



## Full wwPDB EM Validation Report ⓘ

Nov 4, 2025 – 12:14 PM EST

PDB ID : 9N77 / pdb\_00009n77  
EMDB ID : EMD-49087  
Title : SSU processome maturation and disassembly, State K  
Authors : Buzovetsky, O.; Klinge, S.  
Deposited on : 2025-02-05  
Resolution : 3.94 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46



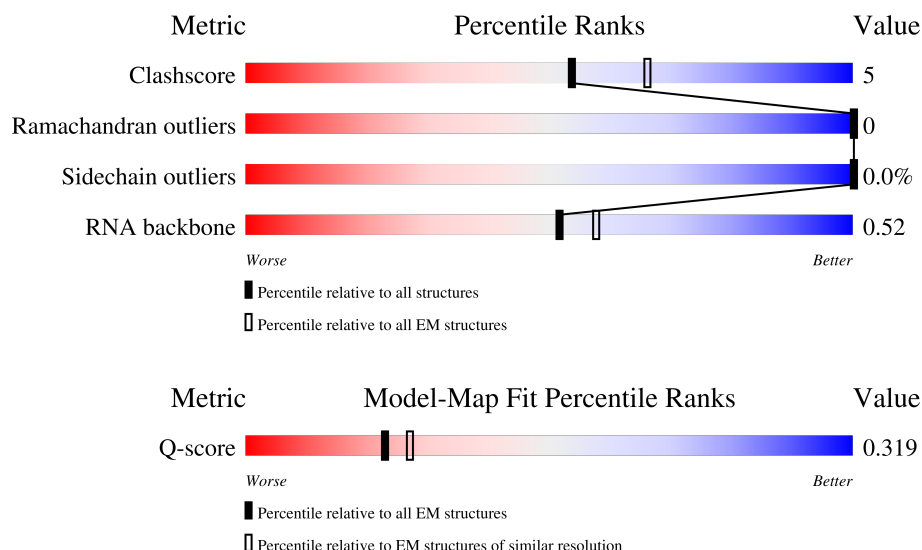
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.94 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	7757 ( 3.44 - 4.43 )

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  $\geq 3$ , 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  $\leq 5\%$ . 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	L0	700	 7% 10% 90%
2	L1	1803	 10% 54% 19% 23%
3	L2	334	 10% 51% 10% 38%

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Mol	Chain	Length	Quality of chain
4	L3	146	
5	L4	261	
6	L5	225	
7	L6	236	
8	L7	190	
9	L8	200	
10	L9	197	
11	LC	143	
12	LD	156	
13	LE	130	
14	LF	135	
15	LG	67	
16	LH	896	
17	LI	713	
18	LJ	513	
19	LK	575	
20	LL	643	
21	LM	1769	
22	LN	776	
23	LO	923	
24	LQ	943	
25	LR	817	
26	LS	594	
27	LT	939	
28	LZ	183	

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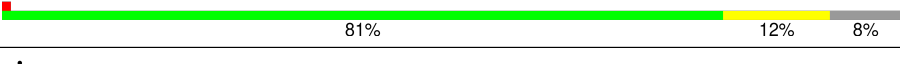

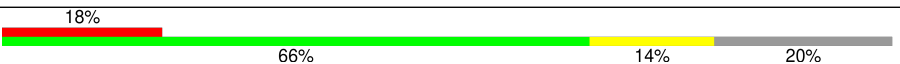

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Mol	Chain	Length	Quality of chain
29	NA	593	
30	NB	610	
31	ND	214	
32	NF	151	
33	NG	137	
34	NL	318	
35	NM	255	
36	NP	144	
37	NQ	82	
38	NS	1267	
39	NV	733	
40	OH	143	
41	OU	152	
42	SA	504	
43	SB	511	
44	SC	327	
44	SD	327	
45	SE	126	
45	SF	126	
46	SG	573	
47	SH	367	
48	SI	1183	
49	SJ	252	
49	SK	252	
50	SL	189	

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Mol	Chain	Length	Quality of chain
51	SM	290	
52	SP	2493	
53	SQ	217	
54	SR	145	
55	SS	899	
56	ST	810	
57	SU	552	
58	SV	206	
59	SW	274	
60	SY	250	
61	SZ	483	



## 2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 190271 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5'ETS rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L0	67	Total	C	N	O	P	0	0
			1437	641	258	471	67		

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L1	1388	Total	C	N	O	P	0	0
			29608	13236	5278	9706	1388		

- Molecule 3 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L2	207	Total	C	N	O	P	0	0
			4394	1964	760	1462	208		

- Molecule 4 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L3	106	Total	C	N	O	S	0	0
			862	545	159	156	2		

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L4	244	Total	C	N	O	S	0	0
			1936	1239	359	335	3		

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L5	206	Total	C	N	O	S	0	0
			1635	1027	300	305	3		



- Molecule 7 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L6	216	Total	C	N	O	S	0	0
			1740	1094	335	308	3		

- Molecule 8 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L7	178	Total	C	N	O	S	0	0
			1427	918	251	258			

- Molecule 9 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L8	170	Total	C	N	O	S	0	0
			1348	836	269	241	2		

- Molecule 10 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L9	181	Total	C	N	O	S	0	0
			1470	930	285	254	1		

- Molecule 11 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LC	128	Total	C	N	O	S	0	0
			997	642	178	177			

- Molecule 12 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LD	137	Total	C	N	O	S	0	0
			1112	714	212	183	3		

- Molecule 13 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LE	129	Total	C	N	O	S	0	0
			1022	650	188	181	3		

- Molecule 14 is a protein called 40S ribosomal protein S24-A.



Mol	Chain	Residues	Atoms				AltConf	Trace
14	LF	130	Total	C	N	O		
			1046	662	204	180	0	0

- Molecule 15 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LG	62	Total	C	N	O	S		
			490	302	98	89	1	0	0

- Molecule 16 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LH	806	Total	C	N	O	S		
			6290	4006	1073	1196	15	0	0

- Molecule 17 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LI	600	Total	C	N	O	S		
			3792	2375	679	733	5	0	0

- Molecule 18 is a protein called U3 small nucleolar RNA-associated protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LJ	476	Total	C	N	O	S		
			3773	2376	675	711	11	0	0

- Molecule 19 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LK	132	Total	C	N	O	S		
			1068	681	185	199	3	0	0

- Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LL	487	Total	C	N	O	S		
			3871	2458	662	738	13	0	0

- Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 10.



Mol	Chain	Residues	Atoms				AltConf	Trace
21	LM	1591	Total	C	N	O	0	0
			8005	4823	1591	1591		

- Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LN	663	Total	C	N	O	S	0	0
			5263	3333	913	995	22		

- Molecule 23 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LO	792	Total	C	N	O	S	0	0
			6321	4038	1086	1179	18		

- Molecule 24 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LQ	816	Total	C	N	O	S	0	0
			6494	4152	1089	1226	27		

- Molecule 25 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LR	793	Total	C	N	O	S	0	0
			6207	3931	1044	1203	29		

- Molecule 26 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LS	429	Total	C	N	O	S	0	0
			3172	2001	577	585	9		

- Molecule 27 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LT	864	Total	C	N	O	S	0	0
			5939	3703	1081	1137	18		

- Molecule 28 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	LZ	142	Total	C	N	O	S	0	0
			1173	743	214	210	6		

- Molecule 29 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	NA	330	Total	C	N	O	S	0	0
			2426	1496	436	490	4		

- Molecule 30 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	NB	262	Total	C	N	O	S	0	0
			1645	1010	318	316	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	ND	74	Total	C	N	O	S	0	0
			564	351	115	98			

- Molecule 32 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	NF	141	Total	C	N	O	S	0	0
			1135	725	214	194	2		

- Molecule 33 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	NG	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 34 is a protein called Dimethyladenosine transferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	NL	285	Total	C	N	O	S	0	0
			2285	1461	405	406	13		

- Molecule 35 is a protein called Small ribosomal subunit protein eS1A.



Mol	Chain	Residues	Atoms					AltConf	Trace
35	NM	229	Total	C	N	O	S	0	0
			1828	1156	339	329	4		

- Molecule 36 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	NP	134	Total	C	N	O	S	0	0
			1040	653	193	192	2		

- Molecule 37 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	NQ	79	Total	C	N	O	S	0	0
			595	371	108	111	5		

- Molecule 38 is a protein called Probable ATP-dependent RNA helicase DHR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NS	931	Total	C	N	O	S	0	0
			5051	3071	1001	977	2		

- Molecule 39 is a protein called Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	NV	19	Total	C	N	O	0	0
			149	94	34	21		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
40	OH	120	Total	C	N	O	0	0
			594	354	120	120		

- Molecule 41 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	OU	56	Total	C	N	O	0	0
			278	166	56	56		

- Molecule 42 is a protein called Nucleolar protein 56.



Mol	Chain	Residues	Atoms					AltConf	Trace
42	SA	397	Total	C	N	O	S	1	0
			3100	1964	534	593	9		

- Molecule 43 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SB	422	Total	C	N	O	S	0	0
			3255	2056	555	634	10		

- Molecule 44 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SC	240	Total	C	N	O	S	1	0
			1865	1181	335	339	10		
44	SD	238	Total	C	N	O	S	0	0
			1850	1171	333	336	10		

- Molecule 45 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SE	121	Total	C	N	O	S	0	0
			916	583	158	171	4		
45	SF	121	Total	C	N	O	S	0	0
			916	583	158	171	4		

- Molecule 46 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SG	459	Total	C	N	O	S	0	0
			3672	2331	645	686	10		

- Molecule 47 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

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

- Molecule 48 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SI	787	Total	C	N	O	S	0	0
			6387	4096	1141	1122	28		



- Molecule 49 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	SJ	213	Total	C	N	O	0	0
			1074	648	213	213		
49	SK	229	Total	C	N	O	0	0
			1160	702	229	229		

- Molecule 50 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SL	148	Total	C	N	O	S	0	0
			1171	750	209	202	10		

- Molecule 51 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SM	247	Total	C	N	O	S	0	0
			2009	1260	379	363	7		

- Molecule 52 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SP	1852	Total	C	N	O	S	0	0
			15102	9753	2498	2804	47		

- Molecule 53 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SQ	97	Total	C	N	O	S	0	0
			836	526	155	152	3		

- Molecule 54 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SR	134	Total	C	N	O	S	0	0
			1052	668	204	178	2		

- Molecule 55 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SS	121	Total	C	N	O	S	0	0
			1014	624	199	181	10		



- Molecule 56 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	ST	584	Total	C	N	O	S	0	0
			3341	2039	656	643	3		

- Molecule 57 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	SU	532	Total	C	N	O	0	0
			2703	1639	532	532		

- Molecule 58 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	SV	155	Total	C	N	O	0	0
			852	512	176	164		

- Molecule 59 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SW	210	Total	C	N	O	S	0	0
			1654	1054	300	296	4		

- Molecule 60 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SY	201	Total	C	N	O	S	0	0
			1715	1068	335	306	6		

- Molecule 61 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	SZ	259	Total	C	N	O	0	0
			1314	796	259	259		

- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	L1	45	Total	Mg	0
			45	45	
62	L9	1	Total	Mg	0
			1	1	

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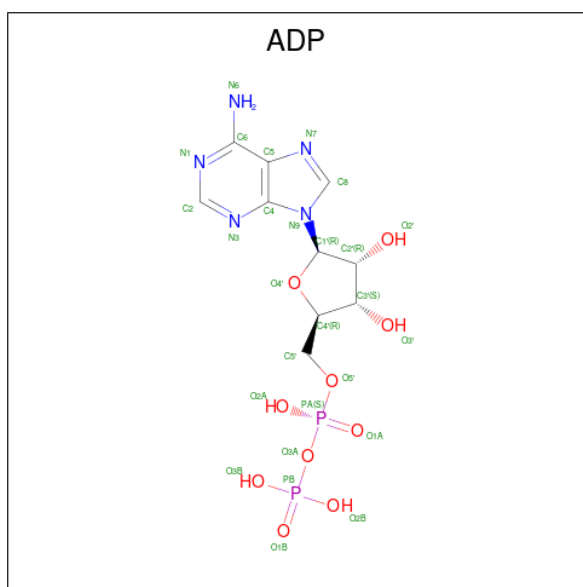
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Mol	Chain	Residues	Atoms		AltConf
62	NS	1	Total	Mg	0
			1	1	
62	SI	1	Total	Mg	0
			1	1	

- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
63	NQ	1	Total	Zn	0
			1	1	
63	SL	1	Total	Zn	0
			1	1	

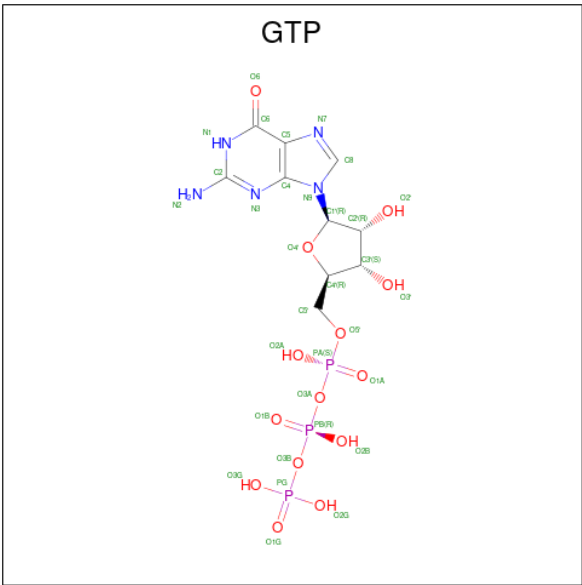
- Molecule 64 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 65 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).





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

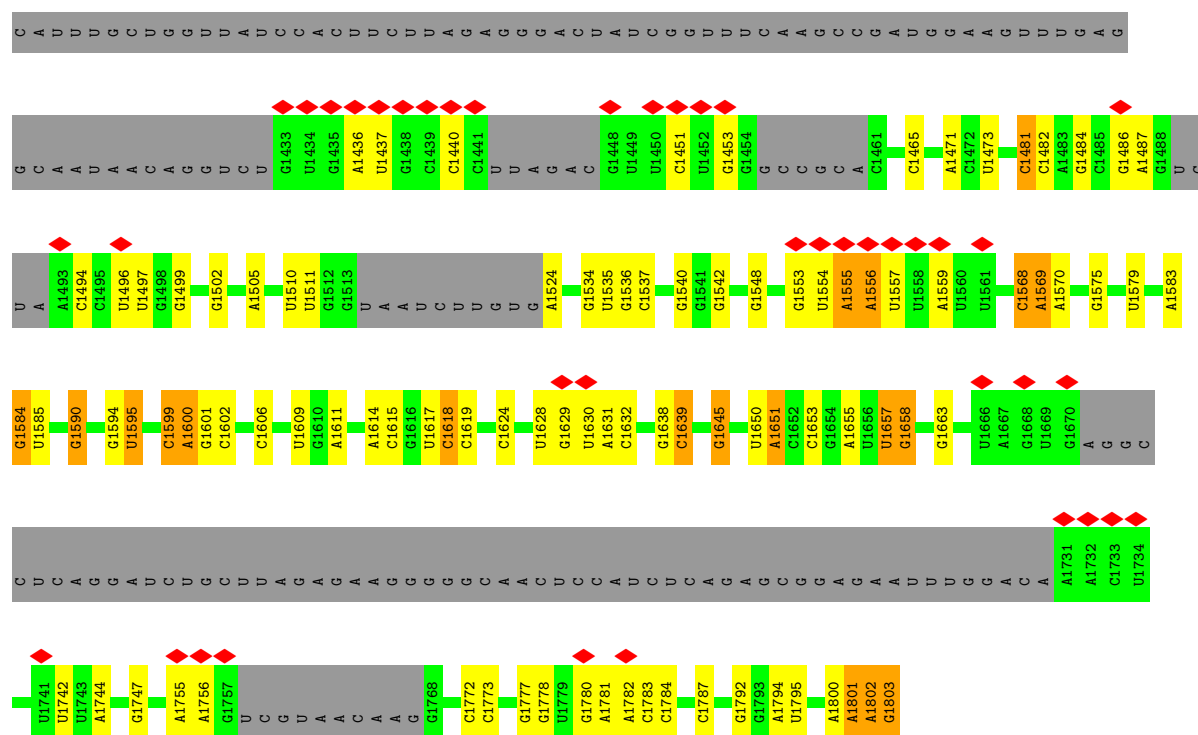




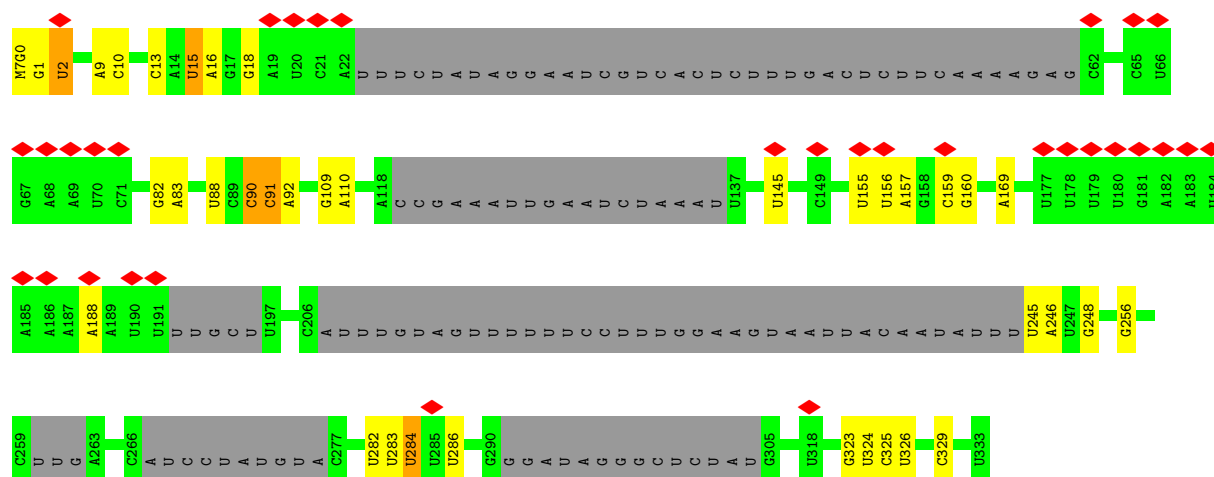




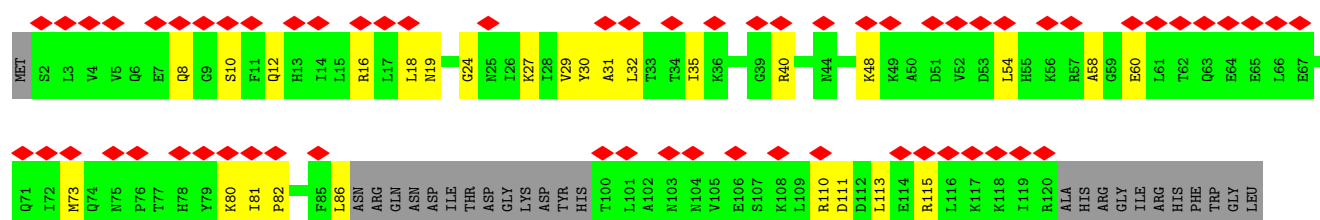
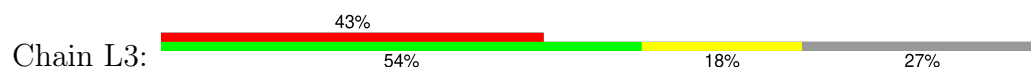




### • Molecule 3: U3 snoRNA



### • Molecule 4: 40S ribosomal protein S18-A





ARG  
VAL  
ARG  
GLY  
GLN  
HIS  
THR  
LYS  
THR  
LYS  
THR  
GLY  
GLY  
ARG  
ARG  
ALA

• Molecule 5: 40S ribosomal protein S4-A

Chain L4:



MET A2 R3 Y27 Y54 A55 L56 E60 D88 E97 Y103 K122 V129 Q130 L131 G132 K133 V136 V139 V140 T141 H142 D143 R148 D171 F172 D176 A177 V181 Y182 I195 D212 S213 L214 D215 N216 V225 K245 LEU SER TLE ALA

GLU GLU ASP ARG ARG ARG ALA GLN GLN GLY LEU

• Molecule 6: 40S ribosomal protein S5

Chain L5:



MET SER ASP THR GLU ALA PRO VAL GLU VAL GLN GLY ASP F14 F15 V16 V17 E18 E19 F20 T21 P22 V23 V24 L25 A26 T27 P28 T29 F30 E31 Q35 A36 Q37 T38 E39 K41 S47 F48 E49 E52 V53 K54 D55 A56 S57 N79 K80 R81 K84 I90 E91 R92

L93 T94 N103 N104 G105 K106 K107 I114 D126 V132 V133 A136 T140 V149 GLY GLY GLY ALA A156 D161 V162 N169 T189 L198 K203 T207 K212 R225

• Molecule 7: 40S ribosomal protein S6-A

Chain L6:



K1 K2 I5 S6 K14 T15 F16 I18 I21 H22 R23 I24 R31 I32 V41 G42 D43 M63 V67 L68 R72 I73 I78 T78 V81 R92 R98 D105 V108 T113 E118 Q119 E120 L124 N140 D151 V157 R160 E161

K164 G165 E166 K167 T168 T170 P173 K174 I175 Q182 K187 Q201 R202 L215 SER GLU ARG LYS ALA ALA LYS LYS ALA ALA ILE ARG LYS ARG ARG ALA SER SER LEU LYS ALA

• Molecule 8: 40S ribosomal protein S7-A

Chain L7:



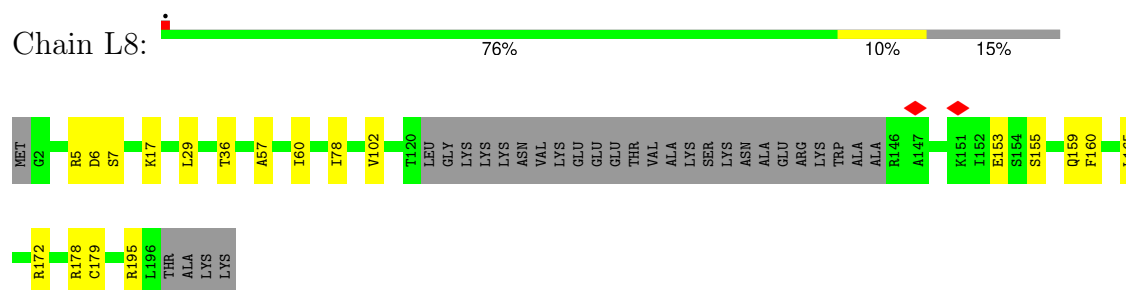
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V62 P63 S66 L67 V73 Q74 T75 K76 L77 T78 R79 E80 L81 E82 K83 K84 F85 Q86 D87 R88 H89 V90 I91 F92 L93 A94 E95 R96 L99 P100 P101 P102 P103 P104 P105 P106 P107 P108 P109 P110 P111 P112 P113 P114 L118 S119 H122 E127 D128 T133 E134 I135 V136

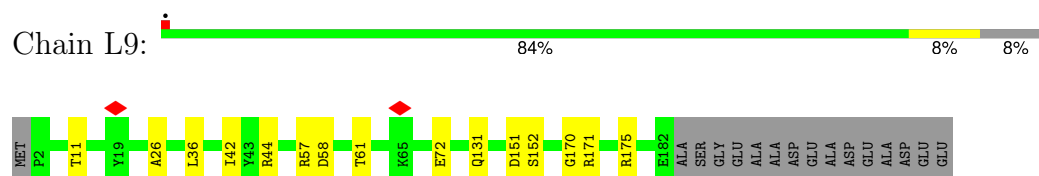
Y142 V152 L153 L154 K157 D158 V159 Q160 L166 E167 S168 F169 V172 T177 I181 T185 P186 S187 E188 T189 H190



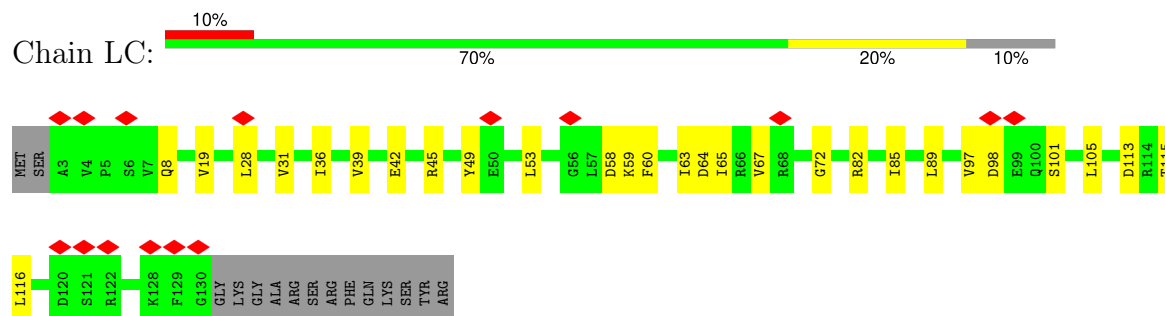
- Molecule 9: 40S ribosomal protein S8-A



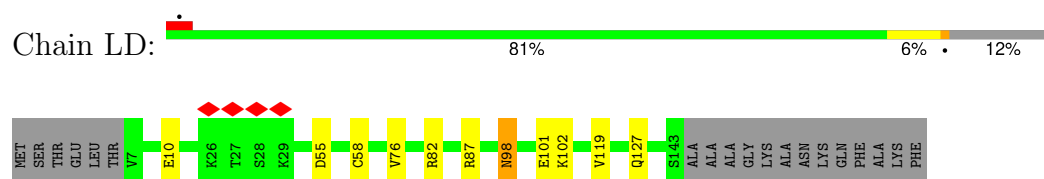
- Molecule 10: 40S ribosomal protein S9-A



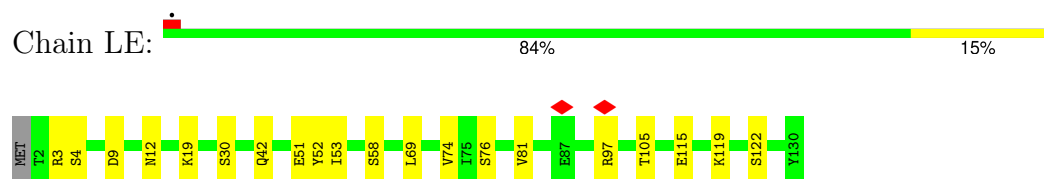
- Molecule 11: 40S ribosomal protein S16-A



- Molecule 12: 40S ribosomal protein S11-A



- Molecule 13: 40S ribosomal protein S22-A



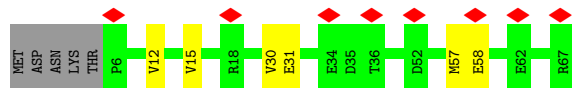
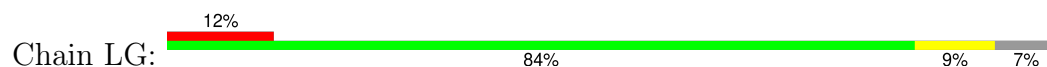
- Molecule 14: 40S ribosomal protein S24-A



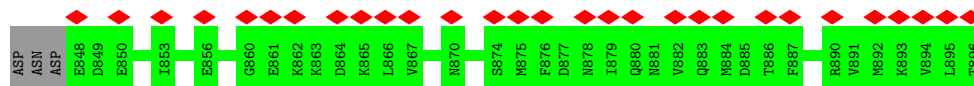
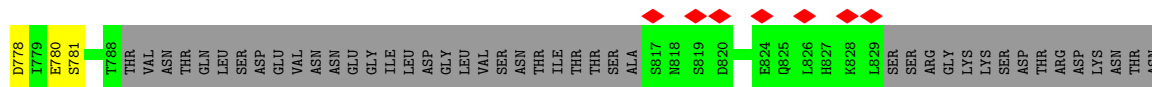
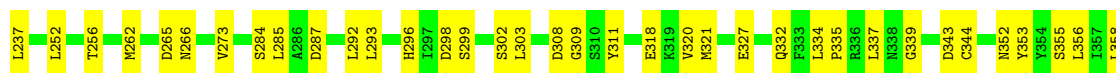
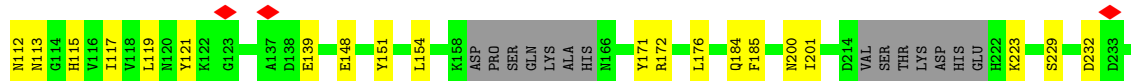




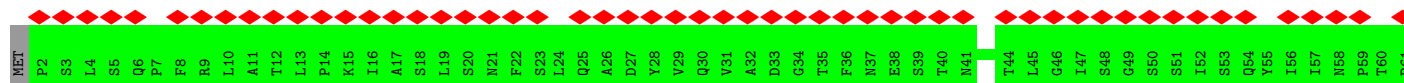
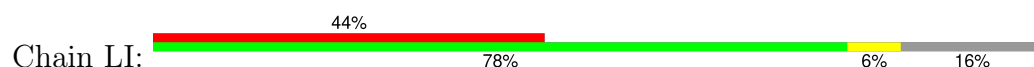
- Molecule 15: 40S ribosomal protein S28-A



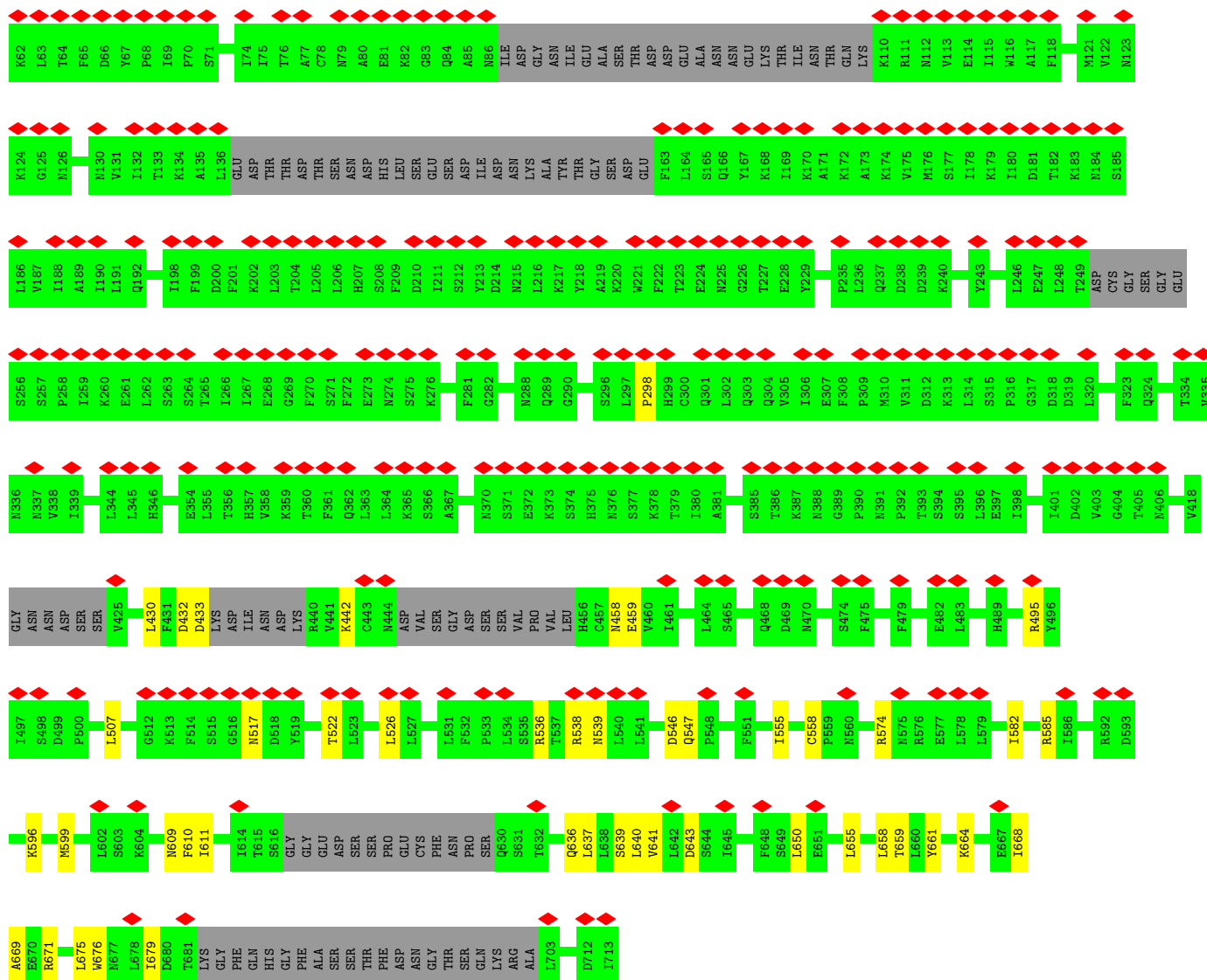
- Molecule 16: NET1-associated nuclear protein 1



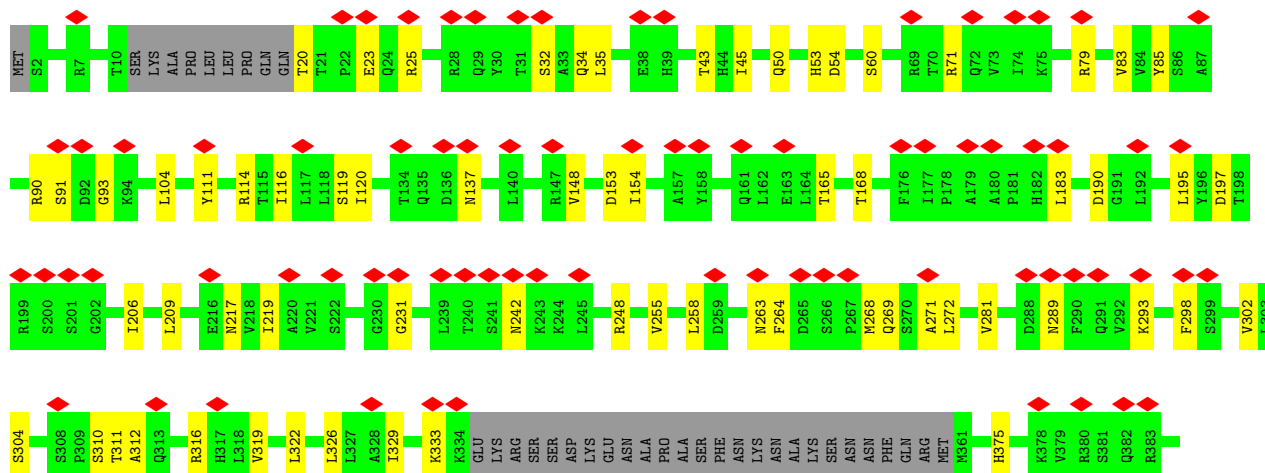
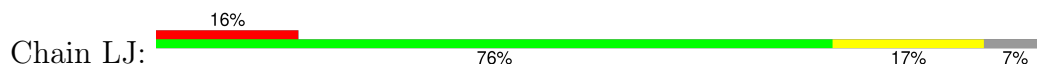
- Molecule 17: U3 small nucleolar RNA-associated protein 8



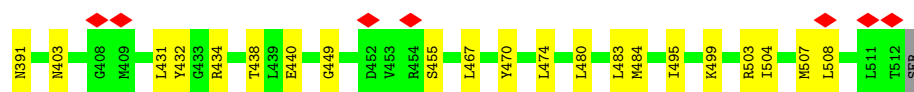




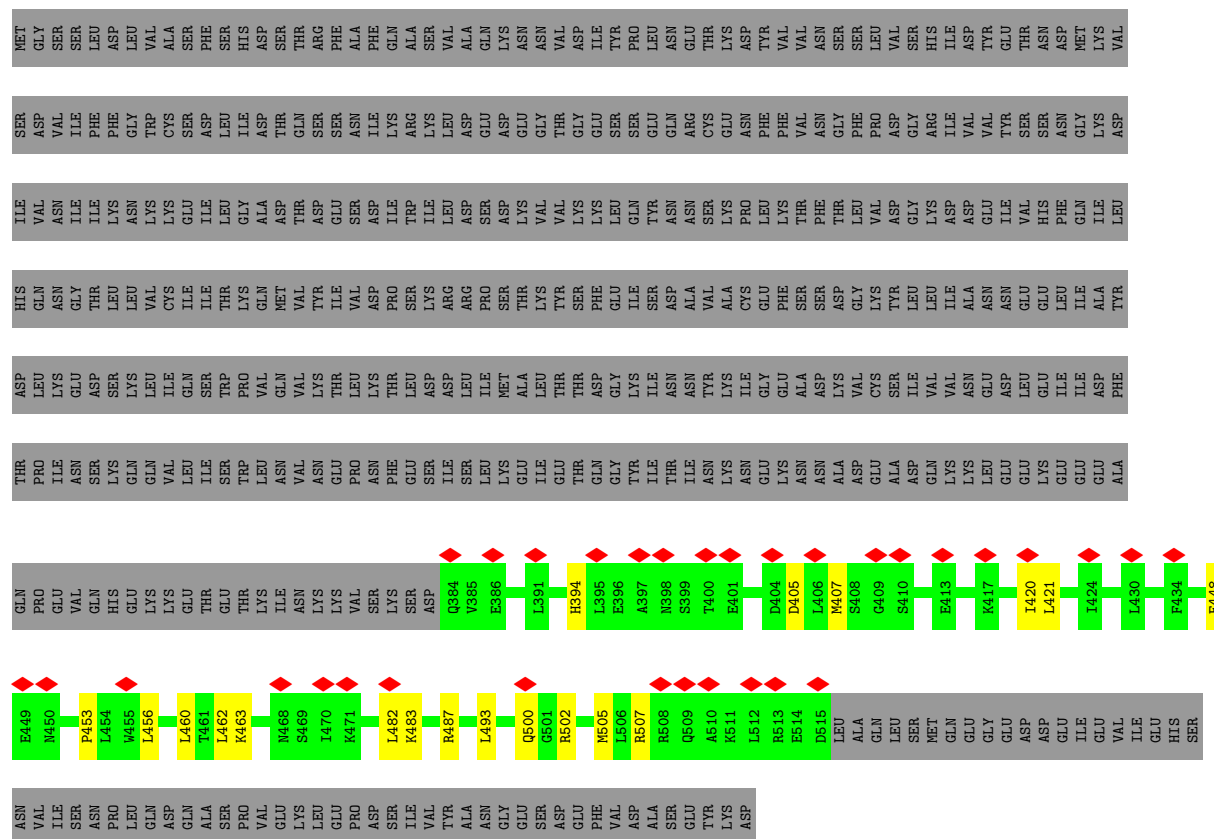
• Molecule 18: U3 small nucleolar RNA-associated protein 15



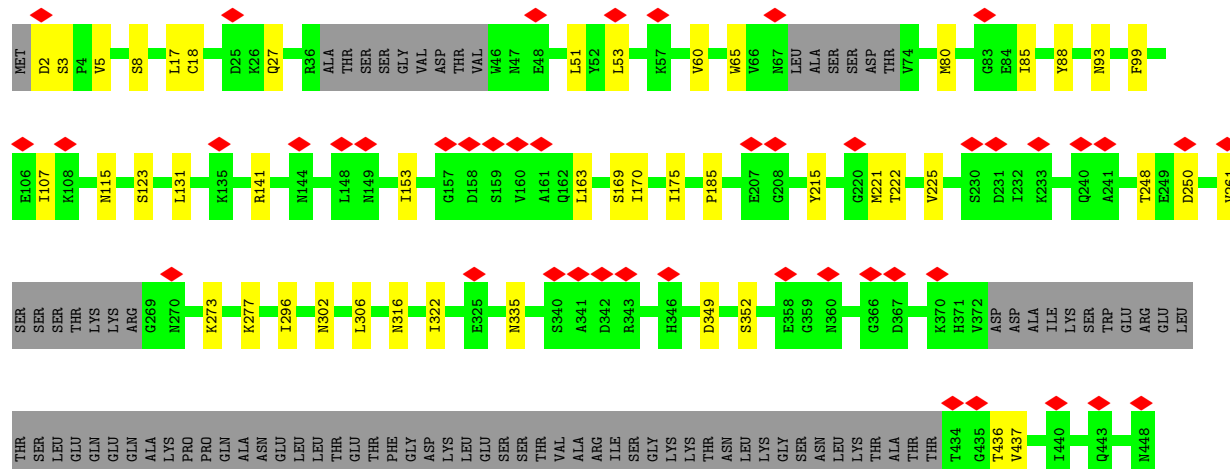




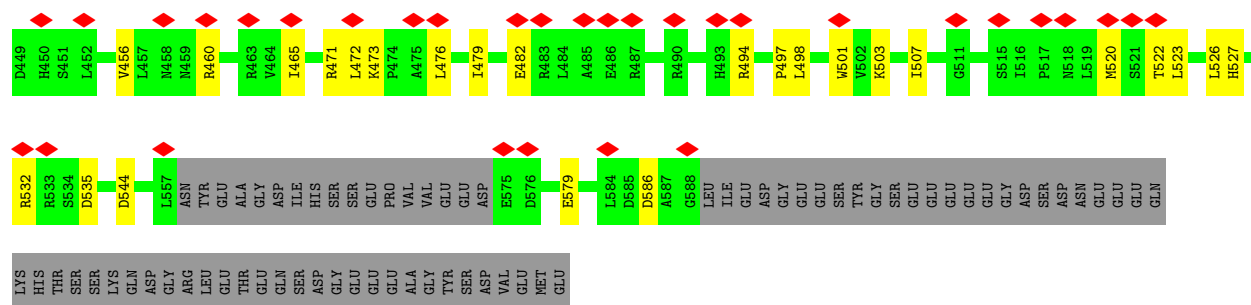
• Molecule 19: U3 small nucleolar RNA-associated protein 9



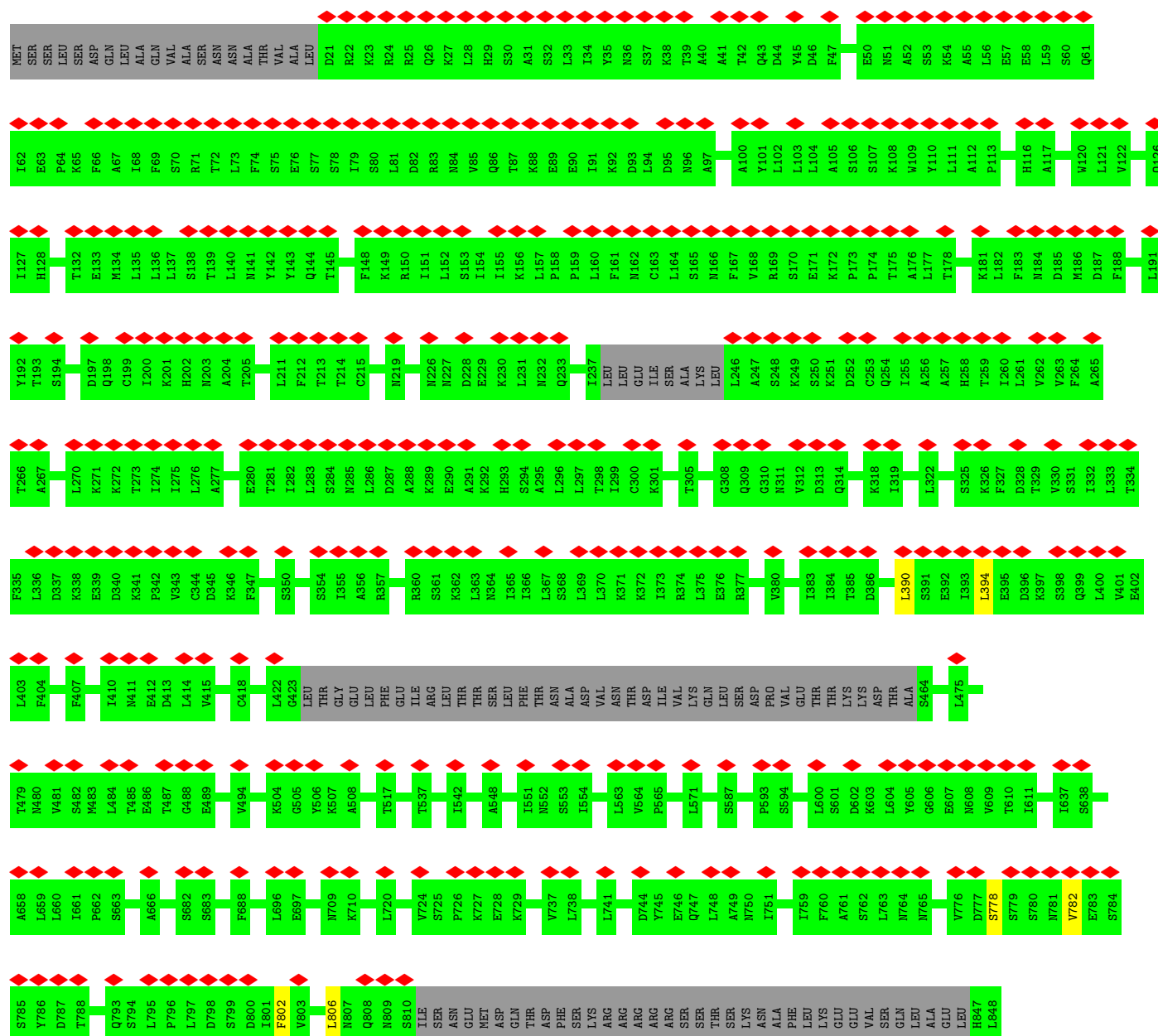
• Molecule 20: U3 small nucleolar RNA-associated protein 5



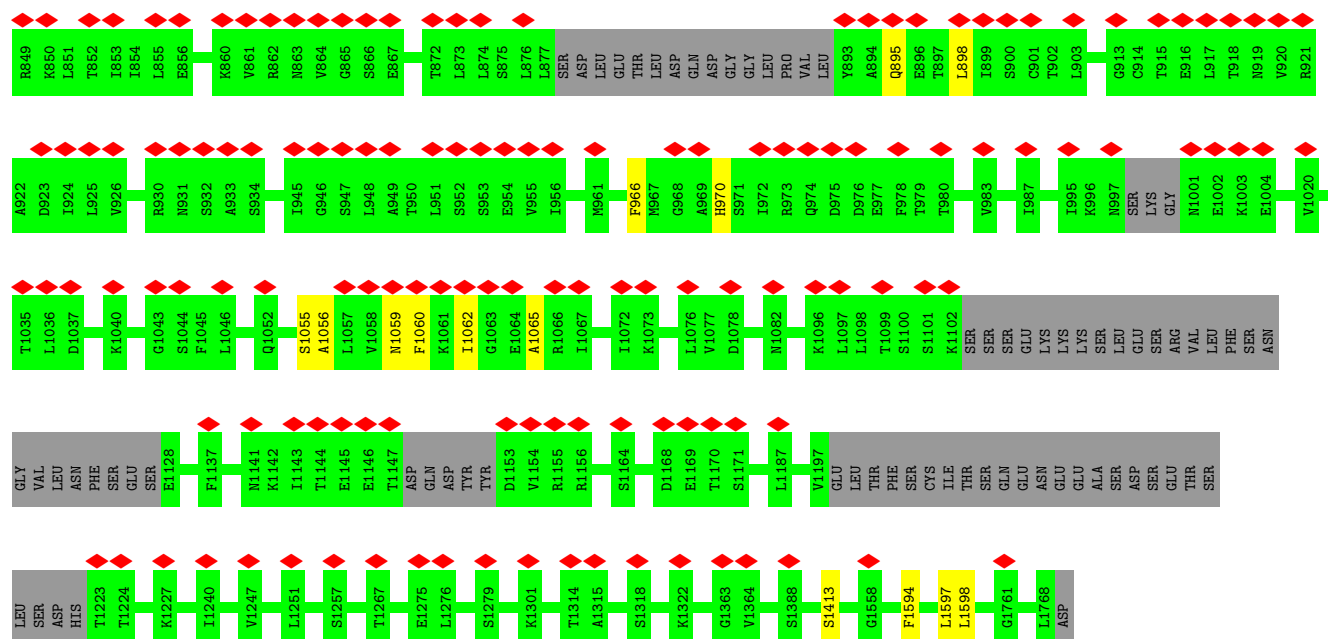




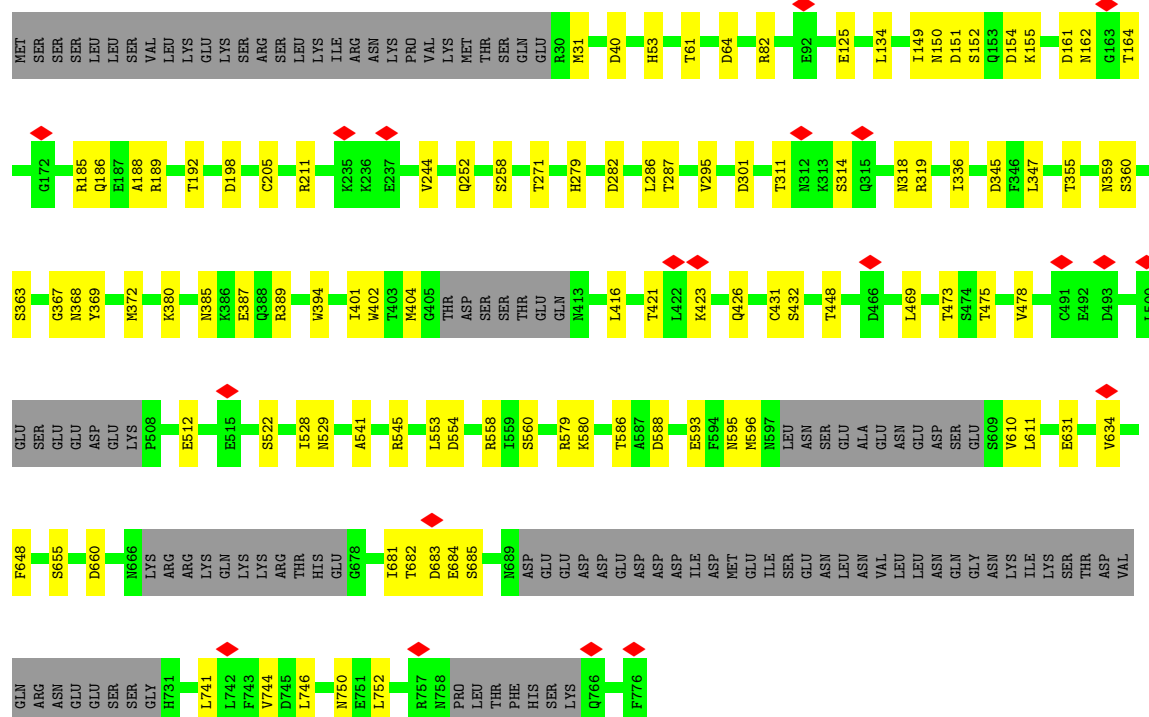
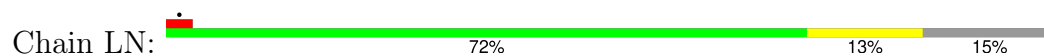
- Molecule 21: U3 small nucleolar RNA-associated protein 10







- Molecule 22: U3 small nucleolar RNA-associated protein 4



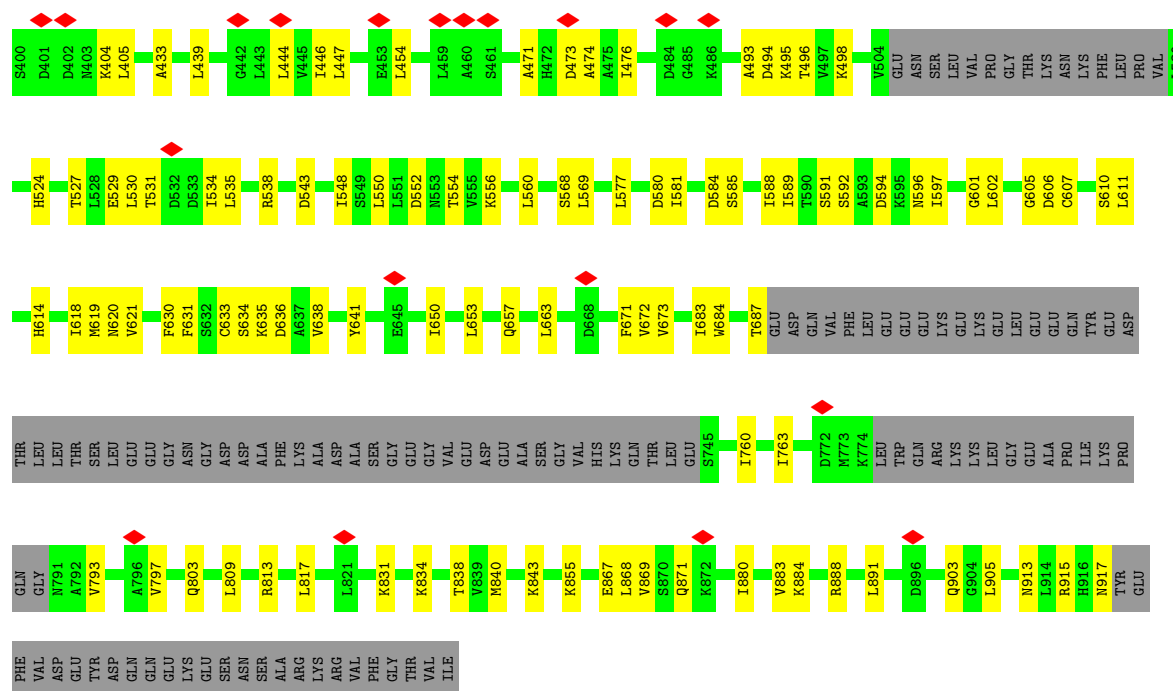
- Molecule 23: Periodic tryptophan protein 2



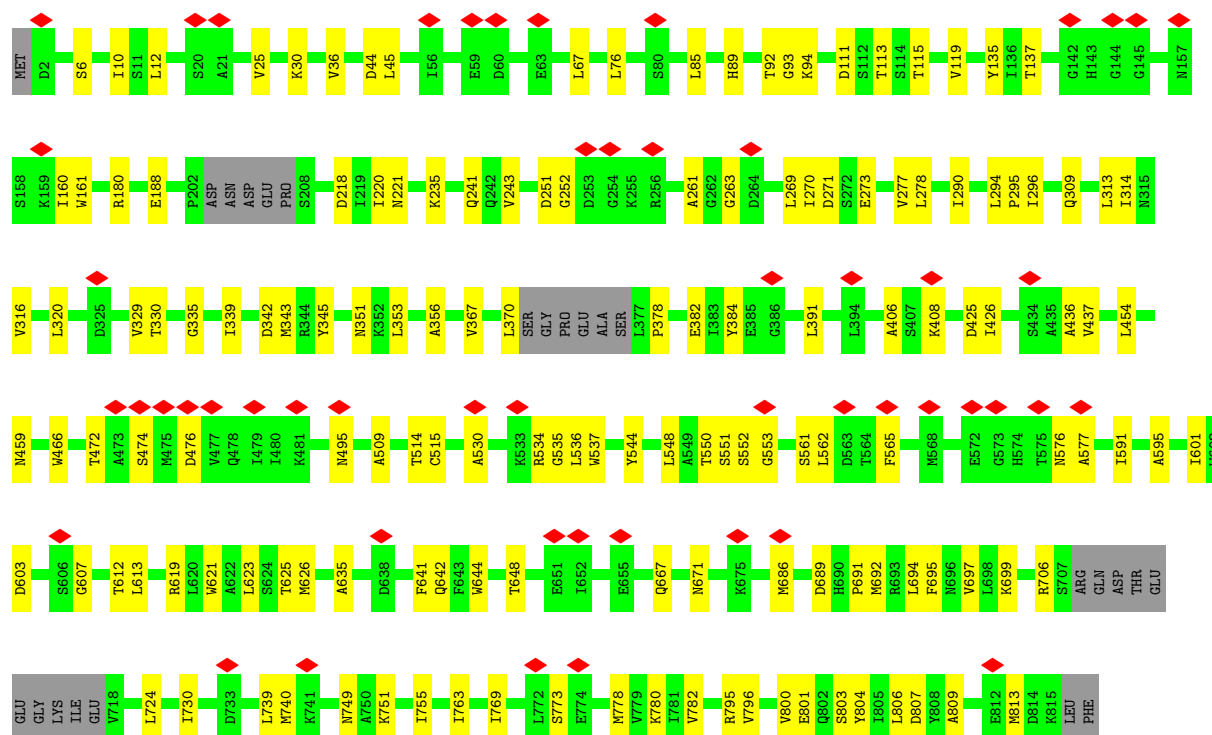
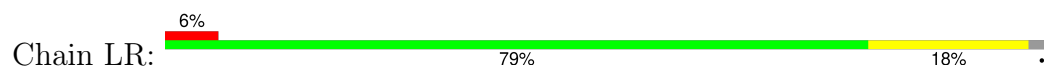








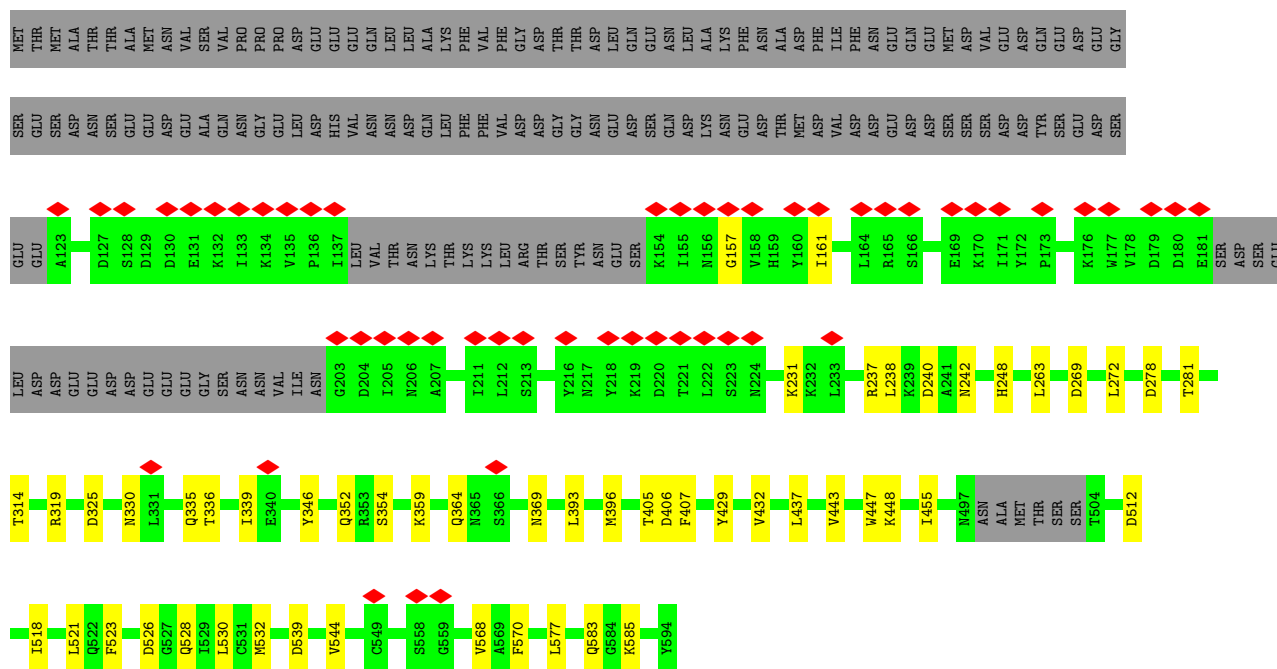
- Molecule 25: U3 small nucleolar RNA-associated protein 13



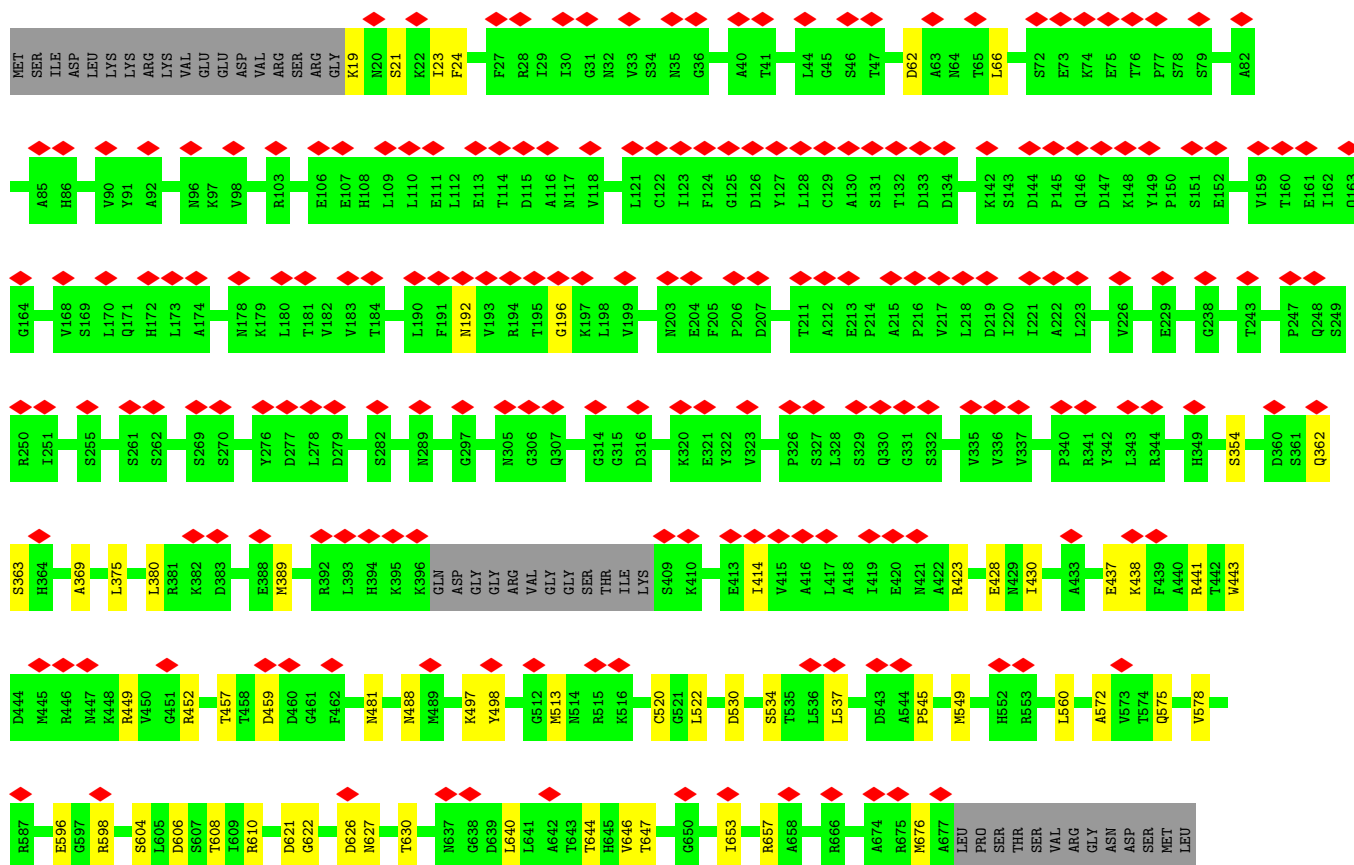
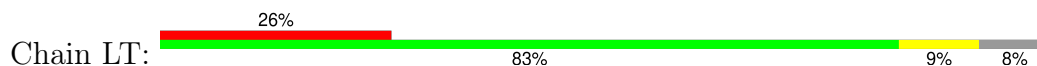
- Molecule 26: U3 small nucleolar RNA-associated protein 18



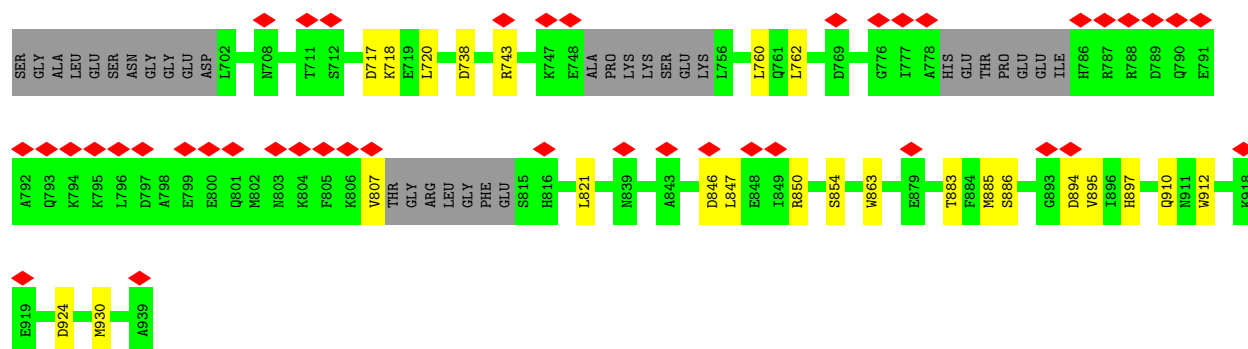




• Molecule 27: U3 small nucleolar RNA-associated protein 21

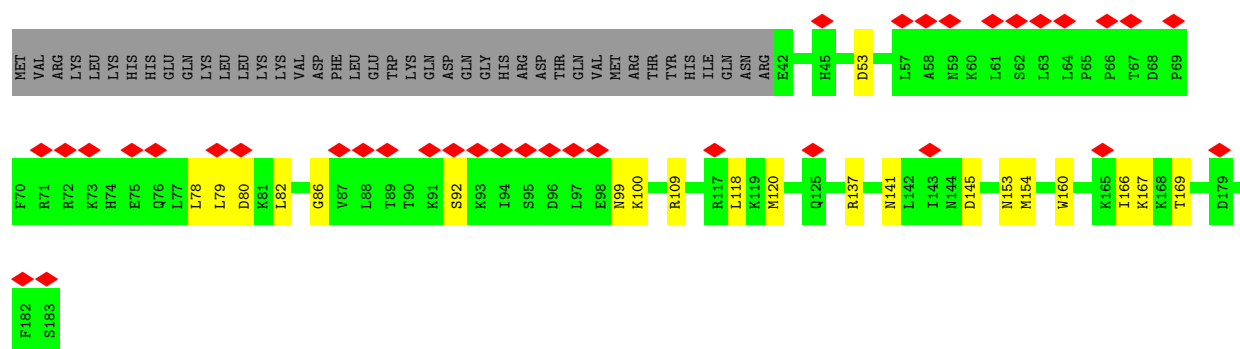






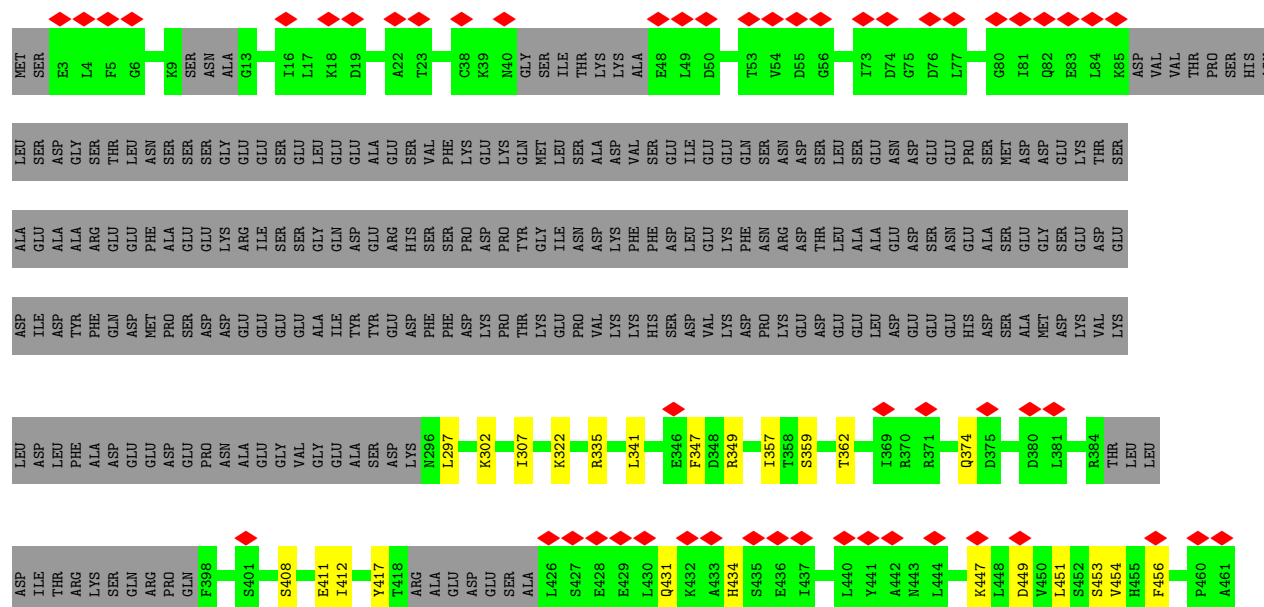
- Molecule 28: U3 small nucleolar ribonucleoprotein protein IMP3

Chain LZ:



- Molecule 29: U3 small nucleolar RNA-associated protein MPP10

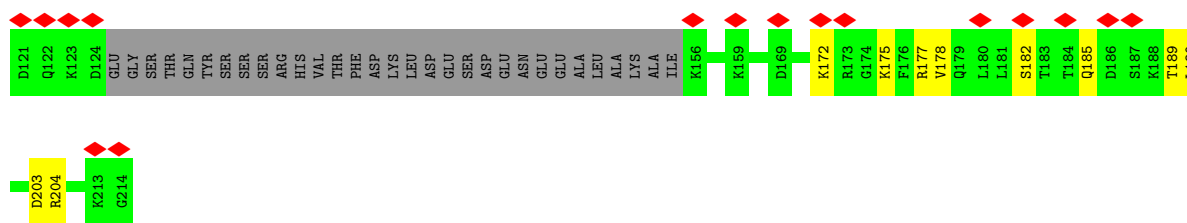
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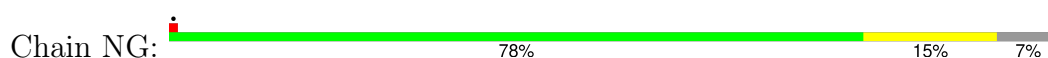




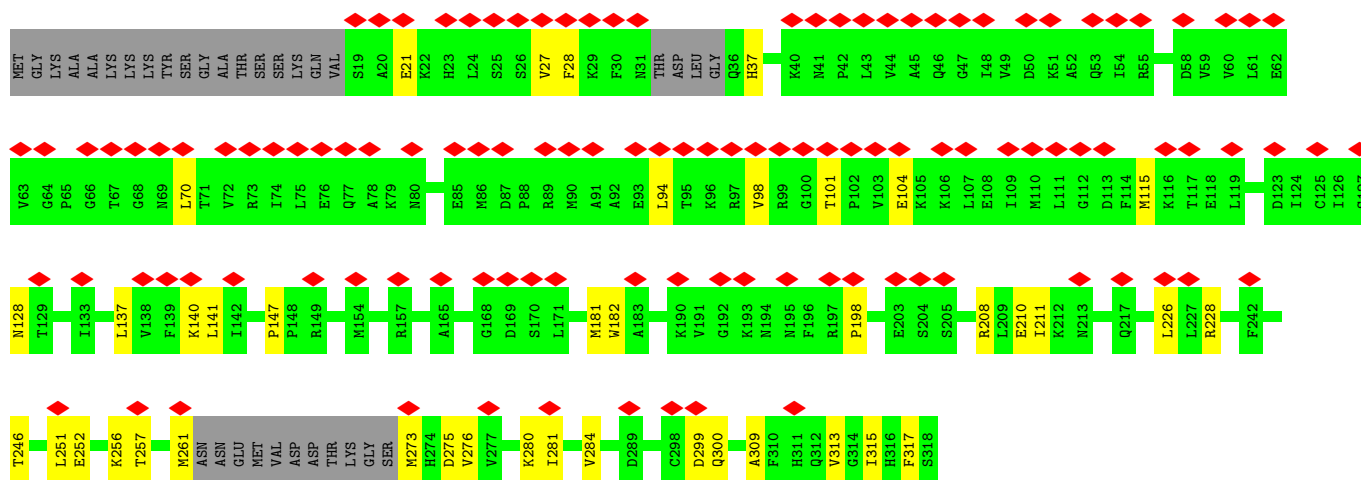
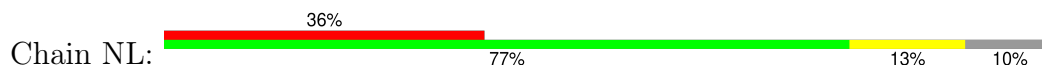
- Molecule 32: 40S ribosomal protein S13



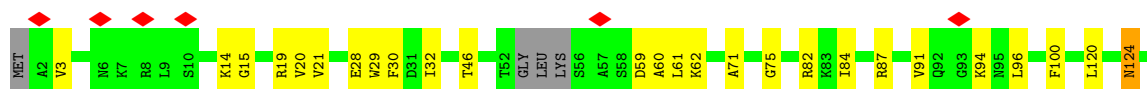
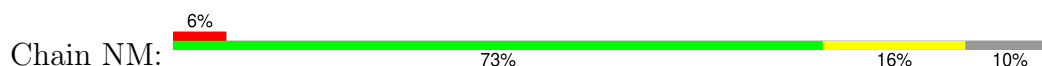
- Molecule 33: 40S ribosomal protein S14-A



- Molecule 34: Dimethyladenosine transferase



- Molecule 35: Small ribosomal subunit protein eS1A



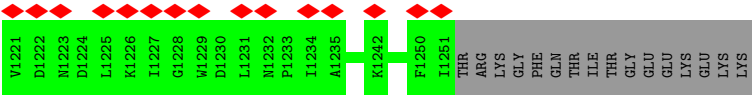




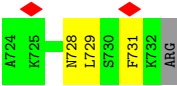
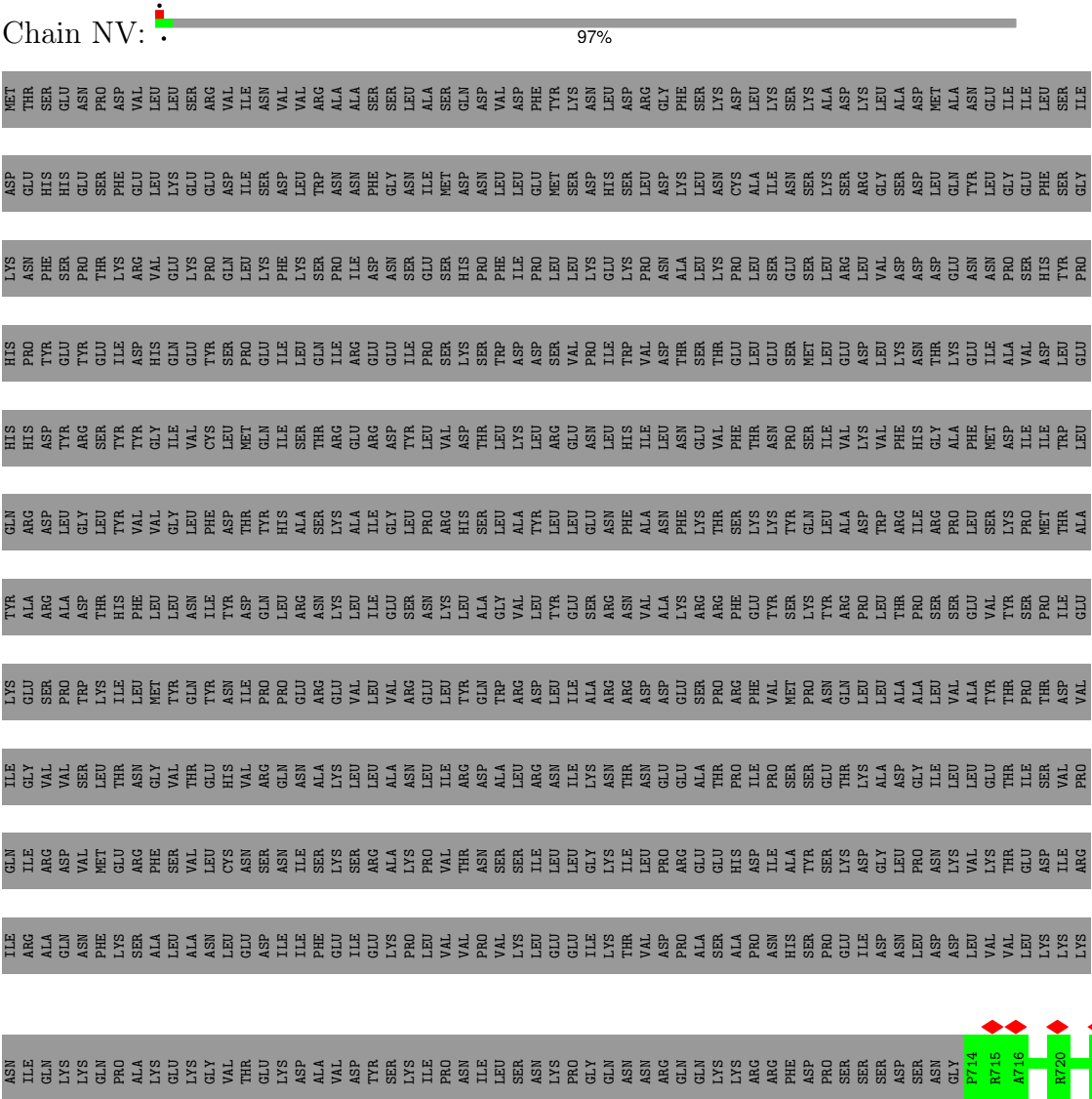


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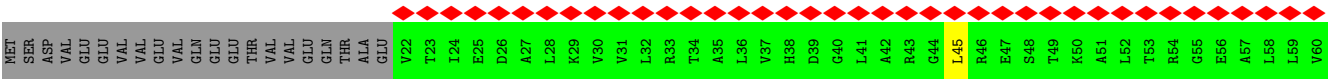
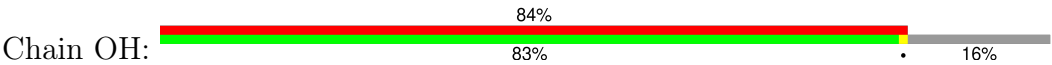




• Molecule 39: Exosome complex exonuclease RRP6

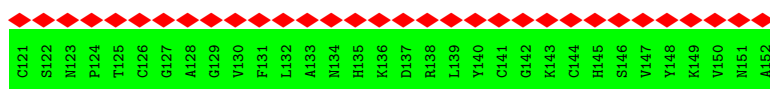
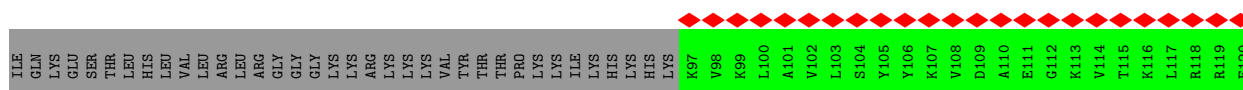
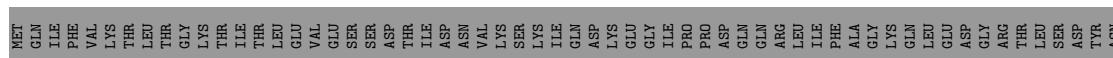


• Molecule 40: 40S ribosomal protein S12

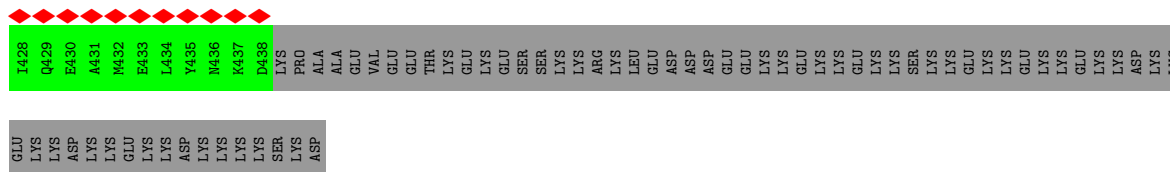
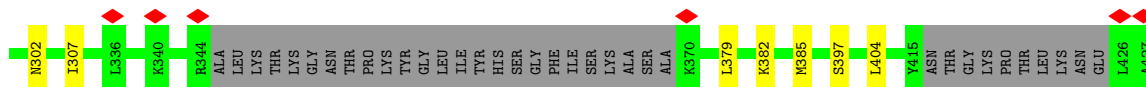
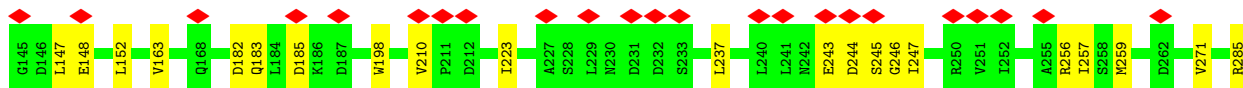
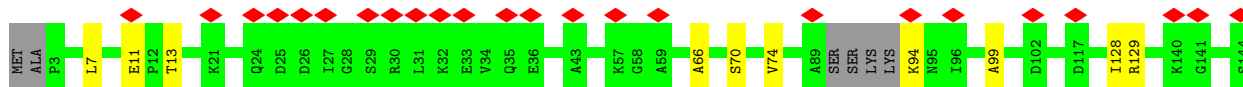




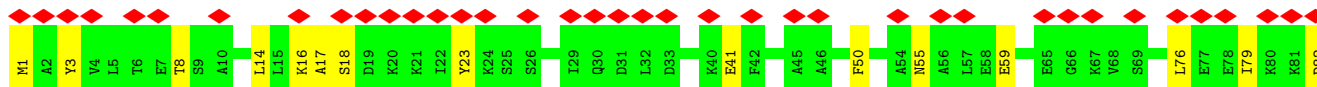
- Molecule 41: Ubiquitin-40S ribosomal protein S31



- Molecule 42: Nucleolar protein 56



- Molecule 43: Nucleolar protein 58



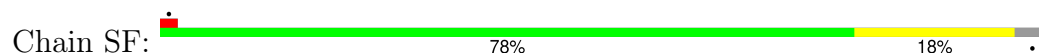




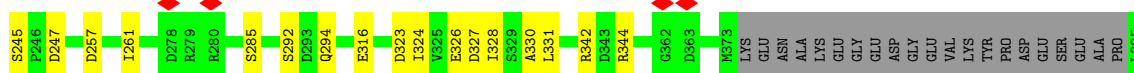
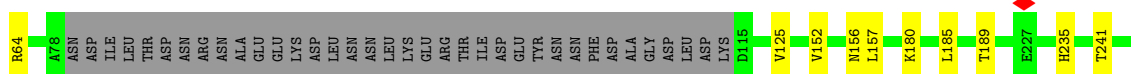
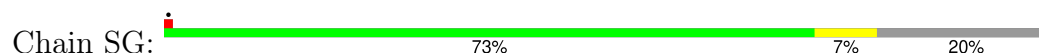




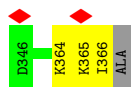
- Molecule 45: 13 kDa ribonucleoprotein-associated protein



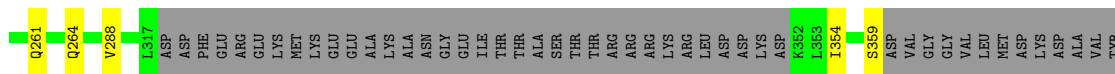
- Molecule 46: Ribosomal RNA-processing protein 9



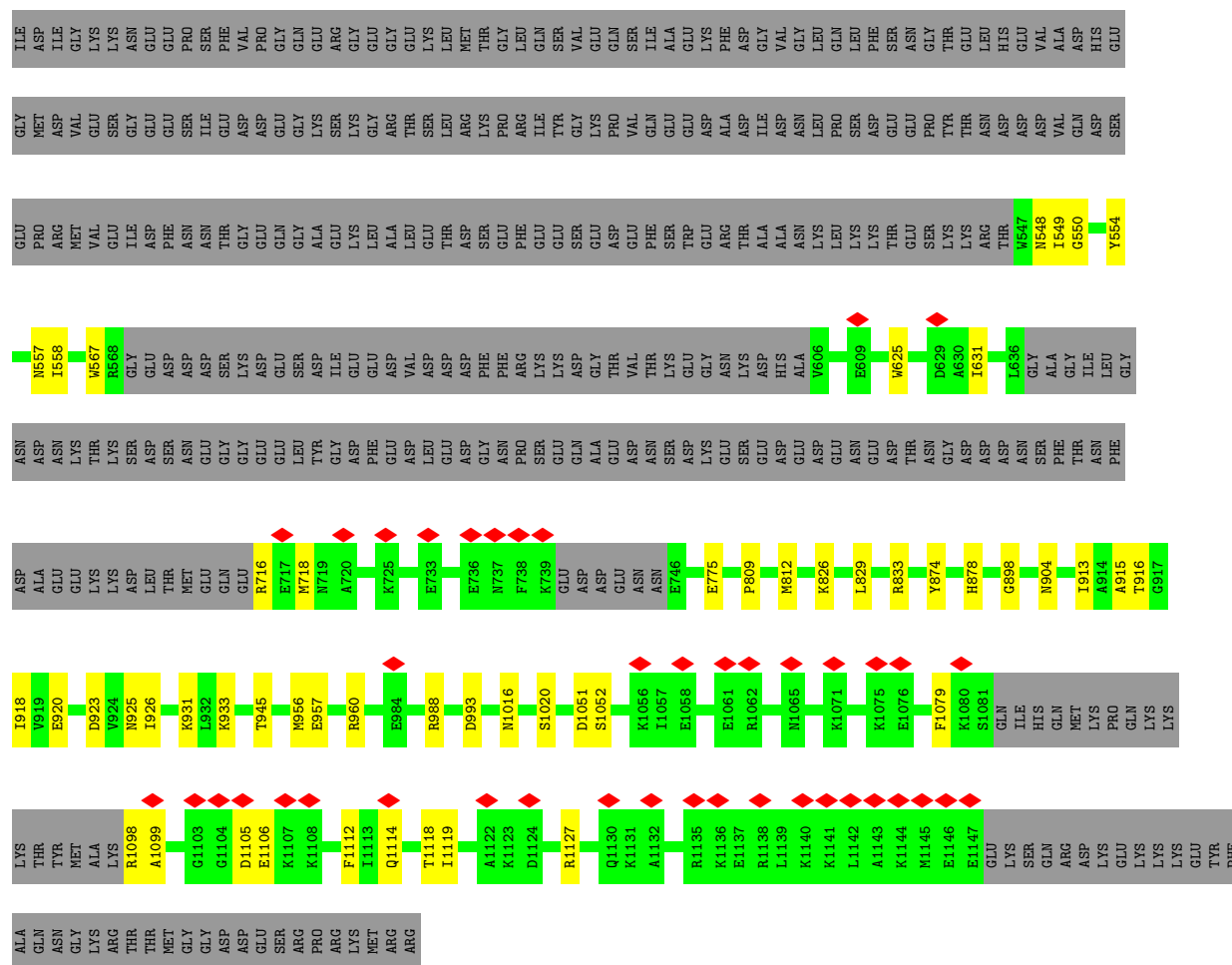
- Molecule 47: RNA 3'-terminal phosphate cyclase-like protein



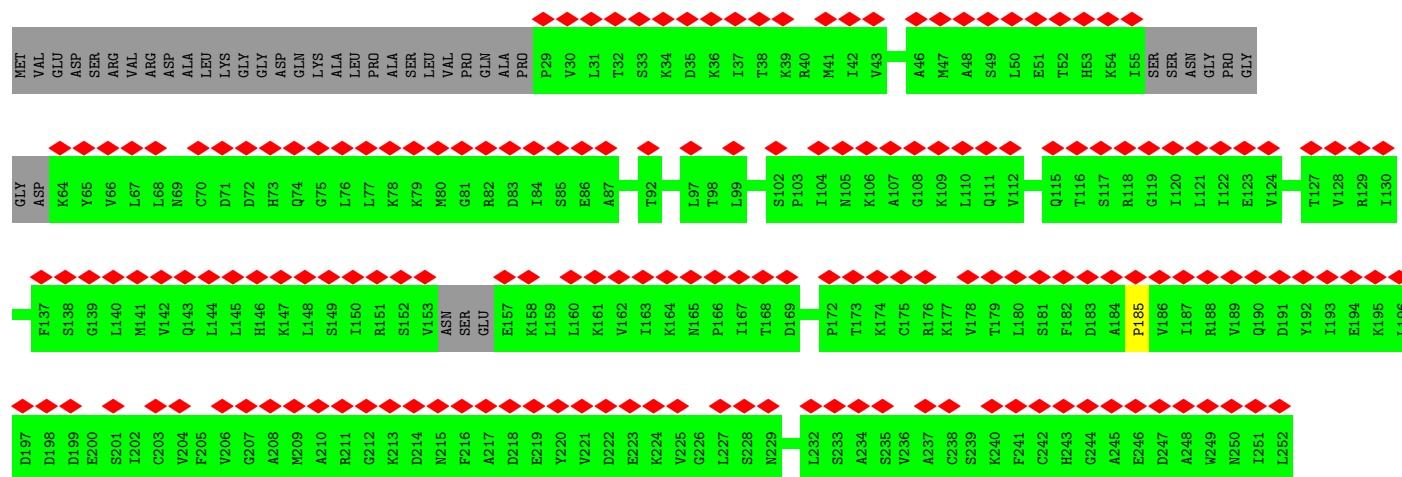
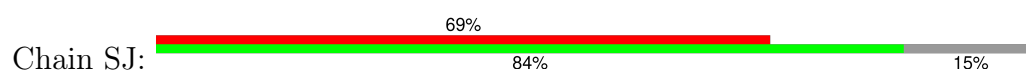
- Molecule 48: Ribosome biogenesis protein BMS1







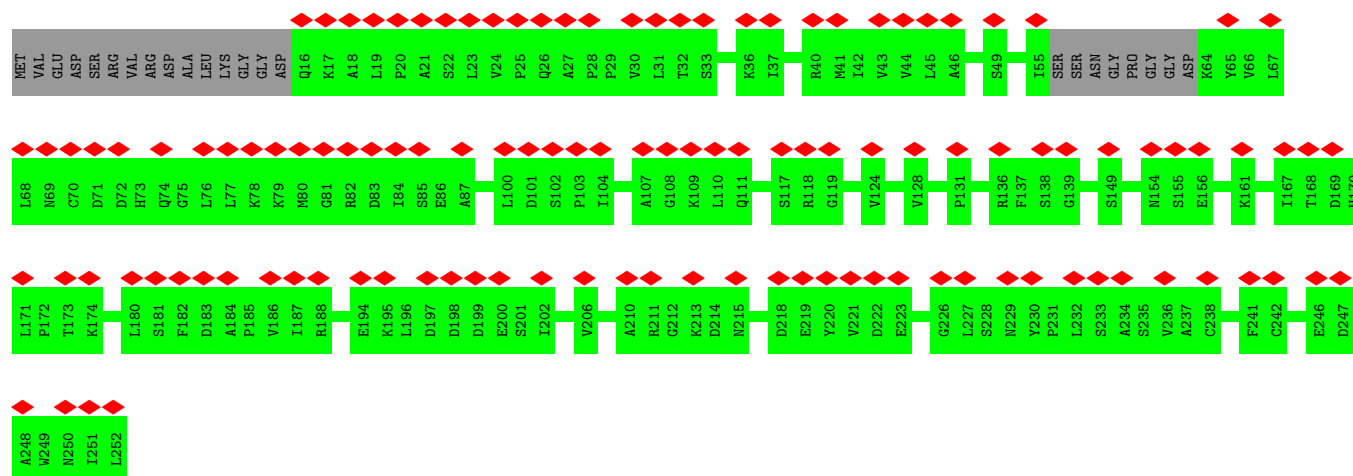
• Molecule 49: Ribosomal RNA small subunit methyltransferase NEP1



• Molecule 49: Ribosomal RNA small subunit methyltransferase NEP1

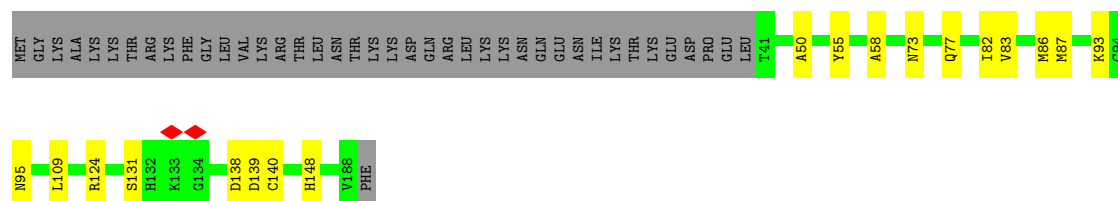






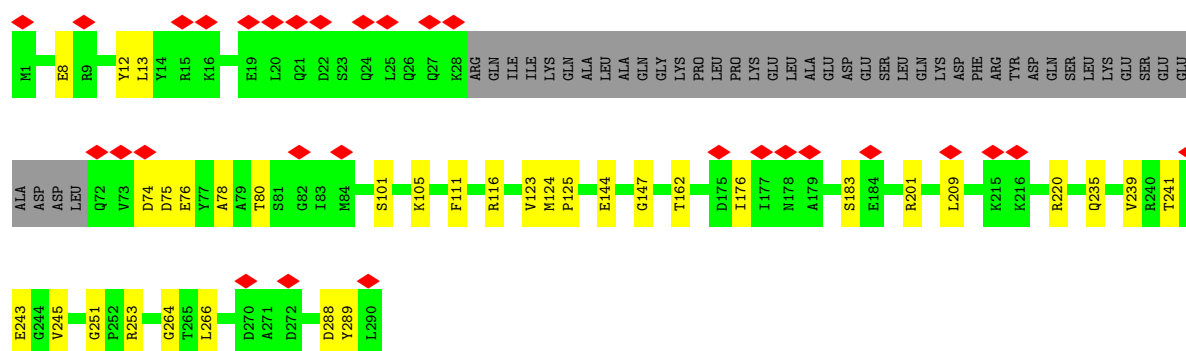
- Molecule 50: rRNA-processing protein FCF1

Chain SL: 69% 10% 22%



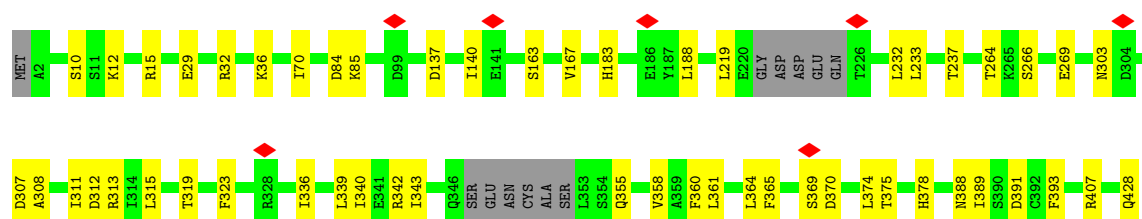
- Molecule 51: U3 small nucleolar ribonucleoprotein protein IMP4

Chain SM: 10% 73% 12% 15%



- Molecule 52: U3 small nucleolar RNA-associated protein 20

Chain SP: 23% 64% 10% 26%



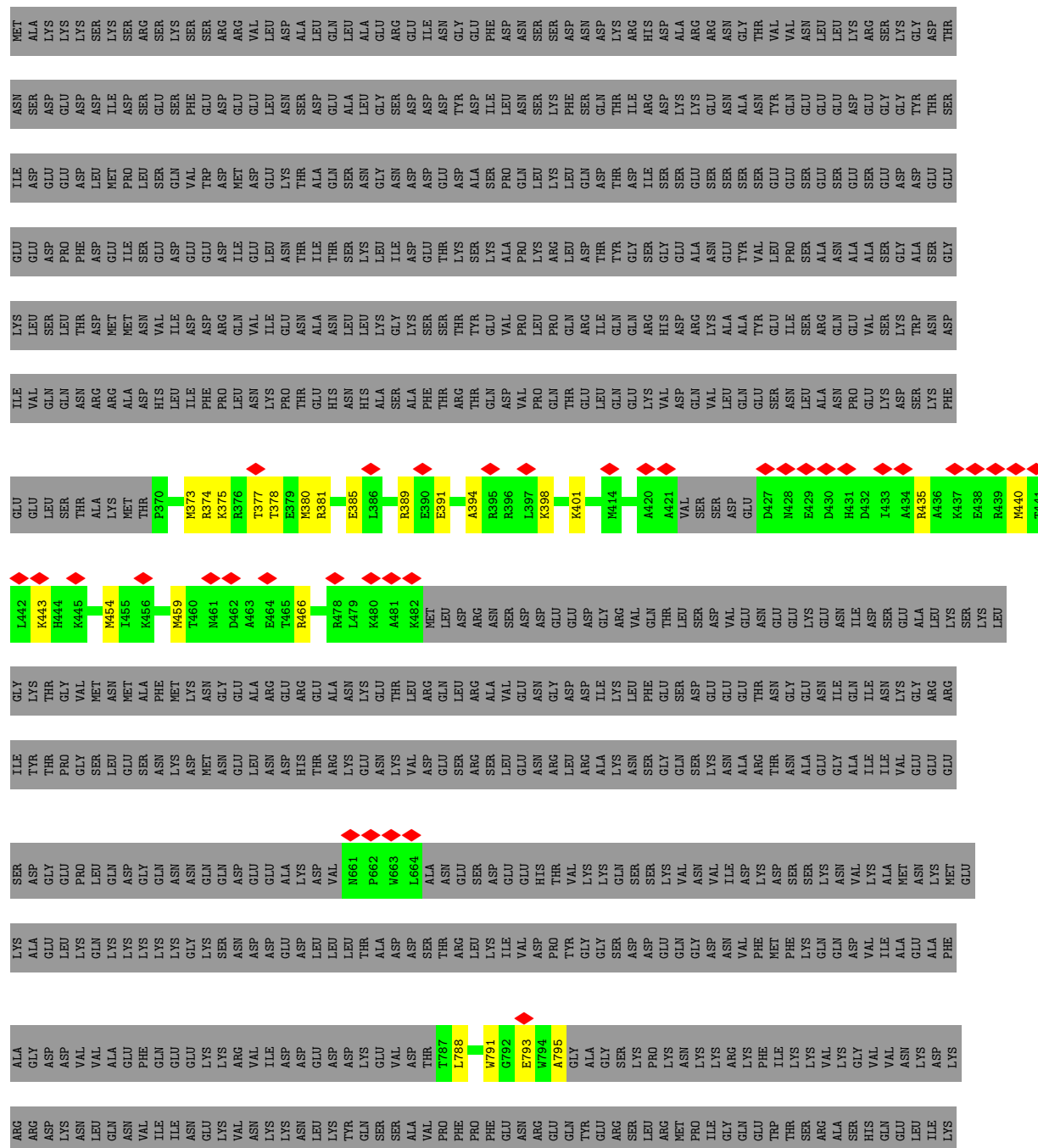










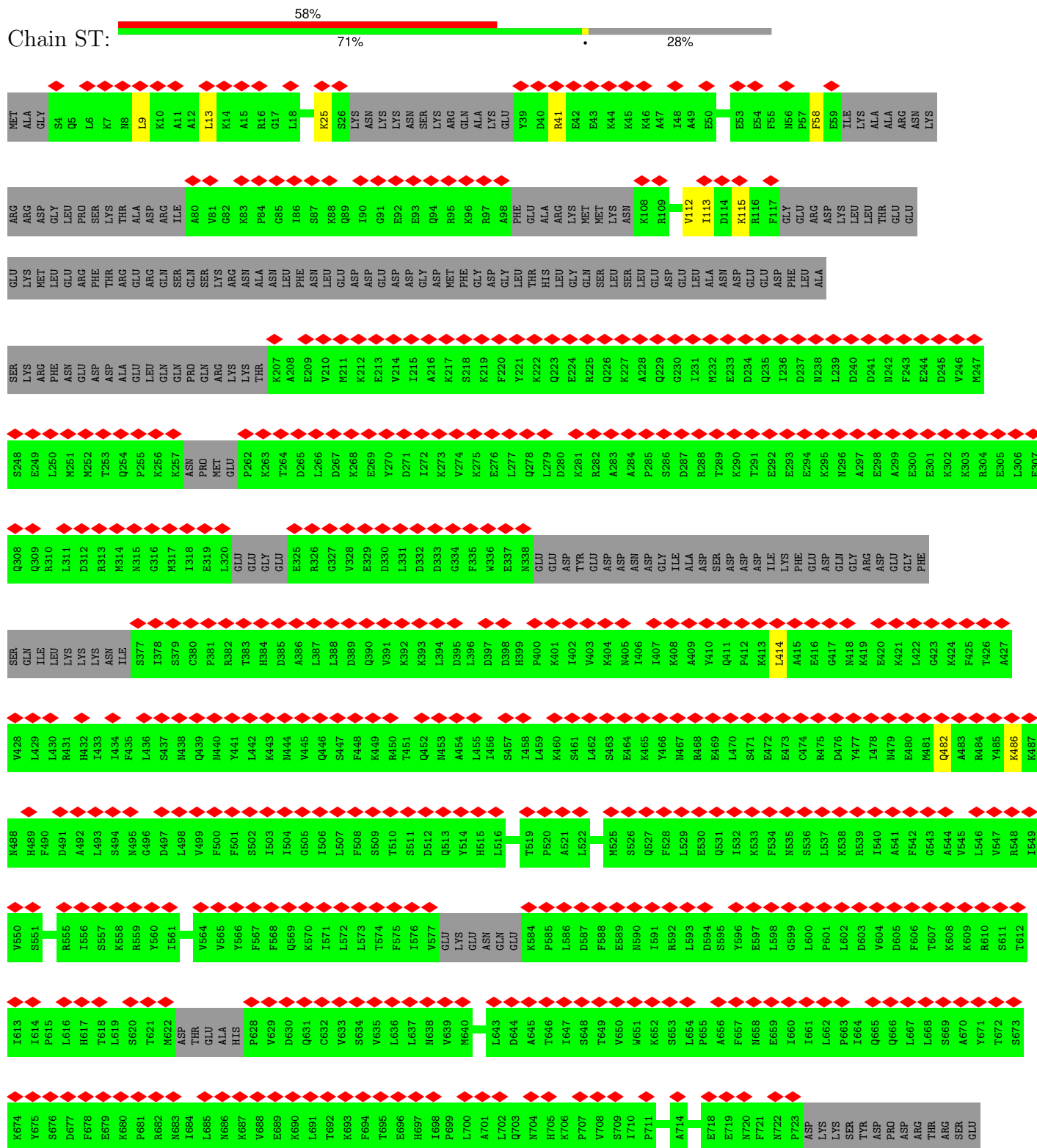




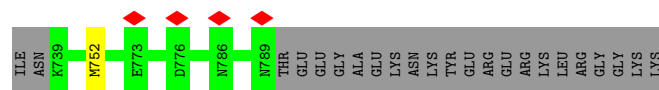
PRO ARG  
ILE MET  
THR THR  
PRO PRO  
GLY GLN  
VAL ILE  
ILE ASP  
PRO PRO  
LEU LEU  
LYS LYS  
ALA ALA  
PHE PHE  
LYS LYS

• Molecule 56: Nucleolar complex protein 14

Chain ST:

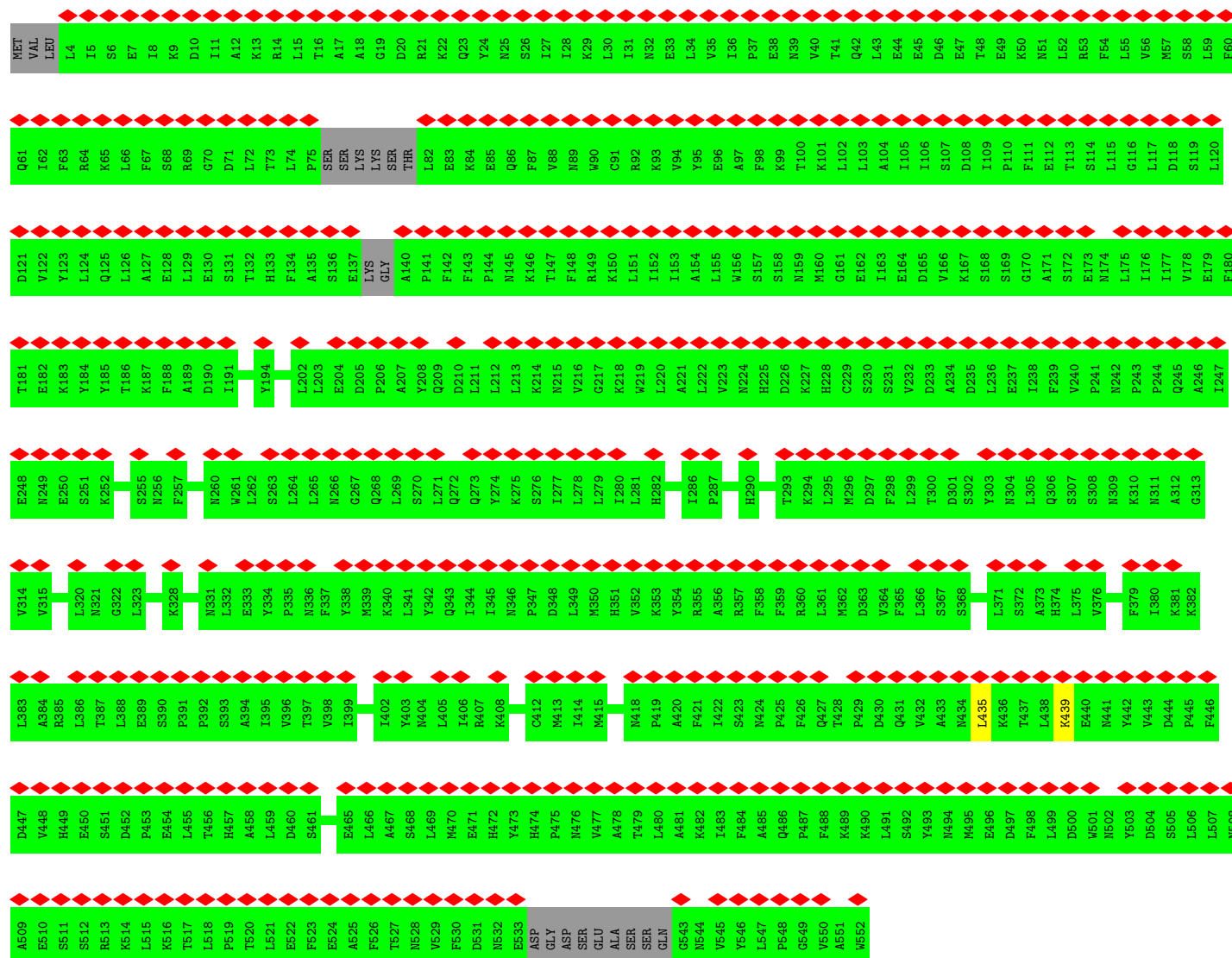






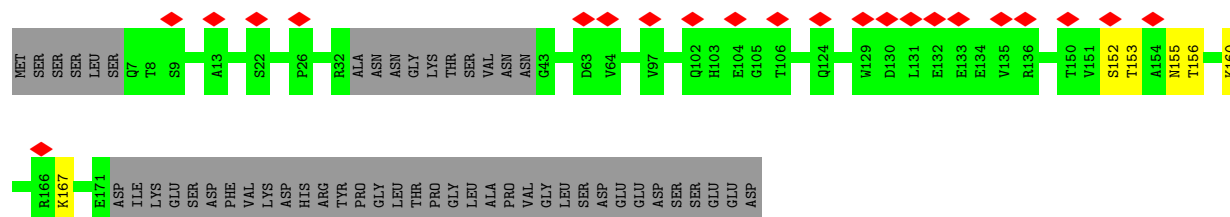
• Molecule 57: Nucleolar complex protein 4

Chain SU: 84% 96%



• Molecule 58: Regulator of rDNA transcription protein 14

Chain SV: 11% 72% 25%













## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19571	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	61.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.411	Depositor
Minimum map value	0.000	Depositor
Average map value	0.102	Depositor
Map value standard deviation	0.184	Depositor
Recommended contour level	0.85	Depositor
Map size (Å)	535.75195, 535.75195, 535.75195	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.063, 1.063, 1.063	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, MG, ADP, M7G, ZN, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	L0	0.11	0/1605	0.23	0/2494
2	L1	0.14	0/33109	0.27	0/51556
3	L2	0.11	0/4868	0.23	0/7561
4	L3	0.40	1/872 (0.1%)	0.64	3/1173 (0.3%)
5	L4	0.15	0/1977	0.32	0/2664
6	L5	0.15	0/1655	0.34	0/2237
7	L6	0.15	0/1764	0.31	0/2359
8	L7	0.17	0/1451	0.41	0/1956
9	L8	0.16	0/1371	0.32	0/1833
10	L9	0.16	0/1495	0.33	0/2003
11	LC	0.19	0/1015	0.47	0/1367
12	LD	0.17	0/1138	0.33	0/1533
13	LE	0.17	0/1039	0.38	0/1395
14	LF	0.17	0/1060	0.33	0/1412
15	LG	0.16	0/492	0.37	0/659
16	LH	0.15	0/6412	0.36	0/8696
17	LI	0.20	1/3835 (0.0%)	0.40	2/5263 (0.0%)
18	LJ	0.13	0/3851	0.32	0/5221
19	LK	0.16	0/1085	0.37	0/1463
20	LL	0.14	0/3939	0.30	0/5341
21	LM	0.12	0/8039	0.30	0/11253
22	LN	0.13	0/5359	0.30	0/7255
23	LO	0.13	0/6463	0.31	0/8748
24	LQ	0.15	0/6620	0.36	2/8936 (0.0%)
25	LR	0.14	0/6313	0.33	0/8551
26	LS	0.15	0/3233	0.33	0/4398
27	LT	0.14	0/6033	0.33	0/8205
28	LZ	0.15	0/1194	0.34	0/1610
29	NA	0.13	0/2442	0.30	0/3281
30	NB	0.13	0/1654	0.31	0/2243
31	ND	0.12	0/568	0.29	0/755
32	NF	0.13	0/1158	0.30	0/1559



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	NG	0.15	0/952	0.30	0/1279
34	NL	0.16	0/2329	0.35	0/3144
35	NM	0.12	0/1853	0.28	0/2484
36	NP	0.12	0/1056	0.29	0/1416
37	NQ	0.14	0/605	0.36	0/817
38	NS	0.14	0/5100	0.39	1/7072 (0.0%)
39	NV	0.23	0/151	0.53	0/196
40	OH	0.10	0/595	0.31	0/827
41	OU	0.15	0/278	0.37	0/386
42	SA	0.14	0/3146	0.30	0/4240
43	SB	0.15	0/3293	0.33	0/4436
44	SC	0.16	0/1903	0.37	0/2567
44	SD	0.14	0/1885	0.34	0/2543
45	SE	0.17	0/928	0.40	0/1262
45	SF	0.16	0/928	0.37	0/1262
46	SG	0.13	0/3744	0.29	0/5040
47	SH	0.15	0/2832	0.32	0/3825
48	SI	0.16	0/6526	0.33	0/8778
49	SJ	0.41	1/1080 (0.1%)	0.59	3/1508 (0.2%)
49	SK	0.11	0/1170	0.28	0/1639
50	SL	0.18	0/1193	0.34	0/1611
51	SM	0.16	0/2046	0.32	0/2759
52	SP	0.12	0/15404	0.29	0/20833
53	SQ	0.17	0/853	0.40	0/1139
54	SR	0.15	0/1069	0.33	0/1427
55	SS	0.15	0/1024	0.39	0/1348
56	ST	0.12	0/3361	0.30	0/4615
57	SU	0.10	0/2726	0.29	0/3825
58	SV	0.12	0/854	0.34	0/1175
59	SW	0.14	0/1682	0.32	0/2264
60	SY	0.15	0/1736	0.36	0/2292
61	SZ	0.11	0/1326	0.28	0/1859
All	All	0.15	3/196737 (0.0%)	0.32	11/274848 (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
38	NS	0	1

All (3) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	SJ	185	PRO	CG-CD	-12.28	1.09	1.50
4	L3	82	PRO	CG-CD	-9.85	1.17	1.50
17	LI	298	PRO	CG-CD	-7.26	1.32	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	SJ	185	PRO	N-CD-CG	-15.08	80.58	103.20
4	L3	82	PRO	N-CD-CG	-12.68	84.18	103.20
17	LI	298	PRO	CA-N-CD	-11.05	96.03	111.50
17	LI	298	PRO	N-CD-CG	-10.20	91.56	103.80
49	SJ	185	PRO	CA-CB-CG	-9.18	87.06	104.50
24	LQ	334	SER	CA-C-N	8.57	132.62	120.28
24	LQ	334	SER	C-N-CA	8.57	132.62	120.28
49	SJ	185	PRO	CA-N-CD	-7.47	101.55	112.00
4	L3	82	PRO	CA-N-CD	-7.34	101.72	112.00
4	L3	82	PRO	CA-CB-CG	-6.96	91.28	104.50
38	NS	428	LEU	N-CA-C	6.82	121.61	111.04

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
38	NS	427	PHE	Peptide

## 5.2 Too-close contacts ⓘ

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	L0	1437	0	722	8	0
2	L1	29608	0	14913	180	0
3	L2	4394	0	2229	17	0
4	L3	862	0	900	15	0
5	L4	1936	0	2019	19	0
6	L5	1635	0	1697	27	0
7	L6	1740	0	1835	34	0
8	L7	1427	0	1499	30	0
9	L8	1348	0	1366	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	L9	1470	0	1554	14	0
11	LC	997	0	1054	23	0
12	LD	1112	0	1179	12	0
13	LE	1022	0	1060	15	0
14	LF	1046	0	1114	13	0
15	LG	490	0	529	5	0
16	LH	6290	0	6113	115	0
17	LI	3792	0	2859	31	0
18	LJ	3773	0	3761	61	0
19	LK	1068	0	1120	20	0
20	LL	3871	0	3876	46	0
21	LM	8005	0	3679	11	0
22	LN	5263	0	5270	63	0
23	LO	6321	0	6235	96	0
24	LQ	6494	0	6544	152	0
25	LR	6207	0	6247	111	0
26	LS	3172	0	3001	38	0
27	LT	5939	0	5096	60	0
28	LZ	1173	0	1208	17	0
29	NA	2426	0	2263	43	0
30	NB	1645	0	1277	20	0
31	ND	564	0	587	11	0
32	NF	1135	0	1197	9	0
33	NG	941	0	979	15	0
34	NL	2285	0	2359	34	0
35	NM	1828	0	1926	35	0
36	NP	1040	0	1057	12	0
37	NQ	595	0	609	5	0
38	NS	5051	0	2958	21	0
39	NV	149	0	172	5	0
40	OH	594	0	298	1	0
41	OU	278	0	135	0	0
42	SA	3100	0	3084	32	0
43	SB	3255	0	3379	46	0
44	SC	1865	0	1908	33	0
44	SD	1850	0	1889	28	0
45	SE	916	0	964	9	0
45	SF	916	0	964	18	0
46	SG	3672	0	3690	23	0
47	SH	2781	0	2878	19	0
48	SI	6387	0	6575	78	0
49	SJ	1074	0	514	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	SK	1160	0	570	0	0
50	SL	1171	0	1229	15	0
51	SM	2009	0	2027	24	0
52	SP	15102	0	15321	151	0
53	SQ	836	0	840	9	0
54	SR	1052	0	1120	17	0
55	SS	1014	0	1045	25	0
56	ST	3341	0	2155	11	0
57	SU	2703	0	1302	1	0
58	SV	852	0	476	5	0
59	SW	1654	0	1742	22	0
60	SY	1715	0	1789	32	0
61	SZ	1314	0	649	2	0
62	L1	45	0	0	0	0
62	L9	1	0	0	0	0
62	NS	1	0	0	0	0
62	SI	1	0	0	0	0
63	NQ	1	0	0	0	0
63	SL	1	0	0	0	0
64	NS	27	0	12	1	0
65	SI	32	0	12	0	0
All	All	190271	0	160630	1730	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 5.

All (1730) 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)
52:SP:1324:ILE:HD12	52:SP:1363:LEU:HD21	1.44	1.00
59:SW:205:ILE:HD11	59:SW:251:ILE:HD11	1.50	0.94
25:LR:601:ILE:HD11	25:LR:613:LEU:HD11	1.50	0.93
24:LQ:212:VAL:HG22	24:LQ:217:LEU:HD13	1.55	0.88
11:LC:98:ASP:OD2	27:LT:488:ASN:ND2	2.06	0.88
42:SA:11:GLU:OE1	42:SA:13:THR:OG1	1.91	0.87
47:SH:302:VAL:HG11	47:SH:329:ILE:HD11	1.54	0.87
48:SI:137:LEU:HD13	48:SI:230:MET:HE1	1.56	0.87
2:L1:127:G:N7	7:L6:202:ARG:NH2	2.25	0.85
45:SE:32:GLN:OE1	45:SE:103:THR:OG1	1.93	0.85
24:LQ:44:SER:OG	24:LQ:48:ASP:O	1.95	0.84
2:L1:493:U:O2'	2:L1:494:U:OP1	1.94	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:619:A:O4'	48:SI:9:ARG:NH1	2.11	0.84
18:LJ:258:LEU:HD21	18:LJ:272:LEU:HD11	1.58	0.83
2:L1:1086:A:OP2	55:SS:443:LYS:NZ	2.12	0.83
48:SI:833:ARG:NE	54:SR:141:GLU:OE1	2.12	0.82
24:LQ:268:LYS:NZ	24:LQ:289:GLU:OE1	2.11	0.82
24:LQ:283:THR:OG1	24:LQ:330:GLN:O	1.98	0.82
6:L5:35:GLN:O	6:L5:38:THR:OG1	1.98	0.81
52:SP:1272:PHE:O	52:SP:1281:ARG:NH1	2.13	0.81
16:LH:677:THR:OG1	16:LH:692:PHE:O	1.97	0.81
18:LJ:507:MET:HE1	19:LK:502:ARG:HA	1.62	0.81
28:LZ:160:TRP:O	28:LZ:167:LYS:NZ	2.12	0.81
30:NB:555:ASN:OD1	30:NB:558:ASN:ND2	2.13	0.81
2:L1:622:A:O2'	2:L1:1032:G:OP2	1.98	0.80
13:LE:30:SER:OG	13:LE:58:SER:O	1.99	0.80
44:SD:309:TYR:OH	60:SY:127:PHE:O	2.00	0.79
1:L0:5:G:OP2	16:LH:703:LYS:NZ	2.16	0.79
22:LN:469:LEU:O	22:LN:473:THR:OG1	2.00	0.79
2:L1:994:G:OP1	2:L1:1778:G:O2'	2.01	0.79
2:L1:902:G:OP2	33:NG:24:ASN:ND2	2.15	0.78
13:LE:97:ARG:NH2	52:SP:1850:LEU:O	2.17	0.78
52:SP:369:SER:O	52:SP:407:ARG:NH2	2.16	0.78
2:L1:133:U:OP2	52:SP:995:ARG:NH1	2.17	0.78
25:LR:137:THR:O	25:LR:180:ARG:NH2	2.17	0.78
16:LH:435:ASP:O	16:LH:762:TYR:OH	2.00	0.78
55:SS:788:LEU:HD21	59:SW:113:TRP:CD1	2.19	0.78
20:LL:349:ASP:O	20:LL:352:SER:OG	2.01	0.78
52:SP:526:TYR:O	52:SP:560:LYS:NZ	2.16	0.78
14:LF:10:ARG:NH2	14:LF:26:ASP:OD2	2.17	0.78
24:LQ:915:ARG:NH2	25:LR:773:SER:OG	2.17	0.77
29:NA:500:LYS:O	29:NA:508:ARG:NH2	2.17	0.77
46:SG:323:ASP:OD1	46:SG:324:ILE:N	2.17	0.77
18:LJ:467:LEU:HD21	18:LJ:484:MET:HE1	1.65	0.77
26:LS:406:ASP:OD2	26:LS:407:PHE:N	2.17	0.77
17:LI:659:THR:OG1	19:LK:507:ARG:NH2	2.17	0.76
24:LQ:230:LYS:NZ	24:LQ:245:MET:SD	2.57	0.76
25:LR:111:ASP:OD2	25:LR:113:THR:OG1	2.03	0.76
2:L1:327:U:O2'	12:LD:10:GLU:OE2	2.03	0.76
44:SD:258:HIS:NE2	44:SD:296:GLU:OE2	2.19	0.76
46:SG:292:SER:OG	46:SG:294:GLN:OE1	2.04	0.76
6:L5:41:LYS:NZ	6:L5:47:SER:OG	2.19	0.76
16:LH:105:HIS:ND1	16:LH:121:TYR:O	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LS:325:ASP:O	26:LS:330:ASN:ND2	2.19	0.76
2:L1:499:U:OP1	30:NB:604:ARG:NH2	2.19	0.76
29:NA:347:PHE:O	29:NA:349:ARG:NH1	2.19	0.76
2:L1:1524:A:N3	2:L1:1590:G:O2'	2.18	0.75
22:LN:586:THR:OG1	22:LN:588:ASP:OD1	2.03	0.75
24:LQ:6:GLN:NE2	24:LQ:687:THR:O	2.18	0.75
44:SD:87:VAL:O	44:SD:100:ARG:N	2.20	0.75
52:SP:583:LEU:O	52:SP:586:THR:OG1	2.03	0.75
43:SB:152:LEU:HD21	44:SD:205:ARG:HG2	1.69	0.75
46:SG:235:HIS:ND1	46:SG:257:ASP:OD2	2.19	0.75
20:LL:302:ASN:ND2	20:LL:316:ASN:OD1	2.20	0.75
20:LL:185:PRO:O	20:LL:215:TYR:OH	2.04	0.75
28:LZ:53:ASP:OD2	29:NA:447:LYS:NZ	2.20	0.74
1:L0:66:C:OP2	16:LH:422:LYS:NZ	2.19	0.74
2:L1:885:G:N2	33:NG:124:ASP:OD2	2.20	0.74
16:LH:693:ASP:OD1	17:LI:495:ARG:NH1	2.19	0.74
2:L1:1638:G:O2'	29:NA:511:ASN:OD1	2.06	0.74
34:NL:37:HIS:ND1	34:NL:198:PRO:O	2.20	0.74
27:LT:762:LEU:HG	29:NA:417:TYR:CZ	2.22	0.74
2:L1:154:G:O6	14:LF:128:LYS:NZ	2.21	0.74
24:LQ:44:SER:HB2	24:LQ:85:LEU:HD11	1.69	0.73
23:LO:363:ALA:HB1	23:LO:390:VAL:HG23	1.69	0.73
55:SS:375:LYS:O	55:SS:378:THR:OG1	2.05	0.73
26:LS:278:ASP:OD2	26:LS:281:THR:OG1	2.05	0.73
52:SP:365:PHE:O	52:SP:369:SER:OG	2.03	0.73
44:SD:278:SER:O	58:SV:160:LYS:NZ	2.20	0.73
46:SG:342:ARG:O	46:SG:344:ARG:NH1	2.20	0.73
24:LQ:344:THR:OG1	24:LQ:352:GLU:O	2.07	0.73
24:LQ:495:LYS:NZ	24:LQ:531:THR:O	2.21	0.73
48:SI:993:ASP:OD2	60:SY:34:TYR:OH	2.05	0.73
2:L1:749:U:O2	52:SP:1683:ARG:NH2	2.22	0.72
26:LS:359:LYS:NZ	26:LS:407:PHE:O	2.22	0.72
19:LK:394:HIS:ND1	19:LK:405:ASP:OD2	2.21	0.72
2:L1:578:U:OP2	48:SI:874:TYR:OH	2.03	0.72
22:LN:448:THR:OG1	22:LN:475:THR:OG1	2.04	0.72
52:SP:469:GLU:OE2	52:SP:471:ASN:ND2	2.23	0.72
2:L1:1101:G:O2'	13:LE:4:SER:OG	2.06	0.72
47:SH:274:LYS:O	47:SH:278:GLN:N	2.23	0.72
24:LQ:471:ALA:O	24:LQ:498:LYS:NZ	2.23	0.72
31:ND:178:VAL:HG23	60:SY:143:MET:HE1	1.71	0.72
22:LN:580:LYS:NZ	22:LN:596:MET:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SP:1586:ILE:HD11	52:SP:1623:LEU:HD11	1.72	0.71
52:SP:1428:THR:OG1	52:SP:1431:PHE:O	2.06	0.71
2:L1:163:G:OP2	2:L1:163:G:N2	2.20	0.71
56:ST:482:GLN:O	56:ST:486:LYS:N	2.24	0.71
45:SE:62:GLU:HA	45:SE:65:LEU:HD13	1.72	0.71
2:L1:912:U:O2'	35:NM:15:GLY:O	2.06	0.71
29:NA:341:LEU:HD13	48:SI:960:ARG:HD2	1.73	0.71
2:L1:575:C:OP1	48:SI:933:LYS:NZ	2.15	0.70
2:L1:334:G:O6	9:L8:5:ARG:NH2	2.24	0.70
18:LJ:248:ARG:NH2	18:LJ:289:ASN:O	2.24	0.70
23:LO:312:GLN:NE2	23:LO:313:THR:HG23	2.06	0.70
24:LQ:634:SER:OG	24:LQ:636:ASP:OD1	2.08	0.70
20:LL:123:SER:O	20:LL:141:ARG:NH1	2.25	0.70
23:LO:16:ARG:NH2	23:LO:699:GLU:O	2.24	0.70
27:LT:608:THR:OG1	27:LT:610:ARG:NH1	2.25	0.70
28:LZ:166:ILE:O	28:LZ:169:THR:OG1	2.09	0.70
30:NB:63:VAL:HG21	60:SY:98:LEU:HD11	1.73	0.70
52:SP:493:ASN:ND2	52:SP:525:ILE:O	2.24	0.70
1:L0:63:G:N7	16:LH:223:LYS:NZ	2.38	0.70
16:LH:503:ASP:OD2	16:LH:571:GLN:NE2	2.25	0.70
43:SB:219:SER:OG	43:SB:220:GLU:OE1	2.08	0.70
43:SB:276:LEU:HD23	43:SB:280:MET:HE2	1.72	0.70
26:LS:530:LEU:HD22	26:LS:532:MET:HE3	1.73	0.69
2:L1:619:A:O5'	48:SI:9:ARG:NH1	2.26	0.69
11:LC:8:GLN:HE21	11:LC:19:VAL:HG23	1.56	0.69
23:LO:73:ILE:HD13	23:LO:102:VAL:HG11	1.74	0.69
43:SB:310:ALA:O	43:SB:372:ARG:NH1	2.26	0.69
2:L1:71:A:OP2	7:L6:164:LYS:NZ	2.24	0.69
3:L2:82:G:O2'	3:L2:83:A:OP2	2.11	0.69
26:LS:429:TYR:O	26:LS:448:LYS:NZ	2.26	0.69
54:SR:74:VAL:HG11	54:SR:104:LEU:HD11	1.73	0.69
2:L1:110:U:OP1	2:L1:753:A:O2'	2.11	0.69
6:L5:38:THR:OG1	6:L5:39:GLU:OE1	2.10	0.69
24:LQ:641:TYR:O	24:LQ:650:ILE:N	2.25	0.69
27:LT:459:ASP:OD2	27:LT:497:LYS:NZ	2.18	0.69
16:LH:107:ILE:HD11	16:LH:119:LEU:HD11	1.75	0.68
18:LJ:507:MET:HE2	18:LJ:507:MET:N	2.07	0.68
25:LR:271:ASP:OD2	25:LR:278:LEU:HD11	1.93	0.68
18:LJ:79:ARG:NH2	18:LJ:114:ARG:O	2.25	0.68
2:L1:1615:C:OP2	6:L5:81:ARG:NH1	2.26	0.68
20:LL:18:CYS:SG	20:LL:65:TRP:NE1	2.66	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SM:243:GLU:OE1	51:SM:243:GLU:N	2.27	0.68
52:SP:643:LYS:NZ	52:SP:683:ASP:OD2	2.26	0.68
43:SB:319:ILE:HD12	43:SB:326:LEU:HD22	1.74	0.68
16:LH:724:ILE:HG21	16:LH:762:TYR:CD2	2.29	0.68
1:L0:90:G:O4'	26:LS:319:ARG:NH2	2.27	0.68
24:LQ:347:SER:OG	24:LQ:350:LYS:O	2.12	0.68
30:NB:28:ASP:OD2	30:NB:32:LYS:NZ	2.26	0.68
23:LO:567:ASP:OD1	23:LO:576:ARG:NH2	2.27	0.68
23:LO:673:ARG:NH1	29:NA:451:LEU:O	2.27	0.68
48:SI:244:MET:HG2	48:SI:812:MET:HE3	1.76	0.68
53:SQ:119:ARG:HD3	53:SQ:174:LEU:HD22	1.76	0.68
2:L1:1638:G:OP2	25:LR:751:LYS:NZ	2.28	0.67
16:LH:16:SER:OG	16:LH:465:ASN:OD1	2.11	0.67
3:L2:245:U:O4	3:L2:246:A:N6	2.28	0.67
6:L5:133:VAL:HG22	6:L5:198:LEU:HD11	1.76	0.67
17:LI:538:ARG:NE	17:LI:539:ASN:OD1	2.28	0.67
4:L3:60:GLU:OE1	18:LJ:60:SER:OG	2.12	0.67
30:NB:598:ILE:HG12	44:SC:156:MET:HE1	1.76	0.67
46:SG:326:GLU:OE2	46:SG:548:ARG:NH1	2.28	0.67
31:ND:182:SER:O	44:SD:294:ARG:NH2	2.28	0.67
5:L4:141:THR:OG1	5:L4:143:ASP:OD1	2.12	0.67
2:L1:761:G:O2'	10:L9:72:GLU:OE2	2.09	0.66
17:LI:676:TRP:O	19:LK:483:LYS:NZ	2.28	0.66
30:NB:598:ILE:N	44:SC:104:ASP:OD2	2.28	0.66
35:NM:87:ARG:NH1	35:NM:100:PHE:O	2.27	0.66
2:L1:1136:U:OP1	24:LQ:596:ASN:ND2	2.28	0.66
3:L2:169:A:OP2	46:SG:180:LYS:NZ	2.23	0.66
23:LO:710:ILE:HG23	27:LT:596:GLU:OE1	1.95	0.66
24:LQ:79:PRO:O	24:LQ:657:GLN:NE2	2.28	0.66
34:NL:257:THR:HG23	38:NS:126:LEU:HD22	1.75	0.66
3:L2:323:G:O2'	60:SY:112:GLN:OE1	2.13	0.66
22:LN:287:THR:HG23	22:LN:336:ILE:HG23	1.76	0.66
2:L1:550:A:OP2	60:SY:3:LYS:NZ	2.27	0.66
35:NM:82:ARG:NH2	35:NM:191:GLU:OE2	2.29	0.66
47:SH:173:LEU:O	47:SH:364:LYS:NZ	2.29	0.66
51:SM:239:VAL:HG23	56:ST:9:LEU:HD23	1.77	0.66
2:L1:187:G:O2'	52:SP:1100:GLN:NE2	2.29	0.66
18:LJ:50:GLN:NE2	18:LJ:91:SER:O	2.28	0.66
24:LQ:580:ASP:OD1	24:LQ:581:ILE:N	2.28	0.66
35:NM:28:GLU:OE2	35:NM:94:LYS:NZ	2.23	0.66
12:LD:101:GLU:OE2	54:SR:13:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LL:115:ASN:OD1	20:LL:131:LEU:N	2.29	0.66
23:LO:845:THR:OG1	24:LQ:903:GLN:NE2	2.29	0.66
24:LQ:588:ILE:HG23	24:LQ:602:LEU:HD11	1.78	0.66
2:L1:1482:C:O2'	11:LC:72:GLY:O	2.11	0.66
25:LR:544:TYR:O	38:NS:247:ASN:ND2	2.28	0.66
20:LL:153:ILE:HG22	20:LL:163:LEU:HD22	1.77	0.65
21:LM:778:SER:O	21:LM:782:VAL:N	2.30	0.65
27:LT:646:VAL:HG13	27:LT:647:THR:HG23	1.78	0.65
27:LT:762:LEU:HG	29:NA:417:TYR:CE1	2.31	0.65
55:SS:374:ARG:O	55:SS:378:THR:HG23	1.95	0.65
52:SP:717:GLN:NE2	52:SP:718:PRO:O	2.30	0.65
48:SI:261:GLN:O	48:SI:264:GLN:NE2	2.29	0.65
24:LQ:592:SER:OG	24:LQ:594:ASP:OD1	2.12	0.65
38:NS:444:MET:O	38:NS:511:SER:N	2.30	0.65
16:LH:27:SER:OG	16:LH:171:TYR:OH	2.14	0.65
30:NB:606:VAL:N	44:SC:302:GLU:OE1	2.29	0.65
35:NM:191:GLU:OE1	35:NM:194:ASN:ND2	2.30	0.65
6:L5:94:THR:HG22	6:L5:114:ILE:HG13	1.79	0.65
19:LK:421:LEU:HD21	19:LK:462:LEU:HD12	1.79	0.65
52:SP:303:ASN:OD1	52:SP:342:ARG:NH1	2.29	0.65
52:SP:894:ASP:OD1	52:SP:932:ARG:NH2	2.30	0.65
2:L1:1555:A:O2'	2:L1:1556:A:O5'	2.14	0.65
24:LQ:330:GLN:OE1	24:LQ:367:ILE:HG21	1.97	0.65
32:NF:83:GLU:OE1	32:NF:84:ILE:HG23	1.96	0.65
52:SP:264:THR:O	52:SP:313:ARG:NH1	2.29	0.65
34:NL:252:GLU:OE2	34:NL:256:LYS:NZ	2.29	0.65
16:LH:753:LYS:NZ	17:LI:430:LEU:O	2.20	0.64
27:LT:459:ASP:O	27:LT:481:ASN:ND2	2.30	0.64
2:L1:902:G:N1	33:NG:51:ASP:OD2	2.30	0.64
33:NG:31:THR:OG1	33:NG:37:GLU:O	2.08	0.64
44:SD:310:GLU:OE1	44:SD:313:HIS:ND1	2.30	0.64
4:L3:16:ARG:NH2	4:L3:19:ASN:OD1	2.30	0.64
25:LR:425:ASP:OD1	25:LR:426:ILE:N	2.31	0.64
45:SF:62:GLU:OE2	46:SG:452:SER:OG	2.14	0.64
5:L4:212:ASP:OD1	5:L4:216:ASN:N	2.30	0.64
35:NM:127:VAL:HG23	35:NM:176:VAL:HG11	1.79	0.64
25:LR:749:ASN:ND2	29:NA:511:ASN:OD1	2.31	0.64
52:SP:452:ASN:C	52:SP:452:ASN:HD22	2.05	0.64
52:SP:871:ASP:OD1	52:SP:889:LYS:NZ	2.30	0.64
48:SI:549:ILE:HD13	48:SI:567:TRP:NE1	2.12	0.64
4:L3:27:LYS:NZ	4:L3:54:LEU:O	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:714:ASP:OD1	16:LH:715:GLU:N	2.31	0.64
36:NP:16:ASN:OD1	36:NP:56:LYS:NZ	2.31	0.64
22:LN:258:SER:OG	22:LN:282:ASP:OD1	2.07	0.64
25:LR:218:ASP:OD2	25:LR:241:GLN:N	2.30	0.64
2:L1:25:C:O2'	2:L1:26:A:OP2	2.16	0.64
2:L1:1609:U:O2'	6:L5:105:GLY:O	2.11	0.64
16:LH:726:GLN:NE2	16:LH:736:THR:O	2.31	0.64
36:NP:38:LYS:O	36:NP:39:THR:OG1	2.12	0.64
48:SI:1105:ASP:OD1	48:SI:1106:GLU:N	2.31	0.64
52:SP:315:LEU:O	52:SP:319:THR:HG23	1.98	0.64
2:L1:802:G:OP1	52:SP:1685:SER:OG	2.09	0.63
44:SD:264:GLN:OE1	44:SD:319:ARG:NH1	2.30	0.63
46:SG:157:LEU:HD11	46:SG:189:THR:HB	1.79	0.63
3:L2:256:G:OP1	42:SA:382:LYS:NZ	2.31	0.63
13:LE:81:VAL:O	13:LE:122:SER:OG	2.16	0.63
27:LT:62:ASP:O	27:LT:66:LEU:N	2.29	0.63
60:SY:97:LYS:O	60:SY:101:THR:HG22	1.98	0.63
2:L1:428:A:N3	2:L1:440:U:O2'	2.26	0.63
3:L2:9:A:O3'	54:SR:40:SER:OG	2.04	0.63
2:L1:227:U:O3'	52:SP:1522:GLN:NE2	2.32	0.63
16:LH:74:LEU:HD21	16:LH:117:ILE:HD13	1.79	0.63
24:LQ:550:LEU:HD12	24:LQ:556:LYS:HZ1	1.64	0.63
35:NM:29:TRP:O	35:NM:94:LYS:NZ	2.29	0.63
51:SM:101:SER:O	51:SM:116:ARG:NH1	2.32	0.63
60:SY:7:ASP:OD1	60:SY:8:VAL:N	2.30	0.63
2:L1:931:C:H1'	35:NM:120:LEU:HD13	1.81	0.63
8:L7:46:ILE:HD13	8:L7:60:ILE:HD13	1.81	0.63
24:LQ:653:LEU:HD13	24:LQ:684:TRP:CH2	2.34	0.63
48:SI:56:VAL:HG22	54:SR:52:ILE:HD12	1.81	0.63
52:SP:1793:LEU:HD12	52:SP:1871:PHE:CD2	2.32	0.63
2:L1:1787:C:OP1	33:NG:127:ARG:NH2	2.31	0.63
18:LJ:34:GLN:OE1	18:LJ:71:ARG:NH2	2.32	0.63
18:LJ:54:ASP:OD2	18:LJ:111:TYR:OH	2.13	0.63
20:LL:482:GLU:OE2	20:LL:522:THR:OG1	2.16	0.63
2:L1:1096:C:N4	13:LE:69:LEU:O	2.30	0.63
2:L1:1632:C:O2'	23:LO:422:PHE:O	2.08	0.63
3:L2:282:U:O2'	3:L2:284:U:O5'	2.17	0.63
24:LQ:134:THR:OG1	24:LQ:149:ASP:OD1	2.16	0.63
24:LQ:397:ILE:HD12	24:LQ:673:VAL:HG23	1.79	0.63
25:LR:92:THR:HG22	25:LR:94:LYS:HE2	1.81	0.63
51:SM:162:THR:OG1	51:SM:264:GLY:O	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:NB:33:ARG:NH2	51:SM:13:LEU:HD13	2.14	0.62
16:LH:262:MET:HE1	16:LH:273:VAL:HG13	1.81	0.62
28:LZ:86:GLY:O	28:LZ:109:ARG:NH2	2.32	0.62
44:SD:123:ILE:O	44:SD:141:TYR:N	2.32	0.62
48:SI:101:ILE:O	48:SI:102:GLN:NE2	2.32	0.62
52:SP:29:GLU:OE1	52:SP:32:ARG:N	2.32	0.62
48:SI:43:MET:HE1	54:SR:38:PHE:CD2	2.35	0.62
58:SV:152:SER:O	58:SV:153:THR:OG1	2.10	0.62
17:LI:599:MET:HE1	17:LI:640:LEU:HB3	1.80	0.62
21:LM:1594:PHE:O	21:LM:1598:LEU:N	2.32	0.62
17:LI:675:LEU:HD11	19:LK:453:PRO:HB3	1.81	0.62
23:LO:430:ARG:NH2	28:LZ:80:ASP:OD2	2.32	0.62
24:LQ:538:ARG:NH2	24:LQ:580:ASP:OD1	2.32	0.62
25:LR:356:ALA:HA	25:LR:391:LEU:HD23	1.79	0.62
44:SC:110:ASN:OD1	44:SC:112:ALA:N	2.31	0.62
52:SP:137:ASP:O	52:SP:140:ILE:HG22	2.00	0.62
52:SP:1786:GLN:OE1	52:SP:1863:LEU:HD21	1.99	0.62
2:L1:1584:G:O2'	2:L1:1585:U:OP2	2.15	0.62
35:NM:59:ASP:OD1	35:NM:60:ALA:N	2.32	0.62
47:SH:337:VAL:N	48:SI:554:TYR:OH	2.32	0.62
22:LN:205:CYS:SG	22:LN:211:ARG:NH1	2.73	0.62
50:SL:138:ASP:OD1	55:SS:435:ARG:NH2	2.33	0.62
2:L1:573:C:OP2	60:SY:11:LYS:NZ	2.32	0.62
2:L1:918:U:O2'	33:NG:35:GLY:O	2.15	0.62
2:L1:1645:G:OP1	56:ST:25:LYS:NZ	2.23	0.62
11:LC:31:VAL:HG12	11:LC:67:VAL:HB	1.81	0.62
13:LE:51:GLU:OE1	13:LE:52:TYR:N	2.33	0.62
17:LI:668:ILE:HD11	19:LK:448:GLU:OE2	2.00	0.62
48:SI:826:LYS:NZ	48:SI:923:ASP:OD2	2.25	0.62
20:LL:248:THR:OG1	20:LL:250:ASP:OD1	2.09	0.62
35:NM:30:PHE:N	35:NM:46:THR:O	2.32	0.62
42:SA:70:SER:O	44:SC:229:LYS:NZ	2.33	0.62
44:SD:304:LEU:HD13	60:SY:133:HIS:CD2	2.34	0.62
17:LI:655:LEU:O	19:LK:507:ARG:NH2	2.32	0.62
27:LT:894:ASP:OD1	27:LT:895:VAL:N	2.33	0.62
14:LF:27:VAL:HG11	14:LF:35:VAL:HG21	1.81	0.61
24:LQ:550:LEU:HD12	24:LQ:556:LYS:NZ	2.15	0.61
34:NL:257:THR:CG2	38:NS:126:LEU:HD22	2.29	0.61
35:NM:124:ASN:C	35:NM:124:ASN:HD22	2.05	0.61
45:SF:120:LYS:O	45:SF:123:THR:OG1	2.18	0.61
52:SP:905:LEU:HD12	52:SP:956:PHE:HE2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SW:205:ILE:HD11	59:SW:251:ILE:CD1	2.28	0.61
16:LH:722:LEU:HD23	16:LH:723:VAL:N	2.14	0.61
20:LL:494:ARG:HG3	20:LL:498:LEU:HD13	1.81	0.61
23:LO:721:VAL:HG13	23:LO:741:MET:HG3	1.82	0.61
25:LR:537:TRP:N	25:LR:551:SER:O	2.33	0.61
25:LR:804:TYR:OH	27:LT:924:ASP:OD1	2.19	0.61
33:NG:66:ASP:OD1	33:NG:70:LYS:NZ	2.25	0.61
8:L7:17:GLU:HG2	8:L7:46:ILE:HG22	1.82	0.61
24:LQ:584:ASP:O	24:LQ:585:SER:OG	2.15	0.61
54:SR:27:ASN:OD1	54:SR:28:ASN:N	2.33	0.61
25:LR:576:ASN:HB3	25:LR:595:ALA:HB3	1.81	0.61
2:L1:537:G:OP1	10:L9:175:ARG:NH2	2.34	0.61
43:SB:115:ASP:OD1	44:SD:322:ARG:NH2	2.34	0.61
47:SH:289:VAL:O	47:SH:317:GLN:NE2	2.34	0.61
52:SP:897:PHE:CZ	52:SP:901:ILE:HD11	2.36	0.61
16:LH:296:HIS:ND1	16:LH:318:GLU:OE1	2.32	0.61
52:SP:1247:LEU:O	52:SP:1251:VAL:HG12	1.99	0.61
2:L1:888:U:O2	2:L1:988:A:O2'	2.18	0.61
18:LJ:504:ILE:HD11	20:LL:503:LYS:HG2	1.83	0.61
8:L7:133:THR:HB	8:L7:154:LEU:HD11	1.82	0.61
18:LJ:153:ASP:OD1	18:LJ:154:ILE:N	2.33	0.61
18:LJ:375:HIS:CE1	26:LS:339:ILE:HD11	2.36	0.61
52:SP:1133:LEU:O	52:SP:1136:THR:OG1	2.16	0.61
16:LH:640:LYS:NZ	16:LH:651:SER:OG	2.34	0.61
17:LI:574:ARG:NH1	17:LI:609:ASN:OD1	2.33	0.61
44:SD:120:GLU:OE2	44:SD:142:ARG:NH2	2.34	0.61
2:L1:1096:C:O4'	13:LE:19:LYS:NZ	2.34	0.61
16:LH:621:LEU:HD13	16:LH:623:PHE:CE1	2.36	0.61
21:LM:390:LEU:O	21:LM:394:LEU:N	2.33	0.61
22:LN:684:GLU:OE1	22:LN:684:GLU:N	2.34	0.61
30:NB:63:VAL:HG21	60:SY:98:LEU:CD1	2.31	0.61
43:SB:3:TYR:OH	43:SB:82:ASP:OD2	2.19	0.61
2:L1:128:U:O4	52:SP:943:ARG:NH1	2.34	0.60
8:L7:17:GLU:CG	8:L7:46:ILE:HG22	2.31	0.60
24:LQ:636:ASP:OD1	24:LQ:638:VAL:HG22	2.00	0.60
44:SD:236:MET:HE3	44:SD:260:PHE:O	2.00	0.60
2:L1:358:U:OP2	38:NS:2:GLY:N	2.35	0.60
16:LH:311:TYR:CE2	26:LS:393:LEU:HD12	2.37	0.60
8:L7:67:LEU:HD22	8:L7:94:ALA:HB2	1.83	0.60
25:LR:235:LYS:NZ	25:LR:273:GLU:O	2.35	0.60
44:SD:89:GLU:OE2	44:SD:100:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SP:1440:LEU:HD13	52:SP:1450:PHE:HB3	1.83	0.60
16:LH:726:GLN:OE1	16:LH:727:GLN:N	2.34	0.60
24:LQ:439:LEU:HD12	24:LQ:444:LEU:HB2	1.83	0.60
25:LR:220:ILE:HD11	25:LR:243:VAL:HG21	1.82	0.60
51:SM:241:THR:HG22	56:ST:13:LEU:HD23	1.83	0.60
16:LH:457:VAL:HB	16:LH:473:LEU:HD11	1.84	0.60
23:LO:564:PHE:N	23:LO:567:ASP:OD2	2.35	0.60
2:L1:904:G:OP1	2:L1:1004:U:O2'	2.14	0.60
2:L1:1143:A:O2'	2:L1:1145:U:OP2	2.16	0.60
23:LO:485:ASN:OD1	23:LO:487:VAL:HG13	2.01	0.60
55:SS:788:LEU:HD22	55:SS:791:TRP:HB3	1.84	0.60
59:SW:204:ARG:NH1	59:SW:250:LEU:O	2.35	0.60
52:SP:311:ILE:HD11	52:SP:343:ILE:HG23	1.84	0.60
16:LH:237:LEU:HD23	16:LH:285:LEU:HD12	1.83	0.60
23:LO:342:GLN:NE2	23:LO:343:GLY:O	2.34	0.60
29:NA:341:LEU:HD11	48:SI:956:MET:SD	2.42	0.60
2:L1:78:A:O2'	7:L6:173:PRO:O	2.19	0.60
11:LC:28:LEU:N	11:LC:64:ASP:OD1	2.33	0.60
43:SB:177:LEU:HD21	43:SB:265:PHE:HB3	1.84	0.60
52:SP:588:ASN:ND2	52:SP:600:THR:OG1	2.34	0.60
52:SP:1763:LEU:N	52:SP:1805:ASP:OD2	2.33	0.60
2:L1:251:A:H2	5:L4:131:LEU:HD12	1.66	0.59
2:L1:934:C:N4	55:SS:391:GLU:O	2.35	0.59
48:SI:1051:ASP:OD1	48:SI:1052:SER:N	2.35	0.59
23:LO:838:THR:O	23:LO:842:ASN:ND2	2.34	0.59
24:LQ:62:LYS:O	24:LQ:111:LYS:NZ	2.34	0.59
48:SI:1079:PHE:CD1	60:SY:67:MET:HE1	2.37	0.59
2:L1:151:G:OP2	14:LF:127:LYS:NZ	2.35	0.59
2:L1:1107:G:OP2	48:SI:18:LYS:NZ	2.33	0.59
8:L7:168:SER:O	8:L7:172:VAL:HG23	2.01	0.59
22:LN:368:ASN:OD1	22:LN:369:TYR:N	2.35	0.59
16:LH:501:THR:OG1	16:LH:503:ASP:OD1	2.19	0.59
29:NA:408:SER:O	29:NA:412:ILE:HD12	2.03	0.59
14:LF:38:ASP:OD1	14:LF:39:GLU:N	2.36	0.59
37:NQ:56:CYS:SG	37:NQ:58:SER:OG	2.60	0.59
46:SG:327:ASP:OD1	46:SG:328:ILE:N	2.35	0.59
52:SP:806:THR:OG1	52:SP:820:THR:OG1	2.08	0.59
23:LO:363:ALA:HB1	23:LO:390:VAL:CG2	2.32	0.59
26:LS:364:GLN:NE2	26:LS:369:ASN:OD1	2.36	0.59
2:L1:1082:C:O2'	2:L1:1083:G:OP1	2.20	0.59
23:LO:485:ASN:O	23:LO:486:SER:OG	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L7:49:ILE:HD11	8:L7:172:VAL:HG22	1.84	0.59
22:LN:345:ASP:OD2	22:LN:360:SER:OG	2.19	0.59
23:LO:726:THR:OG1	23:LO:741:MET:SD	2.56	0.59
42:SA:185:ASP:OD1	42:SA:285:ARG:NE	2.35	0.59
60:SY:32:LYS:O	60:SY:35:VAL:HG12	2.03	0.59
23:LO:779:LEU:HD21	23:LO:821:MET:SD	2.43	0.59
24:LQ:524:HIS:NE2	24:LQ:527:THR:OG1	2.36	0.59
23:LO:739:LEU:HA	23:LO:754:VAL:HG11	1.85	0.58
57:SU:435:LEU:O	57:SU:439:LYS:N	2.35	0.58
27:LT:389:MET:HE1	27:LT:449:ARG:N	2.18	0.58
27:LT:717:ASP:HB3	27:LT:720:LEU:HD23	1.84	0.58
32:NF:62:GLN:HB2	32:NF:65:VAL:HG12	1.83	0.58
34:NL:299:ASP:OD1	34:NL:300:GLN:N	2.35	0.58
2:L1:1584:G:H22	2:L1:1611:A:P	2.27	0.58
3:L2:326:U:OP2	45:SE:42:LYS:NZ	2.33	0.58
16:LH:229:SER:OG	16:LH:232:ASP:O	2.18	0.58
2:L1:1568:C:O2'	2:L1:1569:A:O5'	2.18	0.58
22:LN:595:ASN:N	22:LN:610:VAL:O	2.33	0.58
26:LS:240:ASP:OD1	26:LS:242:ASN:N	2.36	0.58
16:LH:393:ASN:ND2	16:LH:435:ASP:OD2	2.37	0.58
24:LQ:606:ASP:OD1	24:LQ:607:CYS:N	2.37	0.58
2:L1:929:A:OP2	2:L1:931:C:N4	2.33	0.58
6:L5:90:ILE:O	6:L5:94:THR:HG23	2.02	0.58
16:LH:763:ILE:HD12	16:LH:776:PHE:CD2	2.39	0.58
20:LL:88:TYR:OH	20:LL:93:ASN:OD1	2.21	0.58
42:SA:148:GLU:OE2	44:SC:169:LYS:NZ	2.31	0.58
22:LN:681:ILE:HG22	22:LN:683:ASP:H	1.69	0.58
42:SA:256:ARG:NH2	43:SB:50:PHE:O	2.37	0.58
2:L1:1223:A:O2'	56:ST:414:LEU:O	2.21	0.58
34:NL:181:MET:HE1	34:NL:182:TRP:CZ2	2.38	0.58
7:L6:67:VAL:HG21	7:L6:73:ILE:HD11	1.86	0.57
25:LR:603:ASP:O	25:LR:607:GLY:N	2.33	0.57
22:LN:385:ASN:ND2	22:LN:387:GLU:O	2.38	0.57
26:LS:583:GLN:O	26:LS:585:LYS:NZ	2.36	0.57
29:NA:555:ASP:OD1	29:NA:556:THR:N	2.37	0.57
51:SM:75:ASP:OD1	51:SM:76:GLU:N	2.37	0.57
2:L1:1534:G:O2'	2:L1:1536:G:O6	2.22	0.57
24:LQ:843:LYS:NZ	25:LR:706:ARG:O	2.35	0.57
24:LQ:177:LEU:CB	24:LQ:191:LEU:HD21	2.35	0.57
2:L1:1618:C:OP2	23:LO:505:ARG:NH2	2.38	0.57
6:L5:161:ASP:OD1	6:L5:162:VAL:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:31:MET:HE1	22:LN:746:LEU:CD2	2.35	0.57
24:LQ:145:ILE:HD11	24:LQ:166:ILE:HD12	1.86	0.57
24:LQ:618:ILE:HD12	24:LQ:633:CYS:O	2.05	0.57
25:LR:241:GLN:NE2	25:LR:263:GLY:O	2.37	0.57
36:NP:61:VAL:HG13	36:NP:76:LEU:HD11	1.84	0.57
52:SP:1094:PHE:HD2	52:SP:1132:ALA:HB1	1.69	0.57
2:L1:359:A:C5	48:SI:39:MET:HE1	2.40	0.57
2:L1:1152:A:O2'	24:LQ:813:ARG:NH2	2.38	0.57
17:LI:650:LEU:HD12	17:LI:655:LEU:HD11	1.86	0.57
22:LN:314:SER:O	22:LN:318:ASN:N	2.37	0.57
27:LT:846:ASP:OD1	27:LT:847:LEU:N	2.37	0.57
52:SP:1436:ASP:OD2	52:SP:1480:SER:OG	2.18	0.57
22:LN:529:ASN:O	22:LN:545:ARG:NH1	2.37	0.57
29:NA:335:ARG:NH1	48:SI:957:GLU:OE2	2.38	0.57
52:SP:1449:ASP:O	52:SP:1453:ASN:ND2	2.36	0.57
2:L1:994:G:N2	38:NS:134:GLY:O	2.38	0.57
23:LO:195:MET:HE1	23:LO:263:VAL:HG12	1.87	0.57
50:SL:83:VAL:HG21	50:SL:124:ARG:HE	1.69	0.57
59:SW:161:ALA:HB1	59:SW:166:PHE:HD2	1.69	0.57
27:LT:807:VAL:HG21	38:NS:1197:GLN:O	2.04	0.56
2:L1:1064:G:O2'	35:NM:204:ILE:O	2.23	0.56
15:LG:12:VAL:HG22	15:LG:30:VAL:HG12	1.87	0.56
18:LJ:434:ARG:NH2	18:LJ:438:THR:OG1	2.38	0.56
25:LR:667:GLN:OE1	25:LR:671:ASN:ND2	2.31	0.56
34:NL:261:MET:HE1	38:NS:122:ILE:HG21	1.87	0.56
45:SF:64:LEU:HD12	45:SF:67:LEU:HD12	1.87	0.56
52:SP:319:THR:HG22	52:SP:361:LEU:HB2	1.87	0.56
2:L1:60:U:OP2	52:SP:12:LYS:NZ	2.21	0.56
6:L5:49:GLU:N	6:L5:49:GLU:OE1	2.38	0.56
43:SB:14:LEU:HD13	43:SB:79:ILE:HD12	1.88	0.56
44:SC:156:MET:HA	44:SC:156:MET:HE3	1.87	0.56
55:SS:385:GLU:OE2	55:SS:389:ARG:NE	2.37	0.56
22:LN:512:GLU:OE2	22:LN:560:SER:N	2.37	0.56
24:LQ:202:ALA:O	24:LQ:203:HIS:ND1	2.39	0.56
26:LS:335:GLN:HG2	26:LS:336:THR:HG23	1.87	0.56
30:NB:64:LEU:O	60:SY:207:ARG:NH2	2.36	0.56
44:SC:303:GLN:OE1	50:SL:148:HIS:NE2	2.35	0.56
46:SG:503:ASP:OD1	46:SG:504:ASN:N	2.39	0.56
51:SM:235:GLN:NE2	51:SM:251:GLY:O	2.38	0.56
52:SP:1375:ILE:HD12	52:SP:1424:MET:SD	2.45	0.56
9:L8:36:THR:OG1	9:L8:57:ALA:O	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LR:382:GLU:OE1	25:LR:384:TYR:OH	2.23	0.56
26:LS:532:MET:HE1	26:LS:544:VAL:HG23	1.87	0.56
47:SH:67:ILE:O	56:ST:115:LYS:NZ	2.37	0.56
18:LJ:268:MET:HE1	18:LJ:293:LYS:HG3	1.86	0.56
25:LR:561:SER:O	25:LR:565:PHE:N	2.37	0.56
2:L1:858:G:OP1	32:NF:73:ARG:NH1	2.39	0.56
2:L1:1124:A:N6	3:L2:0:M7G:H2'	2.20	0.56
42:SA:66:ALA:HA	44:SC:232:MET:HE1	1.87	0.56
52:SP:183:HIS:CD2	52:SP:188:LEU:HD12	2.41	0.56
2:L1:1773:C:OP1	48:SI:10:LYS:NZ	2.30	0.56
23:LO:423:ARG:NH1	23:LO:460:VAL:O	2.39	0.56
24:LQ:338:ILE:CG1	24:LQ:355:LEU:HD13	2.36	0.56
48:SI:56:VAL:HG23	54:SR:101:GLU:HG3	1.86	0.56
2:L1:886:U:OP2	35:NM:216:LYS:NZ	2.39	0.56
22:LN:426:GLN:OE1	31:ND:190:LEU:HD21	2.06	0.56
23:LO:608:ASN:ND2	27:LT:513:MET:SD	2.79	0.56
25:LR:85:LEU:HD11	25:LR:119:VAL:HG21	1.87	0.56
27:LT:743:ARG:NH1	29:NA:486:ASN:OD1	2.39	0.56
28:LZ:153:ASN:OD1	28:LZ:154:MET:N	2.39	0.56
18:LJ:104:LEU:HD12	18:LJ:120:ILE:O	2.06	0.56
22:LN:380:LYS:NZ	22:LN:634:VAL:O	2.39	0.56
23:LO:841:ASP:OD1	23:LO:842:ASN:N	2.39	0.56
43:SB:55:ASN:ND2	43:SB:59:GLU:OE1	2.38	0.56
2:L1:93:A:O4'	5:L4:3:ARG:NH1	2.38	0.55
2:L1:330:G:OP2	9:L8:172:ARG:NH1	2.39	0.55
7:L6:5:ILE:CG2	7:L6:113:ILE:HD11	2.36	0.55
18:LJ:183:LEU:HB3	18:LJ:195:LEU:HD11	1.87	0.55
20:LL:579:GLU:OE2	22:LN:421:THR:OG1	2.19	0.55
24:LQ:535:LEU:HD21	29:NA:591:ILE:HD12	1.88	0.55
43:SB:195:LEU:HD23	43:SB:205:TYR:HE1	1.70	0.55
52:SP:1812:LEU:HD11	52:SP:1886:PHE:HD2	1.70	0.55
2:L1:447:U:O2'	5:L4:27:TYR:O	2.24	0.55
20:LL:523:LEU:O	20:LL:527:HIS:ND1	2.28	0.55
26:LS:526:ASP:OD2	26:LS:528:GLN:NE2	2.39	0.55
27:LT:604:SER:OG	27:LT:606:ASP:OD1	2.20	0.55
16:LH:265:ASP:OD1	16:LH:266:ASN:N	2.39	0.55
16:LH:657:SER:OG	16:LH:674:THR:OG1	2.24	0.55
17:LI:636:GLN:O	17:LI:639:SER:OG	2.20	0.55
21:LM:966:PHE:O	21:LM:970:HIS:N	2.39	0.55
25:LR:135:TYR:OH	59:SW:81:PHE:O	2.18	0.55
25:LR:686:MET:HE3	25:LR:686:MET:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SP:1189:LEU:HD11	52:SP:1198:PHE:CE2	2.42	0.55
2:L1:207:U:O2	9:L8:178:ARG:NH2	2.39	0.55
9:L8:155:SER:O	9:L8:159:GLN:NE2	2.39	0.55
10:L9:58:ASP:O	10:L9:61:THR:OG1	2.24	0.55
29:NA:335:ARG:NH2	48:SI:957:GLU:OE1	2.39	0.55
44:SD:228:GLN:O	44:SD:231:ARG:NH1	2.39	0.55
52:SP:1738:TYR:CE2	52:SP:1745:ILE:HG21	2.42	0.55
7:L6:157:VAL:HG22	7:L6:175:ILE:HD11	1.87	0.55
16:LH:381:SER:OG	20:LL:349:ASP:OD1	2.23	0.55
25:LR:313:LEU:O	25:LR:330:THR:N	2.38	0.55
29:NA:477:GLU:OE1	29:NA:477:GLU:N	2.39	0.55
52:SP:269:GLU:OE2	52:SP:313:ARG:NH2	2.40	0.55
59:SW:124:LEU:HB3	59:SW:126:LEU:HD23	1.87	0.55
5:L4:103:TYR:O	5:L4:182:TYR:OH	2.25	0.55
8:L7:152:VAL:CG2	8:L7:181:ILE:HD11	2.36	0.55
11:LC:8:GLN:NE2	11:LC:19:VAL:HG23	2.20	0.55
24:LQ:171:CYS:HB2	24:LQ:177:LEU:HD13	1.88	0.55
12:LD:98:ASN:C	12:LD:98:ASN:HD22	2.14	0.55
38:NS:398:HIS:O	38:NS:401:MET:N	2.40	0.55
51:SM:124:MET:HA	51:SM:124:MET:HE3	1.89	0.55
16:LH:661:THR:OG1	16:LH:673:ALA:HB3	2.07	0.55
24:LQ:22:ASN:ND2	24:LQ:85:LEU:O	2.38	0.55
28:LZ:118:LEU:CD2	28:LZ:120:MET:HE3	2.37	0.55
43:SB:3:TYR:O	43:SB:88:ILE:N	2.38	0.55
6:L5:207:THR:O	6:L5:212:LYS:NZ	2.39	0.55
11:LC:49:TYR:O	11:LC:53:LEU:N	2.37	0.55
25:LR:89:HIS:O	25:LR:93:GLY:N	2.39	0.55
43:SB:195:LEU:HD23	43:SB:205:TYR:CE1	2.42	0.55
2:L1:1639:C:OP2	29:NA:511:ASN:ND2	2.40	0.54
6:L5:132:VAL:HG12	6:L5:198:LEU:HD23	1.88	0.54
26:LS:512:ASP:O	60:SY:248:ARG:NH2	2.39	0.54
35:NM:138:PHE:O	35:NM:213:ARG:N	2.40	0.54
2:L1:1228:G:OP2	40:OH:45:LEU:N	2.40	0.54
22:LN:363:SER:O	22:LN:367:GLY:N	2.39	0.54
7:L6:6:SER:O	7:L6:113:ILE:HD12	2.07	0.54
18:LJ:32:SER:OG	18:LJ:333:LYS:NZ	2.40	0.54
52:SP:1137:ILE:CG2	52:SP:1185:LEU:HD11	2.37	0.54
9:L8:160:PHE:CD1	9:L8:165:LEU:HD21	2.43	0.54
12:LD:55:ASP:OD2	12:LD:58:CYS:N	2.40	0.54
18:LJ:20:THR:OG1	18:LJ:25:ARG:NH1	2.40	0.54
20:LL:460:ARG:NH2	20:LL:497:PRO:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LO:150:THR:HG22	23:LO:166:LYS:NZ	2.22	0.54
52:SP:1354:PHE:CE2	52:SP:1363:LEU:HD22	2.42	0.54
52:SP:1652:ASP:OD1	52:SP:1655:ARG:NH1	2.41	0.54
16:LH:95:ASP:OD2	16:LH:97:THR:OG1	2.26	0.54
24:LQ:65:ASP:OD1	24:LQ:66:GLY:N	2.40	0.54
25:LR:295:PRO:O	25:LR:296:ILE:HD13	2.07	0.54
25:LR:534:ARG:O	25:LR:552:SER:OG	2.23	0.54
47:SH:285:LYS:NZ	47:SH:316:GLU:OE1	2.41	0.54
50:SL:109:LEU:HD13	55:SS:440:MET:HE2	1.89	0.54
51:SM:288:ASP:OD1	51:SM:289:TYR:N	2.41	0.54
2:L1:1128:C:N4	47:SH:217:LYS:O	2.41	0.54
16:LH:176:LEU:HD11	16:LH:185:PHE:HB3	1.90	0.54
24:LQ:397:ILE:HD11	24:LQ:663:LEU:HA	1.88	0.54
52:SP:481:TRP:HA	52:SP:484:ILE:HD12	1.89	0.54
2:L1:619:A:O2'	55:SS:459:MET:HE1	2.08	0.54
16:LH:298:ASP:OD1	16:LH:299:SER:N	2.37	0.54
24:LQ:134:THR:HG23	24:LQ:135:ARG:HG3	1.88	0.54
52:SP:615:VAL:HG13	52:SP:619:LEU:HD23	1.90	0.54
52:SP:1616:LEU:O	52:SP:1620:VAL:HG23	2.07	0.54
16:LH:362:GLU:HB3	16:LH:454:ILE:HG21	1.89	0.54
24:LQ:653:LEU:HD12	24:LQ:653:LEU:O	2.08	0.54
24:LQ:552:ASP:OD1	24:LQ:554:THR:OG1	2.13	0.54
52:SP:1275:PHE:O	52:SP:1281:ARG:NH2	2.41	0.54
22:LN:151:ASP:OD1	22:LN:152:SER:N	2.41	0.53
22:LN:394:TRP:CG	22:LN:431:CYS:HG	2.27	0.53
29:NA:408:SER:O	29:NA:411:GLU:N	2.39	0.53
42:SA:210:VAL:HG13	42:SA:247:ILE:HG21	1.90	0.53
44:SD:202:ARG:HD2	45:SE:69:LEU:HD11	1.90	0.53
45:SF:71:CYS:O	45:SF:75:ASN:N	2.41	0.53
51:SM:183:SER:O	51:SM:220:ARG:NE	2.41	0.53
2:L1:251:A:C2	5:L4:131:LEU:HD12	2.43	0.53
2:L1:258:C:OP1	52:SP:898:LYS:NZ	2.41	0.53
24:LQ:105:VAL:O	24:LQ:114:LEU:N	2.39	0.53
24:LQ:803:GLN:NE2	24:LQ:803:GLN:O	2.40	0.53
26:LS:231:LYS:HE3	26:LS:231:LYS:HA	1.90	0.53
44:SC:88:ILE:HG21	44:SC:141:TYR:CE2	2.43	0.53
48:SI:918:ILE:HD11	54:SR:144:ARG:NH2	2.23	0.53
7:L6:32:ILE:HD11	7:L6:63:MET:HE3	1.91	0.53
16:LH:112:ASN:OD1	16:LH:113:ASN:N	2.42	0.53
24:LQ:760:ILE:HA	24:LQ:763:ILE:HG22	1.90	0.53
48:SI:38:LYS:O	48:SI:42:THR:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:304:U:O4'	12:LD:127:GLN:NE2	2.41	0.53
2:L1:618:U:O2'	48:SI:6:LYS:NZ	2.41	0.53
2:L1:1499:G:OP1	36:NP:122:ARG:NH1	2.39	0.53
4:L3:10:SER:O	4:L3:12:GLN:NE2	2.40	0.53
13:LE:115:GLU:OE2	13:LE:119:LYS:NZ	2.42	0.53
22:LN:286:LEU:HD21	22:LN:295:VAL:HG13	1.90	0.53
24:LQ:473:ASP:OD1	24:LQ:474:ALA:N	2.40	0.53
34:NL:276:VAL:HG12	34:NL:280:LYS:HD2	1.90	0.53
39:NV:728:ASN:OD1	39:NV:729:LEU:N	2.41	0.53
43:SB:14:LEU:HD11	43:SB:76:LEU:HD23	1.90	0.53
2:L1:1051:G:O2'	2:L1:1052:U:OP1	2.20	0.53
44:SC:88:ILE:HG21	44:SC:141:TYR:HE2	1.74	0.53
60:SY:106:TYR:CE1	60:SY:110:LEU:HD11	2.43	0.53
2:L1:693:U:O2'	8:L7:95:GLU:OE2	2.27	0.53
16:LH:19:LYS:NZ	16:LH:366:ASN:OD1	2.26	0.53
17:LI:522:THR:HG22	17:LI:526:LEU:HD13	1.91	0.53
25:LR:30:LYS:O	25:LR:45:LEU:N	2.39	0.53
52:SP:1545:VAL:HG12	52:SP:1612:ILE:HD11	1.89	0.53
8:L7:166:LEU:HD21	8:L7:185:ILE:HD11	1.90	0.53
16:LH:355:SER:C	16:LH:356:LEU:HD12	2.33	0.53
22:LN:82:ARG:NH2	22:LN:685:SER:O	2.41	0.53
52:SP:1540:GLN:OE1	52:SP:1540:GLN:N	2.41	0.53
4:L3:29:VAL:HG23	4:L3:30:TYR:CD2	2.44	0.53
11:LC:82:ARG:NH2	11:LC:116:LEU:HD11	2.24	0.53
16:LH:352:ASN:OD1	16:LH:353:TYR:N	2.41	0.53
59:SW:154:LYS:NZ	59:SW:177:LEU:O	2.42	0.53
16:LH:401:GLN:NE2	16:LH:409:LYS:O	2.41	0.53
18:LJ:197:ASP:HB2	18:LJ:206:ILE:HD11	1.89	0.53
34:NL:147:PRO:HG3	34:NL:211:ILE:HG21	1.91	0.53
52:SP:1436:ASP:OD1	52:SP:1437:MET:N	2.41	0.53
2:L1:1102:G:OP1	13:LE:76:SER:OG	2.23	0.53
2:L1:1801:A:C5	59:SW:106:MET:HE1	2.44	0.53
23:LO:452:ASN:OD1	23:LO:453:PHE:N	2.42	0.53
52:SP:976:TYR:O	52:SP:980:ASN:ND2	2.42	0.53
23:LO:120:GLN:NE2	23:LO:141:VAL:HG23	2.24	0.52
24:LQ:577:LEU:N	24:LQ:591:SER:O	2.39	0.52
28:LZ:141:ASN:HD21	29:NA:454:VAL:HG21	1.75	0.52
19:LK:420:ILE:O	19:LK:463:LYS:NZ	2.43	0.52
25:LR:316:VAL:O	25:LR:320:LEU:N	2.36	0.52
27:LT:437:GLU:OE2	27:LT:441:ARG:NH2	2.42	0.52
30:NB:594:GLU:OE1	44:SC:309:TYR:OH	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:NL:27:VAL:HG23	34:NL:28:PHE:CD2	2.44	0.52
48:SI:925:ASN:OD1	48:SI:926:ILE:N	2.42	0.52
18:LJ:53:HIS:NE2	18:LJ:311:THR:O	2.43	0.52
18:LJ:83:VAL:HG13	18:LJ:85:TYR:CE2	2.45	0.52
18:LJ:503:ARG:NH1	19:LK:500:GLN:OE1	2.41	0.52
20:LL:51:LEU:HD22	20:LL:88:TYR:CD1	2.45	0.52
24:LQ:338:ILE:HG13	24:LQ:355:LEU:HD13	1.91	0.52
44:SC:104:ASP:C	44:SC:105:LEU:HD12	2.34	0.52
45:SF:38:ASN:OD1	45:SF:39:GLU:N	2.43	0.52
59:SW:216:ILE:O	59:SW:220:THR:HG22	2.09	0.52
16:LH:46:ILE:CD1	16:LH:385:ILE:HG21	2.39	0.52
18:LJ:449:GLY:O	18:LJ:455:SER:OG	2.26	0.52
20:LL:60:VAL:HG22	20:LL:80:MET:HE1	1.90	0.52
22:LN:432:SER:OG	22:LN:478:VAL:O	2.21	0.52
46:SG:569:ASP:OD1	46:SG:570:GLN:N	2.43	0.52
48:SI:43:MET:HE1	54:SR:38:PHE:CG	2.43	0.52
48:SI:131:ILE:HD11	48:SI:809:PRO:HG3	1.91	0.52
2:L1:419:G:O5'	7:L6:72:ARG:NH2	2.42	0.52
2:L1:1157:A:O2'	2:L1:1159:C:OP1	2.20	0.52
22:LN:279:HIS:HD1	22:LN:301:ASP:CG	2.17	0.52
26:LS:570:PHE:CE2	26:LS:577:LEU:HD13	2.45	0.52
43:SB:18:SER:N	43:SB:41:GLU:OE2	2.42	0.52
52:SP:1261:ILE:HD11	52:SP:1295:VAL:HG21	1.91	0.52
7:L6:5:ILE:HG22	7:L6:113:ILE:HD11	1.91	0.52
24:LQ:321:TYR:CZ	24:LQ:325:ILE:HD11	2.45	0.52
27:LT:428:GLU:OE1	27:LT:452:ARG:NH1	2.43	0.52
36:NP:33:TYR:HH	36:NP:99:SER:HG	1.54	0.52
43:SB:1:MET:O	43:SB:86:THR:N	2.41	0.52
52:SP:1308:LEU:HD23	52:SP:1350:THR:HG21	1.92	0.52
11:LC:31:VAL:HG13	11:LC:36:ILE:CD1	2.40	0.52
17:LI:669:ALA:HB1	19:LK:493:LEU:CD1	2.40	0.52
25:LR:12:LEU:HD11	25:LR:378:PRO:HG2	1.91	0.52
27:LT:530:ASP:O	27:LT:534:SER:N	2.41	0.52
51:SM:144:GLU:OE1	51:SM:147:GLY:N	2.42	0.52
7:L6:18:ILE:HG23	7:L6:23:ARG:HD2	1.92	0.52
7:L6:23:ARG:HH11	7:L6:41:VAL:HG12	1.74	0.52
23:LO:389:SER:OG	23:LO:407:LEU:HD12	2.10	0.52
24:LQ:880:ILE:HG23	25:LR:806:LEU:HD12	1.92	0.52
29:NA:554:VAL:HG21	34:NL:21:GLU:OE1	2.09	0.52
52:SP:1062:LEU:O	52:SP:1065:VAL:HG12	2.10	0.52
52:SP:1602:ASP:O	52:SP:1609:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:LQ:320:SER:O	24:LQ:323:SER:OG	2.22	0.52
24:LQ:404:LYS:C	24:LQ:405:LEU:HD12	2.35	0.52
25:LR:691:PRO:O	25:LR:695:PHE:N	2.41	0.52
26:LS:319:ARG:HD3	26:LS:319:ARG:H	1.75	0.52
48:SI:716:ARG:N	48:SI:718:MET:SD	2.83	0.52
52:SP:1586:ILE:HD11	52:SP:1623:LEU:CD1	2.40	0.52
16:LH:262:MET:HA	16:LH:262:MET:HE3	1.92	0.52
16:LH:343:ASP:OD1	16:LH:344:CYS:N	2.43	0.52
24:LQ:157:TYR:OH	24:LQ:191:LEU:HD12	2.08	0.52
29:NA:588:SER:OG	29:NA:592:LYS:NZ	2.43	0.52
44:SD:198:GLU:OE2	44:SD:200:SER:N	2.43	0.52
48:SI:158:ILE:HD11	48:SI:913:ILE:HD12	1.92	0.52
2:L1:1080:U:O2'	2:L1:1082:C:OP1	2.11	0.51
2:L1:1555:A:O2'	2:L1:1556:A:O4'	2.28	0.51
16:LH:675:ARG:NH1	16:LH:698:VAL:HG12	2.25	0.51
20:LL:296:ILE:HG23	20:LL:296:ILE:O	2.10	0.51
23:LO:331:GLU:O	23:LO:335:GLU:N	2.44	0.51
24:LQ:620:ASN:ND2	24:LQ:663:LEU:O	2.42	0.51
42:SA:210:VAL:CG1	42:SA:247:ILE:HG21	2.39	0.51
43:SB:215:ARG:NH1	43:SB:244:GLY:O	2.42	0.51
48:SI:158:ILE:HD11	48:SI:913:ILE:CD1	2.41	0.51
48:SI:956:MET:HE2	48:SI:956:MET:HA	1.92	0.51
2:L1:600:U:O2	48:SI:44:GLN:NE2	2.41	0.51
22:LN:347:LEU:N	22:LN:359:ASN:O	2.42	0.51
24:LQ:254:GLN:CG	24:LQ:277:ALA:HB3	2.41	0.51
24:LQ:834:LYS:NZ	24:LQ:838:THR:OG1	2.43	0.51
24:LQ:867:GLU:OE2	24:LQ:871:GLN:NE2	2.44	0.51
29:NA:507:ILE:O	29:NA:515:MET:N	2.41	0.51
34:NL:251:LEU:HD23	34:NL:281:ILE:HD11	1.92	0.51
42:SA:94:LYS:HE3	42:SA:94:LYS:HA	1.92	0.51
42:SA:152:LEU:HD23	43:SB:243:MET:CE	2.40	0.51
46:SG:241:THR:HG21	46:SG:285:SER:HA	1.90	0.51
2:L1:763:G:N2	2:L1:774:A:N7	2.58	0.51
23:LO:708:ASP:OD1	23:LO:709:THR:N	2.41	0.51
24:LQ:125:THR:N	24:LQ:139:GLY:O	2.42	0.51
24:LQ:177:LEU:HB3	24:LQ:191:LEU:HD21	1.91	0.51
27:LT:19:LYS:N	27:LT:676:MET:SD	2.83	0.51
43:SB:397:ARG:O	43:SB:401:LEU:HD13	2.11	0.51
52:SP:1151:ILE:HG23	52:SP:1201:LEU:HD13	1.90	0.51
16:LH:478:ASN:OD1	16:LH:479:ASN:N	2.42	0.51
16:LH:508:ILE:HD12	16:LH:531:PHE:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:LQ:614:HIS:ND1	24:LQ:638:VAL:HG23	2.25	0.51
42:SA:302:ASN:ND2	42:SA:397:SER:O	2.43	0.51
60:SY:94:ASP:OD1	60:SY:95:GLN:N	2.42	0.51
16:LH:656:ASP:OD1	16:LH:657:SER:N	2.44	0.51
18:LJ:43:THR:O	18:LJ:304:SER:OG	2.28	0.51
22:LN:149:ILE:HD12	22:LN:155:LYS:O	2.10	0.51
24:LQ:134:THR:HG23	24:LQ:135:ARG:CG	2.41	0.51
59:SW:74:ASP:OD1	59:SW:75:ASP:N	2.39	0.51
2:L1:63:G:O2'	2:L1:170:U:OP1	2.29	0.51
11:LC:63:ILE:HD12	11:LC:65:ILE:HD11	1.92	0.51
16:LH:682:ASN:O	16:LH:686:GLY:N	2.42	0.51
23:LO:263:VAL:HG13	23:LO:277:VAL:HG23	1.92	0.51
43:SB:23:TYR:O	43:SB:112:VAL:HG11	2.11	0.51
2:L1:859:A:OP1	32:NF:73:ARG:NH2	2.37	0.51
23:LO:327:LEU:HD22	23:LO:339:LEU:HD22	1.92	0.51
36:NP:65:ILE:HG22	36:NP:124:ILE:HG23	1.93	0.51
61:SZ:444:VAL:O	61:SZ:448:GLY:N	2.43	0.51
2:L1:1599:C:OP2	48:SI:988:ARG:NH2	2.44	0.51
21:LM:895:GLN:O	21:LM:898:LEU:N	2.43	0.51
23:LO:604:TYR:HE1	23:LO:611:LEU:HD13	1.75	0.51
27:LT:883:THR:O	27:LT:886:SER:OG	2.28	0.51
7:L6:31:ARG:NH1	7:L6:68:LEU:HD22	2.26	0.51
16:LH:778:ASP:O	16:LH:781:SER:N	2.44	0.51
17:LI:611:ILE:HG23	17:LI:658:LEU:HD11	1.92	0.51
18:LJ:168:THR:OG1	18:LJ:190:ASP:OD1	2.24	0.51
24:LQ:170:TRP:CE3	24:LQ:178:ILE:HD12	2.46	0.51
35:NM:124:ASN:C	35:NM:124:ASN:ND2	2.69	0.51
48:SI:1099:ALA:H	60:SY:101:THR:HG21	1.75	0.51
2:L1:434:G:N1	48:SI:56:VAL:O	2.41	0.51
2:L1:1169:G:N1	2:L1:1575:G:OP2	2.38	0.51
25:LR:342:ASP:OD1	25:LR:343:MET:N	2.43	0.51
25:LR:534:ARG:HE	25:LR:535:GLY:H	1.59	0.51
48:SI:775:GLU:OE1	48:SI:775:GLU:N	2.42	0.51
9:L8:195:ARG:NH2	12:LD:10:GLU:O	2.44	0.50
12:LD:98:ASN:O	12:LD:98:ASN:ND2	2.35	0.50
44:SC:305:THR:HG22	44:SC:307:GLU:H	1.76	0.50
48:SI:898:GLY:N	48:SI:915:ALA:O	2.44	0.50
51:SM:74:ASP:OD2	51:SM:201:ARG:NH1	2.44	0.50
52:SP:389:ILE:O	52:SP:389:ILE:HG22	2.11	0.50
55:SS:454:MET:N	55:SS:454:MET:HE2	2.26	0.50
2:L1:125:U:OP1	7:L6:201:GLN:NE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:1594:G:O2'	2:L1:1600:A:N1	2.40	0.50
24:LQ:840:MET:HE2	24:LQ:883:VAL:HG23	1.92	0.50
25:LR:269:LEU:HD11	25:LR:316:VAL:HG13	1.93	0.50
26:LS:272:LEU:HD11	26:LS:314:THR:HG21	1.93	0.50
27:LT:354:SER:N	27:LT:369:ALA:O	2.39	0.50
30:NB:599:LYS:NZ	53:SQ:138:LYS:O	2.44	0.50
51:SM:176:ILE:HD11	56:ST:58:PHE:CE1	2.45	0.50
52:SP:1529:ARG:O	52:SP:1533:MET:N	2.41	0.50
2:L1:188:A:OP2	2:L1:189:C:N4	2.43	0.50
5:L4:181:VAL:HG11	5:L4:225:VAL:HG13	1.92	0.50
16:LH:364:ASN:OD1	16:LH:365:SER:N	2.44	0.50
17:LI:643:ASP:OD1	19:LK:502:ARG:NH2	2.44	0.50
20:LL:2:ASP:OD1	20:LL:3:SER:N	2.44	0.50
27:LT:520:CYS:SG	27:LT:549:MET:HE3	2.52	0.50
34:NL:98:VAL:O	34:NL:101:THR:OG1	2.25	0.50
35:NM:84:ILE:HD12	35:NM:100:PHE:CE2	2.46	0.50
42:SA:163:VAL:HG21	44:SC:205:ARG:HG2	1.93	0.50
42:SA:182:ASP:OD1	42:SA:183:GLN:N	2.44	0.50
23:LO:747:GLU:OE2	27:LT:598:ARG:NH1	2.44	0.50
26:LS:352:GLN:NE2	26:LS:354:SER:O	2.41	0.50
27:LT:885:MET:HE1	27:LT:912:TRP:CH2	2.46	0.50
45:SF:64:LEU:HD21	45:SF:98:ILE:HD12	1.93	0.50
60:SY:111:ARG:NE	60:SY:208:GLU:OE2	2.43	0.50
5:L4:148:ARG:NH2	7:L6:201:GLN:OE1	2.44	0.50
14:LF:47:VAL:CG2	39:NV:729:LEU:HD23	2.41	0.50
16:LH:656:ASP:OD1	16:LH:674:THR:HG21	2.11	0.50
20:LL:465:ILE:HD12	20:LL:501:TRP:NE1	2.27	0.50
22:LN:741:LEU:HD23	22:LN:744:VAL:CG2	2.42	0.50
52:SP:1026:LEU:HD11	52:SP:1061:CYS:SG	2.52	0.50
16:LH:503:ASP:OD1	16:LH:504:GLY:N	2.45	0.50
18:LJ:209:LEU:HD21	18:LJ:242:ASN:OD1	2.11	0.50
22:LN:311:THR:OG1	22:LN:314:SER:OG	2.24	0.50
22:LN:311:THR:HG1	22:LN:314:SER:HG	1.59	0.50
23:LO:17:GLN:OE1	23:LO:17:GLN:N	2.45	0.50
23:LO:150:THR:HG22	23:LO:166:LYS:HZ3	1.76	0.50
34:NL:98:VAL:HG13	34:NL:104:GLU:OE1	2.12	0.50
16:LH:96:ILE:HD12	16:LH:151:TYR:CE1	2.47	0.50
22:LN:189:ARG:HE	58:SV:167:LYS:HD2	1.76	0.50
25:LR:689:ASP:OD2	29:NA:503:LYS:NZ	2.27	0.50
27:LT:530:ASP:HB2	27:LT:537:LEU:HD21	1.93	0.50
36:NP:33:TYR:OH	36:NP:99:SER:OG	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SR:68:ILE:HD13	54:SR:117:ILE:HD11	1.93	0.50
60:SY:120:LYS:O	60:SY:124:GLN:NE2	2.44	0.50
2:L1:68:A:OP1	7:L6:160:ARG:NH2	2.41	0.50
7:L6:2:LYS:HB3	7:L6:108:VAL:HG22	1.93	0.50
52:SP:391:ASP:O	52:SP:428:GLN:NE2	2.45	0.50
12:LD:102:LYS:O	54:SR:13:ARG:NH2	2.45	0.50
18:LJ:431:LEU:HD13	18:LJ:434:ARG:HD3	1.94	0.50
44:SC:173:LEU:HD11	44:SC:256:ASN:HD22	1.76	0.50
52:SP:1647:SER:O	52:SP:1651:ARG:NE	2.45	0.50
52:SP:1678:MET:SD	52:SP:1690:LEU:HD21	2.51	0.50
7:L6:21:GLU:HA	7:L6:24:ILE:HD12	1.92	0.49
10:L9:26:ALA:HB2	50:SL:55:TYR:CE1	2.47	0.49
25:LR:12:LEU:HD11	25:LR:378:PRO:CG	2.42	0.49
27:LT:640:LEU:HD21	27:LT:653:ILE:HG23	1.93	0.49
28:LZ:120:MET:SD	28:LZ:160:TRP:NE1	2.82	0.49
15:LG:58:GLU:OE1	15:LG:58:GLU:N	2.45	0.49
17:LI:432:ASP:OD1	17:LI:433:ASP:N	2.44	0.49
25:LR:160:ILE:O	25:LR:160:ILE:HG22	2.12	0.49
27:LT:630:THR:N	27:LT:644:THR:O	2.43	0.49
27:LT:910:GLN:O	27:LT:910:GLN:NE2	2.45	0.49
48:SI:99:ASN:OD1	48:SI:100:ASP:N	2.46	0.49
8:L7:46:ILE:HD13	8:L7:60:ILE:CD1	2.42	0.49
20:LL:532:ARG:NH2	20:LL:535:ASP:OD2	2.46	0.49
23:LO:349:ASN:N	23:LO:363:ALA:O	2.45	0.49
25:LR:261:ALA:HB1	25:LR:290:ILE:HG21	1.95	0.49
44:SC:85:LYS:NZ	53:SQ:171:SER:O	2.28	0.49
45:SE:110:ILE:O	45:SE:110:ILE:HG12	2.11	0.49
52:SP:358:VAL:HB	52:SP:389:ILE:HD11	1.94	0.49
52:SP:370:ASP:OD1	52:SP:370:ASP:N	2.46	0.49
60:SY:105:ASN:OD1	60:SY:108:ARG:NH2	2.45	0.49
2:L1:43:A:N1	48:SI:41:ARG:NH2	2.60	0.49
2:L1:70:C:P	7:L6:164:LYS:HZ1	2.35	0.49
2:L1:1128:C:O2'	2:L1:1129:U:O5'	2.28	0.49
16:LH:66:LEU:CD2	16:LH:119:LEU:HD13	2.43	0.49
22:LN:40:ASP:OD1	22:LN:40:ASP:N	2.45	0.49
24:LQ:198:GLU:HA	25:LR:667:GLN:NE2	2.28	0.49
27:LT:760:LEU:HB3	29:NA:417:TYR:CZ	2.47	0.49
46:SG:185:LEU:HD13	46:SG:527:VAL:HG11	1.93	0.49
2:L1:1657:U:OP1	2:L1:1658:G:O2'	2.18	0.49
14:LF:51:GLU:OE1	52:SP:36:LYS:N	2.45	0.49
16:LH:327:GLU:OE2	22:LN:319:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LI:596:LYS:HA	17:LI:599:MET:HE2	1.93	0.49
25:LR:25:VAL:HG12	25:LR:294:LEU:HD13	1.93	0.49
28:LZ:141:ASN:ND2	29:NA:454:VAL:HG21	2.28	0.49
31:ND:189:THR:C	31:ND:190:LEU:HD22	2.38	0.49
35:NM:30:PHE:CD2	35:NM:61:LEU:HD21	2.47	0.49
16:LH:56:SER:HB2	16:LH:63:VAL:HG11	1.94	0.49
42:SA:129:ARG:NH1	44:SC:261:LEU:O	2.46	0.49
44:SC:198:GLU:O	44:SC:222:GLU:N	2.45	0.49
45:SF:21:LEU:HD12	45:SF:90:ALA:HB2	1.94	0.49
47:SH:314:ASN:OD1	47:SH:315:LYS:N	2.45	0.49
52:SP:1735:SER:OG	52:SP:1737:ASN:OD1	2.31	0.49
1:L0:9:G:O5'	19:LK:487:ARG:NH1	2.46	0.49
5:L4:181:VAL:CG1	5:L4:225:VAL:HG13	2.42	0.49
13:LE:105:THR:HG23	13:LE:105:THR:O	2.12	0.49
18:LJ:50:GLN:O	18:LJ:53:HIS:N	2.45	0.49
23:LO:102:VAL:HG12	23:LO:113:LEU:CD2	2.43	0.49
29:NA:550:ARG:O	29:NA:554:VAL:HG23	2.12	0.49
43:SB:118:ARG:NH1	44:SD:261:LEU:O	2.46	0.49
17:LI:610:PHE:CE2	17:LI:641:VAL:HG21	2.48	0.49
18:LJ:23:GLU:HB3	18:LJ:268:MET:HE3	1.94	0.49
24:LQ:125:THR:C	24:LQ:126:LEU:HD12	2.38	0.49
24:LQ:128:GLN:O	24:LQ:136:LEU:HD12	2.13	0.49
24:LQ:159:LEU:HD22	24:LQ:189:TRP:CZ3	2.47	0.49
45:SF:33:LEU:HD11	45:SF:100:ALA:HB1	1.95	0.49
52:SP:1720:ILE:O	52:SP:1724:ASN:ND2	2.46	0.49
2:L1:473:A:OP1	10:L9:44:ARG:NH1	2.43	0.49
3:L2:0:M7G:H82	3:L2:1:G:C1'	2.42	0.49
23:LO:415:ASP:OD1	23:LO:420:ARG:N	2.44	0.49
23:LO:721:VAL:HG12	23:LO:745:LEU:HD11	1.94	0.49
24:LQ:569:LEU:CD2	24:LQ:588:ILE:HD11	2.43	0.49
48:SI:130:ASP:OD1	48:SI:131:ILE:N	2.46	0.49
52:SP:430:LYS:NZ	52:SP:754:ASN:OD1	2.35	0.49
52:SP:498:ILE:HG22	52:SP:502:GLU:OE2	2.13	0.49
2:L1:959:U:OP2	37:NQ:20:LYS:NZ	2.45	0.49
8:L7:142:TYR:O	13:LE:42:GLN:NE2	2.44	0.49
16:LH:623:PHE:HD2	16:LH:670:LEU:HD13	1.77	0.49
22:LN:389:ARG:NE	22:LN:404:MET:O	2.40	0.49
24:LQ:494:ASP:OD2	24:LQ:496:THR:OG1	2.30	0.49
18:LJ:432:TYR:O	18:LJ:470:TYR:OH	2.31	0.48
24:LQ:24:VAL:HB	24:LQ:42:ILE:HG23	1.94	0.48
38:NS:124:THR:O	38:NS:124:THR:HG22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:SB:215:ARG:NH2	43:SB:246:GLU:OE2	2.46	0.48
52:SP:728:LEU:HD12	52:SP:729:TRP:CZ3	2.48	0.48
52:SP:892:LEU:HD21	52:SP:928:ILE:HD12	1.95	0.48
3:L2:110:A:O2'	45:SF:46:ARG:NH2	2.46	0.48
16:LH:154:LEU:HD11	16:LH:171:TYR:HB3	1.95	0.48
16:LH:413:SER:OG	16:LH:414:ILE:N	2.46	0.48
23:LO:543:ASN:O	23:LO:547:ALA:N	2.45	0.48
24:LQ:619:MET:HE2	24:LQ:635:LYS:CG	2.44	0.48
27:LT:572:ALA:O	27:LT:575:GLN:NE2	2.46	0.48
30:NB:231:ALA:HB3	30:NB:232:PRO:HD3	1.95	0.48
34:NL:284:VAL:HG13	34:NL:309:ALA:CB	2.43	0.48
48:SI:288:VAL:HG21	48:SI:812:MET:SD	2.53	0.48
51:SM:123:VAL:HG12	51:SM:125:PRO:HD2	1.95	0.48
52:SP:70:ILE:O	52:SP:70:ILE:HG22	2.13	0.48
2:L1:875:G:OP1	35:NM:158:SER:N	2.43	0.48
5:L4:176:ASP:OD1	5:L4:177:ALA:N	2.45	0.48
22:LN:271:THR:HG21	26:LS:443:VAL:HG21	1.94	0.48
22:LN:355:THR:OG1	22:LN:372:MET:O	2.30	0.48
22:LN:746:LEU:HD23	22:LN:752:LEU:HD23	1.94	0.48
23:LO:17:GLN:NE2	23:LO:57:ASN:OD1	2.47	0.48
24:LQ:100:ASP:OD1	24:LQ:101:GLY:N	2.46	0.48
52:SP:457:PHE:CZ	52:SP:485:ILE:HD13	2.49	0.48
52:SP:782:MET:HE3	52:SP:789:ALA:HB1	1.95	0.48
52:SP:898:LYS:HA	52:SP:901:ILE:HD12	1.94	0.48
52:SP:1369:HIS:HA	52:SP:1372:MET:HE2	1.95	0.48
4:L3:48:LYS:HD3	4:L3:54:LEU:HD11	1.94	0.48
24:LQ:217:LEU:HB3	24:LQ:229:TRP:HB2	1.95	0.48
31:ND:172:LYS:NZ	31:ND:175:LYS:O	2.34	0.48
43:SB:159:VAL:HG23	43:SB:162:MET:HG2	1.93	0.48
44:SC:164:ILE:HG22	44:SC:187:VAL:HG11	1.95	0.48
48:SI:196:THR:O	54:SR:140:LYS:NZ	2.41	0.48
52:SP:651:LYS:HG3	52:SP:652:THR:HG23	1.94	0.48
2:L1:154:G:H5'	7:L6:108:VAL:HG21	1.96	0.48
2:L1:214:G:O2'	2:L1:242:U:O4	2.27	0.48
4:L3:32:LEU:HD12	4:L3:35:ILE:HD13	1.94	0.48
15:LG:31:GLU:N	15:LG:31:GLU:OE1	2.46	0.48
24:LQ:653:LEU:HD13	24:LQ:684:TRP:CZ3	2.48	0.48
25:LR:474:SER:OG	25:LR:476:ASP:OD1	2.29	0.48
44:SC:110:ASN:OD1	44:SC:111:MET:N	2.46	0.48
45:SE:74:LYS:HA	45:SE:74:LYS:HE3	1.95	0.48
52:SP:1288:PHE:CE2	52:SP:1302:SER:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SS:380:MET:HE2	55:SS:380:MET:N	2.29	0.48
15:LG:15:VAL:O	15:LG:15:VAL:HG13	2.13	0.48
17:LI:458:ASN:OD1	17:LI:459:GLU:N	2.46	0.48
18:LJ:104:LEU:HD11	18:LJ:119:SER:OG	2.13	0.48
20:LL:85:ILE:O	20:LL:99:PHE:N	2.45	0.48
50:SL:82:ILE:O	50:SL:86:MET:HE3	2.14	0.48
2:L1:1481:C:OP1	36:NP:63:ARG:NH2	2.46	0.48
35:NM:32:ILE:HG12	35:NM:96:LEU:HD12	1.95	0.48
42:SA:7:LEU:HD11	42:SA:128:ILE:CD1	2.44	0.48
10:L9:36:LEU:HD12	10:L9:42:ILE:HD11	1.96	0.48
16:LH:623:PHE:CD2	16:LH:670:LEU:HD13	2.49	0.48
16:LH:728:LEU:HD13	17:LI:442:LYS:HZ1	1.79	0.48
20:LL:153:ILE:HG22	20:LL:163:LEU:CD2	2.43	0.48
24:LQ:135:ARG:NH1	24:LQ:174:GLU:OE2	2.47	0.48
25:LR:595:ALA:HB1	25:LR:619:ARG:HD3	1.95	0.48
50:SL:139:ASP:OD1	50:SL:140:CYS:N	2.47	0.48
22:LN:402:TRP:CE2	22:LN:416:LEU:HD13	2.49	0.48
23:LO:535:LEU:HD13	28:LZ:137:ARG:NH2	2.28	0.48
52:SP:452:ASN:C	52:SP:452:ASN:ND2	2.69	0.48
23:LO:107:ASP:N	23:LO:158:SER:OG	2.47	0.48
25:LR:515:CYS:HB2	25:LR:536:LEU:HD22	1.96	0.48
26:LS:237:ARG:C	26:LS:238:LEU:HD22	2.39	0.48
52:SP:219:LEU:HD21	52:SP:232:LEU:HD12	1.96	0.48
9:L8:160:PHE:CE1	9:L8:165:LEU:HD21	2.48	0.47
16:LH:46:ILE:HD12	16:LH:385:ILE:HG21	1.95	0.47
16:LH:184:GLN:NE2	16:LH:185:PHE:O	2.46	0.47
20:LL:51:LEU:HD22	20:LL:88:TYR:CE1	2.49	0.47
52:SP:339:LEU:O	52:SP:343:ILE:HD12	2.14	0.47
55:SS:394:ALA:O	55:SS:398:LYS:N	2.40	0.47
7:L6:78:THR:O	7:L6:81:VAL:HG22	2.14	0.47
16:LH:537:ASN:OD1	16:LH:538:GLU:N	2.47	0.47
27:LT:375:LEU:HD11	27:LT:414:ILE:HD11	1.95	0.47
29:NA:357:ILE:HG21	51:SM:253:ARG:HH21	1.79	0.47
30:NB:60:GLU:OE2	48:SI:1098:ARG:NE	2.46	0.47
34:NL:251:LEU:HD11	34:NL:315:ILE:CG2	2.45	0.47
50:SL:73:ASN:ND2	55:SS:440:MET:HG2	2.29	0.47
2:L1:1227:A:N6	2:L1:1256:A:O2'	2.47	0.47
3:L2:90:C:O2'	3:L2:91:C:OP1	2.26	0.47
6:L5:132:VAL:HG12	6:L5:198:LEU:CD2	2.44	0.47
16:LH:682:ASN:HB2	16:LH:689:ILE:HD11	1.96	0.47
16:LH:690:ASN:ND2	16:LH:749:ASP:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LO:461:GLN:OE1	23:LO:462:THR:OG1	2.32	0.47
23:LO:467:ASP:OD1	23:LO:468:ALA:N	2.46	0.47
24:LQ:568:SER:C	24:LQ:569:LEU:HD12	2.39	0.47
44:SD:171:LEU:N	44:SD:237:VAL:HG21	2.30	0.47
2:L1:1082:C:HO2'	2:L1:1083:G:P	2.36	0.47
3:L2:15:U:OP1	55:SS:466:ARG:NH2	2.43	0.47
27:LT:192:ASN:O	27:LT:196:GLY:N	2.41	0.47
47:SH:122:THR:HB	47:SH:130:ILE:HD11	1.96	0.47
48:SI:244:MET:CG	48:SI:812:MET:HE3	2.44	0.47
51:SM:8:GLU:O	51:SM:12:TYR:N	2.43	0.47
52:SP:375:THR:O	52:SP:378:HIS:ND1	2.47	0.47
52:SP:1261:ILE:HD11	52:SP:1295:VAL:CG2	2.45	0.47
2:L1:1484:G:N2	2:L1:1606:C:O2	2.47	0.47
22:LN:631:GLU:OE1	22:LN:631:GLU:N	2.47	0.47
25:LR:724:LEU:HD23	25:LR:724:LEU:O	2.13	0.47
27:LT:428:GLU:OE1	27:LT:428:GLU:N	2.45	0.47
35:NM:71:ALA:O	35:NM:75:GLY:N	2.48	0.47
36:NP:77:ASN:OD1	36:NP:96:ALA:N	2.47	0.47
52:SP:1189:LEU:HD12	52:SP:1195:ILE:HD13	1.96	0.47
52:SP:1738:TYR:HE2	52:SP:1745:ILE:HG21	1.79	0.47
55:SS:373:MET:SD	55:SS:374:ARG:N	2.88	0.47
1:L0:87:C:O2	16:LH:332:GLN:NE2	2.47	0.47
2:L1:1540:G:OP2	4:L3:40:ARG:NH2	2.47	0.47
7:L6:5:ILE:HD13	7:L6:16:PHE:CD2	2.50	0.47
16:LH:473:LEU:HD13	16:LH:495:ILE:HD13	1.96	0.47
17:LI:668:ILE:HG23	17:LI:671:ARG:NH2	2.30	0.47
18:LJ:319:VAL:HG22	18:LJ:329:ILE:HD12	1.97	0.47
19:LK:456:LEU:HD11	19:LK:482:LEU:HD21	1.96	0.47
22:LN:192:THR:HG23	22:LN:244:VAL:HG22	1.97	0.47
24:LQ:888:ARG:NH2	25:LR:803:SER:OG	2.43	0.47
43:SB:3:TYR:N	43:SB:86:THR:O	2.41	0.47
44:SD:230:TYR:HD2	44:SD:234:ILE:HD12	1.80	0.47
48:SI:39:MET:HE3	48:SI:39:MET:O	2.14	0.47
2:L1:654:C:O2	2:L1:681:U:N3	2.48	0.47
13:LE:12:ASN:HD22	13:LE:12:ASN:C	2.19	0.47
16:LH:308:ASP:OD1	16:LH:309:GLY:N	2.47	0.47
18:LJ:35:LEU:HD11	18:LJ:326:LEU:HB3	1.96	0.47
21:LM:1062:ILE:HA	21:LM:1065:ALA:HB3	1.96	0.47
22:LN:53:HIS:NE2	22:LN:64:ASP:OD1	2.48	0.47
23:LO:327:LEU:CD2	23:LO:339:LEU:HD22	2.44	0.47
24:LQ:314:ALA:HB1	24:LQ:318:LYS:NZ	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:LQ:399:ILE:HD12	24:LQ:671:PHE:HE1	1.79	0.47
24:LQ:399:ILE:HD11	24:LQ:673:VAL:HG21	1.97	0.47
24:LQ:673:VAL:HG12	24:LQ:683:ILE:CD1	2.44	0.47
25:LR:44:ASP:OD1	25:LR:45:LEU:N	2.47	0.47
44:SC:234:ILE:HG21	44:SC:260:PHE:CD2	2.50	0.47
44:SC:240:VAL:HG23	44:SC:261:LEU:HD13	1.96	0.47
48:SI:107:VAL:HG12	48:SI:354:ILE:HG22	1.96	0.47
5:L4:136:VAL:O	5:L4:136:VAL:HG23	2.14	0.47
6:L5:26:ALA:HB3	11:LC:28:LEU:CD2	2.45	0.47
11:LC:39:VAL:O	11:LC:45:ARG:NH2	2.45	0.47
25:LR:115:THR:HG21	59:SW:78:LYS:HB3	1.95	0.47
29:NA:521:THR:HG22	29:NA:524:ASP:OD2	2.15	0.47
30:NB:270:GLU:O	30:NB:274:ASN:N	2.47	0.47
33:NG:136:ARG:O	59:SW:248:VAL:HG11	2.15	0.47
44:SC:294:ARG:NH1	50:SL:131:SER:OG	2.46	0.47
48:SI:1114:GLN:O	48:SI:1118:THR:HG23	2.14	0.47
2:L1:1124:A:C2	3:L2:0:M7G:HM73	2.50	0.47
7:L6:161:GLU:OE1	7:L6:170:THR:HG22	2.15	0.47
17:LI:675:LEU:HD22	19:LK:456:LEU:HD22	1.96	0.47
42:SA:7:LEU:HD12	42:SA:99:ALA:HB3	1.97	0.47
52:SP:336:ILE:H	52:SP:336:ILE:HD12	1.79	0.47
52:SP:772:ILE:HG23	52:SP:773:LEU:HD22	1.96	0.47
24:LQ:41:LEU:HD13	24:LQ:354:VAL:HG11	1.96	0.47
30:NB:577:LYS:HG2	30:NB:582:VAL:HG22	1.97	0.47
35:NM:20:VAL:HG23	35:NM:21:VAL:HG23	1.96	0.47
43:SB:228:PRO:HD2	43:SB:231:ILE:HD13	1.95	0.47
60:SY:167:THR:HG22	60:SY:169:ASP:H	1.79	0.47
10:L9:11:THR:HG22	10:L9:11:THR:O	2.14	0.46
21:LM:1594:PHE:O	21:LM:1597:LEU:N	2.48	0.46
23:LO:373:ASP:O	23:LO:377:GLY:N	2.46	0.46
29:NA:587:ASP:OD2	29:NA:589:THR:OG1	2.30	0.46
35:NM:124:ASN:ND2	35:NM:124:ASN:O	2.40	0.46
44:SC:117:VAL:HG13	44:SC:118:TYR:HD1	1.80	0.46
48:SI:1119:ILE:HD12	53:SQ:190:LYS:HG3	1.96	0.46
2:L1:931:C:C1'	35:NM:120:LEU:HD13	2.45	0.46
2:L1:1100:G:O2'	13:LE:74:VAL:O	2.20	0.46
6:L5:136:ALA:O	6:L5:140:THR:HG22	2.15	0.46
16:LH:284:SER:OG	16:LH:287:ASP:OD1	2.34	0.46
18:LJ:90:ARG:HE	18:LJ:137:ASN:HB3	1.81	0.46
20:LL:436:THR:OG1	20:LL:471:ARG:NH2	2.49	0.46
24:LQ:535:LEU:HD21	29:NA:591:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LS:532:MET:HE1	26:LS:544:VAL:CG2	2.45	0.46
27:LT:885:MET:HE1	27:LT:912:TRP:CZ2	2.51	0.46
48:SI:625:TRP:CH2	48:SI:631:ILE:HD11	2.49	0.46
51:SM:124:MET:HE2	51:SM:266:LEU:HD11	1.96	0.46
52:SP:1645:SER:O	52:SP:1651:ARG:NH1	2.48	0.46
4:L3:81:ILE:HD13	4:L3:86:LEU:HD21	1.96	0.46
6:L5:26:ALA:HB3	11:LC:28:LEU:HD23	1.96	0.46
13:LE:3:ARG:NH2	13:LE:9:ASP:OD2	2.49	0.46
16:LH:612:SER:HB2	16:LH:662:VAL:HG22	1.98	0.46
22:LN:161:ASP:OD2	22:LN:162:ASN:N	2.48	0.46
22:LN:401:ILE:O	22:LN:416:LEU:HD12	2.14	0.46
24:LQ:188:LEU:O	24:LQ:197:ILE:N	2.44	0.46
24:LQ:261:PHE:O	24:LQ:262:ILE:HD13	2.14	0.46
28:LZ:160:TRP:C	28:LZ:167:LYS:HZ1	2.16	0.46
34:NL:246:THR:HG21	38:NS:133:LEU:O	2.15	0.46
47:SH:299:VAL:O	47:SH:302:VAL:HG12	2.15	0.46
52:SP:436:PHE:HA	52:SP:439:VAL:HG22	1.97	0.46
2:L1:493:U:HO2'	2:L1:494:U:P	2.28	0.46
7:L6:161:GLU:OE2	7:L6:168:THR:HG22	2.15	0.46
8:L7:7:LYS:NZ	8:L7:39:ARG:O	2.47	0.46
8:L7:152:VAL:HG23	8:L7:181:ILE:HD11	1.97	0.46
20:LL:8:SER:OG	20:LL:17:LEU:HD11	2.16	0.46
20:LL:437:VAL:HG21	20:LL:456:VAL:HG13	1.97	0.46
25:LR:536:LEU:HD23	25:LR:550:THR:HB	1.96	0.46
36:NP:75:LYS:O	36:NP:79:LEU:HD23	2.15	0.46
48:SI:90:VAL:HG11	48:SI:98:LEU:HD23	1.96	0.46
22:LN:648:PHE:O	22:LN:655:SER:N	2.45	0.46
23:LO:711:LEU:HD23	23:LO:712:PHE:C	2.40	0.46
24:LQ:263:THR:HG22	24:LQ:270:SER:HA	1.97	0.46
25:LR:495:ASN:N	25:LR:509:ALA:O	2.43	0.46
26:LS:512:ASP:O	60:SY:250:ARG:NH1	2.49	0.46
33:NG:103:ARG:NH1	59:SW:178:ASP:O	2.49	0.46
46:SG:504:ASN:O	46:SG:506:ARG:NH1	2.49	0.46
52:SP:984:ILE:HD12	52:SP:1035:TYR:HB2	1.98	0.46
2:L1:163:G:H21	2:L1:163:G:P	2.37	0.46
2:L1:1473:U:OP2	6:L5:189:THR:OG1	2.34	0.46
7:L6:98:ARG:NH1	7:L6:105:ASP:OD1	2.49	0.46
12:LD:55:ASP:OD1	12:LD:82:ARG:NH1	2.47	0.46
25:LR:769:ILE:HD11	27:LT:897:HIS:CD2	2.50	0.46
27:LT:850:ARG:NH1	27:LT:850:ARG:O	2.48	0.46
38:NS:435:ALA:HB3	38:NS:438:SER:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:1227:A:HB1	2:L1:1256:A:C2'	2.28	0.46
18:LJ:219:ILE:HD13	18:LJ:258:LEU:HB3	1.97	0.46
24:LQ:159:LEU:HD22	24:LQ:189:TRP:CE3	2.51	0.46
25:LR:576:ASN:CB	25:LR:595:ALA:HB3	2.45	0.46
38:NS:419:GLY:N	64:NS:1301:ADP:O1B	2.41	0.46
38:NS:662:MET:N	38:NS:737:LEU:O	2.47	0.46
45:SE:48:ILE:C	45:SE:104:THR:HG23	2.41	0.46
47:SH:65:ILE:HG23	56:ST:112:VAL:HA	1.98	0.46
52:SP:725:ASN:OD1	52:SP:726:LYS:N	2.47	0.46
52:SP:1613:ALA:HB1	52:SP:1639:ILE:HD11	1.96	0.46
2:L1:1502:G:N2	2:L1:1505:A:OP2	2.43	0.46
14:LF:47:VAL:HG22	39:NV:729:LEU:HD23	1.96	0.46
20:LL:437:VAL:CG2	20:LL:456:VAL:HG13	2.46	0.46
21:LM:802:PHE:O	21:LM:806:LEU:N	2.41	0.46
22:LN:286:LEU:HD23	22:LN:287:THR:N	2.31	0.46
24:LQ:619:MET:HE2	24:LQ:635:LYS:HG2	1.97	0.46
25:LR:548:LEU:HB2	25:LR:562:LEU:HD21	1.98	0.46
29:NA:374:GLN:OE1	51:SM:245:VAL:HG23	2.16	0.46
44:SC:175:ALA:HB1	44:SC:181:VAL:HG21	1.98	0.46
52:SP:307:ASP:OD1	52:SP:308:ALA:N	2.46	0.46
52:SP:1247:LEU:CD2	52:SP:1268:ILE:HD13	2.45	0.46
2:L1:501:U:O4	53:SQ:133:LYS:NZ	2.49	0.46
2:L1:1638:G:OP2	2:L1:1638:G:N2	2.48	0.46
8:L7:134:GLU:O	8:L7:154:LEU:HD12	2.16	0.46
9:L8:153:GLU:OE2	9:L8:153:GLU:N	2.43	0.46
16:LH:19:LYS:HZ1	16:LH:366:ASN:CG	2.16	0.46
16:LH:780:GLU:O	16:LH:781:SER:OG	2.29	0.46
23:LO:53:GLU:OE1	23:LO:53:GLU:N	2.49	0.46
23:LO:710:ILE:HG23	27:LT:596:GLU:CD	2.41	0.46
23:LO:821:MET:HA	23:LO:821:MET:HE3	1.98	0.46
24:LQ:227:LYS:NZ	24:LQ:244:GLU:OE1	2.23	0.46
25:LR:339:ILE:HG23	25:LR:621:TRP:NE1	2.31	0.46
28:LZ:78:LEU:O	28:LZ:82:LEU:HD23	2.15	0.46
44:SD:151:LEU:HD12	44:SD:241:PHE:CE2	2.51	0.46
8:L7:47:ARG:HG2	8:L7:49:ILE:HG23	1.97	0.46
20:LL:5:VAL:HG23	20:LL:306:LEU:HD11	1.97	0.46
23:LO:33:VAL:HG23	23:LO:33:VAL:O	2.16	0.46
23:LO:157:ASP:OD2	23:LO:159:ARG:NH1	2.49	0.46
24:LQ:474:ALA:HB1	24:LQ:493:ALA:HB3	1.98	0.46
27:LT:621:ASP:OD1	27:LT:622:GLY:N	2.50	0.46
30:NB:221:ALA:HB3	30:NB:222:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:NG:29:HIS:NE2	33:NG:38:THR:HG23	2.31	0.46
35:NM:3:VAL:HG22	35:NM:3:VAL:O	2.16	0.46
60:SY:35:VAL:HG22	60:SY:39:GLN:OE1	2.16	0.46
2:L1:438:A:H1'	2:L1:465:G:H22	1.80	0.45
16:LH:627:ASP:OD1	16:LH:628:ASP:N	2.49	0.45
18:LJ:34:GLN:OE1	18:LJ:34:GLN:N	2.50	0.45
23:LO:145:HIS:ND1	23:LO:167:ASP:OD2	2.43	0.45
24:LQ:184:GLY:O	24:LQ:202:ALA:N	2.44	0.45
27:LT:21:SER:O	27:LT:657:ARG:NH1	2.50	0.45
42:SA:11:GLU:OE2	42:SA:147:LEU:HD22	2.16	0.45
43:SB:177:LEU:HD21	43:SB:265:PHE:CB	2.45	0.45
46:SG:125:VAL:HG22	46:SG:125:VAL:O	2.16	0.45
46:SG:235:HIS:CD2	46:SG:261:ILE:HD12	2.51	0.45
7:L6:98:ARG:NH2	7:L6:105:ASP:OD1	2.49	0.45
11:LC:28:LEU:O	11:LC:65:ILE:N	2.47	0.45
16:LH:640:LYS:NZ	16:LH:652:GLU:OE2	2.42	0.45
16:LH:769:ASN:OD1	16:LH:770:TYR:N	2.50	0.45
23:LO:151:SER:OG	23:LO:195:MET:O	2.33	0.45
23:LO:164:THR:OG1	23:LO:195:MET:O	2.34	0.45
23:LO:673:ARG:NE	28:LZ:145:ASP:OD2	2.46	0.45
45:SF:21:LEU:HD12	45:SF:90:ALA:CB	2.46	0.45
52:SP:1102:PRO:HA	52:SP:1106:LEU:HD23	1.97	0.45
52:SP:1345:LEU:HD21	52:SP:1393:MET:SD	2.56	0.45
2:L1:1190:C:N4	2:L1:1197:C:O2	2.49	0.45
2:L1:1595:U:OP1	48:SI:945:THR:OG1	2.28	0.45
4:L3:80:LYS:HD3	4:L3:80:LYS:N	2.31	0.45
7:L6:120:GLU:OE1	7:L6:120:GLU:N	2.50	0.45
17:LI:546:ASP:OD1	17:LI:546:ASP:N	2.46	0.45
43:SB:1:MET:HE2	43:SB:16:LYS:CE	2.46	0.45
44:SC:111:MET:HE2	44:SC:111:MET:HA	1.98	0.45
8:L7:17:GLU:HG3	8:L7:46:ILE:HG22	1.98	0.45
11:LC:65:ILE:HG21	11:LC:85:ILE:HD13	1.97	0.45
25:LR:12:LEU:N	25:LR:641:PHE:O	2.49	0.45
26:LS:523:PHE:HE2	26:LS:530:LEU:HD12	1.80	0.45
33:NG:18:ARG:N	33:NG:29:HIS:O	2.50	0.45
2:L1:1105:C:OP2	54:SR:14:LYS:NZ	2.44	0.45
2:L1:1802:A:O2'	35:NM:145:LYS:O	2.32	0.45
3:L2:283:U:O4	21:LM:1413:SER:N	2.48	0.45
5:L4:171:ASP:OD1	5:L4:172:PHE:N	2.45	0.45
16:LH:555:VAL:HG13	16:LH:555:VAL:O	2.15	0.45
21:LM:1056:ALA:O	21:LM:1060:PHE:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:LQ:322:SER:HA	24:LQ:325:ILE:HD12	1.97	0.45
24:LQ:568:SER:O	24:LQ:569:LEU:HD12	2.16	0.45
26:LS:432:VAL:HG11	26:LS:447:TRP:CZ2	2.52	0.45
34:NL:226:LEU:HD23	34:NL:226:LEU:C	2.42	0.45
34:NL:284:VAL:HG13	34:NL:309:ALA:HB3	1.98	0.45
48:SI:1079:PHE:CG	60:SY:67:MET:HE1	2.51	0.45
52:SP:701:LEU:HD21	52:SP:795:ASP:HB3	1.97	0.45
55:SS:375:LYS:O	55:SS:378:THR:N	2.49	0.45
22:LN:541:ALA:HB3	22:LN:553:LEU:HB2	1.98	0.45
24:LQ:631:PHE:HD2	24:LQ:672:VAL:HG11	1.82	0.45
25:LR:796:VAL:O	25:LR:800:VAL:HG23	2.16	0.45
37:NQ:67:THR:OG1	37:NQ:70:LYS:O	2.29	0.45
2:L1:621:A:O2'	2:L1:1106:U:O2'	2.23	0.45
2:L1:1098:U:O2'	50:SL:77:GLN:O	2.31	0.45
4:L3:111:ASP:O	4:L3:115:ARG:HG2	2.17	0.45
5:L4:129:VAL:HG22	5:L4:139:VAL:HG12	1.98	0.45
8:L7:114:ARG:O	8:L7:118:LEU:HD23	2.17	0.45
11:LC:60:PHE:HE1	11:LC:89:LEU:HD13	1.82	0.45
18:LJ:467:LEU:CD2	18:LJ:484:MET:HE1	2.41	0.45
22:LN:150:ASN:ND2	22:LN:198:ASP:OD1	2.49	0.45
25:LR:801:GLU:OE1	27:LT:930:MET:HE3	2.17	0.45
29:NA:449:ASP:O	29:NA:453:SER:N	2.50	0.45
34:NL:115:MET:HE1	34:NL:137:LEU:HA	1.99	0.45
42:SA:259:MET:HE1	44:SD:212:LYS:HA	1.98	0.45
7:L6:14:LYS:HB3	7:L6:124:LEU:HD21	1.98	0.45
8:L7:59:ALA:HB1	8:L7:93:LEU:HD22	1.99	0.45
23:LO:69:LEU:HD12	23:LO:81:LEU:HD11	1.98	0.45
24:LQ:103:ILE:N	24:LQ:117:PHE:O	2.42	0.45
25:LR:345:TYR:CE2	25:LR:353:LEU:HD21	2.51	0.45
26:LS:396:MET:HE1	26:LS:437:LEU:O	2.16	0.45
43:SB:124:LEU:HD11	43:SB:128:LEU:CD1	2.47	0.45
46:SG:330:ALA:O	46:SG:331:LEU:HD22	2.17	0.45
47:SH:220:GLN:OE1	47:SH:220:GLN:N	2.50	0.45
52:SP:1061:CYS:O	52:SP:1064:SER:OG	2.34	0.45
59:SW:187:VAL:HG23	59:SW:251:ILE:HD12	1.99	0.45
16:LH:435:ASP:OD1	16:LH:436:PHE:N	2.47	0.45
24:LQ:399:ILE:HD11	24:LQ:673:VAL:CG2	2.47	0.45
24:LQ:496:THR:HG22	24:LQ:529:GLU:OE1	2.17	0.45
24:LQ:610:SER:C	24:LQ:611:LEU:HD22	2.42	0.45
25:LR:270:ILE:HG13	25:LR:277:VAL:HG22	1.98	0.45
25:LR:454:LEU:N	25:LR:466:TRP:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:NM:61:LEU:HD22	35:NM:96:LEU:CD2	2.47	0.45
43:SB:76:LEU:HD13	43:SB:98:ILE:HD11	1.98	0.45
2:L1:277:U:O2'	2:L1:278:U:OP1	2.32	0.45
7:L6:18:ILE:HD12	7:L6:23:ARG:HD2	1.98	0.45
24:LQ:868:LEU:HD23	25:LR:809:ALA:HB1	1.99	0.45
25:LR:339:ILE:HG23	25:LR:621:TRP:HE1	1.82	0.45
25:LR:495:ASN:OD1	35:NM:14:LYS:NZ	2.23	0.45
28:LZ:99:ASN:OD1	28:LZ:100:LYS:N	2.50	0.45
16:LH:12:LEU:HD23	16:LH:12:LEU:H	1.82	0.44
22:LN:61:THR:HG21	22:LN:681:ILE:HG23	1.98	0.44
22:LN:682:THR:OG1	22:LN:684:GLU:OE1	2.34	0.44
23:LO:210:SER:OG	23:LO:212:ASP:OD1	2.33	0.44
24:LQ:338:ILE:HG12	24:LQ:355:LEU:HD13	1.99	0.44
25:LR:730:ILE:HG22	25:LR:730:ILE:O	2.17	0.44
34:NL:210:GLU:N	34:NL:210:GLU:OE1	2.49	0.44
34:NL:228:ARG:NH1	38:NS:130:SER:O	2.50	0.44
38:NS:515:ILE:N	38:NS:556:ILE:O	2.42	0.44
44:SD:234:ILE:HG22	44:SD:235:GLY:O	2.17	0.44
10:L9:57:ARG:HG2	50:SL:87:MET:HE3	1.99	0.44
22:LN:164:THR:OG1	22:LN:185:ARG:NE	2.46	0.44
23:LO:385:GLU:OE1	23:LO:421:ASN:ND2	2.43	0.44
35:NM:161:ILE:H	35:NM:161:ILE:HD12	1.82	0.44
44:SD:195:TYR:HD1	44:SD:220:ILE:HD11	1.82	0.44
45:SF:17:THR:HG21	45:SF:82:PRO:HD3	1.99	0.44
2:L1:992:A:OP2	2:L1:1011:G:N1	2.42	0.44
16:LH:64:LYS:HE2	16:LH:66:LEU:HD11	1.99	0.44
16:LH:339:GLY:H	16:LH:358:LEU:HD23	1.81	0.44
22:LN:31:MET:HE3	22:LN:750:ASN:HA	1.99	0.44
25:LR:591:ILE:HD12	25:LR:623:LEU:HD11	1.98	0.44
35:NM:175:GLU:OE1	35:NM:187:LYS:NZ	2.50	0.44
38:NS:126:LEU:O	38:NS:126:LEU:HD23	2.17	0.44
42:SA:385:MET:HB3	42:SA:404:LEU:HD21	1.98	0.44
46:SG:152:VAL:HG12	46:SG:562:GLY:HA2	2.00	0.44
48:SI:1112:PHE:CG	53:SQ:178:MET:HE1	2.52	0.44
52:SP:340:ILE:HD13	52:SP:361:LEU:HD21	1.99	0.44
52:SP:625:ILE:HG21	52:SP:642:ILE:HD11	1.99	0.44
52:SP:1189:LEU:HD22	52:SP:1194:SER:HB2	1.99	0.44
2:L1:1584:G:HO2'	2:L1:1585:U:P	2.38	0.44
3:L2:2:U:OP1	34:NL:208:ARG:NH1	2.49	0.44
17:LI:555:ILE:HD13	17:LI:582:ILE:HG13	1.99	0.44
18:LJ:312:ALA:HB3	18:LJ:316:ARG:HH11	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LZ:118:LEU:HD23	28:LZ:120:MET:HE3	2.00	0.44
2:L1:557:G:O3'	48:SI:931:LYS:NZ	2.51	0.44
9:L8:6:ASP:OD1	9:L8:7:SER:N	2.51	0.44
24:LQ:653:LEU:HD13	24:LQ:684:TRP:CZ2	2.53	0.44
24:LQ:869:VAL:HA	25:LR:813:MET:HB3	2.00	0.44
25:LR:345:TYR:CZ	25:LR:353:LEU:HD21	2.53	0.44
43:SB:276:LEU:CD2	43:SB:280:MET:HE2	2.45	0.44
52:SP:312:ASP:OD1	52:SP:313:ARG:N	2.51	0.44
52:SP:464:PHE:O	52:SP:468:ALA:HB2	2.17	0.44
52:SP:1261:ILE:HD12	52:SP:1291:LEU:CD1	2.47	0.44
2:L1:327:U:H1'	12:LD:10:GLU:OE2	2.18	0.44
18:LJ:508:LEU:HD22	20:LL:526:LEU:CD2	2.47	0.44
24:LQ:212:VAL:CG2	24:LQ:217:LEU:HD13	2.36	0.44
24:LQ:530:LEU:HD13	24:LQ:550:LEU:HD21	1.99	0.44
24:LQ:891:LEU:HB3	25:LR:800:VAL:HG22	1.99	0.44
27:LT:738:ASP:OD1	27:LT:738:ASP:N	2.51	0.44
52:SP:1173:LEU:O	52:SP:1177:SER:OG	2.16	0.44
2:L1:930:A:OP2	2:L1:931:C:N4	2.43	0.44
4:L3:24:GLY:HA2	4:L3:58:ALA:HB3	2.00	0.44
4:L3:27:LYS:O	4:L3:31:ALA:N	2.41	0.44
16:LH:302:SER:C	16:LH:303:LEU:HD22	2.43	0.44
24:LQ:905:LEU:HD11	25:LR:782:VAL:HG13	2.00	0.44
25:LR:577:ALA:O	25:LR:595:ALA:N	2.51	0.44
26:LS:248:HIS:N	26:LS:269:ASP:OD2	2.47	0.44
42:SA:163:VAL:HG21	44:SC:205:ARG:CG	2.47	0.44
42:SA:385:MET:SD	45:SF:63:ILE:HD13	2.58	0.44
2:L1:577:G:OP1	29:NA:322:LYS:NZ	2.50	0.44
2:L1:862:A:OP2	32:NF:64:ARG:NH2	2.51	0.44
2:L1:899:G:H4'	33:NG:46:MET:HE1	2.00	0.44
2:L1:1140:G:N7	56:ST:41:ARG:NH2	2.66	0.44
2:L1:1614:A:OP2	6:L5:84:LYS:NZ	2.51	0.44
14:LF:8:ARG:NH1	46:SG:316:GLU:OE1	2.51	0.44
20:LL:472:LEU:HD23	20:LL:473:LYS:O	2.18	0.44
24:LQ:817:LEU:HD22	24:LQ:855:LYS:NZ	2.32	0.44
25:LR:309:GLN:O	25:LR:335:GLY:N	2.49	0.44
27:LT:362:GLN:O	27:LT:363:SER:OG	2.23	0.44
29:NA:431:GLN:HA	29:NA:434:HIS:HB2	2.00	0.44
31:ND:178:VAL:HG23	60:SY:143:MET:CE	2.42	0.44
33:NG:13:VAL:HG23	33:NG:76:ILE:HA	1.99	0.44
42:SA:198:TRP:HB3	42:SA:271:VAL:HG22	2.00	0.44
8:L7:73:VAL:HG22	8:L7:73:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L8:78:ILE:CG2	9:L8:102:VAL:HG21	2.48	0.44
23:LO:492:SER:OG	23:LO:493:TRP:N	2.51	0.44
24:LQ:597:ILE:HD13	24:LQ:621:VAL:HG21	1.99	0.44
25:LR:251:ASP:OD1	25:LR:252:GLY:N	2.46	0.44
25:LR:314:ILE:HG22	25:LR:329:VAL:HA	2.00	0.44
25:LR:406:ALA:HB1	25:LR:437:VAL:HG12	1.99	0.44
43:SB:152:LEU:HD21	44:SD:205:ARG:CG	2.45	0.44
8:L7:63:PRO:O	8:L7:67:LEU:N	2.49	0.43
10:L9:26:ALA:HB2	50:SL:55:TYR:CD1	2.53	0.43
22:LN:152:SER:OG	22:LN:154:ASP:OD1	2.30	0.43
22:LN:554:ASP:O	22:LN:558:ARG:N	2.51	0.43
24:LQ:601:GLY:O	24:LQ:605:GLY:N	2.50	0.43
52:SP:1020:ASN:ND2	52:SP:1024:GLN:OE1	2.51	0.43
52:SP:1088:LYS:O	52:SP:1091:ILE:HG22	2.17	0.43
12:LD:119:VAL:HG23	12:LD:119:VAL:O	2.18	0.43
16:LH:302:SER:O	16:LH:303:LEU:HD22	2.18	0.43
16:LH:414:ILE:H	16:LH:414:ILE:HD12	1.83	0.43
16:LH:471:GLN:NE2	16:LH:472:TYR:O	2.51	0.43
21:LM:1055:SER:O	21:LM:1059:ASN:N	2.45	0.43
25:LR:778:MET:HE3	25:LR:782:VAL:CG2	2.47	0.43
42:SA:223:ILE:HD11	42:SA:237:LEU:HD22	1.99	0.43
47:SH:65:ILE:HD11	47:SH:74:VAL:CG1	2.49	0.43
52:SP:491:LEU:HD23	52:SP:491:LEU:H	1.83	0.43
55:SS:793:GLU:N	55:SS:793:GLU:OE1	2.51	0.43
58:SV:155:ASN:OD1	58:SV:156:THR:N	2.51	0.43
19:LK:505:MET:HE1	20:LL:507:ILE:HA	2.00	0.43
20:LL:222:THR:HG23	20:LL:222:THR:O	2.18	0.43
20:LL:225:VAL:HG23	20:LL:225:VAL:O	2.18	0.43
22:LN:579:ARG:NH1	22:LN:660:ASP:OD1	2.50	0.43
24:LQ:127:LEU:HD22	24:LQ:136:LEU:HD11	1.99	0.43
24:LQ:183:ASP:OD1	24:LQ:184:GLY:N	2.51	0.43
26:LS:346:TYR:CZ	26:LS:393:LEU:HD13	2.52	0.43
27:LT:522:LEU:HD12	27:LT:545:PRO:HB3	2.00	0.43
28:LZ:79:LEU:HD23	28:LZ:92:SER:O	2.18	0.43
43:SB:195:LEU:HD21	43:SB:208:ILE:HG21	2.00	0.43
48:SI:102:GLN:N	48:SI:359:SER:OG	2.48	0.43
52:SP:10:SER:O	52:SP:15:ARG:NH2	2.49	0.43
55:SS:374:ARG:O	55:SS:377:THR:OG1	2.29	0.43
2:L1:512:A:OP1	10:L9:170:GLY:N	2.42	0.43
2:L1:1257:U:O2'	61:SZ:312:TYR:O	2.35	0.43
16:LH:200:ASN:OD1	16:LH:201:ILE:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LJ:104:LEU:HD12	18:LJ:120:ILE:C	2.42	0.43
25:LR:552:SER:OG	25:LR:553:GLY:N	2.51	0.43
25:LR:739:LEU:HD23	25:LR:763:ILE:HD11	2.00	0.43
34:NL:275:ASP:OD1	34:NL:276:VAL:HG23	2.19	0.43
34:NL:280:LYS:NZ	34:NL:313:VAL:HG22	2.33	0.43
34:NL:313:VAL:HG22	34:NL:313:VAL:O	2.18	0.43
43:SB:98:ILE:HG23	43:SB:107:VAL:HG21	2.00	0.43
51:SM:74:ASP:O	51:SM:78:ALA:N	2.51	0.43
52:SP:389:ILE:O	52:SP:393:PHE:N	2.51	0.43
2:L1:96:G:H21	2:L1:426:G:H5'	1.84	0.43
2:L1:1078:C:P	55:SS:394:ALA:HB1	2.58	0.43
5:L4:181:VAL:HG21	5:L4:195:ILE:HG13	2.00	0.43
8:L7:46:ILE:HD11	8:L7:58:LEU:HB3	2.00	0.43
8:L7:133:THR:CB	8:L7:154:LEU:HD11	2.48	0.43
24:LQ:17:ILE:HD12	24:LQ:360:ASN:O	2.19	0.43
25:LR:269:LEU:HD11	25:LR:316:VAL:CG1	2.48	0.43
38:NS:400:ILE:O	38:NS:404:ILE:N	2.46	0.43
44:SC:325:LEU:HD21	50:SL:131:SER:HB3	1.99	0.43
48:SI:956:MET:HE2	56:ST:752:MET:CE	2.49	0.43
2:L1:1473:U:O2'	6:L5:103:ASN:OD1	2.36	0.43
18:LJ:391:ASN:ND2	18:LJ:403:ASN:OD1	2.51	0.43
23:LO:707:ASN:OD1	23:LO:708:ASP:N	2.51	0.43
24:LQ:321:TYR:CE2	24:LQ:325:ILE:HD11	2.54	0.43
25:LR:345:TYR:HE1	25:LR:367:VAL:HG21	1.84	0.43
27:LT:23:ILE:HG23	27:LT:24:PHE:CD2	2.53	0.43
50:SL:50:ALA:HB1	50:SL:58:ALA:HB2	2.00	0.43
52:SP:1534:LEU:HD23	52:SP:1544:ALA:HB3	2.00	0.43
2:L1:512:A:O2'	10:L9:131:GLN:OE1	2.20	0.43
6:L5:79:ASN:ND2	23:LO:510:GLU:OE1	2.51	0.43
12:LD:76:VAL:HG21	12:LD:87:ARG:HB2	2.01	0.43
14:LF:35:VAL:CG2	14:LF:40:LEU:HD21	2.49	0.43
16:LH:662:VAL:HG12	16:LH:672:VAL:HG23	2.01	0.43
17:LI:507:LEU:HD23	17:LI:536:ARG:HG2	2.01	0.43
23:LO:848:PHE:O	23:LO:852:THR:HG22	2.19	0.43
25:LR:642:GLN:OE1	25:LR:644:TRP:CD1	2.72	0.43
31:ND:203:ASP:OD1	31:ND:204:ARG:N	2.51	0.43
43:SB:8:THR:CG2	43:SB:124:LEU:HD21	2.49	0.43
43:SB:211:THR:HG21	43:SB:226:ILE:HD11	2.00	0.43
52:SP:457:PHE:CE2	52:SP:485:ILE:HD13	2.54	0.43
52:SP:1421:LEU:O	52:SP:1425:VAL:HG23	2.18	0.43
55:SS:795:ALA:O	59:SW:127:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:139:C:OP2	7:L6:187:LYS:NZ	2.50	0.43
7:L6:23:ARG:NH1	7:L6:41:VAL:HG12	2.33	0.43
8:L7:86:GLN:O	8:L7:88:ARG:NH1	2.52	0.43
14:LF:5:VAL:HB	39:NV:731:PHE:CE1	2.54	0.43
23:LO:760:ILE:HD12	23:LO:760:ILE:H	1.84	0.43
34:NL:275:ASP:OD1	34:NL:276:VAL:N	2.51	0.43
35:NM:141:ALA:HB1	35:NM:207:LEU:HD12	2.01	0.43
45:SF:13:ASP:O	45:SF:17:THR:HG23	2.19	0.43
52:SP:233:LEU:O	52:SP:237:THR:HG22	2.19	0.43
52:SP:1384:LEU:O	52:SP:1388:SER:N	2.47	0.43
2:L1:154:G:OP2	14:LF:131:ARG:NH1	2.42	0.43
5:L4:56:LEU:N	5:L4:60:GLU:OE1	2.48	0.43
22:LN:593:GLU:O	22:LN:611:LEU:HD23	2.19	0.43
23:LO:298:LEU:HD23	29:NA:472:PRO:HG2	2.01	0.43
24:LQ:760:ILE:HG21	24:LQ:831:LYS:HG2	2.00	0.43
25:LR:436:ALA:HB3	25:LR:459:ASN:OD1	2.18	0.43
25:LR:642:GLN:OE1	25:LR:644:TRP:NE1	2.51	0.43
27:LT:549:MET:HE2	27:LT:560:LEU:HD21	2.01	0.43
30:NB:33:ARG:HH22	51:SM:13:LEU:HD13	1.82	0.43
34:NL:313:VAL:HG13	34:NL:315:ILE:HG12	1.99	0.43
44:SC:302:GLU:OE2	44:SC:302:GLU:HA	2.18	0.43
52:SP:606:THR:HA	52:SP:609:ILE:HD12	2.01	0.43
54:SR:57:LEU:HD11	54:SR:73:ARG:HG3	2.00	0.43
2:L1:487:G:N7	48:SI:1127:ARG:NH1	2.67	0.43
2:L1:885:G:H2'	2:L1:886:U:C6	2.54	0.43
24:LQ:621:VAL:HG13	24:LQ:630:PHE:CD1	2.54	0.43
24:LQ:793:VAL:O	24:LQ:797:VAL:HG23	2.19	0.43
25:LR:780:LYS:HE2	25:LR:780:LYS:HA	2.00	0.43
34:NL:273:MET:HE3	34:NL:276:VAL:HG21	2.00	0.43
42:SA:7:LEU:HD11	42:SA:128:ILE:HD13	2.01	0.43
52:SP:360:PHE:CE2	52:SP:364:LEU:HD11	2.54	0.43
52:SP:1465:ALA:O	52:SP:1469:LEU:HD23	2.18	0.43
53:SQ:106:LEU:O	53:SQ:146:ARG:NH2	2.52	0.43
2:L1:572:C:N4	48:SI:878:HIS:O	2.52	0.42
2:L1:934:C:H41	55:SS:394:ALA:HB3	1.84	0.42
2:L1:1030:A:OP1	55:SS:401:LYS:NZ	2.42	0.42
2:L1:1129:U:O2	2:L1:1129:U:O2'	2.37	0.42
8:L7:75:THR:HG23	8:L7:76:LYS:N	2.33	0.42
10:L9:42:ILE:HD12	10:L9:42:ILE:H	1.84	0.42
17:LI:637:LEU:O	17:LI:641:VAL:HG23	2.19	0.42
25:LR:591:ILE:HD11	25:LR:625:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:NB:59:ASP:O	48:SI:1098:ARG:N	2.51	0.42
35:NM:62:LYS:HZ1	35:NM:91:VAL:HG22	1.84	0.42
43:SB:76:LEU:CD1	43:SB:98:ILE:HD11	2.49	0.42
52:SP:1919:ILE:O	52:SP:1922:ILE:HG22	2.18	0.42
2:L1:1803:G:OP2	55:SS:381:ARG:NH2	2.52	0.42
4:L3:18:LEU:HD22	4:L3:73:MET:CE	2.49	0.42
17:LI:679:ILE:HD12	19:LK:460:LEU:HD11	2.01	0.42
23:LO:286:LEU:O	23:LO:295:ILE:N	2.50	0.42
24:LQ:275:GLN:NE2	24:LQ:338:ILE:O	2.52	0.42
24:LQ:362:ILE:HB	24:LQ:385:ILE:HD12	2.01	0.42
24:LQ:433:ALA:HB1	24:LQ:447:LEU:HD12	2.00	0.42
25:LR:625:THR:O	25:LR:626:MET:HE2	2.20	0.42
26:LS:263:LEU:HD23	26:LS:263:LEU:C	2.44	0.42
27:LT:821:LEU:HD11	27:LT:863:TRP:HB3	2.01	0.42
38:NS:593:HIS:N	38:NS:821:CYS:O	2.50	0.42
43:SB:95:ALA:O	43:SB:98:ILE:HG22	2.19	0.42
43:SB:312:SER:O	43:SB:372:ARG:NH2	2.51	0.42
46:SG:61:ASP:OD1	46:SG:64:ARG:NH2	2.51	0.42
48:SI:918:ILE:HD11	54:SR:144:ARG:HH21	1.83	0.42
50:SL:93:LYS:NZ	50:SL:95:ASN:OD1	2.47	0.42
2:L1:1059:U:OP2	2:L1:1059:U:H4'	2.20	0.42
2:L1:1568:C:HO2'	2:L1:1569:A:P	2.42	0.42
8:L7:122:HIS:CD2	8:L7:177:THR:HG22	2.53	0.42
16:LH:621:LEU:C	16:LH:621:LEU:HD12	2.44	0.42
18:LJ:302:VAL:HG22	18:LJ:322:LEU:CD2	2.49	0.42
23:LO:102:VAL:HG12	23:LO:113:LEU:HD23	2.01	0.42
24:LQ:254:GLN:HG2	24:LQ:277:ALA:HB3	2.00	0.42
24:LQ:262:ILE:HD11	24:LQ:343:TRP:HB3	2.00	0.42
34:NL:94:LEU:O	34:NL:98:VAL:HG12	2.19	0.42
52:SP:84:ASP:OD1	52:SP:85:LYS:N	2.52	0.42
53:SQ:189:ARG:O	53:SQ:192:ASN:N	2.49	0.42
16:LH:386:ASN:ND2	16:LH:467:GLN:OE1	2.42	0.42
18:LJ:90:ARG:O	18:LJ:93:GLY:N	2.50	0.42
18:LJ:375:HIS:NE2	26:LS:339:ILE:HD11	2.34	0.42
22:LN:681:ILE:HG22	22:LN:683:ASP:N	2.33	0.42
23:LO:553:ILE:HD11	23:LO:609:GLU:HA	2.01	0.42
24:LQ:543:ASP:OD1	24:LQ:560:LEU:HD13	2.19	0.42
45:SE:29:ASN:HB3	60:SY:246:LYS:HE3	2.01	0.42
2:L1:1611:A:OP1	6:L5:107:LYS:NZ	2.49	0.42
6:L5:27:THR:O	6:L5:29:ILE:HD12	2.20	0.42
16:LH:474:THR:HG22	16:LH:511:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LL:221:MET:N	20:LL:221:MET:SD	2.92	0.42
24:LQ:631:PHE:CE2	24:LQ:672:VAL:HG21	2.54	0.42
25:LR:408:LYS:HA	25:LR:436:ALA:HB1	2.00	0.42
31:ND:177:ARG:HG3	60:SY:134:THR:HG22	2.02	0.42
32:NF:26:PHE:CE2	32:NF:66:ILE:HG23	2.54	0.42
45:SF:21:LEU:HD11	45:SF:87:LEU:HA	2.01	0.42
46:SG:245:SER:OG	46:SG:247:ASP:OD1	2.35	0.42
48:SI:549:ILE:HD13	48:SI:567:TRP:CE2	2.54	0.42
52:SP:1719:LYS:HE2	52:SP:1719:LYS:HA	2.01	0.42
59:SW:166:PHE:HE1	59:SW:225:VAL:HG22	1.84	0.42
9:L8:17:LYS:HZ2	38:NS:26:ILE:HB	1.84	0.42
9:L8:29:LEU:C	9:L8:29:LEU:HD12	2.44	0.42
16:LH:401:GLN:OE1	16:LH:411:SER:N	2.53	0.42
16:LH:442:ILE:HD12	16:LH:770:TYR:CE2	2.55	0.42
22:LN:125:GLU:O	22:LN:134:LEU:N	2.53	0.42
24:LQ:446:ILE:C	24:LQ:447:LEU:HD22	2.45	0.42
25:LR:36:VAL:O	25:LR:36:VAL:HG13	2.19	0.42
25:LR:692:MET:N	25:LR:692:MET:SD	2.93	0.42
27:LT:717:ASP:OD1	27:LT:718:LYS:N	2.52	0.42
51:SM:80:THR:O	51:SM:80:THR:HG22	2.20	0.42
52:SP:794:VAL:HG12	52:SP:845:TYR:CG	2.55	0.42
59:SW:233:ILE:HG22	59:SW:240:ILE:HG22	2.01	0.42
2:L1:168:A:OP1	7:L6:140:ASN:ND2	2.45	0.42
6:L5:92:ARG:NH2	6:L5:169:ASN:OD1	2.46	0.42
16:LH:334:LEU:CD2	16:LH:337:LEU:HD11	2.50	0.42
18:LJ:45:ILE:HD13	18:LJ:319:VAL:HG12	2.02	0.42
22:LN:522:SER:HA	22:LN:528:ILE:HD11	2.02	0.42
24:LQ:589:ILE:HG22	24:LQ:597:ILE:HD11	2.02	0.42
25:LR:769:ILE:HD11	27:LT:897:HIS:HD2	1.85	0.42
44:SC:307:GLU:HG2	44:SC:308:PRO:HA	2.02	0.42
52:SP:1095:SER:HA	52:SP:1136:THR:HG22	2.01	0.42
53:SQ:142:GLU:N	53:SQ:142:GLU:OE2	2.52	0.42
4:L3:110:ARG:NH1	4:L3:113:LEU:HD23	2.34	0.42
18:LJ:231:GLY:O	18:LJ:255:VAL:HG22	2.19	0.42
23:LO:828:ILE:HG21	27:LT:930:MET:HG2	2.01	0.42
29:NA:412:ILE:HD12	29:NA:412:ILE:H	1.85	0.42
37:NQ:8:LEU:HD22	37:NQ:9:HIS:CE1	2.55	0.42
44:SD:236:MET:HE3	44:SD:236:MET:HA	2.00	0.42
47:SH:365:LYS:NZ	48:SI:920:GLU:OE2	2.53	0.42
2:L1:991:G:N1	2:L1:1012:U:OP2	2.44	0.42
6:L5:225:ARG:NH1	15:LG:57:MET:HE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:500:PHE:CE1	16:LH:507:MET:HE2	2.55	0.42
18:LJ:474:LEU:HD13	18:LJ:480:LEU:HD23	2.02	0.42
20:LL:169:SER:OG	20:LL:170:ILE:N	2.53	0.42
23:LO:150:THR:N	23:LO:164:THR:O	2.51	0.42
23:LO:675:MET:HE1	29:NA:456:PHE:CD1	2.54	0.42
24:LQ:357:THR:OG1	24:LQ:361:THR:O	2.32	0.42
25:LR:514:THR:HG22	25:LR:530:ALA:HB2	2.01	0.42
34:NL:251:LEU:HD13	34:NL:317:PHE:CE1	2.55	0.42
35:NM:217:LEU:O	35:NM:217:LEU:HD23	2.20	0.42
42:SA:244:ASP:OD1	42:SA:245:SER:N	2.53	0.42
44:SC:171:LEU:N	44:SC:237:VAL:HG21	2.34	0.42
48:SI:123:ASP:O	48:SI:904:ASN:ND2	2.43	0.42
48:SI:161:HIS:NE2	48:SI:916:THR:HG21	2.35	0.42
52:SP:663:LEU:HD12	52:SP:696:VAL:HG22	2.01	0.42
2:L1:424:C:O2	2:L1:427:C:N4	2.53	0.42
7:L6:182:GLN:OE1	7:L6:182:GLN:N	2.53	0.42
8:L7:152:VAL:HG21	8:L7:181:ILE:HD11	2.01	0.42
9:L8:60:ILE:HG21	9:L8:179:CYS:SG	2.60	0.42
11:LC:58:ASP:OD1	11:LC:59:LYS:N	2.53	0.42
18:LJ:231:GLY:O	18:LJ:255:VAL:N	2.53	0.42
23:LO:261:ALA:HB1	23:LO:279:PHE:HB3	2.02	0.42
23:LO:717:LEU:HD11	27:LT:578:VAL:HG11	2.02	0.42
25:LR:10:ILE:HD12	25:LR:370:LEU:HD22	2.02	0.42
25:LR:67:LEU:HD11	25:LR:76:LEU:HD11	2.02	0.42
29:NA:359:SER:O	29:NA:362:THR:OG1	2.25	0.42
29:NA:555:ASP:O	29:NA:559:LYS:N	2.48	0.42
34:NL:98:VAL:O	34:NL:98:VAL:HG22	2.19	0.42
43:SB:215:ARG:NH1	43:SB:242:SER:OG	2.53	0.42
43:SB:230:GLU:HG2	43:SB:231:ILE:HD12	2.02	0.42
44:SD:304:LEU:HD13	60:SY:133:HIS:HD2	1.79	0.42
6:L5:16:VAL:HG12	27:LT:498:TYR:CD1	2.55	0.41
8:L7:74:GLN:O	8:L7:78:THR:HG22	2.20	0.41
11:LC:65:ILE:HG21	11:LC:85:ILE:CD1	2.50	0.41
23:LO:558:ASP:OD1	27:LT:423:ARG:NH1	2.46	0.41
24:LQ:175:ASP:OD1	24:LQ:175:ASP:N	2.51	0.41
25:LR:612:THR:O	25:LR:612:THR:HG23	2.20	0.41
44:SC:277:ASP:OD1	44:SC:279:THR:OG1	2.22	0.41
59:SW:222:THR:O	59:SW:223:ARG:NH1	2.49	0.41
2:L1:871:G:H2'	2:L1:872:G:C8	2.55	0.41
23:LO:354:SER:OG	23:LO:356:ASP:OD1	2.22	0.41
24:LQ:190:ASP:HB2	24:LQ:197:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:LQ:589:ILE:CG2	24:LQ:597:ILE:HD11	2.50	0.41
25:LR:694:LEU:HA	25:LR:697:VAL:HG12	2.02	0.41
26:LS:512:ASP:OD1	26:LS:512:ASP:N	2.54	0.41
31:ND:177:ARG:CG	60:SY:134:THR:HG22	2.50	0.41
32:NF:132:VAL:HG22	32:NF:132:VAL:O	2.20	0.41
43:SB:209:ILE:H	43:SB:209:ILE:HD12	1.85	0.41
46:SG:156:ASN:HA	46:SG:544:ALA:HB1	2.03	0.41
2:L1:896:U:O2	33:NG:41:ARG:NH1	2.42	0.41
2:L1:1650:U:H2'	2:L1:1651:A:O4'	2.20	0.41
6:L5:37:GLN:N	11:LC:53:LEU:HD11	2.35	0.41
16:LH:16:SER:HG	16:LH:465:ASN:CG	2.24	0.41
16:LH:86:GLU:OE2	16:LH:113:ASN:ND2	2.52	0.41
16:LH:320:VAL:HG22	16:LH:335:PRO:HA	2.02	0.41
16:LH:657:SER:HG	16:LH:674:THR:HG1	1.55	0.41
18:LJ:495:ILE:HG22	18:LJ:499:LYS:HE2	2.03	0.41
20:LL:520:MET:SD	20:LL:520:MET:N	2.91	0.41
23:LO:17:GLN:NE2	23:LO:58:ILE:O	2.51	0.41
24:LQ:137:ILE:CD1	24:LQ:147:VAL:HG22	2.50	0.41
24:LQ:176:TRP:CZ3	24:LQ:188:LEU:HD21	2.55	0.41
26:LS:405:THR:HG21	26:LS:455:ILE:O	2.21	0.41
26:LS:568:VAL:HG23	26:LS:577:LEU:HD11	2.02	0.41
29:NA:297:LEU:O	29:NA:302:LYS:NZ	2.53	0.41
14:LF:51:GLU:HA	14:LF:51:GLU:OE2	2.21	0.41
16:LH:148:GLU:HG2	16:LH:148:GLU:O	2.21	0.41
16:LH:321:MET:HE1	16:LH:356:LEU:HD11	2.03	0.41
23:LO:70:LEU:HD23	23:LO:70:LEU:C	2.45	0.41
24:LQ:197:ILE:HG22	24:LQ:198:GLU:HG3	2.02	0.41
25:LR:699:LYS:HD3	25:LR:755:ILE:HD11	2.02	0.41
27:LT:430:ILE:HB	27:LT:443:TRP:HB2	2.02	0.41
43:SB:14:LEU:CD1	43:SB:79:ILE:HD12	2.50	0.41
51:SM:111:PHE:CE1	51:SM:209:LEU:HD23	2.56	0.41
59:SW:117:TYR:N	59:SW:118:PRO:CD	2.83	0.41
5:L4:54:TYR:OH	5:L4:97:GLU:OE2	2.38	0.41
8:L7:8:ILE:HG21	8:L7:13:PRO:HB3	2.02	0.41
8:L7:136:VAL:N	8:L7:153:LEU:O	2.50	0.41
10:L9:151:ASP:OD1	10:L9:152:SER:N	2.53	0.41
20:LL:85:ILE:HD11	20:LL:107:ILE:HG12	2.03	0.41
24:LQ:913:ASN:O	24:LQ:917:ASN:N	2.54	0.41
25:LR:25:VAL:HG11	25:LR:296:ILE:HD11	2.02	0.41
25:LR:220:ILE:CD1	25:LR:243:VAL:HG21	2.49	0.41
25:LR:343:MET:SD	25:LR:635:ALA:HB2	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LT:854:SER:HB2	27:LT:895:VAL:HG21	2.03	0.41
34:NL:70:LEU:HD13	34:NL:128:ASN:OD1	2.20	0.41
52:SP:163:SER:O	52:SP:167:VAL:HG23	2.20	0.41
60:SY:44:LYS:O	60:SY:48:LEU:N	2.53	0.41
1:L0:278:G:N2	26:LS:539:ASP:OD2	2.47	0.41
2:L1:1132:A:N7	47:SH:206:ASN:ND2	2.66	0.41
2:L1:1555:A:HO2'	2:L1:1556:A:P	2.43	0.41
6:L5:55:ASP:OD2	6:L5:57:SER:OG	2.38	0.41
11:LC:113:ASP:OD1	11:LC:115:THR:N	2.43	0.41
16:LH:292:LEU:C	16:LH:293:LEU:HD12	2.45	0.41
20:LL:27:GLN:HB2	20:LL:53:LEU:HD12	2.03	0.41
22:LN:252:GLN:NE2	22:LN:318:ASN:OD1	2.54	0.41
23:LO:331:GLU:HB2	23:LO:338:ILE:HD11	2.02	0.41
23:LO:582:THR:HG23	23:LO:684:VAL:HG22	2.03	0.41
24:LQ:308:LEU:HD23	24:LQ:312:GLU:HB3	2.02	0.41
24:LQ:454:LEU:HD23	24:LQ:471:ALA:HB3	2.02	0.41
25:LR:472:THR:HG22	25:LR:474:SER:H	1.86	0.41
35:NM:61:LEU:HD22	35:NM:96:LEU:HD22	2.02	0.41
39:NV:729:LEU:HD12	39:NV:729:LEU:C	2.46	0.41
42:SA:7:LEU:CD1	42:SA:99:ALA:HB3	2.51	0.41
52:SP:374:LEU:O	52:SP:378:HIS:N	2.54	0.41
3:L2:92:A:H2'	43:SB:323:GLU:OE2	2.21	0.41
11:LC:97:VAL:HG12	11:LC:98:ASP:N	2.35	0.41
13:LE:53:ILE:HD13	37:NQ:24:LEU:HD11	2.03	0.41
16:LH:723:VAL:O	16:LH:723:VAL:HG13	2.20	0.41
23:LO:30:LEU:HD13	23:LO:39:VAL:HG22	2.02	0.41
23:LO:187:PHE:HE2	23:LO:206:ILE:HG21	1.86	0.41
24:LQ:534:ILE:CG2	24:LQ:548:ILE:HD11	2.50	0.41
25:LR:6:SER:H	25:LR:648:THR:HG22	1.86	0.41
27:LT:380:LEU:HD23	27:LT:380:LEU:O	2.20	0.41
34:NL:140:LYS:HE2	34:NL:141:LEU:HD12	2.03	0.41
45:SF:60:PRO:HD2	45:SF:63:ILE:HD11	2.02	0.41
45:SF:110:ILE:HG13	45:SF:114:ILE:HD11	2.02	0.41
52:SP:455:GLU:OE1	52:SP:455:GLU:N	2.52	0.41
58:SV:155:ASN:OD1	58:SV:156:THR:HG23	2.20	0.41
1:L0:6:A:O2'	1:L0:7:A:OP2	2.32	0.41
2:L1:1078:C:OP1	55:SS:394:ALA:HB1	2.21	0.41
5:L4:133:LYS:O	5:L4:136:VAL:HG22	2.21	0.41
16:LH:661:THR:HG22	16:LH:708:ASP:HA	2.02	0.41
18:LJ:507:MET:HE1	19:LK:502:ARG:CA	2.42	0.41
20:LL:277:LYS:NZ	20:LL:322:ILE:O	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LL:476:LEU:HD13	20:LL:479:ILE:HD11	2.03	0.41
23:LO:263:VAL:HG13	23:LO:277:VAL:CG2	2.49	0.41
24:LQ:809:LEU:O	24:LQ:809:LEU:HD23	2.21	0.41
25:LR:188:GLU:OE1	25:LR:221:ASN:ND2	2.45	0.41
30:NB:540:ILE:HA	48:SI:150:MET:HE2	2.02	0.41
43:SB:110:ASP:OD1	43:SB:111:ALA:N	2.52	0.41
48:SI:100:ASP:OD1	48:SI:101:ILE:N	2.54	0.41
48:SI:126:ASN:OD1	48:SI:1020:SER:OG	2.30	0.41
52:SP:1069:VAL:O	52:SP:1069:VAL:HG22	2.20	0.41
56:ST:113:ILE:O	56:ST:113:ILE:HG13	2.20	0.41
2:L1:867:G:H21	32:NF:87:ASP:HB3	1.86	0.41
16:LH:89:VAL:HG22	16:LH:110:PHE:O	2.20	0.41
16:LH:664:LEU:H	16:LH:664:LEU:HD23	1.86	0.41
17:LI:661:TYR:O	17:LI:664:LYS:HB3	2.21	0.41
18:LJ:263:ASN:O	18:LJ:310:SER:OG	2.37	0.41
18:LJ:263:ASN:ND2	18:LJ:269:GLN:OE1	2.49	0.41
18:LJ:264:PHE:HZ	18:LJ:271:ALA:HB2	1.85	0.41
18:LJ:495:ILE:HD11	20:LL:544:ASP:OD2	2.21	0.41
18:LJ:507:MET:SD	19:LK:505:MET:HB2	2.61	0.41
19:LK:407:MET:HE2	19:LK:407:MET:HA	2.03	0.41
20:LL:163:LEU:HG	20:LL:175:ILE:HD11	2.03	0.41
20:LL:586:ASP:OD2	22:LN:423:LYS:NZ	2.48	0.41
23:LO:30:LEU:CD1	23:LO:39:VAL:HG22	2.50	0.41
23:LO:62:ASP:OD1	23:LO:71:ILE:HG22	2.20	0.41
23:LO:217:VAL:HG12	23:LO:219:GLU:OE2	2.21	0.41
23:LO:261:ALA:HB2	23:LO:281:SER:HB3	2.03	0.41
23:LO:432:GLN:O	23:LO:449:SER:OG	2.38	0.41
23:LO:497:ILE:CD1	23:LO:532:VAL:HG11	2.51	0.41
23:LO:610:VAL:HG12	23:LO:611:LEU:N	2.36	0.41
24:LQ:95:ALA:HB2	24:LQ:129:PHE:CZ	2.56	0.41
24:LQ:137:ILE:HD12	24:LQ:147:VAL:HG22	2.03	0.41
24:LQ:355:LEU:O	24:LQ:355:LEU:HD12	2.21	0.41
24:LQ:614:HIS:CD2	24:LQ:618:ILE:HD13	2.56	0.41
27:LT:626:ASP:OD1	27:LT:627:ASN:N	2.53	0.41
29:NA:307:ILE:HD11	48:SI:1016:ASN:CG	2.46	0.41
31:ND:185:GLN:O	31:ND:189:THR:HG23	2.21	0.41
36:NP:22:LEU:HD13	36:NP:28:LEU:HD22	2.03	0.41
47:SH:11:PHE:CZ	47:SH:332:ILE:HD11	2.56	0.41
48:SI:43:MET:HE1	54:SR:38:PHE:CB	2.51	0.41
48:SI:548:ASN:OD1	48:SI:550:GLY:N	2.54	0.41
48:SI:557:ASN:OD1	48:SI:558:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SP:264:THR:HG22	52:SP:266:SER:H	1.86	0.41
52:SP:323:PHE:CD1	52:SP:736:LEU:HD13	2.56	0.41
52:SP:355:GLN:NE2	52:SP:388:ASN:O	2.54	0.41
52:SP:1761:ILE:HG22	52:SP:1762:SER:O	2.21	0.41
52:SP:1809:GLU:OE2	52:SP:1812:LEU:HD12	2.21	0.41
60:SY:32:LYS:O	60:SY:36:LYS:NZ	2.52	0.41
5:L4:122:LYS:NZ	5:L4:143:ASP:OD2	2.43	0.41
16:LH:252:LEU:HB3	16:LH:256:THR:HG21	2.03	0.41
18:LJ:217:ASN:CG	18:LJ:219:ILE:HD11	2.46	0.41
18:LJ:440:GLU:HG3	18:LJ:483:LEU:HD11	2.02	0.41
22:LN:186:GLN:NE2	22:LN:188:ALA:O	2.52	0.41
23:LO:739:LEU:CA	23:LO:754:VAL:HG11	2.50	0.41
42:SA:257:ILE:HG13	42:SA:257:ILE:O	2.20	0.41
42:SA:307:ILE:HD11	42:SA:379:LEU:HD11	2.02	0.41
52:SP:1563:ARG:NE	52:SP:1622:GLY:O	2.49	0.41
11:LC:42:GLU:OE2	11:LC:45:ARG:NH1	2.53	0.40
11:LC:101:SER:O	11:LC:105:LEU:HD13	2.21	0.40
20:LL:261:VAL:O	20:LL:273:LYS:NZ	2.49	0.40
23:LO:154:TRP:CZ2	23:LO:161:ILE:HD11	2.56	0.40
24:LQ:217:LEU:O	24:LQ:229:TRP:N	2.50	0.40
24:LQ:233:ILE:H	24:LQ:233:ILE:HD12	1.86	0.40
26:LS:518:ILE:HG21	26:LS:521:LEU:HD21	2.03	0.40
2:L1:194:U:O2'	2:L1:195:G:O5'	2.20	0.40
16:LH:598:LYS:NZ	16:LH:635:PHE:O	2.49	0.40
24:LQ:884:LYS:HE3	25:LR:807:ASP:OD1	2.21	0.40
25:LR:161:TRP:CH2	59:SW:73:VAL:HG22	2.56	0.40
26:LS:157:GLY:O	26:LS:161:ILE:N	2.40	0.40
32:NF:87:ASP:OD1	32:NF:88:LEU:N	2.52	0.40
43:SB:1:MET:HE3	43:SB:17:ALA:O	2.21	0.40
47:SH:365:LYS:NZ	47:SH:366:ILE:O	2.54	0.40
52:SP:1907:ASN:HB3	52:SP:1910:VAL:HG12	2.03	0.40
2:L1:514:G:N7	10:L9:171:ARG:NH2	2.69	0.40
16:LH:139:GLU:OE2	16:LH:172:ARG:NH1	2.54	0.40
16:LH:321:MET:HE3	16:LH:356:LEU:HD21	2.03	0.40
16:LH:459:ILE:O	16:LH:468:VAL:HG12	2.21	0.40
16:LH:573:CYS:SG	16:LH:574:LEU:N	2.94	0.40
18:LJ:281:VAL:HG22	18:LJ:298:PHE:HE2	1.86	0.40
23:LO:792:ILE:HG23	23:LO:793:GLU:N	2.36	0.40
25:LR:692:MET:HE2	29:NA:519:GLU:CD	2.47	0.40
45:SF:17:THR:HG21	45:SF:82:PRO:CD	2.52	0.40
52:SP:1604:GLU:HG3	52:SP:1605:THR:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L6:78:THR:HG22	7:L6:92:ARG:HD2	2.02	0.40
16:LH:77:ILE:HG23	16:LH:115:HIS:ND1	2.37	0.40
16:LH:671:ILE:HD11	16:LH:750:LEU:HD11	2.03	0.40
17:LI:558:CYS:O	17:LI:585:ARG:NH2	2.43	0.40
18:LJ:148:VAL:HG12	18:LJ:165:THR:HG22	2.02	0.40
23:LO:717:LEU:H	23:LO:717:LEU:HD23	1.85	0.40
24:LQ:454:LEU:HD21	24:LQ:476:ILE:HG12	2.02	0.40
24:LQ:589:ILE:HG21	24:LQ:621:VAL:HG11	2.02	0.40
25:LR:595:ALA:HA	25:LR:619:ARG:HG3	2.03	0.40
25:LR:795:ARG:O	25:LR:796:VAL:HB	2.22	0.40
27:LT:438:LYS:NZ	27:LT:457:THR:OG1	2.46	0.40
31:ND:172:LYS:HZ1	31:ND:175:LYS:C	2.23	0.40
33:NG:48:VAL:HG21	33:NG:53:ASP:HB2	2.02	0.40
36:NP:44:GLU:OE1	36:NP:44:GLU:N	2.54	0.40
38:NS:429:TYR:O	38:NS:435:ALA:HA	2.20	0.40
42:SA:74:VAL:HG13	42:SA:74:VAL:O	2.22	0.40
42:SA:163:VAL:O	42:SA:163:VAL:HG22	2.22	0.40
44:SD:319:ARG:HD2	44:SD:321:MET:HE2	2.03	0.40
45:SE:26:GLN:HA	45:SE:29:ASN:OD1	2.21	0.40
46:SG:419:ASN:ND2	46:SG:421:ASN:OD1	2.55	0.40
48:SI:83:THR:OG1	48:SI:119:GLU:OE1	2.38	0.40
48:SI:829:LEU:HD21	48:SI:915:ALA:HB1	2.04	0.40
52:SP:897:PHE:CE1	52:SP:901:ILE:HD11	2.56	0.40
2:L1:1159:C:OP2	51:SM:105:LYS:NZ	2.38	0.40
17:LI:517:ASN:O	17:LI:547:GLN:NE2	2.55	0.40
18:LJ:116:ILE:HG23	18:LJ:116:ILE:O	2.21	0.40
25:LR:351:ASN:O	25:LR:367:VAL:HG23	2.21	0.40
25:LR:740:MET:HE3	25:LR:763:ILE:HD13	2.04	0.40
35:NM:19:ARG:NH1	35:NM:21:VAL:O	2.55	0.40
35:NM:156:ALA:HB3	35:NM:161:ILE:HD11	2.02	0.40
42:SA:243:GLU:O	42:SA:246:GLY:N	2.51	0.40
45:SF:64:LEU:CD2	45:SF:98:ILE:HD12	2.51	0.40
47:SH:136:GLY:O	47:SH:293:GLN:NE2	2.55	0.40
52:SP:323:PHE:HB2	52:SP:364:LEU:HD13	2.03	0.40
52:SP:991:LEU:HB3	52:SP:1047:LEU:HD13	2.04	0.40
52:SP:1416:GLU:O	52:SP:1419:SER:N	2.55	0.40
59:SW:187:VAL:HG12	59:SW:229:SER:HB3	2.03	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L3	102/146 (70%)	102 (100%)	0	0	100	100
5	L4	242/261 (93%)	240 (99%)	2 (1%)	0	100	100
6	L5	202/225 (90%)	197 (98%)	5 (2%)	0	100	100
7	L6	214/236 (91%)	211 (99%)	3 (1%)	0	100	100
8	L7	174/190 (92%)	171 (98%)	3 (2%)	0	100	100
9	L8	166/200 (83%)	162 (98%)	4 (2%)	0	100	100
10	L9	179/197 (91%)	176 (98%)	3 (2%)	0	100	100
11	LC	126/143 (88%)	123 (98%)	3 (2%)	0	100	100
12	LD	135/156 (86%)	133 (98%)	2 (2%)	0	100	100
13	LE	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
14	LF	128/135 (95%)	125 (98%)	3 (2%)	0	100	100
15	LG	60/67 (90%)	60 (100%)	0	0	100	100
16	LH	788/896 (88%)	768 (98%)	20 (2%)	0	100	100
17	LI	582/713 (82%)	574 (99%)	8 (1%)	0	100	100
18	LJ	470/513 (92%)	461 (98%)	9 (2%)	0	100	100
19	LK	130/575 (23%)	129 (99%)	1 (1%)	0	100	100
20	LL	475/643 (74%)	465 (98%)	10 (2%)	0	100	100
21	LM	1573/1769 (89%)	1547 (98%)	26 (2%)	0	100	100
22	LN	649/776 (84%)	634 (98%)	15 (2%)	0	100	100
23	LO	786/923 (85%)	771 (98%)	15 (2%)	0	100	100
24	LQ	806/943 (86%)	787 (98%)	19 (2%)	0	100	100
25	LR	785/817 (96%)	767 (98%)	18 (2%)	0	100	100
26	LS	420/594 (71%)	410 (98%)	10 (2%)	0	100	100
27	LT	852/939 (91%)	835 (98%)	17 (2%)	0	100	100
28	LZ	140/183 (76%)	140 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	NA	312/593 (53%)	311 (100%)	1 (0%)	0	100	100
30	NB	248/610 (41%)	244 (98%)	4 (2%)	0	100	100
31	ND	70/214 (33%)	69 (99%)	1 (1%)	0	100	100
32	NF	139/151 (92%)	137 (99%)	2 (1%)	0	100	100
33	NG	125/137 (91%)	122 (98%)	3 (2%)	0	100	100
34	NL	279/318 (88%)	276 (99%)	3 (1%)	0	100	100
35	NM	225/255 (88%)	222 (99%)	3 (1%)	0	100	100
36	NP	130/144 (90%)	126 (97%)	4 (3%)	0	100	100
37	NQ	77/82 (94%)	75 (97%)	2 (3%)	0	100	100
38	NS	917/1267 (72%)	898 (98%)	19 (2%)	0	100	100
39	NV	17/733 (2%)	17 (100%)	0	0	100	100
40	OH	118/143 (82%)	117 (99%)	1 (1%)	0	100	100
41	OU	54/152 (36%)	54 (100%)	0	0	100	100
42	SA	390/504 (77%)	387 (99%)	3 (1%)	0	100	100
43	SB	420/511 (82%)	411 (98%)	9 (2%)	0	100	100
44	SC	237/327 (72%)	231 (98%)	6 (2%)	0	100	100
44	SD	234/327 (72%)	232 (99%)	2 (1%)	0	100	100
45	SE	119/126 (94%)	114 (96%)	5 (4%)	0	100	100
45	SF	119/126 (94%)	118 (99%)	1 (1%)	0	100	100
46	SG	453/573 (79%)	443 (98%)	10 (2%)	0	100	100
47	SH	358/367 (98%)	352 (98%)	6 (2%)	0	100	100
48	SI	773/1183 (65%)	760 (98%)	13 (2%)	0	100	100
49	SJ	207/252 (82%)	204 (99%)	3 (1%)	0	100	100
49	SK	225/252 (89%)	222 (99%)	3 (1%)	0	100	100
50	SL	146/189 (77%)	140 (96%)	6 (4%)	0	100	100
51	SM	243/290 (84%)	242 (100%)	1 (0%)	0	100	100
52	SP	1832/2493 (74%)	1806 (99%)	26 (1%)	0	100	100
53	SQ	95/217 (44%)	92 (97%)	3 (3%)	0	100	100
54	SR	130/145 (90%)	129 (99%)	1 (1%)	0	100	100
55	SS	113/899 (13%)	110 (97%)	3 (3%)	0	100	100
56	ST	562/810 (69%)	557 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	SU	524/552 (95%)	520 (99%)	4 (1%)	0	100	100
58	SV	151/206 (73%)	148 (98%)	3 (2%)	0	100	100
59	SW	204/274 (74%)	200 (98%)	4 (2%)	0	100	100
60	SY	193/250 (77%)	187 (97%)	6 (3%)	0	100	100
61	SZ	255/483 (53%)	253 (99%)	2 (1%)	0	100	100
All	All	21005/28525 (74%)	20635 (98%)	370 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L3	96/129 (74%)	95 (99%)	1 (1%)	73	81
5	L4	208/222 (94%)	208 (100%)	0	100	100
6	L5	179/191 (94%)	179 (100%)	0	100	100
7	L6	185/201 (92%)	185 (100%)	0	100	100
8	L7	158/170 (93%)	158 (100%)	0	100	100
9	L8	137/161 (85%)	137 (100%)	0	100	100
10	L9	156/166 (94%)	156 (100%)	0	100	100
11	LC	107/119 (90%)	107 (100%)	0	100	100
12	LD	124/137 (90%)	123 (99%)	1 (1%)	79	84
13	LE	110/111 (99%)	110 (100%)	0	100	100
14	LF	109/113 (96%)	109 (100%)	0	100	100
15	LG	55/60 (92%)	55 (100%)	0	100	100
16	LH	696/826 (84%)	696 (100%)	0	100	100
17	LI	244/657 (37%)	244 (100%)	0	100	100
18	LJ	421/454 (93%)	421 (100%)	0	100	100
19	LK	124/533 (23%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	LL	438/574 (76%)	437 (100%)	1 (0%)	92	93
21	LM	43/1633 (3%)	43 (100%)	0	100	100
22	LN	603/713 (85%)	603 (100%)	0	100	100
23	LO	695/812 (86%)	695 (100%)	0	100	100
24	LQ	723/832 (87%)	722 (100%)	1 (0%)	92	95
25	LR	698/719 (97%)	698 (100%)	0	100	100
26	LS	319/528 (60%)	319 (100%)	0	100	100
27	LT	494/819 (60%)	494 (100%)	0	100	100
28	LZ	132/172 (77%)	132 (100%)	0	100	100
29	NA	235/535 (44%)	235 (100%)	0	100	100
30	NB	99/538 (18%)	99 (100%)	0	100	100
31	ND	57/196 (29%)	57 (100%)	0	100	100
32	NF	121/128 (94%)	121 (100%)	0	100	100
33	NG	96/105 (91%)	96 (100%)	0	100	100
34	NL	257/283 (91%)	257 (100%)	0	100	100
35	NM	203/224 (91%)	202 (100%)	1 (0%)	86	89
36	NP	107/116 (92%)	107 (100%)	0	100	100
37	NQ	68/71 (96%)	68 (100%)	0	100	100
38	NS	135/1140 (12%)	135 (100%)	0	100	100
39	NV	14/671 (2%)	14 (100%)	0	100	100
40	OH	2/119 (2%)	2 (100%)	0	100	100
41	OU	1/135 (1%)	1 (100%)	0	100	100
42	SA	328/435 (75%)	328 (100%)	0	100	100
43	SB	352/433 (81%)	352 (100%)	0	100	100
44	SC	200/240 (83%)	200 (100%)	0	100	100
44	SD	198/240 (82%)	198 (100%)	0	100	100
45	SE	100/104 (96%)	100 (100%)	0	100	100
45	SF	100/104 (96%)	100 (100%)	0	100	100
46	SG	399/503 (79%)	399 (100%)	0	100	100
47	SH	307/312 (98%)	307 (100%)	0	100	100
48	SI	692/1039 (67%)	692 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	SJ	9/222 (4%)	9 (100%)	0	100	100
49	SK	12/222 (5%)	12 (100%)	0	100	100
50	SL	131/169 (78%)	131 (100%)	0	100	100
51	SM	220/258 (85%)	220 (100%)	0	100	100
52	SP	1725/2307 (75%)	1724 (100%)	1 (0%)	92	95
53	SQ	91/200 (46%)	91 (100%)	0	100	100
54	SR	113/120 (94%)	113 (100%)	0	100	100
55	SS	105/808 (13%)	105 (100%)	0	100	100
56	ST	125/732 (17%)	125 (100%)	0	100	100
57	SU	27/506 (5%)	27 (100%)	0	100	100
58	SV	20/192 (10%)	20 (100%)	0	100	100
59	SW	183/238 (77%)	183 (100%)	0	100	100
60	SY	191/234 (82%)	191 (100%)	0	100	100
61	SZ	14/424 (3%)	14 (100%)	0	100	100
All	All	14291/25355 (56%)	14285 (100%)	6 (0%)	100	100

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L3	8	GLN
12	LD	98	ASN
20	LL	335	ASN
24	LQ	230	LYS
35	NM	124	ASN
52	SP	452	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
5	L4	67	GLN
5	L4	69	HIS
5	L4	112	HIS
5	L4	142	HIS
5	L4	216	ASN
6	L5	35	GLN
6	L5	63	GLN

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Mol	Chain	Res	Type
6	L5	104	ASN
6	L5	131	GLN
6	L5	200	ASN
9	L8	44	HIS
10	L9	112	GLN
11	LC	8	GLN
11	LC	74	HIS
12	LD	138	ASN
13	LE	24	GLN
14	LF	29	HIS
14	LF	110	GLN
16	LH	184	GLN
16	LH	255	ASN
17	LI	597	GLN
18	LJ	51	HIS
18	LJ	64	GLN
18	LJ	121	ASN
18	LJ	135	GLN
18	LJ	382	GLN
19	LK	474	HIS
20	LL	168	HIS
20	LL	302	ASN
20	LL	324	ASN
20	LL	346	HIS
20	LL	458	ASN
20	LL	499	ASN
22	LN	329	HIS
22	LN	385	ASN
22	LN	467	ASN
22	LN	574	HIS
23	LO	91	HIS
23	LO	132	GLN
23	LO	142	HIS
23	LO	203	GLN
23	LO	254	HIS
23	LO	303	ASN
23	LO	344	HIS
23	LO	597	ASN
24	LQ	194	HIS
24	LQ	200	HIS
24	LQ	276	ASN
24	LQ	657	GLN

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Mol	Chain	Res	Type
24	LQ	871	GLN
25	LR	157	ASN
25	LR	433	HIS
26	LS	330	ASN
26	LS	388	HIS
26	LS	472	GLN
26	LS	593	HIS
27	LT	473	ASN
27	LT	793	GLN
27	LT	897	HIS
27	LT	916	HIS
28	LZ	74	HIS
28	LZ	135	HIS
29	NA	434	HIS
30	NB	558	ASN
34	NL	23	HIS
35	NM	16	GLN
35	NM	194	ASN
36	NP	64	HIS
37	NQ	9	HIS
38	NS	16	HIS
38	NS	103	HIS
42	SA	183	GLN
42	SA	276	GLN
42	SA	297	HIS
43	SB	334	HIS
43	SB	344	HIS
45	SE	26	GLN
46	SG	311	GLN
46	SG	322	HIS
47	SH	126	ASN
48	SI	24	GLN
48	SI	55	HIS
48	SI	878	HIS
48	SI	1055	HIS
48	SI	1063	HIS
51	SM	168	HIS
51	SM	208	HIS
52	SP	46	HIS
52	SP	53	GLN
52	SP	183	HIS
52	SP	346	GLN

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Mol	Chain	Res	Type
52	SP	452	ASN
52	SP	588	ASN
52	SP	1020	ASN
52	SP	1100	GLN
52	SP	1483	HIS
52	SP	1502	ASN
52	SP	1508	GLN
52	SP	1630	ASN
52	SP	1707	HIS
52	SP	1816	HIS
52	SP	1883	HIS
53	SQ	135	HIS
54	SR	18	HIS
54	SR	48	HIS
54	SR	63	GLN
55	SS	431	HIS
55	SS	457	HIS
60	SY	12	GLN
60	SY	200	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L0	63/700 (9%)	11 (17%)	0
2	L1	1369/1803 (75%)	281 (20%)	10 (0%)
3	L2	198/334 (59%)	23 (11%)	1 (0%)
All	All	1630/2837 (57%)	315 (19%)	11 (0%)

All (315) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L0	7	A
1	L0	61	U
1	L0	63	G
1	L0	64	U
1	L0	83	U
1	L0	85	G
1	L0	86	C
1	L0	90	G
1	L0	279	A
1	L0	280	A

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Mol	Chain	Res	Type
1	L0	281	G
2	L1	2	A
2	L1	9	U
2	L1	10	G
2	L1	15	U
2	L1	24	U
2	L1	25	C
2	L1	26	A
2	L1	34	G
2	L1	46	A
2	L1	47	A
2	L1	60	U
2	L1	65	A
2	L1	68	A
2	L1	76	A
2	L1	104	A
2	L1	114	C
2	L1	127	G
2	L1	129	U
2	L1	134	U
2	L1	136	C
2	L1	137	U
2	L1	140	A
2	L1	142	G
2	L1	144	U
2	L1	145	A
2	L1	159	U
2	L1	166	C
2	L1	186	C
2	L1	187	G
2	L1	189	C
2	L1	190	C
2	L1	193	U
2	L1	195	G
2	L1	204	G
2	L1	205	U
2	L1	226	A
2	L1	233	C
2	L1	234	G
2	L1	241	U
2	L1	242	U
2	L1	260	U

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Mol	Chain	Res	Type
2	L1	261	U
2	L1	265	A
2	L1	275	C
2	L1	276	C
2	L1	278	U
2	L1	279	G
2	L1	280	U
2	L1	299	A
2	L1	314	C
2	L1	316	A
2	L1	322	G
2	L1	337	G
2	L1	338	C
2	L1	344	A
2	L1	352	A
2	L1	359	A
2	L1	360	A
2	L1	361	C
2	L1	400	A
2	L1	401	A
2	L1	402	C
2	L1	404	G
2	L1	423	G
2	L1	424	C
2	L1	425	A
2	L1	426	G
2	L1	437	A
2	L1	438	A
2	L1	439	U
2	L1	444	C
2	L1	448	C
2	L1	453	U
2	L1	460	A
2	L1	467	G
2	L1	477	A
2	L1	487	G
2	L1	494	U
2	L1	495	C
2	L1	496	G
2	L1	501	U
2	L1	502	U
2	L1	505	A

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Mol	Chain	Res	Type
2	L1	506	A
2	L1	511	A
2	L1	515	A
2	L1	519	C
2	L1	520	A
2	L1	532	U
2	L1	534	A
2	L1	538	A
2	L1	542	A
2	L1	545	A
2	L1	563	U
2	L1	564	G
2	L1	565	C
2	L1	570	A
2	L1	578	U
2	L1	580	A
2	L1	583	C
2	L1	585	A
2	L1	586	G
2	L1	594	A
2	L1	595	G
2	L1	611	U
2	L1	619	A
2	L1	620	A
2	L1	622	A
2	L1	624	G
2	L1	629	U
2	L1	652	G
2	L1	654	C
2	L1	687	G
2	L1	688	G
2	L1	765	G
2	L1	766	U
2	L1	774	A
2	L1	785	U
2	L1	786	C
2	L1	787	G
2	L1	788	A
2	L1	789	A
2	L1	790	U
2	L1	793	A
2	L1	794	U

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Mol	Chain	Res	Type
2	L1	803	A
2	L1	804	A
2	L1	809	A
2	L1	811	A
2	L1	812	A
2	L1	813	U
2	L1	859	A
2	L1	860	U
2	L1	862	A
2	L1	863	A
2	L1	876	G
2	L1	881	A
2	L1	886	U
2	L1	898	A
2	L1	899	G
2	L1	914	G
2	L1	921	U
2	L1	926	A
2	L1	933	A
2	L1	934	C
2	L1	935	U
2	L1	944	A
2	L1	960	U
2	L1	962	C
2	L1	966	A
2	L1	969	C
2	L1	992	A
2	L1	993	A
2	L1	1005	A
2	L1	1007	C
2	L1	1011	G
2	L1	1020	A
2	L1	1026	A
2	L1	1028	C
2	L1	1029	U
2	L1	1032	G
2	L1	1040	G
2	L1	1052	U
2	L1	1053	G
2	L1	1058	U
2	L1	1059	U
2	L1	1060	U

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Mol	Chain	Res	Type
2	L1	1062	A
2	L1	1076	A
2	L1	1078	C
2	L1	1081	A
2	L1	1083	G
2	L1	1092	A
2	L1	1096	C
2	L1	1097	U
2	L1	1098	U
2	L1	1099	U
2	L1	1100	G
2	L1	1109	G
2	L1	1114	G
2	L1	1119	G
2	L1	1128	C
2	L1	1130	G
2	L1	1131	A
2	L1	1139	A
2	L1	1158	C
2	L1	1159	C
2	L1	1167	G
2	L1	1179	G
2	L1	1189	A
2	L1	1191	U
2	L1	1192	C
2	L1	1193	A
2	L1	1195	C
2	L1	1197	C
2	L1	1200	G
2	L1	1202	A
2	L1	1205	C
2	L1	1207	C
2	L1	1227	A
2	L1	1229	G
2	L1	1232	U
2	L1	1254	U
2	L1	1266	U
2	L1	1267	G
2	L1	1268	G
2	L1	1270	G
2	L1	1273	G
2	L1	1275	A

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Mol	Chain	Res	Type
2	L1	1276	U
2	L1	1436	A
2	L1	1437	U
2	L1	1440	C
2	L1	1451	C
2	L1	1453	G
2	L1	1465	C
2	L1	1471	A
2	L1	1481	C
2	L1	1486	G
2	L1	1487	A
2	L1	1494	C
2	L1	1496	U
2	L1	1497	U
2	L1	1510	U
2	L1	1511	U
2	L1	1535	U
2	L1	1537	C
2	L1	1542	G
2	L1	1548	G
2	L1	1553	G
2	L1	1554	U
2	L1	1555	A
2	L1	1556	A
2	L1	1557	U
2	L1	1559	A
2	L1	1569	A
2	L1	1570	A
2	L1	1579	U
2	L1	1583	A
2	L1	1584	G
2	L1	1590	G
2	L1	1595	U
2	L1	1599	C
2	L1	1600	A
2	L1	1601	G
2	L1	1602	C
2	L1	1617	U
2	L1	1618	C
2	L1	1619	C
2	L1	1624	C
2	L1	1628	U

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Mol	Chain	Res	Type
2	L1	1629	G
2	L1	1630	U
2	L1	1631	A
2	L1	1639	C
2	L1	1645	G
2	L1	1651	A
2	L1	1653	C
2	L1	1655	A
2	L1	1657	U
2	L1	1658	G
2	L1	1663	G
2	L1	1742	U
2	L1	1744	A
2	L1	1747	G
2	L1	1755	A
2	L1	1756	A
2	L1	1772	C
2	L1	1777	G
2	L1	1780	G
2	L1	1781	A
2	L1	1782	A
2	L1	1783	C
2	L1	1784	C
2	L1	1792	G
2	L1	1794	A
2	L1	1795	U
2	L1	1800	A
2	L1	1801	A
2	L1	1802	A
2	L1	1803	G
3	L2	2	U
3	L2	10	C
3	L2	13	C
3	L2	15	U
3	L2	16	A
3	L2	18	G
3	L2	88	U
3	L2	90	C
3	L2	91	C
3	L2	109	G
3	L2	145	U
3	L2	155	U

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Mol	Chain	Res	Type
3	L2	156	U
3	L2	157	A
3	L2	159	C
3	L2	160	G
3	L2	188	A
3	L2	248	G
3	L2	284	U
3	L2	286	U
3	L2	324	U
3	L2	325	C
3	L2	329	C

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	L1	277	U
2	L1	278	U
2	L1	493	U
2	L1	585	A
2	L1	793	A
2	L1	811	A
2	L1	1051	G
2	L1	1082	C
2	L1	1555	A
2	L1	1568	C
3	L2	156	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
26	SEP	LS	128	26	3,4,10	0.68	0	2,4,14	0.79	0



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SEP	LS	128	26	-	0/1/2/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 50 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
64	ADP	NS	1301	62	24,29,29	0.95	3 (12%)	29,45,45	1.31	3 (10%)
65	GTP	SI	2001	62	29,34,34	0.90	0	35,54,54	0.71	0

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	ADP	NS	1301	62	-	2/12/32/32	0/3/3/3
65	GTP	SI	2001	62	-	1/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	NS	1301	ADP	O4'-C1'	2.07	1.43	1.40
64	NS	1301	ADP	PA-O3A	2.03	1.61	1.59
64	NS	1301	ADP	C2-N3	2.01	1.35	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	NS	1301	ADP	N3-C2-N1	-4.15	123.03	128.67
64	NS	1301	ADP	C4-C5-N7	-2.45	106.75	109.34
64	NS	1301	ADP	C4'-O4'-C1'	2.09	111.84	109.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
64	NS	1301	ADP	O4'-C4'-C5'-O5'
64	NS	1301	ADP	C3'-C4'-C5'-O5'
65	SI	2001	GTP	PA-O3A-PB-O1B

There are no ring outliers.

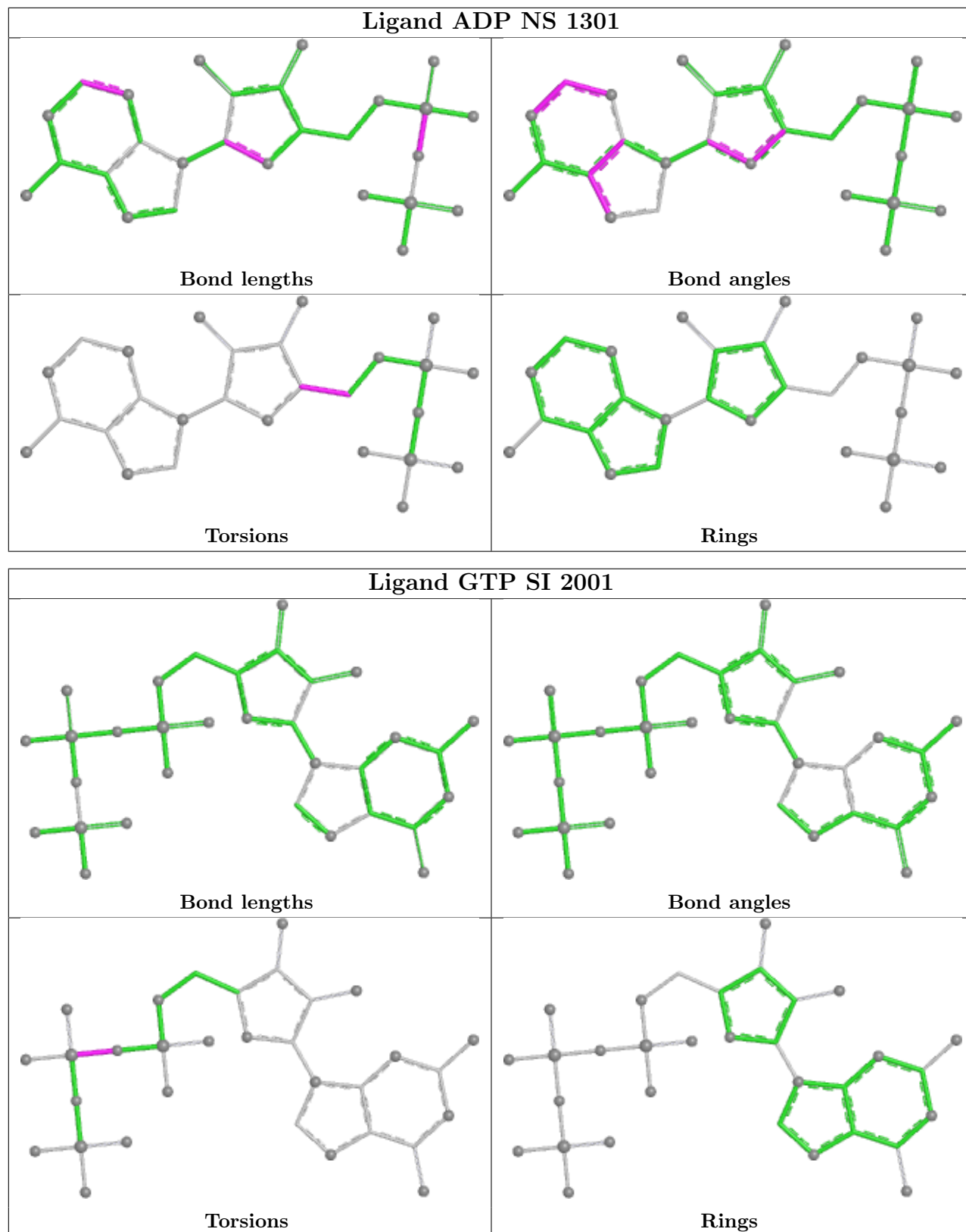
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	NS	1301	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.





## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



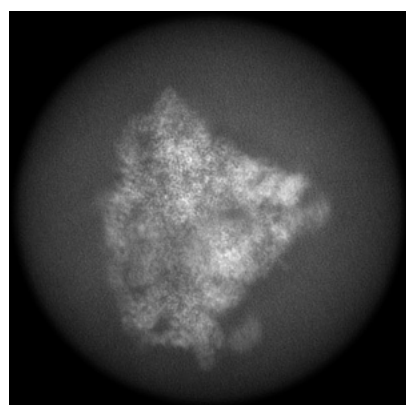
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49087. These allow visual inspection of the internal detail of the map and identification of artifacts.

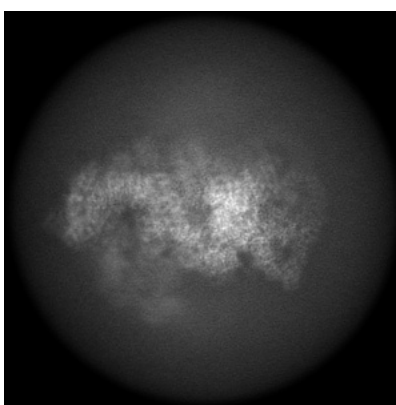
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

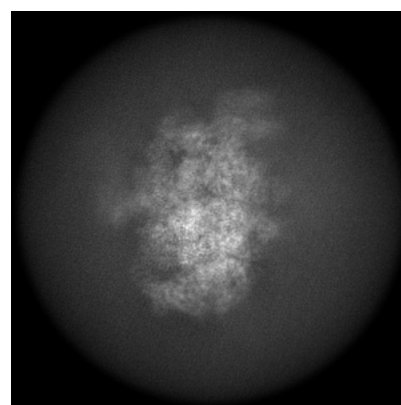
#### 6.1.1 Primary map



X



Y

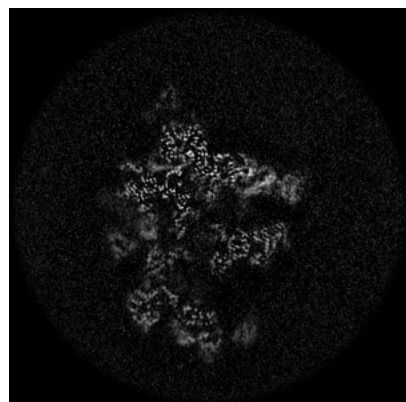


Z

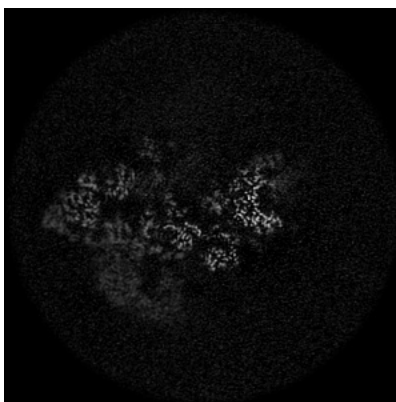
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

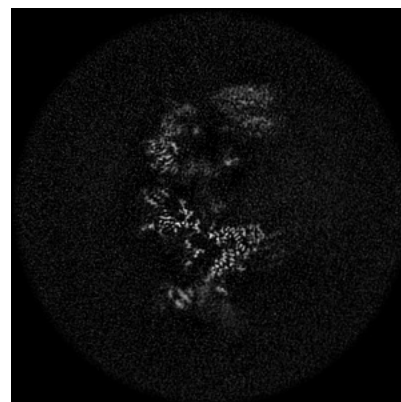
#### 6.2.1 Primary map



X Index: 252



Y Index: 252



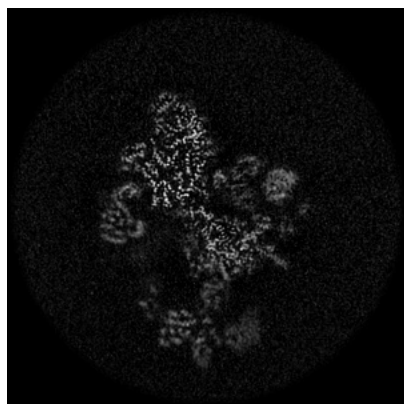
Z Index: 252



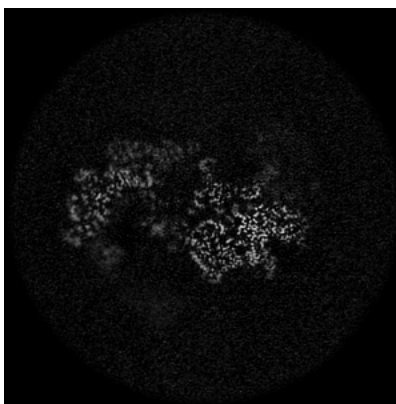
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

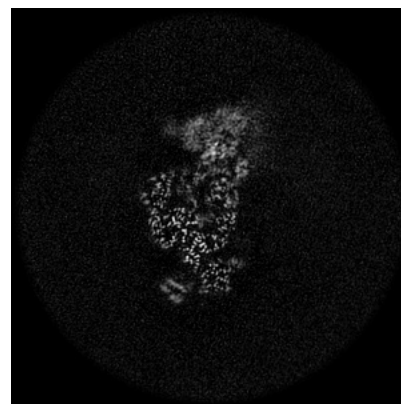
### 6.3.1 Primary map



X Index: 227



Y Index: 228

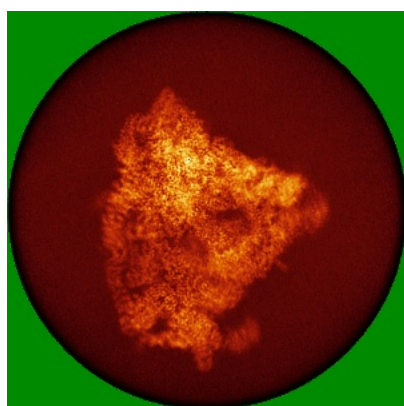


Z Index: 284

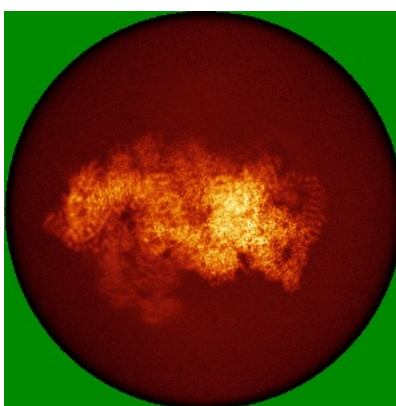
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

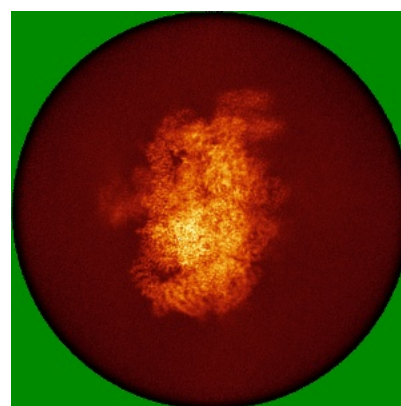
### 6.4.1 Primary map



X



Y



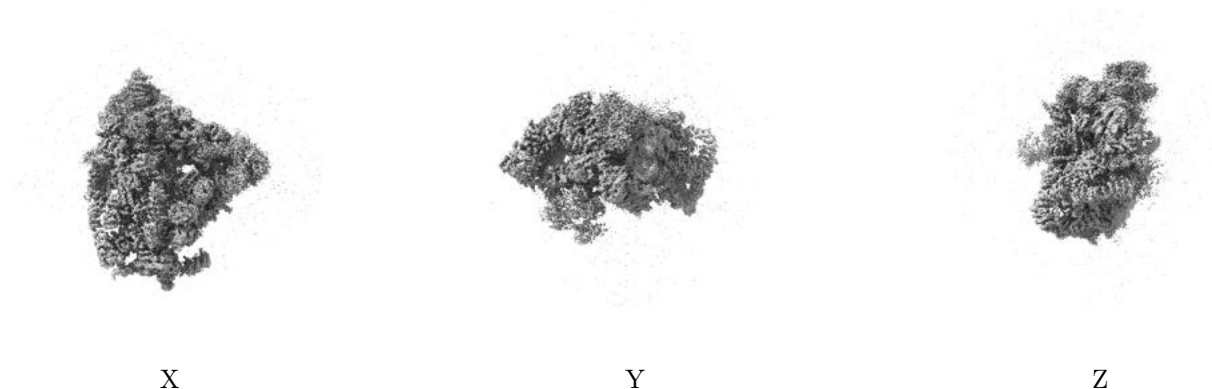
Z

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



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

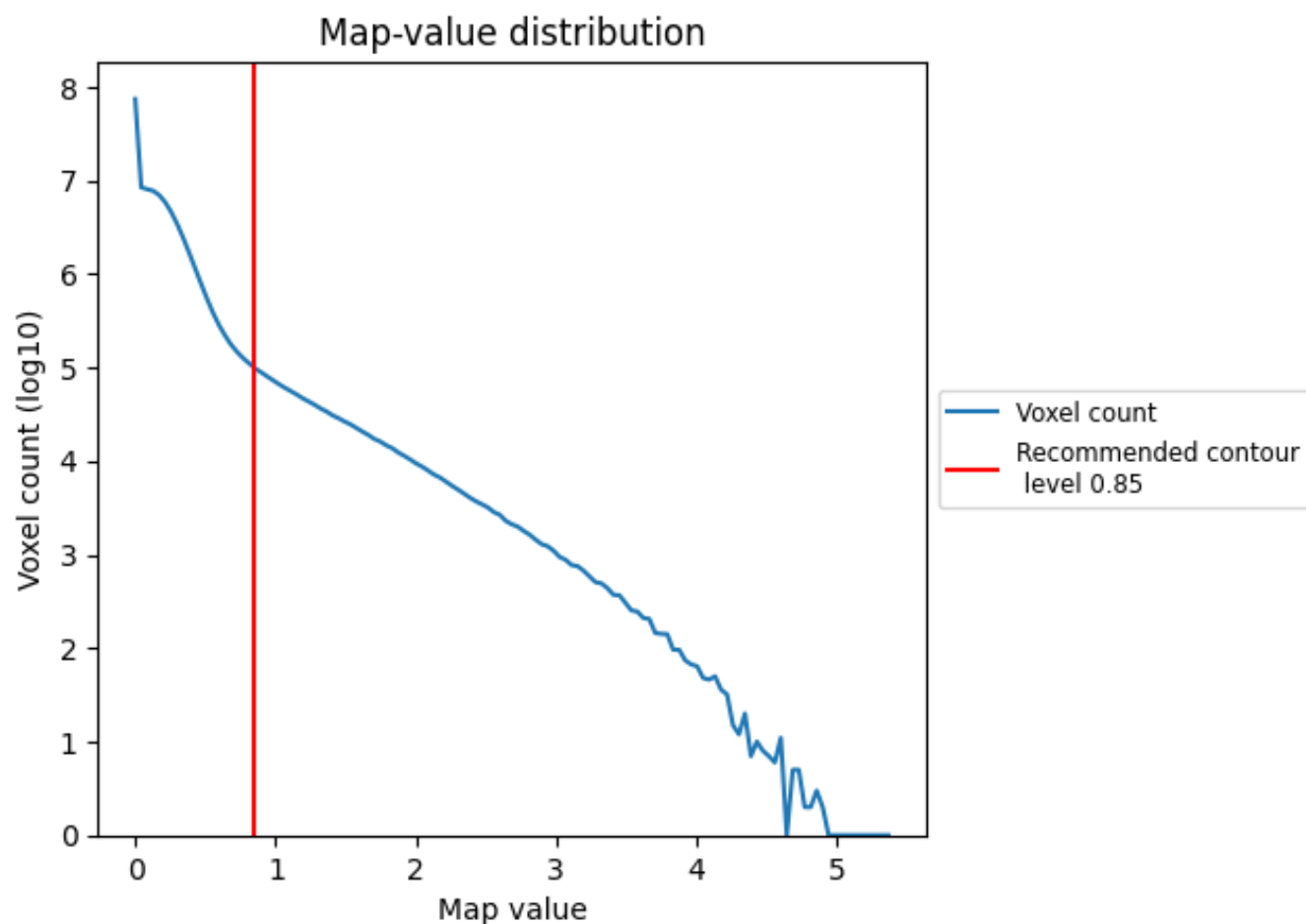
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

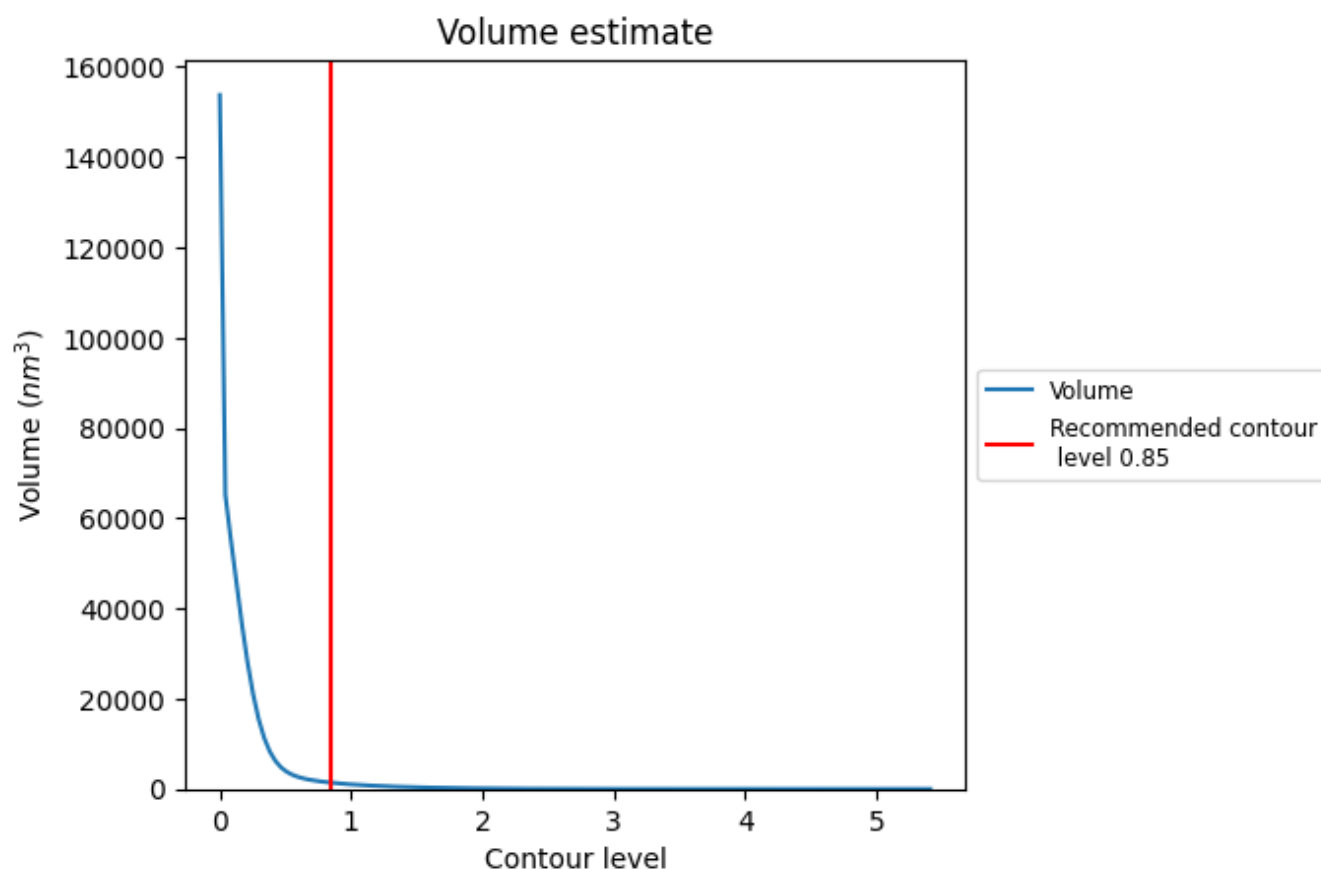
### 7.1 Map-value distribution [i](#)



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](#)

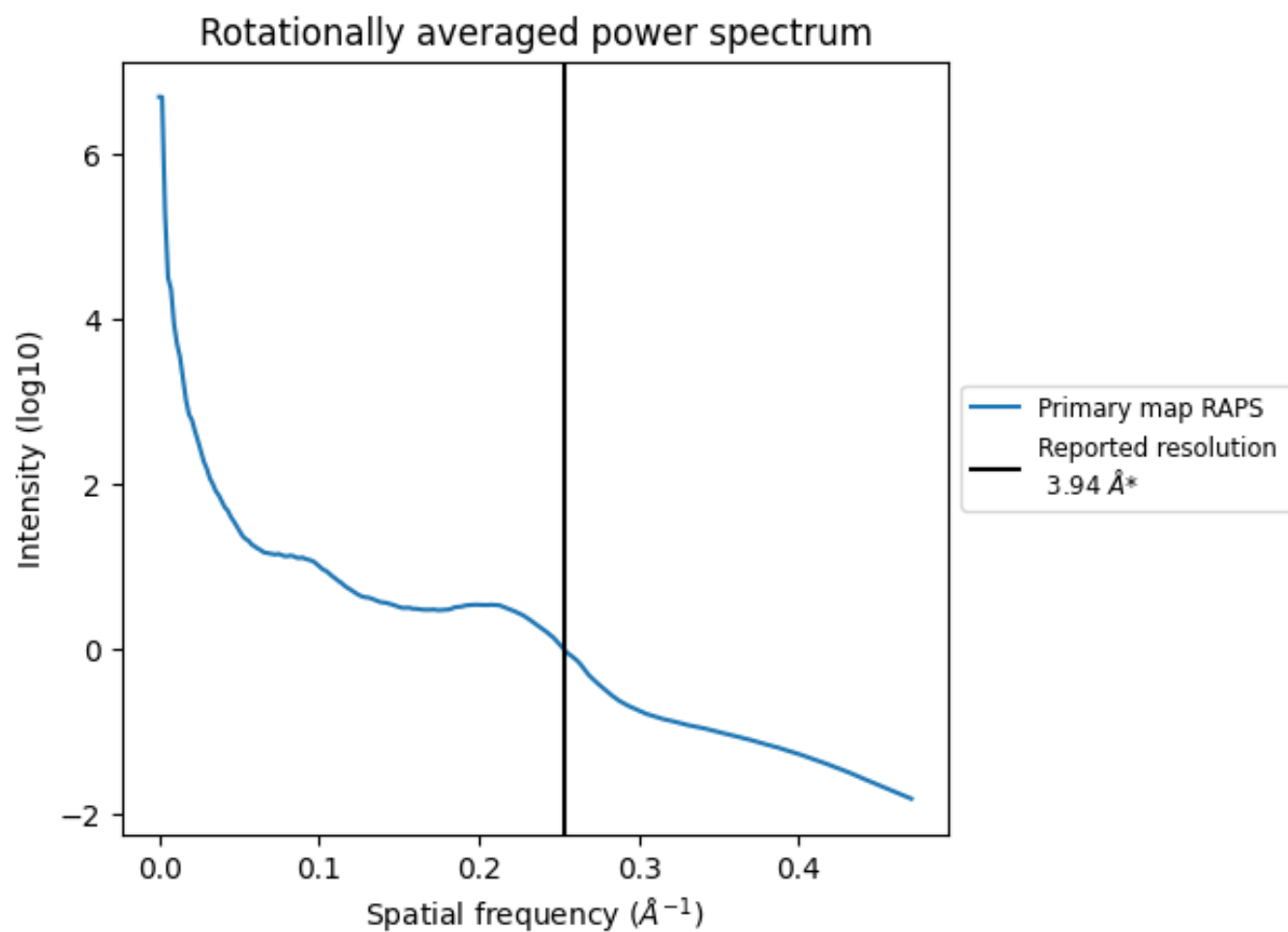


The volume at the recommended contour level is  $1387 \text{ nm}^3$ ; this corresponds to an approximate mass of 1253 kDa.

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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.254 Å<sup>-1</sup>



## 8 Fourier-Shell correlation

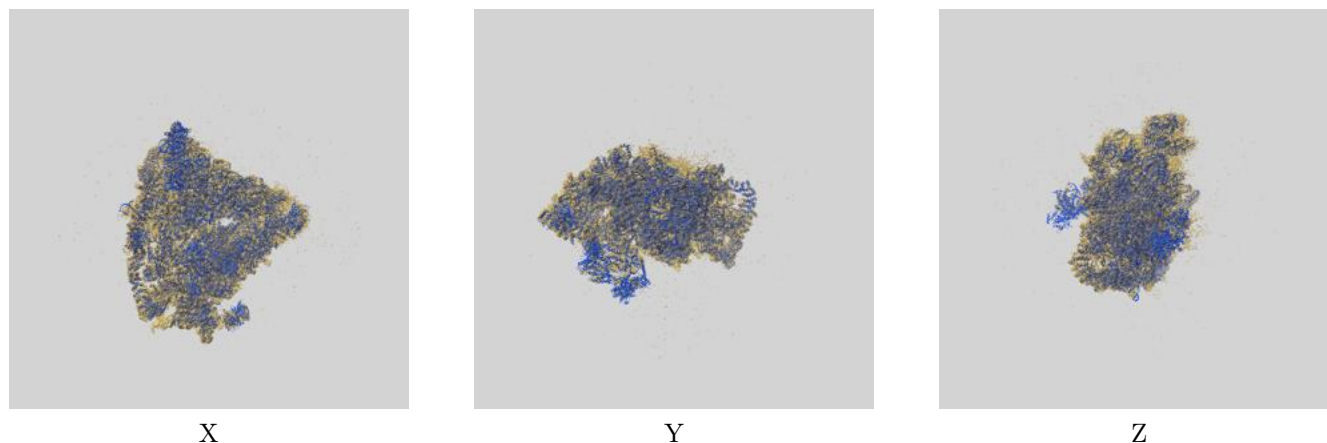
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49087 and PDB model 9N77. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

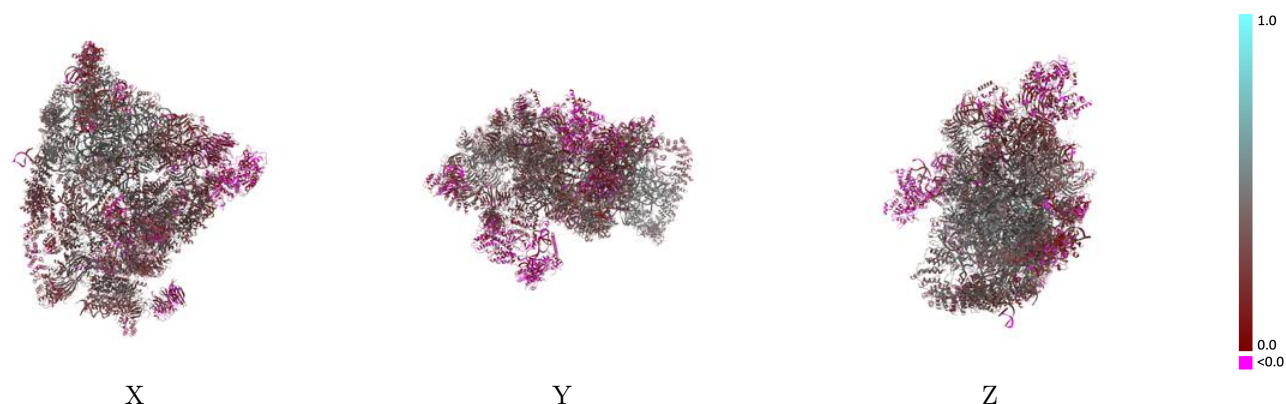
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.85 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.

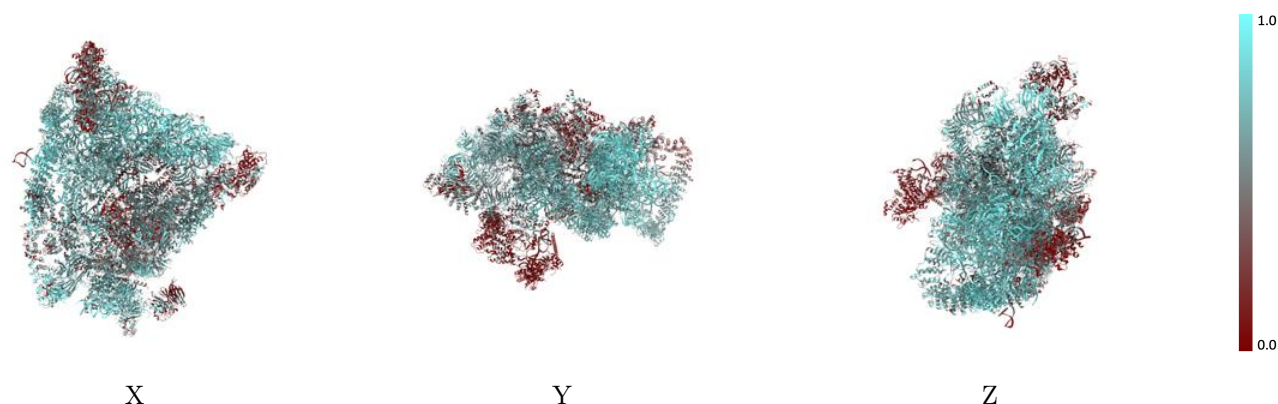


## 9.2 Q-score mapped to coordinate model [i](#)



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

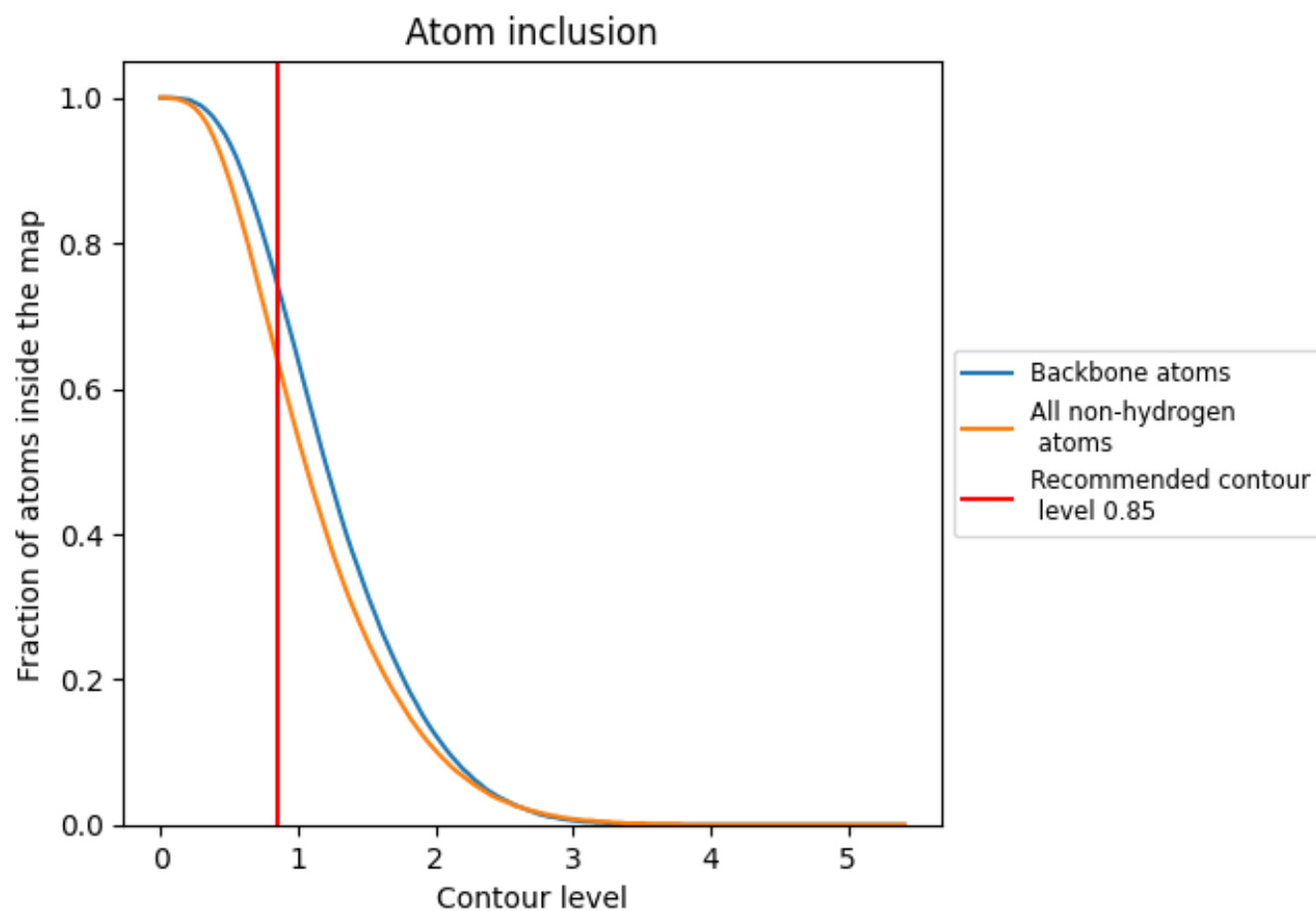
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.85).



## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 74% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.85) and Q-score for the entire model and for each chain.





























































Chain	Atom inclusion	Q-score
All	 0.6390	 0.3190
L0	 0.7340	 0.2780
L1	 0.7980	 0.3520
L2	 0.7400	 0.3060
L3	 0.3350	 0.2680
L4	 0.8160	 0.4920
L5	 0.6980	 0.3470
L6	 0.7620	 0.4410
L7	 0.4290	 0.2210
L8	 0.8310	 0.4780
L9	 0.7930	 0.4560
LC	 0.6420	 0.3790
LD	 0.8420	 0.4800
LE	 0.7810	 0.4460
LF	 0.8460	 0.4570
LG	 0.6510	 0.3730
LH	 0.7080	 0.3450
LI	 0.4300	 0.1790
LJ	 0.5980	 0.2650
LK	 0.5620	 0.2140
LL	 0.6130	 0.2840
LM	 0.6300	 0.2630
LN	 0.7200	 0.3600
LO	 0.5820	 0.3400
LQ	 0.6550	 0.3230
LR	 0.7900	 0.1750
LS	 0.6910	 0.3630
LT	 0.5720	 0.3020
LZ	 0.5160	 0.3190
NA	 0.5510	 0.3030
NB	 0.4970	 0.2870
ND	 0.4810	 0.2610
NF	 0.7900	 0.4100
NG	 0.8720	 0.2370
NL	 0.4810	 0.2900



*Continued on next page...*



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Chain	Atom inclusion	Q-score
NM	 0.7880	 0.2510
NP	 0.3640	 0.3170
NQ	 0.7450	 0.3820
NS	 0.3610	 0.1360
NV	 0.5100	 0.4330
OH	 0.0000	 0.0150
OU	 0.0000	 0.0290
SA	 0.6110	 0.3290
SB	 0.5600	 0.2990
SC	 0.7300	 0.4450
SD	 0.5360	 0.2910
SE	 0.7110	 0.3590
SF	 0.7550	 0.4400
SG	 0.7790	 0.4350
SH	 0.7710	 0.4390
SI	 0.7590	 0.4360
SJ	 0.2170	 0.1120
SK	 0.4550	 0.2320
SL	 0.7600	 0.4480
SM	 0.6620	 0.4080
SP	 0.5310	 0.3400
SQ	 0.6190	 0.4140
SR	 0.8050	 0.4710
SS	 0.5380	 0.3060
ST	 0.2170	 0.1670
SU	 0.1600	 0.1410
SV	 0.7140	 0.3010
SW	 0.7840	 0.2430
SY	 0.5630	 0.3350
SZ	 0.0410	 0.0380