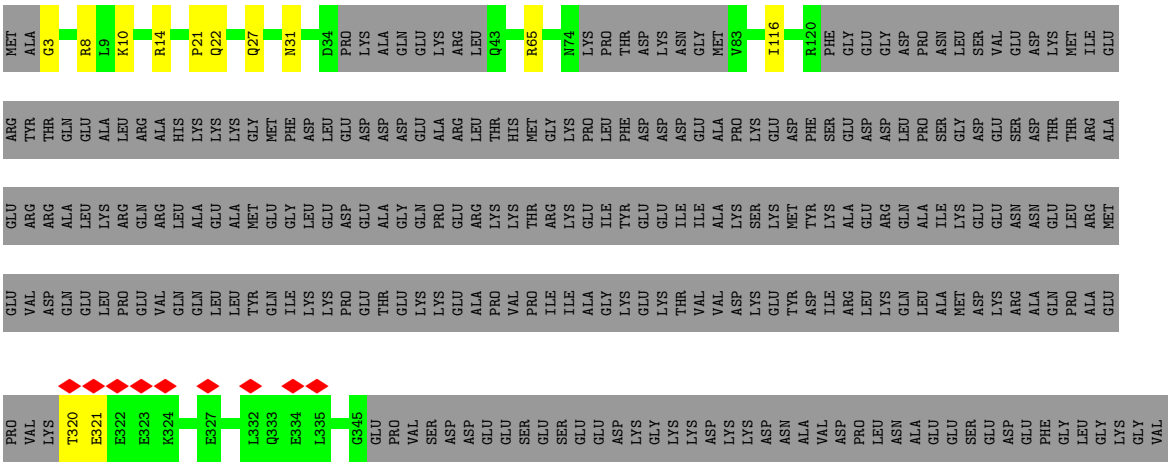
• Molecule 1: Periodic tryptophan protein 2-like protein

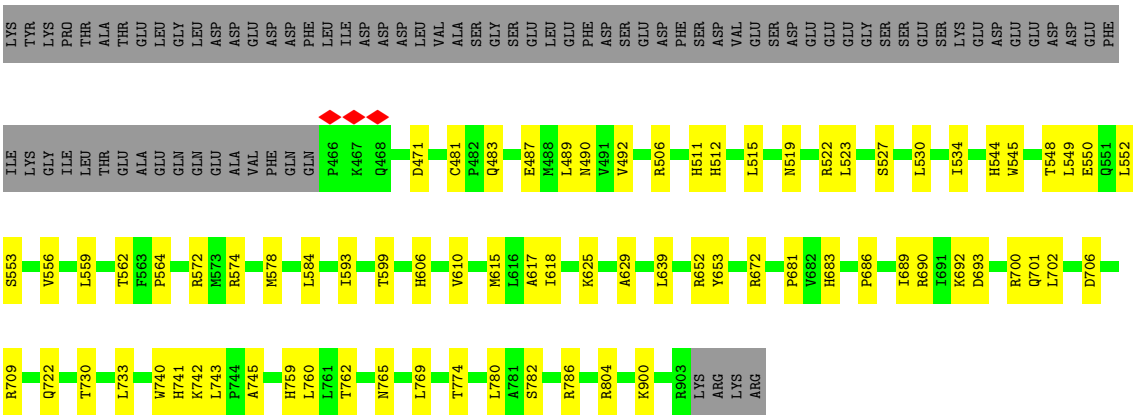
Chain UA: 82% 11% 7%



• Molecule 2: Nucleolar complex protein 14

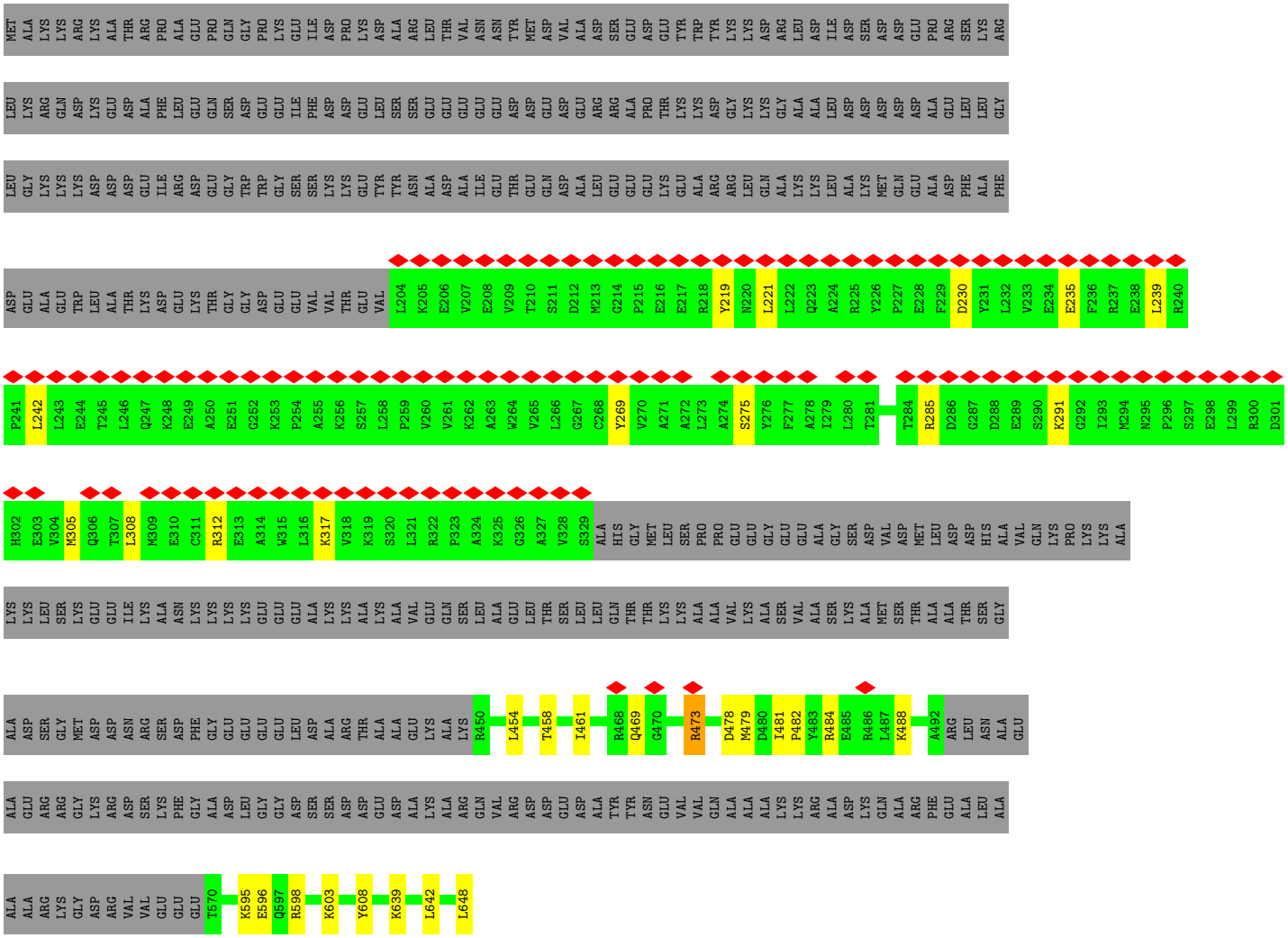
Chain UB: 53% 10% 38%





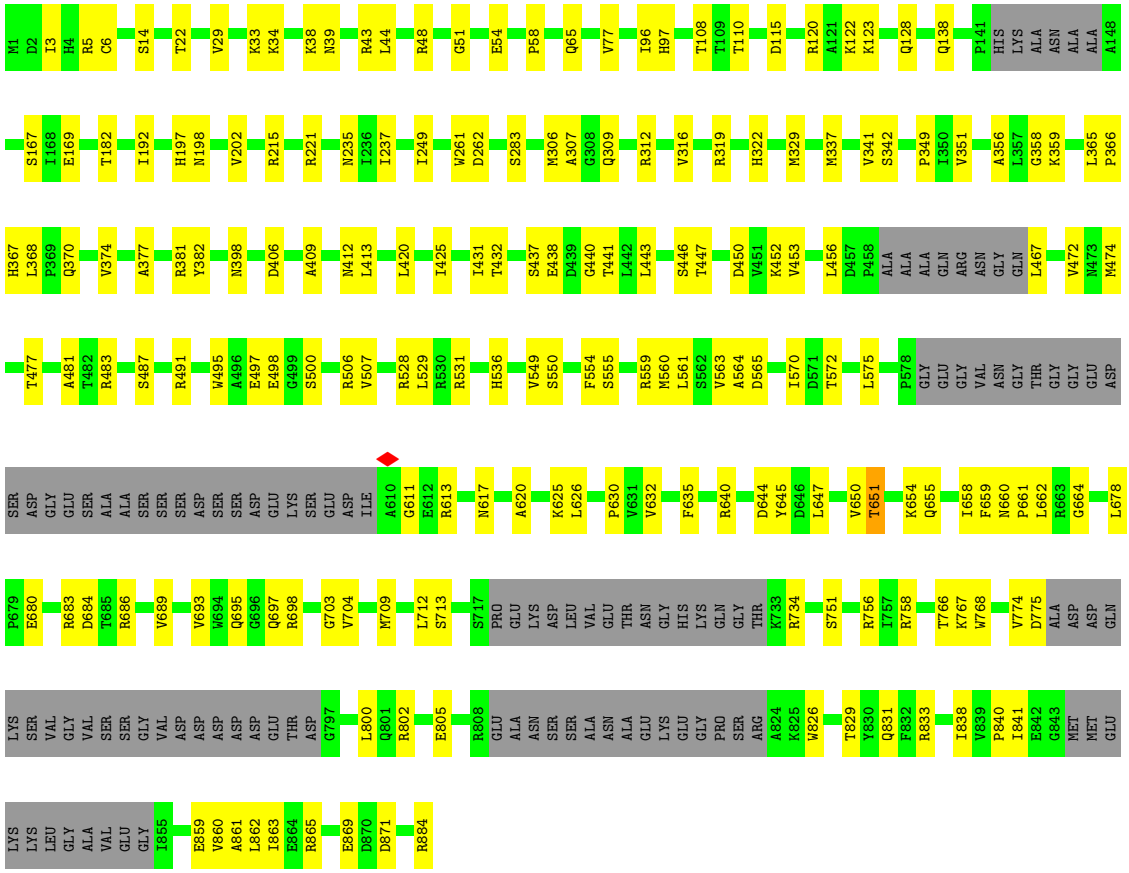
• Molecule 3: Sas10 C-terminal domain-containing protein

Chain UC:



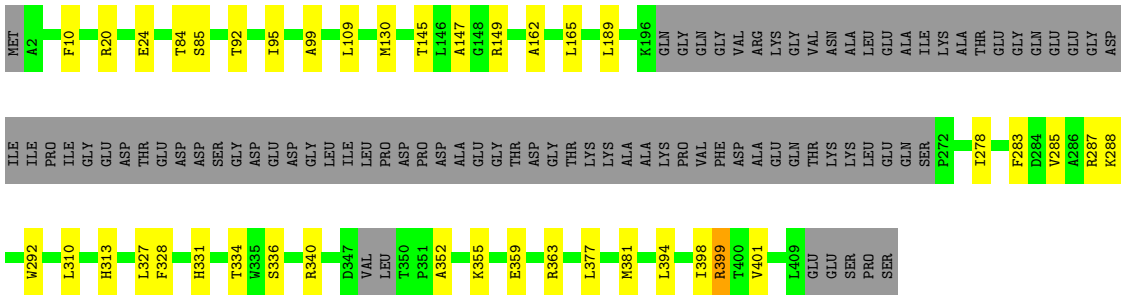
• Molecule 4: UTP4

Chain UD:



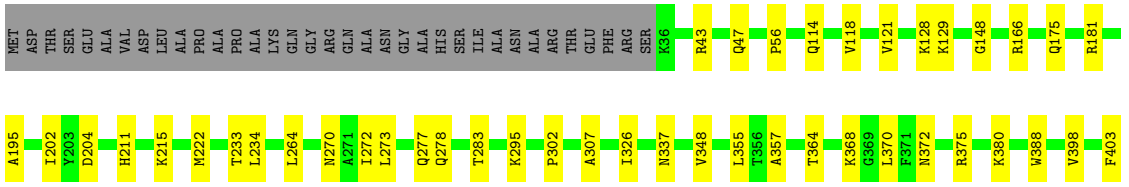
- Molecule 5: U3 snoRNP protein

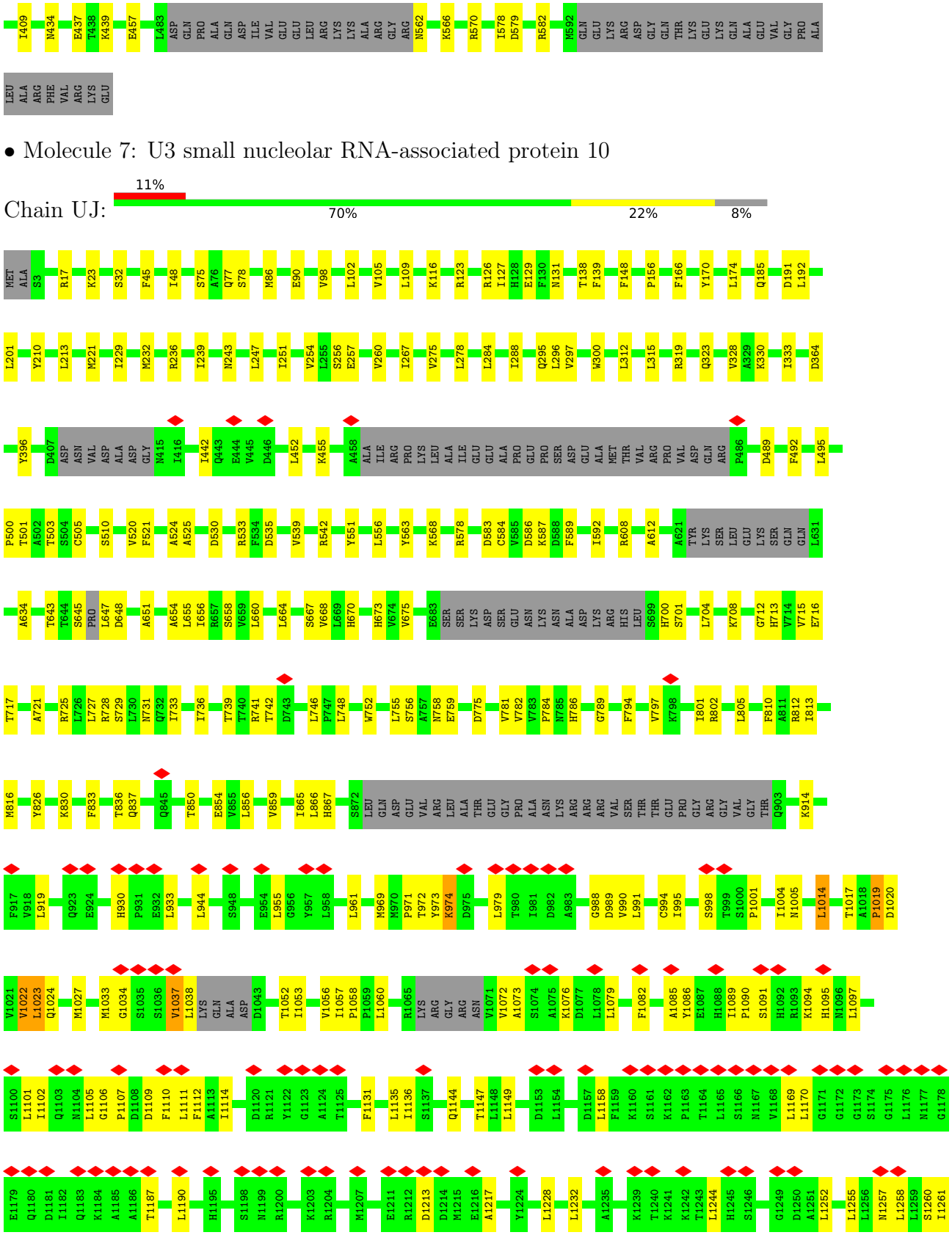
Chain UF: 70% 9% 20%



- Molecule 6: U three protein 7

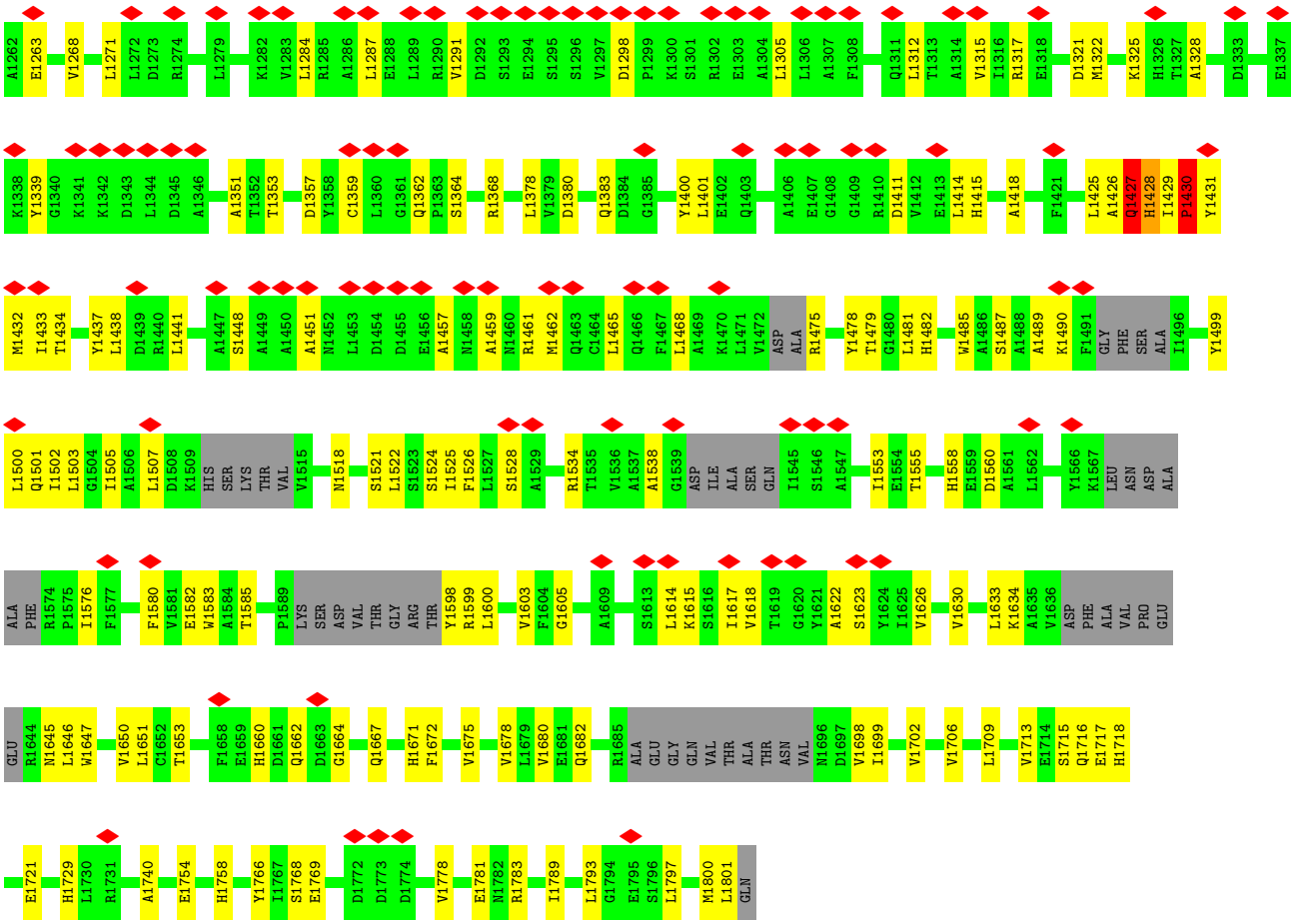
Chain UG: 76% 10% 14%





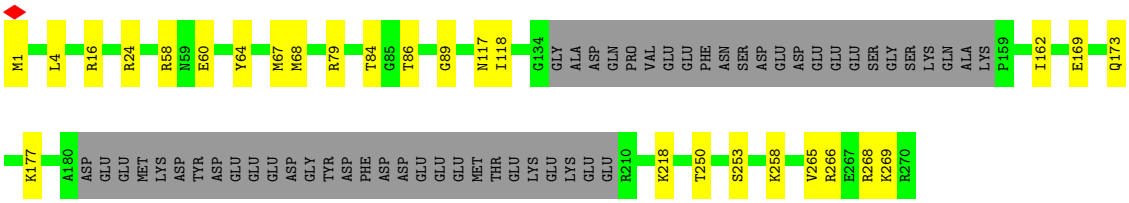
• Molecule 7: U3 small nucleolar RNA-associated protein 10

Chain UJ:



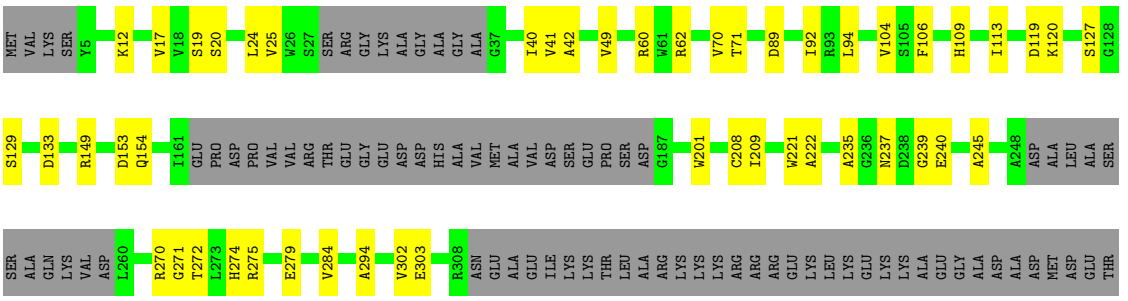
- Molecule 8: U3 small nucleolar RNA-associated protein 11

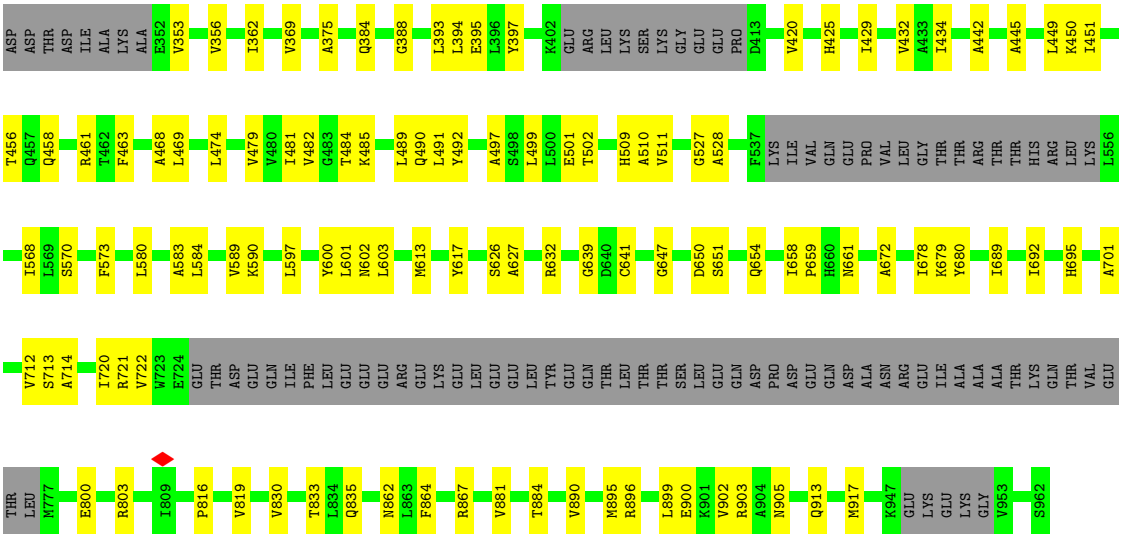
Chain UK: 70% 10% 20%



- Molecule 9: Small-subunit processome Utp12 domain-containing protein

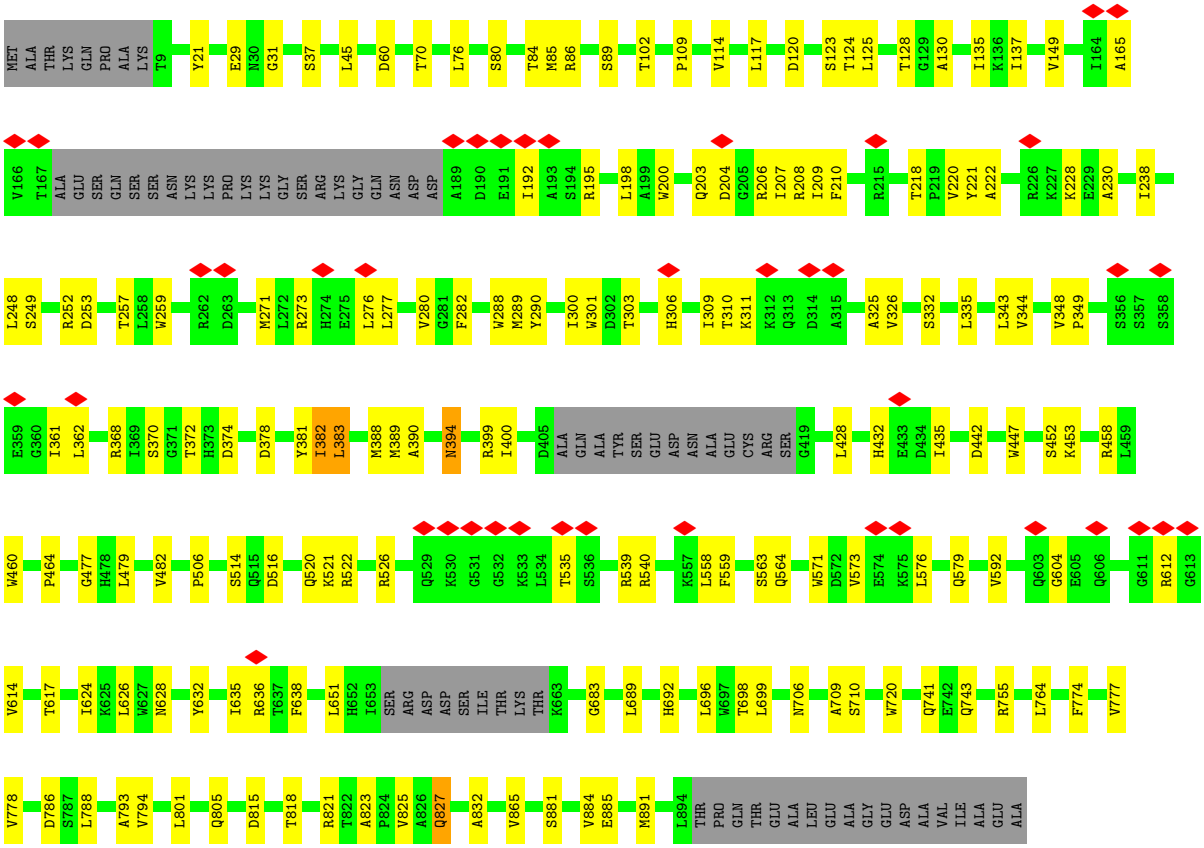
Chain UL: 65% 16% 18%





• Molecule 10: U3 small nucleolar RNA-associated protein 13 C-terminal domain-containing protein

Chain UM:



• Molecule 11: UTP14

Chain UN:

MET PRO GLY ARG GLN ALA HIS GLY ARG PRO LEU LEU PRO SER LEU GLY SER SER SER GLY GLY GLY LYS SER LYS LYS SER ARG SER LYS ALA ARG ARG SER ALA GLN SER LYS ALA LEU ASP ALA PHE ALA LEU ALA ALA GLU GLN VAL PRO GLU SER ARG SER LYS GLY VAL ARG LEU

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

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

GLU ASP ASP ALA ILE ASP LEU ALA THR ALA LEU ASP GLN TYR GLU SER SER GLU GLU GLY GLU GLU GLY GLU GLU SER GLU SER GLU GLU ASP ASP GLU GLU SER GLU GLU GLU ASP SER ASP GLU GLU ASP ASP PRO SER LYS LEU ASP ALA LEU GLN SER MET ILE ALA GLY PHE

ALA GLY GLU ASP GLU GLU SER GLY GLY GLU GLY GLU ALA LYS PRO SER GLY LYS GLN LYS LEU SER LEU LYS ASP LEU GLY LEU VAL GLY VAL LYS ASP P274 D275 M276 K277 R278 S279 L282 M283 K288 ALA THR LYS PRO GLY SER S295 P301 T329 N346 A354

P359 L369 E370 I373 S380 TRP SER GLN PRO LYS VAL GLU ALA GLY ALA TRP SER LYS PRO ASP ASP GLU GLY SER SER LYS PRO ARG LYS ALA PRO LYS GLY ARG PRO GLU GLU ILE ASP VAL THR ASP LEU ALA LEU ALA GLY LYS PRO ALA LYS ALA LYS ALA ASN GLY GLN

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

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

LYS GLU LYS ARG LYS D863 K878 H889 P907 E908 W909 M910 T911 K912 E913 T914 Q927 P932 M933 Y938

- Molecule 12: U3 small nucleolar RNA-associated protein 15 C-terminal domain-containing protein

Chain UO: 77% 13% 10%

MET A2 V6 P14 E23 Q24 R25 Y26 W27 I44 A51 SER LEU GLY THR THR ALA LEU VAL SER SER SER LEU VAL ALA ALA ALA LYS T69 N70 V75 T76 A77 I83 K93 R97 F98 D99 C104 R112 A116 G121 Q130 A134

Q145 P146 V147 W148 V149 C163 T180 R181 N203 V206 D218 A219 R220 M227 I235 L247 S251 I255 L260 I269 Q273 Q284 G285 R286 I317 I323 T324 A325 R332 H333 M338 Q339 V342 L343 S350 GLY PRO ALA ALA ASP

ARG GLU ARG GLU ARG GLU ARG VAL GLU ALA ALA MET ALA LYS GLY PRO GLU ALA ILE ALA LYS LEU ASP ALA ALA LYS ALA LYS ARG K385 R386 A387 P406 R415 G416 R417 D449 I452 R463 R467 Q471 E475 V478 I479 L482 P492 R495

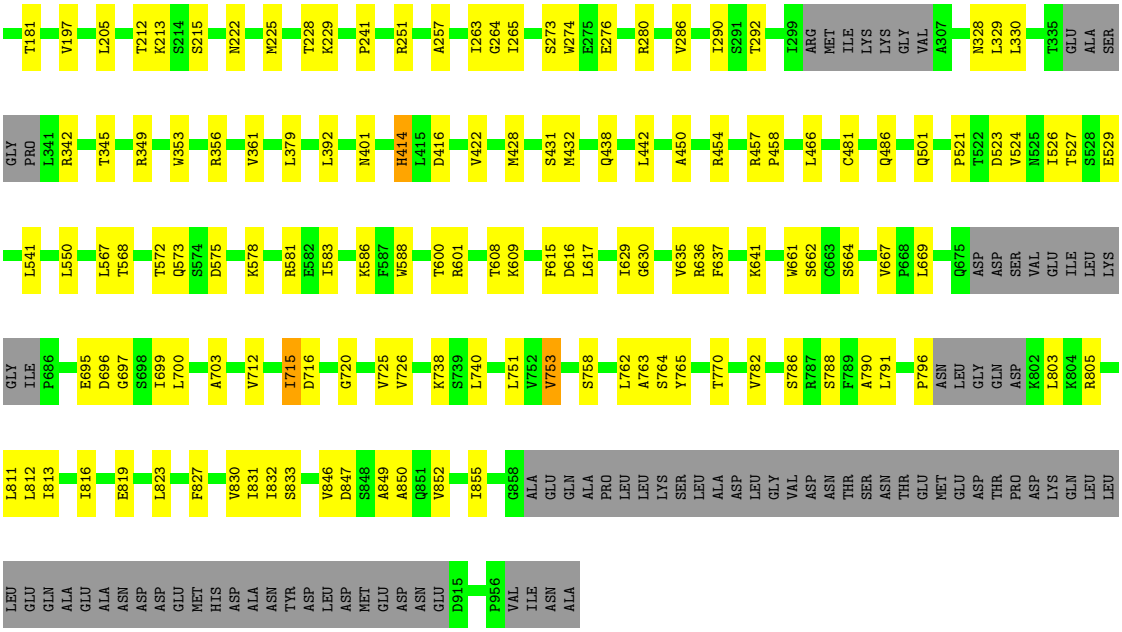
V499 L505 I506 D507 V513 S516 L526 L527 A528 R532 A540 V554 E555 ALA GLN

- Molecule 13: UTP17

Chain UQ: 66% 16% 18%

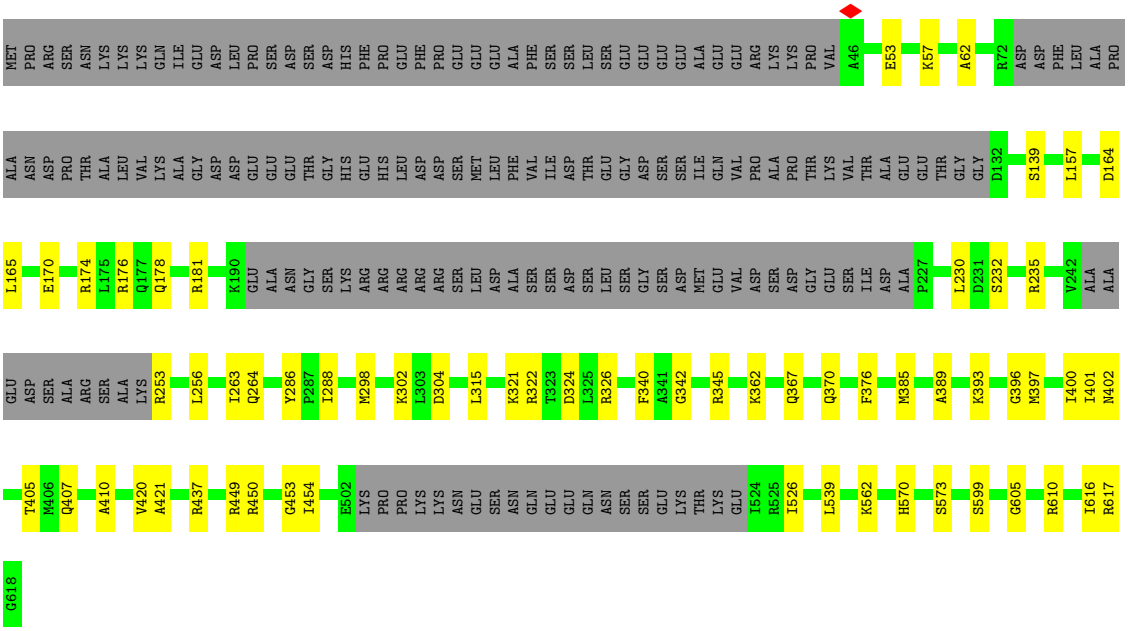
MET VAL SER THR MET GLU THR ASN GLY ASP THR ALA SER LEU LYS ARG LYS ARG GLU PRO LYS ASP ASP PRO HIS SER LEU GLN LYS LYS HIS ARG HIS ARG SER ARG SER LYS PRO GLN ASP ALA ALA THR ALA ASP SER VAL ALA ASN LEU ASN SER ASN SER LEU ALA VAL GLN PRO

ILE ASP GLY ASN SER GLY PRO LEU GLN LEU ALA THR THR ASP ARG LEU ALA S78 M89 I95 I104 I105 T106 Y107 I111 Q112 V113 T116 T130 ARG THR ASN ASP LEU ASP GLU P138 S146 A147 L148 D154 Y155 L156 W157 V158 I165 I168 N169 W170 T171



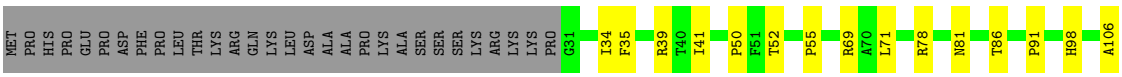
- Molecule 14: UTP18

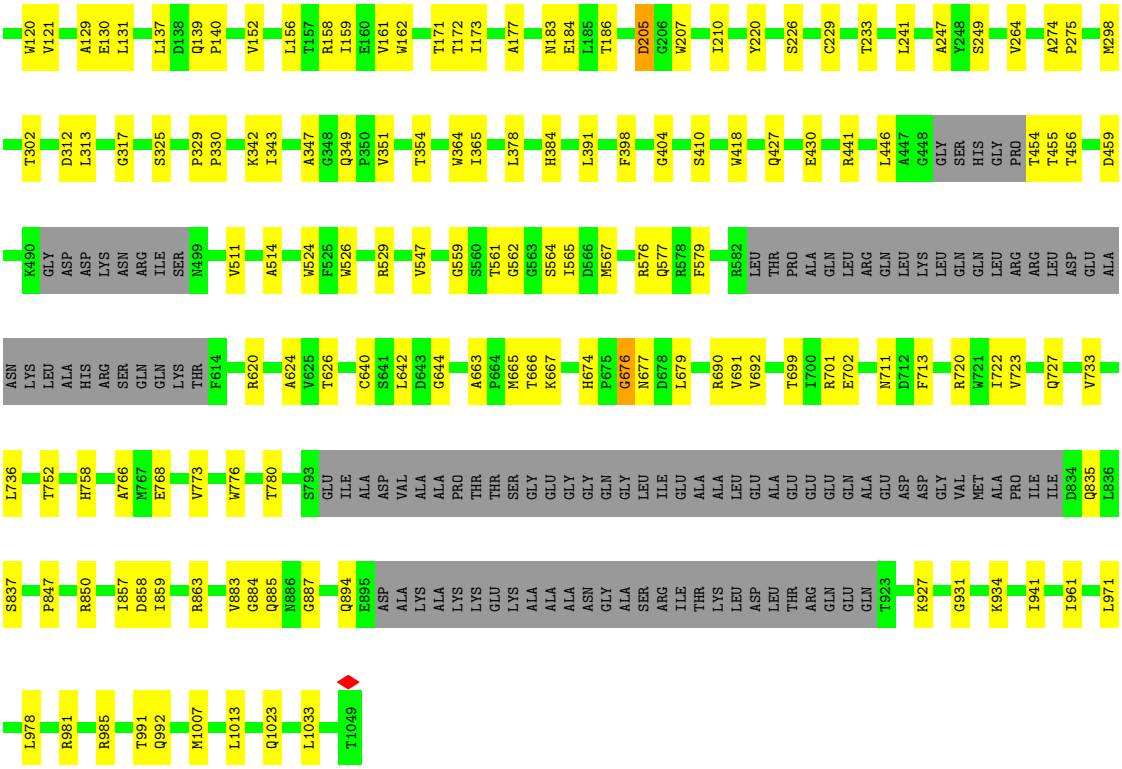
Chain UR: 62% 10% 28%



- Molecule 15: Putative U3 snoRNP protein

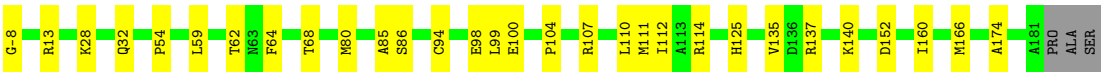
Chain UU: 71% 15% 13%





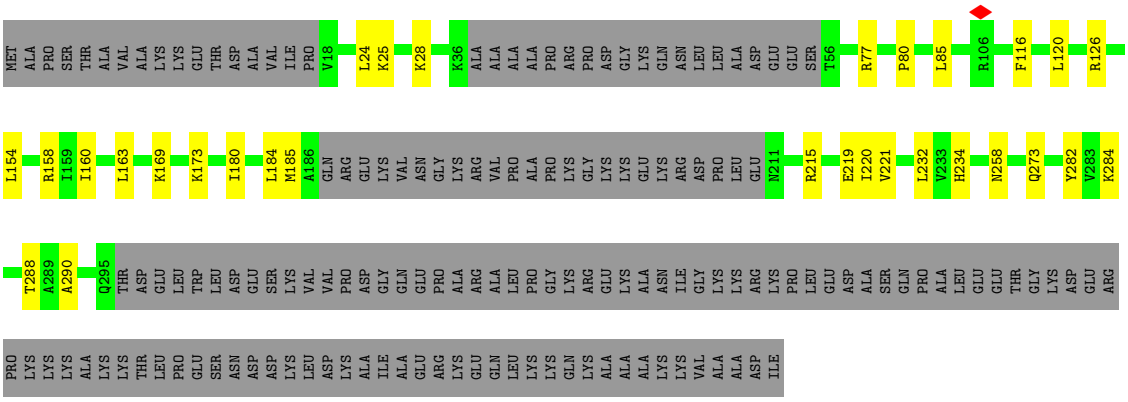
- Molecule 16: UTP24

Chain UX: 83% 16%



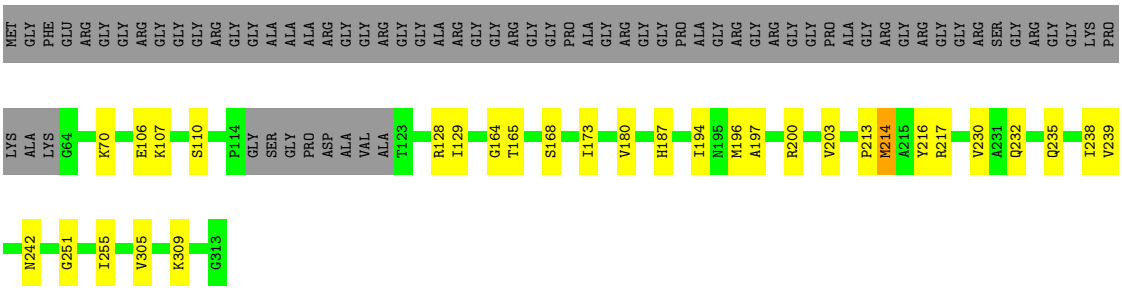
- Molecule 17: Ribosome biogenesis protein C8F11.04

Chain UZ: 52% 8% 40%



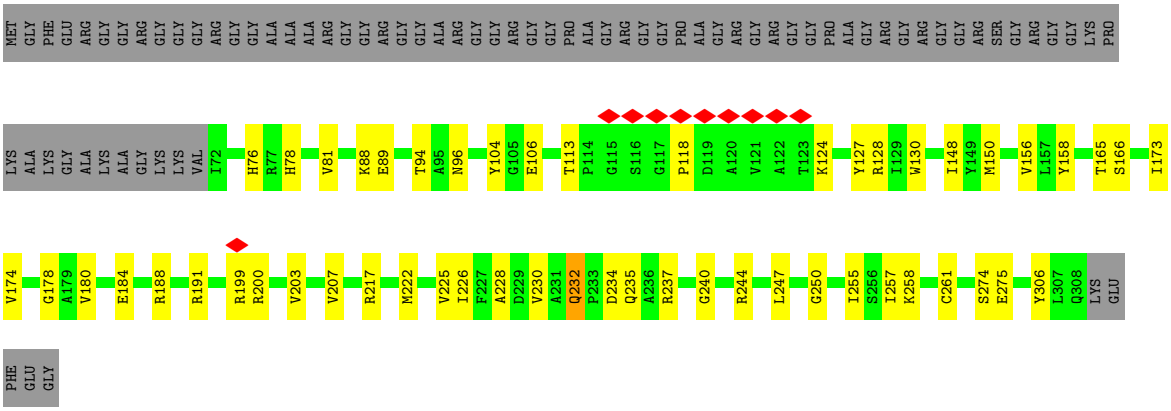
- Molecule 18: rRNA 2'-O-methyltransferase fibrillarin

Chain CA: 67% 10% 23%



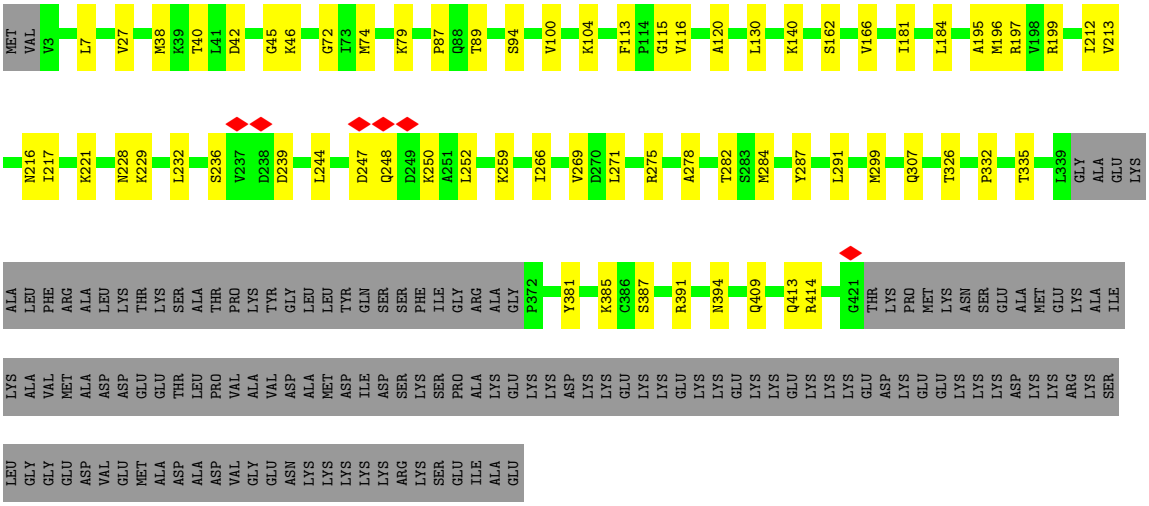
• Molecule 18: rRNA 2'-O-methyltransferase fibrillarin

Chain CB:



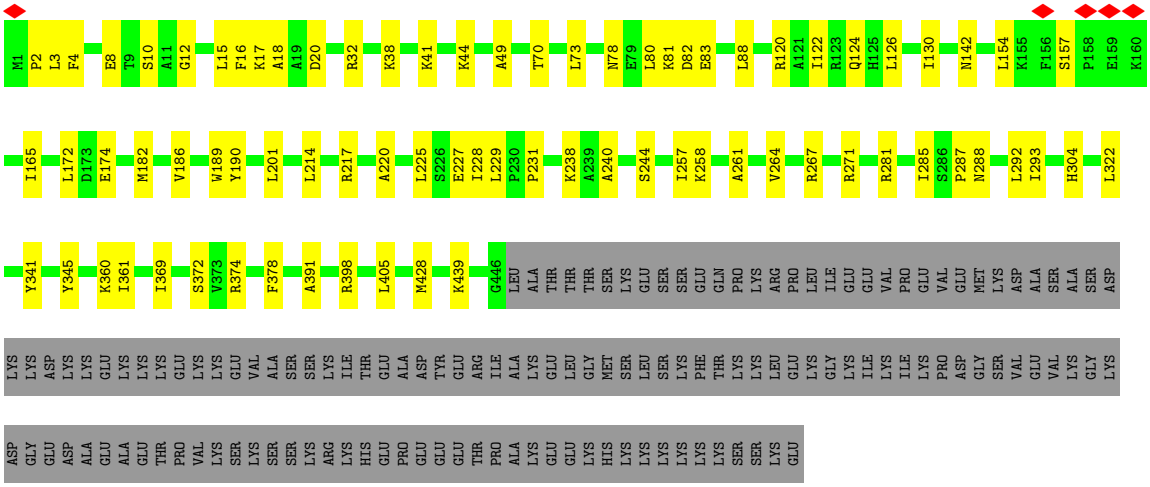
• Molecule 19: Nucleolar protein 56

Chain CC:



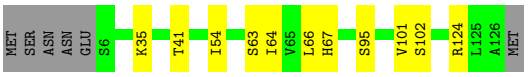
• Molecule 20: Nucleolar protein 58

Chain CD:



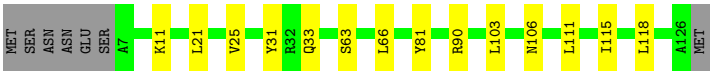
• Molecule 21: H/ACA ribonucleoprotein complex subunit 2

Chain CE:



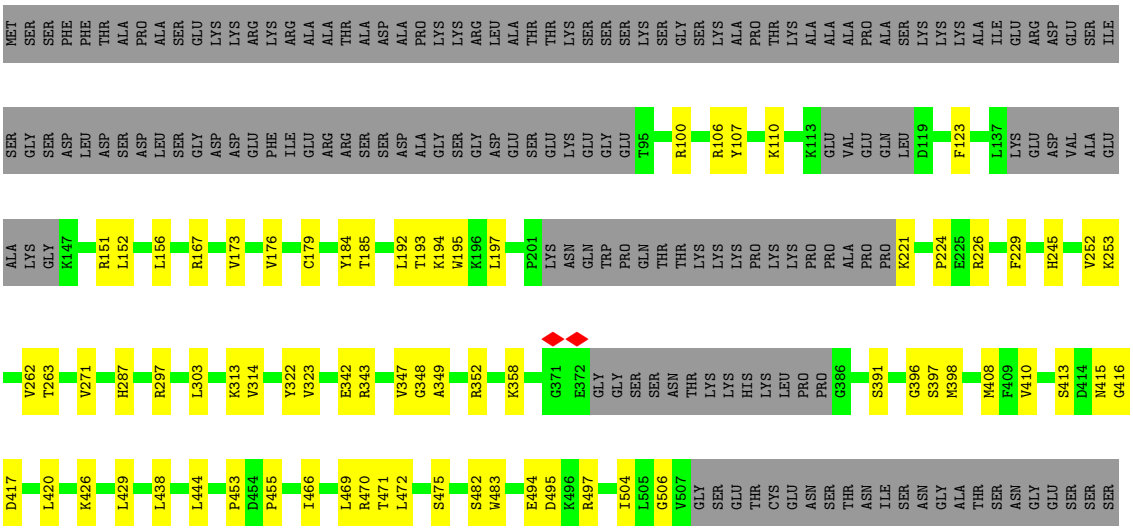
• Molecule 21: H/ACA ribonucleoprotein complex subunit 2

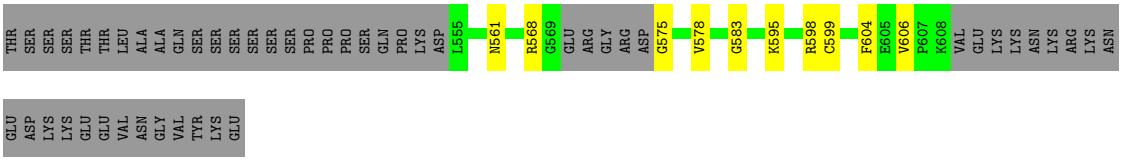
Chain CF:



• Molecule 22: Ribosomal RNA-processing protein

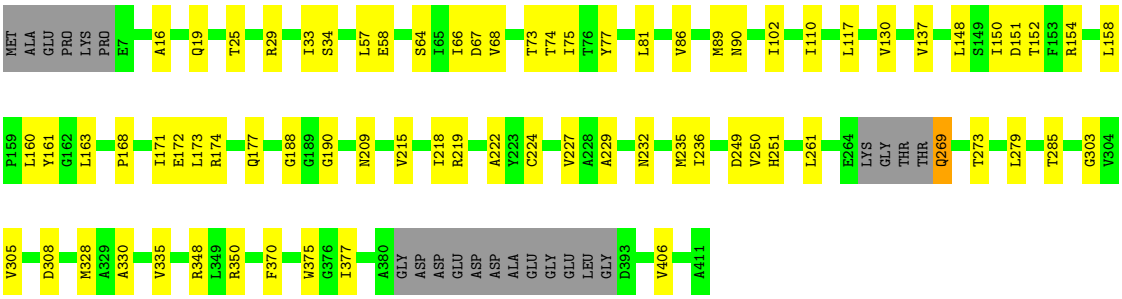
Chain CG:





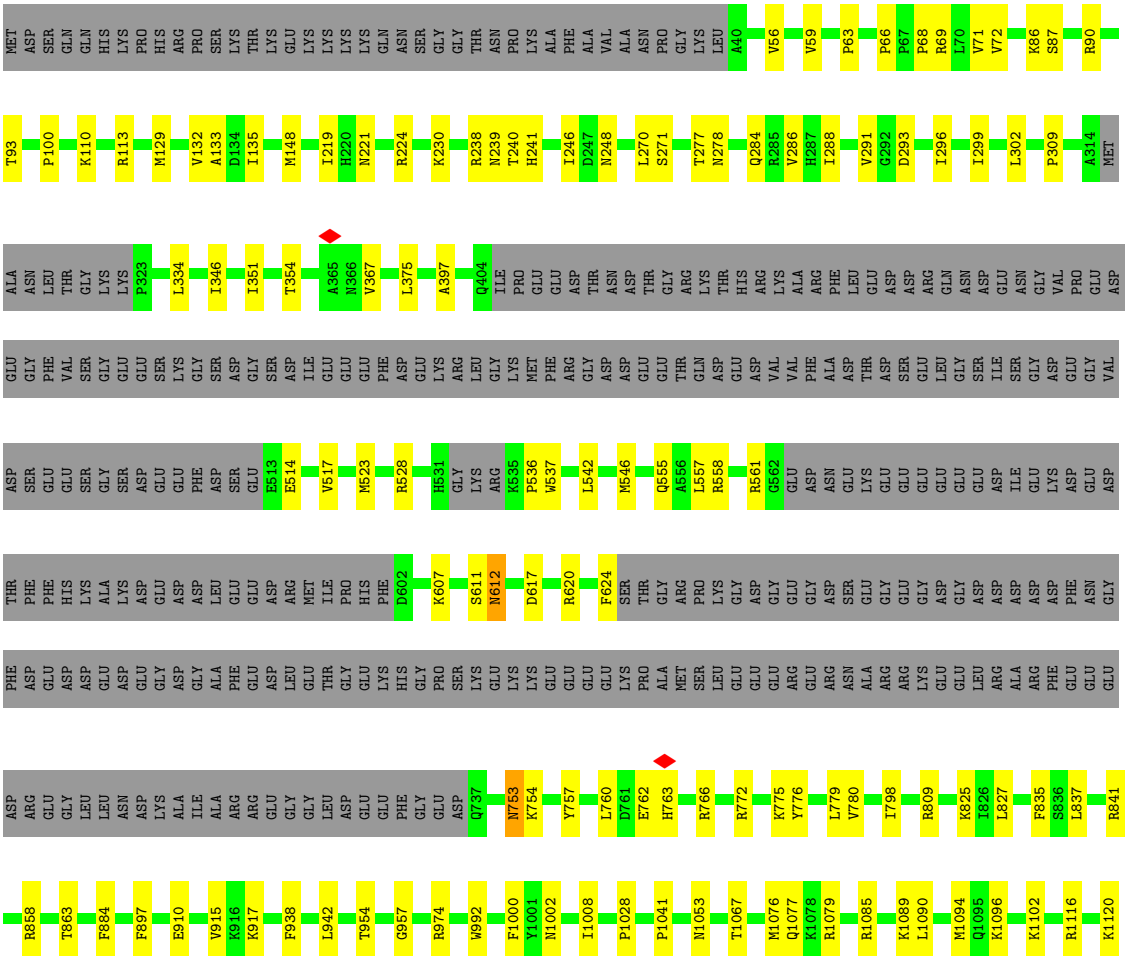
- Molecule 23: RNA 3'-terminal phosphate cyclase-like protein

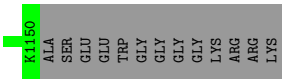
Chain CH: 77% 18% 5%



- Molecule 24: Bms1-type G domain-containing protein

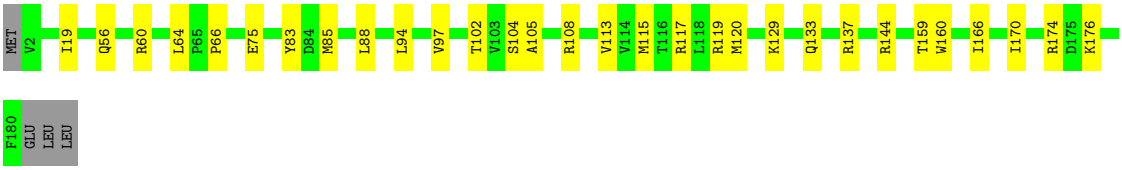
Chain CI: 62% 10% 28%





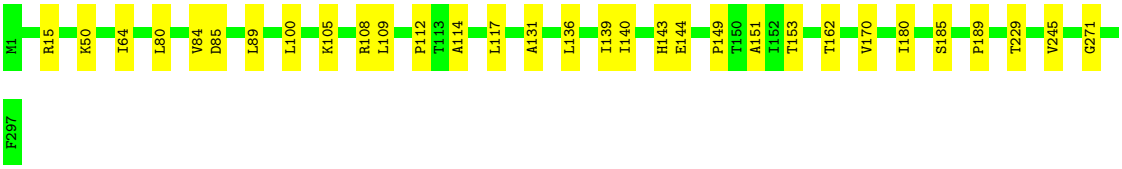
• Molecule 25: U3 small nucleolar ribonucleoprotein protein IMP3

Chain CJ:



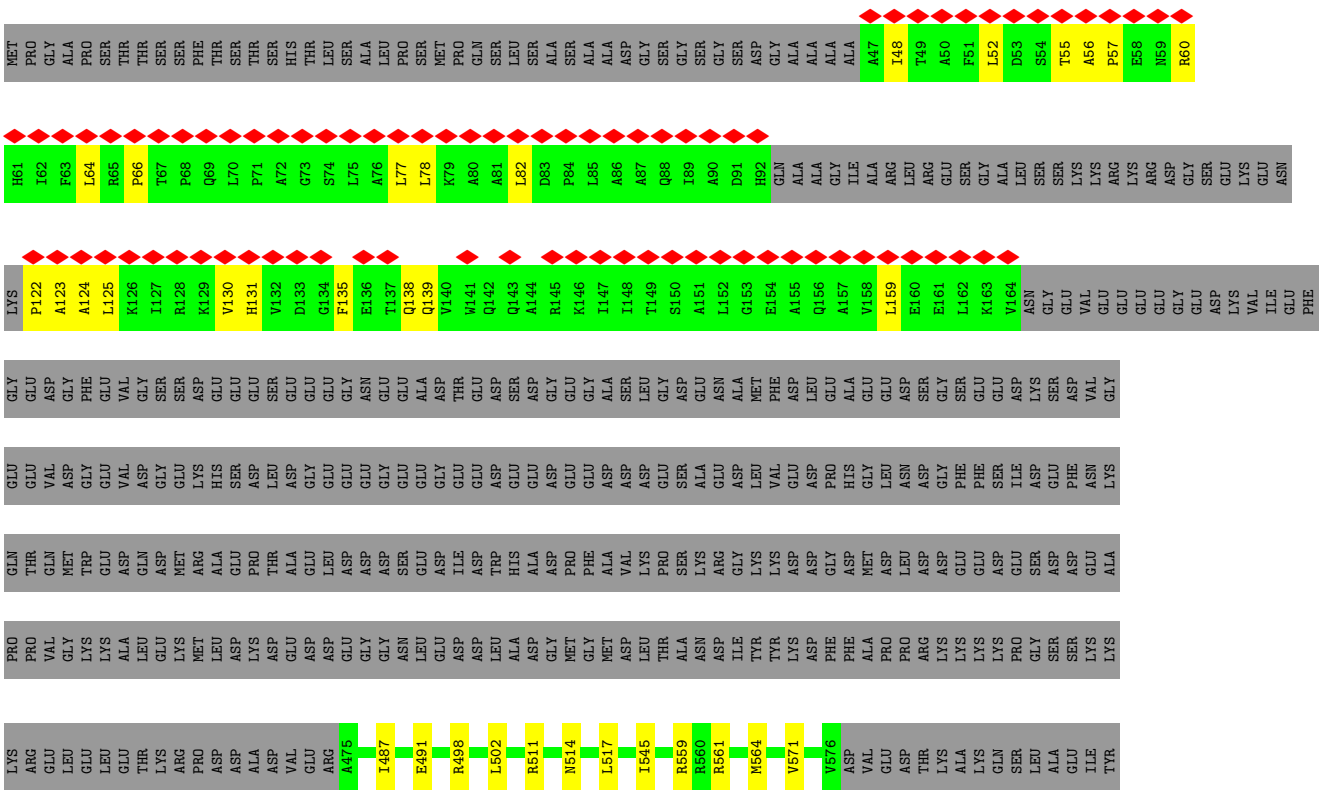
• Molecule 26: U3 small nucleolar ribonucleoprotein protein IMP4

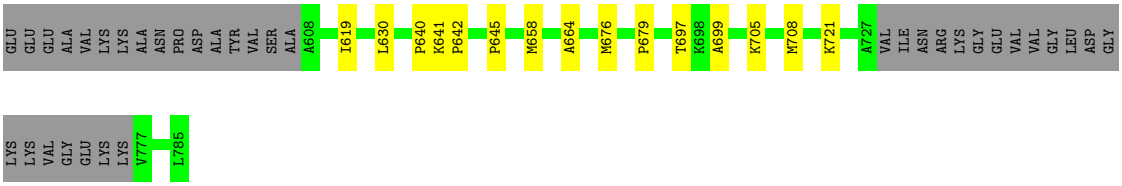
Chain CK:



• Molecule 27: mpp10

Chain CL:



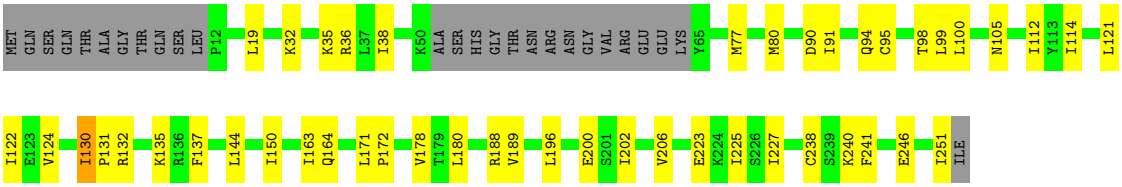


• Molecule 28: DDB1- and CUL4-associated factor 13

Chain CM: 84% 15%

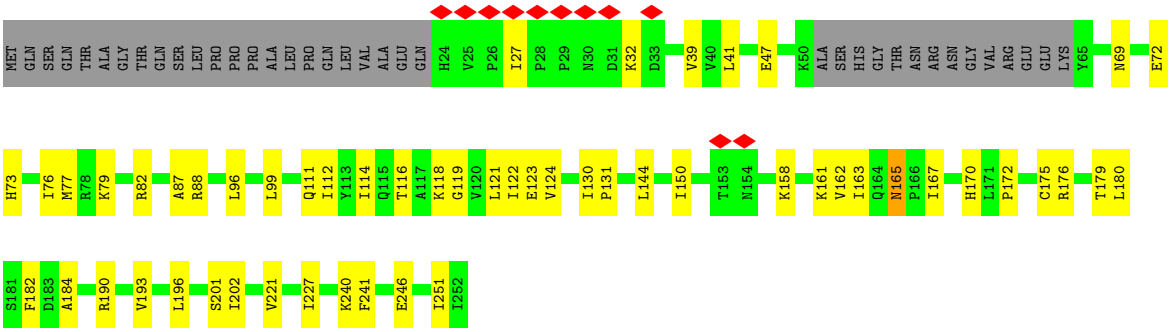
• Molecule 29: Nucleolar essential protein 1

Chain CN: 71% 18% 10%



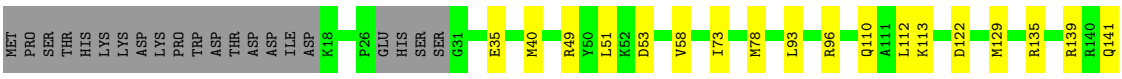
• Molecule 29: Nucleolar essential protein 1

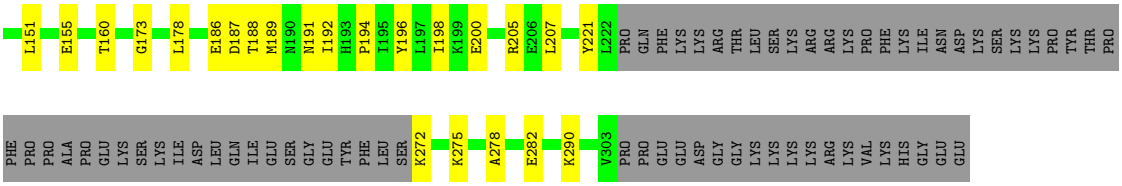
Chain CO: 63% 21% 15%



• Molecule 30: KRR1 small subunit processome component

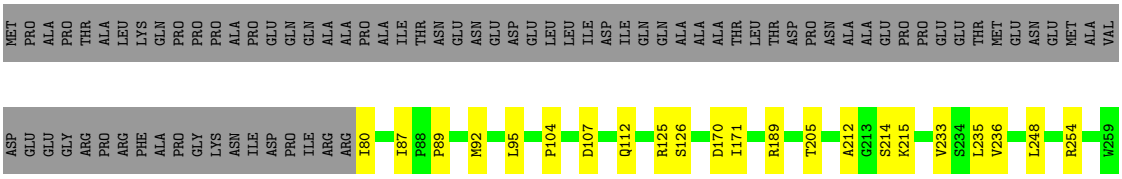
Chain CP: 60% 13% 28%





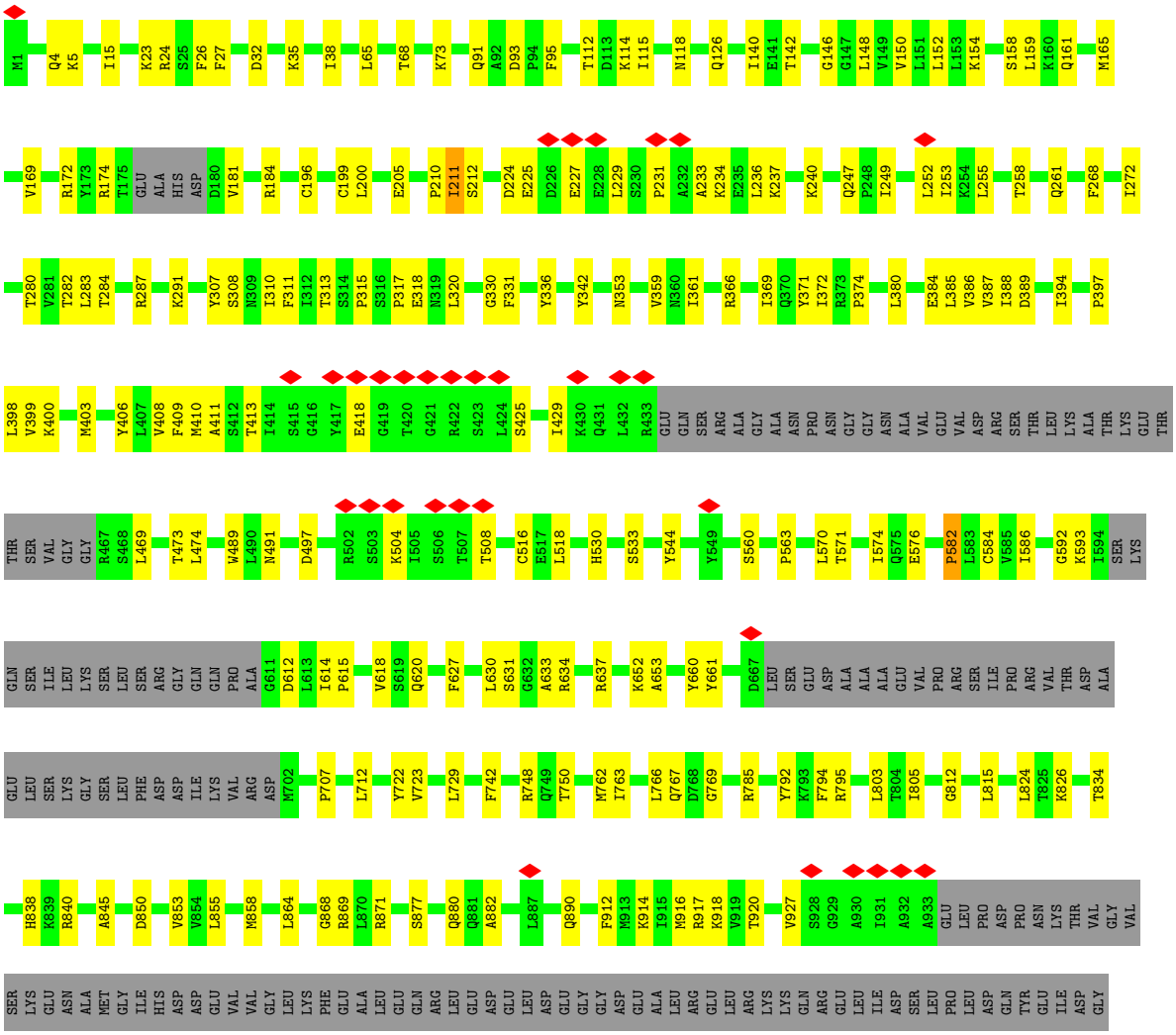
• Molecule 31: Pre-rRNA-processing protein PNO1

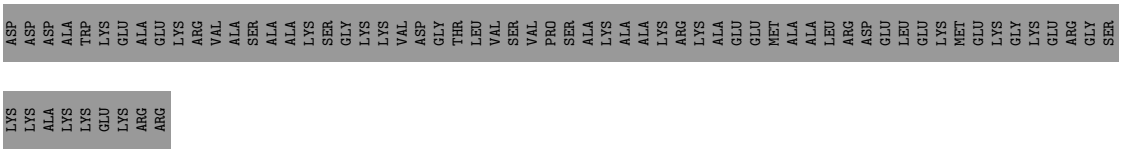
Chain CQ:



• Molecule 32: RNA cytidine acetyltransferase

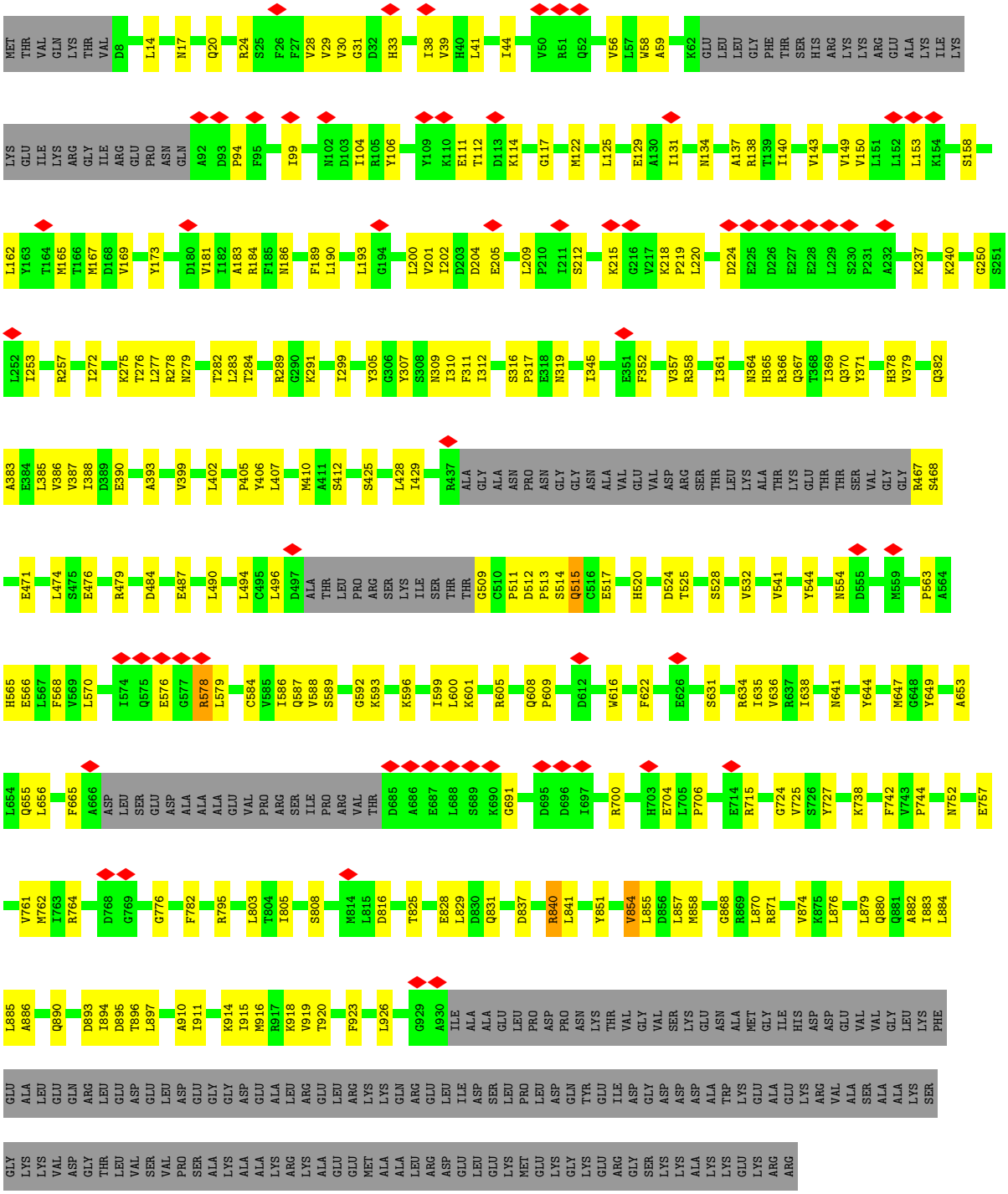
Chain CR:





• Molecule 32: RNA cytidine acetyltransferase

Chain CS:



- Molecule 33: Fcf2 pre-rRNA processing C-terminal domain-containing protein

Chain CT: 58% 6% 35%

MET ALA THR THR LEU GLY LEU PRO ASP GLU GLU ILE ASP ARG LEU LEU ALA GLU ALA GLU ALA ARG LEU ALA GLY SER GLY ASP ALA ASP ALA GLY ALA ILE ALA LEU ALA LYS PRO ALA ALA SER LYS PRO LEU THR VAL ALA ALA PRO ALA ALA PRO LYS ALA GLY GLU GLN THR VAL

PRO GLN VAL LYS LYS ALA GLU E68 L69 P74 P77 GLN LYS LYS LYS G82 P83 P84 Y91 L108 K123 K124 Y134 T139 I140 I141 V162 Y178 Y192 R202 LYS

- Molecule 34: Small ribosomal subunit protein eS1

Chain Ca: 70% 18% 12%

MET ALA VAL GLY LYS ASN LYS R8 K11 T25 R26 W29 I32 K33 A36 V40 R41 D42 V43 R50 L54 K55 L73 R82 K83 I84 K85 L86 R87 V88 D89 C96 L97 T98 R111 K116 T126 T129 Y133 L134 L135 R136 L137

K144 I164 C179 V185 L188 I189 P190 E191 V192 I204 Y205 Q208 H211 K214 V215 K216 L217 L218 K219 H232 GLY GLU SER SER GLU GLU ALA GLY GLN LYS VAL GLU ARG GLU PHE ARG GLU GLN VAL LEU GLU SER VAL

- Molecule 35: 40S ribosomal protein S4

Chain Cb: 66% 22% 12%

MET ALA ARG GLY PRO LYS LYS H8 L19 L20 D21 K22 M42 F47 R51 Y58 K62 A63 Q67 V72 R77 I80 T81 G85 F86 M87 D88 V89 I90 K94 R100 T105 R108 R113 D116 E117 K120 Y121 K122 K125 V126

K127 R128 L139 V140 T141 H142 D143 A144 R145 T146 K155 V160 I169 T170 D171 F172 I173 T177 L180 I183 G190 T196 G203 D212 A213 L214 D215 V225 G229 S230 L237 P238 K239 GLY LYS GLY VAL LYS LEU THR ILE ALA GLU GLU ARG ASP

GLN ARG ARG ALA ARG ALA LEU ALA ALA ALA GLY HIS

- Molecule 36: 40S ribosomal protein s5-like protein

Chain Cc: 79% 11% 9%

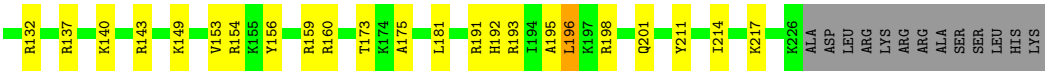
MET SER GLU GLY GLU VAL GLU VAL ALA GLN PRO GLN Y13 R32 I38 E39 I40 R41 D42 I43 S44 Q50 I57 N73 N82 S83 L84 M85 M86 H87 N91 G92 K93 K94 R99 N115 S133 T134 R135 ILE GLY SER ALA GLY THR VAL ARG R144 T163

T176 E179 C180 L181 R212

- Molecule 37: 40S ribosomal protein S6

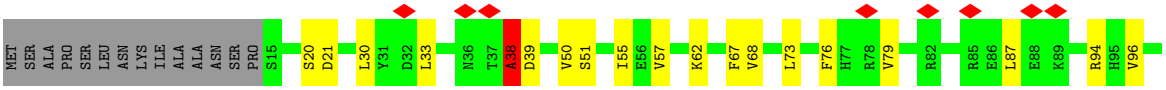
Chain Cd: 71% 23% 5%

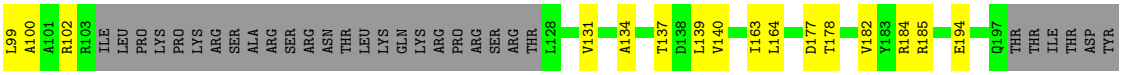
M1 K2 N10 L15 D20 E21 R22 K23 L24 R25 H26 D29 K30 R31 M32 E35 P40 R51 N56 D57 P62 N71 R74 L75 L76 L77 S78 E79 R85 P86 D89 R92 K93 R94 R98 G99 C100 I101 V102 L106 S107 V108 I113



• Molecule 38: 40S ribosomal protein S7

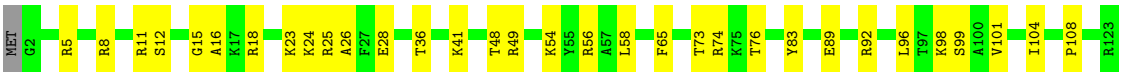
Chain Ce:

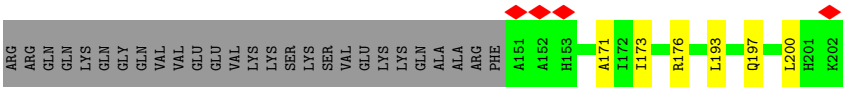




• Molecule 39: 40S ribosomal protein S8

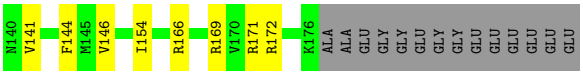
Chain Cf:





• Molecule 40: 40S ribosomal protein s9-like protein

Chain Cg:

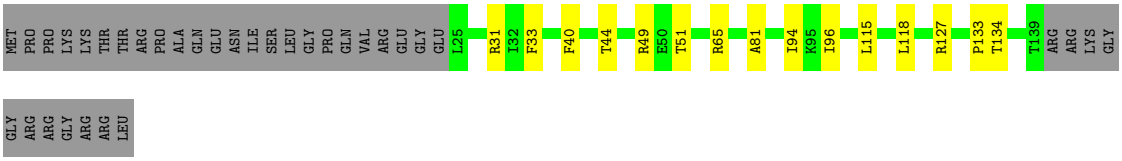


• Molecule 41: 40S ribosomal protein S13-like protein

Chain Ch:

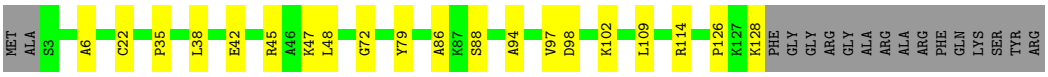
• Molecule 42: 40S ribosomal protein S14-like protein

Chain Ci:



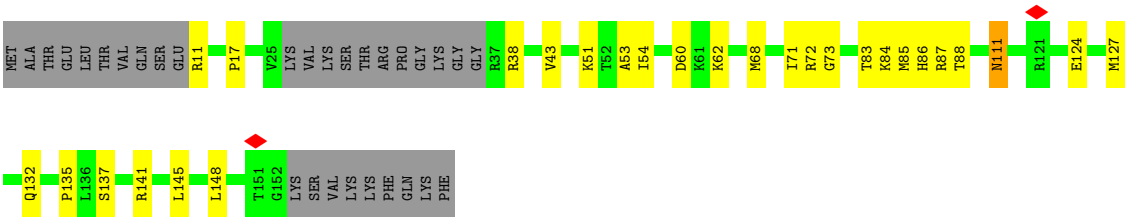
• Molecule 43: 40S ribosomal protein S16-like protein

Chain Cj: 74% 14% 12%



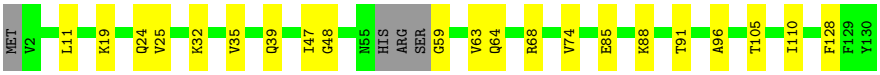
• Molecule 44: 40S ribosomal protein S11-like protein

Chain Ck: 64% 17% 19%



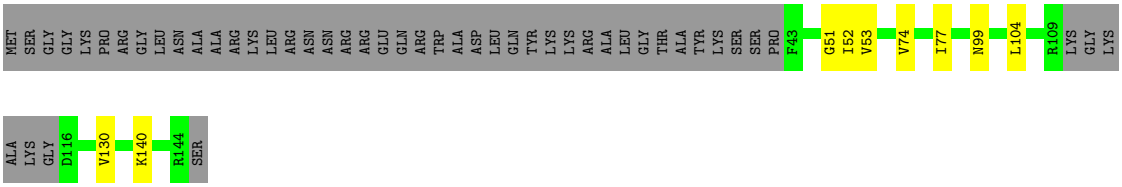
• Molecule 45: 40S ribosomal protein S22-like protein

Chain Cm: 81% 16%



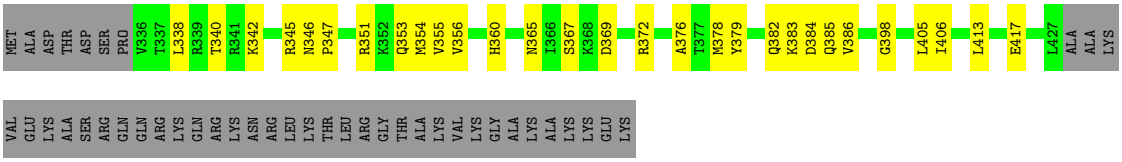
• Molecule 46: 40S ribosomal protein s23-like protein

Chain Cn: 60% 6% 34%



• Molecule 47: Small ribosomal subunit protein eS24

Chain Co: 46% 21% 32%



- Molecule 48: 40S ribosomal protein S28-like protein

Chain Cp: 79% 10% 10%

MET ASP SER SER LYS A6 K9 F10 V11 K12 V13 V29 R30 V31 N52 D53 T54 R66 LEU ARG

- Molecule 49: Faf1

Chain CU: 50% 6% 43%

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

SER ASP VAL ASN SER GLY GLU GLY ASP GLU TRP ASP GLY ILE SER GLY ASP GLU ASP GLY THR GLU SER GLU GLY ASP GLU SER ASP ASP GLU PRO HIS V94 V98 N102 ASP SER SER ALA A107 M111 E115 D126 R129 K130 SER SER SER SER LYS PRO LYS PRO

SER LYS LYS SER THR ASP ASP SER PHE P148 L161 Q162 R163 E167 S179 T189 G190 T191 T205 R209 I219 R257 E258 V259 LYS LYS LYS LYS THR VAL ARG LYS ARG ARG GLU R271 L275 P276 M281 V300 R301 GLY PRO GLN GLY ARG GLY LYS ARG

ARG ARG

- Molecule 50: 35s rna

Chain C1: 44% 20% • 33%

G1 G2 G3 G4 G5 G6 A7 C11 C12 G13 G14 G15 U16 C17 G18 C19 C20 G24 G25 C26 U32 C33 C34 G C36 A40 G41 U45 A53 A G55 U59 A60 G61 U62 C63 C64 C65 G66 G67 U68 A71 U72 A73 C74 G75 U76 C77 G78 G81

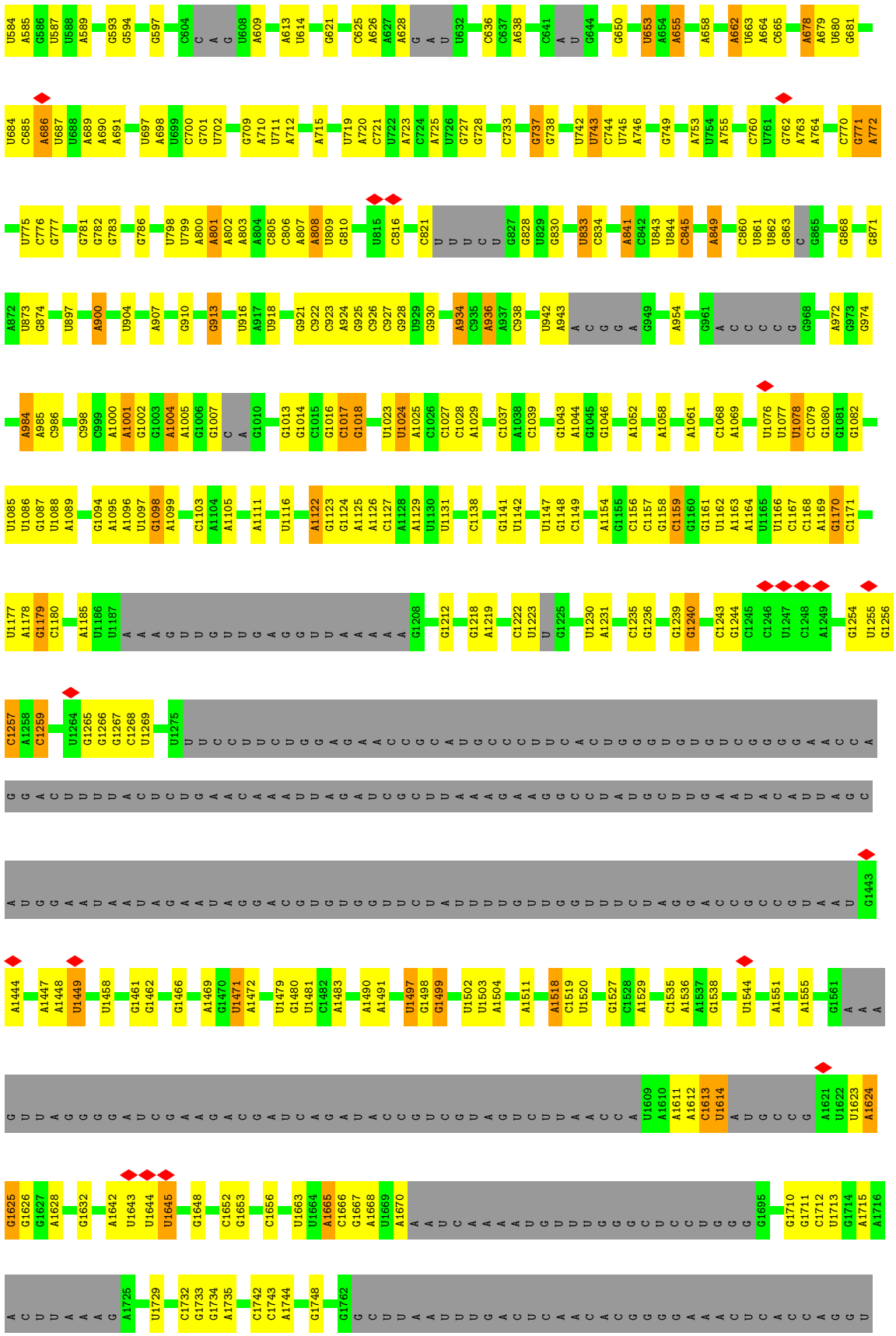
U85 C86 G89 A90 G93 C96 C97 U104 A105 G121 C126 C127 G128 G129 C130 G131 A132 G133 C134 A135 C136 A143 G149 C C150 G152 G155 C158 C159 G162 C163 G164 C165 A166 C167 C168 G169 C170 G171 G176 G177 C182 C183 U193 C203

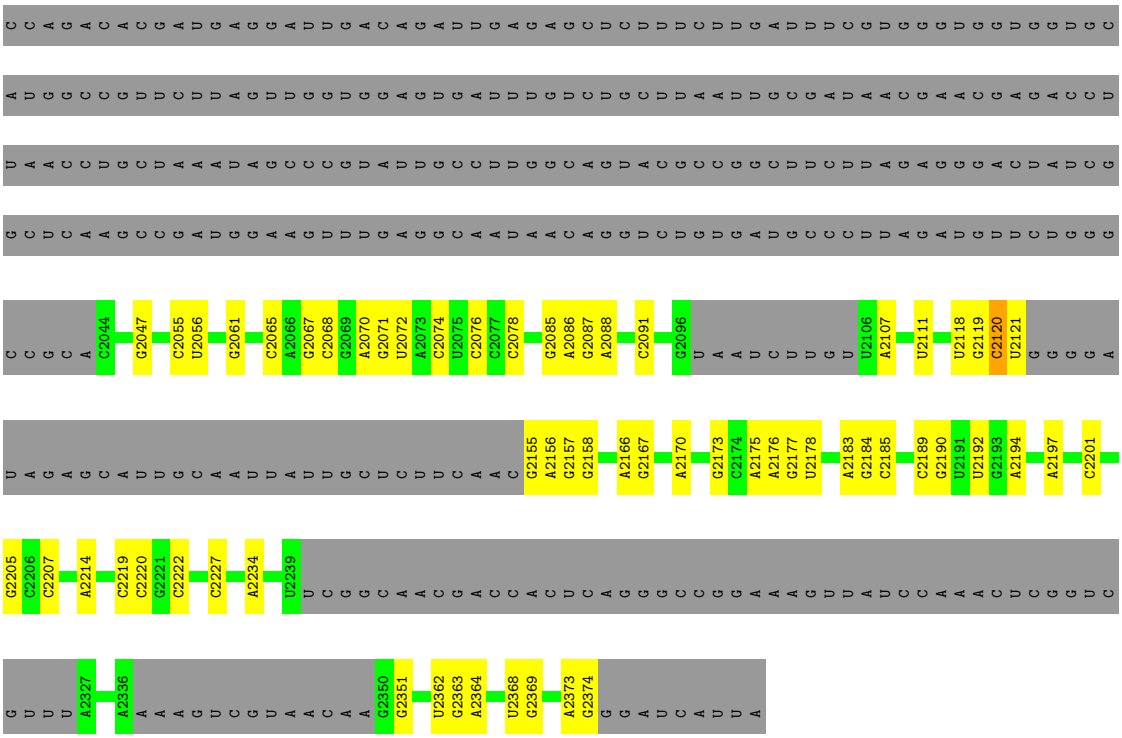
U204 C205 C206 U207 A208 A209 G210 G211 C212 G213 A221 U222 A223 C224 C225 G228 U G U231 G234 C235 C236 G237 U242 U243 G244 G251 G254 G255 U256 G257 C258 U259 G265 C266 U267 G268 G269 G273 C276 U277 A278 U281 C282 A283 A284 A285 C291 G292

G295 U307 U308 G309 G310 G311 G312 A313 A314 U319 A320 G321 C322 G323 G324 C325 U326 G327 A328 G329 C330 C331 U332 C333 U334 C346 C347 U348 C349 U350 U351 G352 G353 G354 G366 U372 C373 C378 U382 G383 C384 A385 G386 U394 U397 C398 G399 C400 C401 U402

G403 U416 A426 A435 A436 A439 G440 A441 U442 G443 C454 C459 G462 C463 G464 C465 A466 C467 C468 G469 G472 U483 G484 G491 C492 G495 C498 G499 C500 U501 A502 C507 U A G C G C C U G C G C A G C C A583

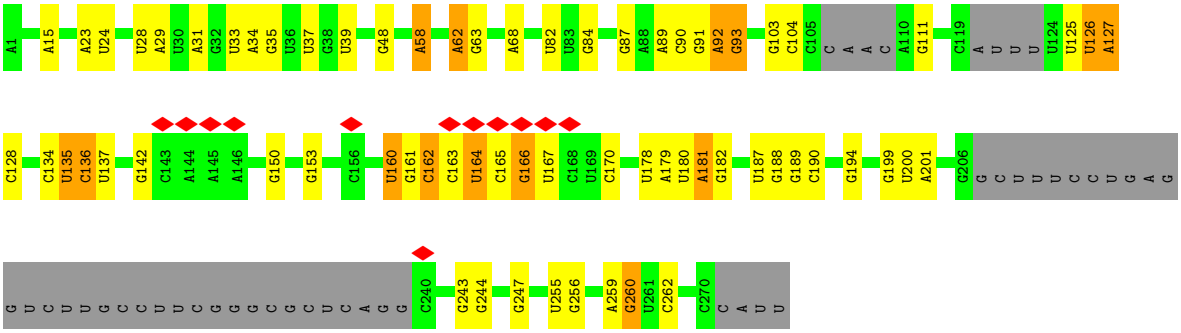
U G U A A C U A G A G U G A A C U C G G C C G C C U G A A A C A C G G G C C G G C A580


U584 A585 G586 U587 U588 A589 G593 G594 G597 C604 C A G U608 A609 A613 U614 G621 C625 A626 A627 A628 G A U U632 C636 C637 A638 C641 A U G644 G650 U653 A654 A655 A658 A662 U663 A664 C665 A678 A679 U680 G681
U684 C685 A686 U687 U688 A689 A690 A691 U697 A698 U699 C700 G701 U702 G709 A710 U711 A712 A715 U719 A720 C721 U722 A723 C724 A725 U726 G727 G728 C733 G737 G738 U742 U743 C744 U745 A746 G749 A753 U754 A755 C760 U761 G762 A763 A764 C770 G771 A772
U775 C776 G777 G781 G782 G783 G786 U798 U799 A800 A801 A802 A803 A804 C805 C806 A807 A808 U809 G810 U815 C816 C821 U U U C U G827 G828 U829 G830 U833 C834 A841 C842 U843 U844 C845 A849 C860 U861 U862 G863 C G865 G868 G871
A872 U873 G874 U897 A900 U904 A907 G910 G913 U916 A917 U918 G921 C922 C923 A924 G925 G926 C927 G928 U929 G930 A934 C935 A936 A937 C938 U942 A943 A C G G A G949 A954 G961 A C C C C G G968 A972 G973 G974
A984 A985 C986 C998 C999 A1000 A1001 G1002 G1003 A1004 A1005 G1006 G1007 C A G1010 G1013 G1014 C1015 G1016 C1017 G1018 U1023 U1024 A1025 C1026 C1027 C1028 A1029 C1037 A1038 C1039 G1043 A1044 G1045 G1046 A1052 A1058 A1061 C1068 A1069 U1076 U1077 U1078 C1079 G1080 G1081 G1082
U1085 U1086 G1087 U1088 A1089 G1094 A1095 A1096 U1097 G1098 A1099 C1103 A1104 A1105 A1111 U1116 A1122 G1123 G1124 A1125 A1126 C1127 A1128 A1129 U1130 U1131 C1138 G1141 U1142 U1147 G1148 C1149 A1154 G1155 C1156 C1157 G1158 C1159 G1160 G1161 U1162 A1163 A1164 U1165 U1166 C1167 C1168 A1169 G1170 C1171
U1177 A1178 G1179 C1180 A1185 U1186 U1187 A A A G U U U G U U U G A G G G U U U A A A A A G1208 G1212 G1218 A1219 C1222 U1223 U G1225 U1230 A1231 C1235 G1236 G1239 G1240 C1243 G1244 C1245 C1246 U1247 C1248 A1249 G1254 U1255 G1256
C1257 A1258 C1259 U1264 G1265 G1266 G1267 C1268 U1269 U1275 U U U C C C U U C U U G G G A G A A A C C C G C A U G G C C C U U G G G U G G U U G G U G A C A C C U U A A U G C C U U U G G C A C C U G G G U C C U U U G G A A A C C U A A G G U A A U U A A G G C
A U U G G A A U A A A G A A U A G G A C C C G A A A U G G A A G A A G G G C C A A U U U C C C U U U G G C C U U U C C U A A G G G U U G G U U G G A A A C C U G G C C C G U A A G1443
A1444 A1447 A1448 U1449 U1458 G1461 G1462 G1466 A1469 G1470 U1471 A1472 U1479 G1480 U1481 C1482 A1483 A1490 A1491 U1497 G1498 G1499 U1502 U1503 A1504 A1511 A1518 C1519 U1520 G1527 C1528 A1529 C1535 A1536 A1537 G1538 U1544 A1551 A1555 G1561 A A A
G U U A G G G G A U C G A A G A C C G A U C U U G G U U A A C C A U1609 A1610 A1611 A1612 C1613 U1614 A U G C C G A1621 U1622 U1623 A1624
G1625 G1626 G1627 A1628 G1632 A1642 U1643 U1644 U1645 G1648 C1652 G1653 C1656 U1663 U1664 A1665 C1666 G1667 A1668 U1669 A1670 A A U C A A A A U U U U G G G G C U C C U G G G G1695 G1710 G1711 C1712 U1713 G1714 A1715 A1716
A C U U A A A G A1725 U1729 C1732 G1733 G1734 A1735 C1742 C1743 A1744 G1748 G1762 G C U U A A A U U U U G A C U C A A C C A C C G G G C U C C A A A C U C A C C A G G U



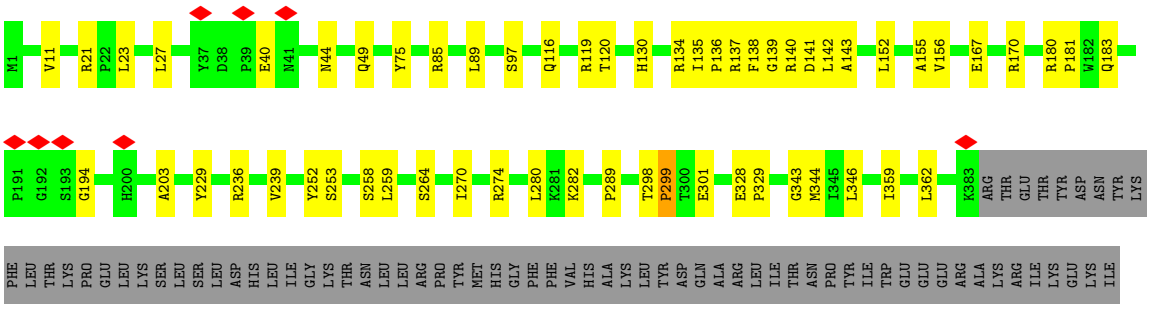
• Molecule 51: u3 rna

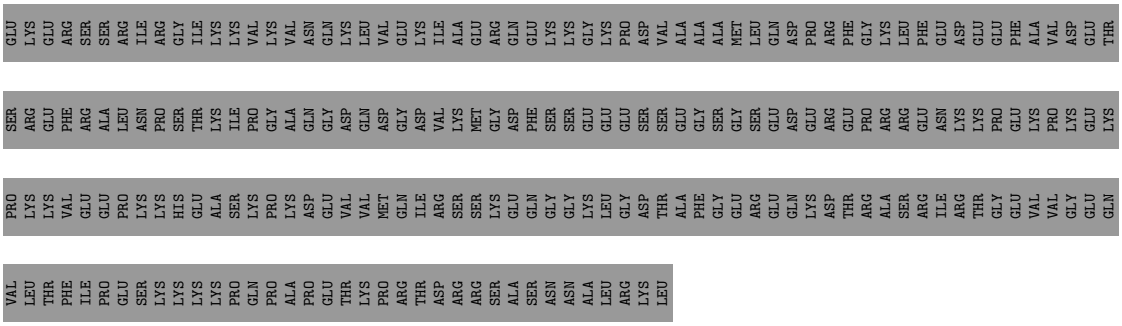
Chain C2:



• Molecule 52: Ribosome biogenesis protein ENP2

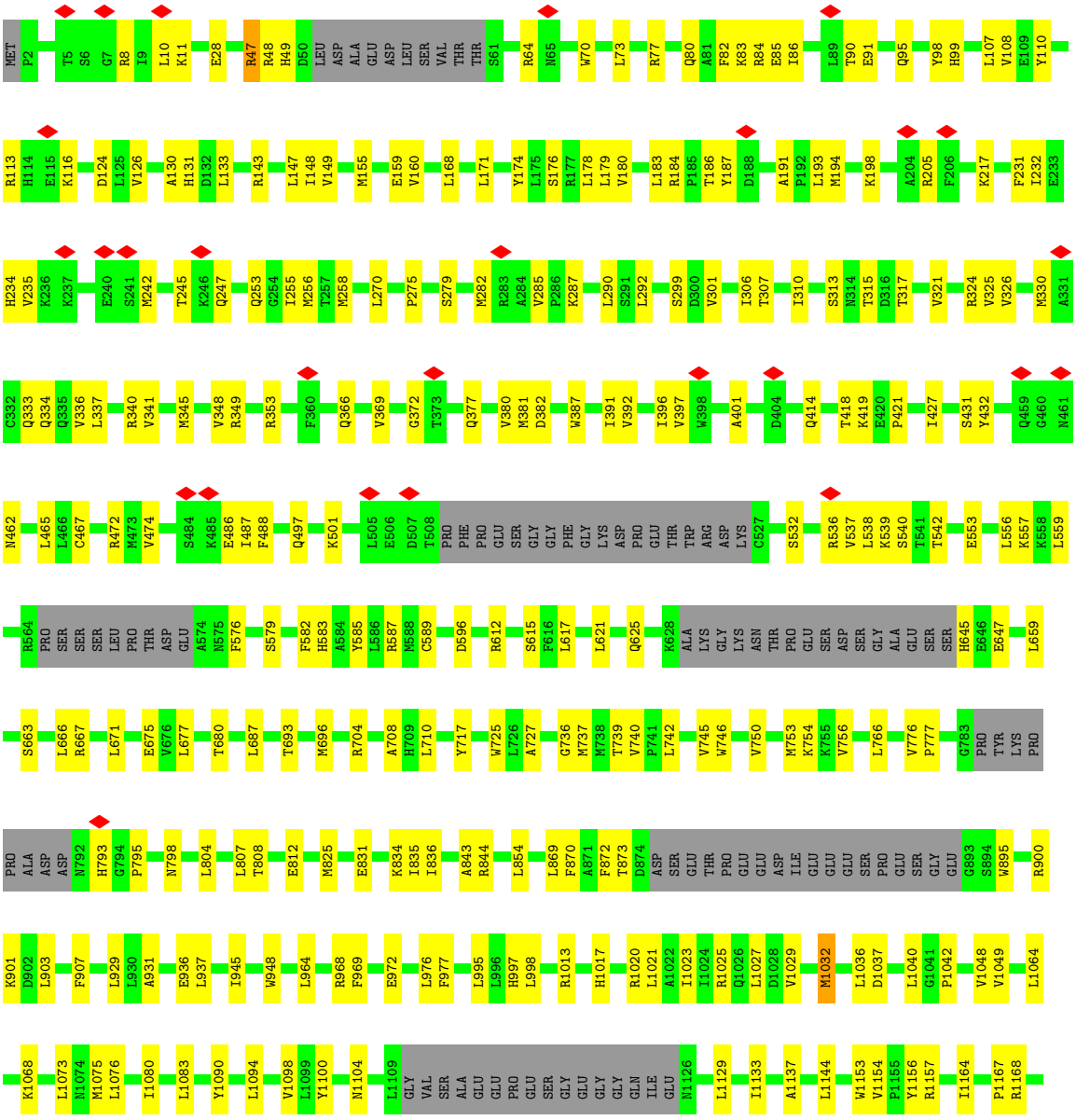
Chain CW:

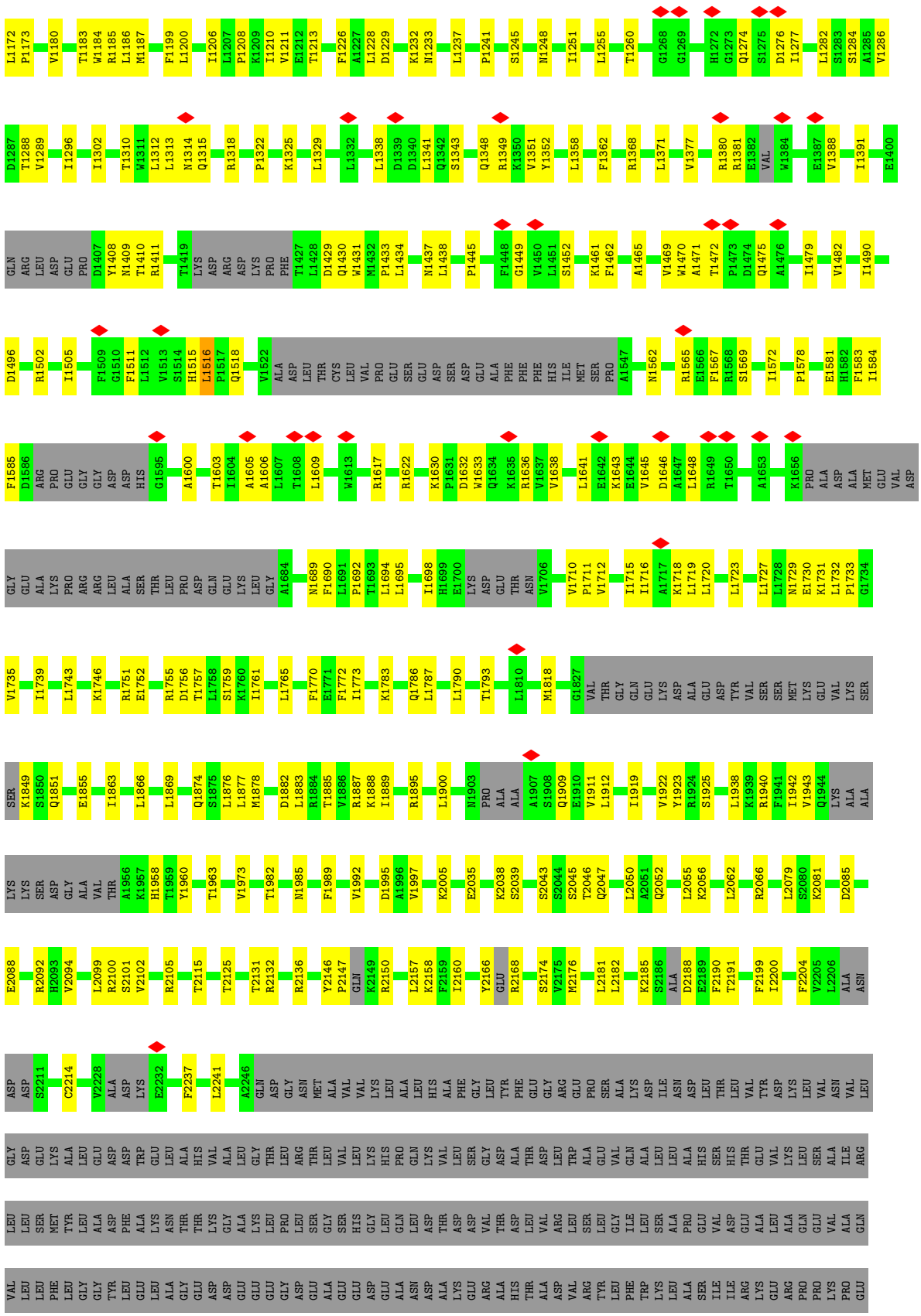


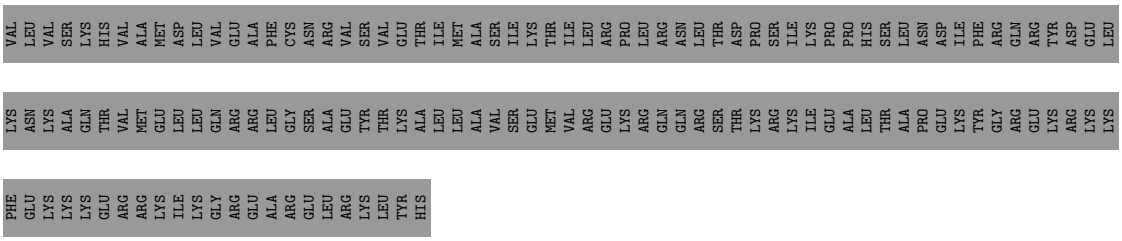


- Molecule 53: UTP20

Chain UT:

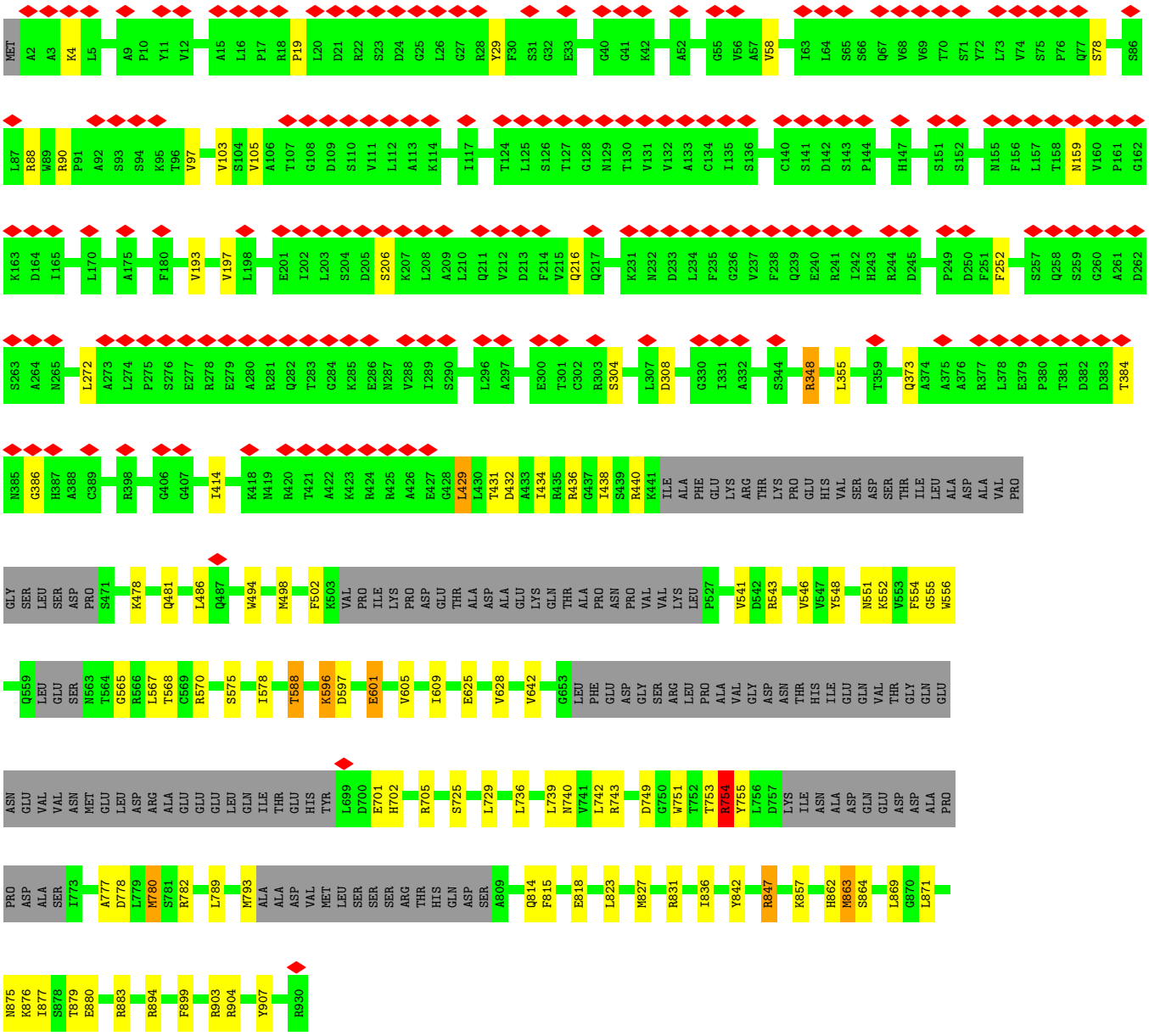



L1172 P1173 V1180 T1183 W1184 R1185 L1186 M1187 F1199 L1200 I1206 L1207 P1208 K1209 I1210 V1211 E1212 T1213 F1226 A1227 L1228 D1229 K1232 N1233 L1237 P1241 S1245 N1248 I1251 L1255 T1260 G1268 G1269 H1272 G1273 Q1274 S1275 D1276 I1277 L1282 S1283 S1284 A1285 V1286
D1287 T1288 V1289 I1296 I1302 T1310 W1311 L1312 L1313 N1314 Q1315 R1318 P1322 K1325 L1329 L1332 L1338 D1339 D1340 L1341 Q1342 S1343 Q1348 R1349 K1350 V1351 Y1352 L1358 F1362 R1368 L1371 V1377 R1380 R1381 E1382 VAL W1384 E1387 V1388 I1391 E1400
GLN ARG LEU ASP GLU PRO D1407 Y1408 N1409 T1410 R1411 T1419 LYS ASP ARG ASP LYS PRO PHE T1427 L1428 D1429 Q1430 W1431 M1432 P1433 L1434 N1437 L1438 P1445 F1448 G1449 V1450 L1451 S1452 K1461 F1462 A1465 V1469 W1470 A1471 T1472 P1473 D1474 Q1475 A1476 I1479 V1482 I1490
D1496 R1502 I1505 F1509 G1510 F1511 L1512 V1513 S1514 H1515 L1516 P1517 Q1518 V1522 ALA ASP LEU THR CYS LEU VAL PRO GLU SER GLU ASP SER ASP GLU ALA PHE PHE PHE HIS ILE MET SER PRO A1547 N1562 R1565 E1566 F1567 R1568 S1569 I1572 P1578 E1581 H1582 F1583 I1584
F1585 D1586 ARG PRO GLU GLY GLY GLY ASP ASP HIS G1595 A1600 T1603 I1604 A1605 A1606 L1607 T1608 L1609 W1613 R1617 R1622 K1630 P1631 D1632 W1633 Q1634 K1635 R1636 V1637 V1638 L1641 E1642 K1643 E1644 V1645 D1646 A1647 L1648 R1649 T1650 A1653 K1656 PRO ALA ASP ALA MET GLU VAL ASP
GLY GLU ALA LYS PRO ARG ARG LEU ALA SER THR LEU PRO ASP GLN GLU LYS LEU GLY A1684 N1689 F1690 L1691 P1692 T1693 L1694 L1695 I1698 H1699 E1700 LYS ASP GLU THR ASN V1706 V1710 P1711 V1712 I1715 I1716 A1717 K1718 L1719 L1720 L1723 L1727 L1728 N1729 E1730 K1731 L1732 P1733 G1734
V1735 I1739 L1743 K1746 R1751 E1752 R1755 D1756 T1757 L1758 S1759 K1760 I1761 L1765 F1770 E1771 F1772 I1773 K1783 Q1786 L1787 L1790 T1793 L1810 M1818 G1827 VAL THR GLY GLN GLU LYS ASP ALA GLU ASP TYR VAL SER SER MET LYS GLU VAL LYS SER
SER K1849 S1850 Q1851 E1855 I1863 L1866 L1869 Q1874 S1875 L1876 L1877 M1878 D1882 L1883 R1884 T1885 V1886 R1887 K1888 I1889 R1895 L1900 N1903 PRO ALA ALA A1907 S1908 Q1909 E1910 V1911 L1912 I1919 V1922 Y1923 R1924 S1925 L1938 K1939 R1940 F1941 I1942 V1943 Q1944 LYS ALA ALA
LYS LYS SER ASP GLY ALA VAL THR A1956 K1957 H1958 T1959 Y1960 T1963 V1973 T1982 N1985 F1989 V1992 D1995 A1996 V1997 K2005 E2035 K2038 S2039 S2043 S2044 S2045 T2046 Q2047 L2050 A2051 Q2052 L2055 K2056 L2062 R2066 L2079 S2080 K2081 D2085
E2088 R2092 H2093 V2094 L2099 R2100 S2101 V2102 R2105 T2115 T2125 T2131 R2132 R2136 Y2146 P2147 GLN K2149 R2150 L2157 K2158 F2159 I2160 Y2166 GLU R2168 S2174 V2175 M2176 L2181 L2182 K2185 S2186 ALA D2188 E2189 F2190 T2191 F2199 I2200 F2204 V2205 L2206 ALA ASN
ASP ASP S2211 C2214 V2228 ALA ASP LYS E2232 F2237 L2241 A2246 GLN ASP GLY ASN MET ALA VAL VAL LYS LEU ALA LEU HIS ALA PHE GLY LEU TYR PHE GLU GLY ARG GLU PRO ALA GLU VAL GLN ALA LYS ASP ILE ASN ASP LEU THR VAL TYR ASP LYS LEU LEU VAL ASN VAL LEU
GLY ASP GLU LYS ALA LEU GLU ASP ASP TRP GLU LEU ALA HIS VAL ALA LEU GLY THR LEU ARG THR LEU VAL LEU LYS HIS PRO GLN LYS VAL LEU SER GLY ASP ALA THR ASP LEU TRP ALA GLU VAL GLN ALA LEU LEU ALA HIS SER HIS THR GLU VAL LYS LEU SER ALA ILE ARG
LEU LEU SER MET TYR LEU ALA ASP PHE ALA LYS ASN THR THR LYS GLY ALA LYS LEU PRO LEU SER GLY SER HIS GLY LEU GLN LEU ASP THR ASP ASP VAL THR ASP LEU VAL ARG LEU SER LEU GLY ILE LEU SER ALA PRO GLU VAL ASP THR ASP GLU VAL ALA ALA GLN GLU VAL ALA
VAL LEU LEU PHE LEU GLY GLY TYR LEU GLU LEU ALA GLU ASP GLU ALA GLU GLU GLU GLY ASP GLU ALA GLU ASP GLU ALA ASN ASP ALA LYS GLU ARG ALA HIS THR ALA ASP VAL ARG TYR LEU PHE TRP LYS LEU ALA SER ILE ILE ARG LYS GLU ARG PRO PRO LYS PRO GLU



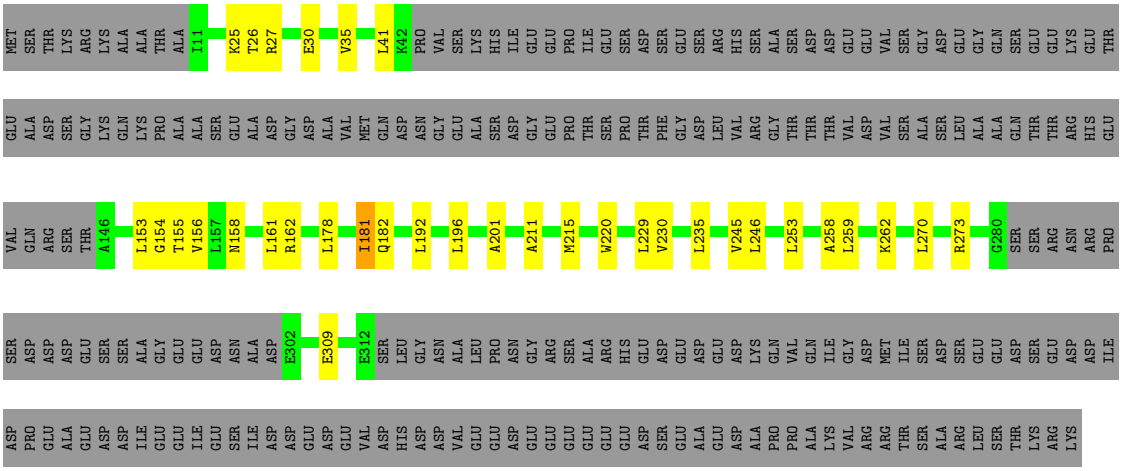
- Molecule 54: UTP8

Chain UH:



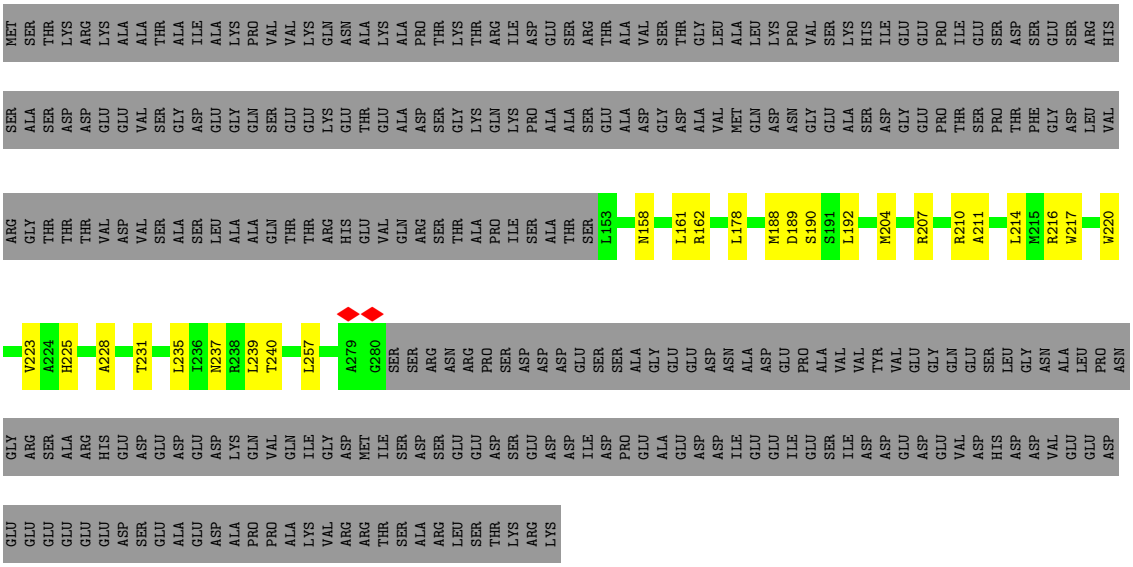
- Molecule 55: Small-subunit processome Utp12 domain-containing protein

Chain UE:



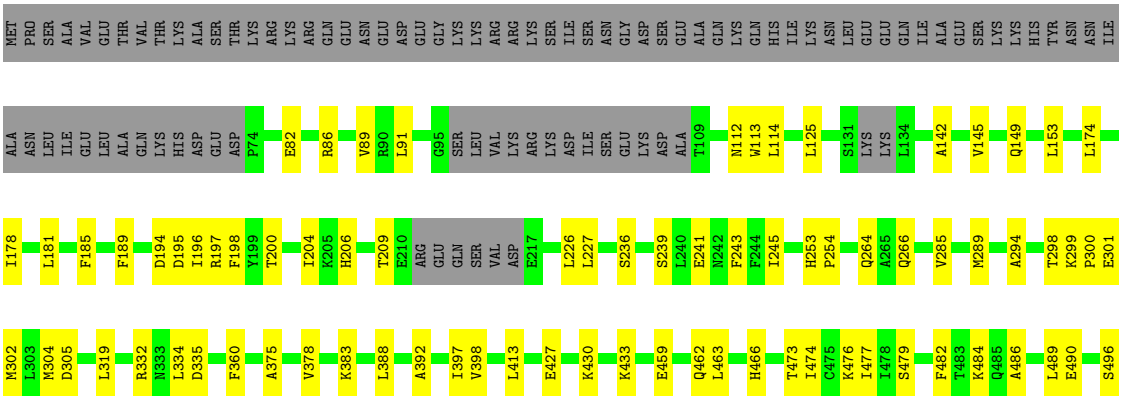
• Molecule 55: Small-subunit processome Utp12 domain-containing protein

Chain UI: 25% 6% 69%



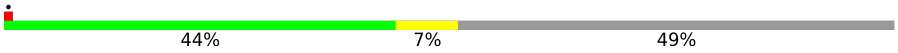
• Molecule 56: CCAAT-binding factor domain-containing protein

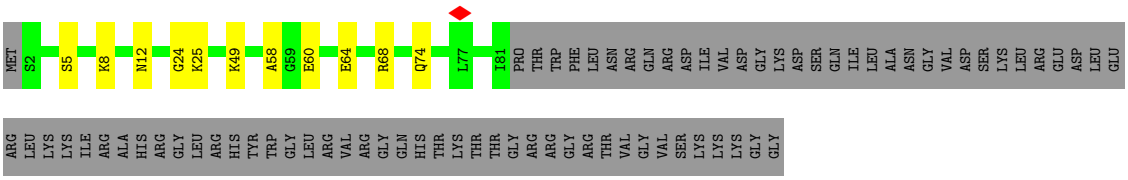
Chain US: 67% 15% 18%



• Molecule 57: Putative ribosomal protein

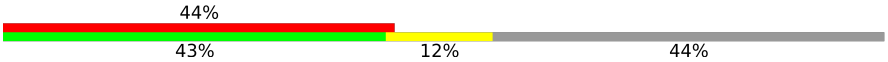
Chain Cl:

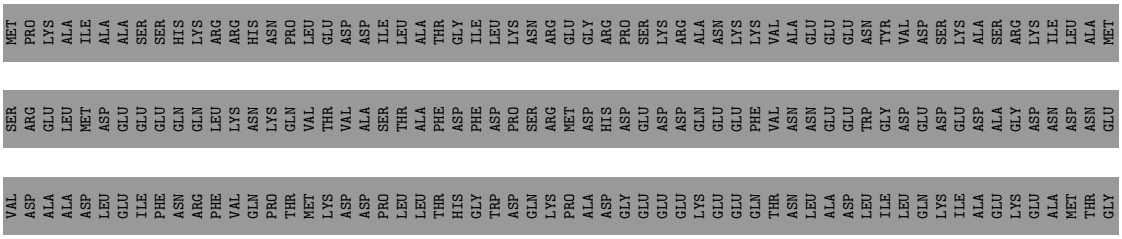


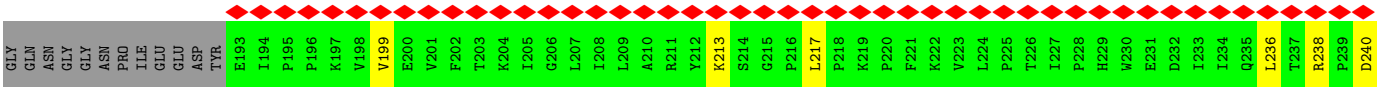


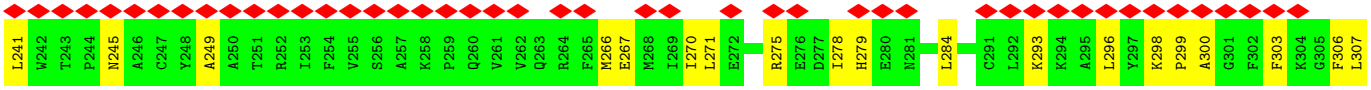
• Molecule 58: Bystin-like protein

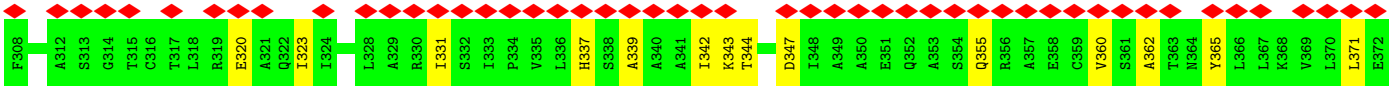
Chain CX:

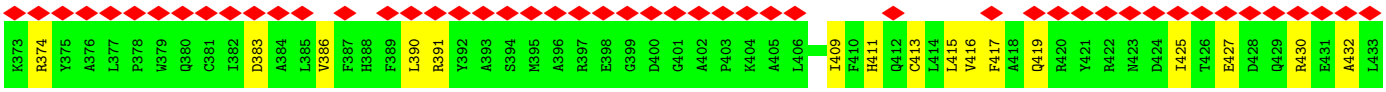


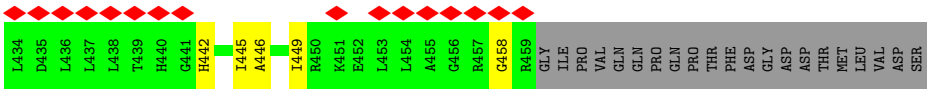






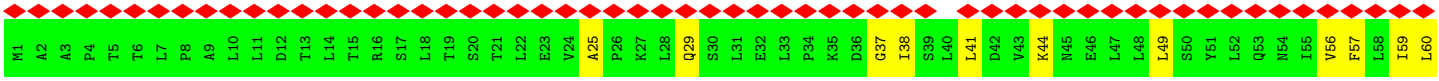






• Molecule 59: U3 small nucleolar ribonucleoprotein protein lcp5-like protein

Chain CY:



I61 K62 L63 R64 E65 A66 K67 Y68 S69 A70 R71 S72 E73 R74 K75 S76 D77 E78 Q79 S80 L81 S82 D83 L84 V85 V86 R87 K88 L89 V90 E91 L92 R93 L94 Y95 L96 E97 K98 G99 T100 R101 P102 L103 E104 D105 K106 L107 R108 F109 Q110 I111 D112 K113 V114 L115 R116 A117 A118 D119 D120

A121 E122 R123 K124 A125 K126 A127 A128 E129 E130 A131 E132 K133 A134 K135 C136 Q137 K138 S139 D140 D141 GLU SER SER SER GLU SER GLN SER ASP SER GLU GLU GLU GLU SER GLY ASP MET ASP SER LYS VAL ASN GLY LEU SER GLY ALA ARG THR GLU ASP LEU LEU HIS ARG PRO ASN LEU

SER ASN PHE GLN ARG PRO ALA ALA ALA THR LYS VAL THR LYS GLU LYS ASP ASN SER GLY VAL TYR ARG PRO PRO ARG ILE ALA PRO ILE ALA MET PRO THR ASN ASP ARG ARG ASP LYS ALA GLU ARG ARG PRO LEU LYS S228 L231 I235 A236 D237 G250 G257 Y275

T278 E286 R291 A292 K293 R294 M297 S301 G302 R303 L314 G315 E316 R320 R323 L324 T325 K326 A327 K328 S329 S330 GLY GLY GLY THR LYS ALA LEU LEU GLU LYS SER ARG LYS ARG THR ILE ASP THR VAL ASN GLY SER ARG GLY SER GLY VAL ALA MET G360

K365 K368 V369 R374 K379 GLY ARG

• Molecule 60: Protein BFR2

Chain CZ: 38% 36% 10% 54%

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

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

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

MET SER SER SER GLN SER ALA SER GLU ASP GLU LYS GLU ASN MET LEU GLU GLU ASP LEU GLU MET ASP SER GLN ASP PHE ASP MET ASP GLY SER GLU GLU GLY SER GLU LEU GLY GLU ASP GLY VAL ARG LEU PHE ASP ASP GLU ALA GLU GLU SER VAL GLU GLU GLY GLU SER

ALA GLU ASP ASP GLU GLU ARG PHE GLU ASP LYS ASP ASP GLU ASN GLU SER SER HIS GLU ASP ASP ASP GLU GLU GLU GLY GLU ASP VAL GLU ASN GLU Q272 S273 E274 K275 E276 D277 G278 D279 D280 E281 R282 A283 K284 L285 R286 R287 L288 A289 T290 E291 G292 E293 K294 A297 E298 A299 M300 S301

Q302 A303 A304 R305 A306 D307 A308 E309 K310 G311 L312 R315 K316 Q317 R318 R319 A320 F321 D322 S323 I324 L325 N326 L327 R328 I329 R330 L331 Q332 K333 A334 L335 I336 A337 A338 N339 S340 F341 H342 V343 V344 E345 K346 A347 E348 G349 Q350 D351 S352 T353 E354 A355 Y356 Q357 A358 A359 E360 E361 A362

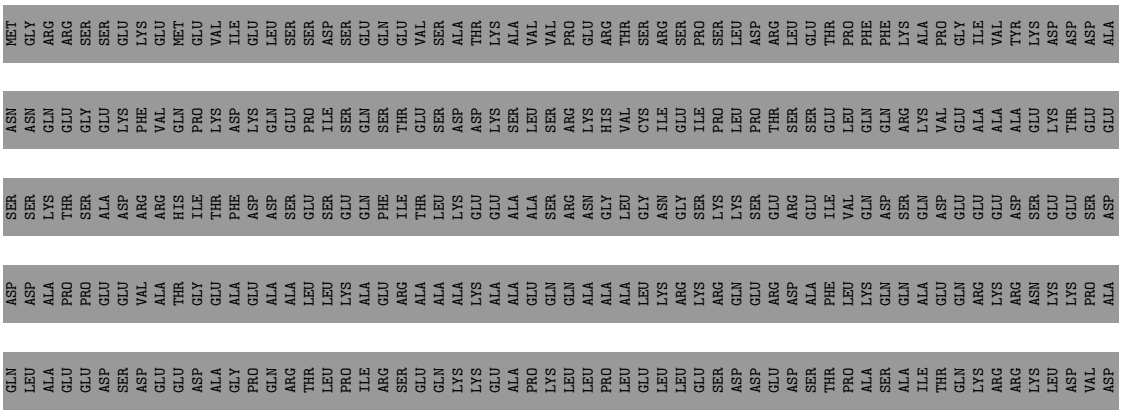
A363 I364 K365 L366 W367 N368 T369 I370 A371 S372 V373 R374 H375 H376 F377 M378 P379 E380 S381 C382 Q383 T384 K385 V386 G387 E388 K389 R390 K391 R392 E393 I394 E395 L396 D397 T398 A399 N400 Q401 E402 I403 W404 E405 T406 M407 E408 E409 V410 E411 E412 V413 V414 M415 S416 H417 R418 R419 K420 V421 L422

D423 K424 W425 S426 N427 K428 V429 K430 K431 S432 N433 A434 G435 L436 N437 T438 R439 K440 L441 V442 N443 S444 E445 G446 Q447 T448 L449 V450 A451 A452 L453 D454 E455 Q456 I457 M458 S459 S460 E461 R462 L463 I464 K465 K466 A467 R468 T469 P470 R471 S472 C473 A474 P475 V476 Q477 A478 A479 K480 K481 V482

E483 E484 D485 P486 A487 I488 Y489 D490 D491 A492 D493 F494 Y495 Q496 L497 L498 L499 K500 E501 L502 V503 E504 Q505 R506 S507 A508 D509 T510 GLY LEU ALA GLY GLU GLY VAL ALA THR VAL ARG TRP ALA ALA LEU LYS GLU THR LYS THR ARG LYS ASN VAL ASP R536 R537 A538 S539 K540 G541 R542

• Molecule 61: UTP16

Chain UP: 12% • 85%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70904	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.452	Depositor
Minimum map value	-0.240	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	501.59998, 501.59998, 501.59998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	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: MG, ADP, A2M, OMC, GTP, SEP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	UA	0.32	0/6555	0.60	3/8909 (0.0%)
2	UB	0.26	0/4592	0.60	1/6178 (0.0%)
3	UC	0.42	0/2001	0.70	0/2680
4	UD	0.30	0/6250	0.62	2/8465 (0.0%)
5	UF	0.27	0/2665	0.57	1/3606 (0.0%)
6	UG	0.29	0/3838	0.58	2/5181 (0.0%)
7	UJ	0.30	0/12938	0.68	6/17550 (0.0%)
8	UK	0.25	0/1709	0.47	0/2261
9	UL	0.28	0/6299	0.69	1/8531 (0.0%)
10	UM	0.23	0/6680	0.59	2/9090 (0.0%)
11	UN	0.28	0/1425	0.52	1/1913 (0.1%)
12	UO	0.29	0/3895	0.60	0/5302
13	UQ	0.33	0/6136	0.66	2/8348 (0.0%)
14	UR	0.29	0/3557	0.57	1/4805 (0.0%)
15	UU	0.29	0/6947	0.60	4/9452 (0.0%)
16	UX	0.29	0/1503	0.63	0/2022
17	UZ	0.22	0/1857	0.63	0/2526
18	CA	0.31	0/1814	0.57	1/2456 (0.0%)
18	CB	0.26	0/1853	0.62	0/2511
19	CC	0.24	0/2911	0.53	0/3937
20	CD	0.25	0/3412	0.60	2/4617 (0.0%)
21	CE	0.26	0/891	0.52	0/1214
21	CF	0.25	0/876	0.54	0/1195
22	CG	0.27	0/3307	0.65	0/4462
23	CH	0.29	0/2939	0.59	1/3988 (0.0%)
24	CI	0.28	0/6813	0.56	2/9182 (0.0%)
25	CJ	0.29	0/1462	0.49	0/1967
26	CK	0.28	0/2376	0.54	0/3214
27	CL	0.26	0/2504	0.53	1/3377 (0.0%)
28	CM	0.30	0/3573	0.59	0/4829
29	CN	0.34	0/1797	0.66	0/2443
29	CO	0.29	0/1714	0.66	0/2325

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	CP	0.25	0/1923	0.52	0/2577
31	CQ	0.22	0/1436	0.51	0/1932
32	CR	0.25	0/6809	0.66	3/9215 (0.0%)
32	CS	0.29	0/6722	0.70	6/9099 (0.1%)
33	CT	0.24	0/1053	0.49	0/1413
34	Ca	0.28	0/1850	0.68	6/2486 (0.2%)
35	Cb	0.30	0/1890	0.75	0/2548
36	Cc	0.26	0/1485	0.52	0/2008
37	Cd	0.29	0/1850	0.68	4/2474 (0.2%)
38	Ce	0.30	0/1298	0.74	2/1750 (0.1%)
39	Cf	0.25	0/1429	0.61	0/1915
40	Cg	0.28	0/1265	0.56	0/1694
41	Ch	0.23	0/557	0.62	0/749
42	Ci	0.24	0/819	0.52	0/1107
43	Cj	0.28	0/958	0.55	0/1293
44	Ck	0.21	0/1107	0.52	0/1486
45	Cm	0.27	0/1001	0.56	0/1345
46	Cn	0.30	0/712	0.61	0/954
47	Co	0.26	0/754	0.74	0/1011
48	Cp	0.28	0/461	0.52	0/620
49	CU	0.23	0/1350	0.49	0/1810
50	C1	0.24	0/37474	0.30	0/58363
51	C2	0.23	0/5434	0.29	0/8459
52	CW	0.25	0/3004	0.65	0/4085
53	UT	0.28	0/16312	0.71	6/22073 (0.0%)
54	UH	0.58	0/6301	0.99	5/8526 (0.1%)
55	UE	0.29	0/1374	0.69	2/1852 (0.1%)
55	UI	0.29	0/1005	0.75	0/1352
56	US	0.30	0/3765	0.68	2/5100 (0.0%)
57	Cl	0.20	0/638	0.67	2/857 (0.2%)
58	CX	0.23	0/2180	0.58	0/2956
59	CY	0.25	0/2111	0.60	1/2816 (0.0%)
60	CZ	0.26	0/2298	0.62	1/3080 (0.0%)
61	UP	0.26	0/428	0.56	0/570
All	All	0.29	0/236142	0.59	73/328111 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	UJ	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	UQ	0	1
15	UU	0	1
17	UZ	0	1
18	CB	0	1
20	CD	0	2
22	CG	0	2
28	CM	0	1
29	CO	0	1
32	CS	0	2
38	Ce	0	1
52	CW	0	1
53	UT	0	2
54	UH	0	2
All	All	0	20

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	UJ	1427	GLN	CA-C-N	9.54	139.76	121.54
7	UJ	1427	GLN	C-N-CA	9.54	139.76	121.54
53	UT	1032	MET	CA-CB-CG	8.23	130.57	114.10
32	CS	578	ARG	CA-C-N	8.18	131.78	120.65
32	CS	578	ARG	C-N-CA	8.18	131.78	120.65
24	CI	753	ASN	CA-C-N	7.61	136.07	121.54
24	CI	753	ASN	C-N-CA	7.61	136.07	121.54
23	CH	90	ASN	N-CA-C	-7.59	105.19	114.75
13	UQ	170	TRP	CA-C-N	7.05	135.00	121.54
13	UQ	170	TRP	C-N-CA	7.05	135.00	121.54
34	Ca	54	LEU	CA-C-N	6.99	134.89	121.54
34	Ca	54	LEU	C-N-CA	6.99	134.89	121.54
54	UH	348	ARG	NE-CZ-NH2	6.92	125.42	119.20
18	CA	214	MET	CB-CG-SD	-6.65	92.75	112.70
34	Ca	33	LYS	CA-C-N	6.49	139.40	120.97
34	Ca	33	LYS	C-N-CA	6.49	139.40	120.97
38	Ce	38	ALA	CA-C-N	6.40	133.22	121.70
38	Ce	38	ALA	C-N-CA	6.40	133.22	121.70
5	UF	399	ARG	CA-CB-CG	6.37	126.83	114.10
32	CS	738	LYS	CA-CB-CG	-6.33	101.44	114.10
53	UT	113	ARG	CB-CG-CD	6.30	125.79	111.30
32	CS	405	PRO	CA-N-CD	-6.20	103.32	112.00
2	UB	544	HIS	N-CA-C	5.99	118.09	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	Cl	74	GLN	CA-C-N	-5.93	115.69	123.34
57	Cl	74	GLN	C-N-CA	-5.93	115.69	123.34
9	UL	271	GLY	N-CA-C	5.88	118.80	110.74
11	UN	889	HIS	N-CA-C	5.87	120.88	113.25
53	UT	812	GLU	N-CA-CB	5.84	120.08	110.39
32	CR	794	PHE	N-CA-C	-5.76	106.09	113.01
4	UD	651	THR	CA-C-N	5.72	128.74	120.38
4	UD	651	THR	C-N-CA	5.72	128.74	120.38
15	UU	264	VAL	N-CA-C	-5.70	107.26	112.96
7	UJ	1618	VAL	N-CA-C	-5.68	107.20	112.83
32	CS	738	LYS	CG-CD-CE	-5.68	98.22	111.30
55	UE	181	ILE	CA-C-N	-5.67	111.69	120.31
55	UE	181	ILE	C-N-CA	-5.67	111.69	120.31
7	UJ	1430	PRO	CA-N-CD	-5.63	104.11	112.00
6	UG	277	GLN	CA-C-N	5.61	128.06	120.38
6	UG	277	GLN	C-N-CA	5.61	128.06	120.38
59	CY	291	ARG	N-CA-CB	5.59	118.94	110.28
32	CS	515	GLN	CA-CB-CG	5.54	125.17	114.10
34	Ca	43	VAL	CA-C-N	-5.52	113.38	120.72
34	Ca	43	VAL	C-N-CA	-5.52	113.38	120.72
7	UJ	974	LYS	CA-CB-CG	5.46	125.03	114.10
14	UR	324	ASP	CB-CA-C	5.43	120.23	111.05
60	CZ	411	GLU	N-CA-CB	5.40	118.65	110.28
53	UT	113	ARG	CA-CB-CG	5.39	124.89	114.10
1	UA	487	SER	CA-C-N	5.38	131.00	120.99
1	UA	487	SER	C-N-CA	5.38	131.00	120.99
1	UA	172	ASP	CA-CB-CG	5.37	117.97	112.60
15	UU	171	THR	CA-C-N	5.26	128.69	121.33
15	UU	171	THR	C-N-CA	5.26	128.69	121.33
32	CR	211	ILE	N-CA-C	5.26	120.28	109.34
54	UH	780	MET	CB-CG-SD	5.26	128.47	112.70
7	UJ	23	LYS	CB-CG-CD	5.23	123.33	111.30
15	UU	676	GLY	N-CA-C	-5.21	107.48	114.25
37	Cd	113	ILE	CA-C-N	-5.18	117.33	122.77
37	Cd	113	ILE	C-N-CA	-5.18	117.33	122.77
56	US	245	ILE	CA-C-N	5.17	131.42	121.54
56	US	245	ILE	C-N-CA	5.17	131.42	121.54
54	UH	863	MET	CA-CB-CG	5.14	124.38	114.10
53	UT	1241	PRO	CA-C-N	5.11	128.49	120.82
53	UT	1241	PRO	C-N-CA	5.11	128.49	120.82
27	CL	56	ALA	N-CA-C	5.10	121.08	109.81
54	UH	216	GLN	OE1-CD-NE2	-5.09	117.51	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	UM	382	ILE	CA-C-N	5.08	134.20	121.80
10	UM	382	ILE	C-N-CA	5.08	134.20	121.80
20	CD	231	PRO	CA-C-N	5.08	131.25	121.54
20	CD	231	PRO	C-N-CA	5.08	131.25	121.54
37	Cd	193	ARG	CG-CD-NE	-5.08	100.83	112.00
54	UH	373	GLN	OE1-CD-NE2	-5.07	117.53	122.60
32	CR	582	PRO	CA-N-CD	-5.05	104.93	112.00
37	Cd	196	LEU	CA-CB-CG	5.03	133.89	116.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	CB	232	GLN	Peptide
20	CD	157	SER	Peptide
20	CD	189	TRP	Peptide
22	CG	179	CYS	Peptide
22	CG	348	GLY	Peptide
28	CM	304	ASP	Peptide
29	CO	165	ASN	Peptide
32	CS	840	ARG	Sidechain
32	CS	854	VAL	Peptide
52	CW	299	PRO	Peptide
38	Ce	38	ALA	Peptide
54	UH	754	ARG	Peptide
54	UH	847	ARG	Sidechain
7	UJ	1427	GLN	Peptide
7	UJ	1768	SER	Peptide
13	UQ	849	ALA	Peptide
53	UT	1516	LEU	Peptide
53	UT	47	ARG	Peptide
15	UU	205	ASP	Peptide
17	UZ	273	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	UA	6411	0	6306	66	0
2	UB	4506	0	4633	65	0
3	UC	1970	0	2023	24	0
4	UD	6108	0	6108	128	0
5	UF	2599	0	2650	27	0
6	UG	3765	0	3800	35	0
7	UJ	12725	0	13039	251	0
8	UK	1695	0	1828	22	0
9	UL	6175	0	6188	95	0
10	UM	6545	0	6547	110	0
11	UN	1401	0	1455	22	0
12	UO	3811	0	3861	50	0
13	UQ	6008	0	6033	92	0
14	UR	3495	0	3506	43	0
15	UU	6778	0	6782	93	0
16	UX	1480	0	1554	22	0
17	UZ	1815	0	1896	21	0
18	CA	1778	0	1830	21	0
18	CB	1816	0	1847	35	0
19	CC	2866	0	2960	43	0
20	CD	3355	0	3483	46	0
21	CE	879	0	918	10	0
21	CF	864	0	900	9	0
22	CG	3245	0	3262	57	0
23	CH	2888	0	2979	49	0
24	CI	6666	0	6825	84	0
25	CJ	1434	0	1482	20	0
26	CK	2329	0	2373	22	0
27	CL	2466	0	2532	36	0
28	CM	3501	0	3498	45	0
29	CN	1762	0	1807	30	0
29	CO	1683	0	1726	35	0
30	CP	1893	0	1993	26	0
31	CQ	1413	0	1479	12	0
32	CR	6677	0	6809	128	0
32	CS	6591	0	6674	154	0
33	CT	1035	0	1063	12	0
34	Ca	1821	0	1936	28	0
35	Cb	1851	0	1905	42	0
36	Cc	1464	0	1504	15	0
37	Cd	1819	0	1920	45	0
38	Ce	1279	0	1322	22	0
39	Cf	1398	0	1401	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	Cg	1248	0	1365	23	0
41	Ch	546	0	580	11	0
42	Ci	808	0	831	11	0
43	Cj	943	0	1002	15	0
44	Ck	1082	0	1138	20	0
45	Cm	985	0	1021	15	0
46	Cn	702	0	750	7	0
47	Co	741	0	785	25	0
48	Cp	458	0	489	7	0
49	CU	1337	0	1376	15	0
50	C1	33584	0	17007	212	0
51	C2	4869	0	2465	22	0
52	CW	2932	0	2866	42	0
53	UT	15998	0	16397	338	0
54	UH	6198	0	6272	69	0
55	UE	1362	0	1440	28	0
55	UI	996	0	1054	19	0
56	US	3672	0	3679	58	0
57	Cl	633	0	676	9	0
58	CX	2130	0	2219	36	0
59	CY	2095	0	2185	44	0
60	CZ	2270	0	2273	50	0
61	UP	422	0	457	7	0
62	UX	1	0	0	0	0
63	CI	32	0	12	0	0
64	CI	1	0	0	0	0
65	CS	27	0	11	3	0
All	All	228132	0	212987	2905	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (2905) 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)
24:CI:286:VAL:O	24:CI:293:ASP:HA	1.31	1.30
4:UD:441:THR:HA	4:UD:456:LEU:O	1.43	1.17
54:UH:555:GLY:O	54:UH:567:LEU:HA	1.47	1.12
53:UT:1168:ARG:O	53:UT:1172:LEU:HB2	1.50	1.08
15:UU:159:ILE:O	15:UU:172:THR:HA	1.53	1.07
23:CH:269:GLN:N	23:CH:269:GLN:HE21	1.59	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Co:360:HIS:O	47:Co:398:GLY:HA2	1.66	0.95
56:US:285:VAL:O	56:US:289:MET:HB2	1.67	0.93
22:CG:221:LYS:N	51:C2:180:U:HO2'	1.66	0.92
3:UC:461:ILE:HD13	56:US:477:ILE:HG22	1.50	0.92
16:UX:94:CYS:SG	16:UX:125:HIS:CE1	2.67	0.88
7:UJ:727:LEU:O	7:UJ:731:ASN:HB2	1.74	0.87
36:Cc:86:MET:HE3	36:Cc:87:HIS:H	1.43	0.83
20:CD:122:ILE:O	20:CD:126:LEU:HB2	1.79	0.83
1:UA:195:ARG:HH12	50:C1:285:A:H5"	1.44	0.81
14:UR:264:GLN:OE1	14:UR:617:ARG:NH1	2.15	0.80
39:Cf:23:LYS:HG3	39:Cf:25:ARG:HH12	1.47	0.79
53:UT:901:LYS:HE2	53:UT:937:LEU:HB2	1.64	0.79
59:CY:115:LEU:HA	60:CZ:315:ARG:HH12	1.46	0.79
12:UO:317:ILE:HG22	12:UO:338:MET:HG2	1.64	0.78
8:UK:64:TYR:H	8:UK:67:MET:HE2	1.50	0.77
4:UD:3:ILE:HD11	4:UD:862:LEU:HB2	1.67	0.77
37:Cd:2:LYS:O	37:Cd:108:VAL:HA	1.85	0.75
4:UD:115:ASP:HB2	4:UD:122:LYS:HB2	1.68	0.75
22:CG:349:ALA:HB1	22:CG:397:SER:HB2	1.69	0.75
9:UL:678:ILE:HB	9:UL:692:ILE:HB	1.69	0.74
13:UQ:635:VAL:HG23	13:UQ:669:LEU:HD11	1.69	0.74
7:UJ:654:ALA:O	7:UJ:658:SER:HB2	1.87	0.74
24:CI:542:LEU:O	24:CI:546:MET:HB2	1.87	0.74
2:UB:743:LEU:HG	56:US:462:GLN:HE21	1.52	0.73
59:CY:106:LYS:HB2	60:CZ:433:ASN:HB2	1.68	0.73
18:CA:180:VAL:HB	18:CA:203:VAL:HG12	1.70	0.73
53:UT:1638:VAL:HG21	53:UT:1711:PRO:HB2	1.70	0.73
4:UD:128:GLN:NE2	18:CB:274:SER:OG	2.20	0.73
13:UQ:225:MET:HA	13:UQ:228:THR:HG22	1.71	0.73
32:CS:776:GLY:HA3	32:CS:816:ASP:HB2	1.71	0.72
53:UT:1013:ARG:O	53:UT:1017:HIS:HB3	1.89	0.72
13:UQ:813:ILE:HD11	13:UQ:855:ILE:HD12	1.72	0.72
23:CH:269:GLN:N	23:CH:269:GLN:NE2	2.36	0.72
53:UT:621:LEU:HG	53:UT:625:GLN:HE22	1.55	0.72
60:CZ:566:GLU:HA	60:CZ:569:ILE:HG12	1.72	0.72
53:UT:307:THR:HG22	53:UT:348:VAL:HG11	1.72	0.71
59:CY:286:GLU:O	59:CY:291:ARG:NH1	2.23	0.71
32:CR:868:GLY:HA2	32:CR:871:ARG:HB2	1.73	0.71
47:Co:382:GLN:HG3	47:Co:384:ASP:H	1.54	0.71
24:CI:754:LYS:HA	24:CI:757:TYR:HB2	1.71	0.71
59:CY:106:LYS:HG3	60:CZ:429:VAL:HG12	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:120:ARG:HD2	61:UP:330:ARG:HG3	1.73	0.71
7:UJ:675:VAL:HG23	7:UJ:729:SER:HA	1.73	0.71
47:Co:346:ASN:HB2	47:Co:353:GLN:HE22	1.55	0.71
54:UH:555:GLY:O	54:UH:567:LEU:CA	2.34	0.71
52:CW:116:GLN:HB2	52:CW:120:THR:HB	1.72	0.71
15:UU:677:ASN:HB3	15:UU:679:LEU:HD13	1.73	0.70
3:UC:461:ILE:HD13	56:US:477:ILE:CG2	2.22	0.70
50:C1:60:A:H62	54:UH:876:LYS:HA	1.56	0.70
2:UB:745:ALA:H	56:US:462:GLN:HE22	1.36	0.70
29:CO:121:LEU:HD11	29:CO:167:ILE:HD13	1.72	0.70
4:UD:420:LEU:HD21	4:UD:467:LEU:HG	1.73	0.70
7:UJ:1033:MET:HA	7:UJ:1037:VAL:HG23	1.73	0.70
50:C1:68:U:H3	54:UH:883:ARG:HH21	1.38	0.70
1:UA:316:ALA:O	1:UA:320:GLY:O	2.10	0.69
53:UT:753:MET:HE3	53:UT:766:LEU:HD22	1.74	0.69
5:UF:394:LEU:HB3	5:UF:398:ILE:HD11	1.73	0.69
35:Cb:72:VAL:HG12	35:Cb:90:ILE:HG12	1.74	0.69
53:UT:108:VAL:HG23	53:UT:147:LEU:HD22	1.74	0.69
7:UJ:1783:ARG:NH1	53:UT:49:HIS:O	2.26	0.69
22:CG:106:ARG:NH2	59:CY:325:THR:O	2.26	0.69
27:CL:52:LEU:O	27:CL:55:THR:C	2.36	0.69
13:UQ:442:LEU:HB3	13:UQ:805:ARG:HD2	1.75	0.69
29:CO:246:GLU:HG2	29:CO:251:ILE:HB	1.73	0.69
32:CR:310:ILE:HG22	32:CR:385:LEU:HB3	1.75	0.69
7:UJ:1600:LEU:HD21	7:UJ:1650:VAL:HB	1.75	0.69
52:CW:130:HIS:O	60:CZ:551:LYS:NZ	2.26	0.69
52:CW:270:ILE:HB	52:CW:280:LEU:HB2	1.75	0.69
53:UT:1490:ILE:HA	53:UT:1505:ILE:HD11	1.74	0.69
39:Cf:98:LYS:HD2	39:Cf:176:ARG:HG2	1.75	0.68
10:UM:389:MET:O	10:UM:400:ILE:HA	1.93	0.68
22:CG:107:TYR:HA	22:CG:110:LYS:HD2	1.74	0.68
35:Cb:183:ILE:O	35:Cb:190:GLY:N	2.26	0.68
7:UJ:971:PRO:HA	7:UJ:974:LYS:HG2	1.75	0.68
32:CR:311:PHE:HB2	32:CR:386:VAL:HG12	1.75	0.68
34:Ca:214:LYS:NZ	50:C1:1471:U:OP1	2.27	0.68
54:UH:554:PHE:O	54:UH:570:ARG:NH1	2.26	0.68
4:UD:368:LEU:HD11	4:UD:865:ARG:HB3	1.76	0.68
58:CX:267:GLU:HA	58:CX:271:LEU:HD23	1.76	0.68
4:UD:167:SER:OG	4:UD:169:GLU:OE1	2.10	0.68
4:UD:237:ILE:HD11	61:UP:346:LEU:HD22	1.75	0.68
47:Co:346:ASN:HB3	47:Co:351:ARG:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:UE:161:LEU:HD21	55:UE:196:LEU:HB2	1.74	0.68
15:UU:722:ILE:HG12	15:UU:736:LEU:HD11	1.76	0.68
7:UJ:1079:LEU:HD13	7:UJ:1114:ILE:HG13	1.77	0.67
29:CO:196:LEU:HD21	29:CO:202:ILE:HB	1.75	0.67
32:CS:134:ASN:OD1	32:CS:554:ASN:ND2	2.27	0.67
5:UF:310:LEU:O	5:UF:313:HIS:ND1	2.20	0.67
7:UJ:833:PHE:O	7:UJ:837:GLN:NE2	2.28	0.67
7:UJ:1187:THR:HA	7:UJ:1244:LEU:HD21	1.76	0.67
12:UO:339:GLN:NE2	57:Cl:5:SER:OG	2.28	0.67
12:UO:415:ARG:NH1	50:C1:131:G:N7	2.43	0.67
53:UT:675:GLU:HA	53:UT:687:LEU:HD11	1.76	0.67
2:UB:700:ARG:NH2	2:UB:706:ASP:OD2	2.28	0.67
2:UB:27:GLN:O	2:UB:31:ASN:ND2	2.28	0.67
2:UB:550:GLU:OE2	56:US:524:PHE:N	2.28	0.67
23:CH:219:ARG:HD2	49:CU:111:MET:HE3	1.77	0.67
54:UH:58:VAL:HG21	54:UH:103:VAL:HG11	1.76	0.67
32:CS:879:LEU:HD11	52:CW:299:PRO:HG2	1.76	0.67
39:Cf:99:SER:N	39:Cf:173:ILE:O	2.27	0.67
53:UT:1646:ASP:OD1	53:UT:1718:LYS:NZ	2.26	0.67
2:UB:629:ALA:HB1	2:UB:709:ARG:HH11	1.61	0.66
23:CH:218:ILE:O	23:CH:250:VAL:HA	1.94	0.66
32:CS:641:ASN:HB3	32:CS:644:TYR:HB2	1.77	0.66
60:CZ:280:ASP:OD2	60:CZ:284:LYS:NZ	2.28	0.66
18:CB:78:HIS:HD2	18:CB:148:ILE:HG12	1.60	0.66
4:UD:865:ARG:NH2	4:UD:871:ASP:OD2	2.28	0.66
53:UT:1605:ALA:HB2	53:UT:1643:LYS:HB3	1.78	0.66
3:UC:648:LEU:HA	16:UX:140:LYS:HD3	1.77	0.66
7:UJ:542:ARG:NH2	7:UJ:551:TYR:OH	2.28	0.66
53:UT:1434:LEU:O	53:UT:1438:LEU:HB2	1.95	0.66
29:CO:193:VAL:HA	29:CO:196:LEU:HD13	1.76	0.66
53:UT:2046:THR:HB	53:UT:2081:LYS:HE3	1.78	0.66
7:UJ:701:SER:HB2	7:UJ:704:LEU:HD12	1.75	0.66
14:UR:253:ARG:NH1	14:UR:599:SER:O	2.29	0.66
29:CN:77:MET:HA	29:CN:80:MET:HB2	1.76	0.66
7:UJ:1411:ASP:O	7:UJ:1415:HIS:ND1	2.28	0.66
38:Ce:51:SER:HB3	38:Ce:67:PHE:HB2	1.77	0.66
18:CB:156:VAL:HG12	18:CB:225:VAL:HB	1.78	0.66
7:UJ:866:LEU:HD22	7:UJ:933:LEU:HD11	1.77	0.65
22:CG:575:GLY:N	22:CG:606:VAL:O	2.29	0.65
7:UJ:645:SER:O	7:UJ:647:LEU:N	2.30	0.65
7:UJ:1500:LEU:HA	7:UJ:1503:LEU:HD12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Cd:71:ASN:HD21	52:CW:85:ARG:HH12	1.43	0.65
14:UR:345:ARG:HH21	50:C1:76:U:H4'	1.62	0.65
4:UD:341:VAL:HG22	4:UD:351:VAL:HG12	1.77	0.65
4:UD:559:ARG:NH2	4:UD:575:LEU:O	2.29	0.65
24:CI:1085:ARG:HE	24:CI:1089:LYS:HD3	1.62	0.65
53:UT:91:GLU:HB2	53:UT:95:GLN:HE21	1.61	0.65
10:UM:372:THR:HG22	10:UM:374:ASP:H	1.62	0.65
50:C1:1122:A:H5'	50:C1:1127:C:H41	1.62	0.65
4:UD:128:GLN:HE21	18:CB:274:SER:HG	1.45	0.65
7:UJ:1034:GLY:HA2	7:UJ:1038:LEU:HD12	1.79	0.65
32:CR:742:PHE:HB3	32:CR:762:MET:HG2	1.78	0.65
1:UA:524:GLN:HE21	1:UA:536:PHE:HB3	1.62	0.65
9:UL:240:GLU:OE2	9:UL:272:THR:OG1	2.13	0.65
17:UZ:85:LEU:HD12	17:UZ:258:ASN:HD22	1.61	0.65
32:CR:240:LYS:HA	32:CR:253:ILE:HD12	1.78	0.65
32:CS:137:ALA:HA	32:CS:490:LEU:HD21	1.79	0.65
9:UL:509:HIS:HB3	9:UL:528:ALA:HB3	1.79	0.64
10:UM:288:TRP:HA	10:UM:301:TRP:O	1.96	0.64
29:CN:112:ILE:HG23	29:CN:124:VAL:HB	1.79	0.64
55:UE:178:LEU:HA	55:UE:181:ILE:HG12	1.80	0.64
53:UT:1877:LEU:HD12	53:UT:1958:HIS:HB2	1.78	0.64
10:UM:651:LEU:HB3	10:UM:706:ASN:HD21	1.63	0.64
13:UQ:641:LYS:NZ	13:UQ:662:SER:OG	2.31	0.64
19:CC:7:LEU:HD11	19:CC:130:LEU:HD23	1.79	0.64
53:UT:275:PRO:HD3	53:UT:321:VAL:HG22	1.79	0.64
7:UJ:826:TYR:HA	7:UJ:865:ILE:HD11	1.80	0.64
7:UJ:1023:LEU:HD11	7:UJ:1060:LEU:HD22	1.79	0.64
29:CN:121:LEU:HB3	29:CN:163:ILE:O	1.97	0.64
34:Ca:87:ARG:NH1	34:Ca:89:ASP:OD1	2.30	0.64
35:Cb:140:VAL:HG12	35:Cb:146:THR:HG22	1.80	0.64
53:UT:313:SER:O	53:UT:353:ARG:NH1	2.31	0.64
53:UT:1343:SER:O	53:UT:1348:GLN:NE2	2.31	0.64
15:UU:71:LEU:H	15:UU:86:THR:HB	1.62	0.64
9:UL:24:LEU:HD22	9:UL:41:VAL:HG22	1.80	0.64
59:CY:37:GLY:HA2	60:CZ:310:LYS:HZ3	1.61	0.64
8:UK:268:ARG:NH2	14:UR:539:LEU:O	2.31	0.64
9:UL:303:GLU:HG2	9:UL:362:ILE:HG22	1.79	0.64
20:CD:304:HIS:ND1	51:C2:93:G:OP2	2.31	0.64
32:CR:283:LEU:HD11	32:CR:474:LEU:HG	1.80	0.64
53:UT:427:ILE:O	53:UT:431:SER:HB2	1.96	0.64
1:UA:561:THR:OG1	25:CJ:144:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:CK:89:LEU:HD11	26:CK:117:LEU:HB2	1.80	0.64
10:UM:332:SER:HB2	10:UM:348:VAL:HB	1.78	0.64
32:CR:287:ARG:NH2	32:CR:418:GLU:OE1	2.30	0.64
2:UB:760:LEU:HA	2:UB:765:ASN:HD22	1.63	0.63
12:UO:325:ALA:HB2	12:UO:332:ARG:HB2	1.80	0.63
14:UR:302:LYS:NZ	14:UR:304:ASP:OD2	2.31	0.63
30:CP:58:VAL:HG22	30:CP:112:LEU:HD21	1.80	0.63
53:UT:1173:PRO:HA	53:UT:1213:THR:HG22	1.79	0.63
4:UD:483:ARG:NH1	4:UD:550:SER:O	2.31	0.63
53:UT:1251:ILE:HA	53:UT:1255:LEU:HD13	1.79	0.63
24:CI:69:ARG:NH1	24:CI:230:LYS:O	2.26	0.63
53:UT:1716:ILE:HG21	53:UT:1735:VAL:HG11	1.81	0.63
7:UJ:1432:MET:HG3	27:CL:139:GLN:HB2	1.80	0.63
9:UL:221:TRP:HE1	9:UL:237:ASN:HB3	1.62	0.63
32:CR:172:ARG:HB3	32:CR:174:ARG:HE	1.63	0.63
4:UD:425:ILE:HD11	4:UD:452:LYS:HD2	1.80	0.63
15:UU:159:ILE:O	15:UU:172:THR:CA	2.39	0.63
29:CO:227:ILE:HD12	29:CO:240:LYS:HD2	1.80	0.63
7:UJ:1503:LEU:HD13	7:UJ:1526:PHE:HE1	1.64	0.63
8:UK:258:LYS:NZ	50:C1:213:G:OP2	2.32	0.63
29:CN:99:LEU:HD21	29:CN:238:CYS:HB3	1.80	0.63
58:CX:266:MET:HE1	58:CX:306:PHE:HB2	1.80	0.63
6:UG:579:ASP:O	6:UG:582:ARG:N	2.31	0.63
15:UU:863:ARG:NH2	27:CL:664:ALA:O	2.32	0.63
32:CR:812:GLY:HA2	32:CR:815:LEU:HD12	1.79	0.63
37:Cd:214:ILE:HG13	37:Cd:217:LYS:HE3	1.81	0.63
52:CW:141:ASP:OD1	52:CW:142:LEU:N	2.32	0.63
1:UA:408:ALA:HB3	1:UA:418:ARG:HB2	1.79	0.63
3:UC:305:MET:N	3:UC:305:MET:SD	2.71	0.63
7:UJ:1053:ILE:HG23	7:UJ:1057:ILE:HD12	1.80	0.63
31:CQ:189:ARG:NH1	31:CQ:235:LEU:O	2.32	0.63
32:CS:24:ARG:NH1	32:CS:140:ILE:O	2.32	0.63
53:UT:1229:ASP:O	53:UT:1233:ASN:ND2	2.31	0.63
15:UU:298:MET:HE3	15:UU:313:LEU:HD21	1.80	0.63
32:CS:278:ARG:HG2	32:CS:467:ARG:HA	1.81	0.63
7:UJ:1038:LEU:HD21	7:UJ:1089:ILE:HD13	1.82	0.62
10:UM:335:LEU:HD11	10:UM:343:LEU:HB3	1.80	0.62
16:UX:94:CYS:SG	16:UX:125:HIS:HE1	2.14	0.62
32:CS:742:PHE:HB3	32:CS:762:MET:HB3	1.80	0.62
6:UG:337:ASN:HB3	6:UG:380:LYS:HD2	1.81	0.62
15:UU:50:PRO:HB2	15:UU:342:LYS:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:UU:312:ASP:O	15:UU:317:GLY:HA2	2.00	0.62
27:CL:697:THR:HG22	27:CL:699:ALA:H	1.63	0.62
53:UT:2055:LEU:HD22	53:UT:2094:VAL:HG12	1.81	0.62
7:UJ:297:VAL:HG11	7:UJ:328:VAL:HG23	1.82	0.62
9:UL:451:ILE:HB	9:UL:461:ARG:HB2	1.82	0.62
9:UL:896:ARG:NH1	9:UL:900:GLU:OE1	2.31	0.62
16:UX:100:GLU:OE2	28:CM:351:ARG:NH2	2.32	0.62
32:CR:114:LYS:NZ	50:C1:1001:A:OP1	2.29	0.62
4:UD:374:VAL:HG11	4:UD:863:ILE:HD11	1.81	0.62
32:CS:700:ARG:HH11	32:CS:704:GLU:HB3	1.65	0.62
12:UO:227:MET:HE1	12:UO:260:LEU:HB3	1.79	0.62
23:CH:172:GLU:OE2	23:CH:174:ARG:NH2	2.33	0.62
37:Cd:85:ARG:NH2	50:C1:743:U:O2'	2.29	0.62
53:UT:1866:LEU:HD11	53:UT:1900:LEU:HD11	1.80	0.62
3:UC:291:LYS:HB3	27:CL:66:PRO:HD2	1.82	0.62
20:CD:70:THR:HG23	20:CD:73:LEU:H	1.64	0.62
30:CP:135:ARG:NH1	50:C1:1611:A:OP1	2.33	0.62
6:UG:403:PHE:O	28:CM:8:ARG:NH2	2.33	0.62
11:UN:276:MET:HG2	53:UT:2200:ILE:HD13	1.82	0.62
4:UD:366:PRO:HB3	4:UD:704:VAL:HG21	1.81	0.62
7:UJ:756:SER:HA	7:UJ:802:ARG:HH21	1.65	0.62
9:UL:890:VAL:HA	10:UM:891:MET:HG2	1.81	0.62
2:UB:8:ARG:NH2	26:CK:180:ILE:O	2.32	0.62
4:UD:617:ASN:HB3	4:UD:620:ALA:HB2	1.80	0.62
7:UJ:1534:ARG:HA	7:UJ:1538:ALA:HB3	1.82	0.62
9:UL:94:LEU:HB2	9:UL:104:VAL:HG22	1.81	0.62
32:CR:792:TYR:O	32:CR:795:ARG:HB2	1.99	0.62
56:US:266:GLN:NE2	56:US:302:MET:SD	2.73	0.62
32:CR:210:PRO:O	32:CR:212:SER:N	2.33	0.61
50:C1:926:C:H5"	52:CW:194:GLY:HA3	1.82	0.61
4:UD:481:ALA:HA	4:UD:497:GLU:HA	1.83	0.61
15:UU:55:PRO:HG2	20:CD:439:LYS:HE3	1.81	0.61
32:CS:237:LYS:HA	32:CS:240:LYS:HZ3	1.64	0.61
32:CS:402:LEU:O	32:CS:406:TYR:OH	2.18	0.61
54:UH:642:VAL:HG13	54:UH:729:LEU:HD23	1.82	0.61
7:UJ:1362:GLN:O	7:UJ:1368:ARG:NH1	2.32	0.61
21:CF:21:LEU:HD23	21:CF:118:LEU:HD23	1.82	0.61
29:CN:36:ARG:HH21	29:CN:172:PRO:HG3	1.65	0.61
50:C1:1257:C:H3'	53:UT:2100:ARG:HH22	1.66	0.61
52:CW:40:GLU:O	52:CW:44:ASN:HB2	2.00	0.61
53:UT:85:GLU:OE1	53:UT:110:TYR:OH	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:US:82:GLU:OE1	56:US:86:ARG:NH1	2.27	0.61
22:CG:167:ARG:NH2	51:C2:127:A:N1	2.43	0.61
34:Ca:164:ILE:HD11	34:Ca:205:TYR:HB3	1.81	0.61
53:UT:149:VAL:HA	53:UT:193:LEU:HD11	1.82	0.61
4:UD:29:VAL:HB	4:UD:33:LYS:HD2	1.82	0.61
7:UJ:1102:ILE:HD11	7:UJ:1114:ILE:HD12	1.82	0.61
29:CO:176:ARG:HH21	29:CO:196:LEU:HD12	1.65	0.61
53:UT:292:LEU:HD11	53:UT:336:VAL:HG21	1.82	0.61
24:CI:291:VAL:HG13	24:CI:1008:ILE:HD11	1.83	0.61
32:CR:313:THR:HA	32:CR:372:ILE:O	2.01	0.61
47:Co:345:ARG:NH1	47:Co:345:ARG:O	2.33	0.61
2:UB:701:GLN:NE2	2:UB:702:LEU:O	2.34	0.61
4:UD:235:ASN:OD1	14:UR:393:LYS:NZ	2.27	0.61
25:CJ:64:LEU:HD11	27:CL:619:ILE:HG13	1.81	0.61
32:CS:31:GLY:HA3	32:CS:204:ASP:HB3	1.83	0.61
40:Cg:141:VAL:HG23	40:Cg:144:PHE:HB2	1.83	0.61
42:Ci:33:PHE:HB3	42:Ci:40:PHE:HB2	1.83	0.61
7:UJ:535:ASP:OD1	7:UJ:542:ARG:NH2	2.32	0.61
12:UO:463:ARG:NH2	13:UQ:524:VAL:O	2.33	0.61
15:UU:624:ALA:HB3	15:UU:642:LEU:HD12	1.82	0.61
25:CJ:102:THR:HG23	25:CJ:105:ALA:H	1.64	0.61
29:CO:180:LEU:HD11	29:CO:241:PHE:HE2	1.66	0.61
32:CR:318:GLU:OE2	32:CR:353:ASN:ND2	2.34	0.61
41:Ch:94:LYS:NZ	50:C1:1538:G:OP1	2.33	0.61
37:Cd:160:ARG:NH2	50:C1:655:A:OP1	2.34	0.61
29:CO:114:ILE:HB	29:CO:122:ILE:HB	1.83	0.61
32:CR:317:PRO:HA	32:CR:320:LEU:HB2	1.81	0.61
10:UM:699:LEU:HA	10:UM:709:ALA:O	2.01	0.60
13:UQ:222:ASN:HB2	13:UQ:225:MET:HE3	1.82	0.60
32:CS:284:THR:HG22	32:CS:412:SER:HB3	1.82	0.60
53:UT:372:GLY:HA2	53:UT:421:PRO:HG3	1.82	0.60
2:UB:519:ASN:OD1	2:UB:522:ARG:NH2	2.34	0.60
9:UL:468:ALA:HA	9:UL:484:THR:HG22	1.83	0.60
10:UM:80:SER:OG	10:UM:84:THR:OG1	2.19	0.60
10:UM:252:ARG:HD3	10:UM:276:LEU:HD23	1.83	0.60
12:UO:6:VAL:HB	55:UE:27:ARG:HH21	1.65	0.60
13:UQ:213:LYS:NZ	50:C1:45:U:O4	2.32	0.60
32:CS:162:LEU:HD11	32:CS:190:LEU:HD23	1.82	0.60
32:CS:406:TYR:O	32:CS:467:ARG:NH2	2.34	0.60
53:UT:387:TRP:HA	53:UT:391:ILE:HD12	1.83	0.60
12:UO:104:CYS:O	12:UO:116:ALA:HA	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:UL:647:GLY:O	9:UL:679:LYS:NZ	2.35	0.60
13:UQ:422:VAL:O	13:UQ:431:SER:N	2.32	0.60
30:CP:40:MET:HA	30:CP:78:MET:O	2.01	0.60
44:Ck:17:PRO:HG2	44:Ck:68:MET:HE3	1.83	0.60
10:UM:271:MET:O	10:UM:273:ARG:NH1	2.34	0.60
29:CO:112:ILE:HB	29:CO:124:VAL:HB	1.84	0.60
60:CZ:378:MET:HE2	60:CZ:382:CYS:HB2	1.82	0.60
6:UG:562:ASN:O	6:UG:566:LYS:NZ	2.34	0.60
7:UJ:86:MET:HE2	7:UJ:90:GLU:HB3	1.82	0.60
7:UJ:656:ILE:HD13	7:UJ:660:LEU:HD21	1.83	0.60
15:UU:404:GLY:HA3	15:UU:758:HIS:HB2	1.84	0.60
18:CA:70:LYS:NZ	33:CT:139:THR:OG1	2.31	0.60
18:CB:96:ASN:OD1	18:CB:200:ARG:NH2	2.34	0.60
20:CD:2:PRO:HB2	20:CD:4:PHE:HE2	1.66	0.60
58:CX:199:VAL:HA	58:CX:236:LEU:HD21	1.83	0.60
7:UJ:1073:ALA:HA	7:UJ:1076:LYS:HD2	1.82	0.60
13:UQ:95:ILE:HG21	13:UQ:148:LEU:HD13	1.84	0.60
19:CC:89:THR:HG23	19:CC:115:GLY:HA3	1.83	0.60
19:CC:212:ILE:HG23	19:CC:213:VAL:HG23	1.82	0.60
35:Cb:94:LYS:NZ	47:Co:347:PRO:O	2.34	0.60
1:UA:706:PHE:O	15:UU:677:ASN:ND2	2.35	0.60
10:UM:335:LEU:HD21	10:UM:343:LEU:HD23	1.84	0.60
18:CB:130:TRP:HH2	18:CB:173:ILE:HD11	1.66	0.60
24:CI:536:PRO:HB2	24:CI:537:TRP:HD1	1.67	0.60
37:Cd:2:LYS:NZ	50:C1:738:G:OP1	2.32	0.60
53:UT:176:SER:HB2	53:UT:217:LYS:HG2	1.83	0.60
53:UT:1098:VAL:HG21	53:UT:1144:LEU:HD21	1.84	0.60
4:UD:120:ARG:NH1	4:UD:498:GLU:OE1	2.35	0.60
12:UO:97:ARG:NH2	12:UO:134:ALA:O	2.35	0.60
13:UQ:466:LEU:HB3	13:UQ:833:SER:HB2	1.83	0.60
32:CR:291:LYS:HE3	32:CR:411:ALA:HB1	1.83	0.60
2:UB:549:LEU:HD23	2:UB:552:LEU:HD21	1.84	0.60
13:UQ:197:VAL:HG21	13:UQ:274:TRP:HE1	1.66	0.60
13:UQ:568:THR:HG21	55:UE:258:ALA:HB1	1.83	0.60
15:UU:52:THR:HG21	15:UU:98:HIS:HA	1.84	0.60
25:CJ:104:SER:OG	25:CJ:108:ARG:NH1	2.35	0.60
39:Cf:83:TYR:HB2	39:Cf:200:LEU:HD21	1.84	0.60
42:Ci:31:ARG:HH12	50:C1:1504:A:H5'	1.67	0.60
53:UT:64:ARG:NH1	53:UT:91:GLU:O	2.35	0.60
5:UF:398:ILE:HA	5:UF:401:VAL:HG22	1.84	0.59
7:UJ:741:ARG:NE	7:UJ:781:VAL:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:UM:522:ARG:NH2	10:UM:535:THR:OG1	2.35	0.59
13:UQ:457:ARG:NH2	50:C1:40:A:OP1	2.35	0.59
26:CK:108:ARG:NH1	26:CK:114:ALA:O	2.35	0.59
32:CS:370:GLN:NE2	32:CS:371:TYR:O	2.33	0.59
41:Ch:120:SER:OG	41:Ch:124:ARG:NH2	2.35	0.59
41:Ch:135:LEU:HD12	41:Ch:136:PRO:HD2	1.84	0.59
53:UT:872:PHE:HE1	53:UT:903:LEU:HD13	1.67	0.59
2:UB:900:LYS:NZ	50:C1:1185:A:OP1	2.35	0.59
24:CI:59:VAL:O	24:CI:239:ASN:ND2	2.36	0.59
32:CR:491:ASN:ND2	32:CR:497:ASP:OD2	2.35	0.59
4:UD:309:GLN:OE1	14:UR:449:ARG:NH2	2.35	0.59
29:CO:96:LEU:HD21	29:CO:114:ILE:HD11	1.84	0.59
52:CW:298:THR:O	52:CW:301:GLU:N	2.33	0.59
53:UT:80:GLN:HA	53:UT:83:LYS:HG2	1.84	0.59
4:UD:611:GLY:O	4:UD:613:ARG:NH1	2.35	0.59
9:UL:490:GLN:OE1	9:UL:492:TYR:OH	2.20	0.59
10:UM:29:GLU:HG2	10:UM:31:GLY:H	1.67	0.59
32:CS:886:ALA:HA	32:CS:890:GLN:HB2	1.83	0.59
53:UT:310:ILE:O	53:UT:353:ARG:NH1	2.35	0.59
58:CX:293:LYS:HG2	58:CX:331:ILE:HD11	1.83	0.59
7:UJ:1465:LEU:HD13	7:UJ:1468:LEU:HD12	1.83	0.59
8:UK:169:GLU:OE2	8:UK:173:GLN:NE2	2.36	0.59
10:UM:382:ILE:HD11	10:UM:390:ALA:HB2	1.84	0.59
17:UZ:126:ARG:HH12	50:C1:2061:G:H5'	1.67	0.59
37:Cd:35:GLU:OE2	37:Cd:51:ARG:NH1	2.36	0.59
56:US:194:ASP:OD1	56:US:197:ARG:NH2	2.36	0.59
1:UA:227:LYS:HG2	1:UA:244:ARG:HH21	1.67	0.59
4:UD:632:VAL:HG12	4:UD:650:VAL:HB	1.85	0.59
4:UD:651:THR:O	4:UD:654:LYS:N	2.35	0.59
10:UM:378:ASP:HA	10:UM:698:THR:HG21	1.85	0.59
10:UM:521:LYS:HD2	10:UM:576:LEU:HD21	1.84	0.59
18:CA:106:GLU:OE2	18:CA:128:ARG:NH1	2.34	0.59
29:CN:188:ARG:HH21	29:CN:189:VAL:HG12	1.66	0.59
30:CP:191:ASN:OD1	50:C1:1612:A:N6	2.33	0.59
35:Cb:72:VAL:HG22	35:Cb:77:ARG:HG3	1.83	0.59
17:UZ:24:LEU:HG	17:UZ:28:LYS:HZ3	1.67	0.59
29:CN:100:LEU:HA	29:CN:105:ASN:HD22	1.66	0.59
29:CO:167:ILE:HD12	29:CO:170:HIS:HB2	1.82	0.59
32:CR:229:LEU:O	32:CR:234:LYS:NZ	2.35	0.59
53:UT:130:ALA:O	53:UT:133:LEU:C	2.46	0.59
2:UB:530:LEU:O	2:UB:534:ILE:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:869:GLU:O	61:UP:356:ARG:NH1	2.35	0.59
7:UJ:752:TRP:HA	7:UJ:755:LEU:HD12	1.84	0.59
7:UJ:1097:LEU:O	7:UJ:1101:LEU:HB2	2.03	0.59
16:UX:112:ILE:HD11	45:Cm:96:ALA:HB2	1.85	0.59
60:CZ:378:MET:O	60:CZ:383:GLN:NE2	2.27	0.59
7:UJ:1431:TYR:HA	7:UJ:1434:THR:HG23	1.85	0.59
32:CS:608:GLN:NE2	32:CS:609:PRO:O	2.35	0.59
50:C1:462:G:N7	59:CY:374:ARG:NH1	2.51	0.59
53:UT:895:TRP:HB3	53:UT:900:ARG:HE	1.67	0.59
1:UA:95:PHE:HB3	1:UA:115:LEU:HD21	1.85	0.58
1:UA:534:LEU:HB2	1:UA:548:VAL:HG22	1.85	0.58
23:CH:251:HIS:HB3	49:CU:111:MET:HG2	1.84	0.58
35:Cb:80:ILE:HG23	35:Cb:81:THR:HG23	1.85	0.58
35:Cb:146:THR:HG21	50:C1:709:G:H21	1.67	0.58
49:CU:275:LEU:HD12	49:CU:276:PRO:HD2	1.85	0.58
53:UT:397:VAL:O	53:UT:401:ALA:HB2	2.03	0.58
29:CO:77:MET:HE2	29:CO:87:ALA:HB2	1.84	0.58
32:CR:593:LYS:HG2	32:CR:631:SER:HB2	1.85	0.58
41:Ch:124:ARG:NH2	50:C1:1212:G:OP1	2.36	0.58
53:UT:831:GLU:O	53:UT:834:LYS:NZ	2.32	0.58
55:UI:188:MET:O	55:UI:225:HIS:NE2	2.34	0.58
4:UD:647:LEU:HB3	4:UD:659:PHE:HB2	1.85	0.58
7:UJ:1489:ALA:HB2	7:UJ:1503:LEU:HD11	1.85	0.58
10:UM:559:PHE:HD1	10:UM:573:VAL:HG12	1.69	0.58
18:CB:158:TYR:OH	18:CB:166:SER:OG	2.16	0.58
25:CJ:115:MET:HB2	25:CJ:120:MET:HB2	1.85	0.58
32:CR:359:VAL:HB	32:CR:369:ILE:HB	1.85	0.58
53:UT:315:THR:HB	53:UT:353:ARG:HA	1.84	0.58
12:UO:145:GLN:HE22	56:US:413:LEU:HG	1.66	0.58
32:CR:23:LYS:O	32:CR:146:GLY:N	2.37	0.58
37:Cd:98:ARG:NH1	37:Cd:101:ILE:O	2.30	0.58
50:C1:805:C:H5'	53:UT:1318:ARG:HD2	1.84	0.58
4:UD:6:CYS:HB2	4:UD:863:ILE:HG22	1.85	0.58
13:UQ:762:LEU:HD21	54:UH:440:ARG:NH1	2.18	0.58
21:CE:64:ILE:O	21:CE:67:HIS:HE1	1.86	0.58
22:CG:495:ASP:OD1	22:CG:497:ARG:NH1	2.35	0.58
50:C1:314:A:H61	50:C1:326:U:H3	1.51	0.58
53:UT:2182:LEU:O	53:UT:2185:LYS:C	2.46	0.58
12:UO:467:ARG:O	12:UO:471:GLN:HB3	2.04	0.58
24:CI:224:ARG:NH2	50:C1:1013:G:O2'	2.35	0.58
35:Cb:203:GLY:HA2	50:C1:830:G:C2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Cd:132:ARG:NH2	50:C1:733:C:O2'	2.36	0.58
39:Cf:73:THR:HG23	50:C1:841:A:H1'	1.86	0.58
53:UT:1349:ARG:HA	53:UT:1352:TYR:HD2	1.68	0.58
5:UF:352:ALA:HB1	5:UF:355:LYS:HE3	1.86	0.58
12:UO:386:ARG:NH1	12:UO:387:ALA:O	2.37	0.58
26:CK:85:ASP:OD1	27:CL:559:ARG:NH2	2.37	0.58
53:UT:126:VAL:HG12	53:UT:171:LEU:HD11	1.86	0.58
1:UA:308:SER:HB2	15:UU:884:GLY:HA2	1.85	0.58
2:UB:483:GLN:N	2:UB:487:GLU:OE2	2.34	0.58
6:UG:128:LYS:HE2	6:UG:166:ARG:HH11	1.69	0.58
32:CR:661:TYR:HB3	32:CR:766:LEU:HD11	1.86	0.58
42:Ci:94:ILE:HG21	42:Ci:115:LEU:HD21	1.84	0.58
56:US:178:ILE:HG22	56:US:181:LEU:H	1.67	0.58
2:UB:745:ALA:H	56:US:462:GLN:NE2	2.00	0.58
4:UD:689:VAL:HA	4:UD:703:GLY:HA2	1.86	0.58
27:CL:124:ALA:HB1	27:CL:125:LEU:HD23	1.84	0.58
49:CU:111:MET:HE2	49:CU:115:GLU:HB3	1.84	0.58
13:UQ:667:VAL:HG11	13:UQ:715:ILE:HG21	1.86	0.58
43:Cj:126:PRO:HD2	43:Cj:128:LYS:HE3	1.86	0.58
44:Ck:73:GLY:HA3	44:Ck:132:GLN:HB3	1.86	0.58
53:UT:901:LYS:NZ	53:UT:936:GLU:OE2	2.32	0.58
53:UT:2039:SER:HB2	53:UT:2050:LEU:HD21	1.85	0.58
7:UJ:1630:VAL:HG22	7:UJ:1634:LYS:HE3	1.84	0.57
10:UM:592:VAL:HG22	10:UM:617:THR:HG22	1.85	0.57
15:UU:159:ILE:HB	15:UU:173:ILE:HB	1.85	0.57
23:CH:16:ALA:HB1	23:CH:19:GLN:HB2	1.86	0.57
32:CR:310:ILE:HD11	32:CR:369:ILE:HG12	1.87	0.57
32:CS:184:ARG:NE	32:CS:524:ASP:OD1	2.36	0.57
37:Cd:23:LYS:NZ	37:Cd:40:PRO:O	2.36	0.57
4:UD:108:THR:HG23	4:UD:110:THR:H	1.68	0.57
7:UJ:1136:ILE:O	7:UJ:1144:GLN:NE2	2.37	0.57
20:CD:16:PHE:HZ	20:CD:130:ILE:HG12	1.69	0.57
20:CD:360:LYS:NZ	51:C2:87:G:OP2	2.38	0.57
26:CK:229:THR:HG21	27:CL:545:ILE:HD11	1.86	0.57
32:CS:841:LEU:HB3	32:CS:920:THR:HG22	1.86	0.57
39:Cf:58:LEU:HD21	52:CW:75:TYR:HB2	1.84	0.57
45:Cm:25:VAL:HG12	45:Cm:63:VAL:HB	1.85	0.57
53:UT:777:PRO:HA	53:UT:844:ARG:HH21	1.68	0.57
53:UT:869:LEU:HD22	53:UT:907:PHE:HE1	1.68	0.57
53:UT:1818:MET:HE3	53:UT:1869:LEU:HA	1.85	0.57
9:UL:245:ALA:HB2	9:UL:270:ARG:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:CM:86:SER:OG	28:CM:88:ASP:OD1	2.22	0.57
30:CP:51:LEU:HD13	30:CP:78:MET:HE2	1.87	0.57
32:CS:257:ARG:HD3	65:CS:1101:ADP:C6	2.39	0.57
53:UT:740:VAL:O	53:UT:746:TRP:NE1	2.25	0.57
53:UT:1878:MET:SD	53:UT:1925:SER:OG	2.62	0.57
22:CG:221:LYS:N	51:C2:180:U:O2'	2.35	0.57
32:CR:311:PHE:O	32:CR:386:VAL:HA	2.05	0.57
32:CS:279:ASN:OD1	32:CS:468:SER:OG	2.21	0.57
53:UT:976:LEU:HD21	53:UT:995:LEU:HD11	1.85	0.57
4:UD:198:ASN:OD1	4:UD:215:ARG:NH1	2.37	0.57
7:UJ:634:ALA:HA	7:UJ:643:THR:HG22	1.87	0.57
7:UJ:1284:LEU:HA	7:UJ:1287:LEU:HD12	1.85	0.57
9:UL:222:ALA:HB3	9:UL:235:ALA:HB3	1.85	0.57
23:CH:215:VAL:HA	23:CH:285:THR:HA	1.87	0.57
32:CR:387:VAL:HG22	32:CR:409:PHE:HB2	1.86	0.57
32:CR:792:TYR:O	32:CR:795:ARG:CB	2.53	0.57
53:UT:1237:LEU:O	53:UT:1248:ASN:ND2	2.35	0.57
1:UA:155:ARG:HD2	1:UA:199:VAL:HA	1.86	0.57
1:UA:270:LEU:HD13	1:UA:284:MET:HE3	1.85	0.57
1:UA:558:ARG:NH2	51:C2:62:A:OP2	2.37	0.57
9:UL:40:ILE:HG13	9:UL:49:VAL:HG12	1.86	0.57
10:UM:248:LEU:HD21	10:UM:280:VAL:HG22	1.87	0.57
10:UM:479:LEU:HG	10:UM:539:ARG:HH22	1.68	0.57
15:UU:454:THR:HG22	15:UU:455:THR:HG23	1.87	0.57
22:CG:482:SER:OG	22:CG:483:TRP:N	2.38	0.57
47:Co:372:ARG:NH2	47:Co:383:LYS:O	2.37	0.57
53:UT:1511:PHE:HD1	53:UT:1515:HIS:HE1	1.51	0.57
2:UB:3:GLY:O	2:UB:8:ARG:NH1	2.37	0.57
2:UB:606:HIS:HA	2:UB:652:ARG:HH22	1.69	0.57
4:UD:506:ARG:NH1	4:UD:507:VAL:O	2.38	0.57
7:UJ:1426:ALA:HA	7:UJ:1430:PRO:HD3	1.86	0.57
14:UR:396:GLY:HA3	14:UR:420:VAL:HG23	1.86	0.57
23:CH:209:ASN:O	23:CH:350:ARG:NH1	2.36	0.57
29:CN:32:LYS:HA	29:CN:36:ARG:HH22	1.69	0.57
30:CP:139:ARG:NH1	30:CP:189:MET:O	2.35	0.57
32:CS:316:SER:HB3	32:CS:319:ASN:HB2	1.86	0.57
50:C1:928:G:OP2	60:CZ:537:ARG:NH2	2.38	0.57
4:UD:684:ASP:HB2	4:UD:734:ARG:HD3	1.87	0.57
10:UM:271:MET:HG2	10:UM:273:ARG:HH22	1.69	0.57
10:UM:289:MET:O	10:UM:300:ILE:HA	2.04	0.57
52:CW:11:VAL:HG22	52:CW:359:ILE:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:UB:759:HIS:O	2:UB:762:THR:OG1	2.20	0.57
4:UD:406:ASP:HB3	4:UD:409:ALA:HB2	1.86	0.57
9:UL:712:VAL:HG12	9:UL:722:VAL:HG22	1.87	0.57
10:UM:368:ARG:HH12	10:UM:428:LEU:HD13	1.69	0.57
13:UQ:601:ARG:NH2	55:UE:30:GLU:OE2	2.38	0.57
13:UQ:615:PHE:N	13:UQ:629:ILE:O	2.37	0.57
28:CM:72:MET:HE3	28:CM:333:MET:HG2	1.86	0.57
30:CP:93:LEU:HD13	30:CP:96:ARG:HH12	1.70	0.57
37:Cd:57:ASP:HA	37:Cd:106:LEU:HA	1.86	0.57
40:Cg:136:LYS:H	59:CY:250:GLY:HA3	1.69	0.57
53:UT:1274:GLN:HG3	53:UT:1276:ASP:H	1.70	0.57
59:CY:98:LYS:HB2	60:CZ:453:LEU:HD21	1.87	0.57
55:UI:189:ASP:HB3	55:UI:192:LEU:HD13	1.87	0.57
27:CL:571:VAL:HG21	27:CL:645:PRO:HB3	1.86	0.57
32:CS:829:LEU:HD11	32:CS:923:PHE:HD1	1.69	0.57
7:UJ:77:GLN:HE21	14:UR:62:ALA:H	1.53	0.56
7:UJ:323:GLN:NE2	7:UJ:364:ASP:OD2	2.38	0.56
10:UM:344:VAL:HG12	10:UM:368:ARG:HG2	1.87	0.56
11:UN:301:PRO:HG3	53:UT:2125:THR:HB	1.86	0.56
21:CE:64:ILE:O	21:CE:67:HIS:CE1	2.57	0.56
23:CH:86:VAL:HG23	23:CH:89:MET:HB3	1.88	0.56
48:Cp:13:VAL:O	48:Cp:52:ASN:HA	2.05	0.56
4:UD:192:ILE:HG12	4:UD:202:VAL:HG12	1.87	0.56
4:UD:319:ARG:NH2	50:C1:66:G:OP1	2.38	0.56
15:UU:883:VAL:O	15:UU:887:GLY:C	2.48	0.56
26:CK:105:LYS:NZ	50:C1:1743:C:OP2	2.38	0.56
29:CN:35:LYS:NZ	29:CN:200:GLU:O	2.38	0.56
29:CO:158:LYS:HB2	29:CO:161:LYS:HE2	1.86	0.56
32:CS:479:ARG:HE	65:CS:1101:ADP:H4'	1.70	0.56
32:CS:513:PRO:HD3	52:CW:274:ARG:HE	1.69	0.56
50:C1:678:A:H5"	50:C1:679:A:H5"	1.86	0.56
53:UT:431:SER:OG	53:UT:472:ARG:NH2	2.32	0.56
4:UD:316:VAL:HG12	13:UQ:349:ARG:HG2	1.87	0.56
7:UJ:786:HIS:HD2	7:UJ:789:GLY:H	1.52	0.56
9:UL:862:ASN:OD1	9:UL:905:ASN:ND2	2.36	0.56
10:UM:300:ILE:HG22	10:UM:309:ILE:HD12	1.86	0.56
13:UQ:401:ASN:HB2	13:UQ:414:HIS:HB3	1.86	0.56
13:UQ:770:THR:HG22	13:UQ:796:PRO:HB3	1.86	0.56
22:CG:415:ASN:ND2	22:CG:417:ASP:OD2	2.39	0.56
28:CM:300:SER:HB3	28:CM:310:TRP:HE1	1.70	0.56
32:CS:587:GLN:HG3	32:CS:636:VAL:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Ce:33:LEU:HD11	38:Ce:87:LEU:HD11	1.87	0.56
45:Cm:59:GLY:N	50:C1:1449:U:O4	2.37	0.56
53:UT:901:LYS:HD3	53:UT:937:LEU:HD13	1.86	0.56
53:UT:1048:VAL:HG23	53:UT:1049:VAL:HG23	1.87	0.56
53:UT:1743:LEU:HD21	53:UT:1793:THR:HG21	1.86	0.56
15:UU:210:ILE:HD12	15:UU:220:TYR:HB3	1.87	0.56
32:CS:283:LEU:HD11	32:CS:474:LEU:HG	1.86	0.56
32:CS:511:PRO:O	32:CS:649:TYR:OH	2.22	0.56
51:C2:92:A:H4'	51:C2:93:G:H5"	1.88	0.56
53:UT:1032:MET:HG3	53:UT:1083:LEU:HD21	1.86	0.56
56:US:289:MET:HE3	56:US:294:ALA:HB2	1.87	0.56
60:CZ:331:LEU:HD21	60:CZ:366:LEU:HD21	1.87	0.56
4:UD:695:GLN:HB3	4:UD:698:ARG:HB3	1.86	0.56
7:UJ:1667:GLN:HG3	7:UJ:1672:PHE:HB2	1.88	0.56
10:UM:370:SER:OG	10:UM:399:ARG:NH1	2.37	0.56
12:UO:417:ARG:NH2	50:C1:129:G:O6	2.39	0.56
18:CB:76:HIS:HB3	18:CB:81:VAL:HG23	1.88	0.56
20:CD:240:ALA:O	20:CD:244:SER:HB2	2.06	0.56
22:CG:568:ARG:HE	22:CG:575:GLY:HA2	1.71	0.56
23:CH:151:ASP:OD1	23:CH:154:ARG:NH2	2.39	0.56
30:CP:35:GLU:OE1	42:Ci:127:ARG:NH1	2.38	0.56
32:CR:26:PHE:O	32:CR:199:CYS:HA	2.06	0.56
32:CR:785:ARG:HH12	32:CS:840:ARG:HH22	1.54	0.56
32:CS:399:VAL:HG11	32:CS:428:LEU:HD11	1.87	0.56
4:UD:774:VAL:HG11	13:UQ:342:ARG:HH21	1.70	0.56
9:UL:12:LYS:HB2	9:UL:722:VAL:HB	1.88	0.56
13:UQ:241:PRO:HA	13:UQ:257:ALA:HA	1.87	0.56
15:UU:559:GLY:HA2	15:UU:564:SER:O	2.06	0.56
20:CD:38:LYS:HG2	20:CD:41:LYS:HZ3	1.69	0.56
28:CM:304:ASP:O	28:CM:306:THR:N	2.38	0.56
29:CN:38:ILE:HG21	29:CN:171:LEU:HD21	1.87	0.56
53:UT:538:LEU:O	53:UT:587:ARG:NH1	2.39	0.56
53:UT:1698:ILE:HD11	53:UT:1735:VAL:HG12	1.88	0.56
2:UB:534:ILE:HD12	2:UB:552:LEU:HD13	1.85	0.56
4:UD:39:ASN:OD1	4:UD:97:HIS:NE2	2.33	0.56
9:UL:474:LEU:HD12	9:UL:479:VAL:HB	1.87	0.56
12:UO:339:GLN:NE2	57:Cl:5:SER:HG	2.02	0.56
23:CH:73:THR:HG23	23:CH:74:THR:HG23	1.87	0.56
28:CM:189:GLN:OE1	28:CM:230:ASN:ND2	2.39	0.56
39:Cf:16:ALA:HB2	50:C1:938:C:H5"	1.88	0.56
39:Cf:26:ALA:O	39:Cf:49:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:UR:362:LYS:HD3	50:C1:74:C:H1'	1.88	0.56
24:CI:837:LEU:HD13	24:CI:884:PHE:HB3	1.88	0.56
35:Cb:58:TYR:HE1	35:Cb:62:LYS:HE3	1.70	0.56
44:Ck:60:ASP:HB3	44:Ck:87:ARG:HH12	1.70	0.56
47:Co:351:ARG:HD2	47:Co:405:LEU:HD22	1.88	0.56
50:C1:1259:C:OP1	53:UT:2100:ARG:NH1	2.38	0.56
53:UT:253:GLN:HA	53:UT:256:MET:HE2	1.86	0.56
53:UT:1919:ILE:HD12	53:UT:1992:VAL:HG21	1.88	0.56
5:UF:285:VAL:HG11	11:UN:369:LEU:HB2	1.87	0.56
9:UL:119:ASP:OD1	9:UL:120:LYS:N	2.39	0.56
14:UR:405:THR:HG23	14:UR:407:GLN:HG2	1.87	0.56
15:UU:391:LEU:HD21	15:UU:773:VAL:HG11	1.86	0.56
23:CH:33:ILE:HD12	23:CH:75:ILE:HD11	1.88	0.56
43:Cj:94:ALA:HB2	43:Cj:102:LYS:HG3	1.88	0.56
53:UT:1245:SER:HA	53:UT:1248:ASN:HB2	1.88	0.56
7:UJ:319:ARG:NH2	7:UJ:323:GLN:O	2.31	0.56
7:UJ:1228:LEU:HD23	7:UJ:1271:LEU:HD12	1.87	0.56
7:UJ:1716:GLN:NE2	7:UJ:1717:GLU:OE1	2.39	0.56
12:UO:284:GLN:OE1	12:UO:286:ARG:NH1	2.39	0.56
15:UU:78:ARG:O	15:UU:81:ASN:ND2	2.37	0.56
20:CD:3:LEU:HB3	20:CD:18:ALA:HB3	1.87	0.56
24:CI:286:VAL:O	24:CI:293:ASP:CA	2.27	0.56
30:CP:198:ILE:HG22	49:CU:161:LEU:HD11	1.87	0.56
42:Ci:44:THR:HG22	42:Ci:51:THR:HA	1.88	0.56
50:C1:849:A:H61	50:C1:873:U:H3	1.53	0.56
51:C2:134:C:H4'	51:C2:181:A:H61	1.71	0.56
53:UT:1027:LEU:HD12	53:UT:1032:MET:HE2	1.88	0.56
59:CY:293:LYS:HG2	59:CY:297:MET:HE3	1.88	0.56
10:UM:303:THR:O	10:UM:306:HIS:ND1	2.37	0.55
17:UZ:154:LEU:HD23	17:UZ:180:ILE:HB	1.86	0.55
53:UT:870:PHE:HA	53:UT:873:THR:HG22	1.88	0.55
57:Cl:12:ASN:HA	57:Cl:25:LYS:HB2	1.88	0.55
58:CX:213:LYS:O	58:CX:245:ASN:ND2	2.39	0.55
1:UA:121:VAL:HG23	1:UA:144:HIS:HB3	1.88	0.55
4:UD:644:ASP:HA	4:UD:662:LEU:HD12	1.88	0.55
7:UJ:1014:LEU:HD23	7:UJ:1019:PRO:HA	1.88	0.55
7:UJ:1482:HIS:HB3	7:UJ:1522:LEU:HD22	1.88	0.55
10:UM:394:ASN:HA	10:UM:435:ILE:HG23	1.89	0.55
24:CI:221:ASN:ND2	50:C1:1024:U:O4'	2.39	0.55
28:CM:171:SER:HB3	28:CM:203:VAL:HB	1.88	0.55
30:CP:110:GLN:NE2	49:CU:179:SER:O	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CR:112:THR:HA	32:CR:115:ILE:HG12	1.89	0.55
54:UH:642:VAL:HG11	54:UH:725:SER:HB3	1.88	0.55
2:UB:584:LEU:HB3	2:UB:625:LYS:HD3	1.88	0.55
10:UM:222:ALA:HB2	10:UM:230:ALA:HA	1.87	0.55
27:CL:658:MET:HB2	27:CL:676:MET:HE1	1.89	0.55
32:CR:397:PRO:HA	32:CR:400:LYS:HG2	1.87	0.55
32:CR:748:ARG:NH2	32:CR:750:THR:OG1	2.40	0.55
53:UT:1313:LEU:HD13	53:UT:1358:LEU:HD11	1.88	0.55
53:UT:1730:GLU:HG3	53:UT:1731:LYS:HD3	1.88	0.55
59:CY:98:LYS:HB3	60:CZ:441:LEU:HD22	1.89	0.55
6:UG:578:ILE:HA	6:UG:582:ARG:HH21	1.70	0.55
10:UM:45:LEU:HD11	10:UM:76:LEU:HD22	1.88	0.55
24:CI:1116:ARG:HE	50:C1:1078:U:H1'	1.71	0.55
53:UT:754:LYS:HA	53:UT:854:LEU:HD11	1.87	0.55
54:UH:88:ARG:HE	54:UH:97:VAL:HG11	1.71	0.55
1:UA:519:ARG:NH1	1:UA:524:GLN:OE1	2.39	0.55
24:CI:760:LEU:HD23	24:CI:763:HIS:HB3	1.88	0.55
29:CO:144:LEU:HD13	29:CO:150:ILE:HG12	1.89	0.55
32:CR:165:MET:O	32:CR:169:VAL:HA	2.07	0.55
53:UT:1090:TYR:O	53:UT:1094:LEU:HB2	2.06	0.55
53:UT:2182:LEU:O	53:UT:2185:LYS:O	2.25	0.55
54:UH:836:ILE:HD11	55:UI:239:LEU:HD11	1.89	0.55
7:UJ:257:GLU:HA	7:UJ:260:VAL:HG12	1.88	0.55
13:UQ:762:LEU:CD2	54:UH:440:ARG:NH1	2.69	0.55
17:UZ:184:LEU:HD23	17:UZ:220:ILE:HD12	1.89	0.55
22:CG:578:VAL:HB	22:CG:604:PHE:HB2	1.89	0.55
29:CN:227:ILE:HD12	29:CN:240:LYS:HG3	1.89	0.55
32:CS:311:PHE:HB2	32:CS:386:VAL:HG22	1.89	0.55
37:Cd:79:GLU:HG2	37:Cd:86:PRO:HG3	1.87	0.55
39:Cf:83:TYR:OH	44:Ck:11:ARG:NH1	2.29	0.55
50:C1:809:U:O4	53:UT:1622:ARG:NH1	2.40	0.55
53:UT:8:ARG:NH1	53:UT:795:PRO:O	2.37	0.55
53:UT:585:TYR:OH	53:UT:596:ASP:OD1	2.25	0.55
1:UA:445:ILE:HA	1:UA:470:PRO:HB3	1.89	0.55
4:UD:349:PRO:HG2	4:UD:365:LEU:HB2	1.88	0.55
7:UJ:784:PRO:HA	7:UJ:816:MET:HE2	1.88	0.55
15:UU:177:ALA:HB2	15:UU:183:ASN:HB3	1.89	0.55
25:CJ:119:ARG:NH1	50:C1:354:G:H5"	2.22	0.55
28:CM:67:GLN:OE1	45:Cm:68:ARG:NH2	2.40	0.55
32:CR:234:LYS:HA	32:CR:237:LYS:HE3	1.89	0.55
35:Cb:177:THR:HG23	35:Cb:196:THR:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:1471:ALA:O	53:UT:1475:GLN:N	2.31	0.55
6:UG:264:LEU:HD11	6:UG:273:LEU:HD22	1.88	0.55
9:UL:491:LEU:HD12	9:UL:501:GLU:HB2	1.88	0.55
9:UL:917:MET:HG2	10:UM:827:GLN:HG2	1.88	0.55
10:UM:624:ILE:HB	10:UM:638:PHE:HB2	1.89	0.55
14:UR:253:ARG:HH21	14:UR:256:LEU:HD11	1.70	0.55
25:CJ:117:ARG:HG3	50:C1:353:G:H4'	1.89	0.55
39:Cf:101:VAL:HA	39:Cf:171:ALA:O	2.07	0.55
53:UT:70:TRP:NE1	53:UT:124:ASP:OD2	2.40	0.55
4:UD:555:SER:HG	4:UD:559:ARG:H	1.54	0.55
5:UF:285:VAL:HB	11:UN:369:LEU:HD12	1.89	0.55
7:UJ:1555:THR:HA	7:UJ:1558:HIS:CD2	2.42	0.55
12:UO:70:ASN:HD22	12:UO:70:ASN:C	2.13	0.55
12:UO:218:ASP:OD1	12:UO:220:ARG:NH1	2.39	0.55
15:UU:205:ASP:O	15:UU:207:TRP:N	2.40	0.55
15:UU:226:SER:HG	15:UU:229:CYS:HG	1.53	0.55
32:CS:724:GLY:HA2	32:CS:762:MET:O	2.07	0.55
4:UD:450:ASP:OD1	4:UD:477:THR:OG1	2.22	0.55
14:UR:263:ILE:HG12	14:UR:616:ILE:HG12	1.88	0.55
20:CD:288:ASN:HB3	20:CD:372:SER:HB3	1.89	0.55
32:CS:30:VAL:HG22	32:CS:153:LEU:HB2	1.88	0.55
32:CS:524:ASP:O	32:CS:528:SER:HB3	2.06	0.55
39:Cf:89:GLU:HG3	52:CW:138:PHE:HD2	1.71	0.55
40:Cg:57:LEU:HD22	59:CY:314:LEU:HD21	1.89	0.55
50:C1:307:U:H3	50:C1:333:C:H42	1.55	0.55
54:UH:823:LEU:HD11	55:UI:257:LEU:HD23	1.88	0.55
12:UO:273:GLN:NE2	56:US:335:ASP:OD2	2.38	0.54
55:UE:154:GLY:N	56:US:305:ASP:OD2	2.35	0.54
55:UE:201:ALA:HB1	55:UE:245:VAL:HG21	1.88	0.54
56:US:476:LYS:O	56:US:479:SER:N	2.40	0.54
7:UJ:32:SER:HB2	7:UJ:123:ARG:HH11	1.72	0.54
7:UJ:667:SER:HA	7:UJ:673:HIS:HB3	1.89	0.54
7:UJ:715:VAL:HA	7:UJ:748:LEU:HD13	1.87	0.54
7:UJ:1090:PRO:O	7:UJ:1094:LYS:N	2.39	0.54
7:UJ:1650:VAL:HA	7:UJ:1653:THR:HG22	1.87	0.54
32:CR:236:LEU:HG	32:CR:240:LYS:HE3	1.88	0.54
2:UB:487:GLU:HA	2:UB:490:ASN:HD22	1.72	0.54
15:UU:347:ALA:O	15:UU:349:GLN:NE2	2.39	0.54
15:UU:511:VAL:HB	15:UU:524:TRP:HB2	1.87	0.54
15:UU:691:VAL:HB	15:UU:701:ARG:HB2	1.89	0.54
15:UU:992:GLN:NE2	15:UU:1023:GLN:OE1	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Cf:5:ARG:NH2	50:C1:918:U:O4	2.41	0.54
42:Ci:65:ARG:HB3	50:C1:1490:A:H5'	1.90	0.54
52:CW:344:MET:HE2	52:CW:346:LEU:HD11	1.89	0.54
53:UT:348:VAL:HG12	53:UT:804:LEU:HB2	1.89	0.54
53:UT:532:SER:HB3	53:UT:576:PHE:HE1	1.72	0.54
53:UT:1694:LEU:HD12	53:UT:1712:VAL:HB	1.89	0.54
4:UD:437:SER:OG	4:UD:438:GLU:N	2.41	0.54
9:UL:449:LEU:HB3	9:UL:463:PHE:HB2	1.87	0.54
24:CI:68:PRO:HB3	24:CI:113:ARG:HG3	1.89	0.54
28:CM:172:SER:OG	28:CM:176:CYS:SG	2.65	0.54
28:CM:284:ALA:HB3	28:CM:304:ASP:H	1.72	0.54
32:CS:111:GLU:HB2	32:CS:114:LYS:HB2	1.89	0.54
50:C1:1665:A:N3	50:C1:1666:C:N4	2.54	0.54
58:CX:238:ARG:HH21	58:CX:241:LEU:HD23	1.73	0.54
2:UB:574:ARG:HG2	2:UB:593:ILE:HG21	1.89	0.54
7:UJ:1647:TRP:HZ3	7:UJ:1698:VAL:HB	1.72	0.54
10:UM:382:ILE:HB	10:UM:388:MET:HB2	1.89	0.54
20:CD:201:LEU:HD21	20:CD:229:LEU:HD11	1.90	0.54
22:CG:185:THR:OG1	22:CG:193:THR:OG1	2.24	0.54
24:CI:63:PRO:HG2	24:CI:66:PRO:HA	1.89	0.54
32:CS:578:ARG:HG2	32:CS:579:LEU:H	1.72	0.54
35:Cb:143:ASP:OD2	35:Cb:145:ARG:NH2	2.41	0.54
53:UT:290:LEU:HD11	53:UT:334:GLN:HG2	1.90	0.54
53:UT:1496:ASP:O	53:UT:1502:ARG:NE	2.39	0.54
10:UM:60:ASP:OD2	10:UM:86:ARG:NH2	2.40	0.54
12:UO:149:VAL:HB	12:UO:163:CYS:HB2	1.88	0.54
16:UX:54:PRO:HB3	16:UX:85:ALA:HB1	1.88	0.54
20:CD:10:SER:OG	20:CD:142:ASN:OD1	2.19	0.54
20:CD:20:ASP:OD2	20:CD:32:ARG:NH2	2.41	0.54
32:CS:276:THR:O	32:CS:279:ASN:ND2	2.39	0.54
44:Ck:83:THR:HG22	44:Ck:124:GLU:HG3	1.89	0.54
56:US:253:HIS:CD2	56:US:254:PRO:HD2	2.43	0.54
57:Cl:64:GLU:OE1	57:Cl:68:ARG:NH2	2.38	0.54
2:UB:14:ARG:NH1	50:C1:1733:G:OP1	2.40	0.54
7:UJ:1713:VAL:HG22	7:UJ:1715:SER:HB3	1.90	0.54
10:UM:540:ARG:HH22	10:UM:576:LEU:HB3	1.72	0.54
12:UO:492:PRO:HA	12:UO:495:ARG:HB2	1.90	0.54
32:CR:374:PRO:HB2	32:CR:398:LEU:HD13	1.90	0.54
32:CR:570:LEU:HD22	32:CR:653:ALA:HB2	1.90	0.54
34:Ca:136:ARG:NH2	50:C1:1469:A:OP1	2.40	0.54
53:UT:372:GLY:HA3	53:UT:419:LYS:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:1154:VAL:HA	53:UT:1157:ARG:HG2	1.88	0.54
56:US:484:LYS:NZ	56:US:486:ALA:O	2.32	0.54
4:UD:182:THR:O	21:CE:124:ARG:NH2	2.41	0.54
7:UJ:229:ILE:HD11	7:UJ:278:LEU:HD23	1.89	0.54
7:UJ:1754:GLU:HG2	7:UJ:1758:HIS:CE1	2.43	0.54
12:UO:83:ILE:HB	12:UO:93:LYS:HB3	1.89	0.54
23:CH:102:ILE:HD12	23:CH:137:VAL:HG22	1.89	0.54
28:CM:251:GLU:OE1	28:CM:254:ASN:ND2	2.40	0.54
53:UT:1184:TRP:HB3	53:UT:1226:PHE:HE2	1.73	0.54
53:UT:2166:TYR:O	53:UT:2168:ARG:NH1	2.41	0.54
11:UN:907:PRO:O	28:CM:25:ARG:NH2	2.40	0.54
15:UU:690:ARG:HG3	15:UU:702:GLU:HG2	1.89	0.54
26:CK:149:PRO:HD2	26:CK:170:VAL:HG11	1.90	0.54
32:CS:570:LEU:HB3	32:CS:584:CYS:HB3	1.89	0.54
38:Ce:99:LEU:HD21	38:Ce:139:LEU:HD22	1.90	0.54
45:Cm:19:LYS:NZ	50:C1:1666:C:O2'	2.41	0.54
52:CW:97:SER:O	52:CW:116:GLN:NE2	2.41	0.54
53:UT:1606:ALA:HA	53:UT:1609:LEU:HD12	1.89	0.54
32:CS:143:VAL:HG21	32:CS:149:VAL:HG22	1.90	0.54
32:CS:509:GLY:HA2	60:CZ:571:ARG:HD2	1.90	0.54
47:Co:386:VAL:HG22	47:Co:406:ILE:HG12	1.90	0.54
48:Cp:13:VAL:O	48:Cp:52:ASN:N	2.41	0.54
53:UT:1876:LEU:HD23	53:UT:1889:ILE:HD11	1.89	0.54
54:UH:754:ARG:HA	55:UI:210:ARG:HB2	1.89	0.54
1:UA:364:ILE:HD13	1:UA:399:THR:HG21	1.91	0.53
4:UD:549:VAL:HA	4:UD:565:ASP:HA	1.89	0.53
7:UJ:1699:ILE:HA	7:UJ:1702:VAL:HG12	1.89	0.53
8:UK:1:MET:HB2	8:UK:4:LEU:HB2	1.90	0.53
28:CM:216:VAL:HG21	28:CM:242:CYS:HB2	1.90	0.53
32:CS:752:ASN:ND2	32:CS:757:GLU:O	2.39	0.53
39:Cf:36:THR:O	39:Cf:96:LEU:N	2.39	0.53
45:Cm:11:LEU:HD22	45:Cm:74:VAL:HG13	1.90	0.53
50:C1:313:A:N6	50:C1:327:G:O2'	2.41	0.53
53:UT:742:LEU:HB2	53:UT:745:VAL:HG12	1.90	0.53
2:UB:618:ILE:HG23	2:UB:639:LEU:HB3	1.89	0.53
7:UJ:170:TYR:O	7:UJ:174:LEU:HA	2.07	0.53
7:UJ:1478:TYR:HA	7:UJ:1481:LEU:HG	1.90	0.53
20:CD:374:ARG:HE	21:CE:67:HIS:CD2	2.25	0.53
33:CT:84:PRO:O	33:CT:134:TYR:OH	2.25	0.53
35:Cb:155:LYS:NZ	50:C1:828:G:OP1	2.41	0.53
35:Cb:183:ILE:HG12	35:Cb:225:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Cf:48:THR:HG21	39:Cf:54:LYS:HE3	1.90	0.53
44:Ck:86:HIS:CE1	44:Ck:87:ARG:HD2	2.43	0.53
50:C1:808:A:H61	50:C1:821:C:H2'	1.74	0.53
59:CY:57:PHE:HE2	60:CZ:404:TRP:HE3	1.57	0.53
1:UA:558:ARG:HB2	1:UA:566:ALA:HB2	1.89	0.53
7:UJ:1401:LEU:HD22	7:UJ:1418:ALA:HB1	1.89	0.53
10:UM:778:VAL:HG21	10:UM:825:VAL:HG22	1.90	0.53
13:UQ:581:ARG:HE	13:UQ:583:ILE:HD11	1.74	0.53
14:UR:164:ASP:OD1	14:UR:165:LEU:N	2.41	0.53
32:CR:618:VAL:HG11	32:CR:627:PHE:CD2	2.43	0.53
32:CS:59:ALA:HB3	32:CS:125:LEU:HA	1.90	0.53
32:CS:345:ILE:HG22	32:CS:358:ARG:HB3	1.90	0.53
2:UB:782:SER:HB3	2:UB:786:ARG:HH12	1.72	0.53
3:UC:642:LEU:HD21	50:C1:1082:G:H5"	1.89	0.53
9:UL:92:ILE:HB	9:UL:106:PHE:HB2	1.90	0.53
9:UL:654:GLN:HB2	9:UL:672:ALA:HB3	1.91	0.53
11:UN:279:SER:HB2	53:UT:2200:ILE:HD11	1.90	0.53
17:UZ:116:PHE:HB3	17:UZ:120:LEU:HB2	1.89	0.53
22:CG:173:VAL:O	22:CG:561:ASN:ND2	2.42	0.53
27:CL:514:ASN:HB3	27:CL:517:LEU:HD12	1.88	0.53
32:CS:112:THR:O	32:CS:138:ARG:NH1	2.41	0.53
54:UH:827:MET:HE3	54:UH:831:ARG:HH12	1.73	0.53
2:UB:599:THR:HG21	56:US:523:ILE:HD13	1.90	0.53
3:UC:595:LYS:HA	3:UC:598:ARG:HG2	1.90	0.53
7:UJ:116:LYS:HE2	33:CT:69:LEU:HD12	1.91	0.53
7:UJ:1479:THR:HA	7:UJ:1522:LEU:HD11	1.91	0.53
9:UL:485:LYS:HA	9:UL:510:ALA:HA	1.91	0.53
15:UU:562:GLY:O	15:UU:620:ARG:NH2	2.37	0.53
16:UX:80:MET:HE2	16:UX:86:SER:HA	1.88	0.53
50:C1:697:U:H2'	50:C1:698:A:H8	1.73	0.53
53:UT:341:VAL:HG12	53:UT:345:MET:HE2	1.90	0.53
53:UT:1322:PRO:HA	53:UT:1325:LYS:HB2	1.90	0.53
53:UT:1617:ARG:HD3	53:UT:1689:ASN:HD21	1.74	0.53
53:UT:1943:VAL:HG12	53:UT:2005:LYS:HE3	1.89	0.53
7:UJ:1706:VAL:HA	7:UJ:1709:LEU:HG	1.89	0.53
10:UM:774:PHE:HA	10:UM:777:VAL:HG12	1.91	0.53
13:UQ:527:THR:HG23	13:UQ:529:GLU:H	1.73	0.53
14:UR:176:ARG:HG3	15:UU:241:LEU:HD13	1.89	0.53
29:CO:69:ASN:ND2	29:CO:72:GLU:OE1	2.42	0.53
13:UQ:156:LEU:HD23	13:UQ:168:ILE:HD11	1.91	0.53
13:UQ:616:ASP:OD2	13:UQ:617:LEU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:UX:107:ARG:O	16:UX:111:MET:HG3	2.09	0.53
19:CC:195:ALA:HB1	19:CC:216:ASN:HB3	1.91	0.53
35:Cb:100:ARG:NH2	35:Cb:121:TYR:O	2.42	0.53
50:C1:860:C:O2'	50:C1:862:U:OP2	2.26	0.53
53:UT:1638:VAL:HA	53:UT:1641:LEU:HD12	1.91	0.53
53:UT:1645:VAL:HG13	53:UT:1648:LEU:HD12	1.89	0.53
53:UT:1710:VAL:HG12	53:UT:1739:ILE:HG23	1.90	0.53
53:UT:1849:LYS:N	53:UT:1851:GLN:OE1	2.42	0.53
9:UL:701:ALA:HB3	9:UL:714:ALA:HB3	1.89	0.53
18:CB:230:VAL:HG22	18:CB:232:GLN:HG2	1.91	0.53
28:CM:47:VAL:HB	28:CM:379:LEU:HD21	1.91	0.53
29:CO:130:ILE:HD12	29:CO:131:PRO:HD2	1.90	0.53
32:CR:249:ILE:HA	32:CR:252:LEU:HD12	1.90	0.53
32:CR:282:THR:HG23	32:CR:469:LEU:HD11	1.90	0.53
36:Cc:57:ILE:HD11	43:Cj:47:LYS:HG2	1.90	0.53
55:UE:153:LEU:HD11	56:US:302:MET:HG2	1.89	0.53
58:CX:374:ARG:NH2	58:CX:419:GLN:OE1	2.42	0.53
1:UA:544:GLN:OE1	43:Cj:114:ARG:NE	2.42	0.53
5:UF:92:THR:HA	5:UF:95:ILE:HD12	1.90	0.53
5:UF:285:VAL:HA	5:UF:288:LYS:HG2	1.91	0.53
10:UM:815:ASP:O	10:UM:818:THR:OG1	2.26	0.53
17:UZ:215:ARG:HB3	17:UZ:220:ILE:HD11	1.91	0.53
18:CA:238:ILE:O	18:CA:242:ASN:ND2	2.33	0.53
29:CO:175:CYS:HA	29:CO:201:SER:O	2.09	0.53
32:CS:312:ILE:HG12	32:CS:387:VAL:HB	1.89	0.53
41:Ch:104:ARG:NH2	50:C1:1535:C:O2'	2.42	0.53
47:Co:369:ASP:O	47:Co:383:LYS:NZ	2.41	0.53
53:UT:467:CYS:HA	53:UT:537:VAL:HG21	1.91	0.53
54:UH:743:ARG:HH22	54:UH:818:GLU:HG3	1.74	0.53
58:CX:278:ILE:HD13	58:CX:320:GLU:HG3	1.90	0.53
7:UJ:236:ARG:HD2	7:UJ:239:ILE:HD12	1.91	0.53
12:UO:23:GLU:OE2	12:UO:27:TRP:NE1	2.42	0.53
16:UX:114:ARG:NH2	28:CM:349:ASN:OD1	2.40	0.53
20:CD:190:TYR:HD1	20:CD:257:ILE:HG21	1.73	0.53
21:CF:33:GLN:HG2	21:CF:106:ASN:HB3	1.90	0.53
24:CI:620:ARG:HA	24:CI:624:PHE:HB2	1.91	0.53
37:Cd:74:ARG:NH2	50:C1:1004:A2M:OP2	2.41	0.53
54:UH:4:LYS:HZ3	54:UH:601:GLU:HA	1.74	0.53
58:CX:371:LEU:HD21	58:CX:417:PHE:HB2	1.89	0.53
7:UJ:1487:SER:HA	7:UJ:1490:LYS:HE2	1.91	0.52
7:UJ:1499:TYR:HA	7:UJ:1502:ILE:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:UL:589:VAL:HB	9:UL:603:LEU:HB2	1.90	0.52
9:UL:816:PRO:HA	9:UL:819:VAL:HG22	1.91	0.52
12:UO:206:VAL:HG21	12:UO:247:LEU:HD11	1.91	0.52
35:Cb:171:ASP:OD1	35:Cb:172:PHE:N	2.39	0.52
53:UT:148:ILE:HG21	53:UT:168:LEU:HD13	1.91	0.52
53:UT:326:VAL:HG12	53:UT:330:MET:HE1	1.92	0.52
53:UT:1909:GLN:OE1	53:UT:1985:ASN:ND2	2.40	0.52
60:CZ:279:ASP:OD1	60:CZ:282:ARG:NH2	2.42	0.52
1:UA:577:THR:HG21	1:UA:677:GLY:HA2	1.92	0.52
4:UD:377:ALA:HB3	4:UD:382:TYR:HB2	1.90	0.52
4:UD:500:SER:O	4:UD:528:ARG:NH1	2.42	0.52
9:UL:511:VAL:HA	9:UL:527:GLY:HA3	1.90	0.52
15:UU:835:GLN:NE2	15:UU:985:ARG:O	2.43	0.52
21:CE:35:LYS:HB2	21:CE:102:SER:HB3	1.90	0.52
22:CG:313:LYS:NZ	22:CG:322:TYR:OH	2.39	0.52
37:Cd:85:ARG:HH12	50:C1:745:U:H5"	1.73	0.52
50:C1:1016:G:H5"	50:C1:1017:C:H5"	1.90	0.52
7:UJ:556:LEU:HD21	7:UJ:592:ILE:HG23	1.90	0.52
7:UJ:1429:ILE:O	7:UJ:1431:TYR:N	2.41	0.52
12:UO:14:PRO:HA	55:UE:35:VAL:HG13	1.90	0.52
18:CB:234:ASP:OD2	18:CB:237:ARG:NH2	2.43	0.52
22:CG:151:ARG:HH22	22:CG:494:GLU:HB3	1.74	0.52
24:CI:86:LYS:HG3	24:CI:100:PRO:HG3	1.90	0.52
32:CR:196:CYS:HB2	32:CR:489:TRP:CD1	2.45	0.52
32:CR:633:ALA:O	32:CR:723:VAL:HA	2.09	0.52
32:CR:840:ARG:NH2	32:CR:853:VAL:O	2.42	0.52
32:CS:311:PHE:O	32:CS:386:VAL:HA	2.09	0.52
53:UT:737:MET:HE3	53:UT:740:VAL:HG21	1.91	0.52
53:UT:1578:PRO:HA	53:UT:1581:GLU:HG2	1.91	0.52
53:UT:1783:LYS:O	53:UT:1787:LEU:N	2.41	0.52
1:UA:347:VAL:HG11	1:UA:389:GLU:HA	1.90	0.52
6:UG:457:GLU:HB2	11:UN:878:LYS:HB3	1.91	0.52
7:UJ:256:SER:HB2	14:UR:230:LEU:HD23	1.89	0.52
7:UJ:974:LYS:HD2	7:UJ:1017:THR:HG21	1.90	0.52
7:UJ:1600:LEU:HA	7:UJ:1603:VAL:HG22	1.92	0.52
9:UL:113:ILE:HD13	9:UL:129:SER:HB3	1.90	0.52
10:UM:271:MET:HG2	10:UM:273:ARG:HH12	1.75	0.52
14:UR:453:GLY:HA3	14:UR:526:ILE:HG13	1.90	0.52
16:UX:62:THR:HG23	16:UX:99:LEU:HG	1.91	0.52
53:UT:130:ALA:O	53:UT:133:LEU:O	2.28	0.52
53:UT:287:LYS:HD3	53:UT:290:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:2176:MET:HE1	53:UT:2214:CYS:HA	1.91	0.52
53:UT:2199:PHE:HE2	53:UT:2241:LEU:HG	1.73	0.52
54:UH:777:ALA:HA	54:UH:780:MET:HE2	1.92	0.52
4:UD:884:ARG:NH2	50:C1:71:A:O2'	2.35	0.52
7:UJ:752:TRP:NE1	7:UJ:775:ASP:OD1	2.39	0.52
9:UL:590:LYS:NZ	9:UL:602:ASN:OD1	2.43	0.52
10:UM:786:ASP:OD1	10:UM:786:ASP:N	2.42	0.52
24:CI:56:VAL:HG22	46:Cn:52:ILE:HG12	1.92	0.52
29:CN:19:LEU:HB3	56:US:482:PHE:HB2	1.92	0.52
32:CR:826:LYS:HE3	32:CR:927:VAL:HA	1.92	0.52
38:Ce:76:PHE:O	38:Ce:79:VAL:C	2.52	0.52
39:Cf:41:LYS:NZ	50:C1:844:U:O5'	2.38	0.52
44:Ck:38:ARG:NH1	44:Ck:53:ALA:O	2.42	0.52
53:UT:1310:THR:O	53:UT:1314:ASN:ND2	2.43	0.52
1:UA:21:LEU:HB2	1:UA:30:PHE:HB2	1.91	0.52
7:UJ:608:ARG:NH1	7:UJ:668:VAL:O	2.42	0.52
7:UJ:1615:LYS:HE2	7:UJ:1660:HIS:HB2	1.92	0.52
11:UN:329:THR:HG21	11:UN:933:MET:HE1	1.92	0.52
13:UQ:765:TYR:OH	13:UQ:819:GLU:O	2.28	0.52
24:CI:56:VAL:O	50:C1:1018:G:N1	2.38	0.52
26:CK:108:ARG:HH21	26:CK:109:LEU:HD23	1.74	0.52
29:CO:39:VAL:HG11	29:CO:99:LEU:HD11	1.91	0.52
32:CR:389:ASP:HA	32:CR:411:ALA:HB3	1.92	0.52
43:Cj:126:PRO:HB3	50:C1:2166:A:H5"	1.92	0.52
58:CX:390:LEU:HD13	58:CX:432:ALA:HB1	1.91	0.52
58:CX:427:GLU:HA	58:CX:430:ARG:HE	1.73	0.52
2:UB:700:ARG:HH21	2:UB:702:LEU:HA	1.74	0.52
7:UJ:1754:GLU:O	7:UJ:1758:HIS:ND1	2.41	0.52
10:UM:249:SER:OG	10:UM:257:THR:OG1	2.27	0.52
20:CD:361:ILE:HG13	20:CD:405:LEU:HD13	1.91	0.52
20:CD:378:PHE:HB2	21:CE:63:SER:HB3	1.91	0.52
21:CE:63:SER:HA	21:CE:66:LEU:HB2	1.90	0.52
29:CN:246:GLU:HG3	29:CN:251:ILE:HB	1.92	0.52
42:Ci:134:THR:O	50:C1:1471:U:O2'	2.27	0.52
53:UT:1470:TRP:O	53:UT:1475:GLN:NE2	2.40	0.52
55:UI:178:LEU:HD13	55:UI:216:ARG:HH12	1.75	0.52
3:UC:458:THR:HB	56:US:473:THR:OG1	2.10	0.52
6:UG:204:ASP:OD2	16:UX:13:ARG:NH2	2.43	0.52
10:UM:741:GLN:HE21	10:UM:764:LEU:HD21	1.75	0.52
32:CS:41:LEU:HD23	32:CS:44:ILE:HD12	1.91	0.52
32:CS:876:LEU:HB3	32:CS:880:GLN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:310:ILE:HG23	53:UT:353:ARG:HG3	1.92	0.52
60:CZ:539:SER:OG	60:CZ:542:ARG:NH2	2.43	0.52
55:UI:158:ASN:HB2	55:UI:162:ARG:NH1	2.24	0.52
1:UA:162:ASP:OD1	1:UA:207:GLN:NE2	2.38	0.52
7:UJ:1291:VAL:O	7:UJ:1339:TYR:OH	2.22	0.52
13:UQ:273:SER:N	13:UQ:276:GLU:OE2	2.39	0.52
15:UU:137:LEU:HD12	15:UU:158:ARG:HD3	1.92	0.52
15:UU:441:ARG:NH1	51:C2:68:A:OP1	2.43	0.52
30:CP:141:GLN:HG3	49:CU:257:ARG:HH21	1.75	0.52
47:Co:345:ARG:NE	53:UT:73:LEU:O	2.39	0.52
50:C1:849:A:N7	50:C1:874:G:N2	2.58	0.52
53:UT:427:ILE:O	53:UT:431:SER:CB	2.58	0.52
53:UT:1581:GLU:HA	53:UT:1584:ILE:HG12	1.91	0.52
53:UT:1752:GLU:HA	53:UT:1755:ARG:HD2	1.92	0.52
55:UI:220:TRP:HA	55:UI:223:VAL:HG22	1.91	0.52
1:UA:732:LYS:O	1:UA:736:MET:HG3	2.10	0.52
5:UF:287:ARG:HA	5:UF:292:TRP:CD2	2.45	0.52
7:UJ:1001:PRO:HA	7:UJ:1004:ILE:HG12	1.92	0.52
7:UJ:1255:LEU:HD12	7:UJ:1258:LEU:HD12	1.92	0.52
7:UJ:1475:ARG:O	7:UJ:1518:ASN:ND2	2.42	0.52
10:UM:192:ILE:HA	10:UM:195:ARG:HG3	1.90	0.52
10:UM:477:GLY:O	10:UM:539:ARG:NH1	2.43	0.52
14:UR:400:ILE:HB	14:UR:410:ALA:HB3	1.91	0.52
17:UZ:180:ILE:HD13	17:UZ:232:LEU:HD12	1.91	0.52
22:CG:262:VAL:HG11	22:CG:303:LEU:HD11	1.92	0.52
23:CH:375:TRP:O	24:CI:763:HIS:NE2	2.43	0.52
24:CI:1076:MET:HA	24:CI:1079:ARG:HG2	1.92	0.52
27:CL:561:ARG:NH2	27:CL:564:MET:SD	2.83	0.52
53:UT:198:LYS:HA	53:UT:247:GLN:HE22	1.74	0.52
53:UT:1348:GLN:HA	53:UT:1351:VAL:HG22	1.92	0.52
53:UT:1746:LYS:O	53:UT:1751:ARG:NH2	2.41	0.52
53:UT:2136:ARG:HH11	53:UT:2181:LEU:HD11	1.74	0.52
54:UH:702:HIS:CD2	54:UH:705:ARG:HH22	2.28	0.52
58:CX:298:LYS:HD3	58:CX:299:PRO:HD2	1.92	0.52
2:UB:686:PRO:HD2	2:UB:689:ILE:HG13	1.92	0.51
4:UD:840:PRO:HA	4:UD:860:VAL:HG23	1.92	0.51
6:UG:202:ILE:HB	6:UG:211:HIS:HB2	1.91	0.51
10:UM:200:TRP:HZ3	10:UM:210:PHE:HB2	1.75	0.51
10:UM:579:GLN:OE1	10:UM:612:ARG:NH2	2.44	0.51
20:CD:220:ALA:O	20:CD:238:LYS:NZ	2.33	0.51
22:CG:123:PHE:HZ	35:Cb:237:LEU:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:CI:1053:ASN:ND2	50:C1:2068:C:OP1	2.43	0.51
32:CS:634:ARG:HH21	32:CS:636:VAL:HG22	1.75	0.51
35:Cb:183:ILE:O	35:Cb:190:GLY:CA	2.58	0.51
43:Cj:42:GLU:HA	43:Cj:45:ARG:HB2	1.92	0.51
3:UC:639:LYS:HD2	33:CT:123:LYS:HB3	1.92	0.51
7:UJ:1086:TYR:CZ	7:UJ:1094:LYS:HD3	2.45	0.51
7:UJ:1754:GLU:HG2	7:UJ:1758:HIS:HE1	1.75	0.51
7:UJ:1778:VAL:HA	7:UJ:1781:GLU:HG3	1.92	0.51
32:CR:308:SER:N	32:CR:384:GLU:OE2	2.40	0.51
34:Ca:32:ILE:HG22	34:Ca:96:CYS:HB3	1.91	0.51
35:Cb:86:PHE:HD2	35:Cb:87:MET:HG2	1.75	0.51
41:Ch:108:ASP:O	41:Ch:111:SER:OG	2.27	0.51
52:CW:137:ARG:NH1	52:CW:167:GLU:OE2	2.43	0.51
54:UH:588:THR:HG23	54:UH:609:ILE:HD11	1.92	0.51
1:UA:385:VAL:HA	1:UA:401:SER:HB2	1.92	0.51
10:UM:117:LEU:HG	10:UM:128:THR:HG22	1.93	0.51
13:UQ:762:LEU:HD21	54:UH:440:ARG:HH11	1.75	0.51
22:CG:167:ARG:HE	22:CG:598:ARG:HH12	1.56	0.51
32:CR:313:THR:HG22	32:CR:388:ILE:HG22	1.92	0.51
32:CS:99:ILE:HG23	32:CS:104:ILE:HD13	1.92	0.51
40:Cg:55:ARG:NH1	40:Cg:59:THR:OG1	2.43	0.51
53:UT:693:THR:HA	53:UT:696:MET:HE2	1.91	0.51
54:UH:4:LYS:NZ	54:UH:601:GLU:HA	2.26	0.51
54:UH:494:TRP:CD2	54:UH:498:MET:HE1	2.45	0.51
1:UA:774:LEU:HD22	1:UA:819:VAL:HG21	1.92	0.51
2:UB:559:LEU:HA	2:UB:562:THR:HG22	1.92	0.51
7:UJ:495:LEU:HD21	7:UJ:520:VAL:HG21	1.92	0.51
21:CF:63:SER:HA	21:CF:66:LEU:HB2	1.92	0.51
52:CW:21:ARG:O	53:UT:968:ARG:NH2	2.42	0.51
3:UC:608:TYR:OH	40:Cg:31:GLU:OE2	2.25	0.51
24:CI:354:THR:HG22	32:CR:4:GLN:HG2	1.93	0.51
27:CL:82:LEU:HD13	27:CL:130:VAL:HG21	1.93	0.51
28:CM:308:ARG:NH1	28:CM:317:SER:OG	2.43	0.51
40:Cg:171:ARG:HD3	50:C1:1095:A:H5"	1.92	0.51
44:Ck:51:LYS:HD2	44:Ck:54:ILE:HD12	1.93	0.51
50:C1:925:G:OP1	52:CW:119:ARG:NE	2.40	0.51
52:CW:23:LEU:HD12	52:CW:27:LEU:HD23	1.91	0.51
53:UT:1388:VAL:HA	53:UT:1391:ILE:HD12	1.92	0.51
58:CX:360:VAL:HG12	58:CX:362:ALA:H	1.75	0.51
7:UJ:1766:TYR:HA	7:UJ:1769:GLU:HG3	1.93	0.51
9:UL:353:VAL:HA	9:UL:356:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:UO:121:GLY:HA2	12:UO:147:VAL:HG23	1.92	0.51
15:UU:847:PRO:HD2	15:UU:850:ARG:HH21	1.74	0.51
21:CF:106:ASN:HD21	21:CF:111:LEU:HD23	1.75	0.51
22:CG:583:GLY:HA2	22:CG:599:CYS:HA	1.92	0.51
32:CS:20:GLN:HG2	32:CS:220:LEU:HD11	1.93	0.51
32:CS:883:ILE:HG12	32:CS:897:LEU:HD21	1.93	0.51
34:Ca:40:VAL:HB	34:Ca:73:LEU:HD12	1.93	0.51
50:C1:62:U:C2	54:UH:894:ARG:HG3	2.46	0.51
50:C1:1230:U:H2'	50:C1:1231:A:H8	1.75	0.51
53:UT:585:TYR:O	53:UT:589:CYS:CB	2.59	0.51
53:UT:1037:ASP:O	53:UT:1040:LEU:O	2.28	0.51
53:UT:1516:LEU:O	53:UT:1518:GLN:N	2.43	0.51
53:UT:1982:THR:OG1	53:UT:1985:ASN:OD1	2.29	0.51
54:UH:875:ASN:O	54:UH:903:ARG:NH2	2.44	0.51
56:US:204:ILE:HG21	56:US:227:LEU:HD11	1.92	0.51
59:CY:41:LEU:HD11	60:CZ:318:ARG:HH21	1.74	0.51
4:UD:758:ARG:HG2	4:UD:768:TRP:HE3	1.76	0.51
10:UM:70:THR:HB	10:UM:123:SER:HB2	1.92	0.51
13:UQ:104:ILE:HG12	13:UQ:113:VAL:HG22	1.92	0.51
15:UU:140:PRO:HD2	15:UU:156:LEU:HD23	1.92	0.51
18:CA:239:VAL:HG21	18:CA:255:ILE:HD12	1.91	0.51
22:CG:100:ARG:HG3	40:Cg:68:LEU:HD23	1.92	0.51
28:CM:242:CYS:HA	28:CM:259:SER:HA	1.91	0.51
37:Cd:94:ARG:NH2	52:CW:89:LEU:O	2.43	0.51
37:Cd:159:ARG:NH1	50:C1:665:C:OP1	2.44	0.51
54:UH:543:ARG:HA	54:UH:546:VAL:HG22	1.93	0.51
1:UA:29:LEU:HD21	1:UA:322:LEU:HD11	1.91	0.51
2:UB:489:LEU:HA	2:UB:492:VAL:HG12	1.92	0.51
4:UD:96:ILE:HG12	4:UD:536:HIS:HB2	1.92	0.51
4:UD:108:THR:HG21	61:UP:333:PRO:HG2	1.92	0.51
18:CB:222:MET:HG2	20:CD:124:GLN:HA	1.92	0.51
18:CB:226:ILE:HD12	18:CB:247:LEU:HD22	1.93	0.51
19:CC:248:GLN:HA	19:CC:252:LEU:HB2	1.93	0.51
31:CQ:112:GLN:HB3	31:CQ:125:ARG:HB3	1.91	0.51
31:CQ:212:ALA:HB3	31:CQ:215:LYS:HB2	1.92	0.51
37:Cd:30:LYS:H	37:Cd:102:VAL:HG12	1.76	0.51
54:UH:879:THR:HG23	54:UH:880:GLU:HG3	1.92	0.51
55:UE:25:LYS:NZ	55:UE:27:ARG:O	2.44	0.51
59:CY:110:GLN:HA	59:CY:113:LYS:HE3	1.93	0.51
7:UJ:1213:ASP:OD1	7:UJ:1217:ALA:N	2.39	0.51
7:UJ:1380:ASP:OD1	7:UJ:1427:GLN:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CG:252:VAL:HG12	22:CG:263:THR:HG22	1.93	0.51
22:CG:343:ARG:HG3	22:CG:358:LYS:HA	1.93	0.51
24:CI:612:ASN:HD22	24:CI:612:ASN:C	2.17	0.51
24:CI:1094:MET:HE1	33:CT:108:LEU:HD13	1.93	0.51
28:CM:224:LEU:HB2	28:CM:234:ILE:HG22	1.93	0.51
32:CS:33:HIS:NE2	32:CS:205:GLU:OE2	2.40	0.51
32:CS:357:VAL:HG13	32:CS:370:GLN:HE22	1.75	0.51
38:Ce:55:ILE:HD11	38:Ce:185:ARG:HG2	1.92	0.51
53:UT:1783:LYS:HB3	53:UT:1786:GLN:HG3	1.93	0.51
54:UH:355:LEU:HD22	54:UH:414:ILE:HD11	1.93	0.51
4:UD:14:SER:O	4:UD:48:ARG:NH1	2.44	0.51
4:UD:800:LEU:HD13	7:UJ:664:LEU:HD23	1.93	0.51
6:UG:372:ASN:HB3	6:UG:375:ARG:HG2	1.93	0.51
15:UU:274:ALA:HB1	15:UU:302:THR:HG21	1.92	0.51
37:Cd:78:SER:OG	37:Cd:92:ARG:NH1	2.44	0.51
42:Ci:133:PRO:HB3	50:C1:1472:A:H5”	1.91	0.51
53:UT:663:SER:HB3	53:UT:836:ILE:HG21	1.93	0.51
54:UH:754:ARG:HG3	54:UH:755:TYR:H	1.76	0.51
2:UB:689:ILE:O	2:UB:722:GLN:NE2	2.43	0.50
2:UB:701:GLN:HE21	56:US:542:TRP:HA	1.76	0.50
4:UD:443:LEU:HD22	4:UD:456:LEU:HD11	1.93	0.50
7:UJ:664:LEU:O	7:UJ:667:SER:OG	2.29	0.50
15:UU:752:THR:OG1	15:UU:768:GLU:OE2	2.29	0.50
30:CP:49:ARG:HH12	30:CP:53:ASP:HB3	1.76	0.50
32:CR:5:LYS:NZ	32:CR:205:GLU:O	2.42	0.50
50:C1:934:A:H5”	50:C1:936:A:H5’	1.93	0.50
53:UT:176:SER:O	53:UT:180:VAL:HB	2.11	0.50
1:UA:195:ARG:NH1	50:C1:285:A:OP1	2.45	0.50
1:UA:705:GLN:HE21	15:UU:674:HIS:HE1	1.59	0.50
7:UJ:232:MET:HB3	7:UJ:243:ASN:HB3	1.93	0.50
7:UJ:563:TYR:H	7:UJ:568:LYS:NZ	2.09	0.50
11:UN:927:GLN:HE22	28:CM:339:LYS:NZ	2.09	0.50
32:CR:231:PRO:HA	32:CR:234:LYS:HE2	1.91	0.50
38:Ce:38:ALA:HA	38:Ce:39:ASP:HB2	1.93	0.50
38:Ce:50:VAL:HG21	38:Ce:68:VAL:HG22	1.94	0.50
43:Cj:35:PRO:HG2	43:Cj:38:LEU:HD12	1.94	0.50
50:C1:61:G:O6	54:UH:904:ARG:NH1	2.44	0.50
53:UT:1042:PRO:HB2	53:UT:1064:LEU:HD11	1.93	0.50
10:UM:349:PRO:HG3	10:UM:361:ILE:HG21	1.94	0.50
10:UM:520:GLN:HG2	10:UM:539:ARG:HB2	1.93	0.50
16:UX:104:PRO:HA	16:UX:107:ARG:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CS:277:LEU:HB3	32:CS:406:TYR:HA	1.93	0.50
36:Cc:91:ASN:OD1	50:C1:2170:A:O2'	2.26	0.50
53:UT:107:LEU:HD21	53:UT:126:VAL:HG22	1.91	0.50
56:US:86:ARG:HA	56:US:89:VAL:HG22	1.93	0.50
1:UA:538:SER:OG	1:UA:541:GLU:O	2.29	0.50
2:UB:584:LEU:HD22	2:UB:625:LYS:HB2	1.92	0.50
7:UJ:521:PHE:O	7:UJ:525:ALA:HB2	2.11	0.50
10:UM:257:THR:OG1	10:UM:259:TRP:NE1	2.44	0.50
17:UZ:77:ARG:NH2	50:C1:373:C:O2'	2.45	0.50
29:CN:225:ILE:HD11	29:CN:241:PHE:HZ	1.76	0.50
32:CS:14:LEU:HA	32:CS:17:ASN:HD22	1.77	0.50
32:CS:565:HIS:CD2	32:CS:589:SER:HB2	2.47	0.50
35:Cb:160:VAL:HG11	35:Cb:169:ILE:HD12	1.92	0.50
40:Cg:50:ILE:HD13	40:Cg:78:LEU:HD21	1.93	0.50
40:Cg:126:LEU:HD23	40:Cg:129:GLN:HE21	1.77	0.50
54:UH:502:PHE:HD1	54:UH:541:VAL:HG21	1.76	0.50
1:UA:633:ALA:HB2	6:UG:175:GLN:HE21	1.76	0.50
4:UD:570:ILE:HD11	4:UD:626:LEU:HD11	1.94	0.50
4:UD:833:ARG:NH2	50:C1:64:C:OP1	2.44	0.50
12:UO:235:ILE:HD13	12:UO:251:SER:HB3	1.93	0.50
13:UQ:567:LEU:HD11	13:UQ:573:GLN:HG2	1.93	0.50
22:CG:184:TYR:HE1	22:CG:194:LYS:HG3	1.75	0.50
26:CK:80:LEU:HB3	26:CK:84:VAL:HG22	1.94	0.50
32:CS:725:VAL:HG12	32:CS:762:MET:HB2	1.94	0.50
35:Cb:42:MET:HE1	35:Cb:47:PHE:HD1	1.77	0.50
44:Ck:137:SER:O	44:Ck:141:ARG:NH1	2.44	0.50
45:Cm:32:LYS:HA	45:Cm:35:VAL:HG12	1.94	0.50
4:UD:686:ARG:NH1	50:C1:63:C:O2	2.44	0.50
7:UJ:654:ALA:O	7:UJ:658:SER:CB	2.58	0.50
10:UM:865:VAL:HG12	27:CL:679:PRO:HG3	1.94	0.50
19:CC:385:LYS:NZ	51:C2:194:G:OP1	2.37	0.50
21:CE:41:THR:HG23	21:CE:102:SER:HB2	1.93	0.50
22:CG:152:LEU:HB3	22:CG:156:LEU:HD23	1.94	0.50
32:CR:317:PRO:HD3	32:CR:371:TYR:CZ	2.47	0.50
32:CR:570:LEU:HB3	32:CR:584:CYS:HB3	1.92	0.50
35:Cb:19:LEU:HD11	35:Cb:108:ARG:HD2	1.94	0.50
41:Ch:108:ASP:OD1	41:Ch:111:SER:OG	2.30	0.50
51:C2:126:U:H4'	51:C2:127:A:H5"	1.94	0.50
2:UB:733:LEU:HD22	2:UB:780:LEU:HD21	1.94	0.50
4:UD:425:ILE:HD13	4:UD:431:ILE:HD11	1.92	0.50
6:UG:148:GLY:O	6:UG:166:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:UJ:794:PHE:HA	7:UJ:797:VAL:HG22	1.92	0.50
7:UJ:1500:LEU:HB3	7:UJ:1553:ILE:HG12	1.94	0.50
9:UL:71:THR:OG1	9:UL:113:ILE:O	2.25	0.50
9:UL:864:PHE:O	9:UL:867:ARG:O	2.30	0.50
13:UQ:846:VAL:HG22	13:UQ:852:VAL:HG12	1.93	0.50
23:CH:160:LEU:HA	23:CH:163:LEU:HD12	1.94	0.50
23:CH:222:ALA:HB2	23:CH:279:LEU:HD13	1.93	0.50
26:CK:89:LEU:HB2	26:CK:136:LEU:HD13	1.93	0.50
28:CM:95:ASP:OD1	28:CM:95:ASP:N	2.45	0.50
32:CR:181:VAL:HG22	32:CR:563:PRO:HG3	1.92	0.50
32:CR:284:THR:O	32:CR:473:THR:HA	2.11	0.50
32:CR:366:ARG:NH1	32:CS:383:ALA:O	2.42	0.50
50:C1:372:U:H3	50:C1:394:U:H3	1.59	0.50
53:UT:645:HIS:ND1	53:UT:647:GLU:OE1	2.40	0.50
53:UT:2092:ARG:NE	53:UT:2131:THR:OG1	2.44	0.50
2:UB:743:LEU:HG	56:US:462:GLN:NE2	2.25	0.50
7:UJ:201:LEU:HD11	7:UJ:254:VAL:HG13	1.94	0.50
7:UJ:296:LEU:HD22	7:UJ:312:LEU:HG	1.94	0.50
7:UJ:988:GLY:HA2	7:UJ:991:LEU:HB2	1.94	0.50
7:UJ:1425:LEU:HA	7:UJ:1429:ILE:HD11	1.94	0.50
7:UJ:1448:SER:O	7:UJ:1461:ARG:NH2	2.44	0.50
9:UL:25:VAL:HB	9:UL:40:ILE:HB	1.93	0.50
15:UU:885:GLN:NE2	15:UU:894:GLN:OE1	2.44	0.50
53:UT:2157:LEU:HA	53:UT:2160:ILE:HG22	1.94	0.50
59:CY:57:PHE:HD1	59:CY:60:LEU:HD12	1.77	0.50
1:UA:704:VAL:O	15:UU:720:ARG:NH2	2.43	0.50
7:UJ:1534:ARG:HG3	7:UJ:1598:TYR:HB3	1.94	0.50
22:CG:472:LEU:HB3	22:CG:475:SER:HB2	1.93	0.50
23:CH:232:ASN:O	23:CH:236:ILE:HG12	2.12	0.50
32:CR:914:LYS:HA	32:CR:917:ARG:HG2	1.93	0.50
5:UF:10:PHE:HB2	11:UN:912:LYS:HD3	1.94	0.49
9:UL:209:ILE:O	10:UM:743:GLN:NE2	2.44	0.49
32:CS:162:LEU:HA	32:CS:165:MET:HB2	1.94	0.49
32:CS:183:ALA:HB1	32:CS:186:ASN:HD21	1.77	0.49
32:CS:622:PHE:HZ	32:CS:782:PHE:HB2	1.77	0.49
32:CS:727:TYR:HE1	32:CS:762:MET:HE3	1.77	0.49
43:Cj:97:VAL:HG12	43:Cj:98:ASP:H	1.77	0.49
53:UT:617:LEU:HD12	53:UT:666:LEU:HG	1.94	0.49
56:US:142:ALA:HA	56:US:145:VAL:HG22	1.94	0.49
56:US:206:HIS:HA	56:US:209:THR:HG22	1.93	0.49
2:UB:471:ASP:OD2	2:UB:506:ARG:NH2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:UJ:1623:SER:OG	7:UJ:1671:HIS:NE2	2.37	0.49
7:UJ:1800:MET:HG2	7:UJ:1801:LEU:HD12	1.94	0.49
10:UM:635:ILE:HG22	10:UM:636:ARG:HG3	1.94	0.49
15:UU:131:LEU:HD23	15:UU:162:TRP:CD2	2.46	0.49
15:UU:343:ILE:HG22	15:UU:354:THR:HG22	1.94	0.49
24:CI:93:THR:HG21	24:CI:334:LEU:HB2	1.93	0.49
28:CM:26:ASN:HB3	28:CM:31:LEU:HD22	1.94	0.49
29:CN:164:GLN:HB3	50:C1:2158:G:H5"	1.93	0.49
30:CP:160:THR:HG22	30:CP:173:GLY:HA3	1.94	0.49
53:UT:1036:LEU:HD22	53:UT:1094:LEU:HD11	1.93	0.49
53:UT:1100:TYR:O	53:UT:1104:ASN:ND2	2.45	0.49
7:UJ:758:ASN:OD1	7:UJ:759:GLU:N	2.45	0.49
7:UJ:1357:ASP:O	7:UJ:1368:ARG:NH2	2.45	0.49
7:UJ:1427:GLN:HB3	7:UJ:1428:HIS:ND1	2.27	0.49
7:UJ:1672:PHE:HA	7:UJ:1675:VAL:HG22	1.94	0.49
10:UM:442:ASP:HB3	10:UM:447:TRP:HB2	1.94	0.49
16:UX:110:LEU:HG	16:UX:114:ARG:HD2	1.94	0.49
19:CC:196:MET:HA	19:CC:199:ARG:HE	1.77	0.49
22:CG:123:PHE:HB2	35:Cb:105:THR:HG23	1.93	0.49
23:CH:209:ASN:HD21	23:CH:348:ARG:HB2	1.77	0.49
29:CO:190:ARG:HA	29:CO:193:VAL:HG22	1.93	0.49
32:CR:767:GLN:HG3	32:CR:769:GLY:H	1.76	0.49
32:CR:824:LEU:HB2	32:CR:869:ARG:HG3	1.94	0.49
4:UD:51:GLY:HA2	4:UD:77:VAL:HG23	1.94	0.49
7:UJ:1058:PRO:HG3	7:UJ:1105:LEU:HA	1.94	0.49
7:UJ:1284:LEU:HD21	7:UJ:1328:ALA:HA	1.94	0.49
14:UR:322:ARG:NH2	50:C1:133:G:H22	2.11	0.49
22:CG:151:ARG:HH12	22:CG:494:GLU:HA	1.76	0.49
32:CR:272:ILE:HG23	32:CR:307:TYR:HE2	1.76	0.49
32:CS:250:GLY:HA2	32:CS:253:ILE:HG22	1.94	0.49
32:CS:596:LYS:HA	32:CS:599:ILE:HD12	1.94	0.49
34:Ca:191:GLU:OE1	34:Ca:211:HIS:ND1	2.45	0.49
36:Cc:99:ARG:NH1	50:C1:2111:U:OP1	2.41	0.49
53:UT:1338:LEU:O	53:UT:1381:ARG:NH1	2.45	0.49
53:UT:1692:PRO:HA	53:UT:1695:LEU:HD12	1.95	0.49
2:UB:782:SER:HB3	2:UB:786:ARG:NH1	2.28	0.49
11:UN:354:ALA:HB2	19:CC:87:PRO:HG3	1.94	0.49
13:UQ:615:PHE:H	13:UQ:630:GLY:HA2	1.77	0.49
19:CC:299:MET:HG3	19:CC:307:GLN:HB2	1.95	0.49
26:CK:131:ALA:HB2	26:CK:139:ILE:HD11	1.94	0.49
32:CR:571:THR:HG22	32:CR:582:PRO:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CS:39:VAL:HG11	32:CS:94:PRO:HB3	1.94	0.49
34:Ca:26:ARG:HA	34:Ca:50:ARG:HH11	1.76	0.49
35:Cb:125:LYS:H	35:Cb:142:HIS:CD2	2.30	0.49
35:Cb:180:LEU:N	35:Cb:229:GLY:O	2.44	0.49
38:Ce:163:ILE:HA	38:Ce:194:GLU:O	2.12	0.49
40:Cg:36:ASN:HD21	40:Cg:38:ARG:NH2	2.11	0.49
53:UT:1479:ILE:HA	53:UT:1482:VAL:HG12	1.94	0.49
54:UH:736:LEU:O	54:UH:740:ASN:ND2	2.35	0.49
59:CY:316:GLU:O	59:CY:320:ARG:HG3	2.12	0.49
60:CZ:325:LEU:HD21	60:CZ:502:LEU:HB2	1.95	0.49
7:UJ:191:ASP:OD1	7:UJ:192:LEU:N	2.46	0.49
9:UL:60:ARG:HD2	9:UL:62:ARG:HH11	1.78	0.49
24:CI:346:ILE:HG12	24:CI:351:ILE:HG12	1.94	0.49
28:CM:422:GLU:O	28:CM:426:SER:HB2	2.13	0.49
32:CS:309:ASN:ND2	32:CS:382:GLN:O	2.45	0.49
50:C1:1029:A:H61	50:C1:1046:G:H1'	1.78	0.49
54:UH:789:LEU:HG	54:UH:793:MET:HE1	1.94	0.49
59:CY:96:LEU:HD23	59:CY:100:THR:HG21	1.94	0.49
2:UB:512:HIS:O	2:UB:519:ASN:ND2	2.38	0.49
13:UQ:466:LEU:HB2	13:UQ:832:ILE:HG12	1.95	0.49
14:UR:562:LYS:NZ	50:C1:237:G:OP1	2.43	0.49
15:UU:565:ILE:HB	15:UU:579:PHE:HB2	1.95	0.49
16:UX:13:ARG:HB3	25:CJ:19:ILE:HG13	1.95	0.49
19:CC:40:THR:HG22	19:CC:42:ASP:H	1.76	0.49
32:CR:158:SER:HA	32:CR:161:GLN:HB3	1.95	0.49
32:CS:38:ILE:HG12	32:CS:150:VAL:HG11	1.95	0.49
32:CS:570:LEU:HD22	32:CS:653:ALA:HB2	1.95	0.49
34:Ca:190:PRO:HG2	34:Ca:192:VAL:HG13	1.94	0.49
51:C2:35:G:OP2	51:C2:35:G:N2	2.36	0.49
59:CY:291:ARG:HA	59:CY:294:ARG:HG2	1.95	0.49
2:UB:692:LYS:HD3	2:UB:693:ASP:H	1.76	0.49
7:UJ:973:TYR:HD2	7:UJ:979:LEU:HB2	1.78	0.49
7:UJ:1524:SER:O	7:UJ:1583:TRP:NE1	2.46	0.49
8:UK:173:GLN:HB3	8:UK:177:LYS:NZ	2.28	0.49
9:UL:240:GLU:OE1	9:UL:274:HIS:ND1	2.46	0.49
13:UQ:521:PRO:HG3	55:UE:26:THR:HG21	1.94	0.49
15:UU:931:GLY:O	15:UU:934:LYS:C	2.56	0.49
18:CB:217:ARG:HH12	20:CD:8:GLU:HB2	1.76	0.49
19:CC:244:LEU:HD11	19:CC:250:LYS:HG2	1.95	0.49
20:CD:227:GLU:HG3	20:CD:228:ILE:HG23	1.94	0.49
32:CS:129:GLU:HA	32:CS:167:MET:HG2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CS:134:ASN:O	32:CS:138:ARG:HG2	2.13	0.49
34:Ca:36:ALA:HA	34:Ca:41:ARG:HH12	1.78	0.49
50:C1:799:U:O4	50:C1:800:A:N6	2.46	0.49
53:UT:419:LYS:HG3	53:UT:421:PRO:HD2	1.94	0.49
53:UT:1433:PRO:O	53:UT:1437:ASN:ND2	2.46	0.49
53:UT:1585:PHE:HD1	53:UT:1636:ARG:HH22	1.61	0.49
54:UH:862:HIS:C	54:UH:863:MET:HE2	2.37	0.49
7:UJ:492:PHE:CD1	7:UJ:533:ARG:HD2	2.48	0.49
7:UJ:1232:LEU:HD21	7:UJ:1252:LEU:HD22	1.94	0.49
9:UL:490:GLN:HG2	9:UL:502:THR:HG23	1.93	0.49
11:UN:910:MET:HE3	11:UN:914:THR:HG21	1.95	0.49
23:CH:249:ASP:OD1	23:CH:249:ASP:N	2.46	0.49
32:CR:68:THR:HG21	32:CR:73:LYS:HD3	1.95	0.49
32:CR:282:THR:HA	32:CR:410:MET:HB2	1.93	0.49
32:CR:388:ILE:HD11	32:CR:410:MET:HE3	1.95	0.49
32:CR:592:GLY:HA3	32:CR:631:SER:HA	1.95	0.49
32:CS:364:ASN:OD1	32:CS:365:HIS:ND1	2.42	0.49
35:Cb:212:ASP:O	35:Cb:215:ASP:N	2.45	0.49
37:Cd:160:ARG:O	37:Cd:173:THR:HA	2.13	0.49
41:Ch:136:PRO:HG2	41:Ch:139:TRP:HB2	1.94	0.49
51:C2:160:U:H2'	51:C2:161:G:H8	1.78	0.49
52:CW:167:GLU:HB2	52:CW:181:PRO:HB2	1.95	0.49
53:UT:279:SER:OG	53:UT:324:ARG:NH1	2.45	0.49
9:UL:429:ILE:HA	9:UL:445:ALA:HB2	1.93	0.49
15:UU:184:GLU:HG3	15:UU:186:THR:HG23	1.95	0.49
15:UU:526:TRP:O	15:UU:529:ARG:NH1	2.39	0.49
32:CS:828:GLU:HA	32:CS:831:GLN:HG3	1.95	0.49
35:Cb:116:ASP:O	35:Cb:120:LYS:HG3	2.13	0.49
53:UT:270:LEU:H	53:UT:317:THR:HG21	1.78	0.49
53:UT:431:SER:HG	53:UT:472:ARG:HH22	1.60	0.49
53:UT:964:LEU:HD11	53:UT:998:LEU:HD11	1.95	0.49
53:UT:1349:ARG:NH1	53:UT:1429:ASP:OD2	2.46	0.49
59:CY:118:ALA:HB2	60:CZ:311:GLY:HA3	1.93	0.49
61:UP:308:LYS:NZ	61:UP:309:ASN:O	2.40	0.49
4:UD:262:ASP:HB2	14:UR:450:ARG:HE	1.78	0.48
7:UJ:801:ILE:HB	7:UJ:805:LEU:HD11	1.94	0.48
8:UK:117:ASN:HB3	51:C2:260:G:H4'	1.95	0.48
18:CB:188:ARG:HA	18:CB:191:ARG:HD3	1.95	0.48
25:CJ:137:ARG:NH1	25:CJ:160:TRP:O	2.46	0.48
34:Ca:25:THR:O	34:Ca:50:ARG:NH1	2.46	0.48
34:Ca:126:THR:HG22	34:Ca:136:ARG:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:C2:162:C:O2'	51:C2:164:U:OP2	2.30	0.48
4:UD:54:GLU:OE1	4:UD:65:GLN:NE2	2.45	0.48
4:UD:680:GLU:HG3	4:UD:683:ARG:HH22	1.78	0.48
5:UF:359:GLU:O	5:UF:363:ARG:HG3	2.13	0.48
7:UJ:1268:VAL:HG11	7:UJ:1287:LEU:HD21	1.95	0.48
9:UL:597:LEU:HB2	49:CU:98:VAL:HG21	1.94	0.48
13:UQ:264:GLY:HA2	13:UQ:280:ARG:O	2.12	0.48
18:CA:214:MET:HE3	18:CA:217:ARG:NH1	2.28	0.48
22:CG:287:HIS:CE1	22:CG:313:LYS:HD2	2.48	0.48
24:CI:607:LYS:O	24:CI:611:SER:HB3	2.14	0.48
26:CK:185:SER:OG	50:C1:2207:C:OP1	2.31	0.48
32:CR:38:ILE:HD11	32:CR:152:LEU:HD21	1.95	0.48
32:CS:744:PRO:HA	32:CS:761:VAL:O	2.12	0.48
38:Ce:50:VAL:HG23	38:Ce:51:SER:H	1.77	0.48
50:C1:1623:U:H5"	50:C1:1624:A:H2'	1.95	0.48
53:UT:191:ALA:HA	53:UT:194:MET:HB3	1.94	0.48
53:UT:1756:ASP:O	53:UT:1759:SER:OG	2.27	0.48
7:UJ:1001:PRO:O	7:UJ:1005:ASN:ND2	2.38	0.48
10:UM:563:SER:OG	10:UM:564:GLN:N	2.46	0.48
21:CF:25:VAL:HG22	21:CF:103:LEU:HD11	1.94	0.48
24:CI:827:LEU:H	24:CI:863:THR:HG22	1.78	0.48
32:CS:29:VAL:HA	32:CS:202:ILE:O	2.12	0.48
37:Cd:2:LYS:HB2	37:Cd:108:VAL:HG22	1.95	0.48
47:Co:345:ARG:O	47:Co:351:ARG:O	2.31	0.48
53:UT:1729:ASN:HA	53:UT:1732:LEU:HD22	1.95	0.48
53:UT:1751:ARG:O	53:UT:1755:ARG:HG3	2.13	0.48
54:UH:847:ARG:NH2	55:UI:231:THR:O	2.44	0.48
58:CX:413:CYS:HA	58:CX:416:VAL:HG12	1.95	0.48
1:UA:264:HIS:HB2	1:UA:305:ILE:HD13	1.95	0.48
7:UJ:1522:LEU:HA	7:UJ:1525:ILE:HG12	1.94	0.48
9:UL:835:GLN:OE1	10:UM:821:ARG:NH2	2.39	0.48
10:UM:85:MET:HE3	10:UM:109:PRO:HG3	1.96	0.48
11:UN:275:ASP:OD1	11:UN:275:ASP:N	2.45	0.48
16:UX:152:ASP:OD1	16:UX:152:ASP:N	2.45	0.48
20:CD:304:HIS:CD2	20:CD:322:LEU:HD22	2.48	0.48
22:CG:391:SER:HB3	22:CG:438:LEU:HD11	1.96	0.48
23:CH:219:ARG:HA	23:CH:251:HIS:O	2.13	0.48
32:CR:425:SER:O	32:CR:429:ILE:HB	2.14	0.48
50:C1:927:C:H3'	60:CZ:537:ARG:HH22	1.78	0.48
53:UT:1277:ILE:HG21	53:UT:1282:LEU:HD13	1.94	0.48
54:UH:575:SER:HA	54:UH:578:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:758:ARG:HD2	4:UD:768:TRP:HB3	1.95	0.48
7:UJ:256:SER:O	7:UJ:295:GLN:NE2	2.46	0.48
7:UJ:850:THR:O	7:UJ:854:GLU:HG2	2.13	0.48
13:UQ:568:THR:HG22	55:UE:262:LYS:HZ2	1.77	0.48
14:UR:288:ILE:HD12	14:UR:315:LEU:HD11	1.95	0.48
14:UR:570:HIS:ND1	14:UR:573:SER:OG	2.34	0.48
18:CB:228:ALA:HB3	18:CB:255:ILE:HG13	1.96	0.48
18:CB:258:LYS:HZ1	18:CB:261:CYS:HB2	1.78	0.48
23:CH:25:THR:HG21	23:CH:57:LEU:HD11	1.95	0.48
24:CI:246:ILE:HB	24:CI:798:ILE:HB	1.95	0.48
31:CQ:170:ASP:OD1	31:CQ:214:SER:OG	2.27	0.48
32:CR:748:ARG:NH2	32:CR:750:THR:O	2.46	0.48
45:Cm:105:THR:HG22	45:Cm:110:ILE:HG12	1.94	0.48
50:C1:781:G:H2'	50:C1:782:G:H8	1.77	0.48
53:UT:1064:LEU:HD23	53:UT:1068:LYS:HB3	1.95	0.48
53:UT:2005:LYS:HD2	53:UT:2050:LEU:HD11	1.95	0.48
1:UA:316:ALA:O	1:UA:320:GLY:C	2.57	0.48
4:UD:249:ILE:HB	4:UD:261:TRP:HB2	1.94	0.48
9:UL:275:ARG:NH2	9:UL:279:GLU:O	2.47	0.48
20:CD:4:PHE:O	20:CD:88:LEU:HA	2.13	0.48
28:CM:282:HIS:O	28:CM:408:LYS:NZ	2.46	0.48
32:CR:834:THR:O	32:CR:838:HIS:ND1	2.42	0.48
34:Ca:204:ILE:O	50:C1:1648:G:O2'	2.31	0.48
45:Cm:85:GLU:HA	49:CU:300:VAL:HG21	1.96	0.48
50:C1:2067:G:N2	50:C1:2189:C:O2	2.45	0.48
56:US:236:SER:O	56:US:239:SER:OG	2.29	0.48
60:CZ:392:ARG:NH1	60:CZ:406:THR:OG1	2.47	0.48
1:UA:316:ALA:O	1:UA:321:GLN:HB2	2.13	0.48
7:UJ:1429:ILE:HD12	7:UJ:1433:ILE:HD11	1.95	0.48
10:UM:699:LEU:HD12	10:UM:710:SER:HB3	1.95	0.48
12:UO:499:VAL:HG23	55:UE:259:LEU:HD22	1.95	0.48
15:UU:978:LEU:HD22	15:UU:991:THR:HG23	1.96	0.48
28:CM:225:PHE:HA	28:CM:232:PRO:HA	1.95	0.48
28:CM:319:ASP:HA	28:CM:395:ARG:HH12	1.78	0.48
38:Ce:20:SER:OG	38:Ce:21:ASP:N	2.46	0.48
53:UT:1076:LEU:O	53:UT:1080:ILE:HG12	2.14	0.48
54:UH:701:GLU:OE1	54:UH:705:ARG:NH2	2.39	0.48
59:CY:25:ALA:HB2	60:CZ:369:THR:HG23	1.95	0.48
55:UI:158:ASN:HB2	55:UI:162:ARG:HH12	1.78	0.48
1:UA:787:MET:HE2	1:UA:787:MET:HB3	1.73	0.48
4:UD:358:GLY:O	4:UD:751:SER:OG	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:UJ:275:VAL:HG12	7:UJ:315:LEU:HD21	1.96	0.48
7:UJ:1662:GLN:HG3	7:UJ:1664:GLY:H	1.78	0.48
15:UU:713:PHE:HA	15:UU:723:VAL:O	2.14	0.48
18:CA:164:GLY:HA3	18:CA:196:MET:HE2	1.95	0.48
49:CU:163:ARG:O	49:CU:167:GLU:HG2	2.14	0.48
4:UD:122:LYS:HE2	4:UD:123:LYS:HE2	1.95	0.48
4:UD:775:ASP:OD1	13:UQ:345:THR:OG1	2.31	0.48
7:UJ:1434:THR:HA	7:UJ:1437:TYR:CE2	2.48	0.48
24:CI:133:ALA:O	24:CI:238:ARG:NH2	2.43	0.48
24:CI:762:GLU:O	24:CI:766:ARG:HB3	2.14	0.48
46:Cn:53:VAL:O	46:Cn:99:ASN:HA	2.14	0.48
53:UT:414:GLN:O	53:UT:418:THR:OG1	2.23	0.48
53:UT:1472:THR:HA	53:UT:1475:GLN:HB2	1.96	0.48
53:UT:1562:ASN:O	53:UT:1565:ARG:O	2.31	0.48
7:UJ:1383:GLN:HE21	7:UJ:1428:HIS:HB3	1.79	0.48
10:UM:692:HIS:CG	10:UM:696:LEU:HD21	2.49	0.48
19:CC:284:MET:HE3	20:CD:267:ARG:NE	2.29	0.48
24:CI:942:LEU:HB3	27:CL:517:LEU:HD11	1.96	0.48
32:CS:586:ILE:HG12	32:CS:638:ILE:HG13	1.94	0.48
37:Cd:15:LEU:HD22	50:C1:737:G:H4'	1.96	0.48
52:CW:136:PRO:HG2	60:CZ:544:LEU:HD22	1.95	0.48
52:CW:152:LEU:HD23	52:CW:170:ARG:HG2	1.95	0.48
56:US:112:ASN:OD1	56:US:113:TRP:N	2.47	0.48
4:UD:554:PHE:HE1	4:UD:561:LEU:HD13	1.79	0.47
7:UJ:1158:LEU:HD21	7:UJ:1170:LEU:HD21	1.96	0.47
10:UM:208:ARG:HH12	10:UM:221:TYR:HE1	1.61	0.47
13:UQ:158:VAL:O	13:UQ:165:ILE:HA	2.13	0.47
13:UQ:812:LEU:HA	13:UQ:823:LEU:O	2.14	0.47
17:UZ:158:ARG:HD3	17:UZ:185:MET:HE3	1.95	0.47
24:CI:1116:ARG:HG2	24:CI:1120:LYS:HE3	1.96	0.47
30:CP:151:LEU:O	30:CP:155:GLU:HG3	2.14	0.47
32:CR:331:PHE:HB3	32:CR:336:TYR:HB2	1.96	0.47
32:CR:574:ILE:HG22	32:CR:576:GLU:H	1.78	0.47
32:CS:868:GLY:HA2	32:CS:871:ARG:HB2	1.96	0.47
36:Cc:176:THR:HG22	36:Cc:179:GLU:HG2	1.96	0.47
37:Cd:32:MET:HG3	37:Cd:100:CYS:HB2	1.96	0.47
37:Cd:159:ARG:HD3	37:Cd:175:ALA:HB2	1.96	0.47
53:UT:1911:VAL:HG11	53:UT:1973:VAL:HG21	1.95	0.47
53:UT:2079:LEU:HD22	53:UT:2115:THR:HG21	1.95	0.47
1:UA:97:SER:HB3	1:UA:115:LEU:HD23	1.95	0.47
7:UJ:501:THR:HG22	7:UJ:503:THR:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:UM:628:ASN:HB2	10:UM:635:ILE:HD11	1.94	0.47
11:UN:282:LEU:HD22	53:UT:2158:LYS:HE3	1.96	0.47
18:CA:251:GLY:O	18:CA:305:VAL:HA	2.14	0.47
20:CD:292:LEU:O	20:CD:398:ARG:NH1	2.47	0.47
24:CI:302:LEU:O	24:CI:776:TYR:HB3	2.14	0.47
27:CL:721:LYS:NZ	50:C1:1729:U:OP1	2.41	0.47
32:CS:212:SER:O	32:CS:215:LYS:NZ	2.45	0.47
32:CS:512:ASP:OD1	32:CS:514:SER:OG	2.27	0.47
32:CS:851:TYR:HA	32:CS:854:VAL:HB	1.96	0.47
37:Cd:137:ARG:HB2	37:Cd:140:LYS:HG3	1.96	0.47
40:Cg:139:VAL:HG13	59:CY:257:GLY:HA3	1.96	0.47
47:Co:385:GLN:HA	47:Co:413:LEU:HD13	1.96	0.47
53:UT:621:LEU:O	53:UT:625:GLN:NE2	2.47	0.47
53:UT:677:LEU:HD23	53:UT:680:THR:HG23	1.95	0.47
56:US:300:PRO:HD2	56:US:332:ARG:HH11	1.76	0.47
58:CX:374:ARG:HH21	58:CX:416:VAL:HG23	1.78	0.47
60:CZ:330:ARG:HA	60:CZ:333:LYS:HD3	1.95	0.47
60:CZ:572:LEU:O	60:CZ:576:LEU:HB3	2.13	0.47
2:UB:21:PRO:HB3	50:C1:1732:C:H1'	1.97	0.47
3:UC:221:LEU:HB3	27:CL:64:LEU:HD11	1.96	0.47
6:UG:439:LYS:NZ	50:C1:426:A:OP2	2.47	0.47
15:UU:927:LYS:HB3	15:UU:927:LYS:HE2	1.74	0.47
23:CH:188:GLY:O	23:CH:273:THR:OG1	2.31	0.47
24:CI:938:PHE:HA	27:CL:511:ARG:HH22	1.80	0.47
28:CM:261:ASP:OD2	28:CM:263:ASN:ND2	2.47	0.47
30:CP:207:LEU:HD11	30:CP:221:TYR:HB2	1.96	0.47
36:Cc:82:ASN:OD1	36:Cc:94:LYS:NZ	2.47	0.47
44:Ck:111:ASN:HD22	44:Ck:111:ASN:C	2.18	0.47
50:C1:331:C:N4	50:C1:332:U:O4	2.47	0.47
53:UT:1090:TYR:HB3	53:UT:1094:LEU:HD13	1.96	0.47
53:UT:1286:VAL:HA	53:UT:1289:VAL:HG22	1.97	0.47
53:UT:1765:LEU:HD23	53:UT:1773:ILE:HD11	1.96	0.47
4:UD:283:SER:HB3	4:UD:329:MET:HG3	1.96	0.47
7:UJ:284:LEU:HD13	7:UJ:288:ILE:HG21	1.96	0.47
7:UJ:1053:ILE:HD13	7:UJ:1082:PHE:HZ	1.78	0.47
12:UO:323:ILE:HB	12:UO:333:HIS:HB2	1.97	0.47
15:UU:752:THR:N	15:UU:766:ALA:O	2.37	0.47
22:CG:314:VAL:HG13	22:CG:323:VAL:HB	1.96	0.47
29:CO:180:LEU:HD11	29:CO:241:PHE:CE2	2.48	0.47
39:Cf:76:THR:HG22	39:Cf:108:PRO:HG2	1.96	0.47
48:Cp:13:VAL:O	48:Cp:52:ASN:CA	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:945:ILE:HA	53:UT:948:TRP:HE3	1.78	0.47
58:CX:296:LEU:HD13	58:CX:331:ILE:HD12	1.96	0.47
59:CY:44:LYS:HB3	60:CZ:321:PHE:HZ	1.79	0.47
4:UD:626:LEU:HD12	4:UD:630:PRO:HG3	1.95	0.47
7:UJ:166:PHE:CG	7:UJ:185:GLN:HG3	2.49	0.47
7:UJ:755:LEU:O	7:UJ:802:ARG:NH2	2.47	0.47
8:UK:24:ARG:NH2	50:C1:2091:C:OP2	2.48	0.47
10:UM:604:GLY:HA2	10:UM:636:ARG:HE	1.80	0.47
13:UQ:847:ASP:O	13:UQ:850:ALA:HA	2.15	0.47
15:UU:69:ARG:NH1	15:UU:91:PRO:O	2.47	0.47
18:CA:194:ILE:HD11	19:CC:162:SER:HB3	1.96	0.47
22:CG:416:GLY:HA2	22:CG:466:ILE:HG13	1.95	0.47
25:CJ:66:PRO:HB2	26:CK:64:ILE:HD12	1.96	0.47
43:Cj:45:ARG:HA	43:Cj:48:LEU:HD12	1.96	0.47
46:Cn:130:VAL:HG13	46:Cn:140:LYS:HD3	1.97	0.47
47:Co:382:GLN:HB3	47:Co:385:GLN:HG2	1.95	0.47
53:UT:1960:TYR:HA	53:UT:1963:THR:HG22	1.97	0.47
4:UD:709:MET:O	4:UD:826:TRP:HA	2.14	0.47
8:UK:68:MET:HE2	51:C2:58:A:H5'	1.96	0.47
17:UZ:126:ARG:NH1	50:C1:2061:G:OP1	2.47	0.47
20:CD:17:LYS:N	20:CD:44:LYS:O	2.37	0.47
23:CH:160:LEU:HD23	23:CH:335:VAL:HB	1.95	0.47
24:CI:753:ASN:O	24:CI:754:LYS:HG2	2.14	0.47
29:CN:91:ILE:HD12	29:CN:94:GLN:HE21	1.79	0.47
29:CN:130:ILE:HD11	29:CN:137:PHE:HD1	1.79	0.47
32:CR:660:TYR:HB2	32:CR:712:LEU:HD13	1.95	0.47
43:Cj:86:ALA:HB1	43:Cj:109:LEU:HD13	1.97	0.47
47:Co:346:ASN:CB	47:Co:351:ARG:O	2.62	0.47
53:UT:299:SER:OG	53:UT:340:ARG:NH1	2.47	0.47
59:CY:62:LYS:HB3	60:CZ:341:PHE:HD2	1.80	0.47
55:UI:211:ALA:HB1	55:UI:214:LEU:HB2	1.96	0.47
2:UB:769:LEU:HD23	2:UB:774:THR:HG22	1.95	0.47
4:UD:549:VAL:HG21	4:UD:563:VAL:HB	1.95	0.47
4:UD:560:MET:HE1	4:UD:661:PRO:HB2	1.97	0.47
4:UD:693:VAL:HG21	4:UD:838:ILE:HG22	1.96	0.47
5:UF:287:ARG:HD2	5:UF:327:LEU:HD11	1.97	0.47
9:UL:395:GLU:OE1	9:UL:397:TYR:OH	2.29	0.47
9:UL:469:LEU:HD11	9:UL:485:LYS:HG2	1.97	0.47
10:UM:276:LEU:HD21	34:Ca:50:ARG:HD2	1.96	0.47
12:UO:513:VAL:HG11	55:UE:270:LEU:HD21	1.95	0.47
13:UQ:106:THR:HG22	13:UQ:111:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:UQ:154:ASP:O	13:UQ:169:ASN:ND2	2.48	0.47
13:UQ:379:LEU:HB3	13:UQ:392:LEU:HB3	1.96	0.47
15:UU:711:ASN:HD21	15:UU:727:GLN:NE2	2.13	0.47
17:UZ:282:TYR:HB3	17:UZ:290:ALA:HB1	1.97	0.47
18:CB:235:GLN:HG2	18:CB:255:ILE:HD11	1.96	0.47
21:CF:11:LYS:HA	21:CF:81:TYR:HB2	1.97	0.47
24:CI:277:THR:HG22	24:CI:278:ASN:H	1.78	0.47
24:CI:917:LYS:NZ	50:C1:1142:U:OP1	2.42	0.47
27:CL:52:LEU:O	27:CL:57:PRO:HD2	2.14	0.47
31:CQ:87:ILE:HG12	31:CQ:95:LEU:HD22	1.97	0.47
32:CR:729:LEU:HD21	32:CR:805:ILE:HD11	1.95	0.47
32:CR:912:PHE:O	32:CR:916:MET:HG2	2.14	0.47
40:Cg:169:ARG:HA	40:Cg:172:ARG:HE	1.80	0.47
2:UB:572:ARG:HG3	2:UB:610:VAL:HG22	1.97	0.47
4:UD:841:ILE:HG13	4:UD:859:GLU:HB3	1.95	0.47
6:UG:570:ARG:HH12	50:C1:325:C:H3'	1.80	0.47
7:UJ:782:VAL:O	7:UJ:812:ARG:NH2	2.48	0.47
15:UU:644:GLY:HA3	15:UU:663:ALA:HA	1.96	0.47
22:CG:184:TYR:CE1	22:CG:194:LYS:HG3	2.49	0.47
23:CH:168:PRO:HA	23:CH:171:ILE:HB	1.97	0.47
24:CI:246:ILE:HG21	24:CI:270:LEU:HD22	1.95	0.47
24:CI:825:LYS:NZ	50:C1:1162:U:O3'	2.47	0.47
26:CK:143:HIS:HB2	26:CK:151:ALA:HB3	1.96	0.47
32:CS:601:LYS:O	32:CS:605:ARG:HG2	2.15	0.47
36:Cc:133:SER:OG	36:Cc:144:ARG:NH2	2.48	0.47
53:UT:242:MET:SD	53:UT:245:THR:OG1	2.65	0.47
53:UT:687:LEU:HD12	53:UT:725:TRP:HH2	1.80	0.47
3:UC:230:ASP:OD1	27:CL:60:ARG:NH2	2.47	0.47
4:UD:698:ARG:HD2	4:UD:709:MET:SD	2.54	0.47
6:UG:114:GLN:HB3	6:UG:129:LYS:HE2	1.97	0.47
7:UJ:500:PRO:HB3	7:UJ:539:VAL:HA	1.96	0.47
7:UJ:1558:HIS:HB2	7:UJ:1605:GLY:HA3	1.97	0.47
10:UM:89:SER:OG	10:UM:102:THR:OG1	2.30	0.47
13:UQ:450:ALA:HB2	13:UQ:458:PRO:HG2	1.97	0.47
18:CB:156:VAL:HG23	18:CB:180:VAL:HG23	1.97	0.47
23:CH:177:GLN:HB3	23:CH:190:GLY:HA2	1.97	0.47
31:CQ:233:VAL:HA	31:CQ:236:VAL:HG12	1.95	0.47
32:CR:224:ASP:HB3	32:CR:227:GLU:HG3	1.95	0.47
32:CS:158:SER:HB2	32:CS:691:GLY:HA3	1.96	0.47
38:Ce:76:PHE:O	38:Ce:79:VAL:O	2.33	0.47
44:Ck:84:LYS:NZ	44:Ck:124:GLU:OE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:CX:344:THR:O	58:CX:347:ASP:C	2.58	0.47
2:UB:527:SER:HB3	2:UB:559:LEU:HD22	1.97	0.47
4:UD:697:GLN:OE1	4:UD:713:SER:N	2.48	0.47
6:UG:348:VAL:HA	6:UG:357:ALA:O	2.15	0.47
7:UJ:1105:LEU:HD13	7:UJ:1110:PHE:CD2	2.50	0.47
7:UJ:1667:GLN:CD	7:UJ:1713:VAL:HB	2.39	0.47
9:UL:375:ALA:O	9:UL:384:GLN:HB2	2.14	0.47
9:UL:695:HIS:NE2	9:UL:713:SER:OG	2.39	0.47
14:UR:178:GLN:OE1	14:UR:181:ARG:NH1	2.48	0.47
15:UU:35:PHE:HB3	15:UU:776:TRP:HB3	1.97	0.47
15:UU:121:VAL:HB	15:UU:129:ALA:HB3	1.97	0.47
22:CG:444:LEU:HD11	22:CG:455:PRO:HA	1.97	0.47
29:CN:100:LEU:HD13	29:CN:105:ASN:HD21	1.80	0.47
32:CR:516:CYS:HB3	32:CR:570:LEU:HD11	1.97	0.47
42:Ci:49:ARG:HG3	50:C1:1504:A:H1'	1.97	0.47
53:UT:1855:GLU:HB2	53:UT:1895:ARG:HG3	1.97	0.47
56:US:174:LEU:HD21	56:US:226:LEU:HD21	1.96	0.47
5:UF:20:ARG:NH1	5:UF:24:GLU:OE2	2.48	0.46
5:UF:278:ILE:HG23	11:UN:373:ILE:HD12	1.97	0.46
7:UJ:586:ASP:OD1	7:UJ:587:LYS:N	2.48	0.46
7:UJ:712:GLY:O	7:UJ:716:GLU:HG3	2.15	0.46
9:UL:133:ASP:OD1	9:UL:149:ARG:NH1	2.41	0.46
9:UL:481:ILE:HD11	9:UL:489:LEU:HB3	1.97	0.46
10:UM:755:ARG:HG3	10:UM:793:ALA:HB1	1.97	0.46
14:UR:157:LEU:O	14:UR:174:ARG:NH1	2.42	0.46
15:UU:120:TRP:CD1	15:UU:130:GLU:HG2	2.50	0.46
18:CB:191:ARG:HH11	20:CD:154:LEU:HD22	1.80	0.46
19:CC:113:PHE:HB2	19:CC:116:VAL:HG12	1.97	0.46
19:CC:332:PRO:O	19:CC:335:THR:OG1	2.27	0.46
26:CK:140:ILE:HA	26:CK:153:THR:O	2.15	0.46
30:CP:290:LYS:NZ	50:C1:900:A:OP1	2.39	0.46
51:C2:164:U:O2	51:C2:166:G:N2	2.45	0.46
53:UT:1313:LEU:HD23	53:UT:1313:LEU:HA	1.82	0.46
7:UJ:648:ASP:OD1	7:UJ:651:ALA:N	2.44	0.46
9:UL:568:ILE:HA	9:UL:584:LEU:HD23	1.97	0.46
13:UQ:292:THR:HG23	13:UQ:361:VAL:HG12	1.96	0.46
15:UU:723:VAL:HG22	15:UU:733:VAL:HG22	1.96	0.46
32:CS:364:ASN:OD1	32:CS:365:HIS:N	2.48	0.46
35:Cb:100:ARG:HH12	35:Cb:122:LYS:HA	1.80	0.46
46:Cn:53:VAL:O	46:Cn:99:ASN:N	2.47	0.46
47:Co:346:ASN:ND2	47:Co:351:ARG:HE	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Co:365:ASN:ND2	50:C1:1105:A:N3	2.62	0.46
50:C1:1097:U:H2'	50:C1:1098:G:C8	2.50	0.46
53:UT:116:LYS:NZ	53:UT:159:GLU:OE2	2.46	0.46
53:UT:776:VAL:HG11	53:UT:843:ALA:HB3	1.98	0.46
53:UT:1757:THR:O	53:UT:1761:ILE:HG12	2.14	0.46
55:UE:156:VAL:HG21	56:US:301:GLU:HG2	1.96	0.46
56:US:185:PHE:HA	56:US:189:PHE:HD2	1.79	0.46
3:UC:285:ARG:NH1	27:CL:138:GLN:OE1	2.45	0.46
6:UG:278:GLN:HA	6:UG:302:PRO:HB3	1.97	0.46
7:UJ:1102:ILE:HD13	7:UJ:1105:LEU:HD12	1.97	0.46
16:UX:135:VAL:HG13	16:UX:160:ILE:HD11	1.97	0.46
19:CC:94:SER:N	50:C1:454:C:OP1	2.48	0.46
19:CC:217:ILE:HG22	19:CC:221:LYS:NZ	2.30	0.46
24:CI:129:MET:HA	24:CI:132:VAL:HG12	1.97	0.46
32:CS:201:VAL:HG22	32:CS:212:SER:HB3	1.97	0.46
39:Cf:74:ARG:HH12	53:UT:1025:ARG:CZ	2.29	0.46
40:Cg:166:ARG:HH21	40:Cg:172:ARG:NH1	2.14	0.46
47:Co:376:ALA:O	47:Co:379:TYR:O	2.34	0.46
53:UT:366:GLN:HA	53:UT:369:VAL:HG22	1.98	0.46
53:UT:474:VAL:HG21	53:UT:540:SER:HB3	1.97	0.46
53:UT:2150:ARG:HH22	53:UT:2190:PHE:HE1	1.61	0.46
55:UE:155:THR:HA	55:UE:158:ASN:HD22	1.79	0.46
2:UB:65:ARG:HD2	50:C1:2047:G:H5'	1.96	0.46
4:UD:453:VAL:HG23	4:UD:472:VAL:HB	1.96	0.46
6:UG:434:ASN:HB3	6:UG:437:GLU:HG3	1.98	0.46
7:UJ:45:PHE:HA	7:UJ:48:ILE:HD12	1.97	0.46
7:UJ:991:LEU:O	7:UJ:995:ILE:HG13	2.15	0.46
7:UJ:1190:LEU:HB2	7:UJ:1244:LEU:HD22	1.96	0.46
10:UM:137:ILE:HD11	10:UM:198:LEU:HD22	1.96	0.46
13:UQ:116:THR:HA	13:UQ:432:MET:SD	2.56	0.46
14:UR:253:ARG:NH2	14:UR:256:LEU:HD11	2.30	0.46
15:UU:427:GLN:NE2	50:C1:256:U:OP1	2.47	0.46
23:CH:64:SER:HB3	23:CH:77:TYR:HE1	1.81	0.46
39:Cf:11:ARG:NH1	39:Cf:15:GLY:O	2.48	0.46
54:UH:555:GLY:N	54:UH:568:THR:O	2.49	0.46
56:US:427:GLU:HA	56:US:430:LYS:HG3	1.98	0.46
57:Cl:8:LYS:NZ	57:Cl:60:GLU:O	2.49	0.46
1:UA:588:LEU:HD23	1:UA:678:VAL:HB	1.97	0.46
1:UA:594:LYS:HE2	1:UA:595:TYR:CZ	2.51	0.46
7:UJ:260:VAL:HB	7:UJ:295:GLN:HE21	1.81	0.46
7:UJ:396:TYR:HE2	7:UJ:442:ILE:HD11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:UJ:1500:LEU:HD23	7:UJ:1553:ILE:HG12	1.96	0.46
10:UM:207:ILE:HB	10:UM:220:VAL:HB	1.96	0.46
20:CD:258:LYS:HB3	20:CD:258:LYS:HE3	1.77	0.46
23:CH:81:LEU:HG	24:CI:910:GLU:HG2	1.96	0.46
24:CI:1085:ARG:O	24:CI:1089:LYS:HG2	2.15	0.46
28:CM:258:ALA:HB2	28:CM:289:VAL:HB	1.96	0.46
50:C1:3:G:H1	50:C1:32:U:H3	1.63	0.46
53:UT:377:GLN:HA	53:UT:380:VAL:HG12	1.98	0.46
54:UH:308:ASP:HB3	54:UH:348:ARG:HH12	1.80	0.46
55:UE:182:GLN:HB3	55:UE:220:TRP:CD1	2.51	0.46
59:CY:95:TYR:HD1	60:CZ:453:LEU:HD13	1.80	0.46
60:CZ:539:SER:H	60:CZ:542:ARG:HH21	1.64	0.46
1:UA:845:LEU:HD23	15:UU:1013:LEU:HD22	1.98	0.46
12:UO:255:ILE:HG12	12:UO:269:ILE:HB	1.97	0.46
13:UQ:392:LEU:HD22	13:UQ:428:MET:HE3	1.98	0.46
17:UZ:169:LYS:HE2	17:UZ:173:LYS:HD3	1.97	0.46
24:CI:1096:LYS:HG3	33:CT:178:TYR:HB2	1.97	0.46
30:CP:188:THR:HG23	30:CP:194:PRO:HD3	1.97	0.46
32:CR:612:ASP:HB3	32:CR:615:PRO:HD2	1.97	0.46
39:Cf:193:LEU:O	39:Cf:197:GLN:HG3	2.16	0.46
40:Cg:128:ARG:HH21	50:C1:1058:A:H4'	1.81	0.46
43:Cj:72:GLY:O	50:C1:2065:C:O2'	2.29	0.46
58:CX:365:TYR:HE1	58:CX:409:ILE:HG12	1.81	0.46
4:UD:625:LYS:HB3	7:UJ:670:HIS:CD2	2.50	0.46
9:UL:632:ARG:NH1	9:UL:641:CYS:SG	2.87	0.46
13:UQ:811:LEU:HD21	13:UQ:855:ILE:HD13	1.97	0.46
14:UR:421:ALA:HB2	14:UR:437:ARG:HG3	1.98	0.46
19:CC:228:ASN:OD1	19:CC:229:LYS:N	2.48	0.46
20:CD:78:ASN:HD22	20:CD:81:LYS:HD2	1.80	0.46
25:CJ:83:TYR:OH	26:CK:15:ARG:NH1	2.42	0.46
32:CS:218:LYS:NZ	32:CS:219:PRO:O	2.38	0.46
32:CS:805:ILE:O	32:CS:808:SER:OG	2.24	0.46
32:CS:825:THR:N	32:CS:828:GLU:OE1	2.36	0.46
34:Ca:129:THR:HG22	34:Ca:133:TYR:H	1.81	0.46
34:Ca:129:THR:OG1	34:Ca:179:CYS:O	2.33	0.46
49:CU:126:ASP:O	49:CU:129:ARG:NH1	2.41	0.46
52:CW:143:ALA:HB3	52:CW:152:LEU:HB2	1.98	0.46
53:UT:232:ILE:HA	53:UT:235:VAL:HG22	1.97	0.46
54:UH:780:MET:HG2	54:UH:815:PHE:HZ	1.81	0.46
8:UK:268:ARG:HH11	21:CE:95:SER:HB3	1.81	0.46
9:UL:24:LEU:HD11	9:UL:388:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:UO:99:ASP:HA	57:Cl:25:LYS:HD3	1.97	0.46
15:UU:325:SER:HB2	15:UU:446:LEU:HG	1.98	0.46
25:CJ:108:ARG:HA	25:CJ:113:VAL:HG11	1.97	0.46
30:CP:272:LYS:HA	30:CP:275:LYS:HE2	1.98	0.46
32:CS:310:ILE:HB	32:CS:369:ILE:HG13	1.97	0.46
45:Cm:47:ILE:HD11	45:Cm:63:VAL:HG11	1.97	0.46
50:C1:464:G:H2'	59:CY:369:VAL:HG21	1.97	0.46
2:UB:545:TRP:HB3	2:UB:548:THR:HB	1.98	0.46
7:UJ:1614:LEU:HD13	7:UJ:1617:ILE:H	1.81	0.46
12:UO:475:GLU:OE2	12:UO:516:SER:OG	2.32	0.46
20:CD:217:ARG:HH11	20:CD:244:SER:HB3	1.81	0.46
29:CO:73:HIS:HB3	29:CO:76:ILE:HG12	1.97	0.46
32:CS:275:LYS:HD3	32:CS:307:TYR:HE1	1.81	0.46
37:Cd:195:ALA:HA	37:Cd:198:ARG:HG2	1.97	0.46
50:C1:1462:G:H22	50:C1:1536:A:H2	1.64	0.46
53:UT:86:ILE:O	53:UT:90:THR:N	2.41	0.46
59:CY:49:LEU:HD11	60:CZ:373:VAL:HG12	1.97	0.46
55:UI:161:LEU:HD23	55:UI:192:LEU:HB3	1.98	0.46
7:UJ:1359:CYS:HB3	7:UJ:1400:TYR:CE1	2.52	0.46
7:UJ:1524:SER:HB2	7:UJ:1583:TRP:CD2	2.51	0.46
10:UM:689:LEU:HB3	10:UM:720:TRP:CH2	2.51	0.46
13:UQ:700:LEU:O	13:UQ:715:ILE:HG12	2.16	0.46
14:UR:286:TYR:HB2	14:UR:288:ILE:HG12	1.98	0.46
14:UR:605:GLY:HA2	14:UR:610:ARG:O	2.16	0.46
29:CN:132:ARG:HB2	29:CO:88:ARG:HH12	1.81	0.46
32:CS:566:GLU:OE2	32:CS:715:ARG:NH2	2.49	0.46
32:CS:914:LYS:O	32:CS:918:LYS:HG3	2.16	0.46
34:Ca:144:LYS:HD3	34:Ca:208:GLN:HA	1.97	0.46
38:Ce:30:LEU:HA	38:Ce:33:LEU:HD12	1.98	0.46
38:Ce:134:ALA:HA	38:Ce:137:THR:HG22	1.97	0.46
1:UA:199:VAL:N	1:UA:213:VAL:O	2.49	0.45
1:UA:339:HIS:CE1	1:UA:365:LYS:HD2	2.51	0.45
3:UC:473:ARG:HD2	29:CO:182:PHE:HB3	1.99	0.45
4:UD:650:VAL:HA	4:UD:655:GLN:O	2.16	0.45
5:UF:99:ALA:HB1	5:UF:109:LEU:HD21	1.97	0.45
7:UJ:17:ARG:O	7:UJ:126:ARG:NH2	2.49	0.45
9:UL:302:VAL:HG22	9:UL:369:VAL:HG11	1.97	0.45
21:CF:90:ARG:NH2	22:CG:397:SER:OG	2.50	0.45
24:CI:514:GLU:HA	24:CI:517:VAL:HG22	1.97	0.45
32:CS:224:ASP:OD1	32:CS:224:ASP:N	2.49	0.45
32:CS:803:LEU:HD22	32:CS:882:ALA:HB2	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Ch:147:SER:HA	41:Ch:150:VAL:HG22	1.98	0.45
53:UT:750:VAL:HA	53:UT:753:MET:HG3	1.98	0.45
1:UA:847:GLN:HE21	15:UU:1007:MET:HE1	1.82	0.45
4:UD:766:THR:HG23	4:UD:767:LYS:HG3	1.98	0.45
7:UJ:492:PHE:HD1	7:UJ:533:ARG:HD2	1.80	0.45
7:UJ:988:GLY:HA3	7:UJ:1022:VAL:HG13	1.97	0.45
10:UM:777:VAL:HG21	10:UM:794:VAL:HG21	1.98	0.45
12:UO:338:MET:HE3	12:UO:342:VAL:HB	1.97	0.45
32:CS:385:LEU:HD13	32:CS:407:LEU:HD23	1.98	0.45
32:CS:593:LYS:HG3	32:CS:631:SER:HB2	1.98	0.45
44:Ck:127:MET:HG3	44:Ck:148:LEU:HD13	1.97	0.45
50:C1:923:C:H2'	50:C1:924:A:C8	2.51	0.45
52:CW:183:GLN:O	52:CW:229:TYR:OH	2.29	0.45
2:UB:672:ARG:HB3	2:UB:690:ARG:HH22	1.81	0.45
4:UD:58:PRO:HB3	4:UD:337:MET:HE1	1.99	0.45
7:UJ:700:HIS:HA	7:UJ:701:SER:HA	1.71	0.45
7:UJ:1534:ARG:HD2	7:UJ:1599:ARG:HG3	1.98	0.45
12:UO:554:VAL:HA	55:UE:230:VAL:HB	1.98	0.45
17:UZ:284:LYS:NZ	17:UZ:288:THR:O	2.48	0.45
18:CA:165:THR:O	18:CA:168:SER:OG	2.31	0.45
24:CI:71:VAL:HG22	24:CI:135:ILE:HB	1.98	0.45
25:CJ:85:MET:HE1	27:CL:630:LEU:HD22	1.98	0.45
29:CO:47:GLU:HG2	29:CO:118:LYS:HE2	1.99	0.45
32:CR:544:TYR:CE1	32:CR:637:ARG:HD2	2.51	0.45
32:CS:520:HIS:HD2	32:CS:568:PHE:HE2	1.63	0.45
35:Cb:58:TYR:CE1	35:Cb:62:LYS:HE3	2.51	0.45
36:Cc:38:ILE:HD11	36:Cc:115:ASN:HD22	1.82	0.45
39:Cf:23:LYS:HZ1	39:Cf:25:ARG:HH22	1.64	0.45
53:UT:1302:ILE:HG21	53:UT:1338:LEU:HD23	1.97	0.45
58:CX:343:LYS:O	58:CX:347:ASP:HB2	2.16	0.45
2:UB:741:HIS:CD2	2:UB:742:LYS:HG2	2.52	0.45
4:UD:561:LEU:O	4:UD:572:THR:HA	2.16	0.45
4:UD:829:THR:HG22	4:UD:831:GLN:H	1.81	0.45
13:UQ:578:LYS:HA	13:UQ:581:ARG:HG3	1.96	0.45
23:CH:305:VAL:HG12	23:CH:308:ASP:H	1.81	0.45
23:CH:328:MET:HE2	23:CH:330:ALA:HB3	1.97	0.45
32:CR:544:TYR:CZ	32:CR:637:ARG:HD2	2.51	0.45
32:CS:14:LEU:HD13	32:CS:200:LEU:HD21	1.98	0.45
36:Cc:40:ILE:HG22	36:Cc:42:ASP:H	1.82	0.45
39:Cf:11:ARG:HB2	50:C1:907:A:H5"	1.97	0.45
42:Ci:96:ILE:HD11	42:Ci:115:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:C1:954:A:N3	59:CY:320:ARG:NH1	2.61	0.45
52:CW:252:TYR:CZ	52:CW:259:LEU:HD13	2.52	0.45
53:UT:131:HIS:HD2	53:UT:174:TYR:CD1	2.34	0.45
53:UT:282:MET:HB2	53:UT:337:LEU:HD21	1.99	0.45
53:UT:1645:VAL:HA	53:UT:1648:LEU:HD12	1.98	0.45
56:US:319:LEU:HD11	56:US:360:PHE:HB2	1.99	0.45
58:CX:442:HIS:H	58:CX:446:ALA:HB2	1.82	0.45
60:CZ:412:GLU:HA	60:CZ:415:MET:HG3	1.98	0.45
1:UA:23:SER:HB3	1:UA:28:HIS:HB2	1.97	0.45
2:UB:10:LYS:HG3	26:CK:245:VAL:HG11	1.97	0.45
4:UD:221:ARG:HH12	14:UR:454:ILE:HG13	1.82	0.45
4:UD:554:PHE:CE1	4:UD:561:LEU:HD13	2.51	0.45
7:UJ:1651:LEU:HD22	7:UJ:1702:VAL:HG23	1.98	0.45
9:UL:284:VAL:HA	9:UL:294:ALA:O	2.17	0.45
13:UQ:89:MET:HA	13:UQ:107:TYR:HA	1.99	0.45
18:CA:173:ILE:O	33:CT:91:TYR:OH	2.34	0.45
19:CC:409:GLN:O	19:CC:413:GLN:HG3	2.17	0.45
23:CH:68:VAL:HG22	23:CH:75:ILE:HG22	1.99	0.45
32:CS:837:ASP:HB3	32:CS:857:LEU:HD21	1.99	0.45
53:UT:82:PHE:CE2	53:UT:86:ILE:HD13	2.51	0.45
60:CZ:560:ASP:OD1	60:CZ:562:ARG:NH2	2.50	0.45
7:UJ:1680:VAL:HG22	7:UJ:1729:HIS:CE1	2.51	0.45
12:UO:44:ILE:HA	12:UO:77:ALA:HB2	1.98	0.45
13:UQ:703:ALA:HB2	13:UQ:712:VAL:HG22	1.98	0.45
15:UU:576:ARG:HA	15:UU:576:ARG:HD3	1.74	0.45
24:CI:523:MET:HE1	32:CS:366:ARG:HH12	1.81	0.45
31:CQ:89:PRO:HA	31:CQ:92:MET:HE1	1.99	0.45
32:CS:358:ARG:HH11	32:CS:370:GLN:HB2	1.82	0.45
47:Co:338:LEU:HD11	47:Co:378:MET:HE2	1.97	0.45
50:C1:801:A:H1'	53:UT:1322:PRO:HG2	1.99	0.45
50:C1:1613:C:H4'	50:C1:1614:U:H5'	1.98	0.45
53:UT:1919:ILE:HA	53:UT:1922:VAL:HG12	1.98	0.45
54:UH:478:LYS:HA	54:UH:481:GLN:HG3	1.97	0.45
4:UD:381:ARG:NH2	4:UD:398:ASN:O	2.49	0.45
4:UD:440:GLY:O	4:UD:456:LEU:O	2.34	0.45
4:UD:452:LYS:HD3	55:UE:309:GLU:OE2	2.17	0.45
7:UJ:1481:LEU:HB3	7:UJ:1485:TRP:HZ3	1.80	0.45
10:UM:540:ARG:NH2	10:UM:576:LEU:HB3	2.32	0.45
13:UQ:600:THR:HG21	13:UQ:661:TRP:HB2	1.98	0.45
15:UU:941:ILE:HG21	15:UU:981:ARG:HD2	1.97	0.45
19:CC:217:ILE:HG22	19:CC:221:LYS:HZ1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CS:870:LEU:HB3	32:CS:874:VAL:HG12	1.98	0.45
38:Ce:177:ASP:OD1	38:Ce:177:ASP:N	2.48	0.45
39:Cf:8:ARG:NH2	39:Cf:28:GLU:OE2	2.48	0.45
39:Cf:99:SER:CA	39:Cf:173:ILE:O	2.65	0.45
44:Ck:43:VAL:HG21	44:Ck:145:LEU:HD11	1.99	0.45
50:C1:2175:A:H2'	50:C1:2176:A:C8	2.51	0.45
52:CW:280:LEU:HD12	52:CW:282:LYS:HD3	1.99	0.45
53:UT:1153:TRP:O	53:UT:1156:TYR:N	2.47	0.45
53:UT:1727:LEU:HA	53:UT:1730:GLU:HG2	1.99	0.45
4:UD:697:GLN:O	4:UD:712:LEU:HB2	2.17	0.45
7:UJ:1052:THR:O	7:UJ:1056:VAL:HB	2.17	0.45
8:UK:266:ARG:HH12	50:C1:205:C:N4	2.14	0.45
12:UO:75:VAL:HG11	12:UO:343:LEU:HD22	1.99	0.45
15:UU:249:SER:HA	15:UU:275:PRO:HB3	1.99	0.45
20:CD:428:MET:HE3	50:C1:251:G:H1'	1.99	0.45
23:CH:34:SER:HA	23:CH:74:THR:HG22	1.98	0.45
32:CS:576:GLU:HA	60:CZ:297:ALA:HB1	1.98	0.45
37:Cd:153:VAL:HA	37:Cd:156:TYR:HB2	1.98	0.45
53:UT:536:ARG:HH12	53:UT:825:MET:HE1	1.81	0.45
53:UT:1200:LEU:HD22	53:UT:1206:ILE:HG21	1.99	0.45
53:UT:1368:ARG:HA	53:UT:1371:LEU:HD12	1.98	0.45
54:UH:429:LEU:H	54:UH:429:LEU:HG	1.70	0.45
58:CX:425:ILE:O	58:CX:430:ARG:NH1	2.49	0.45
59:CY:301:SER:HB2	59:CY:303:ARG:HH11	1.82	0.45
7:UJ:1507:LEU:HD11	7:UJ:1560:ASP:HB3	1.97	0.45
7:UJ:1528:SER:HB3	7:UJ:1583:TRP:HZ2	1.82	0.45
9:UL:393:LEU:HD13	9:UL:395:GLU:HG3	1.98	0.45
9:UL:510:ALA:O	9:UL:528:ALA:N	2.38	0.45
13:UQ:572:THR:HG23	13:UQ:575:ASP:H	1.82	0.45
19:CC:46:LYS:NZ	50:C1:439:A:OP1	2.40	0.45
20:CD:261:ALA:HA	20:CD:264:VAL:HG12	1.98	0.45
23:CH:224:CYS:HB3	23:CH:227:VAL:HG23	1.97	0.45
24:CI:1028:PRO:HG2	50:C1:1161:G:H5"	1.99	0.45
26:CK:112:PRO:HG2	26:CK:189:PRO:HD3	1.98	0.45
30:CP:205:ARG:HD3	30:CP:205:ARG:HA	1.78	0.45
32:CS:517:GLU:N	32:CS:517:GLU:OE2	2.50	0.45
36:Cc:44:SER:HA	48:Cp:54:ILE:HB	1.98	0.45
44:Ck:135:PRO:HA	44:Ck:141:ARG:HG3	1.99	0.45
53:UT:969:PHE:HZ	53:UT:1023:ILE:HD11	1.81	0.45
53:UT:1180:VAL:HG23	53:UT:1185:ARG:HH22	1.82	0.45
53:UT:1569:SER:HA	53:UT:1572:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:1632:ASP:HB3	53:UT:1633:TRP:CE3	2.52	0.45
54:UH:842:TYR:HB2	54:UH:871:LEU:HD13	1.98	0.45
1:UA:2:LYS:NZ	15:UU:676:GLY:O	2.44	0.45
1:UA:486:GLY:HA3	1:UA:513:VAL:HG11	1.99	0.45
2:UB:481:CYS:HB2	2:UB:511:HIS:CD2	2.52	0.45
4:UD:564:ALA:HB1	4:UD:630:PRO:HG2	1.99	0.45
9:UL:432:VAL:HA	9:UL:442:ALA:O	2.17	0.45
10:UM:452:SER:OG	10:UM:453:LYS:N	2.49	0.45
17:UZ:120:LEU:HD21	17:UZ:221:VAL:HG13	1.99	0.45
19:CC:236:SER:OG	19:CC:239:ASP:OD1	2.23	0.45
23:CH:158:LEU:HA	23:CH:161:TYR:HD2	1.82	0.45
23:CH:377:ILE:HG21	24:CI:542:LEU:HD23	1.98	0.45
24:CI:72:VAL:HG11	24:CI:129:MET:HB3	1.98	0.45
50:C1:495:G:OP2	50:C1:495:G:N2	2.38	0.45
52:CW:156:VAL:HA	52:CW:203:ALA:HA	1.99	0.45
57:Cl:49:LYS:HD3	57:Cl:49:LYS:HA	1.72	0.45
1:UA:216:ASP:OD1	1:UA:216:ASP:N	2.50	0.44
2:UB:681:PRO:HB2	2:UB:683:HIS:HE2	1.82	0.44
4:UD:802:ARG:HA	4:UD:805:GLU:HG2	1.98	0.44
8:UK:253:SER:HB3	8:UK:265:VAL:H	1.80	0.44
9:UL:626:SER:OG	9:UL:627:ALA:N	2.50	0.44
10:UM:165:ALA:C	10:UM:195:ARG:HH22	2.25	0.44
10:UM:383:LEU:HD11	10:UM:464:PRO:HG3	1.99	0.44
13:UQ:803:LEU:HD23	13:UQ:830:VAL:HG11	1.98	0.44
14:UR:367:GLN:O	14:UR:370:GLN:C	2.60	0.44
15:UU:665:MET:HG3	15:UU:666:THR:HG22	1.98	0.44
30:CP:129:MET:HE1	30:CP:186:GLU:HA	1.97	0.44
31:CQ:171:ILE:HG23	31:CQ:236:VAL:HG21	1.99	0.44
32:CS:291:LYS:NZ	32:CS:412:SER:O	2.50	0.44
32:CS:926:LEU:HD23	32:CS:926:LEU:HA	1.83	0.44
35:Cb:122:LYS:HE2	35:Cb:145:ARG:NH2	2.33	0.44
39:Cf:65:PHE:HD2	39:Cf:104:ILE:HD13	1.82	0.44
58:CX:430:ARG:HH12	58:CX:458:GLY:HA2	1.82	0.44
60:CZ:403:ILE:O	60:CZ:407:MET:HG3	2.18	0.44
60:CZ:575:THR:HG22	60:CZ:579:GLN:HB2	1.97	0.44
2:UB:553:SER:HA	2:UB:556:VAL:HG22	1.99	0.44
4:UD:5:ARG:HH12	54:UH:904:ARG:HH11	1.64	0.44
4:UD:640:ARG:HH12	4:UD:660:ASN:ND2	2.15	0.44
7:UJ:1351:ALA:HB2	7:UJ:1378:LEU:HD23	1.98	0.44
8:UK:162:ILE:HD13	61:UP:321:ARG:HH21	1.83	0.44
9:UL:680:TYR:O	9:UL:689:ILE:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:UU:71:LEU:HD11	15:UU:106:ALA:HB2	1.98	0.44
18:CB:184:GLU:O	18:CB:207:VAL:HA	2.18	0.44
19:CC:181:ILE:HG13	19:CC:184:LEU:HD23	1.99	0.44
20:CD:293:ILE:HG21	20:CD:369:ILE:HD11	1.98	0.44
24:CI:772:ARG:HE	24:CI:775:LYS:HE2	1.81	0.44
24:CI:915:VAL:HG21	24:CI:992:TRP:HB3	2.00	0.44
27:CL:705:LYS:HA	27:CL:708:MET:HE3	1.98	0.44
30:CP:196:TYR:O	30:CP:200:GLU:HG2	2.17	0.44
32:CS:916:MET:HA	32:CS:919:VAL:HG22	2.00	0.44
34:Ca:134:LEU:HG	34:Ca:218:LEU:HD12	1.99	0.44
35:Cb:125:LYS:HB3	35:Cb:142:HIS:HD2	1.80	0.44
38:Ce:184:ARG:HH22	38:Ce:185:ARG:HE	1.65	0.44
44:Ck:85:MET:HG3	44:Ck:88:THR:HB	1.99	0.44
50:C1:1013:G:H2'	50:C1:1014:G:H8	1.82	0.44
52:CW:119:ARG:NH1	52:CW:135:ILE:O	2.49	0.44
53:UT:1037:ASP:O	53:UT:1040:LEU:C	2.61	0.44
53:UT:2043:SER:OG	53:UT:2045:SER:O	2.35	0.44
59:CY:103:LEU:HA	59:CY:106:LYS:HG2	1.99	0.44
1:UA:546:SER:OG	1:UA:547:GLY:N	2.50	0.44
1:UA:724:LEU:HD22	1:UA:749:VAL:HG22	1.99	0.44
4:UD:356:ALA:HB1	4:UD:359:LYS:HB2	1.99	0.44
7:UJ:813:ILE:HA	7:UJ:816:MET:HG3	1.99	0.44
7:UJ:1645:ASN:OD1	7:UJ:1646:LEU:N	2.50	0.44
9:UL:613:MET:HE3	9:UL:613:MET:HB2	1.76	0.44
9:UL:800:GLU:HA	9:UL:803:ARG:HG2	1.99	0.44
13:UQ:146:SER:HA	13:UQ:157:TRP:O	2.16	0.44
18:CB:150:MET:HE2	18:CB:156:VAL:HG11	1.99	0.44
24:CI:299:ILE:HG12	24:CI:779:LEU:HD22	1.98	0.44
32:CR:24:ARG:NH2	32:CR:140:ILE:O	2.50	0.44
32:CS:181:VAL:HG22	32:CS:563:PRO:HB3	1.98	0.44
34:Ca:82:ARG:NH2	34:Ca:188:LEU:O	2.50	0.44
37:Cd:192:HIS:O	37:Cd:196:LEU:HD12	2.17	0.44
53:UT:1284:SER:O	53:UT:1288:THR:HG23	2.17	0.44
53:UT:1645:VAL:HG11	53:UT:1719:LEU:HD22	1.99	0.44
3:UC:239:LEU:HD23	3:UC:242:LEU:HD12	1.98	0.44
9:UL:573:PHE:CE1	9:UL:580:LEU:HD13	2.52	0.44
10:UM:21:TYR:HB2	10:UM:37:SER:HB2	1.98	0.44
10:UM:238:ILE:HA	10:UM:248:LEU:O	2.17	0.44
13:UQ:181:THR:O	13:UQ:229:LYS:NZ	2.46	0.44
13:UQ:356:ARG:HD2	13:UQ:526:ILE:HD12	1.99	0.44
18:CA:180:VAL:O	18:CA:203:VAL:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:CI:87:SER:HB3	24:CI:219:ILE:HG13	1.98	0.44
24:CI:148:MET:HE3	24:CI:148:MET:HB3	1.75	0.44
24:CI:858:ARG:NH2	50:C1:1157:C:O3'	2.51	0.44
26:CK:162:THR:OG1	26:CK:271:GLY:O	2.29	0.44
32:CS:484:ASP:O	32:CS:487:GLU:HG3	2.18	0.44
35:Cb:19:LEU:HB2	35:Cb:51:ARG:NH2	2.31	0.44
50:C1:745:U:H2'	50:C1:746:A:H8	1.83	0.44
53:UT:1377:VAL:HA	53:UT:1380:ARG:HG2	1.97	0.44
53:UT:1600:ALA:O	53:UT:1603:THR:OG1	2.26	0.44
53:UT:1617:ARG:HG2	53:UT:1690:PHE:CZ	2.53	0.44
53:UT:1883:LEU:O	53:UT:1887:ARG:HG3	2.17	0.44
54:UH:755:TYR:OH	55:UI:204:MET:SD	2.61	0.44
5:UF:145:THR:O	5:UF:149:ARG:HG3	2.16	0.44
5:UF:165:LEU:HD13	11:UN:370:GLU:HG2	2.00	0.44
7:UJ:919:LEU:HB3	7:UJ:961:LEU:HB3	2.00	0.44
7:UJ:989:ASP:OD1	7:UJ:990:VAL:N	2.50	0.44
7:UJ:1024:GLN:HA	7:UJ:1027:MET:HE2	1.98	0.44
7:UJ:1622:ALA:O	7:UJ:1626:VAL:HG13	2.17	0.44
10:UM:85:MET:HE1	10:UM:128:THR:HG21	1.98	0.44
12:UO:540:ALA:HA	55:UE:246:LEU:HD12	2.00	0.44
15:UU:858:ASP:OD1	15:UU:859:ILE:N	2.50	0.44
22:CG:176:VAL:HG23	22:CG:185:THR:HG22	1.99	0.44
24:CI:954:THR:O	24:CI:957:GLY:N	2.38	0.44
24:CI:974:ARG:NH1	50:C1:2183:A:OP2	2.50	0.44
37:Cd:76:LEU:O	52:CW:49:GLN:NE2	2.50	0.44
40:Cg:123:ALA:O	40:Cg:127:ILE:HG13	2.17	0.44
42:Ci:81:ALA:HB2	42:Ci:118:LEU:HD23	1.99	0.44
44:Ck:72:ARG:HH22	50:C1:830:G:H2'	1.83	0.44
50:C1:81:G:H1	50:C1:126:C:H42	1.66	0.44
50:C1:686:A:H2'	50:C1:687:U:H4'	1.99	0.44
53:UT:11:LYS:HG2	53:UT:798:ASN:HB3	2.00	0.44
53:UT:736:GLY:O	53:UT:739:THR:OG1	2.29	0.44
53:UT:1017:HIS:HA	53:UT:1020:ARG:HH21	1.83	0.44
53:UT:2085:ASP:HA	53:UT:2088:GLU:HB3	1.98	0.44
56:US:430:LYS:HA	56:US:433:LYS:HG3	1.99	0.44
1:UA:343:MET:HE3	1:UA:357:THR:HG21	1.99	0.44
4:UD:487:SER:HA	4:UD:554:PHE:CD2	2.53	0.44
7:UJ:704:LEU:HB3	7:UJ:708:LYS:NZ	2.32	0.44
9:UL:601:LEU:HD22	9:UL:639:GLY:HA3	1.98	0.44
14:UR:322:ARG:HH22	50:C1:133:G:H22	1.64	0.44
19:CC:287:TYR:CZ	19:CC:291:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:CD:341:TYR:HB3	20:CD:345:TYR:HB2	1.99	0.44
22:CG:398:MET:HA	22:CG:413:SER:HA	1.99	0.44
29:CO:111:GLN:NE2	29:CO:123:GLU:OE2	2.51	0.44
32:CR:785:ARG:HH12	32:CS:840:ARG:NH2	2.14	0.44
32:CR:803:LEU:HD11	32:CR:882:ALA:HB2	2.00	0.44
32:CS:388:ILE:HB	32:CS:410:MET:HG2	1.99	0.44
50:C1:467:C:H4'	50:C1:468:C:H5'	1.99	0.44
50:C1:1239:G:H2'	50:C1:1240:G:H8	1.82	0.44
53:UT:349:ARG:HA	53:UT:349:ARG:HD3	1.84	0.44
53:UT:931:ALA:HB2	53:UT:997:HIS:HD2	1.83	0.44
53:UT:1168:ARG:HA	53:UT:1168:ARG:HD3	1.75	0.44
57:Cl:24:GLY:HA2	57:Cl:58:ALA:HB3	2.00	0.44
6:UG:337:ASN:O	6:UG:380:LYS:NZ	2.48	0.44
7:UJ:109:LEU:HD11	7:UJ:138:THR:HG22	1.99	0.44
7:UJ:330:LYS:HA	7:UJ:333:ILE:HD12	1.99	0.44
7:UJ:721:ALA:O	7:UJ:725:ARG:HG3	2.17	0.44
24:CI:1077:GLN:NE2	50:C1:366:G:OP1	2.41	0.44
32:CR:32:ASP:O	32:CR:154:LYS:NZ	2.50	0.44
32:CR:855:LEU:HA	32:CR:858:MET:HG2	2.00	0.44
32:CR:914:LYS:O	32:CR:918:LYS:HG3	2.18	0.44
32:CS:795:ARG:HA	32:CS:890:GLN:OE1	2.18	0.44
32:CS:883:ILE:HD12	32:CS:911:ILE:HG21	2.00	0.44
37:Cd:20:ASP:OD2	37:Cd:22:ARG:NH1	2.51	0.44
49:CU:189:THR:HG23	49:CU:191:THR:H	1.82	0.44
50:C1:782:G:H2'	50:C1:783:G:C8	2.53	0.44
50:C1:907:A:O2'	50:C1:930:G:N2	2.50	0.44
52:CW:343:GLY:HA2	52:CW:362:LEU:HD22	2.00	0.44
53:UT:306:ILE:HD11	53:UT:341:VAL:HG22	2.00	0.44
53:UT:659:LEU:HA	53:UT:667:ARG:HG3	1.99	0.44
53:UT:1310:THR:HB	53:UT:1351:VAL:HG12	2.00	0.44
55:UI:190:SER:HB2	55:UI:228:ALA:HB2	1.99	0.44
2:UB:116:ILE:HG13	23:CH:58:GLU:HG3	2.00	0.44
4:UD:48:ARG:NE	4:UD:54:GLU:OE2	2.48	0.44
4:UD:122:LYS:HG2	4:UD:123:LYS:HG3	1.98	0.44
7:UJ:810:PHE:HA	7:UJ:813:ILE:HG12	2.00	0.44
9:UL:449:LEU:HD12	9:UL:482:VAL:HG21	2.00	0.44
13:UQ:751:LEU:HD21	13:UQ:791:LEU:HD12	1.99	0.44
13:UQ:827:PHE:HD2	13:UQ:831:ILE:HD11	1.83	0.44
15:UU:692:VAL:HG12	15:UU:699:THR:HA	2.00	0.44
22:CG:106:ARG:HH22	59:CY:329:SER:N	2.15	0.44
22:CG:408:MET:HE2	22:CG:420:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CG:420:LEU:O	22:CG:429:LEU:N	2.51	0.44
25:CJ:159:THR:OG1	25:CJ:160:TRP:N	2.49	0.44
29:CN:135:LYS:HE3	29:CN:135:LYS:HB3	1.85	0.44
30:CP:278:ALA:O	30:CP:282:GLU:HG2	2.17	0.44
32:CR:620:GLN:OE1	37:Cd:25:ARG:NH2	2.50	0.44
32:CS:190:LEU:HA	32:CS:193:LEU:HG	1.99	0.44
34:Ca:219:LYS:HA	34:Ca:219:LYS:HD3	1.77	0.44
35:Cb:128:ARG:O	35:Cb:139:LEU:HA	2.18	0.44
37:Cd:137:ARG:NH2	50:C1:728:G:O6	2.51	0.44
38:Ce:73:LEU:HG	38:Ce:100:ALA:HB2	2.00	0.44
40:Cg:146:VAL:HG11	40:Cg:154:ILE:HD11	2.00	0.44
53:UT:282:MET:HE1	53:UT:325:VAL:HG23	1.99	0.44
53:UT:1997:VAL:HG22	53:UT:2035:GLU:HG2	2.00	0.44
53:UT:2132:ARG:HE	53:UT:2174:SER:HB3	1.81	0.44
56:US:91:LEU:HD11	56:US:114:LEU:HD13	2.00	0.44
56:US:496:SER:H	56:US:499:SER:HB2	1.82	0.44
3:UC:219:TYR:HA	27:CL:60:ARG:HB2	1.99	0.44
6:UG:326:ILE:HD11	6:UG:370:LEU:HD13	1.99	0.44
7:UJ:102:LEU:HA	7:UJ:105:VAL:HG12	2.00	0.44
7:UJ:129:GLU:HG2	7:UJ:156:PRO:HG2	1.99	0.44
9:UL:239:GLY:HA2	9:UL:275:ARG:HE	1.82	0.44
9:UL:492:TYR:HD1	9:UL:499:LEU:HA	1.83	0.44
9:UL:913:GLN:O	9:UL:917:MET:HG3	2.17	0.44
12:UO:463:ARG:HH21	13:UQ:523:ASP:HB3	1.83	0.44
12:UO:478:VAL:HG13	12:UO:505:LEU:HD12	1.99	0.44
16:UX:-8:GLY:N	50:C1:254:G:O6	2.51	0.44
18:CA:107:LYS:HB2	18:CA:129:ILE:HD12	2.00	0.44
18:CA:309:LYS:HE3	18:CA:309:LYS:HB3	1.82	0.44
24:CI:248:ASN:HB3	24:CI:271:SER:HB2	1.99	0.44
29:CO:121:LEU:HD22	29:CO:163:ILE:HB	2.00	0.44
32:CR:795:ARG:HA	32:CR:890:GLN:HG3	1.99	0.44
32:CR:845:ALA:HB1	32:CR:917:ARG:HE	1.83	0.44
35:Cb:63:ALA:O	35:Cb:67:GLN:HG2	2.18	0.44
50:C1:1503:U:H2'	50:C1:1504:A:C8	2.53	0.44
50:C1:2368:U:H2'	50:C1:2369:G:C8	2.53	0.44
53:UT:10:LEU:H	53:UT:205:ARG:NH2	2.16	0.44
53:UT:804:LEU:O	53:UT:808:THR:HG23	2.18	0.44
58:CX:266:MET:O	58:CX:270:ILE:HB	2.18	0.44
3:UC:235:GLU:OE1	3:UC:269:TYR:OH	2.26	0.43
4:UD:65:GLN:HB3	4:UD:370:GLN:HB2	2.00	0.43
4:UD:413:LEU:HD12	54:UH:907:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:UJ:1429:ILE:N	7:UJ:1430:PRO:HD2	2.32	0.43
9:UL:42:ALA:HB1	9:UL:70:VAL:HB	2.00	0.43
9:UL:570:SER:HB3	9:UL:583:ALA:HB3	2.00	0.43
12:UO:70:ASN:C	12:UO:70:ASN:ND2	2.76	0.43
20:CD:287:PRO:HB2	20:CD:391:ALA:HB2	1.99	0.43
22:CG:413:SER:O	22:CG:416:GLY:N	2.51	0.43
29:CO:122:ILE:HG12	29:CO:162:VAL:HG12	2.00	0.43
32:CR:65:LEU:HD22	32:CR:154:LYS:HE3	2.00	0.43
32:CR:126:GLN:HA	32:CR:152:LEU:HD12	1.99	0.43
32:CR:877:SER:H	32:CR:880:GLN:HB2	1.82	0.43
32:CS:885:LEU:HD23	32:CS:890:GLN:HG2	2.00	0.43
35:Cb:85:GLY:N	35:Cb:88:ASP:OD2	2.39	0.43
37:Cd:211:TYR:HA	37:Cd:214:ILE:HG22	1.99	0.43
44:Ck:68:MET:HE1	50:C1:833:U:C4	2.53	0.43
46:Cn:74:VAL:HG11	46:Cn:104:LEU:HD11	2.00	0.43
53:UT:977:PHE:HZ	53:UT:995:LEU:HD21	1.82	0.43
53:UT:1183:THR:O	53:UT:1187:MET:HG3	2.18	0.43
53:UT:1938:LEU:HD21	53:UT:1942:ILE:HD11	2.00	0.43
54:UH:877:ILE:HD12	54:UH:899:PHE:HD2	1.83	0.43
56:US:198:PHE:HE2	56:US:264:GLN:HG3	1.83	0.43
59:CY:81:LEU:HD22	60:CZ:404:TRP:CD2	2.53	0.43
2:UB:615:MET:HE3	2:UB:615:MET:O	2.18	0.43
7:UJ:1459:ALA:HA	7:UJ:1462:MET:HE2	1.98	0.43
8:UK:218:LYS:NZ	50:C1:378:C:OP2	2.41	0.43
9:UL:17:VAL:HG22	9:UL:394:LEU:HD13	2.00	0.43
10:UM:310:THR:HA	10:UM:361:ILE:H	1.82	0.43
10:UM:432:HIS:CE1	10:UM:458:ARG:HD2	2.53	0.43
18:CB:94:THR:O	18:CB:127:TYR:HA	2.19	0.43
24:CI:90:ARG:HH22	32:CR:91:GLN:HB2	1.83	0.43
29:CO:116:THR:HG23	29:CO:119:GLY:H	1.82	0.43
32:CR:255:LEU:HD11	32:CR:330:GLY:HA2	1.99	0.43
32:CS:282:THR:OG1	32:CS:471:GLU:OE1	2.28	0.43
32:CS:310:ILE:HG12	32:CS:385:LEU:HD23	2.00	0.43
32:CS:532:VAL:HG13	32:CS:579:LEU:HD21	2.00	0.43
39:Cf:98:LYS:HB3	50:C1:913:G:H5"	2.01	0.43
50:C1:346:C:O2'	50:C1:347:C:O5'	2.35	0.43
50:C1:2120:C:H1'	50:C1:2155:G:H22	1.83	0.43
53:UT:872:PHE:HE2	53:UT:929:LEU:HD11	1.83	0.43
53:UT:1029:VAL:HA	53:UT:1032:MET:HG2	2.00	0.43
53:UT:1206:ILE:O	53:UT:1210:ILE:HG12	2.18	0.43
53:UT:1358:LEU:HD22	53:UT:1362:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:2047:GLN:NE2	53:UT:2085:ASP:OD1	2.48	0.43
54:UH:739:LEU:O	54:UH:743:ARG:HG3	2.18	0.43
54:UH:862:HIS:CE1	54:UH:864:SER:HB3	2.53	0.43
59:CY:29:GLN:OE1	60:CZ:372:SER:OG	2.35	0.43
59:CY:56:VAL:HG21	60:CZ:370:ILE:HD12	2.01	0.43
60:CZ:367:TRP:HE1	60:CZ:394:ILE:HD12	1.83	0.43
2:UB:804:ARG:NH2	29:CO:184:ALA:O	2.52	0.43
7:UJ:1411:ASP:HB3	7:UJ:1414:LEU:HB3	1.99	0.43
7:UJ:1438:LEU:HA	7:UJ:1441:LEU:HG	2.00	0.43
7:UJ:1718:HIS:HA	7:UJ:1721:GLU:HG2	2.00	0.43
10:UM:638:PHE:HE1	10:UM:683:GLY:HA2	1.82	0.43
11:UN:276:MET:HE1	53:UT:2237:PHE:HB3	2.01	0.43
13:UQ:636:ARG:HH12	55:UE:41:LEU:HB2	1.83	0.43
22:CG:297:ARG:CZ	22:CG:342:GLU:HB2	2.49	0.43
22:CG:347:VAL:HG23	22:CG:398:MET:HE3	1.99	0.43
22:CG:352:ARG:NH1	22:CG:396:GLY:O	2.49	0.43
25:CJ:166:ILE:O	25:CJ:170:ILE:HG13	2.18	0.43
29:CN:130:ILE:HD12	29:CN:131:PRO:HD2	1.99	0.43
37:Cd:21:GLU:O	37:Cd:25:ARG:HD3	2.18	0.43
47:Co:340:THR:HA	47:Co:356:VAL:HG12	2.00	0.43
50:C1:1480:G:H1	50:C1:1502:U:H3	1.65	0.43
53:UT:553:GLU:HA	53:UT:556:LEU:HD12	2.01	0.43
53:UT:1210:ILE:O	53:UT:1213:THR:OG1	2.26	0.43
53:UT:1720:LEU:HD23	53:UT:1723:LEU:HD13	2.00	0.43
54:UH:753:THR:HG23	55:UI:207:ARG:HH21	1.83	0.43
4:UD:432:THR:N	4:UD:446:SER:O	2.44	0.43
7:UJ:489:ASP:HA	7:UJ:492:PHE:HD2	1.83	0.43
9:UL:713:SER:O	9:UL:720:ILE:HA	2.18	0.43
15:UU:561:THR:HA	15:UU:624:ALA:HA	2.00	0.43
16:UX:64:PHE:O	16:UX:68:THR:OG1	2.20	0.43
23:CH:67:ASP:O	23:CH:75:ILE:HA	2.18	0.43
31:CQ:104:PRO:HA	31:CQ:107:ASP:HB3	2.00	0.43
32:CR:15:ILE:HG12	32:CR:148:LEU:HD21	2.00	0.43
32:CS:299:ILE:HG23	32:CS:310:ILE:HD13	1.99	0.43
35:Cb:86:PHE:CD2	35:Cb:87:MET:HG2	2.52	0.43
37:Cd:140:LYS:HA	37:Cd:143:ARG:HG2	1.99	0.43
38:Ce:62:LYS:HB2	38:Ce:94:ARG:HE	1.82	0.43
43:Cj:47:LYS:NZ	43:Cj:79:TYR:OH	2.51	0.43
49:CU:205:THR:O	49:CU:209:ARG:HG3	2.18	0.43
50:C1:176:G:H2'	50:C1:177:G:H8	1.83	0.43
50:C1:2166:A:N1	50:C1:2194:A:H5"	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:717:TYR:HE1	53:UT:727:ALA:HA	1.83	0.43
53:UT:969:PHE:CZ	53:UT:1023:ILE:HD11	2.54	0.43
53:UT:1129:LEU:O	53:UT:1133:ILE:HG12	2.17	0.43
53:UT:1391:ILE:HD11	53:UT:1430:GLN:HA	2.00	0.43
53:UT:1630:LYS:HA	53:UT:1630:LYS:HD2	1.69	0.43
4:UD:774:VAL:HG11	13:UQ:342:ARG:HE	1.84	0.43
5:UF:328:PHE:HB2	5:UF:334:THR:HG21	2.00	0.43
7:UJ:174:LEU:HD13	33:CT:74:PRO:HB2	2.00	0.43
7:UJ:1255:LEU:C	7:UJ:1257:ASN:N	2.76	0.43
7:UJ:1630:VAL:HG23	7:UJ:1678:VAL:HG21	2.00	0.43
9:UL:109:HIS:NE2	9:UL:127:SER:OG	2.43	0.43
12:UO:467:ARG:NH2	12:UO:507:ASP:OD2	2.33	0.43
13:UQ:740:LEU:HD22	13:UQ:816:ILE:HD12	2.01	0.43
17:UZ:28:LYS:HB2	17:UZ:28:LYS:HE2	1.82	0.43
22:CG:253:LYS:HD3	22:CG:253:LYS:HA	1.73	0.43
22:CG:444:LEU:HD22	22:CG:453:PRO:HB2	1.99	0.43
24:CI:284:GLN:HB3	24:CI:296:ILE:HD12	2.01	0.43
24:CI:375:LEU:HD13	32:CR:159:LEU:HG	2.01	0.43
24:CI:1090:LEU:HD22	33:CT:162:VAL:HG22	2.00	0.43
36:Cc:92:GLY:O	50:C1:2192:U:O2'	2.33	0.43
41:Ch:130:LYS:NZ	41:Ch:136:PRO:O	2.32	0.43
50:C1:782:G:H2'	50:C1:783:G:H8	1.83	0.43
50:C1:1239:G:H2'	50:C1:1240:G:C8	2.54	0.43
53:UT:497:GLN:NE2	53:UT:501:LYS:HD2	2.33	0.43
53:UT:1732:LEU:HD23	53:UT:1733:PRO:HD3	2.00	0.43
53:UT:1882:ASP:O	53:UT:1885:THR:OG1	2.35	0.43
58:CX:383:ASP:HA	58:CX:386:VAL:HB	2.01	0.43
1:UA:418:ARG:HD3	1:UA:418:ARG:HA	1.85	0.43
6:UG:43:ARG:O	6:UG:47:GLN:HG3	2.18	0.43
7:UJ:77:GLN:HE21	14:UR:62:ALA:N	2.15	0.43
7:UJ:221:MET:HE1	7:UJ:254:VAL:HG11	2.01	0.43
7:UJ:505:CYS:HA	7:UJ:510:SER:HB3	2.00	0.43
7:UJ:1647:TRP:CZ2	7:UJ:1682:GLN:HB3	2.54	0.43
13:UQ:524:VAL:HG12	13:UQ:526:ILE:H	1.84	0.43
18:CB:180:VAL:HG13	18:CB:203:VAL:HG23	2.00	0.43
18:CB:240:GLY:O	18:CB:244:ARG:HG2	2.19	0.43
19:CC:100:VAL:O	19:CC:120:ALA:HA	2.17	0.43
19:CC:381:TYR:CZ	19:CC:385:LYS:HE2	2.53	0.43
20:CD:214:LEU:HB2	20:CD:225:LEU:HD21	2.00	0.43
27:CL:52:LEU:O	27:CL:55:THR:O	2.36	0.43
29:CO:77:MET:HE1	29:CO:82:ARG:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CS:201:VAL:HG23	32:CS:209:LEU:HB2	2.00	0.43
53:UT:612:ARG:HG2	53:UT:835:ILE:HG23	1.99	0.43
53:UT:1167:PRO:HD2	53:UT:1168:ARG:HG2	2.00	0.43
53:UT:1228:LEU:HG	53:UT:1288:THR:HG21	2.01	0.43
53:UT:1312:LEU:HA	53:UT:1315:GLN:HG2	2.00	0.43
53:UT:1462:PHE:HE2	53:UT:1482:VAL:HG23	1.83	0.43
53:UT:2062:LEU:HB2	53:UT:2101:SER:HB3	2.00	0.43
54:UH:193:VAL:CG1	54:UH:197:VAL:HG21	2.48	0.43
56:US:149:GLN:HG2	56:US:153:LEU:HD22	2.01	0.43
56:US:397:ILE:HD13	56:US:463:LEU:HD22	2.01	0.43
58:CX:355:GLN:HB2	58:CX:391:ARG:HH22	1.84	0.43
6:UG:579:ASP:HA	30:CP:73:ILE:HD11	2.00	0.43
7:UJ:1501:GLN:O	7:UJ:1505:ILE:HG12	2.19	0.43
9:UL:89:ASP:OD1	9:UL:89:ASP:N	2.50	0.43
13:UQ:637:PHE:O	13:UQ:664:SER:N	2.45	0.43
14:UR:326:ARG:HG2	14:UR:342:GLY:HA2	1.99	0.43
15:UU:365:ILE:HB	15:UU:378:LEU:HD22	2.00	0.43
17:UZ:160:ILE:HA	17:UZ:163:LEU:HD23	2.00	0.43
19:CC:27:VAL:HG21	28:CM:335:THR:HG21	2.01	0.43
19:CC:387:SER:O	19:CC:391:ARG:HG3	2.18	0.43
26:CK:117:LEU:HD11	43:Cj:126:PRO:HG2	2.01	0.43
28:CM:423:ARG:NH2	28:CM:431:GLU:O	2.47	0.43
32:CR:614:ILE:HG12	32:CR:634:ARG:HD3	2.00	0.43
32:CR:785:ARG:NH1	32:CS:840:ARG:HH22	2.17	0.43
50:C1:468:C:O2'	50:C1:469:G:O4'	2.37	0.43
53:UT:462:ASN:HA	53:UT:465:LEU:HB2	2.00	0.43
53:UT:1341:LEU:H	53:UT:1381:ARG:HH22	1.67	0.43
55:UE:229:LEU:HD13	55:UE:235:LEU:HD13	1.99	0.43
58:CX:300:ALA:HB2	58:CX:337:HIS:CD2	2.53	0.43
59:CY:231:LEU:O	59:CY:235:ILE:HG12	2.19	0.43
3:UC:317:LYS:HD2	27:CL:159:LEU:HD13	2.01	0.43
6:UG:307:ALA:HB2	6:UG:348:VAL:HG13	2.01	0.43
10:UM:222:ALA:HB3	10:UM:228:LYS:HG3	1.99	0.43
10:UM:280:VAL:HA	10:UM:290:TYR:O	2.18	0.43
11:UN:908:GLU:OE1	28:CM:42:ARG:NH2	2.44	0.43
18:CB:257:ILE:HD13	18:CB:275:GLU:HG2	2.00	0.43
24:CI:288:ILE:HB	24:CI:291:VAL:HB	2.00	0.43
25:CJ:129:LYS:O	25:CJ:133:GLN:HG3	2.18	0.43
28:CM:432:LYS:NZ	50:C1:585:A:OP2	2.41	0.43
29:CO:41:LEU:HD12	29:CO:114:ILE:HG12	2.00	0.43
32:CR:199:CYS:SG	32:CR:212:SER:OG	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CS:390:GLU:HB3	32:CS:393:ALA:HB3	2.00	0.43
35:Cb:127:LYS:HB2	35:Cb:140:VAL:HG23	2.01	0.43
43:Cj:22:CYS:HB2	43:Cj:88:SER:OG	2.19	0.43
51:C2:137:U:H3	51:C2:150:G:H1	1.67	0.43
53:UT:553:GLU:HA	53:UT:556:LEU:HB2	2.01	0.43
53:UT:710:LEU:HD21	53:UT:737:MET:HG2	2.01	0.43
54:UH:252:PHE:CE2	54:UH:272:LEU:HD12	2.54	0.43
54:UH:625:GLU:HA	54:UH:628:VAL:HG12	2.00	0.43
59:CY:56:VAL:HA	59:CY:59:ILE:HD12	1.99	0.43
59:CY:94:LEU:HD21	60:CZ:463:LEU:HD13	2.01	0.43
1:UA:705:GLN:HE22	15:UU:676:GLY:HA3	1.82	0.43
2:UB:519:ASN:O	2:UB:523:LEU:N	2.52	0.43
4:UD:678:LEU:O	4:UD:683:ARG:NH2	2.46	0.43
5:UF:331:HIS:O	5:UF:334:THR:OG1	2.29	0.43
7:UJ:1680:VAL:HG22	7:UJ:1729:HIS:HE1	1.82	0.43
15:UU:233:THR:N	15:UU:247:ALA:O	2.43	0.43
29:CN:178:VAL:HG23	29:CN:223:GLU:HG3	2.00	0.43
32:CR:388:ILE:HD13	32:CR:388:ILE:HG21	1.79	0.43
32:CS:183:ALA:HB1	32:CS:186:ASN:ND2	2.34	0.43
32:CS:361:ILE:HB	32:CS:367:GLN:HG3	2.00	0.43
32:CS:884:LEU:HD13	32:CS:915:ILE:HG21	2.00	0.43
37:Cd:149:LYS:H	37:Cd:149:LYS:HG2	1.49	0.43
39:Cf:24:LYS:HB3	50:C1:984:A:H2	1.84	0.43
45:Cm:24:GLN:HA	45:Cm:63:VAL:O	2.18	0.43
50:C1:60:A:H2'	54:UH:857:LYS:HZ2	1.84	0.43
50:C1:1644:U:O2'	50:C1:1645:U:O2	2.30	0.43
56:US:298:THR:OG1	56:US:299:LYS:N	2.52	0.43
59:CY:323:ARG:O	59:CY:327:ALA:HB3	2.18	0.43
55:UI:235:LEU:O	55:UI:239:LEU:HB2	2.18	0.43
1:UA:3:THR:HG21	1:UA:607:LEU:HD13	2.01	0.43
5:UF:336:SER:OG	5:UF:340:ARG:NH1	2.52	0.43
7:UJ:75:SER:O	7:UJ:78:SER:OG	2.29	0.43
7:UJ:210:TYR:CE1	7:UJ:213:LEU:HB2	2.54	0.43
10:UM:204:ASP:OD2	10:UM:206:ARG:NH2	2.52	0.43
12:UO:25:ARG:NH1	50:C1:85:U:OP2	2.52	0.43
14:UR:401:ILE:HG13	14:UR:407:GLN:C	2.44	0.43
20:CD:15:LEU:HD21	20:CD:80:LEU:HD11	2.01	0.43
22:CG:167:ARG:NE	22:CG:598:ARG:HH12	2.16	0.43
29:CN:144:LEU:HD13	29:CN:150:ILE:HG12	2.01	0.43
40:Cg:127:ILE:HG12	40:Cg:132:ILE:HD11	2.01	0.43
44:Ck:43:VAL:HG11	44:Ck:145:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:C1:221:A:O2'	50:C1:224:C:N4	2.42	0.43
50:C1:1497:U:O2	50:C1:1499:G:N1	2.52	0.43
50:C1:1503:U:H2'	50:C1:1504:A:H8	1.83	0.43
51:C2:160:U:H2'	51:C2:161:G:C8	2.54	0.43
53:UT:108:VAL:HG11	53:UT:143:ARG:HH21	1.82	0.43
53:UT:184:ARG:HD3	53:UT:231:PHE:HD1	1.84	0.43
53:UT:255:ILE:O	53:UT:258:MET:HB3	2.19	0.43
53:UT:557:LYS:HD2	53:UT:557:LYS:HA	1.81	0.43
53:UT:1229:ASP:OD1	53:UT:1232:LYS:NZ	2.36	0.43
53:UT:1863:ILE:HA	53:UT:1866:LEU:HG	2.00	0.43
53:UT:2146:TYR:HA	53:UT:2147:PRO:HD3	1.85	0.43
59:CY:44:LYS:HG3	59:CY:100:THR:HG21	2.01	0.43
1:UA:619:SER:HB3	1:UA:672:GLU:HA	2.01	0.42
1:UA:715:ILE:HG23	1:UA:736:MET:HB3	2.00	0.42
3:UC:308:LEU:HG	3:UC:312:ARG:HE	1.84	0.42
6:UG:355:LEU:HD22	6:UG:368:LYS:HA	2.01	0.42
7:UJ:836:THR:O	7:UJ:914:LYS:NZ	2.41	0.42
7:UJ:1091:SER:O	7:UJ:1095:HIS:ND1	2.44	0.42
9:UL:201:TRP:HA	9:UL:208:CYS:HA	2.00	0.42
9:UL:881:VAL:HA	9:UL:884:THR:HG22	2.01	0.42
10:UM:612:ARG:NH1	10:UM:632:TYR:OH	2.52	0.42
15:UU:961:ILE:HD13	15:UU:971:LEU:HD13	2.00	0.42
18:CA:196:MET:HE3	18:CA:196:MET:HB3	1.91	0.42
29:CN:114:ILE:HB	29:CN:122:ILE:HB	2.01	0.42
32:CR:258:THR:HG23	32:CR:261:GLN:H	1.84	0.42
32:CS:125:LEU:HB3	32:CS:131:ILE:HD11	2.01	0.42
32:CS:541:VAL:HA	32:CS:544:TYR:HB2	2.00	0.42
38:Ce:55:ILE:HG21	38:Ce:182:VAL:HG23	2.01	0.42
39:Cf:89:GLU:OE1	39:Cf:92:ARG:NH2	2.52	0.42
41:Ch:129:TYR:HA	41:Ch:132:VAL:HG12	2.01	0.42
52:CW:119:ARG:NH2	60:CZ:540:LYS:O	2.37	0.42
53:UT:1313:LEU:HD22	53:UT:1358:LEU:HD21	2.01	0.42
53:UT:1712:VAL:HA	53:UT:1715:ILE:HD12	1.99	0.42
53:UT:1723:LEU:HD21	53:UT:1727:LEU:HB2	2.01	0.42
53:UT:1885:THR:HA	53:UT:1888:LYS:NZ	2.34	0.42
55:UI:214:LEU:HA	55:UI:217:TRP:HB2	2.01	0.42
5:UF:130:MET:SD	5:UF:147:ALA:HB2	2.59	0.42
5:UF:377:LEU:HD12	5:UF:381:MET:HE3	2.00	0.42
7:UJ:297:VAL:HG12	7:UJ:300:TRP:HZ3	1.85	0.42
9:UL:19:SER:OG	9:UL:20:SER:N	2.51	0.42
10:UM:506:PRO:HD2	10:UM:526:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:UQ:753:VAL:HG13	13:UQ:763:ALA:HB3	2.01	0.42
15:UU:139:GLN:NE2	15:UU:156:LEU:HB2	2.35	0.42
15:UU:642:LEU:HD22	15:UU:667:LYS:HD3	2.00	0.42
24:CI:555:GLN:HA	24:CI:558:ARG:HB2	2.00	0.42
25:CJ:75:GLU:HG3	25:CJ:94:LEU:HD13	2.01	0.42
32:CR:850:ASP:HB3	32:CR:853:VAL:HG23	2.01	0.42
32:CS:169:VAL:O	32:CS:173:TYR:HD2	2.03	0.42
32:CS:494:LEU:HB2	32:CS:496:LEU:HD13	2.00	0.42
32:CS:644:TYR:HA	32:CS:647:MET:HE1	2.01	0.42
38:Ce:57:VAL:HG11	38:Ce:178:THR:HG23	2.01	0.42
53:UT:1021:LEU:HB3	53:UT:1025:ARG:NH2	2.34	0.42
53:UT:1164:ILE:HD11	53:UT:1186:LEU:HD23	2.00	0.42
53:UT:2066:ARG:HA	53:UT:2105:ARG:HH12	1.84	0.42
54:UH:778:ASP:O	54:UH:782:ARG:HG2	2.19	0.42
2:UB:578:MET:HE1	2:UB:617:ALA:HB1	2.00	0.42
6:UG:222:MET:HG2	6:UG:233:THR:HG22	2.01	0.42
7:UJ:98:VAL:HG11	7:UJ:127:ILE:HD12	2.01	0.42
7:UJ:994:CYS:O	7:UJ:998:SER:HB2	2.19	0.42
7:UJ:1149:LEU:HA	7:UJ:1149:LEU:HD23	1.87	0.42
10:UM:614:VAL:HB	10:UM:626:LEU:HD11	2.00	0.42
12:UO:180:THR:HG22	12:UO:181:ARG:HH11	1.84	0.42
14:UR:170:GLU:O	14:UR:174:ARG:HG2	2.19	0.42
15:UU:567:MET:HE2	15:UU:577:GLN:HB3	2.01	0.42
18:CB:113:THR:H	18:CB:124:LYS:HG3	1.83	0.42
23:CH:110:ILE:HD12	23:CH:110:ILE:HA	1.91	0.42
24:CI:557:LEU:HD11	24:CI:561:ARG:HH21	1.84	0.42
28:CM:422:GLU:O	28:CM:426:SER:CB	2.67	0.42
29:CO:27:ILE:HD11	29:CO:111:GLN:HB2	2.00	0.42
31:CQ:80:ILE:HA	31:CQ:126:SER:HB3	2.01	0.42
32:CR:27:PHE:HB2	32:CR:150:VAL:HG22	2.01	0.42
32:CR:342:TYR:HB3	32:CR:361:ILE:HD13	2.01	0.42
32:CS:837:ASP:HA	32:CS:840:ARG:HG2	2.02	0.42
33:CT:124:LYS:NZ	50:C1:1082:G:N7	2.46	0.42
35:Cb:21:ASP:OD1	35:Cb:22:LYS:N	2.44	0.42
38:Ce:102:ARG:HD2	38:Ce:131:VAL:HG13	2.00	0.42
44:Ck:71:ILE:HG21	44:Ck:145:LEU:HD21	2.00	0.42
50:C1:749:G:H4'	53:UT:704:ARG:HH22	1.85	0.42
53:UT:381:MET:SD	53:UT:382:ASP:N	2.93	0.42
53:UT:432:TYR:OH	53:UT:807:LEU:O	2.34	0.42
53:UT:1583:PHE:HE2	53:UT:1600:ALA:HB2	1.84	0.42
54:UH:78:SER:HB2	54:UH:105:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:CX:411:HIS:CG	58:CX:442:HIS:HB2	2.54	0.42
60:CZ:331:LEU:HD23	60:CZ:331:LEU:HA	1.90	0.42
4:UD:22:THR:HG22	4:UD:43:ARG:H	1.84	0.42
4:UD:647:LEU:O	4:UD:658:ILE:HA	2.19	0.42
5:UF:84:THR:OG1	5:UF:85:SER:N	2.52	0.42
7:UJ:713:HIS:O	7:UJ:717:THR:HB	2.20	0.42
7:UJ:725:ARG:HG2	7:UJ:728:ARG:HH21	1.84	0.42
9:UL:712:VAL:HA	9:UL:721:ARG:O	2.20	0.42
10:UM:253:ASP:OD1	10:UM:253:ASP:N	2.49	0.42
13:UQ:197:VAL:HG21	13:UQ:274:TRP:NE1	2.33	0.42
23:CH:117:LEU:HD21	23:CH:130:VAL:HG21	2.01	0.42
24:CI:240:THR:HG23	24:CI:241:HIS:CD2	2.54	0.42
28:CM:237:VAL:HB	28:CM:443:VAL:HG12	2.01	0.42
28:CM:243:ASN:N	28:CM:258:ALA:O	2.44	0.42
34:Ca:11:LYS:HE2	34:Ca:11:LYS:HB2	1.94	0.42
45:Cm:48:GLY:HA3	45:Cm:64:GLN:O	2.19	0.42
47:Co:346:ASN:HB2	47:Co:353:GLN:NE2	2.27	0.42
50:C1:312:G:O2'	50:C1:328:A:N6	2.52	0.42
53:UT:1408:TYR:HA	53:UT:1411:ARG:HD2	2.01	0.42
1:UA:773:LEU:HD23	1:UA:797:LEU:HD21	2.02	0.42
2:UB:564:PRO:HB2	56:US:513:PRO:HD2	2.02	0.42
4:UD:367:HIS:CD2	4:UD:368:LEU:HG	2.55	0.42
12:UO:449:ASP:HB3	12:UO:452:ILE:HB	2.02	0.42
16:UX:94:CYS:O	16:UX:98:GLU:HG3	2.20	0.42
18:CB:247:LEU:O	20:CD:120:ARG:NH1	2.42	0.42
32:CS:186:ASN:HA	32:CS:189:PHE:HB3	2.02	0.42
35:Cb:116:ASP:OD1	35:Cb:117:GLU:N	2.52	0.42
35:Cb:212:ASP:OD1	35:Cb:213:ALA:N	2.52	0.42
36:Cc:50:GLN:HE21	36:Cc:73:ASN:HA	1.85	0.42
53:UT:256:MET:SD	53:UT:301:VAL:HA	2.60	0.42
53:UT:710:LEU:HD11	53:UT:737:MET:HG2	2.02	0.42
54:UH:869:LEU:HG	55:UE:273:ARG:HH12	1.83	0.42
4:UD:647:LEU:HD23	4:UD:659:PHE:HD1	1.85	0.42
5:UF:162:ALA:HB2	11:UN:359:PRO:HA	2.01	0.42
6:UG:270:ASN:HB3	6:UG:272:ILE:HG12	2.02	0.42
11:UN:283:MET:HE2	53:UT:2204:PHE:HE2	1.84	0.42
13:UQ:550:LEU:HB3	13:UQ:588:TRP:HB2	2.01	0.42
15:UU:418:TRP:CE2	15:UU:430:GLU:HB2	2.55	0.42
15:UU:857:ILE:HG23	31:CQ:254:ARG:HH21	1.84	0.42
15:UU:1013:LEU:HD23	15:UU:1013:LEU:HA	1.90	0.42
16:UX:59:LEU:HD11	16:UX:137:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:UZ:24:LEU:HG	17:UZ:28:LYS:NZ	2.35	0.42
17:UZ:25:LYS:HA	17:UZ:28:LYS:HE2	2.02	0.42
24:CI:148:MET:HE1	24:CI:897:PHE:HB2	2.00	0.42
24:CI:617:ASP:HA	24:CI:620:ARG:HG2	2.02	0.42
32:CS:895:ASP:OD1	32:CS:896:THR:N	2.53	0.42
39:Cf:92:ARG:HH12	52:CW:140:ARG:NH1	2.18	0.42
40:Cg:73:ALA:HB1	40:Cg:77:ARG:NH2	2.35	0.42
60:CZ:272:GLN:HG2	60:CZ:274:GLU:H	1.85	0.42
60:CZ:415:MET:HA	60:CZ:418:ARG:HB3	2.02	0.42
55:UI:239:LEU:HA	55:UI:239:LEU:HD12	1.80	0.42
4:UD:425:ILE:HG21	4:UD:431:ILE:HD11	2.02	0.42
4:UD:487:SER:OG	4:UD:491:ARG:N	2.49	0.42
18:CB:199:ARG:HA	18:CB:199:ARG:HD2	1.76	0.42
19:CC:326:THR:HA	19:CC:394:ASN:HD21	1.84	0.42
22:CG:426:LYS:NZ	59:CY:237:ASP:O	2.52	0.42
24:CI:938:PHE:HA	27:CL:511:ARG:NH2	2.35	0.42
32:CS:58:TRP:HB2	32:CS:106:TYR:HA	2.01	0.42
32:CS:378:HIS:CD2	32:CS:379:VAL:HG13	2.54	0.42
32:CS:525:THR:OG1	32:CS:706:PRO:O	2.31	0.42
32:CS:910:ALA:O	32:CS:914:LYS:HG2	2.20	0.42
40:Cg:129:GLN:HB2	50:C1:1097:U:H4'	2.02	0.42
50:C1:311:G:H21	50:C1:329:A:H62	1.67	0.42
50:C1:781:G:H2'	50:C1:782:G:C8	2.53	0.42
52:CW:170:ARG:NH2	52:CW:180:ARG:O	2.40	0.42
53:UT:585:TYR:O	53:UT:589:CYS:HB3	2.19	0.42
53:UT:2052:GLN:O	53:UT:2056:LYS:HG3	2.19	0.42
56:US:383:LYS:HD2	56:US:383:LYS:HA	1.77	0.42
58:CX:303:PHE:HD1	58:CX:307:LEU:HD13	1.85	0.42
7:UJ:1789:ILE:HD12	7:UJ:1789:ILE:HA	1.93	0.42
8:UK:58:ARG:HH12	8:UK:60:GLU:HA	1.85	0.42
8:UK:79:ARG:HA	8:UK:79:ARG:HD3	1.78	0.42
9:UL:650:ASP:OD1	9:UL:651:SER:N	2.47	0.42
10:UM:120:ASP:OD2	10:UM:124:THR:OG1	2.33	0.42
10:UM:458:ARG:HB3	10:UM:460:TRP:HE1	1.85	0.42
13:UQ:716:ASP:O	13:UQ:720:GLY:HA2	2.20	0.42
15:UU:152:VAL:HG22	15:UU:161:VAL:HG22	2.01	0.42
18:CA:110:SER:HB3	33:CT:141:ILE:HD11	2.02	0.42
19:CC:278:ALA:O	19:CC:282:THR:HG23	2.19	0.42
22:CG:410:VAL:HG12	22:CG:469:LEU:HD21	2.01	0.42
23:CH:406:VAL:HG21	24:CI:809:ARG:HH22	1.84	0.42
32:CR:24:ARG:HH21	32:CR:140:ILE:HG22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CR:93:ASP:OD1	32:CR:93:ASP:N	2.41	0.42
32:CS:272:ILE:HG22	32:CS:305:TYR:HD2	1.85	0.42
37:Cd:85:ARG:NH1	50:C1:745:U:H5"	2.34	0.42
39:Cf:73:THR:O	39:Cf:74:ARG:HD3	2.20	0.42
58:CX:275:ARG:O	58:CX:279:HIS:ND1	2.43	0.42
58:CX:339:ALA:HA	58:CX:342:ILE:HG22	2.02	0.42
1:UA:540:SER:OG	1:UA:541:GLU:N	2.53	0.42
4:UD:756:ARG:CZ	4:UD:758:ARG:HH12	2.33	0.42
7:UJ:1699:ILE:HD13	7:UJ:1740:ALA:HB2	2.02	0.42
8:UK:84:THR:HG22	8:UK:86:THR:HG23	2.01	0.42
9:UL:461:ARG:HE	9:UL:497:ALA:HB2	1.84	0.42
10:UM:311:LYS:HZ3	10:UM:362:LEU:HD22	1.85	0.42
10:UM:325:ALA:HA	10:UM:335:LEU:O	2.19	0.42
10:UM:801:LEU:HD22	10:UM:805:GLN:HB3	2.02	0.42
12:UO:406:PRO:HA	14:UR:321:LYS:HD3	2.02	0.42
13:UQ:738:LYS:HD3	13:UQ:782:VAL:HG22	2.02	0.42
18:CA:230:VAL:HG22	18:CA:232:GLN:HG2	2.01	0.42
22:CG:504:ILE:HG22	22:CG:506:GLY:H	1.84	0.42
24:CI:780:VAL:HG11	32:CR:225:GLU:OE2	2.20	0.42
29:CN:90:ASP:OD1	29:CN:90:ASP:N	2.52	0.42
32:CR:504:LYS:O	32:CR:508:THR:OG1	2.30	0.42
32:CS:635:ILE:O	32:CS:725:VAL:HG23	2.20	0.42
34:Ca:214:LYS:HE2	34:Ca:216:LYS:HD3	2.01	0.42
37:Cd:10:ASN:HD21	53:UT:708:ALA:HB2	1.85	0.42
50:C1:1131:U:O2'	50:C1:1180:C:O2'	2.34	0.42
50:C1:1652:C:H2'	50:C1:1653:G:H8	1.85	0.42
52:CW:229:TYR:CZ	52:CW:236:ARG:HD2	2.54	0.42
53:UT:155:MET:HB3	53:UT:160:VAL:HG11	2.01	0.42
53:UT:392:VAL:O	53:UT:396:ILE:HG12	2.20	0.42
54:UH:749:ASP:OD2	54:UH:751:TRP:NE1	2.53	0.42
56:US:125:LEU:HD23	56:US:125:LEU:HA	1.93	0.42
56:US:375:ALA:HA	56:US:378:VAL:HG22	2.02	0.42
58:CX:284:LEU:HD22	58:CX:323:ILE:HB	2.02	0.42
5:UF:189:LEU:HD23	5:UF:189:LEU:HA	1.90	0.42
6:UG:215:LYS:HG2	50:C1:291:C:C2	2.55	0.42
7:UJ:75:SER:N	7:UJ:78:SER:OG	2.51	0.42
7:UJ:1109:ASP:O	7:UJ:1112:PHE:HB3	2.19	0.42
7:UJ:1793:LEU:HD23	7:UJ:1797:LEU:HD21	2.02	0.42
9:UL:153:ASP:CG	9:UL:154:GLN:H	2.28	0.42
10:UM:381:TYR:CD1	10:UM:389:MET:HE1	2.55	0.42
13:UQ:263:ILE:HD12	13:UQ:329:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:UU:514:ALA:HB2	15:UU:547:VAL:HG13	2.02	0.42
19:CC:72:GLY:HA3	19:CC:104:LYS:HE3	2.02	0.42
19:CC:197:ARG:NH2	20:CD:174:GLU:OE2	2.52	0.42
22:CG:195:TRP:CD1	22:CG:226:ARG:HA	2.55	0.42
23:CH:154:ARG:HE	23:CH:154:ARG:HB3	1.55	0.42
28:CM:93:VAL:HB	28:CM:104:TRP:HB3	2.01	0.42
32:CR:118:ASN:O	32:CR:142:THR:OG1	2.33	0.42
32:CR:229:LEU:HD23	32:CR:233:ALA:HB1	2.01	0.42
32:CR:229:LEU:HB3	32:CR:233:ALA:HB3	2.01	0.42
32:CS:608:GLN:HE21	32:CS:616:TRP:CD1	2.37	0.42
47:Co:342:LYS:HB2	47:Co:355:VAL:HG12	2.02	0.42
50:C1:466:A:OP1	50:C1:467:C:N4	2.42	0.42
50:C1:1235:C:H2'	50:C1:1236:G:H8	1.85	0.42
50:C1:1625:G:H2'	50:C1:1626:G:C8	2.55	0.42
53:UT:1874:GLN:HA	53:UT:1877:LEU:HD23	2.02	0.42
53:UT:2188:ASP:O	53:UT:2191:THR:OG1	2.29	0.42
55:UE:253:LEU:HD12	55:UE:253:LEU:HA	1.92	0.42
57:Cl:25:LYS:HD2	57:Cl:25:LYS:O	2.20	0.42
58:CX:415:LEU:HA	58:CX:449:ILE:HG12	2.01	0.42
60:CZ:394:ILE:HD13	60:CZ:403:ILE:HG12	2.01	0.42
2:UB:116:ILE:HG12	23:CH:66:ILE:HB	2.01	0.41
3:UC:596:GLU:O	3:UC:603:LYS:HB2	2.20	0.41
4:UD:44:LEU:HD21	4:UD:341:VAL:HG11	2.02	0.41
6:UG:398:VAL:HG12	6:UG:409:ILE:HG12	2.01	0.41
7:UJ:612:ALA:HA	7:UJ:664:LEU:HD11	2.01	0.41
10:UM:203:GLN:OE1	34:Ca:29:TRP:HD1	2.03	0.41
15:UU:351:VAL:HA	15:UU:364:TRP:O	2.19	0.41
15:UU:456:THR:HG23	15:UU:459:ASP:H	1.85	0.41
19:CC:269:VAL:HG13	20:CD:281:ARG:HH21	1.85	0.41
20:CD:172:LEU:HD11	20:CD:271:ARG:NH1	2.35	0.41
21:CF:31:TYR:O	21:CF:33:GLN:NE2	2.52	0.41
32:CR:722:TYR:HB2	32:CR:763:ILE:HD11	2.02	0.41
35:Cb:128:ARG:HG2	35:Cb:140:VAL:HG22	2.00	0.41
37:Cd:198:ARG:HA	37:Cd:201:GLN:HG3	2.02	0.41
47:Co:346:ASN:HB3	47:Co:351:ARG:HG3	2.02	0.41
50:C1:625:C:H2'	50:C1:626:A:C8	2.55	0.41
52:CW:139:GLY:HA2	52:CW:155:ALA:HA	2.02	0.41
53:UT:1790:LEU:O	53:UT:1793:THR:OG1	2.35	0.41
1:UA:358:ALA:HB1	1:UA:385:VAL:HG13	2.00	0.41
7:UJ:1478:TYR:HD1	7:UJ:1481:LEU:HD12	1.85	0.41
7:UJ:1524:SER:HB2	7:UJ:1583:TRP:CG	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:UL:434:ILE:HD11	9:UL:712:VAL:HG22	2.02	0.41
9:UL:456:THR:O	9:UL:458:GLN:HG2	2.21	0.41
9:UL:600:TYR:OH	23:CH:303:GLY:HA2	2.21	0.41
13:UQ:212:THR:HG22	13:UQ:215:SER:HB3	2.02	0.41
13:UQ:586:LYS:HE3	13:UQ:601:ARG:HD3	2.01	0.41
13:UQ:790:ALA:HA	13:UQ:812:LEU:O	2.20	0.41
15:UU:329:PRO:HA	15:UU:330:PRO:HD3	1.95	0.41
18:CA:187:HIS:HB3	19:CC:166:VAL:HG23	2.01	0.41
18:CB:250:GLY:HA2	18:CB:306:TYR:O	2.20	0.41
19:CC:74:MET:HE3	19:CC:79:LYS:HB2	2.00	0.41
24:CI:397:ALA:HB2	32:CR:707:PRO:HG3	2.02	0.41
24:CI:1000:PHE:CE2	24:CI:1002:ASN:HB2	2.55	0.41
27:CL:487:ILE:O	27:CL:491:GLU:HG3	2.20	0.41
32:CR:386:VAL:HG13	32:CR:406:TYR:HE2	1.85	0.41
32:CR:518:LEU:HD11	32:CR:586:ILE:HD13	2.02	0.41
37:Cd:137:ARG:HE	50:C1:753:A:P	2.44	0.41
40:Cg:110:LEU:HD23	40:Cg:110:LEU:HA	1.82	0.41
48:Cp:9:LYS:HE3	48:Cp:9:LYS:HB3	1.84	0.41
50:C1:770:C:H42	50:C1:781:G:H1	1.68	0.41
52:CW:264:SER:HA	52:CW:289:PRO:HA	2.02	0.41
53:UT:333:GLN:HG3	53:UT:334:GLN:HG3	2.02	0.41
53:UT:536:ARG:HA	53:UT:539:LYS:HD3	2.02	0.41
53:UT:1349:ARG:HA	53:UT:1349:ARG:HD3	1.94	0.41
53:UT:1912:LEU:HD12	53:UT:1989:PHE:HE2	1.85	0.41
55:UE:211:ALA:O	55:UE:215:MET:HG3	2.20	0.41
56:US:459:GLU:H	56:US:459:GLU:CD	2.29	0.41
59:CY:38:ILE:HG22	59:CY:41:LEU:H	1.84	0.41
1:UA:495:TRP:HB3	1:UA:497:ILE:HG23	2.02	0.41
1:UA:541:GLU:O	1:UA:543:GLN:N	2.53	0.41
7:UJ:930:HIS:H	7:UJ:969:MET:HE3	1.85	0.41
7:UJ:1305:LEU:HD21	7:UJ:1339:TYR:CD2	2.56	0.41
7:UJ:1582:GLU:HA	7:UJ:1585:THR:HG22	2.01	0.41
10:UM:273:ARG:HG3	10:UM:277:LEU:HD11	2.01	0.41
14:UR:389:ALA:HB3	14:UR:397:MET:HB2	2.02	0.41
19:CC:232:LEU:HD23	19:CC:259:LYS:HE3	2.03	0.41
23:CH:148:LEU:HD22	23:CH:152:THR:HG21	2.02	0.41
27:CL:122:PRO:HB2	27:CL:123:ALA:H	1.67	0.41
29:CN:180:LEU:HD13	29:CN:206:VAL:HG22	2.02	0.41
30:CP:113:LYS:HE3	30:CP:113:LYS:HB2	1.82	0.41
34:Ca:137:LEU:HD22	34:Ca:215:VAL:HG22	2.01	0.41
46:Cn:51:GLY:HA2	46:Cn:77:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:583:HIS:HE1	53:UT:615:SER:HB2	1.86	0.41
53:UT:1409:ASN:OD1	53:UT:1410:THR:N	2.53	0.41
53:UT:1770:PHE:HA	53:UT:1773:ILE:HD12	2.02	0.41
53:UT:2099:LEU:HA	53:UT:2102:VAL:HG12	2.01	0.41
56:US:195:ASP:HB3	56:US:243:PHE:HD1	1.84	0.41
59:CY:275:TYR:HA	59:CY:278:THR:HG22	2.03	0.41
60:CZ:536:ARG:HH11	60:CZ:537:ARG:H	1.68	0.41
2:UB:320:THR:OG1	2:UB:321:GLU:N	2.53	0.41
7:UJ:139:PHE:HB3	7:UJ:148:PHE:HD1	1.84	0.41
7:UJ:655:LEU:HG	7:UJ:660:LEU:HD23	2.02	0.41
7:UJ:856:LEU:HA	7:UJ:859:VAL:HG12	2.01	0.41
7:UJ:1131:PHE:O	7:UJ:1135:LEU:HG	2.20	0.41
7:UJ:1553:ILE:HD12	7:UJ:1553:ILE:HA	1.89	0.41
8:UK:64:TYR:HB2	8:UK:67:MET:HG3	2.03	0.41
10:UM:516:ASP:OD1	10:UM:516:ASP:N	2.53	0.41
16:UX:166:MET:HA	16:UX:174:ALA:O	2.20	0.41
18:CA:213:PRO:HA	18:CA:216:TYR:CZ	2.55	0.41
18:CA:235:GLN:HG2	18:CA:255:ILE:HD11	2.03	0.41
18:CB:174:VAL:HG22	18:CB:178:GLY:HA3	2.03	0.41
24:CI:528:ARG:HA	32:CR:247:GLN:HE22	1.85	0.41
28:CM:319:ASP:HA	28:CM:395:ARG:NH1	2.35	0.41
28:CM:394:HIS:C	28:CM:395:ARG:HD2	2.46	0.41
32:CR:200:LEU:HD23	32:CR:200:LEU:HA	1.92	0.41
32:CS:289:ARG:HH12	32:CS:476:GLU:N	2.18	0.41
35:Cb:113:ARG:HH21	53:UT:77:ARG:HE	1.67	0.41
50:C1:662:A:H62	53:UT:793:HIS:CE1	2.37	0.41
53:UT:178:LEU:HD22	53:UT:179:LEU:HD22	2.03	0.41
53:UT:579:SER:O	53:UT:583:HIS:ND1	2.50	0.41
53:UT:717:TYR:CE2	53:UT:756:VAL:HG13	2.54	0.41
53:UT:1260:THR:HG21	53:UT:1296:ILE:HG21	2.02	0.41
53:UT:1732:LEU:HD21	53:UT:1772:PHE:CD1	2.55	0.41
53:UT:1923:TYR:OH	53:UT:1995:ASP:OD2	2.27	0.41
56:US:388:LEU:O	56:US:392:ALA:HB2	2.20	0.41
58:CX:217:LEU:HD11	58:CX:249:ALA:HB1	2.02	0.41
4:UD:529:LEU:O	4:UD:531:ARG:NH1	2.54	0.41
4:UD:660:ASN:O	4:UD:664:GLY:N	2.50	0.41
12:UO:528:ALA:O	12:UO:532:ARG:HG2	2.21	0.41
13:UQ:165:ILE:HD13	13:UQ:205:LEU:HD23	2.01	0.41
25:CJ:56:GLN:O	25:CJ:60:ARG:HG2	2.20	0.41
32:CS:56:VAL:HA	32:CS:122:MET:O	2.20	0.41
45:Cm:128:PHE:HZ	49:CU:281:MET:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Cp:13:VAL:HG13	48:Cp:29:VAL:HG13	2.02	0.41
50:C1:1170:G:H5"	50:C1:1171:C:H5'	2.02	0.41
53:UT:1073:LEU:HD21	53:UT:1137:ALA:HB2	2.03	0.41
54:UH:596:LYS:HB3	54:UH:596:LYS:HE2	1.79	0.41
55:UE:162:ARG:HG3	55:UE:192:LEU:HD21	2.03	0.41
2:UB:672:ARG:HB3	2:UB:690:ARG:NH2	2.35	0.41
4:UD:138:GLN:NE2	4:UD:197:HIS:O	2.41	0.41
4:UD:307:ALA:HB1	13:UQ:328:ASN:ND2	2.36	0.41
6:UG:114:GLN:O	6:UG:118:VAL:HG23	2.21	0.41
7:UJ:1576:ILE:HD12	7:UJ:1580:PHE:HE2	1.85	0.41
9:UL:375:ALA:HB3	9:UL:384:GLN:HB2	2.03	0.41
9:UL:903:ARG:HD3	10:UM:885:GLU:HG2	2.03	0.41
10:UM:209:ILE:HB	10:UM:218:THR:HG23	2.01	0.41
10:UM:326:VAL:HG12	10:UM:335:LEU:HB3	2.01	0.41
11:UN:274:PRO:HA	11:UN:277:LYS:HG3	2.03	0.41
12:UO:203:ASN:HB2	12:UO:219:ALA:HB3	2.02	0.41
13:UQ:786:SER:O	13:UQ:788:SER:N	2.54	0.41
15:UU:39:ARG:HD3	15:UU:41:ILE:HG22	2.02	0.41
19:CC:271:LEU:O	19:CC:275:ARG:HG3	2.21	0.41
27:CL:131:HIS:HB2	27:CL:135:PHE:HE2	1.86	0.41
27:CL:498:ARG:HD3	27:CL:502:LEU:HB3	2.02	0.41
28:CM:339:LYS:HZ3	28:CM:339:LYS:HB2	1.85	0.41
28:CM:378:LEU:HD23	28:CM:378:LEU:HA	1.84	0.41
29:CN:95:CYS:HA	29:CN:98:THR:HG22	2.02	0.41
32:CS:592:GLY:HA3	32:CS:631:SER:HA	2.02	0.41
32:CS:656:LEU:HD22	32:CS:665:PHE:HZ	1.84	0.41
32:CS:855:LEU:HA	32:CS:858:MET:HG2	2.02	0.41
37:Cd:160:ARG:HD3	50:C1:653:U:O2	2.20	0.41
38:Ce:87:LEU:HB3	38:Ce:96:VAL:HG11	2.02	0.41
50:C1:843:U:O2'	50:C1:845:C:OP2	2.31	0.41
53:UT:80:GLN:O	53:UT:84:ARG:HG3	2.20	0.41
53:UT:187:TYR:CE2	53:UT:235:VAL:HG12	2.56	0.41
53:UT:1157:ARG:HD3	53:UT:1199:PHE:CE1	2.56	0.41
58:CX:240:ASP:OD1	58:CX:240:ASP:N	2.52	0.41
58:CX:415:LEU:HD22	58:CX:445:ILE:HG23	2.02	0.41
2:UB:527:SER:HA	2:UB:530:LEU:HG	2.02	0.41
4:UD:644:ASP:OD1	4:UD:645:TYR:N	2.49	0.41
6:UG:283:THR:HG22	6:UG:295:LYS:HG2	2.01	0.41
6:UG:364:THR:HB	6:UG:388:TRP:HB3	2.03	0.41
7:UJ:969:MET:O	7:UJ:972:THR:OG1	2.30	0.41
9:UL:425:HIS:CE1	9:UL:450:LYS:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:UM:120:ASP:CG	10:UM:125:LEU:H	2.29	0.41
10:UM:788:LEU:HD23	10:UM:832:ALA:HA	2.02	0.41
13:UQ:438:GLN:OE1	13:UQ:501:GLN:NE2	2.53	0.41
22:CG:595:LYS:HE3	22:CG:595:LYS:HB2	1.96	0.41
23:CH:150:ILE:HD11	23:CH:173:LEU:HD21	2.03	0.41
24:CI:835:PHE:O	24:CI:841:ARG:HA	2.21	0.41
26:CK:50:LYS:HG2	49:CU:219:ILE:HG22	2.03	0.41
28:CM:73:CYS:SG	28:CM:74:LYS:N	2.94	0.41
28:CM:89:GLY:O	28:CM:108:ALA:N	2.53	0.41
29:CN:99:LEU:HA	29:CN:99:LEU:HD23	1.84	0.41
30:CP:187:ASP:HB3	30:CP:192:ILE:HB	2.03	0.41
32:CS:317:PRO:HG3	32:CS:352:PHE:HA	2.03	0.41
32:CS:425:SER:O	32:CS:429:ILE:HG12	2.21	0.41
37:Cd:29:ASP:O	37:Cd:30:LYS:HD3	2.21	0.41
46:Cn:53:VAL:O	46:Cn:99:ASN:CA	2.68	0.41
53:UT:10:LEU:HD23	53:UT:10:LEU:HA	1.93	0.41
53:UT:184:ARG:HG3	53:UT:234:HIS:CD2	2.56	0.41
53:UT:1694:LEU:HB3	53:UT:1716:ILE:HD11	2.01	0.41
54:UH:486:LEU:HD12	54:UH:486:LEU:HA	1.94	0.41
58:CX:446:ALA:HA	58:CX:449:ILE:HD12	2.02	0.41
2:UB:653:TYR:HA	2:UB:740:TRP:CZ2	2.55	0.41
4:UD:409:ALA:HA	4:UD:412:ASN:HB2	2.02	0.41
6:UG:181:ARG:N	6:UG:195:ALA:O	2.52	0.41
7:UJ:127:ILE:HG23	7:UJ:131:ASN:HB2	2.02	0.41
7:UJ:812:ARG:O	7:UJ:816:MET:HG3	2.21	0.41
7:UJ:944:LEU:HD22	7:UJ:955:LEU:HD22	2.03	0.41
7:UJ:1106:GLY:HA2	7:UJ:1107:PRO:HD3	1.82	0.41
7:UJ:1633:LEU:HG	7:UJ:1647:TRP:HE1	1.85	0.41
8:UK:118:ILE:HD13	51:C2:260:G:H5'	2.03	0.41
9:UL:658:ILE:HA	9:UL:659:PRO:HD3	1.94	0.41
10:UM:482:VAL:HA	10:UM:514:SER:HB2	2.03	0.41
12:UO:482:LEU:HD22	12:UO:526:LEU:HD22	2.03	0.41
13:UQ:416:ASP:OD2	13:UQ:486:GLN:N	2.54	0.41
17:UZ:215:ARG:HE	17:UZ:219:GLU:HB3	1.86	0.41
19:CC:381:TYR:CZ	19:CC:414:ARG:HG3	2.56	0.41
23:CH:261:LEU:HD21	50:C1:1715:A:C5	2.56	0.41
32:CR:184:ARG:HB2	32:CR:560:SER:HB2	2.02	0.41
32:CR:399:VAL:HG12	32:CR:403:MET:HE2	2.02	0.41
32:CS:28:VAL:HG21	32:CS:193:LEU:HD13	2.03	0.41
32:CS:117:GLY:O	65:CS:1101:ADP:O3'	2.39	0.41
32:CS:565:HIS:HA	32:CS:588:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Ca:86:LEU:HB3	34:Ca:98:THR:HB	2.02	0.41
45:Cm:35:VAL:O	45:Cm:39:GLN:HG3	2.21	0.41
50:C1:710:A:H2'	50:C1:711:U:O4'	2.20	0.41
53:UT:133:LEU:HD12	53:UT:133:LEU:HA	1.88	0.41
53:UT:486:GLU:HB3	53:UT:487:ILE:H	1.76	0.41
53:UT:968:ARG:O	53:UT:972:GLU:CB	2.69	0.41
53:UT:1431:TRP:HH2	53:UT:1461:LYS:HD3	1.86	0.41
60:CZ:415:MET:HE2	60:CZ:419:ARG:HD2	2.03	0.41
1:UA:112:VAL:HG22	1:UA:157:LEU:HD13	2.01	0.41
2:UB:512:HIS:HB3	2:UB:515:LEU:HG	2.03	0.41
2:UB:701:GLN:NE2	56:US:542:TRP:HA	2.36	0.41
3:UC:275:SER:HA	27:CL:78:LEU:HD11	2.03	0.41
3:UC:454:LEU:HD21	56:US:398:VAL:HG21	2.03	0.41
3:UC:458:THR:HG22	56:US:474:ILE:HG12	2.02	0.41
4:UD:635:PHE:CE1	4:UD:647:LEU:HD13	2.56	0.41
5:UF:394:LEU:HB2	5:UF:399:ARG:NH2	2.35	0.41
6:UG:234:LEU:HD12	6:UG:264:LEU:HB2	2.02	0.41
7:UJ:733:ILE:O	7:UJ:741:ARG:NH1	2.50	0.41
7:UJ:1076:LYS:HB3	7:UJ:1169:LEU:HG	2.02	0.41
7:UJ:1111:LEU:HD23	7:UJ:1147:THR:HG21	2.03	0.41
7:UJ:1451:ALA:HA	7:UJ:1457:ALA:HB1	2.03	0.41
9:UL:895:MET:O	9:UL:899:LEU:HB2	2.21	0.41
10:UM:114:VAL:HA	10:UM:130:ALA:HA	2.01	0.41
10:UM:200:TRP:CZ3	10:UM:210:PHE:HB2	2.56	0.41
10:UM:248:LEU:HD22	10:UM:282:PHE:CE1	2.56	0.41
13:UQ:353:TRP:NE1	50:C1:72:U:OP1	2.31	0.41
13:UQ:356:ARG:HA	13:UQ:454:ARG:HH12	1.84	0.41
13:UQ:751:LEU:O	13:UQ:764:SER:HA	2.20	0.41
15:UU:34:ILE:HG23	15:UU:780:THR:HG23	2.03	0.41
15:UU:384:HIS:NE2	15:UU:410:SER:OG	2.43	0.41
17:UZ:80:PRO:HB3	17:UZ:234:HIS:ND1	2.35	0.41
18:CB:88:LYS:HD2	18:CB:89:GLU:HB3	2.02	0.41
18:CB:104:TYR:CE2	18:CB:165:THR:HG23	2.56	0.41
19:CC:45:GLY:HA3	50:C1:435:A:N1	2.36	0.41
19:CC:140:LYS:NZ	50:C1:436:A:H62	2.19	0.41
20:CD:165:ILE:HD11	20:CD:285:ILE:HD12	2.02	0.41
25:CJ:88:LEU:HD11	25:CJ:97:VAL:HG22	2.03	0.41
28:CM:64:GLY:O	28:CM:92:LYS:NZ	2.54	0.41
28:CM:253:MET:HG3	28:CM:270:ARG:HH11	1.86	0.41
29:CN:196:LEU:HD21	29:CN:202:ILE:HB	2.01	0.41
29:CO:32:LYS:HD2	29:CO:172:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CO:179:THR:HB	29:CO:221:VAL:HG21	2.02	0.41
30:CP:122:ASP:HB2	30:CP:178:LEU:HD22	2.01	0.41
32:CR:630:LEU:HD12	32:CR:631:SER:H	1.86	0.41
32:CS:742:PHE:HA	32:CS:764:ARG:HD3	2.03	0.41
34:Ca:116:LYS:NZ	50:C1:1518:A:OP1	2.54	0.41
34:Ca:185:VAL:O	34:Ca:189:ILE:HG12	2.21	0.41
36:Cc:83:SER:HB2	36:Cc:163:THR:HG21	2.03	0.41
37:Cd:26:HIS:CG	37:Cd:40:PRO:HG2	2.56	0.41
37:Cd:56:ASN:HD22	37:Cd:62:PRO:HA	1.85	0.41
43:Cj:6:ALA:HA	43:Cj:22:CYS:O	2.21	0.41
50:C1:278:A:OP2	50:C1:278:A:H8	2.03	0.41
50:C1:1177:U:H4'	50:C1:1179:G:H4'	2.02	0.41
50:C1:1243:C:H2'	50:C1:1244:G:C8	2.56	0.41
52:CW:236:ARG:HH22	52:CW:239:VAL:HG23	1.86	0.41
52:CW:328:GLU:HA	52:CW:329:PRO:HD3	1.88	0.41
53:UT:488:PHE:O	53:UT:542:THR:OG1	2.34	0.41
53:UT:1208:PRO:HA	53:UT:1211:VAL:HG22	2.01	0.41
53:UT:1329:LEU:HD22	53:UT:1362:PHE:HE2	1.86	0.41
53:UT:1465:ALA:O	53:UT:1469:VAL:HG22	2.20	0.41
53:UT:1940:ARG:NH2	53:UT:2038:LYS:HG3	2.36	0.41
53:UT:2005:LYS:HB2	53:UT:2005:LYS:HE2	1.89	0.41
54:UH:551:ASN:HB3	54:UH:552:LYS:NZ	2.36	0.41
54:UH:554:PHE:HB3	54:UH:567:LEU:HD11	2.03	0.41
54:UH:814:GLN:O	54:UH:818:GLU:HG2	2.21	0.41
56:US:304:MET:HE2	56:US:334:LEU:HD23	2.03	0.41
56:US:332:ARG:HB2	56:US:334:LEU:HD13	2.02	0.41
59:CY:89:LEU:HB3	60:CZ:489:TYR:CZ	2.56	0.41
1:UA:1:MET:SD	1:UA:581:SER:OG	2.75	0.41
1:UA:795:ARG:HH11	15:UU:1033:LEU:HD12	1.84	0.41
5:UF:283:PHE:O	5:UF:287:ARG:HG3	2.21	0.41
7:UJ:32:SER:HB2	7:UJ:123:ARG:NH1	2.33	0.41
7:UJ:578:ARG:NH1	7:UJ:583:ASP:OD1	2.54	0.41
7:UJ:736:ILE:O	7:UJ:739:THR:OG1	2.35	0.41
7:UJ:826:TYR:O	7:UJ:830:LYS:HG2	2.20	0.41
8:UK:89:GLY:HA3	24:CI:1067:THR:HG22	2.02	0.41
9:UL:617:TYR:OH	9:UL:661:ASN:ND2	2.49	0.41
10:UM:881:SER:O	10:UM:884:VAL:HG12	2.21	0.41
14:UR:298:MET:HE1	14:UR:340:PHE:CG	2.56	0.41
14:UR:402:ASN:HD22	14:UR:405:THR:HG22	1.85	0.41
18:CA:197:ALA:O	18:CA:200:ARG:C	2.64	0.41
19:CC:266:ILE:HG21	19:CC:271:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CG:192:LEU:O	22:CG:229:PHE:HA	2.20	0.41
24:CI:110:LYS:HA	24:CI:309:PRO:HG2	2.03	0.41
32:CR:268:PHE:O	32:CR:272:ILE:HG12	2.21	0.41
32:CR:372:ILE:HD13	32:CR:380:LEU:HD21	2.03	0.41
32:CS:600:LEU:HB3	32:CS:601:LYS:HZ2	1.86	0.41
34:Ca:73:LEU:HD23	34:Ca:84:ILE:HD11	2.03	0.41
39:Cf:12:SER:HA	39:Cf:18:ARG:HH21	1.86	0.41
50:C1:176:G:H2'	50:C1:177:G:C8	2.56	0.41
50:C1:500:C:O2'	50:C1:501:U:O4'	2.39	0.41
50:C1:727:G:H2'	50:C1:728:G:C8	2.55	0.41
52:CW:253:SER:HB3	52:CW:258:SER:HB3	2.03	0.41
53:UT:98:TYR:HD2	53:UT:99:HIS:CE1	2.39	0.41
53:UT:183:LEU:O	53:UT:186:THR:OG1	2.32	0.41
53:UT:285:VAL:HG11	53:UT:337:LEU:HD13	2.03	0.41
53:UT:671:LEU:HD23	53:UT:671:LEU:HA	1.90	0.41
53:UT:1020:ARG:HG2	53:UT:1075:MET:HE1	2.03	0.41
53:UT:1449:GLY:O	53:UT:1452:SER:OG	2.32	0.41
53:UT:1900:LEU:HD13	53:UT:1900:LEU:HA	1.92	0.41
55:UE:229:LEU:HD13	55:UE:235:LEU:HB3	2.02	0.41
4:UD:34:LYS:O	4:UD:38:LYS:HG3	2.20	0.40
4:UD:306:MET:HE2	4:UD:312:ARG:HB2	2.02	0.40
7:UJ:452:LEU:HA	7:UJ:455:LYS:HG2	2.04	0.40
7:UJ:742:THR:O	7:UJ:746:LEU:HG	2.21	0.40
8:UK:16:ARG:HD3	50:C1:1159:C:C4	2.56	0.40
9:UL:899:LEU:HA	9:UL:902:VAL:HG12	2.03	0.40
13:UQ:608:THR:HG23	13:UQ:609:LYS:H	1.85	0.40
14:UR:376:PHE:CD2	14:UR:385:MET:HE3	2.56	0.40
16:UX:28:LYS:O	16:UX:32:GLN:HG3	2.21	0.40
19:CC:38:MET:HE3	19:CC:38:MET:HB3	1.85	0.40
20:CD:182:MET:O	20:CD:186:VAL:HG23	2.21	0.40
22:CG:195:TRP:HD1	22:CG:226:ARG:HA	1.86	0.40
22:CG:197:LEU:HD23	22:CG:224:PRO:HB3	2.03	0.40
24:CI:1041:PRO:HG3	33:CT:192:TYR:CZ	2.55	0.40
32:CR:35:LYS:HB3	32:CR:95:PHE:CD1	2.57	0.40
32:CR:315:PRO:HD3	32:CR:394:ILE:HD11	2.03	0.40
37:Cd:191:ARG:NH2	50:C1:868:G:O6	2.54	0.40
38:Ce:140:VAL:HG21	38:Ce:164:LEU:HD22	2.03	0.40
45:Cm:88:LYS:HA	45:Cm:91:THR:HG22	2.02	0.40
48:Cp:11:VAL:HG22	48:Cp:31:VAL:HB	2.03	0.40
50:C1:208:A:O2'	50:C1:209:A:O4'	2.31	0.40
50:C1:924:A:H5"	52:CW:134:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:UT:47:ARG:O	53:UT:49:HIS:N	2.54	0.40
53:UT:1391:ILE:HG21	53:UT:1433:PRO:HB2	2.02	0.40
53:UT:1585:PHE:HE1	53:UT:1636:ARG:HH12	1.69	0.40
61:UP:345:ALA:HA	61:UP:348:ARG:HG2	2.02	0.40
2:UB:730:THR:OG1	2:UB:780:LEU:HD22	2.21	0.40
3:UC:608:TYR:CG	40:Cg:30:GLY:HA3	2.56	0.40
4:UD:431:ILE:HD13	4:UD:447:THR:HG22	2.03	0.40
4:UD:838:ILE:HA	4:UD:861:ALA:O	2.21	0.40
7:UJ:247:LEU:O	7:UJ:251:ILE:HG12	2.21	0.40
7:UJ:979:LEU:HD12	7:UJ:979:LEU:HA	1.97	0.40
7:UJ:1437:TYR:CZ	7:UJ:1438:LEU:HB2	2.57	0.40
7:UJ:1521:SER:O	7:UJ:1524:SER:OG	2.24	0.40
13:UQ:251:ARG:HD3	13:UQ:251:ARG:HA	1.86	0.40
13:UQ:568:THR:HG22	55:UE:262:LYS:NZ	2.37	0.40
15:UU:666:THR:OG1	15:UU:667:LYS:N	2.53	0.40
22:CG:470:ARG:HD3	22:CG:471:THR:N	2.37	0.40
27:CL:48:ILE:HG23	27:CL:77:LEU:HD11	2.02	0.40
31:CQ:205:THR:HG23	31:CQ:248:LEU:HD21	2.02	0.40
32:CR:652:LYS:HA	32:CR:652:LYS:HD2	1.91	0.40
32:CR:864:LEU:HB2	32:CR:869:ARG:HB3	2.04	0.40
35:Cb:173:ILE:HD12	35:Cb:230:SER:HB3	2.03	0.40
37:Cd:154:ARG:CZ	37:Cd:181:LEU:HD11	2.52	0.40
50:C1:134:C:H41	50:C1:203:C:H42	1.68	0.40
50:C1:1479:U:H2'	50:C1:1480:G:C8	2.57	0.40
52:CW:140:ARG:HD3	52:CW:156:VAL:HG13	2.02	0.40
53:UT:559:LEU:HD11	53:UT:582:PHE:HA	2.01	0.40
54:UH:548:TYR:CE2	54:UH:552:LYS:HE2	2.56	0.40
56:US:463:LEU:HA	56:US:466:HIS:HB2	2.03	0.40
56:US:474:ILE:O	56:US:477:ILE:HG12	2.21	0.40
59:CY:365:LYS:HA	59:CY:368:LYS:HG2	2.02	0.40
1:UA:354:ARG:HA	1:UA:367:TRP:O	2.20	0.40
8:UK:250:THR:OG1	8:UK:269:LYS:NZ	2.36	0.40
9:UL:830:VAL:HA	9:UL:833:THR:HG22	2.02	0.40
12:UO:112:ARG:HH12	36:Cc:32:ARG:HH12	1.70	0.40
12:UO:475:GLU:O	12:UO:479:ILE:HG12	2.21	0.40
13:UQ:286:VAL:HG21	13:UQ:290:ILE:HD11	2.02	0.40
13:UQ:481:CYS:SG	13:UQ:541:LEU:HD13	2.61	0.40
18:CB:106:GLU:OE2	18:CB:128:ARG:NH1	2.54	0.40
18:CB:250:GLY:CA	18:CB:306:TYR:O	2.69	0.40
25:CJ:174:ARG:HH21	25:CJ:176:LYS:HD3	1.86	0.40
27:CL:124:ALA:HA	27:CL:125:LEU:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:CM:79:LEU:HD12	28:CM:336:MET:HB2	2.04	0.40
29:CN:100:LEU:HA	29:CN:105:ASN:ND2	2.33	0.40
32:CS:512:ASP:HB3	32:CS:515:GLN:HG3	2.03	0.40
39:Cf:56:ARG:HH22	50:C1:916:U:P	2.42	0.40
39:Cf:99:SER:HA	39:Cf:173:ILE:O	2.22	0.40
40:Cg:108:GLN:NE2	40:Cg:120:ILE:HG13	2.36	0.40
40:Cg:108:GLN:NE2	40:Cg:124:ARG:HB2	2.37	0.40
44:Ck:62:LYS:NZ	50:C1:910:G:OP1	2.52	0.40
50:C1:333:C:H2'	50:C1:334:U:O4'	2.22	0.40
50:C1:771:G:O2'	50:C1:772:A:O5'	2.30	0.40
54:UH:19:PRO:HD3	54:UH:29:TYR:CZ	2.57	0.40
54:UH:605:VAL:O	54:UH:609:ILE:HG12	2.21	0.40
54:UH:742:LEU:HD23	54:UH:742:LEU:HA	1.88	0.40
56:US:196:ILE:O	56:US:200:THR:OG1	2.32	0.40
1:UA:558:ARG:HA	1:UA:558:ARG:HD2	1.84	0.40
1:UA:620:GLY:H	1:UA:673:VAL:HG23	1.87	0.40
4:UD:474:MET:HE1	4:UD:495:TRP:CZ3	2.56	0.40
6:UG:118:VAL:HA	6:UG:121:VAL:HG12	2.02	0.40
7:UJ:584:CYS:HB2	7:UJ:589:PHE:HZ	1.87	0.40
9:UL:394:LEU:HB2	9:UL:420:VAL:HB	2.03	0.40
10:UM:135:ILE:HB	10:UM:149:VAL:O	2.21	0.40
11:UN:346:ASN:ND2	11:UN:932:PRO:O	2.50	0.40
13:UQ:265:ILE:HD13	13:UQ:330:LEU:HD21	2.03	0.40
15:UU:626:THR:N	15:UU:640:CYS:O	2.50	0.40
19:CC:326:THR:HA	19:CC:394:ASN:ND2	2.36	0.40
20:CD:12:GLY:HA3	20:CD:49:ALA:O	2.21	0.40
21:CF:103:LEU:HD23	21:CF:115:ILE:HD11	2.02	0.40
22:CG:245:HIS:CE1	22:CG:271:VAL:HG12	2.57	0.40
23:CH:229:ALA:HA	23:CH:232:ASN:ND2	2.36	0.40
24:CI:536:PRO:HB2	24:CI:537:TRP:CD1	2.51	0.40
24:CI:1102:LYS:HG3	50:C1:400:C:H5"	2.04	0.40
32:CR:280:THR:HA	32:CR:408:VAL:O	2.21	0.40
32:CR:287:ARG:HH11	32:CR:413:THR:HG22	1.86	0.40
32:CR:530:HIS:O	32:CR:533:SER:OG	2.35	0.40
32:CR:845:ALA:HB2	32:CR:920:THR:HG21	2.04	0.40
50:C1:1266:G:H2'	50:C1:1267:G:H8	1.87	0.40
50:C1:1625:G:N2	50:C1:1663:U:O2	2.54	0.40
53:UT:1470:TRP:CE3	53:UT:1475:GLN:HG2	2.56	0.40
54:UH:88:ARG:NH2	54:UH:90:ARG:HH21	2.20	0.40
54:UH:556:TRP:CE2	54:UH:565:GLY:HA3	2.56	0.40
60:CZ:273:SER:OG	60:CZ:276:GLU:OE2	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:UI:237:ASN:O	55:UI:240:THR:OG1	2.34	0.40
4:UD:322:HIS:NE2	4:UD:342:SER:OG	2.45	0.40
7:UJ:267:ILE:HD13	7:UJ:267:ILE:HA	1.94	0.40
7:UJ:524:ALA:HB1	7:UJ:530:ASP:HB3	2.03	0.40
7:UJ:1085:ALA:O	7:UJ:1089:ILE:HG12	2.21	0.40
7:UJ:1312:LEU:HA	7:UJ:1315:VAL:HG12	2.03	0.40
7:UJ:1317:ARG:NH1	7:UJ:1353:THR:HB	2.37	0.40
7:UJ:1364:SER:O	7:UJ:1368:ARG:HG2	2.21	0.40
9:UL:221:TRP:NE1	9:UL:237:ASN:HB3	2.34	0.40
10:UM:558:LEU:HA	10:UM:571:TRP:O	2.22	0.40
10:UM:823:ALA:O	10:UM:827:GLN:HB2	2.21	0.40
14:UR:53:GLU:O	14:UR:57:LYS:HG2	2.21	0.40
14:UR:232:SER:HA	14:UR:235:ARG:HG2	2.03	0.40
18:CB:118:PRO:HA	51:C2:243:G:H5”	2.02	0.40
20:CD:82:ASP:OD1	20:CD:83:GLU:N	2.54	0.40
21:CE:54:ILE:HB	21:CE:101:VAL:HG22	2.04	0.40
23:CH:29:ARG:NH1	23:CH:370:PHE:O	2.54	0.40
23:CH:235:MET:HB3	23:CH:279:LEU:HD22	2.03	0.40
26:CK:100:LEU:HD13	26:CK:144:GLU:HB3	2.04	0.40
27:CL:641:LYS:HD3	27:CL:642:PRO:HD2	2.04	0.40
29:CO:99:LEU:HD23	29:CO:99:LEU:HA	1.93	0.40
32:CS:893:ASP:OD1	32:CS:894:ILE:N	2.55	0.40
36:Cc:84:LEU:HD11	36:Cc:181:LEU:HD22	2.04	0.40
39:Cf:25:ARG:HA	39:Cf:25:ARG:HD3	1.81	0.40
47:Co:342:LYS:O	47:Co:354:MET:HA	2.21	0.40
47:Co:413:LEU:O	47:Co:417:GLU:CB	2.70	0.40
50:C1:1268:C:H2’	50:C1:1269:U:C6	2.57	0.40
51:C2:135:U:H4’	51:C2:136:C:H4’	2.03	0.40
53:UT:753:MET:HE2	53:UT:753:MET:HB3	1.91	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	UA	834/904 (92%)	800 (96%)	34 (4%)	0	100	100
2	UB	556/907 (61%)	531 (96%)	25 (4%)	0	100	100
3	UC	242/648 (37%)	232 (96%)	10 (4%)	0	100	100
4	UD	761/884 (86%)	731 (96%)	30 (4%)	0	100	100
5	UF	325/414 (78%)	315 (97%)	10 (3%)	0	100	100
6	UG	475/558 (85%)	452 (95%)	22 (5%)	1 (0%)	43	73
7	UJ	1620/1802 (90%)	1532 (95%)	81 (5%)	7 (0%)	30	61
8	UK	211/270 (78%)	207 (98%)	4 (2%)	0	100	100
9	UL	767/962 (80%)	714 (93%)	53 (7%)	0	100	100
10	UM	835/912 (92%)	789 (94%)	45 (5%)	1 (0%)	48	78
11	UN	171/633 (27%)	169 (99%)	2 (1%)	0	100	100
12	UO	497/557 (89%)	475 (96%)	21 (4%)	1 (0%)	43	73
13	UQ	775/960 (81%)	724 (93%)	49 (6%)	2 (0%)	36	67
14	UR	436/618 (71%)	423 (97%)	13 (3%)	0	100	100
15	UU	896/1049 (85%)	847 (94%)	47 (5%)	2 (0%)	43	73
16	UX	188/193 (97%)	177 (94%)	11 (6%)	0	100	100
17	UZ	229/391 (59%)	218 (95%)	11 (5%)	0	100	100
18	CA	238/313 (76%)	225 (94%)	13 (6%)	0	100	100
18	CB	235/313 (75%)	226 (96%)	9 (4%)	0	100	100
19	CC	383/523 (73%)	364 (95%)	18 (5%)	1 (0%)	36	67
20	CD	444/582 (76%)	430 (97%)	14 (3%)	0	100	100
21	CE	119/127 (94%)	116 (98%)	3 (2%)	0	100	100
21	CF	118/127 (93%)	112 (95%)	6 (5%)	0	100	100
22	CG	402/630 (64%)	390 (97%)	12 (3%)	0	100	100
23	CH	383/411 (93%)	375 (98%)	8 (2%)	0	100	100
24	CI	829/1163 (71%)	805 (97%)	23 (3%)	1 (0%)	48	78
25	CJ	177/183 (97%)	177 (100%)	0	0	100	100
26	CK	295/297 (99%)	285 (97%)	10 (3%)	0	100	100
27	CL	310/720 (43%)	294 (95%)	15 (5%)	1 (0%)	36	67
28	CM	443/446 (99%)	422 (95%)	21 (5%)	0	100	100
29	CN	222/252 (88%)	212 (96%)	10 (4%)	0	100	100
29	CO	211/252 (84%)	199 (94%)	11 (5%)	1 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	CP	227/322 (70%)	220 (97%)	7 (3%)	0	100	100
31	CQ	178/259 (69%)	172 (97%)	6 (3%)	0	100	100
32	CR	836/1073 (78%)	793 (95%)	42 (5%)	1 (0%)	48	78
32	CS	826/1073 (77%)	784 (95%)	42 (5%)	0	100	100
33	CT	127/203 (63%)	120 (94%)	7 (6%)	0	100	100
34	Ca	223/255 (88%)	210 (94%)	12 (5%)	1 (0%)	30	61
35	Cb	230/264 (87%)	216 (94%)	14 (6%)	0	100	100
36	Cc	188/212 (89%)	180 (96%)	8 (4%)	0	100	100
37	Cd	224/239 (94%)	214 (96%)	10 (4%)	0	100	100
38	Ce	155/203 (76%)	139 (90%)	16 (10%)	0	100	100
39	Cf	170/202 (84%)	168 (99%)	2 (1%)	0	100	100
40	Cg	157/190 (83%)	155 (99%)	2 (1%)	0	100	100
41	Ch	64/151 (42%)	63 (98%)	1 (2%)	0	100	100
42	Ci	113/150 (75%)	109 (96%)	4 (4%)	0	100	100
43	Cj	124/143 (87%)	119 (96%)	5 (4%)	0	100	100
44	Ck	127/161 (79%)	121 (95%)	6 (5%)	0	100	100
45	Cm	122/130 (94%)	114 (93%)	8 (7%)	0	100	100
46	Cn	92/145 (63%)	90 (98%)	2 (2%)	0	100	100
47	Co	90/136 (66%)	83 (92%)	6 (7%)	1 (1%)	11	39
48	Cp	59/68 (87%)	56 (95%)	3 (5%)	0	100	100
49	CU	168/311 (54%)	161 (96%)	7 (4%)	0	100	100
52	CW	381/668 (57%)	353 (93%)	28 (7%)	0	100	100
53	UT	1981/2612 (76%)	1873 (94%)	104 (5%)	4 (0%)	43	73
54	UH	787/930 (85%)	752 (96%)	29 (4%)	6 (1%)	16	47
55	UE	172/410 (42%)	156 (91%)	16 (9%)	0	100	100
55	UI	126/410 (31%)	120 (95%)	6 (5%)	0	100	100
56	US	443/549 (81%)	424 (96%)	18 (4%)	1 (0%)	43	73
57	Cl	78/156 (50%)	71 (91%)	7 (9%)	0	100	100
58	CX	265/480 (55%)	250 (94%)	15 (6%)	0	100	100
59	CY	258/381 (68%)	251 (97%)	7 (3%)	0	100	100
60	CZ	279/609 (46%)	268 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	UP	52/364 (14%)	50 (96%)	2 (4%)	0	100	100
All	All	23949/32460 (74%)	22823 (95%)	1094 (5%)	32 (0%)	49	78

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	UJ	1428	HIS
7	UJ	1430	PRO
32	CR	211	ILE
34	Ca	55	LYS
13	UQ	171	THR
13	UQ	697	GLY
53	UT	48	ARG
54	UH	304	SER
54	UH	384	THR
54	UH	386	GLY
56	US	241	GLU
6	UG	56	PRO
7	UJ	1019	PRO
7	UJ	1260	SER
12	UO	130	GLN
15	UU	398	PHE
53	UT	1567	PHE
54	UH	159	ASN
54	UH	754	ARG
15	UU	837	SER
19	CC	247	ASP
7	UJ	1072	VAL
10	UM	383	LEU
24	CI	367	VAL
27	CL	640	PRO
53	UT	28	GLU
47	Co	367	SER
54	UH	206	SER
7	UJ	1298	ASP
7	UJ	1022	VAL
53	UT	1445	PRO
29	CO	165	ASN

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	UA	662/774 (86%)	662 (100%)	0	100	100
2	UB	474/788 (60%)	473 (100%)	1 (0%)	87	89
3	UC	208/536 (39%)	200 (96%)	8 (4%)	29	60
4	UD	657/738 (89%)	657 (100%)	0	100	100
5	UF	250/341 (73%)	250 (100%)	0	100	100
6	UG	386/474 (81%)	386 (100%)	0	100	100
7	UJ	1379/1526 (90%)	1369 (99%)	10 (1%)	76	82
8	UK	161/227 (71%)	161 (100%)	0	100	100
9	UL	667/821 (81%)	667 (100%)	0	100	100
10	UM	712/770 (92%)	710 (100%)	2 (0%)	86	87
11	UN	146/522 (28%)	146 (100%)	0	100	100
12	UO	403/456 (88%)	402 (100%)	1 (0%)	87	89
13	UQ	650/817 (80%)	641 (99%)	9 (1%)	59	76
14	UR	359/523 (69%)	359 (100%)	0	100	100
15	UU	677/863 (78%)	677 (100%)	0	100	100
16	UX	152/167 (91%)	152 (100%)	0	100	100
17	UZ	186/329 (56%)	186 (100%)	0	100	100
18	CA	175/228 (77%)	175 (100%)	0	100	100
18	CB	195/228 (86%)	195 (100%)	0	100	100
19	CC	287/435 (66%)	287 (100%)	0	100	100
20	CD	344/489 (70%)	344 (100%)	0	100	100
21	CE	91/108 (84%)	91 (100%)	0	100	100
21	CF	88/108 (82%)	88 (100%)	0	100	100
22	CG	331/525 (63%)	331 (100%)	0	100	100
23	CH	303/320 (95%)	302 (100%)	1 (0%)	86	87
24	CI	681/1009 (68%)	680 (100%)	1 (0%)	88	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	CJ	147/169 (87%)	147 (100%)	0	100	100
26	CK	245/266 (92%)	245 (100%)	0	100	100
27	CL	251/588 (43%)	251 (100%)	0	100	100
28	CM	364/383 (95%)	364 (100%)	0	100	100
29	CN	202/223 (91%)	201 (100%)	1 (0%)	81	85
29	CO	193/223 (86%)	192 (100%)	1 (0%)	81	85
30	CP	202/287 (70%)	202 (100%)	0	100	100
31	CQ	151/215 (70%)	151 (100%)	0	100	100
32	CR	731/916 (80%)	731 (100%)	0	100	100
32	CS	722/916 (79%)	721 (100%)	1 (0%)	88	90
33	CT	108/167 (65%)	108 (100%)	0	100	100
34	Ca	198/223 (89%)	198 (100%)	0	100	100
35	Cb	199/221 (90%)	199 (100%)	0	100	100
36	Cc	149/178 (84%)	149 (100%)	0	100	100
37	Cd	192/204 (94%)	192 (100%)	0	100	100
38	Ce	137/177 (77%)	137 (100%)	0	100	100
39	Cf	139/164 (85%)	139 (100%)	0	100	100
40	Cg	123/162 (76%)	123 (100%)	0	100	100
41	Ch	58/130 (45%)	58 (100%)	0	100	100
42	Ci	78/117 (67%)	78 (100%)	0	100	100
43	Cj	92/115 (80%)	92 (100%)	0	100	100
44	Ck	117/143 (82%)	116 (99%)	1 (1%)	70	80
45	Cm	103/113 (91%)	103 (100%)	0	100	100
46	Cn	70/116 (60%)	70 (100%)	0	100	100
47	Co	79/115 (69%)	79 (100%)	0	100	100
48	Cp	47/61 (77%)	47 (100%)	0	100	100
49	CU	137/260 (53%)	137 (100%)	0	100	100
52	CW	310/587 (53%)	310 (100%)	0	100	100
53	UT	1725/2276 (76%)	1725 (100%)	0	100	100
54	UH	674/788 (86%)	664 (98%)	10 (2%)	57	75
55	UE	148/346 (43%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	UI	108/346 (31%)	108 (100%)	0	100	100
56	US	404/493 (82%)	402 (100%)	2 (0%)	81	85
57	Cl	71/135 (53%)	71 (100%)	0	100	100
58	CX	227/411 (55%)	227 (100%)	0	100	100
59	CY	225/322 (70%)	225 (100%)	0	100	100
60	CZ	238/519 (46%)	238 (100%)	0	100	100
61	UP	44/314 (14%)	44 (100%)	0	100	100
All	All	20032/27511 (73%)	19983 (100%)	49 (0%)	85	89

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	UB	22	GLN
3	UC	469	GLN
3	UC	473	ARG
3	UC	478	ASP
3	UC	479	MET
3	UC	481	ILE
3	UC	482	PRO
3	UC	484	ARG
3	UC	488	LYS
7	UJ	867	HIS
7	UJ	1014	LEU
7	UJ	1020	ASP
7	UJ	1023	LEU
7	UJ	1037	VAL
7	UJ	1261	ILE
7	UJ	1263	GLU
7	UJ	1321	ASP
7	UJ	1322	MET
7	UJ	1325	LYS
10	UM	394	ASN
10	UM	827	GLN
12	UO	70	ASN
13	UQ	414	HIS
13	UQ	695	GLU
13	UQ	696	ASP
13	UQ	699	ILE
13	UQ	715	ILE
13	UQ	725	VAL

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Mol	Chain	Res	Type
13	UQ	726	VAL
13	UQ	753	VAL
13	UQ	758	SER
23	CH	269	GLN
24	CI	612	ASN
29	CN	130	ILE
29	CO	79	LYS
32	CS	655	GLN
44	Ck	111	ASN
54	UH	429	LEU
54	UH	431	THR
54	UH	432	ASP
54	UH	434	ILE
54	UH	436	ARG
54	UH	438	ILE
54	UH	588	THR
54	UH	596	LYS
54	UH	597	ASP
54	UH	601	GLU
56	US	489	LEU
56	US	490	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (214) such sidechains are listed below:

Mol	Chain	Res	Type
1	UA	156	HIS
1	UA	328	GLN
1	UA	381	HIS
1	UA	543	GLN
1	UA	568	ASN
1	UA	846	ASN
2	UB	56	ASN
2	UB	505	GLN
2	UB	557	HIS
2	UB	701	GLN
2	UB	768	HIS
2	UB	783	HIS
2	UB	789	GLN
2	UB	802	HIS
2	UB	863	GLN
3	UC	491	GLN
4	UD	37	GLN

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Mol	Chain	Res	Type
4	UD	128	GLN
4	UD	389	ASN
4	UD	455	HIS
4	UD	536	HIS
4	UD	714	GLN
4	UD	755	GLN
4	UD	801	GLN
4	UD	807	ASN
5	UF	59	ASN
5	UF	319	HIS
6	UG	47	GLN
6	UG	228	HIS
6	UG	239	GLN
6	UG	363	HIS
6	UG	391	GLN
6	UG	393	GLN
7	UJ	77	GLN
7	UJ	91	ASN
7	UJ	103	HIS
7	UJ	158	GLN
7	UJ	268	GLN
7	UJ	295	GLN
7	UJ	350	GLN
7	UJ	404	HIS
7	UJ	909	GLN
7	UJ	1254	ASN
7	UJ	1667	GLN
7	UJ	1745	GLN
7	UJ	1746	GLN
8	UK	23	GLN
9	UL	107	ASN
9	UL	688	GLN
9	UL	870	ASN
9	UL	886	HIS
9	UL	930	GLN
10	UM	160	HIS
10	UM	274	HIS
10	UM	520	GLN
10	UM	628	ASN
10	UM	741	GLN
10	UM	827	GLN
10	UM	857	ASN

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Mol	Chain	Res	Type
11	UN	338	HIS
11	UN	362	GLN
11	UN	927	GLN
12	UO	33	GLN
12	UO	46	HIS
12	UO	70	ASN
12	UO	145	GLN
12	UO	203	ASN
12	UO	271	ASN
12	UO	339	GLN
12	UO	480	ASN
12	UO	531	ASN
13	UQ	98	GLN
13	UQ	473	GLN
13	UQ	501	GLN
13	UQ	718	GLN
14	UR	69	GLN
14	UR	402	ASN
14	UR	440	GLN
14	UR	472	ASN
14	UR	493	ASN
15	UU	236	GLN
15	UU	473	ASN
15	UU	577	GLN
15	UU	711	ASN
15	UU	758	HIS
15	UU	784	HIS
15	UU	969	ASN
16	UX	57	ASN
16	UX	141	HIS
17	UZ	150	HIS
17	UZ	161	ASN
17	UZ	273	GLN
18	CA	235	GLN
18	CA	270	GLN
18	CA	277	GLN
18	CA	289	GLN
18	CB	277	GLN
19	CC	85	ASN
19	CC	272	GLN
20	CD	147	HIS
20	CD	180	ASN

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Mol	Chain	Res	Type
21	CE	67	HIS
21	CF	33	GLN
22	CG	424	GLN
23	CH	177	GLN
24	CI	287	HIS
24	CI	374	GLN
24	CI	749	GLN
24	CI	1011	GLN
24	CI	1063	GLN
26	CK	169	ASN
27	CL	88	GLN
27	CL	662	GLN
27	CL	667	GLN
28	CM	60	GLN
28	CM	77	ASN
28	CM	230	ASN
28	CM	263	ASN
28	CM	368	GLN
28	CM	421	ASN
29	CN	18	GLN
29	CN	105	ASN
29	CN	170	HIS
31	CQ	240	GLN
32	CR	134	ASN
32	CR	353	ASN
32	CR	557	GLN
32	CR	655	GLN
32	CR	734	HIS
32	CR	741	GLN
32	CR	819	ASN
32	CS	17	ASN
32	CS	102	ASN
32	CS	134	ASN
32	CS	186	ASN
32	CS	319	ASN
32	CS	378	HIS
32	CS	431	GLN
32	CS	539	GLN
32	CS	554	ASN
32	CS	565	HIS
32	CS	623	GLN
32	CS	732	GLN

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Mol	Chain	Res	Type
32	CS	741	GLN
32	CS	783	HIS
32	CS	907	GLN
34	Ca	79	HIS
34	Ca	101	HIS
34	Ca	132	HIS
34	Ca	149	GLN
34	Ca	182	HIS
34	Ca	208	GLN
34	Ca	220	GLN
35	Cb	98	ASN
35	Cb	142	HIS
36	Cc	50	GLN
36	Cc	109	HIS
37	Cd	71	ASN
37	Cd	116	GLN
37	Cd	189	HIS
37	Cd	213	GLN
38	Ce	77	HIS
38	Ce	132	HIS
38	Ce	197	GLN
39	Cf	13	HIS
39	Cf	44	HIS
39	Cf	84	HIS
40	Cg	131	HIS
40	Cg	137	GLN
43	Cj	100	HIS
43	Cj	107	GLN
44	Ck	132	GLN
46	Cn	48	HIS
47	Co	353	GLN
48	Cp	44	ASN
49	CU	162	GLN
49	CU	251	ASN
53	UT	49	HIS
53	UT	74	ASN
53	UT	202	HIS
53	UT	247	GLN
53	UT	334	GLN
53	UT	436	GLN
53	UT	625	GLN
53	UT	780	GLN

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Mol	Chain	Res	Type
53	UT	792	ASN
53	UT	1081	ASN
53	UT	1104	ASN
53	UT	1146	GLN
53	UT	1248	ASN
53	UT	1314	ASN
53	UT	1315	GLN
53	UT	1345	GLN
53	UT	1366	GLN
53	UT	1386	GLN
53	UT	1416	ASN
53	UT	1437	ASN
53	UT	1782	GLN
53	UT	2023	ASN
54	UH	232	ASN
54	UH	315	GLN
54	UH	329	ASN
54	UH	373	GLN
54	UH	816	GLN
55	UE	158	ASN
56	US	253	HIS
56	US	462	GLN
56	US	464	GLN
56	US	488	ASN
57	Cl	13	HIS
58	CX	263	GLN
59	CY	364	GLN
60	CZ	554	ASN
55	UI	237	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	C1	1549/2344 (66%)	354 (22%)	23 (1%)
51	C2	225/274 (82%)	57 (25%)	2 (0%)
All	All	1774/2618 (67%)	411 (23%)	25 (1%)

All (411) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	C1	4	G

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Mol	Chain	Res	Type
50	C1	5	G
50	C1	7	A
50	C1	14	G
50	C1	16	U
50	C1	17	C
50	C1	18	G
50	C1	19	C
50	C1	26	C
50	C1	40	A
50	C1	41	G
50	C1	59	U
50	C1	60	A
50	C1	61	G
50	C1	71	A
50	C1	72	U
50	C1	73	A
50	C1	77	C
50	C1	78	G
50	C1	86	C
50	C1	90	A
50	C1	93	G
50	C1	96	C
50	C1	97	C
50	C1	104	U
50	C1	105	A
50	C1	121	G
50	C1	126	C
50	C1	127	C
50	C1	128	G
50	C1	134	C
50	C1	136	C
50	C1	143	A
50	C1	150	C
50	C1	152	G
50	C1	155	G
50	C1	158	C
50	C1	159	C
50	C1	162	G
50	C1	166	A
50	C1	169	G
50	C1	182	C
50	C1	183	C

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Mol	Chain	Res	Type
50	C1	193	U
50	C1	203	C
50	C1	206	C
50	C1	207	U
50	C1	209	A
50	C1	210	G
50	C1	211	G
50	C1	225	C
50	C1	234	G
50	C1	236	C
50	C1	242	U
50	C1	243	U
50	C1	244	G
50	C1	257	G
50	C1	258	C
50	C1	259	U
50	C1	265	G
50	C1	266	C
50	C1	267	U
50	C1	268	G
50	C1	269	G
50	C1	273	G
50	C1	276	C
50	C1	277	U
50	C1	278	A
50	C1	281	U
50	C1	282	C
50	C1	283	A
50	C1	285	A
50	C1	291	C
50	C1	292	G
50	C1	295	G
50	C1	308	U
50	C1	309	G
50	C1	310	G
50	C1	312	G
50	C1	319	U
50	C1	320	A
50	C1	323	G
50	C1	326	U
50	C1	333	C
50	C1	346	C

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Mol	Chain	Res	Type
50	C1	347	C
50	C1	349	C
50	C1	351	U
50	C1	382	U
50	C1	383	G
50	C1	384	C
50	C1	386	G
50	C1	398	C
50	C1	402	U
50	C1	403	G
50	C1	416	U
50	C1	435	A
50	C1	436	A
50	C1	440	G
50	C1	441	A
50	C1	443	G
50	C1	454	C
50	C1	459	C
50	C1	465	C
50	C1	466	A
50	C1	468	C
50	C1	469	G
50	C1	472	G
50	C1	483	U
50	C1	484	G
50	C1	491	G
50	C1	492	C
50	C1	499	G
50	C1	500	C
50	C1	501	U
50	C1	502	A
50	C1	583	A
50	C1	584	U
50	C1	587	U
50	C1	589	A
50	C1	594	G
50	C1	597	G
50	C1	609	A
50	C1	613	A
50	C1	614	U
50	C1	621	G
50	C1	628	A

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Mol	Chain	Res	Type
50	C1	636	C
50	C1	638	A
50	C1	650	G
50	C1	653	U
50	C1	655	A
50	C1	658	A
50	C1	662	A
50	C1	663	U
50	C1	664	A
50	C1	678	A
50	C1	680	U
50	C1	681	G
50	C1	685	C
50	C1	686	A
50	C1	690	A
50	C1	691	A
50	C1	700	C
50	C1	701	G
50	C1	702	U
50	C1	712	A
50	C1	715	A
50	C1	719	U
50	C1	720	A
50	C1	721	C
50	C1	723	A
50	C1	725	A
50	C1	737	G
50	C1	742	U
50	C1	743	U
50	C1	744	C
50	C1	755	A
50	C1	760	C
50	C1	762	G
50	C1	763	A
50	C1	764	A
50	C1	772	A
50	C1	775	U
50	C1	776	C
50	C1	777	G
50	C1	786	G
50	C1	798	U
50	C1	801	A

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Mol	Chain	Res	Type
50	C1	802	A
50	C1	803	A
50	C1	806	C
50	C1	807	A
50	C1	808	A
50	C1	810	G
50	C1	816	C
50	C1	833	U
50	C1	834	C
50	C1	841	A
50	C1	845	C
50	C1	849	A
50	C1	861	U
50	C1	863	G
50	C1	871	G
50	C1	897	U
50	C1	900	A
50	C1	904	U
50	C1	913	G
50	C1	921	G
50	C1	922	C
50	C1	934	A
50	C1	936	A
50	C1	942	U
50	C1	943	A
50	C1	972	A
50	C1	974	G
50	C1	984	A
50	C1	985	A
50	C1	986	C
50	C1	1000	A
50	C1	1001	A
50	C1	1002	G
50	C1	1005	A
50	C1	1007	G
50	C1	1017	C
50	C1	1018	G
50	C1	1023	U
50	C1	1024	U
50	C1	1025	A
50	C1	1027	C
50	C1	1028	C

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Mol	Chain	Res	Type
50	C1	1037	C
50	C1	1039	C
50	C1	1043	G
50	C1	1044	A
50	C1	1052	A
50	C1	1061	A
50	C1	1069	A
50	C1	1076	U
50	C1	1077	U
50	C1	1078	U
50	C1	1079	C
50	C1	1080	G
50	C1	1085	U
50	C1	1086	U
50	C1	1088	U
50	C1	1089	A
50	C1	1094	G
50	C1	1096	A
50	C1	1098	G
50	C1	1099	A
50	C1	1103	C
50	C1	1111	A
50	C1	1116	U
50	C1	1122	A
50	C1	1123	G
50	C1	1124	G
50	C1	1125	A
50	C1	1126	A
50	C1	1129	A
50	C1	1138	C
50	C1	1141	G
50	C1	1147	U
50	C1	1148	G
50	C1	1149	C
50	C1	1154	A
50	C1	1156	C
50	C1	1158	G
50	C1	1159	C
50	C1	1163	A
50	C1	1164	A
50	C1	1166	U
50	C1	1167	C

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Mol	Chain	Res	Type
50	C1	1168	C
50	C1	1169	A
50	C1	1170	G
50	C1	1178	A
50	C1	1179	G
50	C1	1218	G
50	C1	1219	A
50	C1	1222	C
50	C1	1223	U
50	C1	1240	G
50	C1	1254	G
50	C1	1255	U
50	C1	1256	G
50	C1	1257	C
50	C1	1259	C
50	C1	1265	G
50	C1	1444	A
50	C1	1447	A
50	C1	1448	A
50	C1	1449	U
50	C1	1458	U
50	C1	1461	G
50	C1	1466	G
50	C1	1471	U
50	C1	1481	U
50	C1	1483	A
50	C1	1491	A
50	C1	1497	U
50	C1	1498	G
50	C1	1499	G
50	C1	1511	A
50	C1	1518	A
50	C1	1519	C
50	C1	1520	U
50	C1	1527	G
50	C1	1529	A
50	C1	1544	U
50	C1	1551	A
50	C1	1555	A
50	C1	1613	C
50	C1	1614	U
50	C1	1624	A

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Mol	Chain	Res	Type
50	C1	1625	G
50	C1	1628	A
50	C1	1632	G
50	C1	1642	A
50	C1	1643	U
50	C1	1645	U
50	C1	1656	C
50	C1	1665	A
50	C1	1667	G
50	C1	1668	A
50	C1	1670	A
50	C1	1710	G
50	C1	1711	G
50	C1	1712	C
50	C1	1713	U
50	C1	1735	A
50	C1	1742	C
50	C1	1744	A
50	C1	1748	G
50	C1	2055	C
50	C1	2056	U
50	C1	2070	A
50	C1	2071	G
50	C1	2072	U
50	C1	2074	C
50	C1	2076	C
50	C1	2078	C
50	C1	2085	G
50	C1	2086	A
50	C1	2087	G
50	C1	2088	A
50	C1	2107	A
50	C1	2118	U
50	C1	2119	G
50	C1	2120	C
50	C1	2121	U
50	C1	2156	A
50	C1	2157	G
50	C1	2167	G
50	C1	2173	G
50	C1	2177	G
50	C1	2178	U

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Mol	Chain	Res	Type
50	C1	2184	G
50	C1	2185	C
50	C1	2190	G
50	C1	2197	A
50	C1	2201	C
50	C1	2205	G
50	C1	2214	A
50	C1	2220	C
50	C1	2222	C
50	C1	2227	C
50	C1	2234	A
50	C1	2351	G
50	C1	2362	U
50	C1	2363	G
50	C1	2364	A
50	C1	2373	A
50	C1	2374	G
51	C2	15	A
51	C2	24	U
51	C2	28	U
51	C2	29	A
51	C2	31	A
51	C2	33	U
51	C2	34	A
51	C2	37	U
51	C2	39	U
51	C2	48	G
51	C2	58	A
51	C2	62	A
51	C2	63	G
51	C2	82	U
51	C2	84	G
51	C2	89	A
51	C2	90	C
51	C2	91	G
51	C2	92	A
51	C2	93	G
51	C2	103	G
51	C2	104	C
51	C2	111	G
51	C2	125	U
51	C2	126	U

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Mol	Chain	Res	Type
51	C2	127	A
51	C2	128	C
51	C2	135	U
51	C2	136	C
51	C2	142	G
51	C2	153	G
51	C2	160	U
51	C2	162	C
51	C2	163	C
51	C2	164	U
51	C2	165	C
51	C2	166	G
51	C2	167	U
51	C2	170	C
51	C2	178	U
51	C2	179	A
51	C2	181	A
51	C2	182	G
51	C2	187	U
51	C2	188	G
51	C2	189	G
51	C2	190	C
51	C2	199	G
51	C2	200	U
51	C2	201	A
51	C2	244	G
51	C2	247	G
51	C2	255	U
51	C2	256	G
51	C2	259	A
51	C2	260	G
51	C2	262	C

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	C1	89	G
50	C1	135	A
50	C1	150	C
50	C1	209	A
50	C1	277	U
50	C1	281	U

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Mol	Chain	Res	Type
50	C1	319	U
50	C1	397	U
50	C1	593	G
50	C1	684	U
50	C1	689	A
50	C1	771	G
50	C1	802	A
50	C1	1001	A
50	C1	1017	C
50	C1	1068	C
50	C1	1087	G
50	C1	1163	A
50	C1	1712	C
50	C1	1734	G
50	C1	2156	A
50	C1	2177	G
50	C1	2219	C
51	C2	23	A
51	C2	255	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SEP	UA	646	1	8,9,10	0.67	0	8,12,14	1.11	1 (12%)
14	SEP	UR	139	14	8,9,10	1.51	1 (12%)	8,12,14	1.79	2 (25%)
50	OMC	C1	998	50	19,22,23	2.92	8 (42%)	26,31,34	0.67	0
50	A2M	C1	1004	50	22,25,26	3.44	9 (40%)	31,36,39	2.71	10 (32%)

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
1	SEP	UA	646	1	-	4/5/8/10	-
14	SEP	UR	139	14	-	0/5/8/10	-
50	OMC	C1	998	50	-	0/9/27/28	0/2/2/2
50	A2M	C1	1004	50	-	0/9/27/28	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C1	1004	A2M	C2'-C1'	-8.57	1.31	1.53
50	C1	1004	A2M	O4'-C1'	8.40	1.61	1.42
50	C1	1004	A2M	O4'-C4'	-6.57	1.30	1.45
50	C1	998	OMC	C2-N3	6.18	1.48	1.36
50	C1	998	OMC	C6-C5	5.86	1.48	1.35
50	C1	998	OMC	C4-N4	4.91	1.45	1.33
50	C1	998	OMC	C4-N3	4.86	1.44	1.34
50	C1	1004	A2M	C6-N6	4.43	1.45	1.34
50	C1	998	OMC	C2-N1	4.07	1.48	1.40
14	UR	139	SEP	P-O1P	3.27	1.61	1.50
50	C1	998	OMC	C6-N1	3.16	1.45	1.38
50	C1	1004	A2M	O3'-C3'	-3.07	1.35	1.43
50	C1	1004	A2M	C5-C4	-2.98	1.33	1.39
50	C1	1004	A2M	O2'-C2'	2.87	1.50	1.42
50	C1	1004	A2M	C5-N7	-2.75	1.33	1.39
50	C1	998	OMC	O2-C2	-2.74	1.18	1.23
50	C1	998	OMC	C5-C4	2.27	1.48	1.42
50	C1	1004	A2M	C8-N9	-2.26	1.33	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C1	1004	A2M	N6-C6-N1	-7.08	102.84	118.35
50	C1	1004	A2M	C5-C6-N6	6.22	136.96	123.43
50	C1	1004	A2M	N3-C2-N1	-5.51	119.98	128.60
50	C1	1004	A2M	C5-C4-N3	-5.42	119.68	126.75
50	C1	1004	A2M	N9-C8-N7	-4.28	108.06	113.91
50	C1	1004	A2M	C2-N3-C4	3.57	120.17	111.75
50	C1	1004	A2M	N3-C4-N9	3.38	132.66	127.08
14	UR	139	SEP	OG-CB-CA	3.34	111.40	108.14
14	UR	139	SEP	P-OG-CB	-3.26	109.31	118.30
50	C1	1004	A2M	C5-N7-C8	3.10	107.91	103.51
1	UA	646	SEP	OG-CB-CA	2.45	110.53	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C1	1004	A2M	C4-N9-C8	2.19	108.10	105.73
50	C1	1004	A2M	C6-C5-C4	2.14	120.06	117.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	UA	646	SEP	CB-OG-P-O1P
1	UA	646	SEP	CB-OG-P-O2P
1	UA	646	SEP	N-CA-CB-OG
1	UA	646	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	C1	1004	A2M	1	0

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	$\#\|Z\| > 2$
63	GTP	CI	1201	64	30,34,34	0.90	2 (6%)	46,54,54	1.80	11 (23%)
65	ADP	CS	1101	-	27,29,29	2.96	9 (33%)	42,45,45	2.09	15 (35%)

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
63	GTP	CI	1201	64	-	3/22/38/38	0/3/3/3
65	ADP	CS	1101	-	-	0/16/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	CS	1101	ADP	O4'-C1'	8.38	1.61	1.42
65	CS	1101	ADP	C2'-C1'	-7.06	1.30	1.53
65	CS	1101	ADP	O4'-C4'	-6.46	1.30	1.45
65	CS	1101	ADP	C6-N6	4.70	1.45	1.34
65	CS	1101	ADP	O3'-C3'	-2.94	1.36	1.43
65	CS	1101	ADP	O2'-C2'	2.93	1.49	1.43
65	CS	1101	ADP	C5-C4	-2.58	1.34	1.39
65	CS	1101	ADP	C5-N7	-2.51	1.34	1.39
65	CS	1101	ADP	C8-N9	-2.22	1.33	1.37
63	CI	1201	GTP	C5-N7	-2.13	1.35	1.39
63	CI	1201	GTP	C2-N3	2.02	1.38	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
65	CS	1101	ADP	N3-C2-N1	-5.52	119.97	128.60
65	CS	1101	ADP	C5-C4-N3	-5.02	120.20	126.75
63	CI	1201	GTP	C5-C4-N3	-4.91	120.49	128.46
63	CI	1201	GTP	C2-N3-C4	4.47	120.27	112.30
65	CS	1101	ADP	N9-C8-N7	-4.11	108.29	113.91
63	CI	1201	GTP	PB-O3B-PG	-3.71	120.11	132.83
65	CS	1101	ADP	C2-N3-C4	3.35	119.66	111.75
65	CS	1101	ADP	N3-C4-N9	3.35	132.60	127.08
63	CI	1201	GTP	N9-C4-N3	3.20	132.36	125.94
65	CS	1101	ADP	C4-N9-C1'	-3.17	119.03	126.59
63	CI	1201	GTP	PA-O3A-PB	-3.09	122.24	132.83
65	CS	1101	ADP	N6-C6-N1	-3.03	111.73	118.35
65	CS	1101	ADP	PA-O3A-PB	-2.91	122.85	132.83
63	CI	1201	GTP	C2-N1-C6	-2.90	119.81	125.10
65	CS	1101	ADP	C5-N7-C8	2.86	107.57	103.51
63	CI	1201	GTP	N9-C8-N7	-2.78	108.15	113.39
65	CS	1101	ADP	C3'-C2'-C1'	2.58	106.33	101.43
63	CI	1201	GTP	C5-C6-N1	2.56	119.68	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	CI	1201	GTP	C8-N7-C5	2.56	108.87	104.24
65	CS	1101	ADP	C4-N9-C8	2.46	108.40	105.73
65	CS	1101	ADP	C1'-N9-C8	2.41	132.57	127.14
63	CI	1201	GTP	O6-C6-C5	-2.38	120.29	126.60
65	CS	1101	ADP	C5-C6-N6	2.37	128.59	123.43
65	CS	1101	ADP	C4'-O4'-C1'	-2.26	104.49	109.47
65	CS	1101	ADP	C6-C5-C4	2.15	120.07	117.18
63	CI	1201	GTP	C3'-C2'-C1'	2.14	105.50	101.43

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	CI	1201	GTP	PB-O3B-PG-O1G
63	CI	1201	GTP	PB-O3A-PA-O2A
63	CI	1201	GTP	O4'-C4'-C5'-O5'

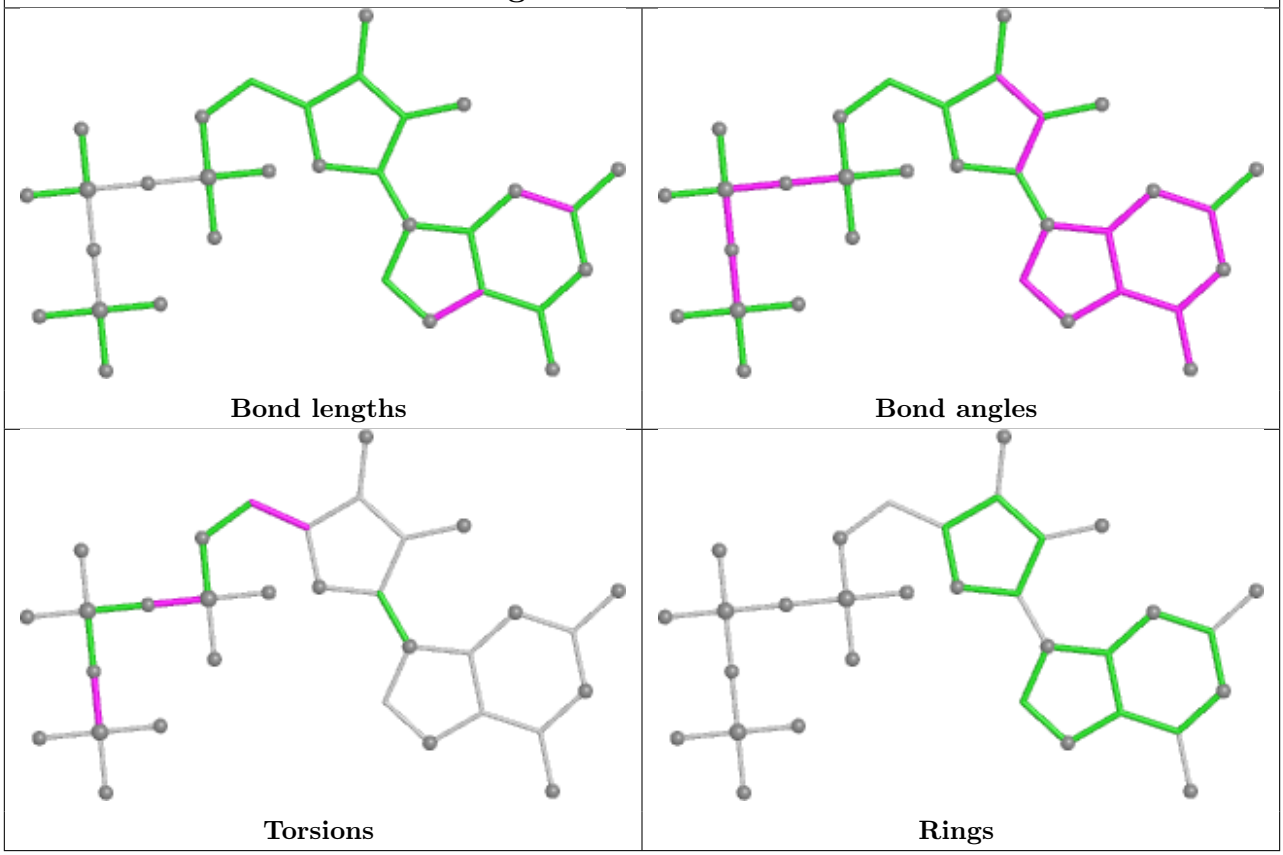
There are no ring outliers.

1 monomer is involved in 3 short contacts:

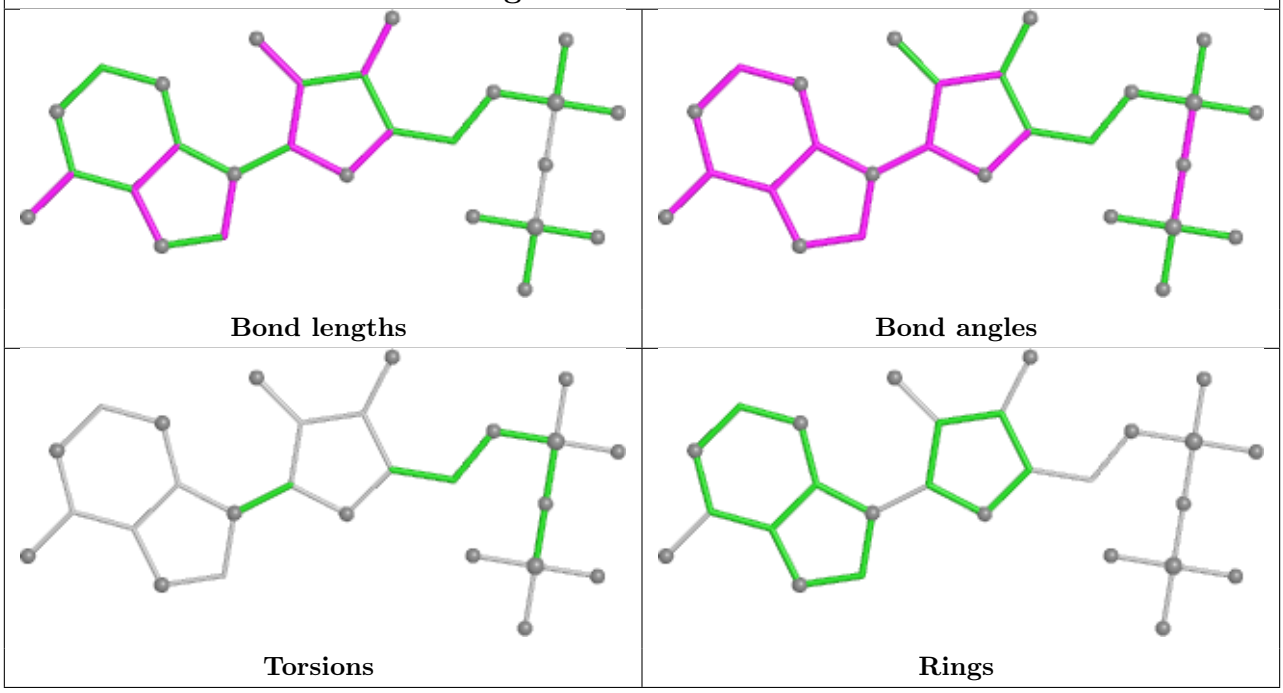
Mol	Chain	Res	Type	Clashes	Symm-Clashes
65	CS	1101	ADP	3	0

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 CI 1201



Ligand ADP CS 1101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

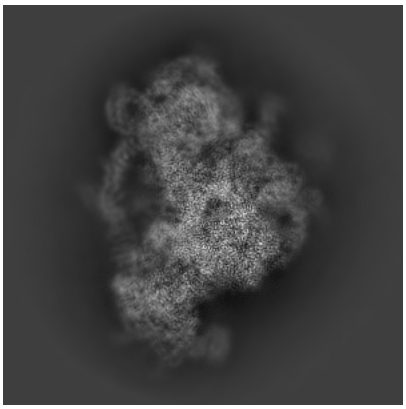
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-66687. These allow visual inspection of the internal detail of the map and identification of artifacts.

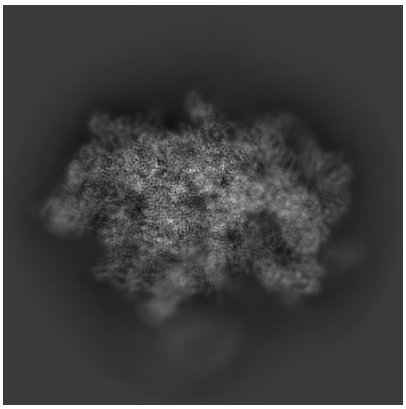
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

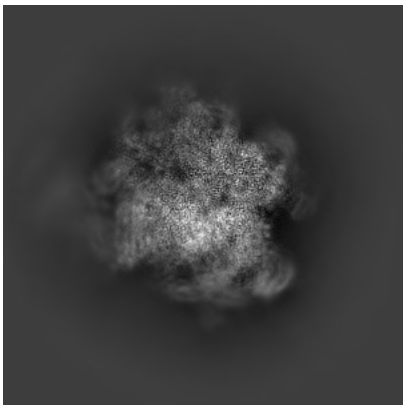
6.1.1 Primary map



X

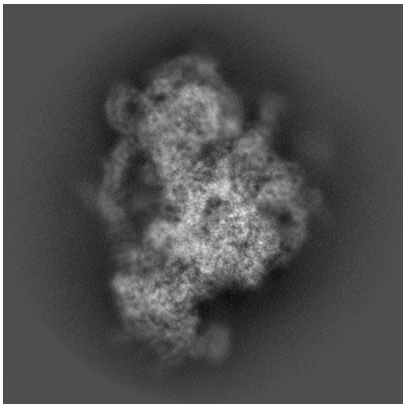


Y

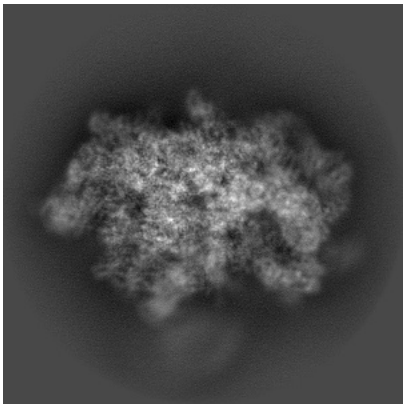


Z

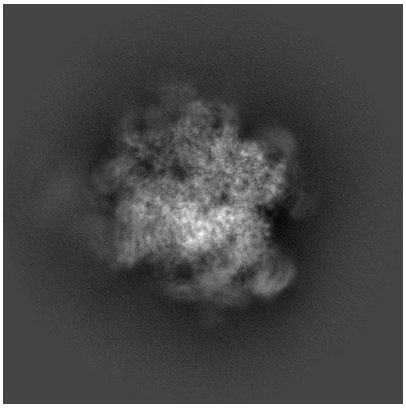
6.1.2 Raw map



X



Y

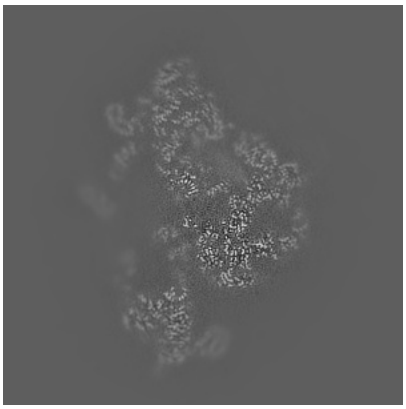


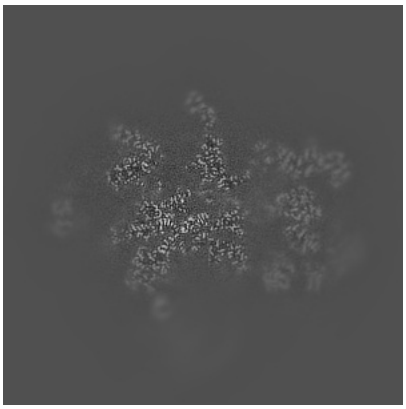
Z

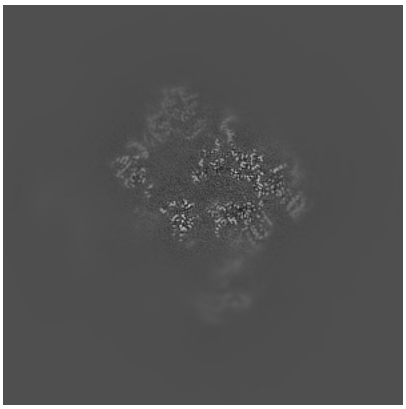
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

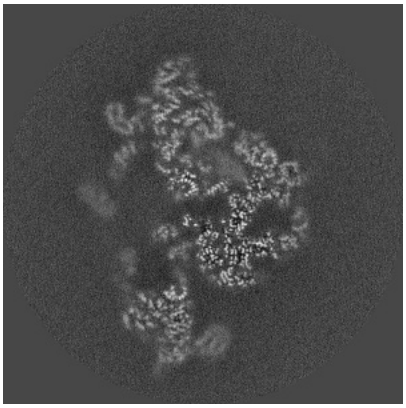
6.2.1 Primary map

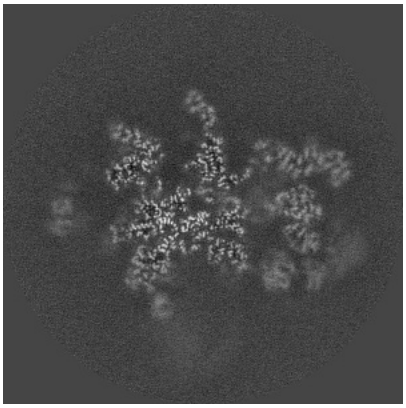

X Index: 240

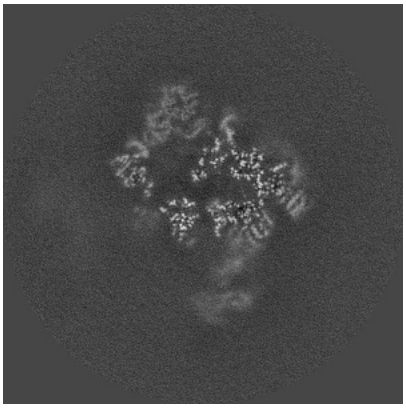

Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240

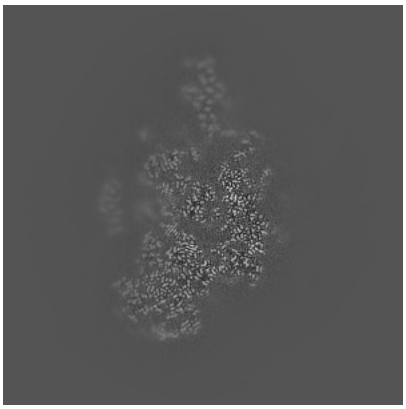

Y Index: 240


Z Index: 240

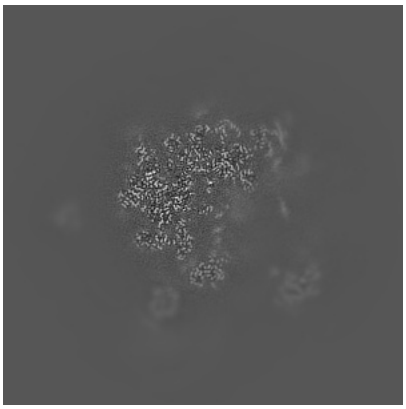
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

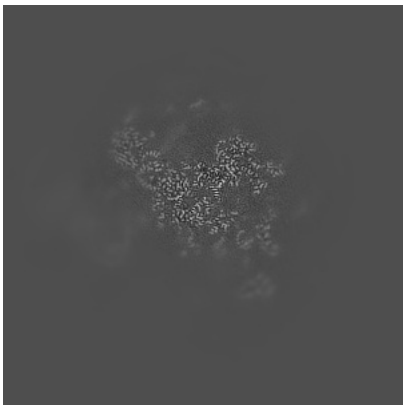
6.3.1 Primary map



X Index: 285

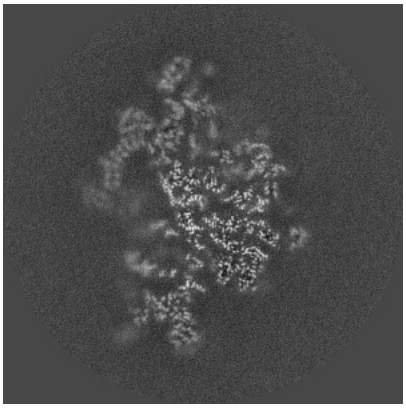


Y Index: 271

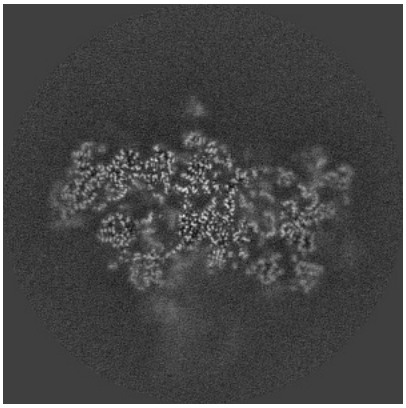


Z Index: 217

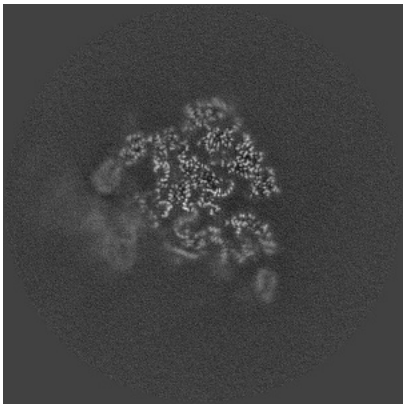
6.3.2 Raw map



X Index: 258



Y Index: 223

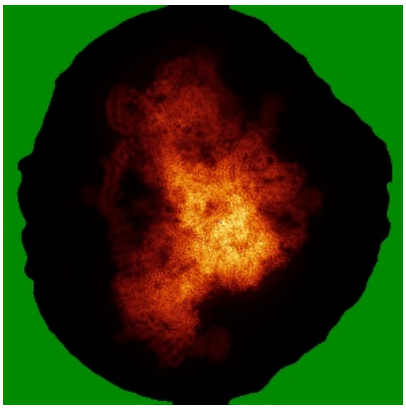


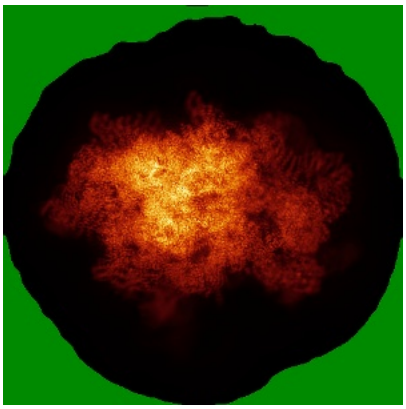
Z Index: 202

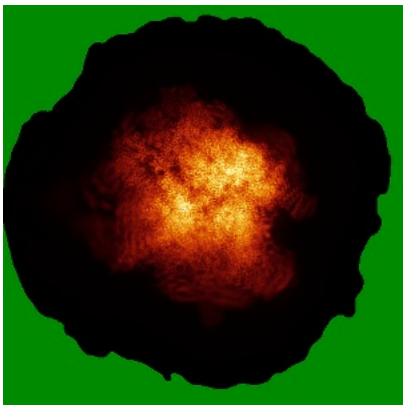
The images above show the largest variance slices of the map in three orthogonal directions.

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

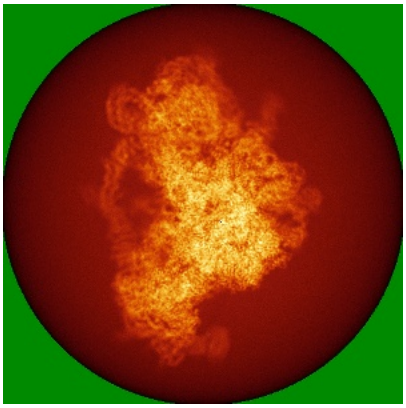
6.4.1 Primary map

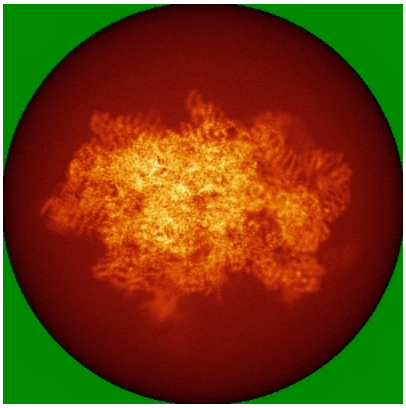

X

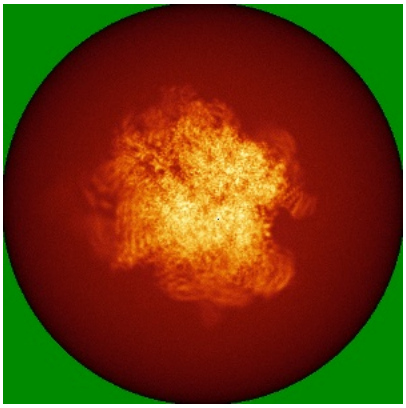

Y


Z

6.4.2 Raw map


X


Y


Z

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

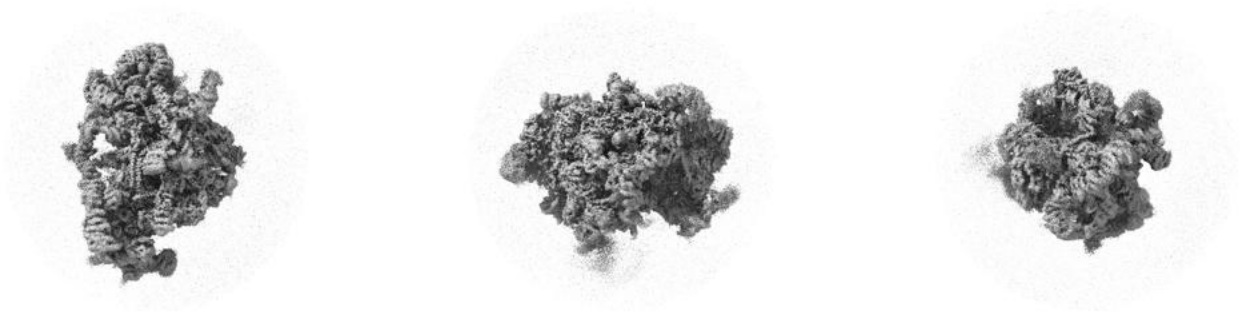
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

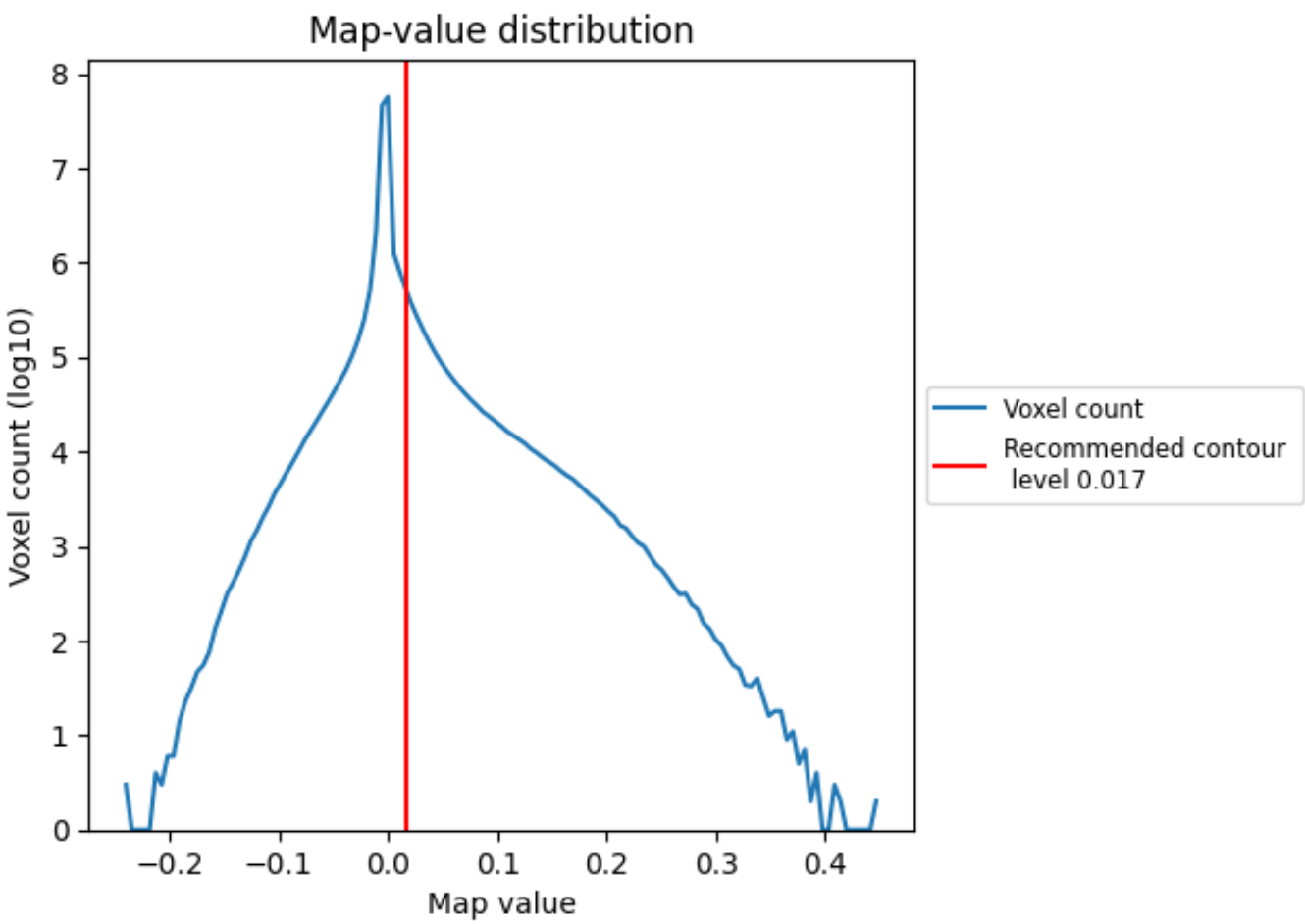
6.6 Mask visualisation (i)

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

7 Map analysis (i)

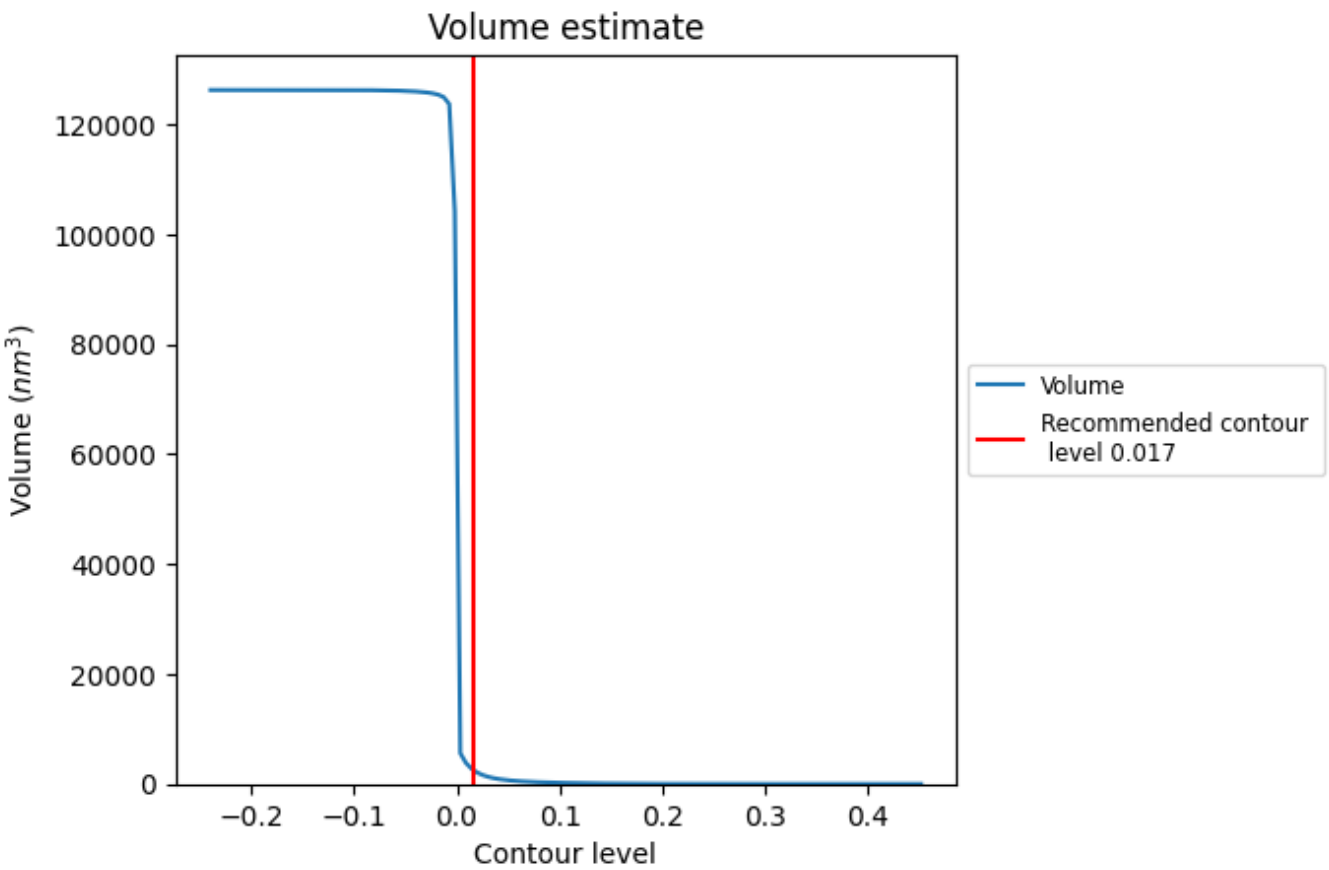
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

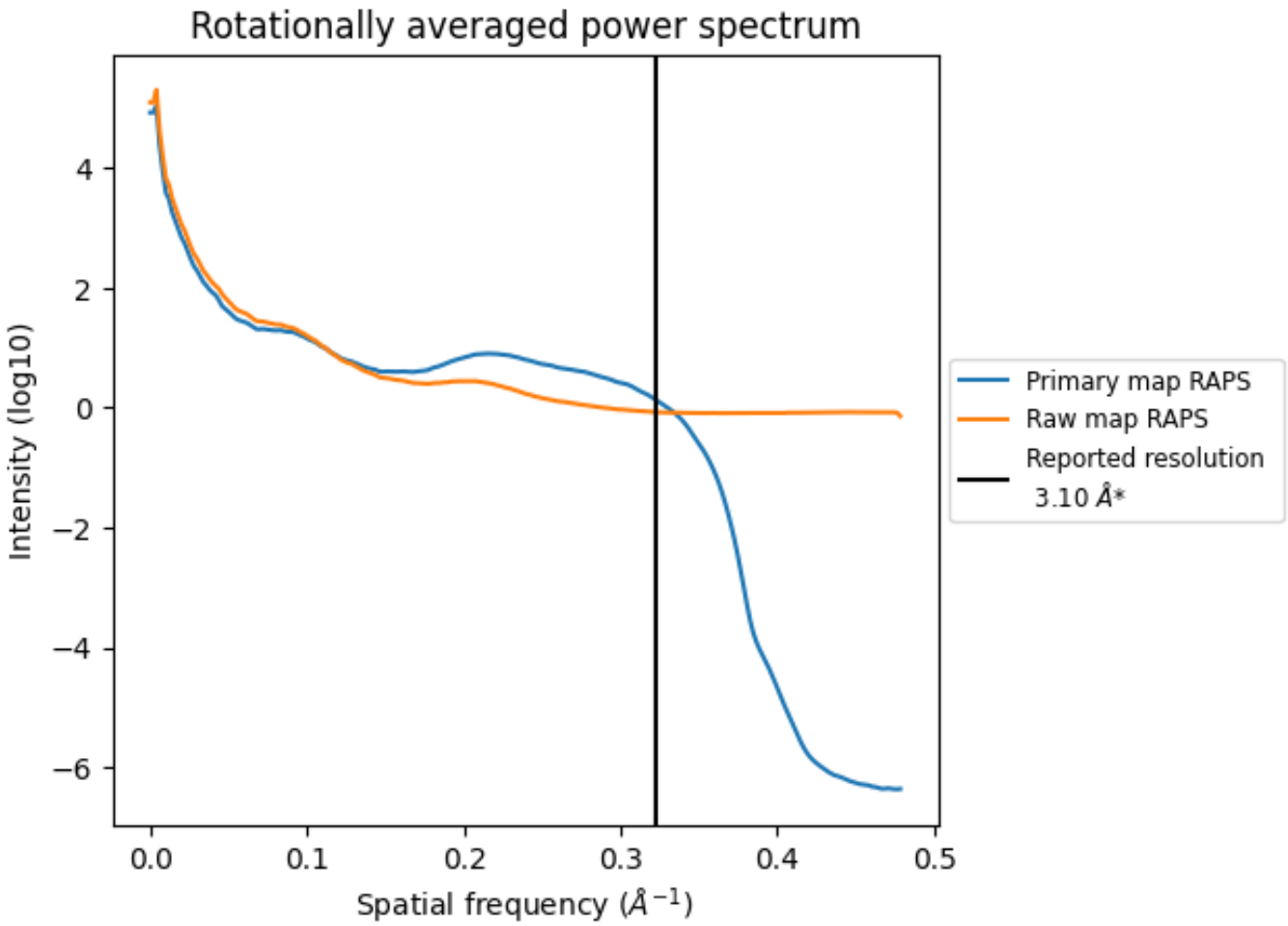
7.2 Volume estimate (i)



The volume at the recommended contour level is 2450 nm^3; this corresponds to an approximate mass of 2213 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)

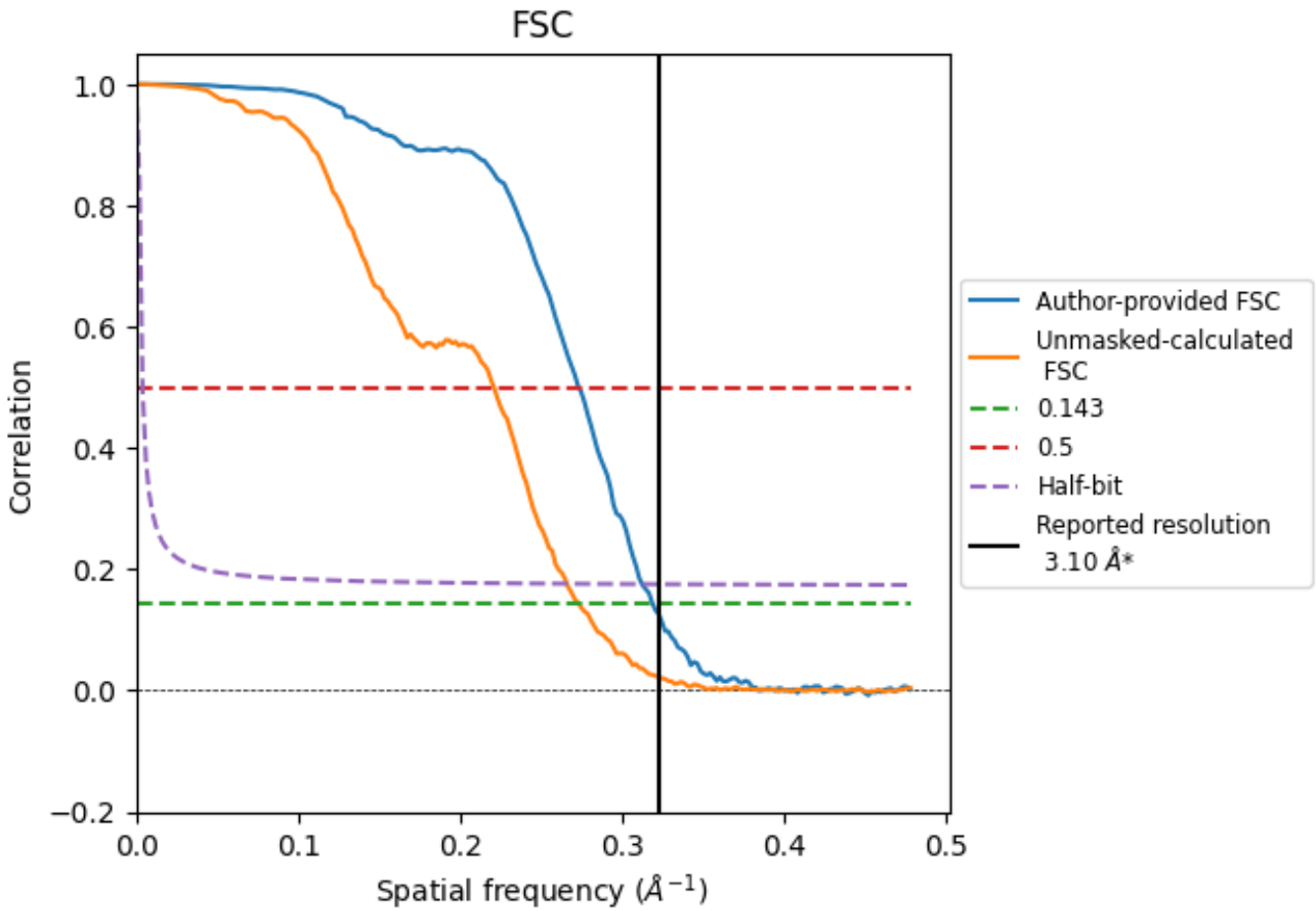


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

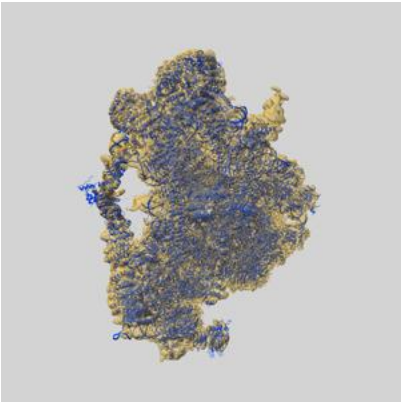
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.65	3.20
Unmasked-calculated*	3.65	4.52	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.65 differs from the reported value 3.1 by more than 10 %

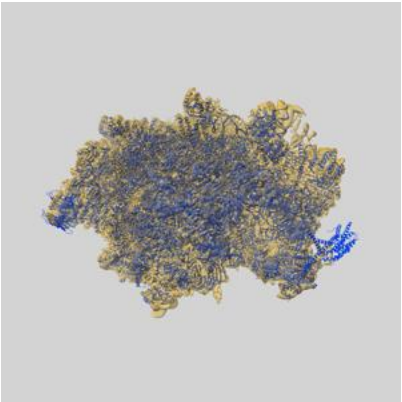
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-66687 and PDB model 9XAH. Per-residue inclusion information can be found in section 3 on page 17.

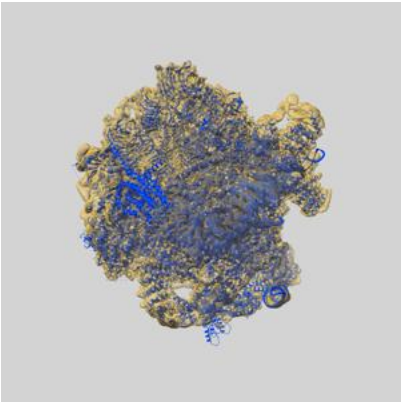
9.1 Map-model overlay (i)



X



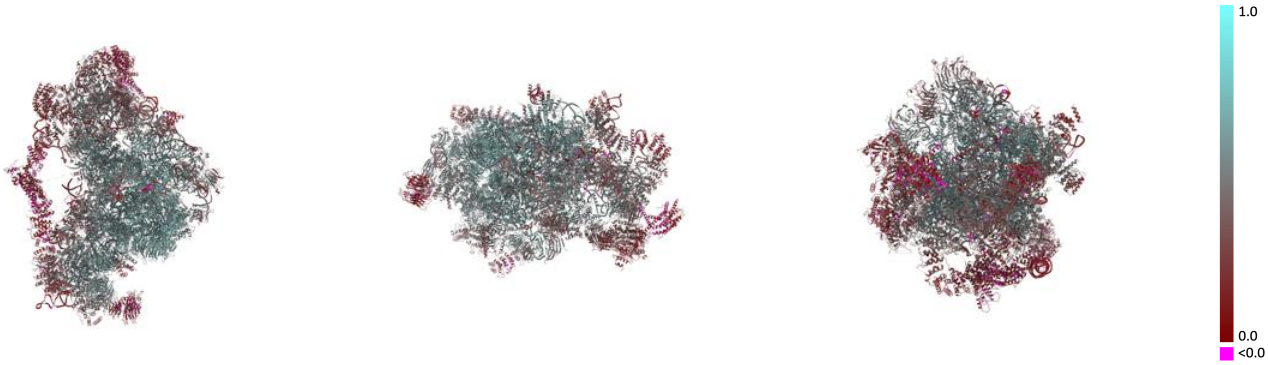
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

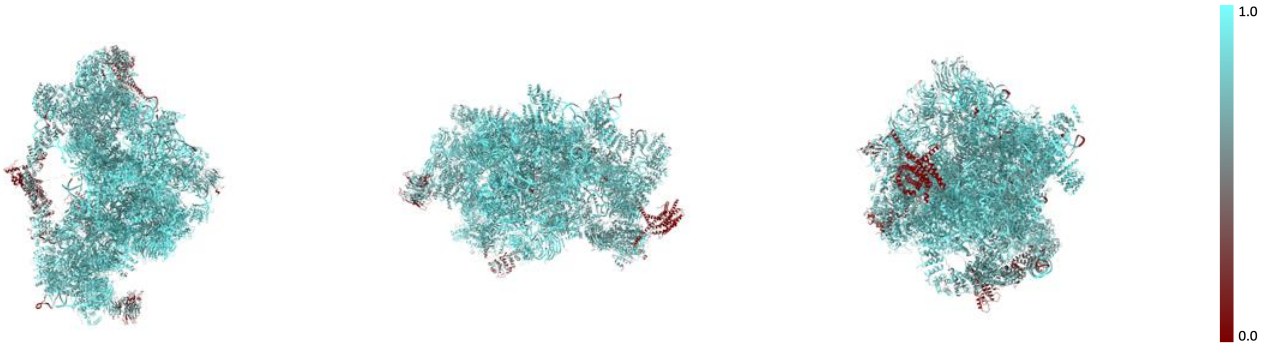
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

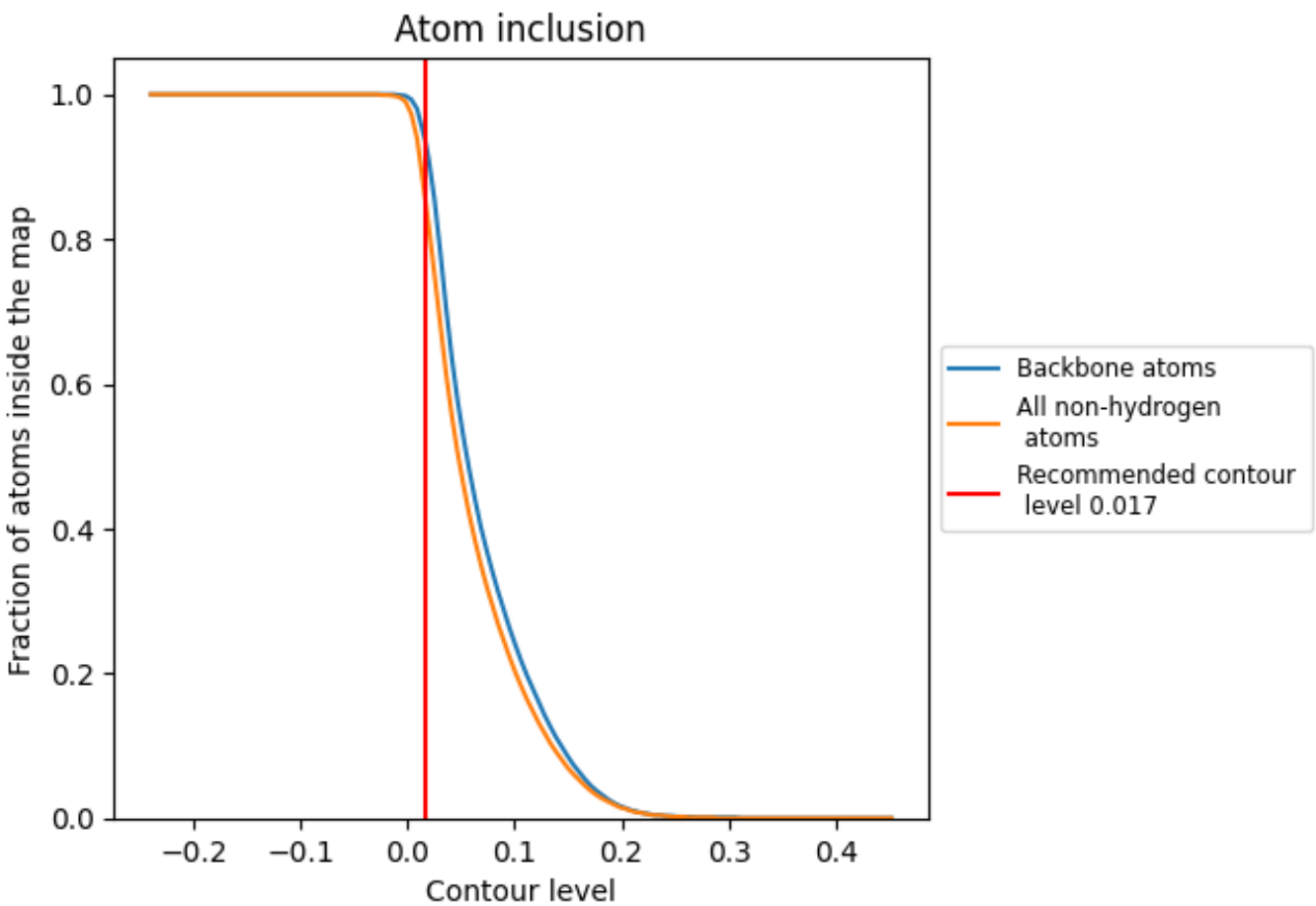
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.017).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8510	0.4430
C1	0.9370	0.4800
C2	0.9080	0.4410
CA	0.9680	0.5950
CB	0.8350	0.4300
CC	0.9110	0.4860
CD	0.8670	0.4490
CE	0.9520	0.5650
CF	0.9430	0.5220
CG	0.8950	0.4700
CH	0.9440	0.5460
CI	0.9370	0.5420
CJ	0.9770	0.6290
CK	0.9630	0.5950
CL	0.6970	0.4320
CM	0.9650	0.6020
CN	0.9050	0.4970
CO	0.8040	0.3920
CP	0.8700	0.4690
CQ	0.8750	0.4330
CR	0.7900	0.3650
CS	0.7150	0.2660
CT	0.9400	0.5600
CU	0.8810	0.5050
CW	0.8440	0.4350
CX	0.2060	0.1360
CY	0.4030	0.2290
CZ	0.1710	0.1500
Ca	0.8780	0.4650
Cb	0.8420	0.4160
Cc	0.9450	0.5690
Cd	0.8650	0.4470
Ce	0.8060	0.3760
Cf	0.8600	0.4380
Cg	0.9540	0.5540

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Chain	Atom inclusion	Q-score
Ch	0.7680	0.3480
Ci	0.9230	0.5110
Cj	0.9700	0.5940
Ck	0.8440	0.3930
Cl	0.7810	0.3770
Cm	0.9130	0.5240
Cn	0.9800	0.6040
Co	0.8350	0.3880
Cp	0.9590	0.5680
UA	0.9710	0.6080
UB	0.8640	0.4170
UC	0.4510	0.3020
UD	0.9120	0.5010
UE	0.8960	0.4720
UF	0.9200	0.4740
UG	0.9610	0.5930
UH	0.6320	0.2580
UI	0.8250	0.3700
UJ	0.7170	0.2780
UK	0.9390	0.5600
UL	0.9150	0.4930
UM	0.7870	0.4050
UN	0.9280	0.5330
UO	0.9460	0.5410
UP	0.8940	0.4770
UQ	0.9150	0.5110
UR	0.9560	0.5790
US	0.8630	0.4150
UT	0.7830	0.3060
UU	0.9670	0.5880
UX	0.9420	0.5660
UZ	0.8700	0.4180