



Full wwPDB EM Validation Report ⓘ

Nov 6, 2025 – 05:12 PM EST

PDB ID : 9N76 / pdb_00009n76
EMDB ID : EMD-49086
Title : SSU processome maturation and disassembly, State J
Authors : Buzovetsky, O.; Klinge, S.
Deposited on : 2025-02-05
Resolution : 4.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

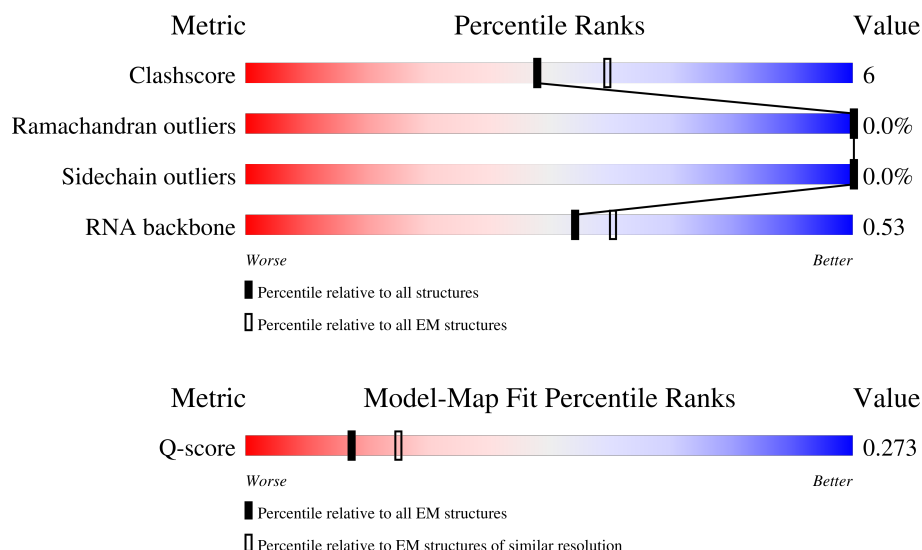
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	5410 (3.70 - 4.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
2	L1	1803	
3	L2	334	

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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	LP	440	
25	LQ	943	
26	LR	817	
27	LS	594	
28	LT	939	

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Mol	Chain	Length	Quality of chain
29	LZ	183	
30	NA	593	
31	NB	610	
32	ND	214	
33	NF	151	
34	NG	137	
35	NH	1237	
36	NI	297	
37	NL	318	
38	NM	255	
39	NP	144	
40	NQ	82	
41	NS	1267	
42	NV	733	
43	OH	143	
44	OU	152	
45	SA	504	
46	SB	511	
47	SC	327	
47	SD	327	
48	SE	126	
48	SF	126	
49	SG	573	
50	SH	367	
51	SI	1183	

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Mol	Chain	Length	Quality of chain
52	SJ	252	
52	SK	252	
53	SL	189	
54	SM	290	
55	SP	2493	
56	SQ	217	
57	SR	145	
58	SS	899	
59	ST	810	
60	SU	552	
61	SV	206	
62	SW	274	
63	SY	250	
64	SZ	483	

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 206690 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	1449	Total	C	N	O	P	0	0
			30918	13821	5521	10127	1449		

- 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		
			6449	4113	1087	1230	19	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	1599	Total	C	N	O	S	0	0
			9274	5735	1730	1797	12		

- 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 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	LP	379	Total	C	N	O	0	0
			1901	1143	379	379		

- Molecule 25 is a protein called U3 small nucleolar RNA-associated protein 12.

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

- Molecule 26 is a protein called U3 small nucleolar RNA-associated protein 13.

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

- Molecule 27 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	LS	463	Total	C	N	O	P	S	0	0
			3662	2326	643	683	1	9		

- Molecule 28 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LT	871	Total	C	N	O	S	0	0
			6787	4306	1170	1289	22		

- Molecule 29 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

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

- Molecule 30 is a protein called U3 small nucleolar RNA-associated protein MPP10.

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

- Molecule 31 is a protein called Something about silencing protein 10.

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

- Molecule 32 is a protein called Bud site selection protein 21.

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

- Molecule 33 is a protein called 40S ribosomal protein S13.

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

- Molecule 34 is a protein called 40S ribosomal protein S14-A.

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

- Molecule 35 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	NH	1077	Total	C	N	O	S	0	0
			8693	5650	1434	1585	24		

- Molecule 36 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	NI	240	Total	C	N	O	S	0	0
			1953	1248	331	366	8		

- Molecule 37 is a protein called Dimethyladenosine transferase.

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

- Molecule 38 is a protein called Small ribosomal subunit protein eS1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NM	237	Total	C	N	O	S	0	0
			1891	1195	350	342	4		

- Molecule 39 is a protein called 40S ribosomal protein S19-A.

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

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

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

- Molecule 41 is a protein called Probable ATP-dependent RNA helicase DHR1.

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

- Molecule 42 is a protein called Exosome complex exonuclease RRP6.

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

- Molecule 43 is a protein called 40S ribosomal protein S12.

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

- Molecule 44 is a protein called Ubiquitin-40S ribosomal protein S31.

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

- Molecule 45 is a protein called Nucleolar protein 56.

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

- Molecule 46 is a protein called Nucleolar protein 58.

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

- Molecule 47 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

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

- Molecule 48 is a protein called 13 kDa ribonucleoprotein-associated protein.

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

- Molecule 49 is a protein called Ribosomal RNA-processing protein 9.

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

- Molecule 50 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

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

- Molecule 51 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SI	758	Total	C	N	O	S	0	0
			6144	3946	1097	1074	27		

- Molecule 52 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

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

- Molecule 53 is a protein called rRNA-processing protein FCF1.

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

- Molecule 54 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

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

- Molecule 55 is a protein called U3 small nucleolar RNA-associated protein 20.

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

- Molecule 56 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SQ	107	Total	C	N	O	S	0	0
			885	555	165	162	3		

- Molecule 57 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 58 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SS	94	Total	C	N	O	S	0	0
			791	491	152	139	9		

- Molecule 59 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	ST	597	Total	C	N	O	S	0	0
			3455	2108	682	662	3		

- Molecule 60 is a protein called Nucleolar complex protein 4.

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

- Molecule 61 is a protein called Regulator of rDNA transcription protein 14.

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

- Molecule 62 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SW	213	Total	C	N	O	S	0	0
			1669	1063	303	299	4		

- Molecule 63 is a protein called U3 small nucleolar RNA-associated protein 11.

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

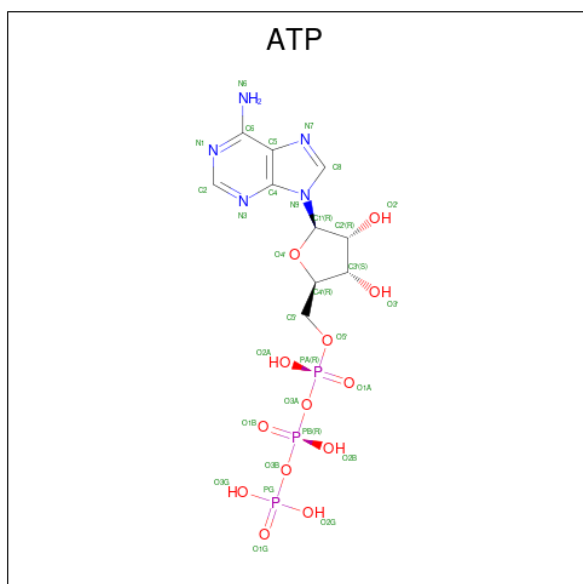
- Molecule 64 is a protein called Essential nuclear protein 1.

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

- Molecule 65 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
65	L1	35	Total	Mg	0
			35	35	
65	NH	1	Total	Mg	0
			1	1	
65	NS	1	Total	Mg	0
			1	1	
65	SI	1	Total	Mg	0
			1	1	

- Molecule 66 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

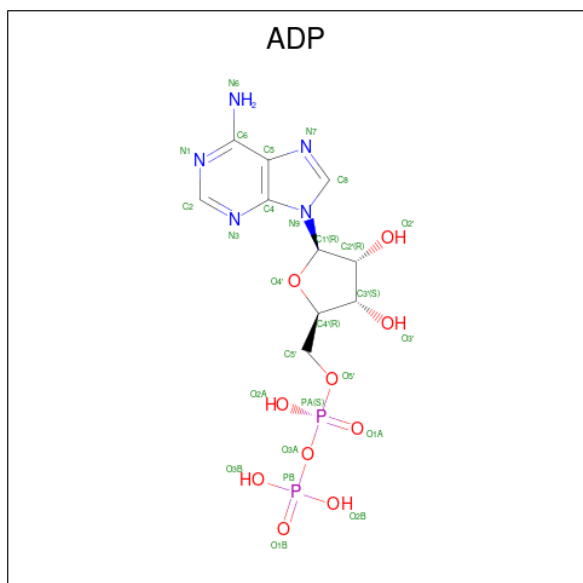


Mol	Chain	Residues	Atoms					AltConf
66	NH	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 67 is ZINC ION (CCD ID: ZN) (formula: Zn).

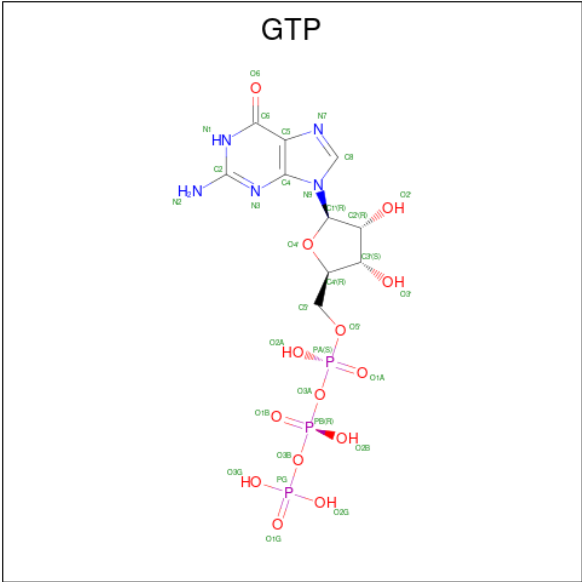
Mol	Chain	Residues	Atoms		AltConf
67	NQ	1	Total	Zn	0
			1	1	
67	SL	1	Total	Zn	0
			1	1	

- Molecule 68 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



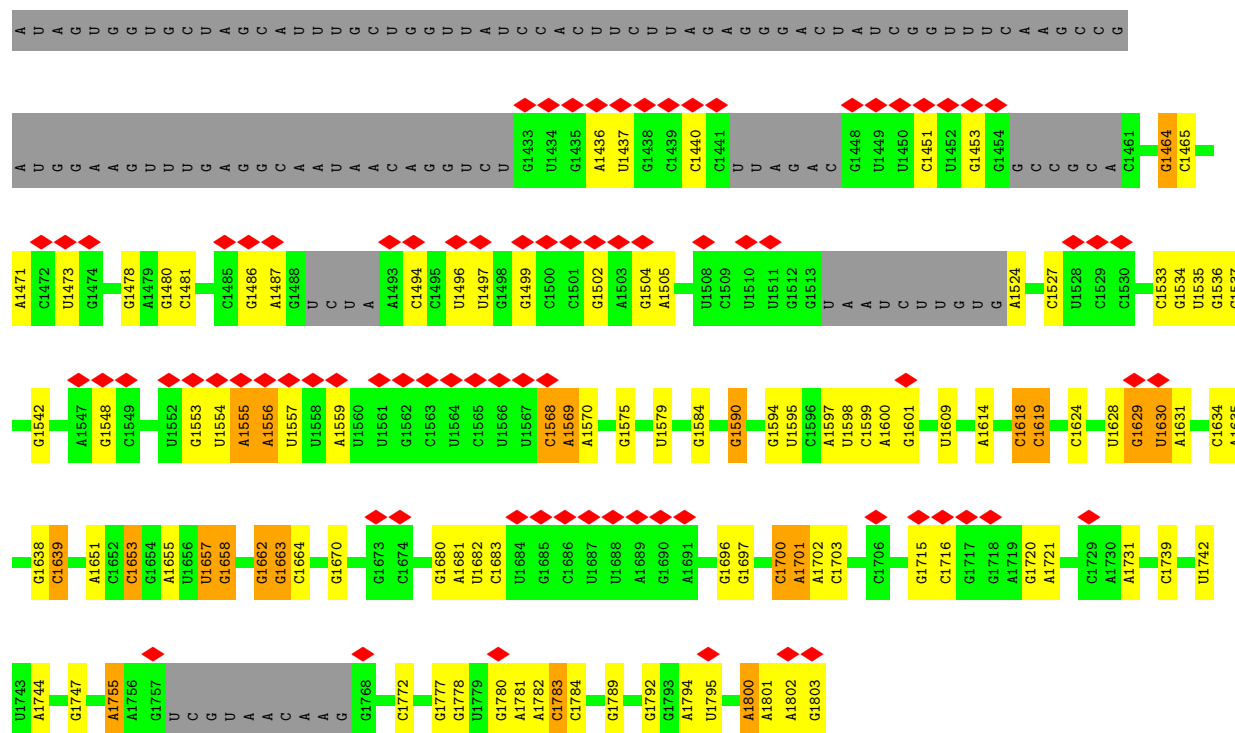
Mol	Chain	Residues	Atoms					AltConf
68	NS	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 69 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

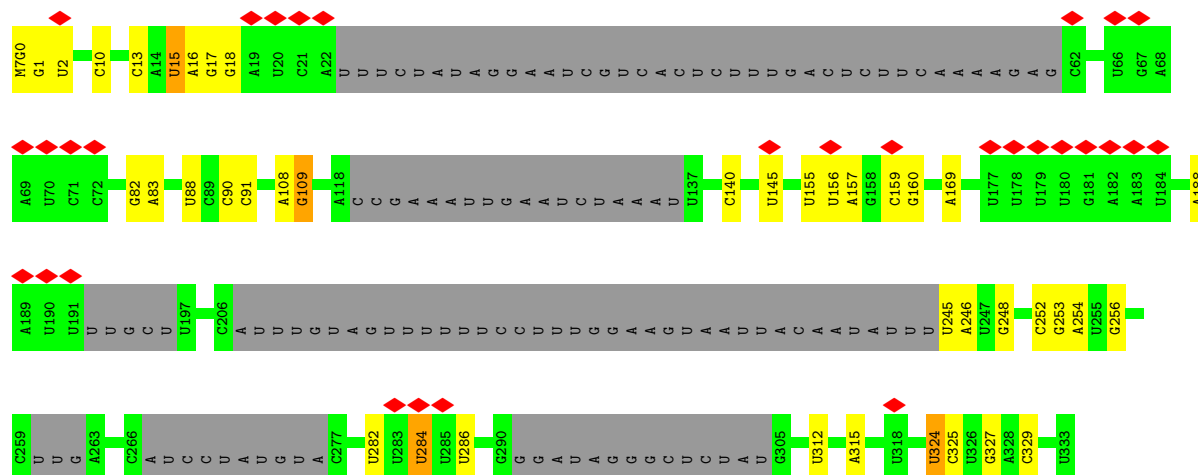


Mol	Chain	Residues	Atoms					AltConf
69	SI	1	Total	C	N	O	P	0
			32	10	5	14	3	

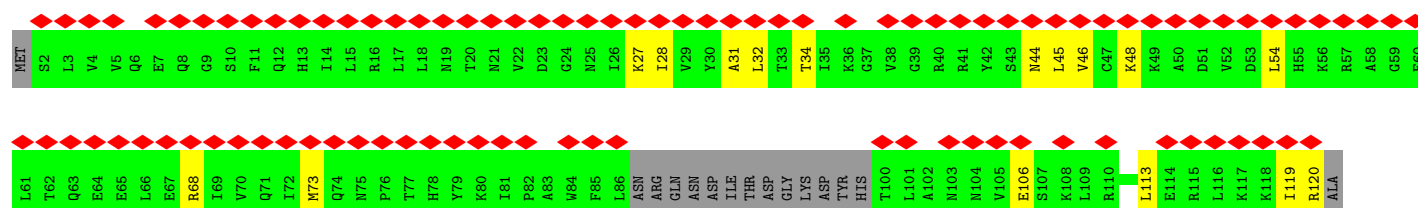




• Molecule 3: U3 snoRNA




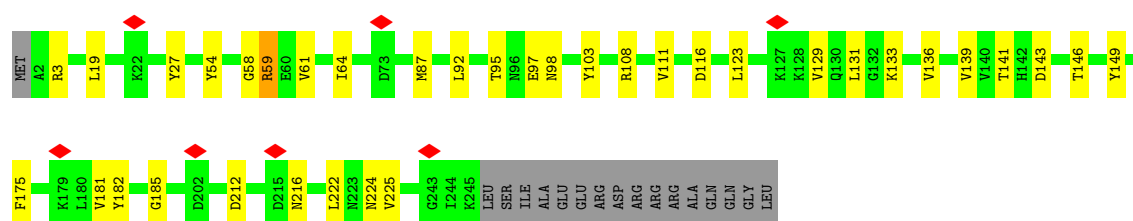
• Molecule 4: 40S ribosomal protein S18-A




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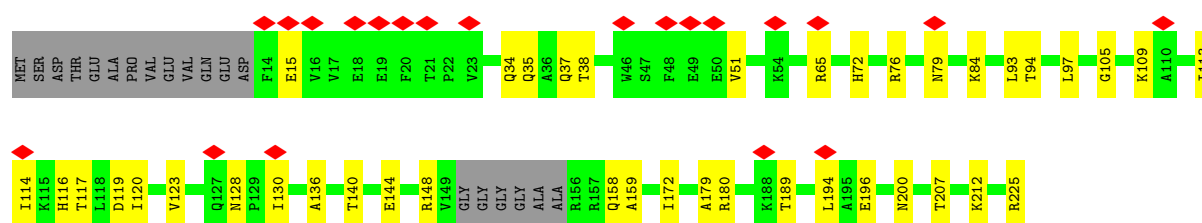
• Molecule 5: 40S ribosomal protein S4-A

Chain L4: 




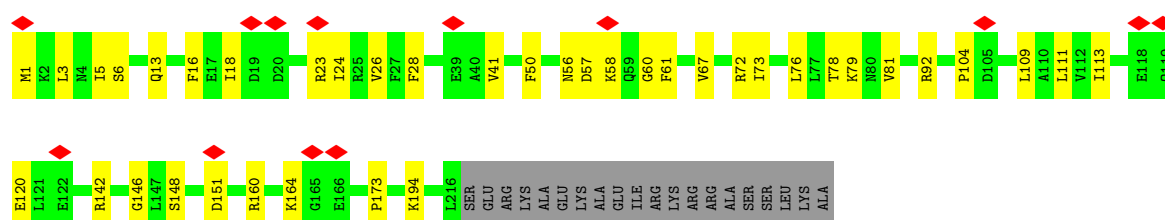
• Molecule 6: 40S ribosomal protein S5

Chain L5: 




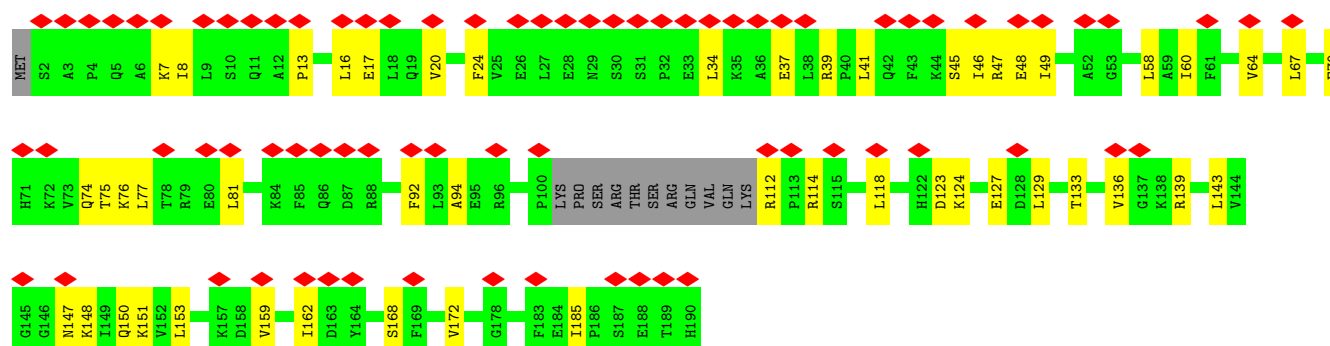
• Molecule 7: 40S ribosomal protein S6-A

Chain L6: 

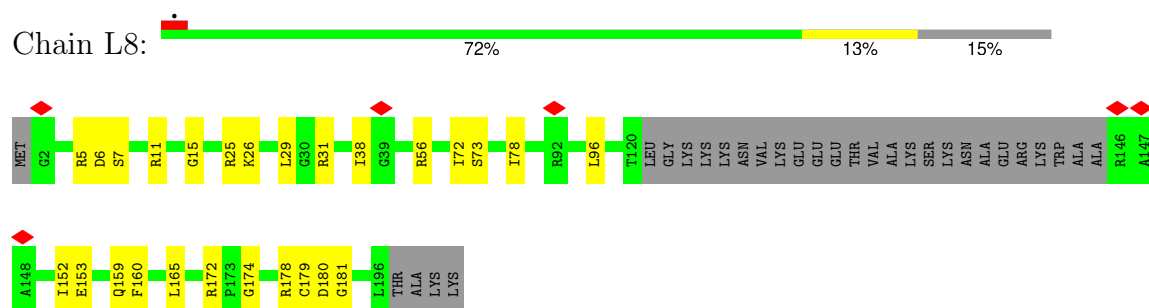


• Molecule 8: 40S ribosomal protein S7-A

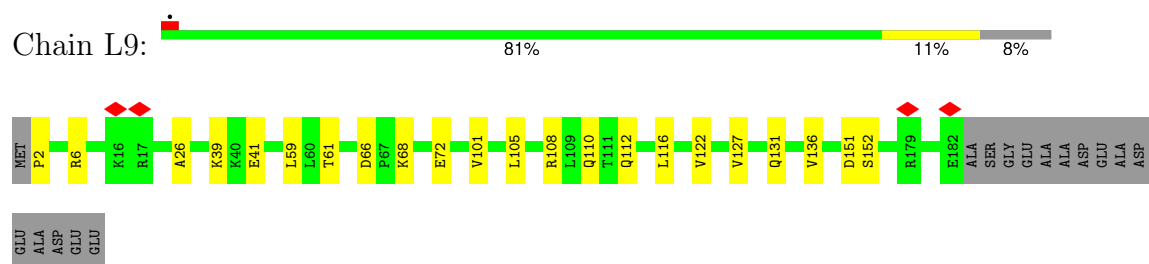
Chain L7: 



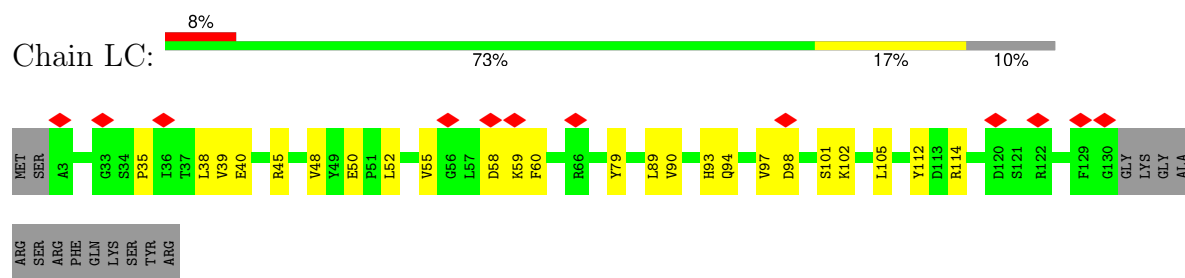
- Molecule 9: 40S ribosomal protein S8-A



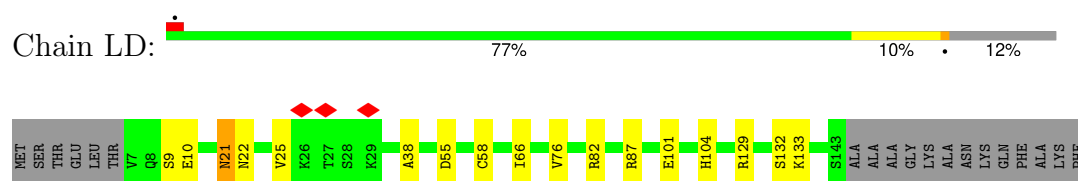
- Molecule 10: 40S ribosomal protein S9-A



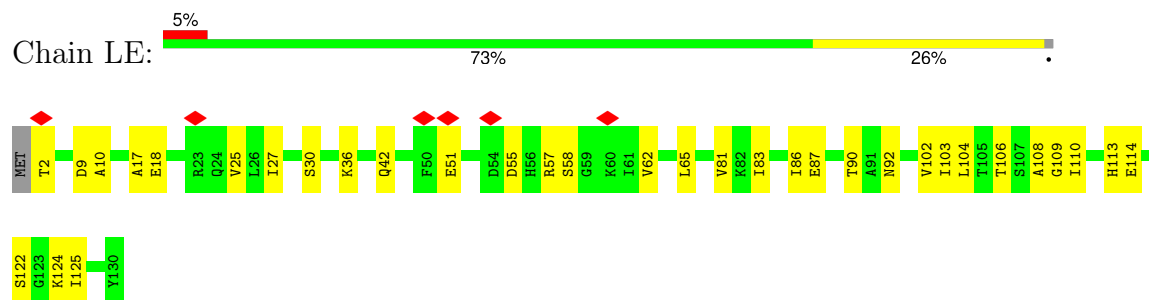
- Molecule 11: 40S ribosomal protein S16-A



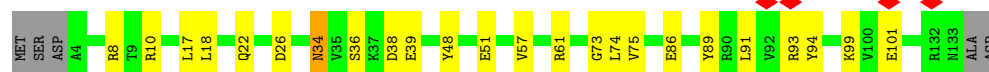
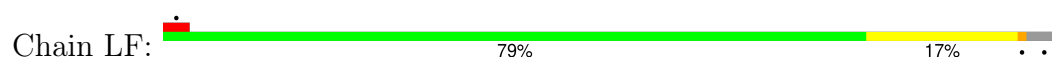
- Molecule 12: 40S ribosomal protein S11-A



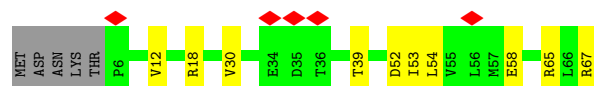
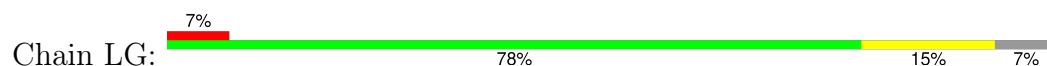
- Molecule 13: 40S ribosomal protein S22-A



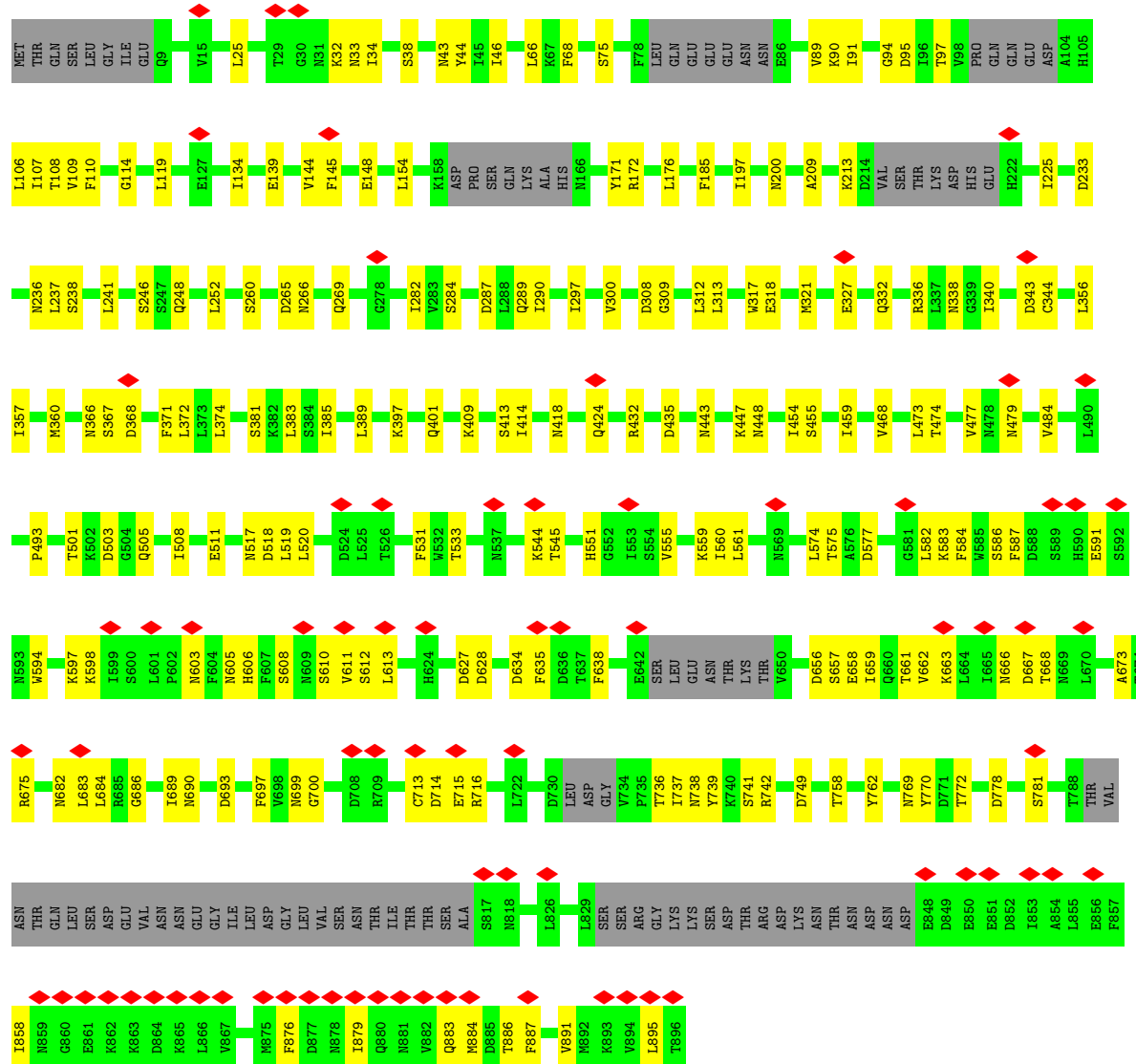
- Molecule 14: 40S ribosomal protein S24-A



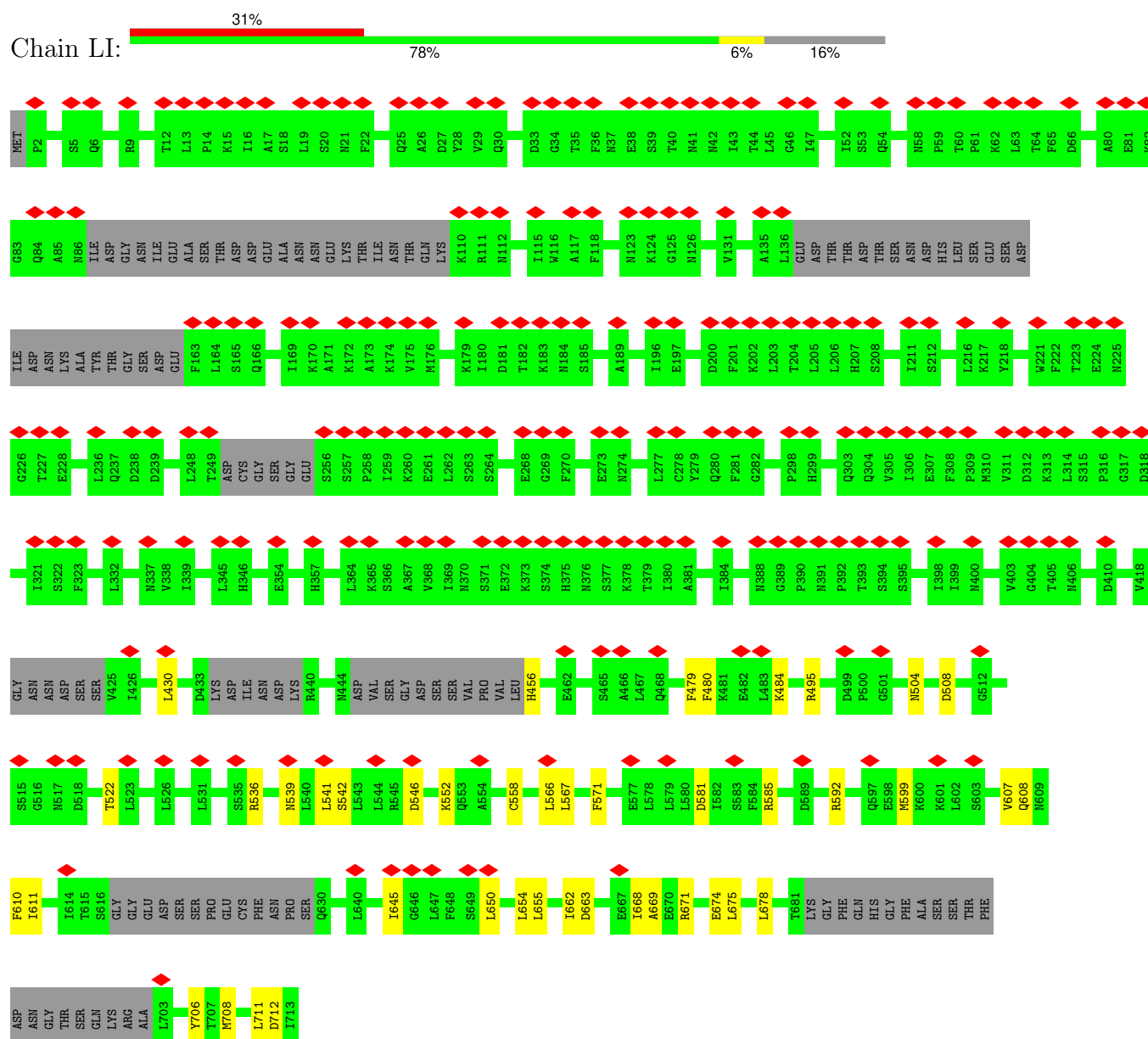
- Molecule 15: 40S ribosomal protein S28-A

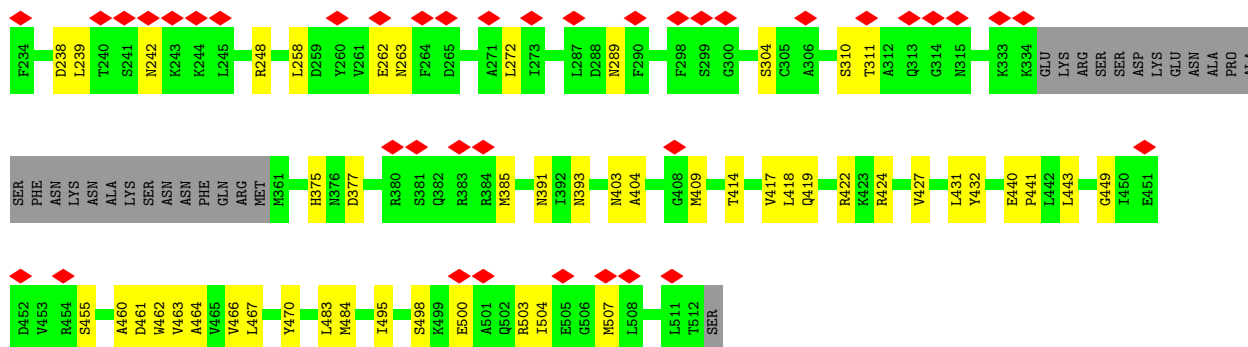


- Molecule 16: NET1-associated nuclear protein 1



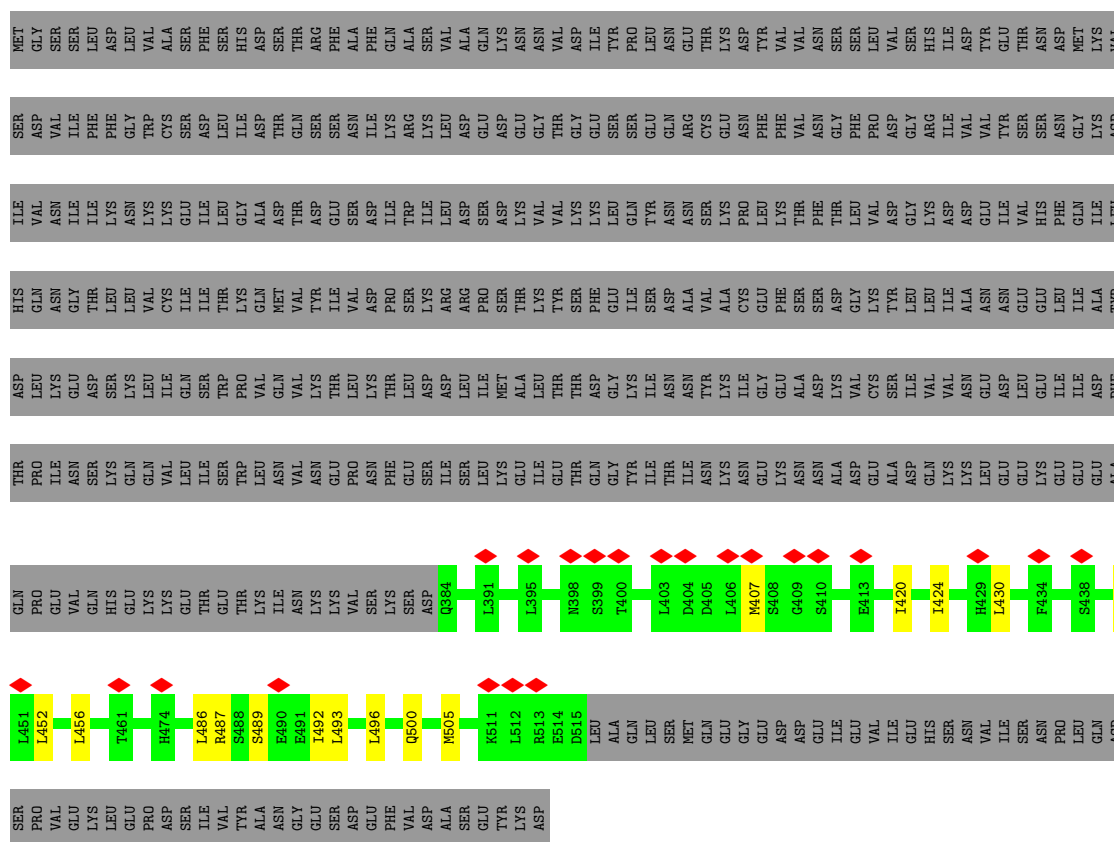
• Molecule 17: U3 small nucleolar RNA-associated protein 8





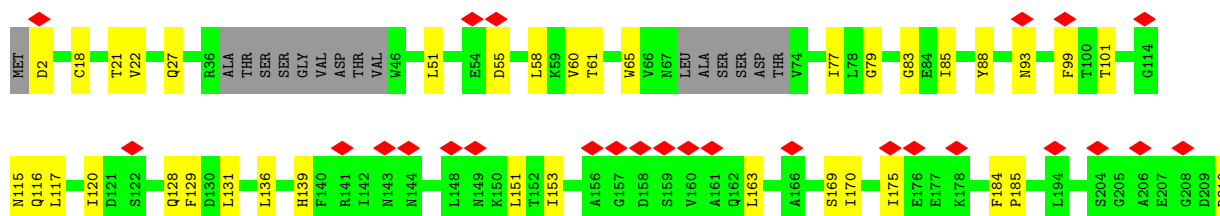
• Molecule 19: U3 small nucleolar RNA-associated protein 9

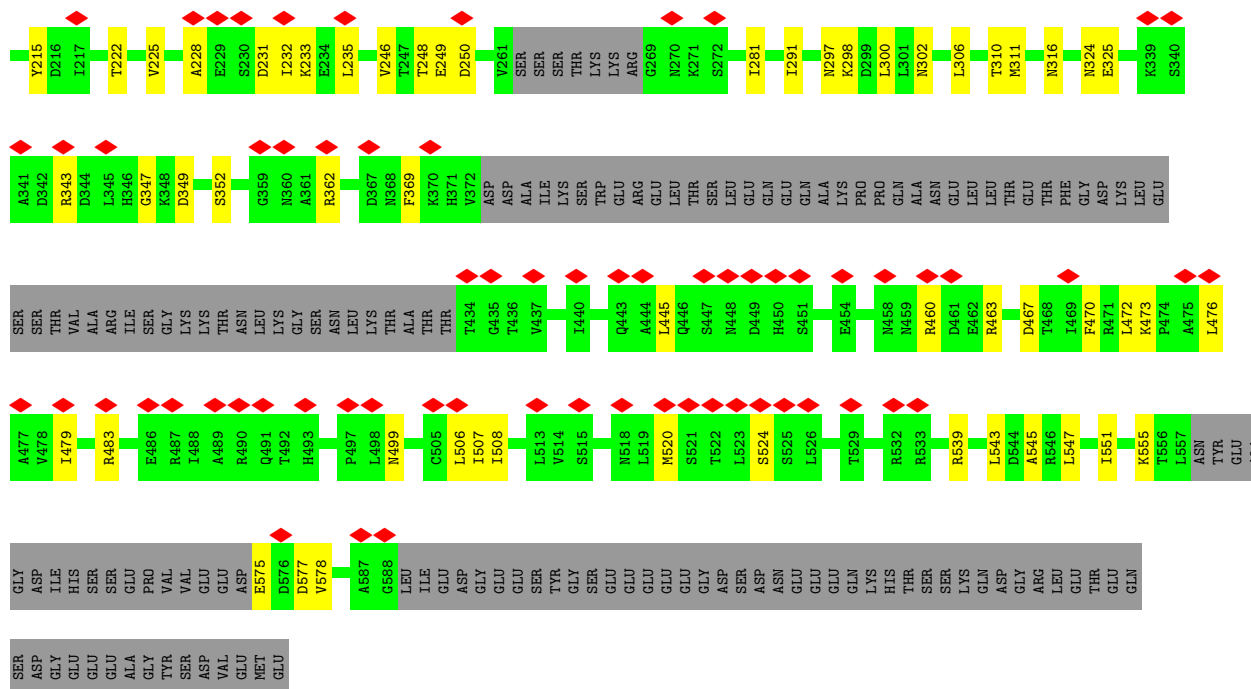
Chain LK: 20% 77%



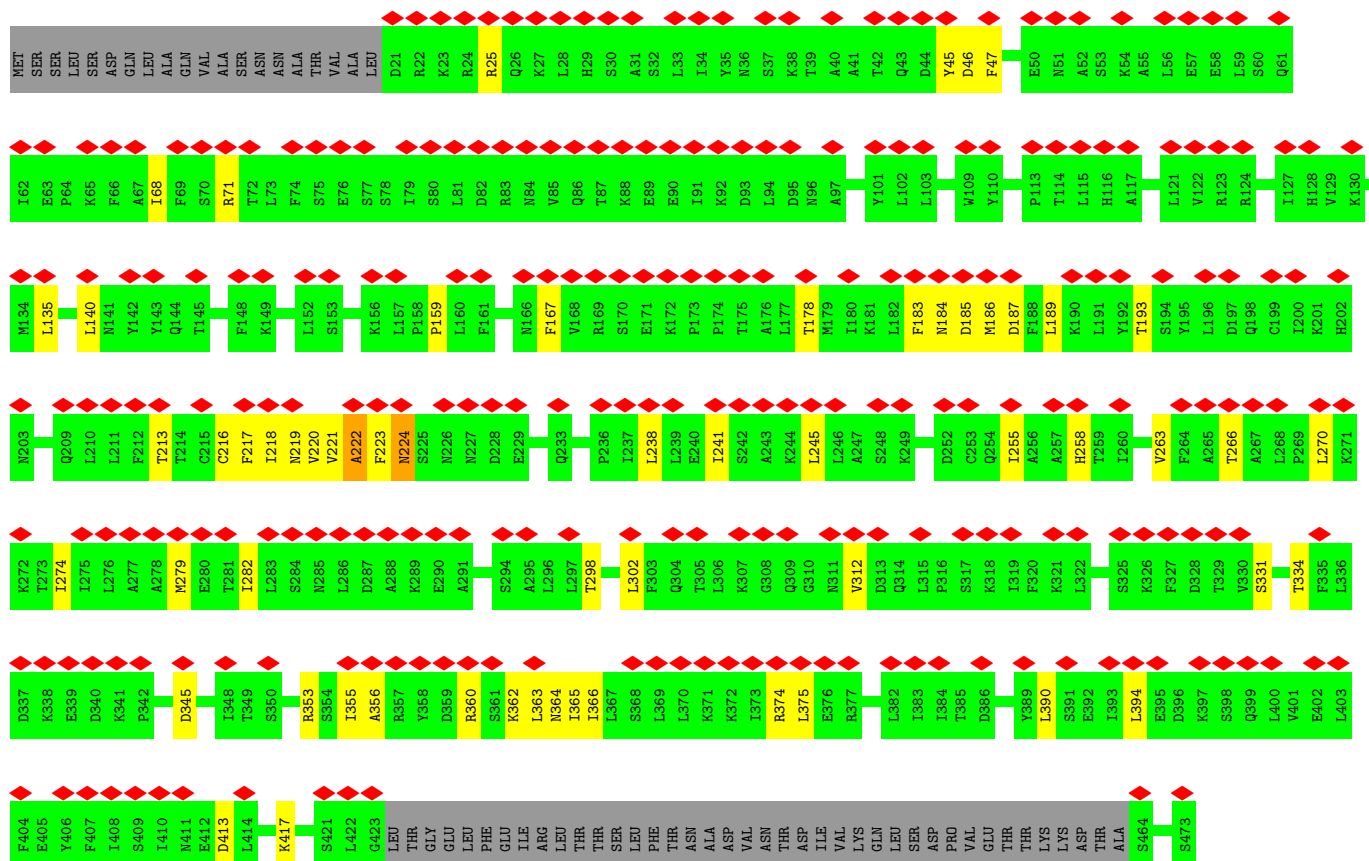
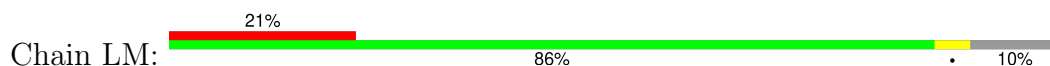
• Molecule 20: U3 small nucleolar RNA-associated protein 5

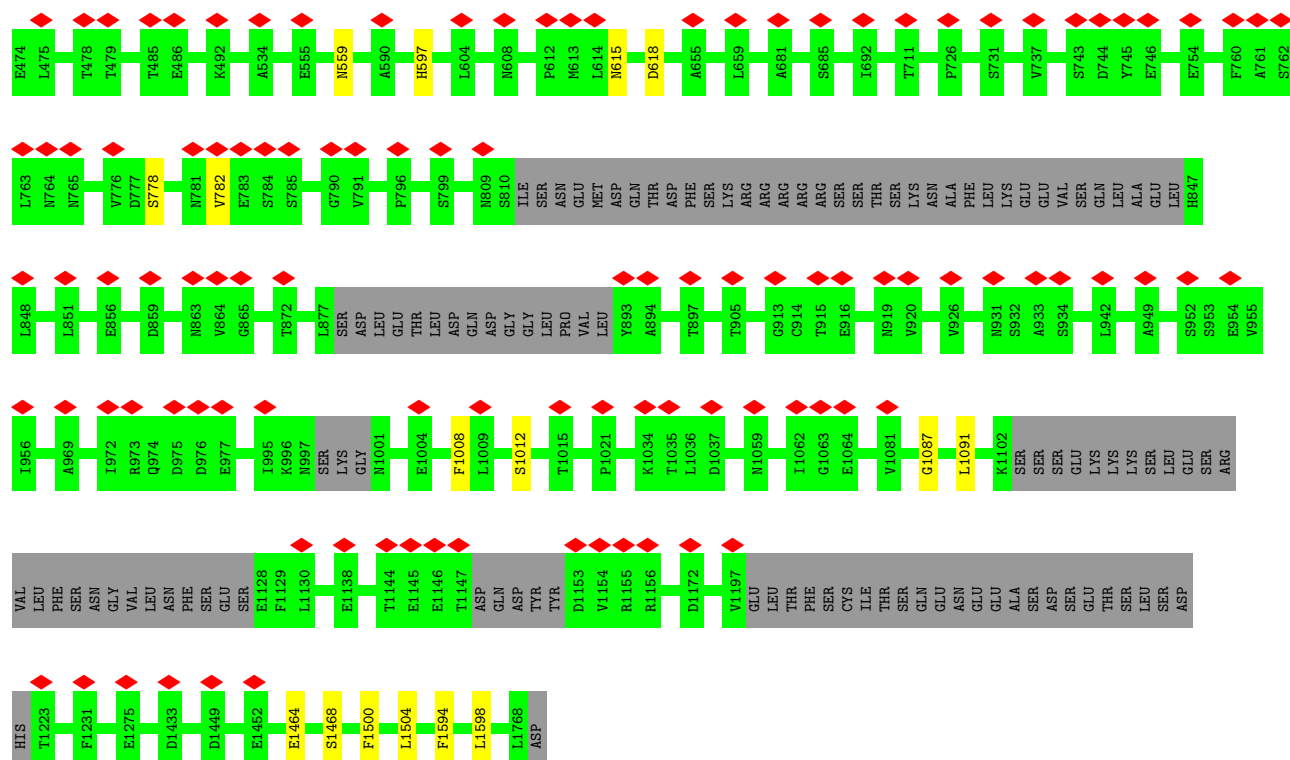
Chain LL: 14% 61% 14% 24%



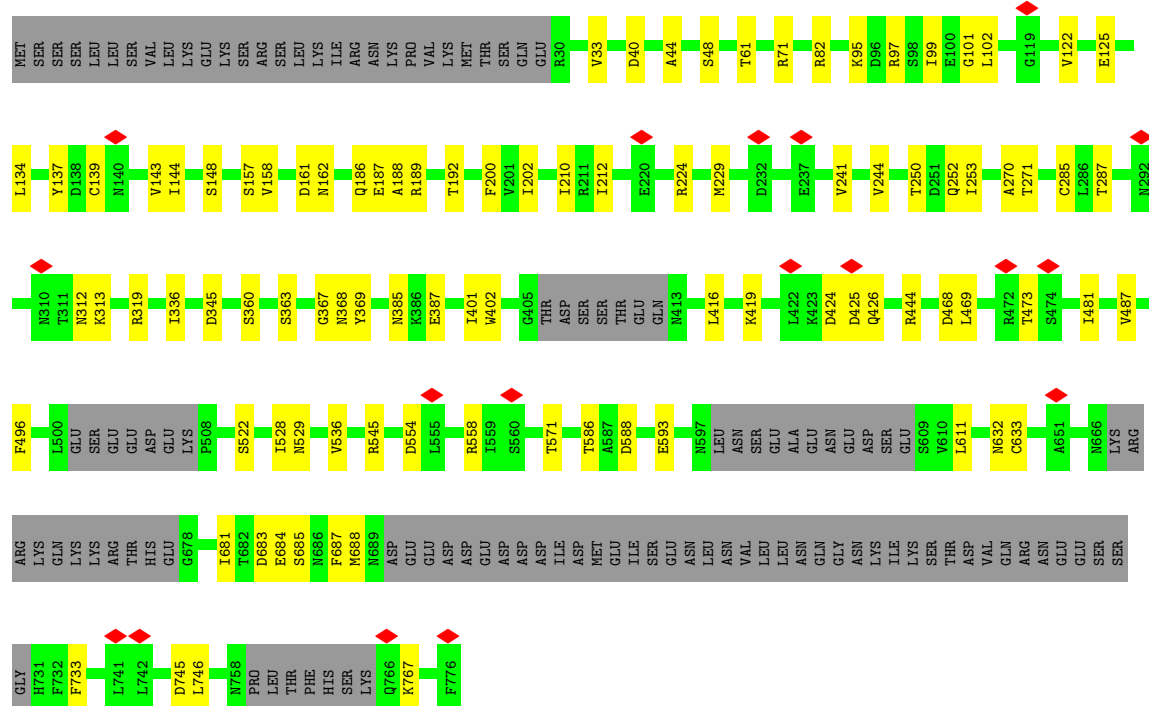
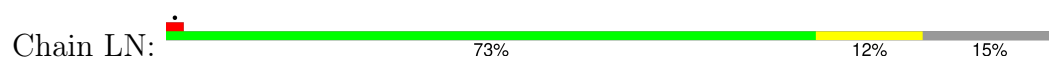


• Molecule 21: U3 small nucleolar RNA-associated protein 10

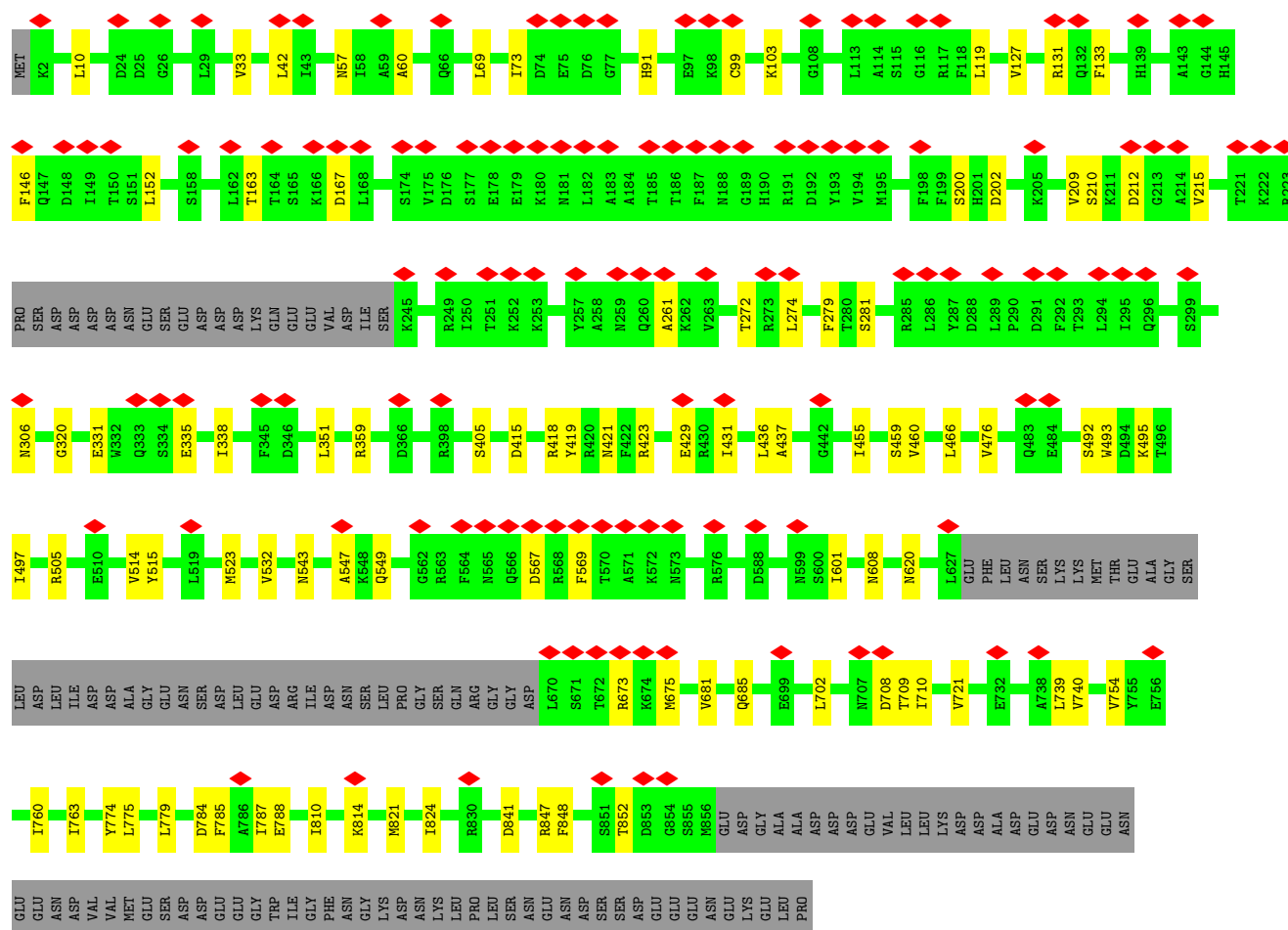
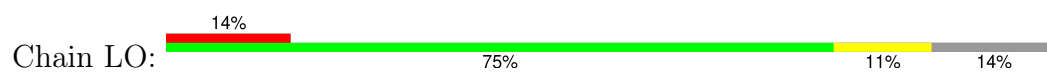




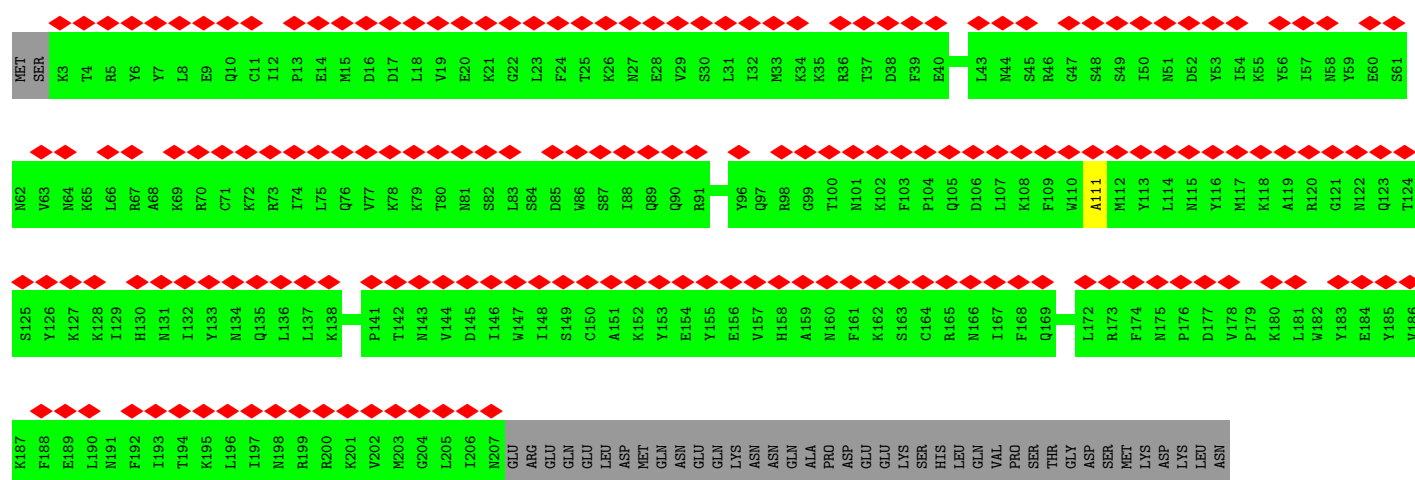
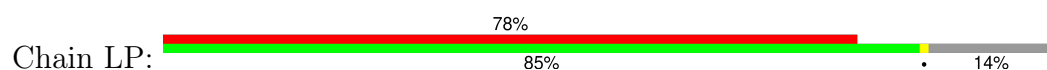
- Molecule 22: U3 small nucleolar RNA-associated protein 4



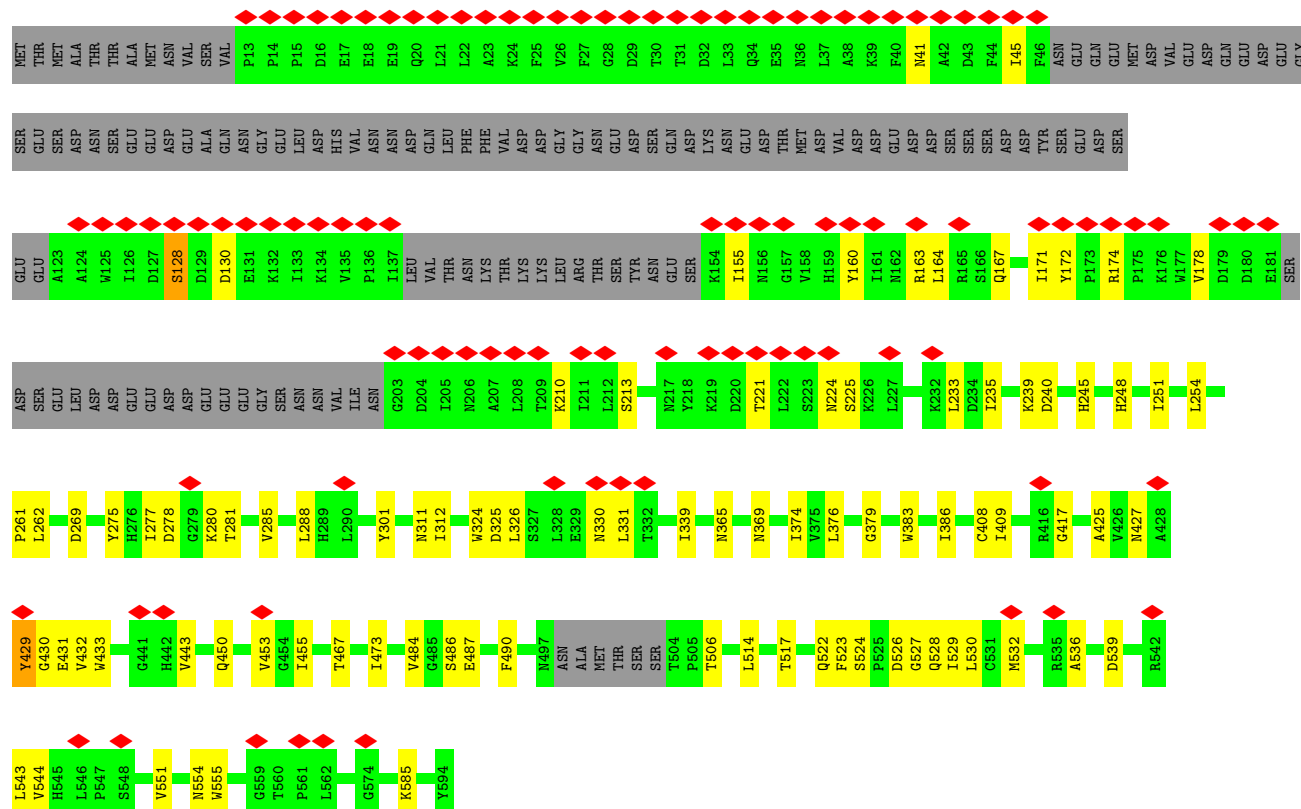
- Molecule 23: Periodic tryptophan protein 2



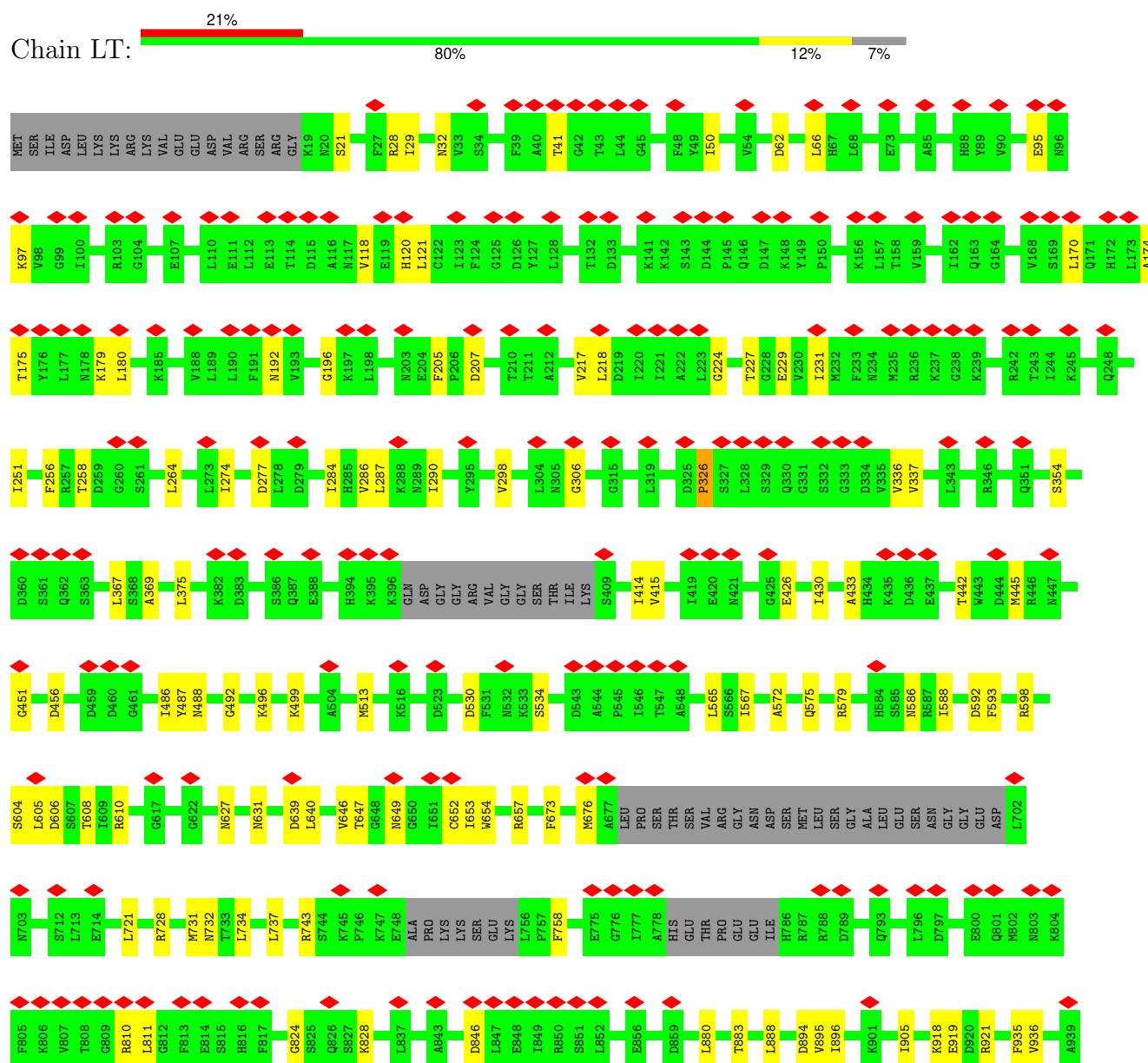
• Molecule 24: U3 small nucleolar RNA-associated protein 6



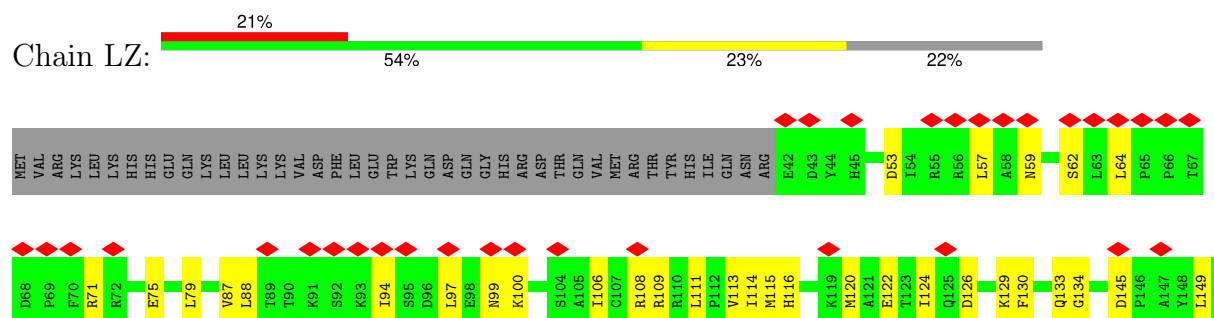


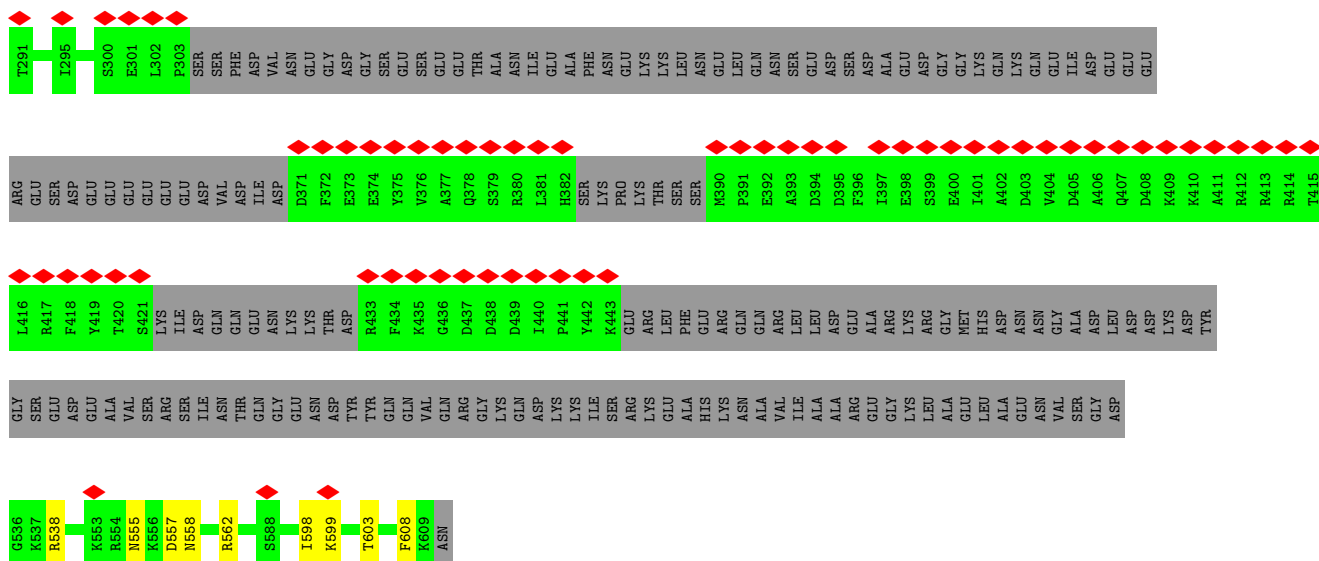


• Molecule 28: U3 small nucleolar RNA-associated protein 21

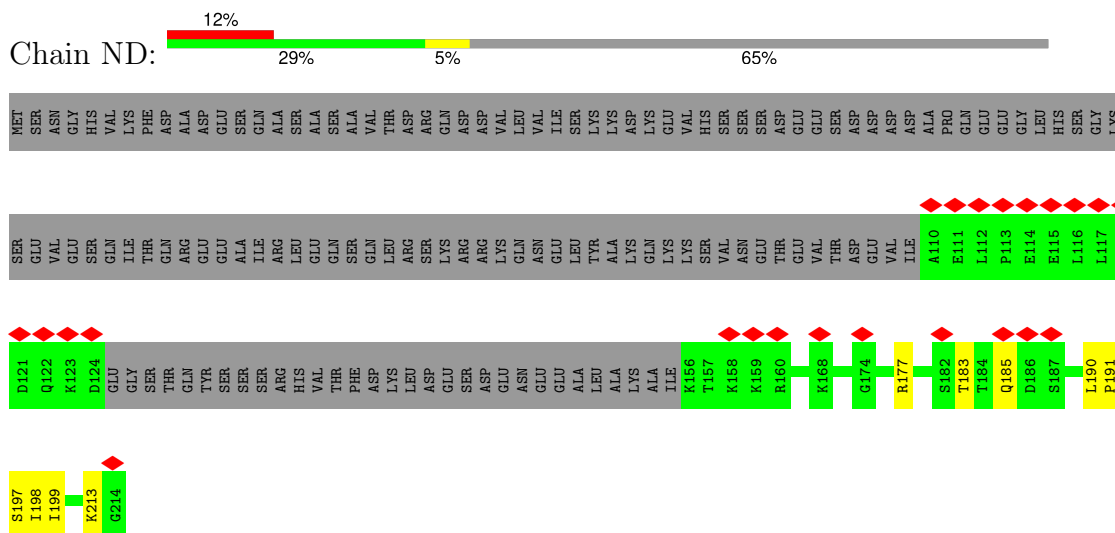


• Molecule 29: U3 small nucleolar ribonucleoprotein protein IMP3

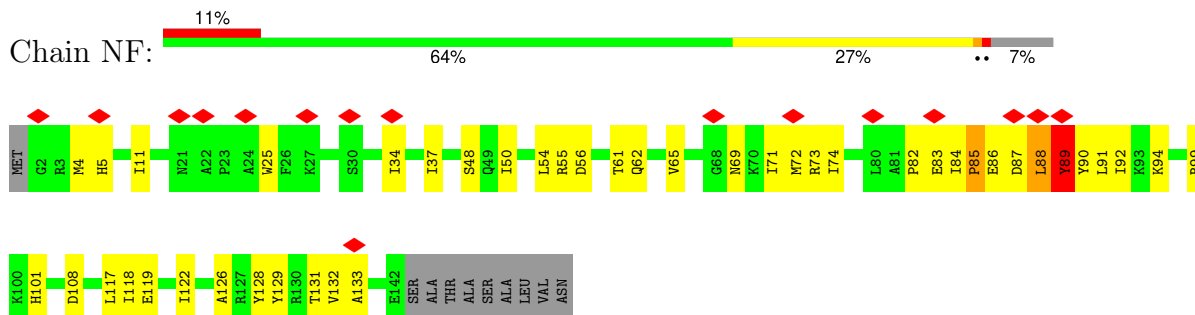




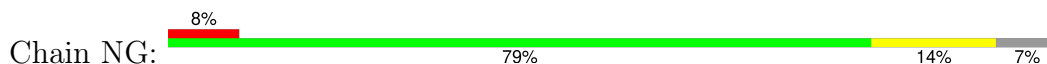
- Molecule 32: Bud site selection protein 21



- Molecule 33: 40S ribosomal protein S13

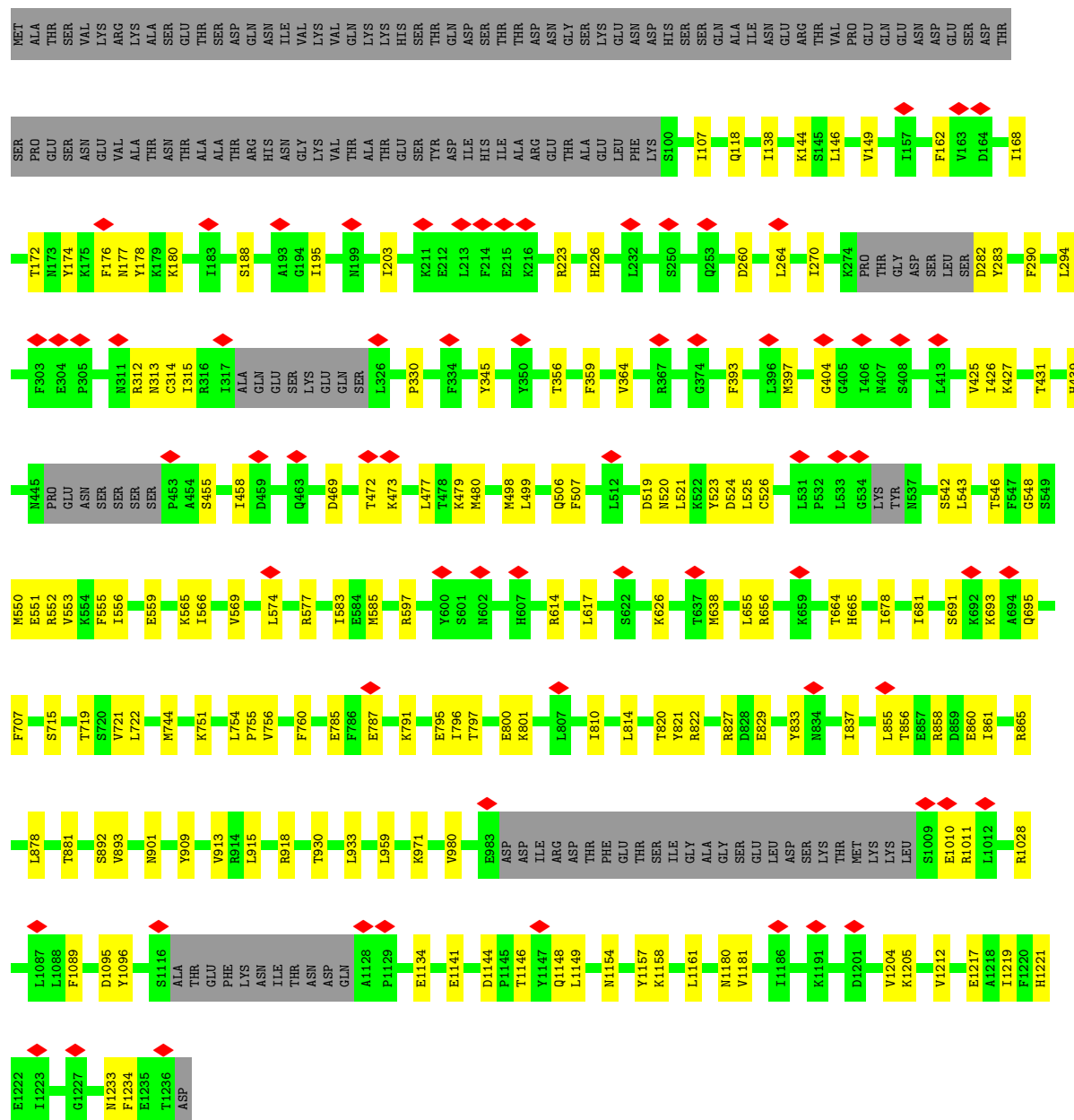
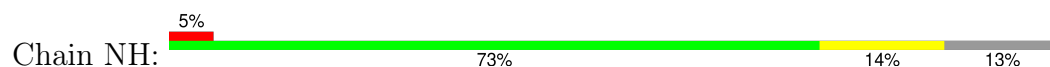


- Molecule 34: 40S ribosomal protein S14-A

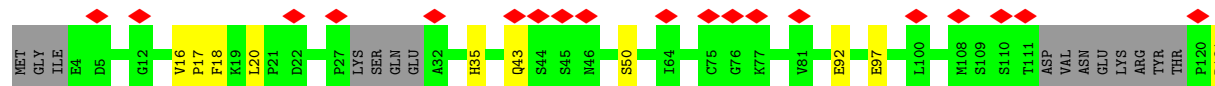


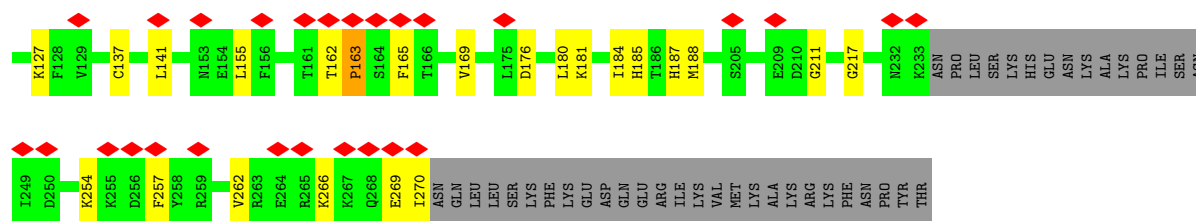


- Molecule 35: U3 small nucleolar RNA-associated protein 22

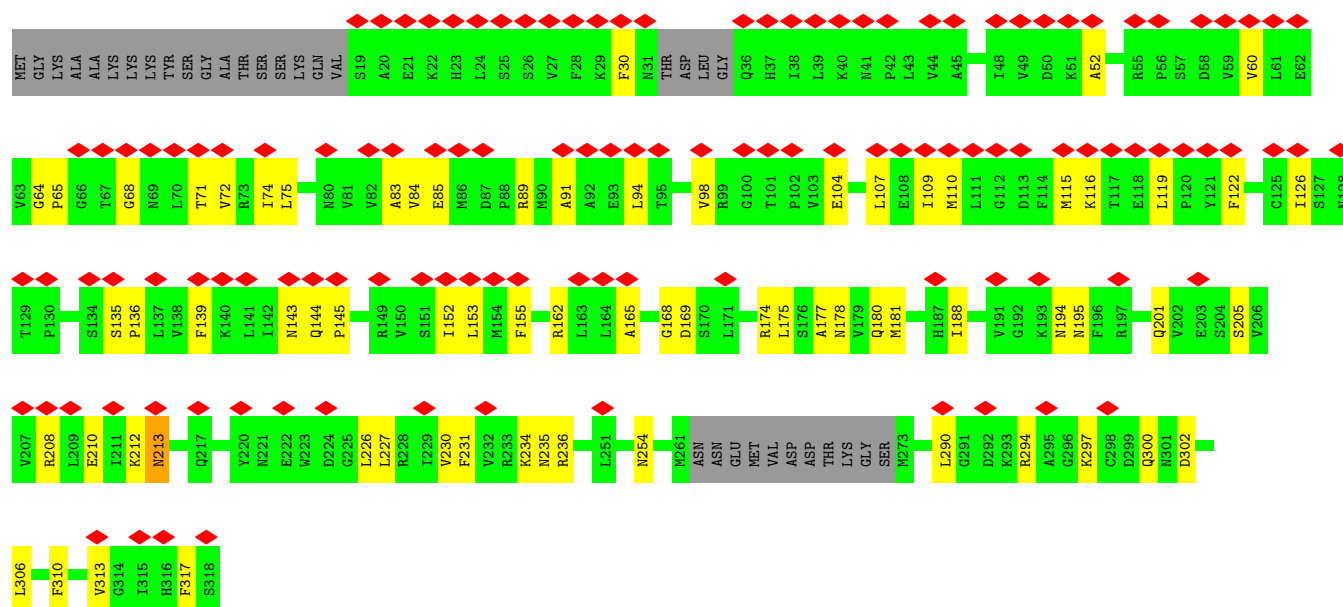


- Molecule 36: Ribosomal RNA-processing protein 7

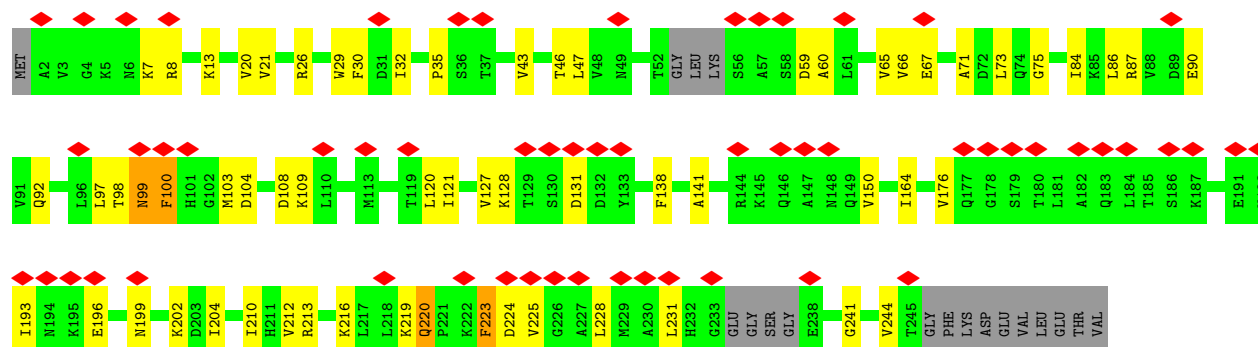




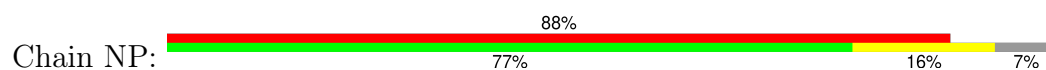
• Molecule 37: Dimethyladenosine transferase

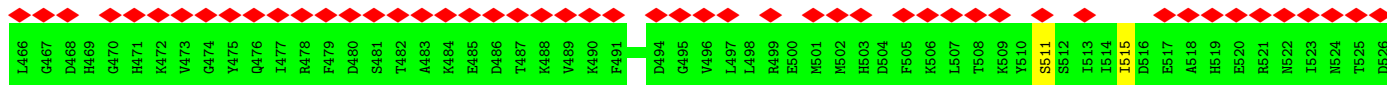


• Molecule 38: Small ribosomal subunit protein eS1A

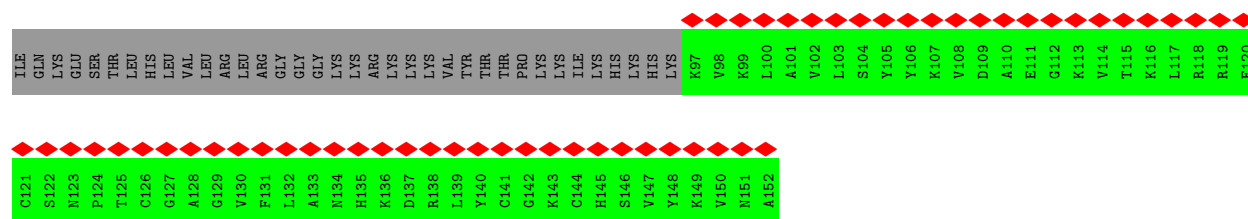


• Molecule 39: 40S ribosomal protein S19-A

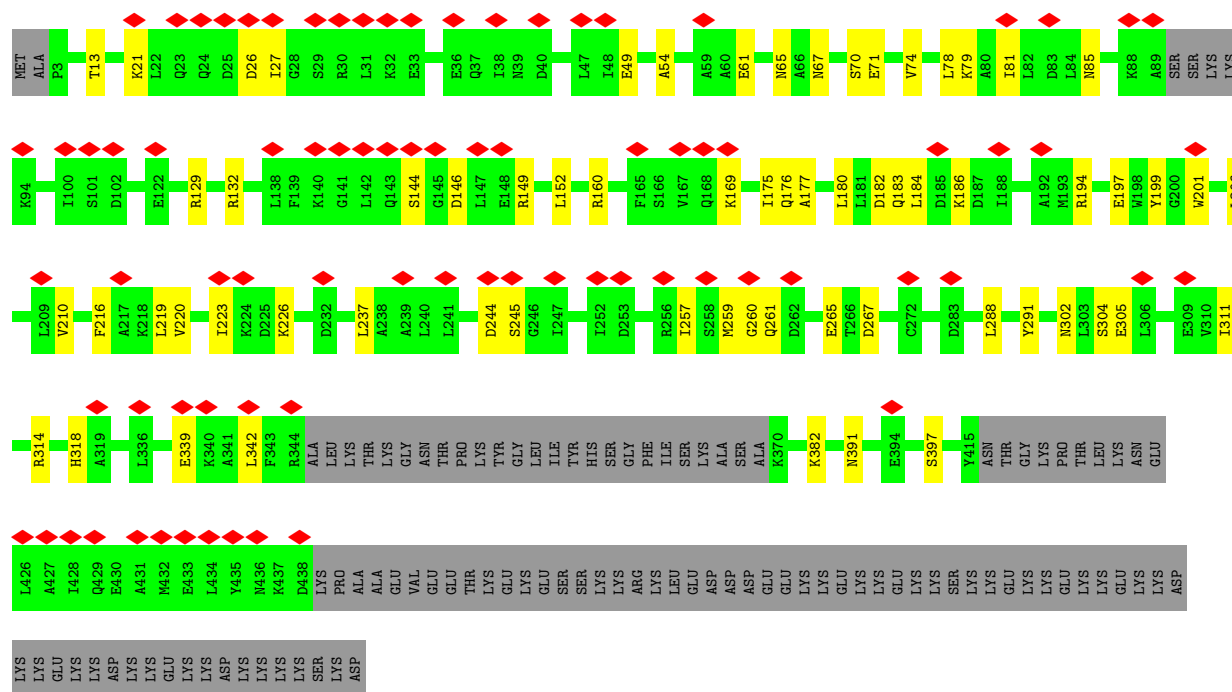




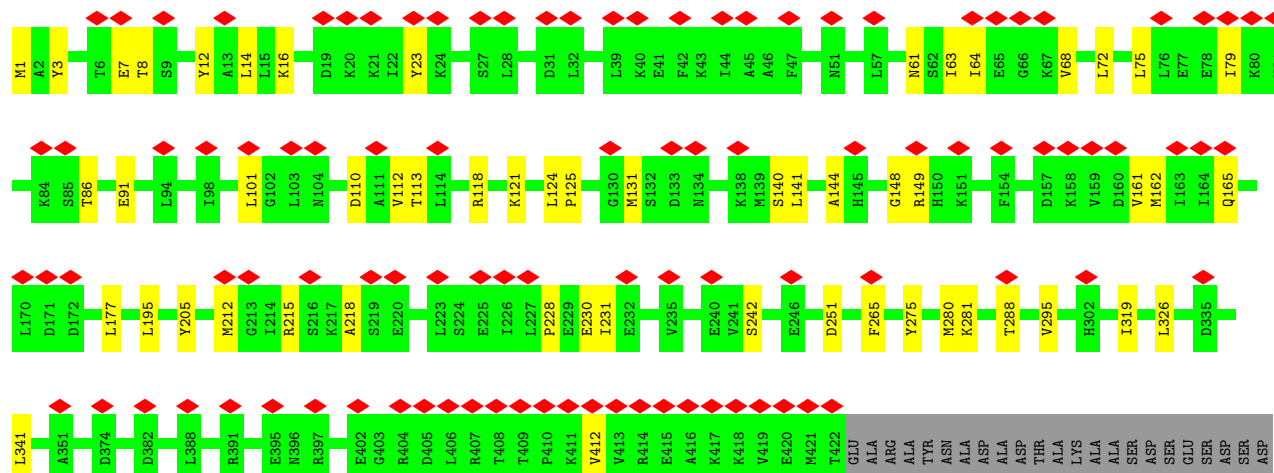
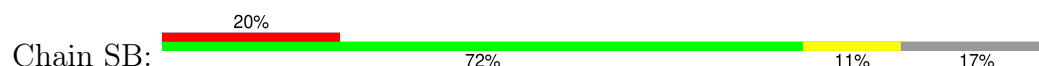




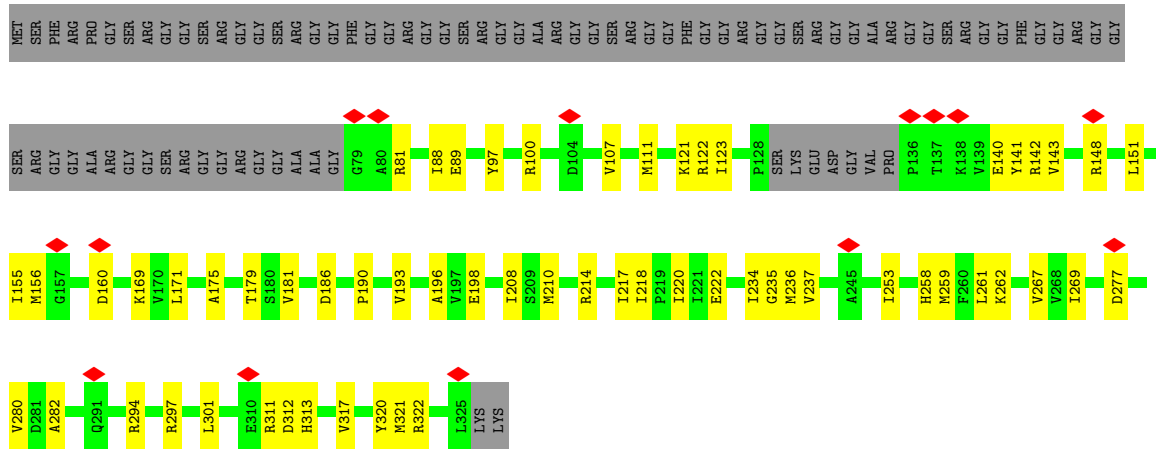
• Molecule 45: Nucleolar protein 56



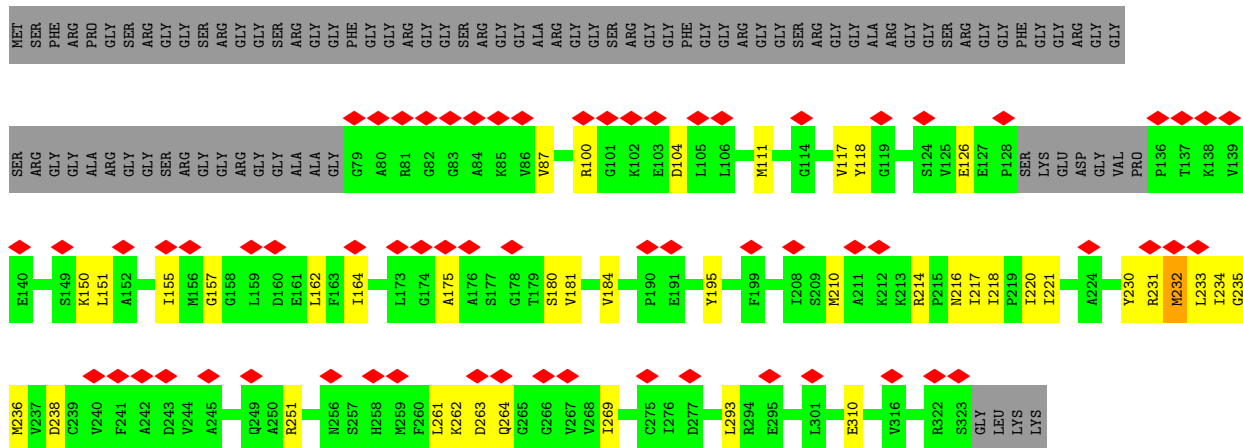
• Molecule 46: Nucleolar protein 58



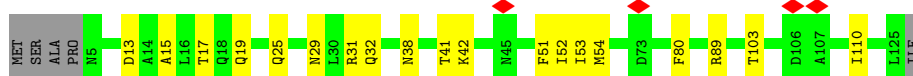
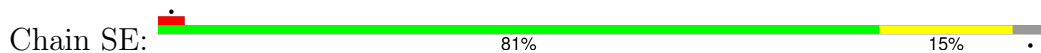
- Molecule 47: rRNA 2'-O-methyltransferase fibrillar



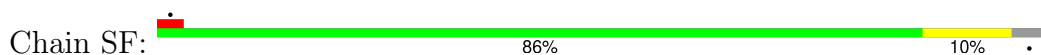
- Molecule 47: rRNA 2'-O-methyltransferase fibrillar

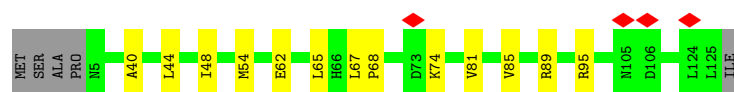


- Molecule 48: 13 kDa ribonucleoprotein-associated protein

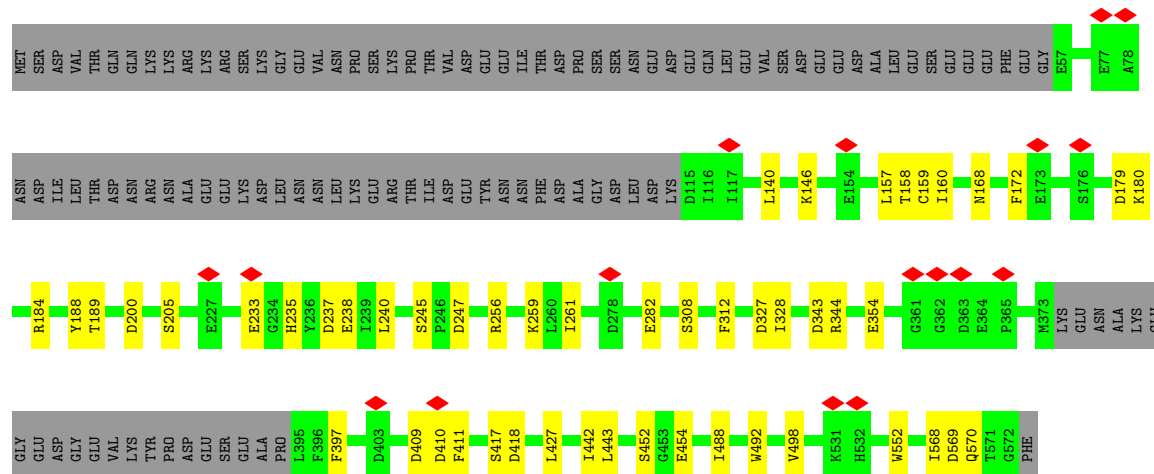


- Molecule 48: 13 kDa ribonucleoprotein-associated protein

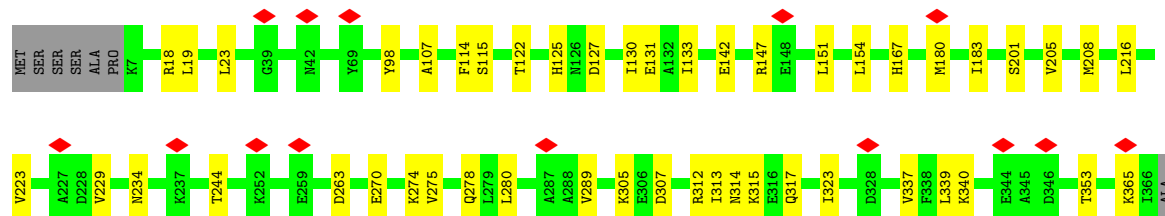
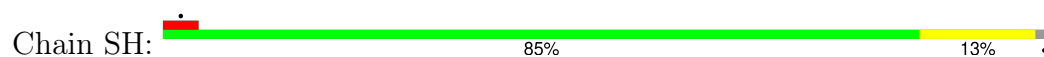




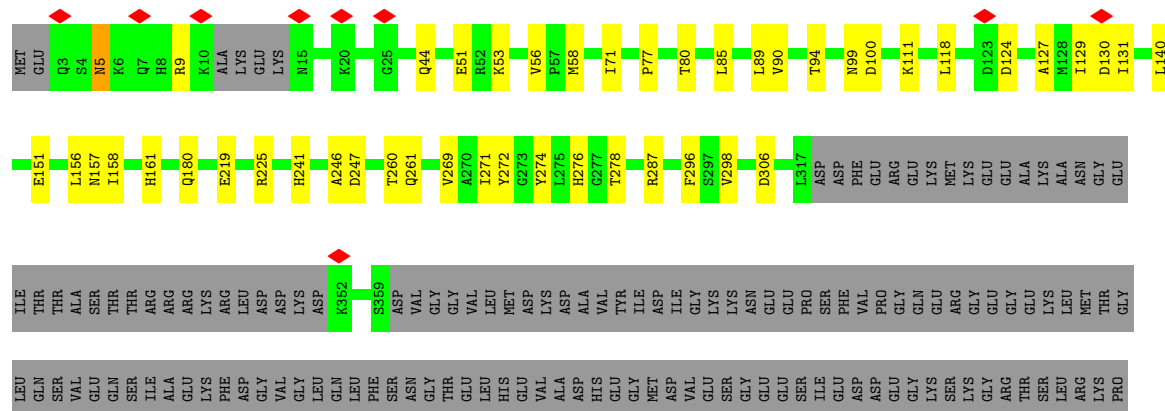
• Molecule 49: Ribosomal RNA-processing protein 9

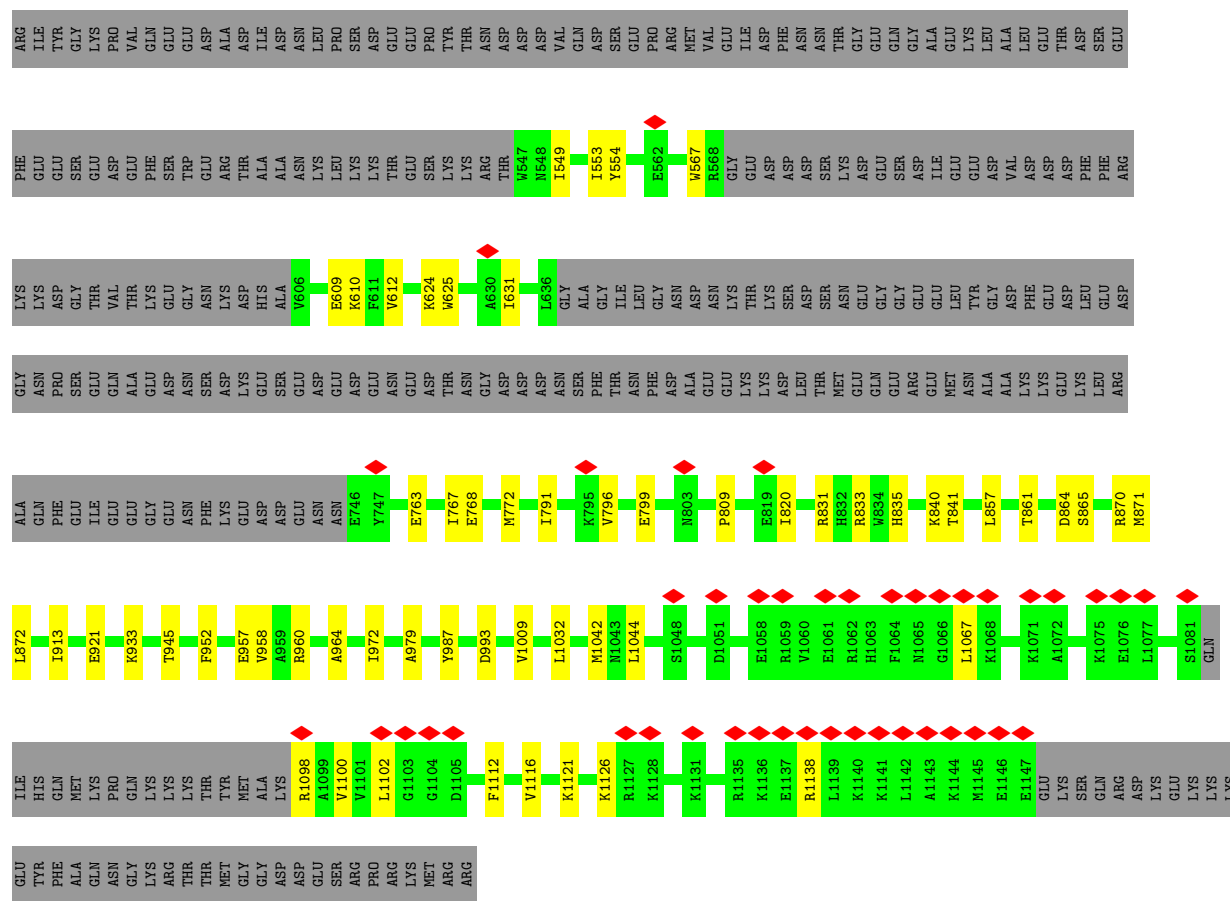


• Molecule 50: RNA 3'-terminal phosphate cyclase-like protein



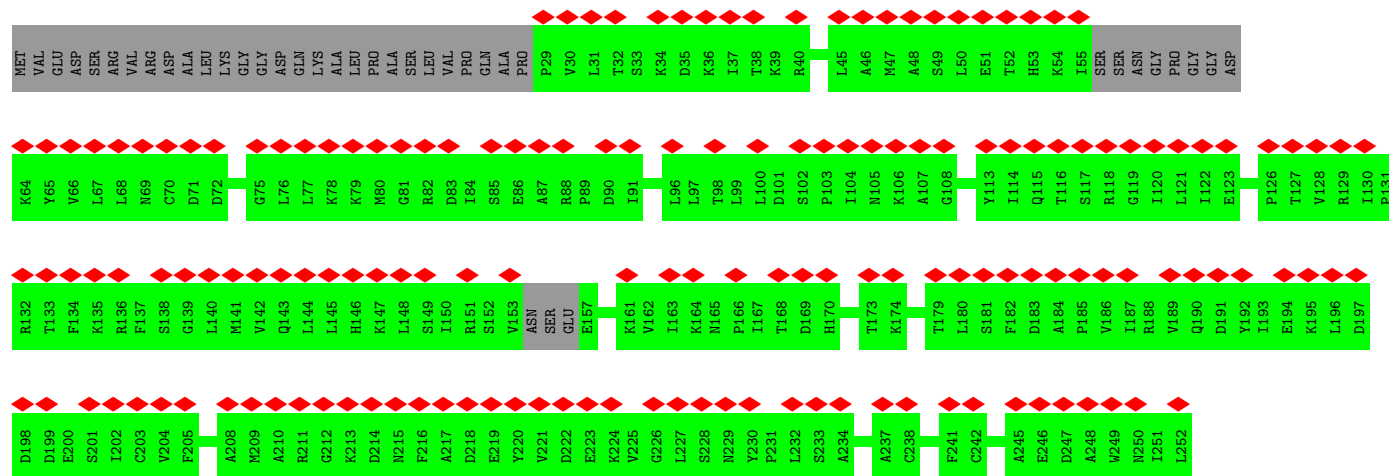
• Molecule 51: Ribosome biogenesis protein BMS1





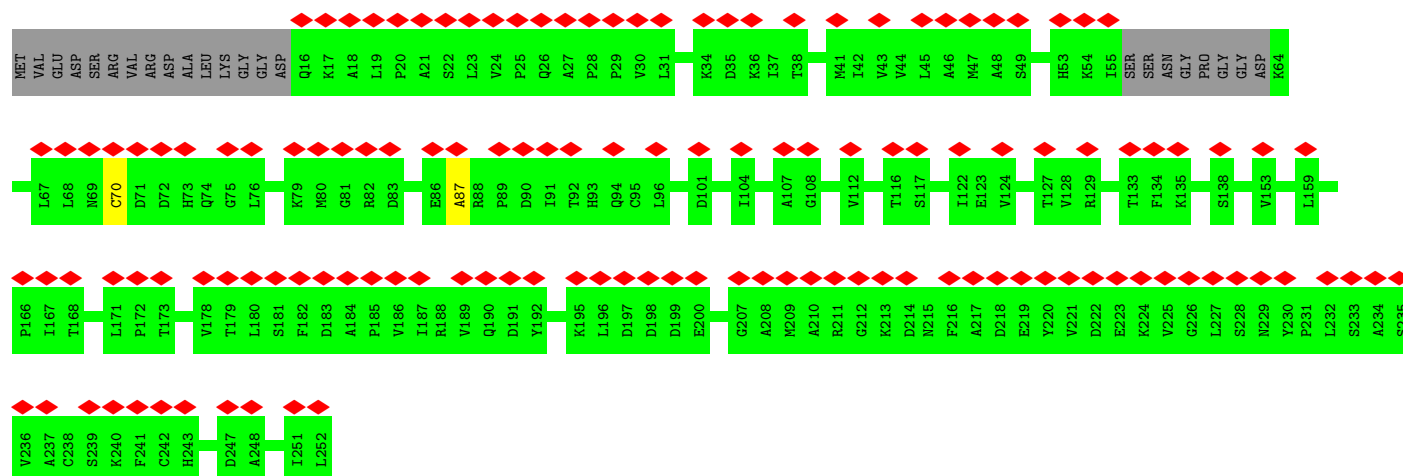
• Molecule 52: Ribosomal RNA small subunit methyltransferase NEP1

Chain SJ:

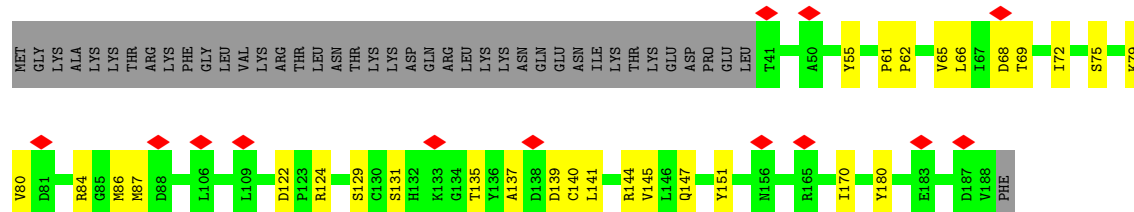


• Molecule 52: Ribosomal RNA small subunit methyltransferase NEP1

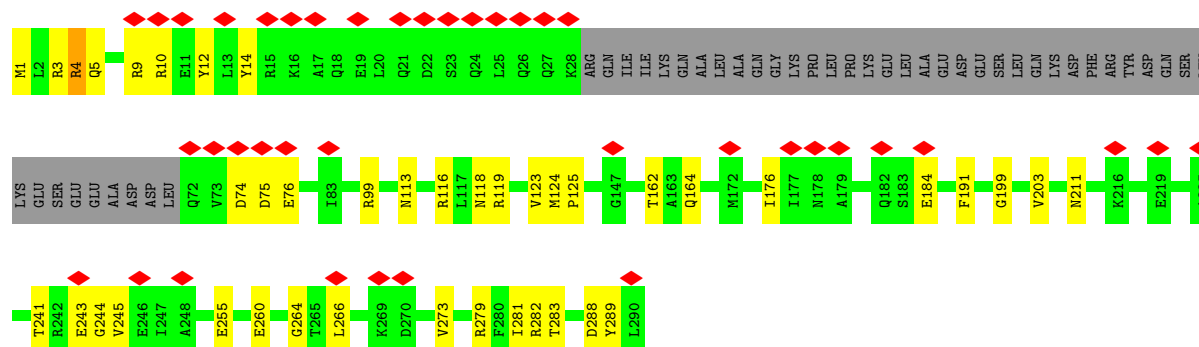
Chain SK:



• Molecule 53: rRNA-processing protein FCF1

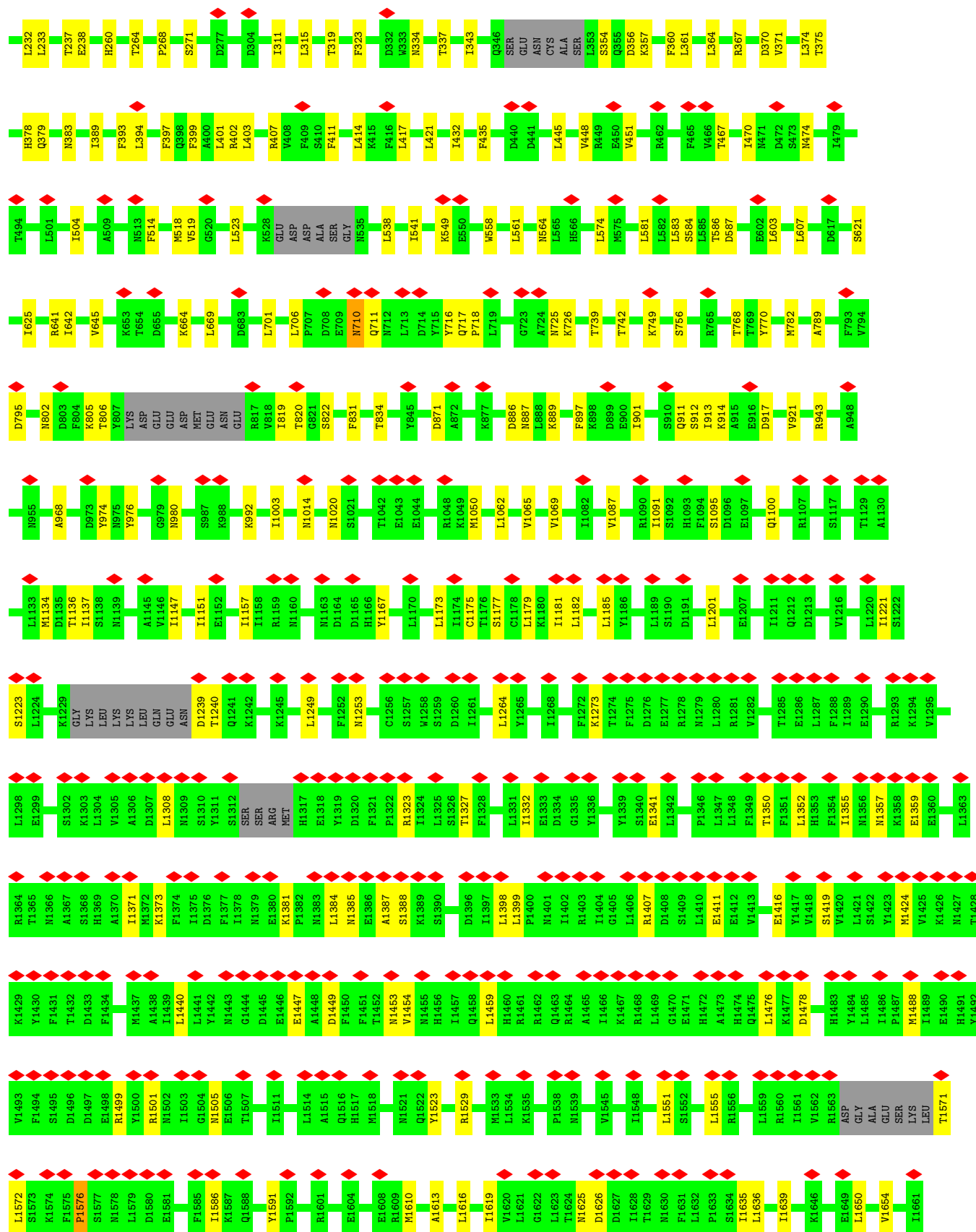


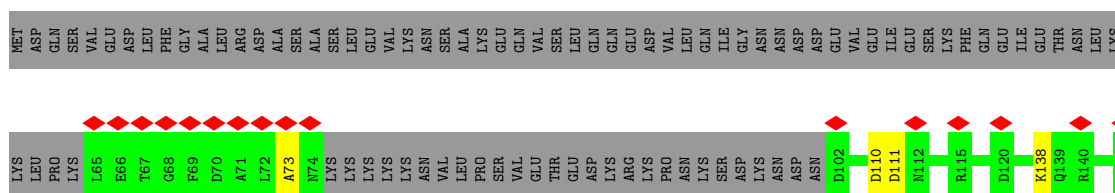
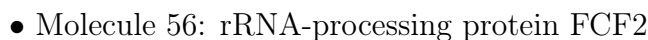
• Molecule 54: U3 small nucleolar ribonucleoprotein protein IMP4



• Molecule 55: U3 small nucleolar RNA-associated protein 20

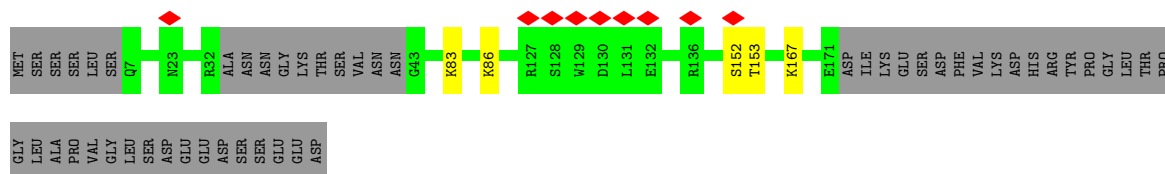




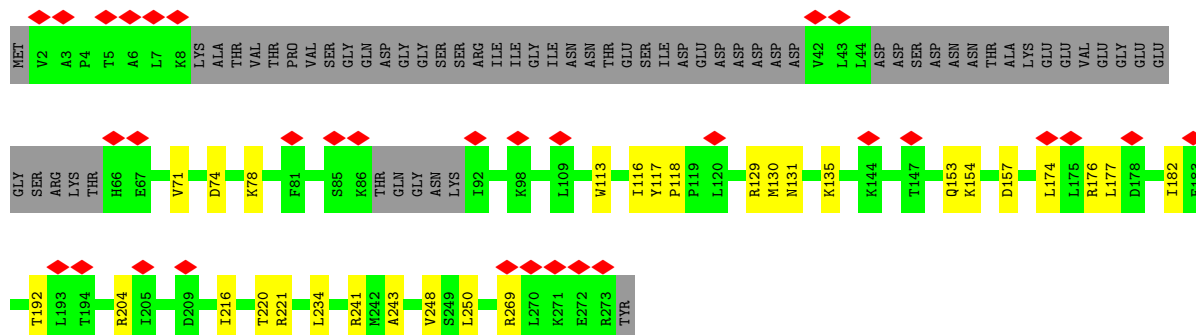




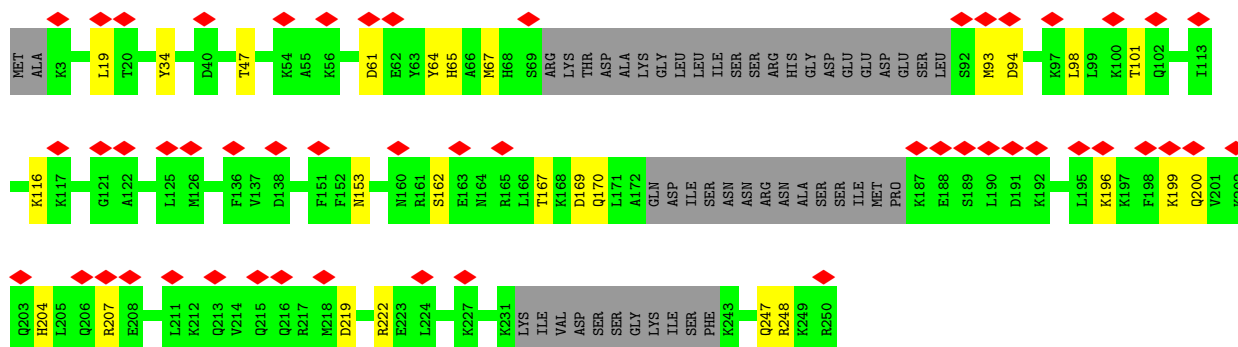




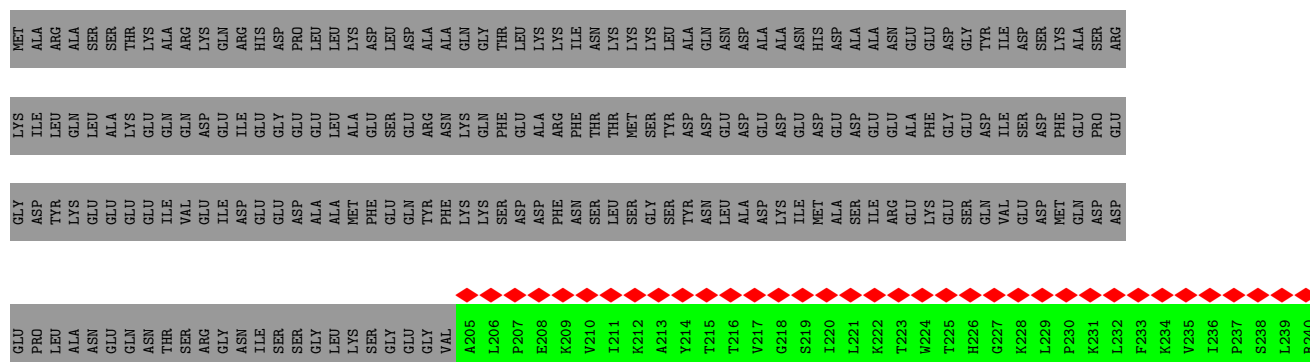
• Molecule 62: Pre-rRNA-processing protein PNO1



• Molecule 63: U3 small nucleolar RNA-associated protein 11



• Molecule 64: Essential nuclear protein 1



VAL ASN	L422	L362	H302	N241
	T423	P363	I303	W242
	F424	F364	Y304	Q243
	A425	S365	R305	D244
Q426	P366	A306	V245	
R427	P367	V307	I246	
Y428	T368	K308	Y247	
K429	T369	K309	T248	
N430	V370	S310	T249	
D431	F371	L311	N250	
I432	I372	Y312	P251	
T433	K373	K313	E252	
Q434	I374	P314	E253	
D435	L375	S315	W254	
Q436	L376	A316	S255	
R437	D377	F317	P256	
D438	K378	F318	H257	
F439	K379	K319	V258	
L440	Y380	G320	V259	
L441	A381	F321	Y260	
E442	L382	L322	E261	
T443	P383	F323	A262	
V444	Y384	P324	T263	
R445	Q385	L325	K264	
Q446	T386	V326	L265	
R447	V387	E327	F266	
G448	D388	T328	V267	
H449	C389	G329	S268	
K450	C390	C330	N269	
D451	V391	N331	L270	
I452	Y392	V332	T271	
G453	Y393	R333	A272	
P454	F394	E334	K273	
E455	M395	A335	E274	
I456	R396	T336	S275	
R457	F397	I337	Q276	
R458	R398	A338		
E459	I399	G339		
L460	L400	S340		
L461	ASP	V341		
A462	ASP	L342		
G463	GLY	A343		
A464	S404	K344		
S465	N405	V345		
R466	G406	S346		
GLU	E407	V347		
PHE	D408	P347		
VAL	A409	V348		
ASP	T410	A349		
PRO	R411	L350		
GLN	V412	H351		
GLU	L413	S352		
ALA	P414	T293		
ASN	V415	S294		
ASP	I416	A354		
LEU	T417	A355		
MET	H418	L356		
ILE	K419	S357		
ASP	A420	Y358		
	F421	L359		
		L360		
		R361		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11394	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	3.863	Depositor
Minimum map value	0.000	Depositor
Average map value	0.094	Depositor
Map value standard deviation	0.169	Depositor
Recommended contour level	0.75	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: ATP, ADP, SEP, GTP, MG, M7G, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L0	0.09	0/1605	0.22	0/2494
2	L1	0.10	0/34578	0.27	0/53850
3	L2	0.09	0/4868	0.23	0/7561
4	L3	0.16	0/872	0.35	0/1173
5	L4	0.16	0/1977	0.42	1/2664 (0.0%)
6	L5	0.16	0/1655	0.39	0/2237
7	L6	0.16	0/1764	0.35	0/2359
8	L7	0.20	0/1451	0.49	0/1956
9	L8	0.13	0/1371	0.34	0/1833
10	L9	0.18	0/1495	0.40	1/2003 (0.0%)
11	LC	0.19	0/1015	0.45	0/1367
12	LD	0.16	0/1138	0.41	0/1533
13	LE	0.19	0/1039	0.45	0/1395
14	LF	0.17	0/1060	0.42	0/1412
15	LG	0.17	0/492	0.42	0/659
16	LH	0.17	0/6576	0.42	0/8902
17	LI	0.14	0/3835	0.35	0/5263
18	LJ	0.15	0/3851	0.37	0/5221
19	LK	0.14	0/1085	0.32	0/1463
20	LL	0.14	0/3939	0.36	0/5341
21	LM	0.13	0/9356	0.35	2/12933 (0.0%)
22	LN	0.13	0/5359	0.35	2/7255 (0.0%)
23	LO	0.12	0/6463	0.31	0/8748
24	LP	0.13	0/1907	0.34	0/2667
25	LQ	0.15	0/6620	0.39	0/8936
26	LR	0.13	0/6313	0.33	0/8551
27	LS	0.17	0/3735	0.41	2/5064 (0.0%)
28	LT	0.15	0/6921	0.34	1/9362 (0.0%)
29	LZ	0.22	0/1194	0.48	0/1610
30	NA	0.17	0/2442	0.38	0/3281
31	NB	0.12	0/1654	0.33	0/2243
32	ND	0.15	0/568	0.39	0/755

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	NF	0.36	0/1158	0.58	1/1559 (0.1%)
34	NG	0.15	0/952	0.36	0/1279
35	NH	0.14	0/8899	0.34	1/12035 (0.0%)
36	NI	0.17	0/1994	0.41	1/2684 (0.0%)
37	NL	0.18	0/2329	0.40	0/3144
38	NM	0.25	0/1915	0.51	0/2563
39	NP	0.13	0/1056	0.33	0/1416
40	NQ	0.17	0/605	0.43	0/817
41	NS	0.20	0/5100	0.44	1/7072 (0.0%)
42	NV	0.19	0/151	0.46	0/196
43	OH	0.09	0/595	0.27	0/827
44	OU	0.10	0/278	0.28	0/386
45	SA	0.13	0/3146	0.32	0/4240
46	SB	0.15	0/3293	0.34	0/4436
47	SC	0.17	0/1903	0.41	0/2567
47	SD	0.17	0/1885	0.37	0/2543
48	SE	0.17	0/928	0.38	0/1262
48	SF	0.17	0/928	0.43	0/1262
49	SG	0.12	0/3744	0.31	0/5040
50	SH	0.15	0/2832	0.38	0/3825
51	SI	0.15	0/6281	0.35	0/8457
52	SJ	0.12	0/1080	0.32	0/1508
52	SK	0.14	0/1170	0.37	0/1639
53	SL	0.16	0/1193	0.40	0/1611
54	SM	0.17	0/2046	0.36	0/2759
55	SP	0.13	0/15404	0.33	1/20833 (0.0%)
56	SQ	0.14	0/901	0.37	0/1204
57	SR	0.15	0/1069	0.38	0/1427
58	SS	0.15	0/799	0.37	0/1050
59	ST	0.13	0/3475	0.31	0/4761
60	SU	0.12	0/2726	0.31	0/3825
61	SV	0.13	0/854	0.37	0/1175
62	SW	0.16	0/1696	0.37	0/2282
63	SY	0.18	0/1736	0.43	0/2292
64	SZ	0.12	0/1326	0.31	0/1859
All	All	0.14	0/213645	0.35	14/297926 (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
21	LM	0	2
33	NF	0	2
38	NM	0	4
41	NS	0	4
47	SD	0	1
48	SF	0	1
54	SM	0	1
All	All	0	15

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	NF	89	TYR	CA-CB-CG	8.98	130.07	113.90
21	LM	222	ALA	CA-C-N	8.80	136.08	122.08
21	LM	222	ALA	C-N-CA	8.80	136.08	122.08
36	NI	163	PRO	CA-N-CD	-8.79	99.69	112.00
28	LT	326	PRO	CA-N-CD	-8.35	100.31	112.00
22	LN	224	ARG	CA-C-N	8.01	135.14	122.17
22	LN	224	ARG	C-N-CA	8.01	135.14	122.17
10	L9	2	PRO	CA-N-CD	-7.54	101.44	112.00
5	L4	59	ARG	CG-CD-NE	-7.26	96.03	112.00
55	SP	1576	PRO	CA-N-CD	-6.95	102.27	112.00
41	NS	1101	PRO	CA-N-CD	-5.84	103.82	112.00
27	LS	429	TYR	CA-C-N	5.73	132.63	121.41
27	LS	429	TYR	C-N-CA	5.73	132.63	121.41
35	NH	330	PRO	CA-N-CD	-5.63	104.11	112.00

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	LM	222	ALA	Peptide
21	LM	224	ASN	Peptide
33	NF	88	LEU	Peptide
33	NF	89	TYR	Sidechain
38	NM	219	LYS	Peptide
38	NM	220	GLN	Peptide
38	NM	223	PHE	Peptide
38	NM	99	ASN	Peptide
41	NS	424	VAL	Peptide
41	NS	427	PHE	Peptide

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Mol	Chain	Res	Type	Group
41	NS	428	LEU	Peptide
41	NS	430	GLU	Peptide
47	SD	232	MET	Peptide
48	SF	89	ARG	Sidechain
54	SM	4	ARG	Sidechain

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	7	0
2	L1	30918	0	15571	213	0
3	L2	4394	0	2229	19	0
4	L3	862	0	900	15	0
5	L4	1936	0	2019	30	0
6	L5	1635	0	1697	29	0
7	L6	1740	0	1835	36	0
8	L7	1427	0	1499	35	0
9	L8	1348	0	1366	17	0
10	L9	1470	0	1554	15	0
11	LC	997	0	1054	19	0
12	LD	1112	0	1179	15	0
13	LE	1022	0	1060	25	0
14	LF	1046	0	1114	18	0
15	LG	490	0	529	8	0
16	LH	6449	0	6398	141	0
17	LI	3792	0	2859	37	0
18	LJ	3773	0	3761	66	0
19	LK	1068	0	1120	18	0
20	LL	3871	0	3876	77	0
21	LM	9274	0	6159	53	0
22	LN	5263	0	5270	67	0
23	LO	6321	0	6235	68	0
24	LP	1901	0	836	3	0
25	LQ	6494	0	6544	127	0
26	LR	6207	0	6247	87	0
27	LS	3662	0	3639	67	0
28	LT	6787	0	6685	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	LZ	1173	0	1208	33	0
30	NA	2426	0	2263	56	0
31	NB	1645	0	1277	21	0
32	ND	564	0	587	13	0
33	NF	1135	0	1197	47	0
34	NG	941	0	979	15	0
35	NH	8693	0	8806	112	0
36	NI	1953	0	1933	25	0
37	NL	2285	0	2359	48	0
38	NM	1891	0	1995	56	0
39	NP	1040	0	1057	17	0
40	NQ	595	0	610	19	0
41	NS	5051	0	2958	30	0
42	NV	149	0	172	2	0
43	OH	594	0	298	1	0
44	OU	278	0	135	0	0
45	SA	3100	0	3084	43	0
46	SB	3255	0	3379	41	0
47	SC	1865	0	1908	48	0
47	SD	1850	0	1889	37	0
48	SE	916	0	964	14	0
48	SF	916	0	964	10	0
49	SG	3672	0	3690	32	0
50	SH	2781	0	2878	34	0
51	SI	6144	0	6331	91	0
52	SJ	1074	0	514	0	0
52	SK	1160	0	570	1	0
53	SL	1171	0	1229	20	0
54	SM	2009	0	2027	34	0
55	SP	15102	0	15321	176	0
56	SQ	885	0	866	12	0
57	SR	1052	0	1120	13	0
58	SS	791	0	815	14	0
59	ST	3455	0	2276	22	0
60	SU	2703	0	1302	0	0
61	SV	852	0	476	3	0
62	SW	1669	0	1747	24	0
63	SY	1715	0	1789	21	0
64	SZ	1314	0	649	1	0
65	L1	35	0	0	0	0
65	NH	1	0	0	0	0
65	NS	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	SI	1	0	0	0	0
66	NH	31	0	12	1	0
67	NQ	1	0	0	0	0
67	SL	1	0	0	0	0
68	NS	27	0	12	0	0
69	SI	32	0	12	0	0
All	All	206690	0	177615	2188	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 6.

All (2188) 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)
8:L7:67:LEU:HD22	8:L7:94:ALA:HB2	1.45	0.98
2:L1:446:A:OP1	5:L4:59:ARG:NH1	2.04	0.90
37:NL:98:VAL:HG11	37:NL:107:LEU:HD23	1.52	0.89
35:NH:787:GLU:OE2	38:NH:199:ASN:ND2	2.05	0.89
23:LO:841:ASP:OD1	25:LQ:903:GLN:NE2	2.08	0.86
2:L1:23:G:O6	2:L1:603:U:O2	1.94	0.86
2:L1:1662:G:OP1	41:NS:247:ASN:ND2	2.08	0.86
41:NS:426:GLN:N	41:NS:429:TYR:O	2.10	0.85
16:LH:574:LEU:HD23	16:LH:613:LEU:HD21	1.58	0.85
27:LS:455:ILE:HD12	27:LS:484:VAL:HG12	1.59	0.85
16:LH:716:ARG:NH2	16:LH:772:THR:OG1	2.11	0.84
12:LD:55:ASP:OD1	12:LD:82:ARG:NH1	2.11	0.83
25:LQ:180:THR:OG1	25:LQ:207:CYS:SG	2.35	0.83
4:L3:113:LEU:HD13	59:ST:751:THR:HG22	1.60	0.83
48:SE:32:GLN:OE1	48:SE:103:THR:OG1	1.95	0.83
26:LR:542:CYS:SG	26:LR:587:GLN:NE2	2.52	0.83
46:SB:14:LEU:HD13	46:SB:79:ILE:HD12	1.61	0.82
2:L1:1034:C:HO2'	13:LE:2:THR:N	1.77	0.82
23:LO:119:LEU:HD12	23:LO:163:THR:HG21	1.62	0.82
55:SP:1699:LYS:O	55:SP:1702:HIS:ND1	2.10	0.82
30:NA:340:LEU:O	51:SI:960:ARG:NH2	2.11	0.82
49:SG:452:SER:OG	49:SG:454:GLU:OE1	1.97	0.82
2:L1:609:U:O3'	57:SR:19:ARG:NH2	2.14	0.81
33:NH:56:ASP:OD2	40:NQ:52:THR:OG1	1.99	0.81
35:NH:617:LEU:HD13	35:NH:678:ILE:HD11	1.62	0.81
46:SB:68:VAL:HG23	46:SB:72:LEU:HD23	1.62	0.81
55:SP:1610:MET:HE3	55:SP:1654:VAL:HG22	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L0:86:C:N4	16:LH:318:GLU:OE2	2.14	0.80
30:NA:339:ALA:O	30:NA:342:THR:OG1	2.00	0.80
6:L5:196:GLU:OE2	6:L5:200:ASN:ND2	2.14	0.80
8:L7:143:LEU:O	13:LE:42:GLN:NE2	2.15	0.80
47:SC:81:ARG:O	56:SQ:152:ILE:HD11	1.81	0.80
11:LC:98:ASP:OD2	28:LT:488:ASN:ND2	2.15	0.80
25:LQ:79:PRO:O	25:LQ:657:GLN:NE2	2.14	0.80
6:L5:35:GLN:O	6:L5:38:THR:OG1	2.00	0.80
18:LJ:61:THR:OG1	18:LJ:80:PHE:O	2.00	0.80
2:L1:1004:U:O2	62:SW:241:ARG:NH2	2.15	0.80
25:LQ:472:HIS:NE2	25:LQ:492:SER:OG	2.14	0.80
2:L1:1162:C:OP1	6:L5:148:ARG:NH2	2.15	0.80
2:L1:1524:A:N3	2:L1:1590:G:O2'	2.15	0.80
16:LH:883:GLN:O	16:LH:886:THR:OG1	2.00	0.79
2:L1:293:U:O2'	5:L4:133:LYS:NZ	2.12	0.79
2:L1:433:C:N4	2:L1:436:A:OP1	2.15	0.79
16:LH:742:ARG:NH2	16:LH:758:THR:OG1	2.16	0.79
30:NA:428:GLU:OE1	30:NA:431:GLN:NE2	2.15	0.79
63:SY:219:ASP:OD1	63:SY:222:ARG:NH2	2.16	0.79
22:LN:586:THR:OG1	22:LN:588:ASP:OD1	2.01	0.79
54:SM:113:ASN:ND2	54:SM:211:ASN:OD1	2.16	0.78
14:LF:8:ARG:NH1	49:SG:354:GLU:OE1	2.15	0.78
23:LO:848:PHE:O	23:LO:852:THR:OG1	2.01	0.78
41:NS:420:LYS:O	41:NS:424:VAL:N	2.16	0.78
2:L1:622:A:O2'	2:L1:1032:G:OP1	2.02	0.78
2:L1:225:A:O2'	55:SP:1407:ARG:NH2	2.16	0.78
54:SM:12:TYR:OH	54:SM:76:GLU:OE2	2.01	0.78
2:L1:433:C:OP1	51:SI:53:LYS:NZ	2.17	0.77
2:L1:885:G:N2	34:NG:124:ASP:OD2	2.17	0.77
2:L1:524:U:O2'	2:L1:527:A:N7	2.16	0.77
2:L1:265:A:OP2	7:L6:194:LYS:NZ	2.17	0.77
2:L1:814:A:O2'	33:NF:73:ARG:NH2	2.17	0.77
2:L1:358:U:OP2	41:NS:2:GLY:N	2.18	0.77
14:LF:10:ARG:NH1	14:LF:26:ASP:OD2	2.16	0.77
31:NB:19:ASN:ND2	31:NB:22:GLY:O	2.18	0.77
2:L1:899:G:OP2	38:NM:13:LYS:NZ	2.18	0.77
23:LO:608:ASN:ND2	28:LT:513:MET:SD	2.58	0.76
17:LI:567:LEU:HD22	17:LI:599:MET:HE1	1.66	0.76
50:SH:340:LYS:NZ	51:SI:768:GLU:OE1	2.17	0.76
16:LH:520:LEU:HD11	18:LJ:464:ALA:HB2	1.68	0.76
25:LQ:181:SER:OG	25:LQ:183:ASP:OD1	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LZ:126:ASP:OD2	63:SY:65:HIS:NE2	2.16	0.76
20:LL:302:ASN:ND2	20:LL:316:ASN:OD1	2.19	0.76
2:L1:460:A:O2'	5:L4:27:TYR:OH	2.03	0.76
2:L1:867:G:N2	33:NF:87:ASP:OD1	2.18	0.76
29:LZ:59:ASN:O	29:LZ:62:SER:OG	2.03	0.76
13:LE:30:SER:OG	13:LE:58:SER:O	2.03	0.76
33:NF:128:TYR:O	33:NF:131:THR:OG1	2.04	0.76
45:SA:194:ARG:NH1	46:SB:165:GLN:OE1	2.19	0.76
55:SP:379:GLN:NE2	55:SP:383:ASN:OD1	2.19	0.76
28:LT:456:ASP:OD1	28:LT:487:TYR:OH	2.04	0.76
45:SA:291:TYR:OH	46:SB:251:ASP:OD1	2.03	0.76
8:L7:47:ARG:NH1	8:L7:48:GLU:O	2.19	0.75
53:SL:124:ARG:NH1	55:SP:1851:GLU:O	2.19	0.75
2:L1:330:G:OP2	9:L8:172:ARG:NH1	2.20	0.75
18:LJ:54:ASP:OD2	18:LJ:111:TYR:OH	2.05	0.75
2:L1:331:A:OP1	9:L8:56:ARG:NH1	2.20	0.75
46:SB:7:GLU:OE2	47:SD:231:ARG:NE	2.19	0.75
50:SH:142:GLU:O	50:SH:147:ARG:NH2	2.20	0.75
22:LN:345:ASP:OD2	22:LN:360:SER:OG	2.04	0.75
25:LQ:628:HIS:ND1	25:LQ:645:GLU:OE2	2.20	0.75
25:LQ:888:ARG:NH2	26:LR:807:ASP:OD2	2.20	0.75
2:L1:134:U:O2'	55:SP:992:LYS:NZ	2.18	0.74
31:NB:555:ASN:OD1	31:NB:558:ASN:ND2	2.19	0.74
18:LJ:377:ASP:OD1	20:LL:343:ARG:NH1	2.20	0.74
50:SH:365:LYS:NZ	51:SI:921:GLU:OE2	2.19	0.74
29:LZ:174:ARG:O	29:LZ:176:GLN:NE2	2.19	0.74
7:L6:18:ILE:HG21	7:L6:24:ILE:HD11	1.70	0.74
30:NA:335:ARG:NH2	51:SI:957:GLU:OE1	2.20	0.74
2:L1:246:G:N2	12:LD:38:ALA:O	2.20	0.74
29:LZ:151:THR:OG1	29:LZ:153:ASN:OD1	2.05	0.74
47:SD:111:MET:SD	47:SD:216:ASN:ND2	2.61	0.74
62:SW:154:LYS:NZ	62:SW:177:LEU:O	2.21	0.74
2:L1:487:G:O5'	51:SI:1126:LYS:NZ	2.21	0.73
2:L1:151:G:O2'	7:L6:13:GLN:NE2	2.21	0.73
16:LH:594:TRP:O	20:LL:362:ARG:NH2	2.22	0.73
26:LR:137:THR:O	26:LR:180:ARG:NH2	2.21	0.73
48:SE:25:GLN:NE2	48:SE:29:ASN:OD1	2.21	0.73
16:LH:605:ASN:OD1	16:LH:606:HIS:ND1	2.20	0.73
41:NS:428:LEU:HA	41:NS:430:GLU:H	1.53	0.73
59:ST:16:ARG:O	59:ST:44:LYS:NZ	2.21	0.73
2:L1:1635:A:O3'	26:LR:795:ARG:NH2	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SD:220:ILE:HD13	47:SD:234:ILE:HD11	1.70	0.73
2:L1:71:A:OP2	7:L6:164:LYS:NZ	2.21	0.73
21:LM:413:ASP:OD2	21:LM:417:LYS:NZ	2.21	0.73
51:SI:833:ARG:NE	57:SR:141:GLU:OE1	2.20	0.73
2:L1:1639:C:OP2	30:NA:511:ASN:ND2	2.22	0.73
27:LS:325:ASP:O	27:LS:330:ASN:ND2	2.22	0.73
55:SP:583:LEU:O	55:SP:586:THR:OG1	2.06	0.73
55:SP:549:LYS:NZ	55:SP:584:SER:O	2.16	0.72
16:LH:505:GLN:O	16:LH:533:THR:OG1	2.05	0.72
16:LH:327:GLU:OE2	22:LN:319:ARG:NH2	2.22	0.72
33:NF:87:ASP:O	33:NF:91:LEU:N	2.21	0.72
11:LC:39:VAL:HG11	11:LC:48:VAL:HG11	1.71	0.72
22:LN:681:ILE:HG22	22:LN:683:ASP:H	1.53	0.72
35:NH:1205:LYS:NZ	35:NH:1217:GLU:OE2	2.23	0.72
23:LO:495:LYS:NZ	23:LO:515:TYR:O	2.22	0.72
26:LR:159:LYS:NZ	62:SW:71:VAL:O	2.23	0.72
2:L1:1464:G:O2'	54:SM:99:ARG:NH1	2.21	0.72
62:SW:129:ARG:NH1	62:SW:131:ASN:OD1	2.23	0.72
8:L7:17:GLU:HG3	8:L7:46:ILE:HG22	1.72	0.71
56:SQ:167:LYS:O	56:SQ:170:LYS:NZ	2.22	0.71
2:L1:934:C:O4'	58:SS:392:ARG:NH2	2.22	0.71
11:LC:50:GLU:OE2	11:LC:112:TYR:OH	2.07	0.71
23:LO:455:ILE:HD11	23:LO:476:VAL:HG21	1.73	0.71
28:LT:354:SER:O	28:LT:631:ASN:ND2	2.21	0.71
51:SI:118:LEU:HD23	51:SI:131:ILE:HD13	1.72	0.71
3:L2:324:U:OP1	63:SY:116:LYS:NZ	2.23	0.71
37:NL:213:ASN:O	37:NL:213:ASN:ND2	2.22	0.71
22:LN:687:PHE:O	22:LN:688:MET:HE2	1.91	0.71
62:SW:220:THR:HG21	62:SW:243:ALA:HB2	1.71	0.71
16:LH:284:SER:OG	16:LH:287:ASP:OD1	2.08	0.71
31:NB:60:GLU:CD	51:SI:1100:VAL:HG12	2.16	0.71
55:SP:710:ASN:ND2	55:SP:710:ASN:O	2.23	0.71
2:L1:1480:G:OP1	39:NP:63:ARG:NH2	2.24	0.71
6:L5:94:THR:CG2	6:L5:114:ILE:HD13	2.21	0.71
16:LH:714:ASP:OD1	16:LH:715:GLU:N	2.24	0.71
16:LH:598:LYS:NZ	16:LH:635:PHE:O	2.24	0.71
45:SA:302:ASN:ND2	45:SA:397:SER:O	2.23	0.70
2:L1:1618:C:OP2	23:LO:505:ARG:NH2	2.24	0.70
51:SI:831:ARG:NH1	51:SI:835:HIS:O	2.23	0.70
55:SP:587:ASP:OD1	55:SP:664:LYS:NZ	2.22	0.70
8:L7:7:LYS:NZ	8:L7:39:ARG:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:1011:G:O2'	41:NS:134:GLY:O	2.08	0.70
12:LD:101:GLU:OE2	57:SR:13:ARG:NH2	2.24	0.70
14:LF:99:LYS:NZ	14:LF:101:GLU:OE1	2.25	0.70
45:SA:146:ASP:OD2	45:SA:149:ARG:NE	2.24	0.70
3:L2:82:G:O2'	3:L2:83:A:OP2	2.09	0.70
5:L4:54:TYR:OH	5:L4:97:GLU:OE2	2.09	0.70
2:L1:1473:U:OP2	6:L5:189:THR:OG1	2.09	0.70
17:LI:552:LYS:NZ	17:LI:581:ASP:OD2	2.24	0.70
2:L1:530:C:O2	14:LF:61:ARG:NH1	2.25	0.70
38:NМ:141:ALA:HB2	38:NМ:210:ILE:HD13	1.73	0.70
13:LE:92:ASN:O	53:SL:79:LYS:NZ	2.24	0.69
24:LP:111:ALA:HB1	56:SQ:73:ALA:HB2	1.74	0.69
48:SF:62:GLU:HA	48:SF:65:LEU:HD13	1.74	0.69
2:L1:351:C:O4'	57:SR:13:ARG:NH2	2.24	0.69
33:NФ:87:ASP:N	33:NФ:89:TYR:HB2	2.07	0.69
50:SH:18:ARG:NE	51:SI:609:GLU:OE1	2.25	0.69
2:L1:641:G:N7	8:L7:112:ARG:NH2	2.39	0.69
2:L1:1504:G:OP1	39:NP:97:SER:OG	2.09	0.69
51:SI:1100:VAL:HG13	51:SI:1102:LEU:HD21	1.74	0.69
2:L1:870:C:O2	40:NQ:51:GLN:NE2	2.24	0.69
47:SC:277:ASP:OD2	47:SC:280:VAL:HG12	1.92	0.69
49:SG:235:HIS:CD2	49:SG:261:ILE:HD12	2.27	0.69
2:L1:494:U:OP2	51:SI:1138:ARG:NH1	2.26	0.69
16:LH:658:GLU:OE1	16:LH:675:ARG:NH2	2.26	0.69
22:LN:481:ILE:HD11	22:LN:487:VAL:HG23	1.75	0.69
18:LJ:258:LEU:HD21	18:LJ:272:LEU:HD11	1.73	0.69
20:LL:18:CYS:SG	20:LL:65:TRP:NE1	2.66	0.69
21:LM:312:VAL:O	21:LM:353:ARG:NH1	2.25	0.69
22:LN:424:ASP:OD2	22:LN:444:ARG:NH1	2.26	0.69
33:NФ:101:HIS:NE2	33:NФ:108:ASP:OD2	2.24	0.69
54:SM:116:ARG:NH1	54:SM:118:ASN:OD1	2.26	0.69
41:NS:424:VAL:HA	41:NS:429:TYR:CB	2.22	0.69
16:LH:38:SER:OG	16:LH:43:ASN:OD1	2.02	0.69
20:LL:55:ASP:HB3	20:LL:58:LEU:HD13	1.75	0.69
25:LQ:414:LEU:HD22	25:LQ:447:LEU:HD11	1.75	0.69
2:L1:1008:G:OP1	34:NG:135:ARG:NH2	2.25	0.68
35:NH:526:CYS:SG	35:NH:614:ARG:NH2	2.65	0.68
27:LS:278:ASP:OD2	27:LS:281:THR:OG1	2.10	0.68
20:LL:233:LYS:NZ	20:LL:248:THR:O	2.25	0.68
21:LM:218:ILE:HD12	21:LM:263:VAL:HG21	1.75	0.68
2:L1:593:U:OP2	10:L9:39:LYS:NZ	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:48:ASP:OD1	25:LQ:49:VAL:N	2.27	0.68
16:LH:432:ARG:NH1	16:LH:700:GLY:O	2.26	0.68
23:LO:423:ARG:NH1	23:LO:460:VAL:O	2.26	0.68
25:LQ:135:ARG:NH2	25:LQ:174:GLU:OE1	2.26	0.68
18:LJ:484:MET:HE2	20:LL:551:ILE:HD11	1.75	0.68
27:LS:486:SER:OG	27:LS:490:PHE:O	2.12	0.68
54:SM:164:GLN:NE2	54:SM:260:GLU:OE2	2.27	0.68
21:LM:216:CYS:O	21:LM:220:VAL:N	2.26	0.68
25:LQ:250:LYS:NZ	25:LQ:254:GLN:O	2.24	0.68
33:NF:118:ILE:HG22	33:NF:122:ILE:HD11	1.75	0.68
2:L1:187:G:O2'	55:SP:1100:GLN:NE2	2.27	0.68
2:L1:1003:A:OP1	62:SW:269:ARG:NH2	2.26	0.68
25:LQ:51:ILE:O	25:LQ:59:LEU:HD12	1.94	0.68
35:NH:827:ARG:NH1	35:NH:829:GLU:OE2	2.27	0.68
47:SD:100:ARG:NH1	47:SD:104:ASP:OD2	2.27	0.68
2:L1:896:U:OP1	38:NM:26:ARG:NH2	2.28	0.67
28:LT:284:ILE:HG23	28:LT:337:VAL:HG11	1.77	0.67
26:LR:586:LYS:NZ	41:NS:253:GLU:OE1	2.21	0.67
55:SP:29:GLU:OE1	55:SP:32:ARG:N	2.25	0.67
25:LQ:352:GLU:OE1	25:LQ:364:TYR:OH	2.06	0.67
27:LS:517:THR:HG22	27:LS:536:ALA:HB2	1.76	0.67
2:L1:959:U:OP2	40:NQ:20:LYS:NZ	2.27	0.67
3:L2:312:U:O2'	45:SA:339:GLU:OE2	2.11	0.67
16:LH:336:ARG:NH1	16:LH:479:ASN:O	2.26	0.67
39:NP:38:LYS:O	39:NP:39:THR:OG1	2.12	0.67
2:L1:1614:A:OP2	6:L5:84:LYS:NZ	2.26	0.67
15:LG:65:ARG:NE	25:LQ:750:GLU:OE2	2.27	0.67
17:LI:611:ILE:HG21	17:LI:654:LEU:HD21	1.77	0.67
18:LJ:484:MET:CE	20:LL:547:LEU:HD11	2.24	0.67
30:NA:567:ASN:O	37:NL:116:LYS:NZ	2.24	0.67
47:SC:123:ILE:HD12	56:SQ:152:ILE:HG22	1.75	0.67
62:SW:216:ILE:O	62:SW:220:THR:HG22	1.95	0.67
28:LT:174:ALA:O	28:LT:175:THR:OG1	2.09	0.67
29:LZ:156:ASP:O	54:SM:3:ARG:NH1	2.27	0.67
35:NH:800:GLU:CD	35:NH:837:ILE:HD13	2.20	0.67
41:NS:423:GLN:O	41:NS:426:GLN:N	2.26	0.67
45:SA:261:GLN:OE1	46:SB:149:ARG:NH1	2.28	0.67
46:SB:161:VAL:HG23	46:SB:162:MET:HE3	1.76	0.67
55:SP:1449:ASP:O	55:SP:1453:ASN:ND2	2.28	0.67
51:SI:871:MET:CE	51:SI:1009:VAL:HG11	2.25	0.67
2:L1:414:C:OP1	51:SI:111:LYS:NZ	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LE:81:VAL:O	13:LE:122:SER:OG	2.12	0.66
27:LS:526:ASP:O	27:LS:528:GLN:NE2	2.28	0.66
25:LQ:128:GLN:NE2	25:LQ:129:PHE:O	2.28	0.66
33:NF:119:GLU:HA	33:NF:122:ILE:HD12	1.77	0.66
17:LI:663:ASP:OD1	19:LK:500:GLN:NE2	2.28	0.66
20:LL:88:TYR:OH	20:LL:93:ASN:OD1	2.14	0.66
46:SB:110:ASP:OD1	46:SB:113:THR:HG23	1.95	0.66
51:SI:1100:VAL:HG13	51:SI:1102:LEU:CD2	2.26	0.66
25:LQ:578:SER:OG	25:LQ:591:SER:OG	2.05	0.66
2:L1:958:U:O2'	33:NF:55:ARG:NH2	2.28	0.66
25:LQ:143:SER:OG	25:LQ:160:ARG:NH1	2.28	0.66
26:LR:15:ILE:HD13	26:LR:379:LEU:HD11	1.75	0.66
49:SG:237:ASP:OD2	49:SG:238:GLU:N	2.27	0.66
55:SP:354:SER:OG	55:SP:356:ASP:OD1	2.13	0.66
45:SA:180:LEU:HD22	45:SA:288:LEU:HD13	1.77	0.66
2:L1:385:A:OP1	9:L8:25:ARG:NH2	2.28	0.66
2:L1:953:G:OP2	33:NF:94:LYS:NZ	2.29	0.65
25:LQ:564:LYS:NZ	50:SH:270:GLU:OE2	2.28	0.65
35:NH:542:SER:O	35:NH:546:THR:HG23	1.96	0.65
2:L1:93:A:O4'	5:L4:3:ARG:NH1	2.29	0.65
8:L7:159:VAL:HG23	8:L7:185:ILE:HG21	1.78	0.65
12:LD:55:ASP:OD2	12:LD:58:CYS:N	2.29	0.65
18:LJ:500:GLU:O	18:LJ:504:ILE:HD12	1.95	0.65
55:SP:1591:TYR:CD1	55:SP:1616:LEU:HD11	2.31	0.65
16:LH:586:SER:OG	16:LH:597:LYS:NZ	2.27	0.65
55:SP:1332:ILE:HG23	55:SP:1373:LYS:HE3	1.79	0.65
2:L1:1555:A:O2'	2:L1:1556:A:O5'	2.15	0.65
4:L3:44:ASN:OD1	4:L3:48:LYS:NZ	2.29	0.65
8:L7:77:LEU:O	8:L7:81:LEU:HD12	1.96	0.65
11:LC:114:ARG:NH1	23:LO:549:GLN:OE1	2.29	0.65
12:LD:21:ASN:O	12:LD:21:ASN:ND2	2.27	0.65
25:LQ:220:THR:HG23	25:LQ:259:ILE:HD11	1.77	0.65
41:NS:428:LEU:CA	41:NS:430:GLU:H	2.08	0.65
3:L2:253:G:N2	3:L2:254:A:N1	2.44	0.65
15:LG:18:ARG:O	25:LQ:747:LYS:NZ	2.30	0.65
27:LS:417:GLY:HA2	27:LS:473:ILE:HD12	1.78	0.65
16:LH:435:ASP:O	16:LH:762:TYR:OH	2.09	0.65
31:NB:64:LEU:O	63:SY:207:ARG:NH2	2.29	0.65
2:L1:1082:C:O2'	2:L1:1083:G:OP1	2.13	0.65
2:L1:1226:A:O2'	2:L1:1256:A:N1	2.27	0.65
2:L1:1629:G:O2'	2:L1:1630:U:O4'	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LF:48:TYR:CD2	14:LF:75:VAL:HG21	2.32	0.65
28:LT:367:LEU:HD21	28:LT:375:LEU:HD11	1.78	0.65
21:LM:356:ALA:O	21:LM:360:ARG:NH1	2.30	0.65
2:L1:350:U:OP1	2:L1:351:C:O2'	2.12	0.64
18:LJ:418:LEU:HD23	18:LJ:462:TRP:NE1	2.13	0.64
25:LQ:910:GLN:OE1	25:LQ:911:GLN:NE2	2.30	0.64
47:SD:155:ILE:HD11	47:SD:162:LEU:HD13	1.80	0.64
2:L1:1178:G:N7	59:ST:753:LYS:NZ	2.44	0.64
15:LG:30:VAL:HG11	15:LG:54:LEU:HD21	1.78	0.64
51:SI:129:ILE:HD13	51:SI:158:ILE:HD13	1.79	0.64
20:LL:115:ASN:OD1	20:LL:131:LEU:N	2.30	0.64
21:LM:186:MET:HE1	21:LM:224:ASN:HD21	1.62	0.64
22:LN:200:PHE:HB3	22:LN:212:ILE:HD11	1.79	0.64
2:L1:460:A:HO2'	5:L4:27:TYR:HH	1.46	0.64
54:SM:74:ASP:OD2	54:SM:75:ASP:N	2.31	0.64
16:LH:477:VAL:HG11	18:LJ:424:ARG:NH1	2.12	0.64
17:LI:678:LEU:HD22	20:LL:545:ALA:HB1	1.80	0.64
25:LQ:223:ASP:OD2	25:LQ:224:SER:N	2.30	0.64
27:LS:376:LEU:HD22	27:LS:386:ILE:HD12	1.80	0.64
62:SW:113:TRP:CZ3	62:SW:130:MET:HE2	2.32	0.64
16:LH:343:ASP:OD2	16:LH:344:CYS:N	2.31	0.64
17:LI:706:TYR:OH	17:LI:708:MET:SD	2.53	0.64
20:LL:139:HIS:ND1	20:LL:139:HIS:O	2.30	0.64
51:SI:871:MET:HE1	51:SI:1009:VAL:HG11	1.79	0.64
2:L1:359:A:OP2	41:NS:5:ARG:NH2	2.31	0.64
5:L4:185:GLY:N	5:L4:224:ASN:OD1	2.31	0.64
23:LO:69:LEU:HD21	23:LO:127:VAL:HB	1.80	0.63
2:L1:1527:C:OP1	6:L5:109:LYS:NZ	2.31	0.63
18:LJ:53:HIS:NE2	18:LJ:311:THR:O	2.31	0.63
47:SC:156:MET:HA	47:SC:156:MET:HE3	1.79	0.63
2:L1:982:U:OP2	37:NL:236:ARG:NH1	2.30	0.63
21:LM:778:SER:O	21:LM:782:VAL:N	2.32	0.63
23:LO:673:ARG:NE	29:LZ:145:ASP:OD2	2.30	0.63
8:L7:168:SER:O	8:L7:172:VAL:HG23	1.98	0.63
17:LI:669:ALA:HB3	19:LK:493:LEU:HD21	1.80	0.63
20:LL:575:GLU:O	22:LN:419:LYS:NZ	2.31	0.63
29:LZ:162:ASP:OD2	29:LZ:163:ASN:N	2.30	0.63
50:SH:154:LEU:O	59:ST:805:LEU:HD21	1.97	0.63
2:L1:498:G:OP1	31:NB:599:LYS:NZ	2.31	0.63
11:LC:101:SER:O	11:LC:105:LEU:HD23	1.98	0.63
27:LS:427:ASN:N	27:LS:431:GLU:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:NA:563:ILE:HG12	37:NL:109:ILE:HD11	1.81	0.63
26:LR:579:GLN:NE2	26:LR:620:LEU:O	2.32	0.63
35:NH:574:LEU:HD11	35:NH:678:ILE:HG13	1.81	0.63
37:NL:52:ALA:CB	37:NL:126:ILE:HD11	2.29	0.63
16:LH:574:LEU:HD13	16:LH:584:PHE:CD2	2.34	0.63
19:LK:505:MET:HE1	20:LL:507:ILE:CG1	2.29	0.63
30:NA:297:LEU:O	30:NA:302:LYS:NZ	2.26	0.62
38:NM:141:ALA:HB2	38:NM:210:ILE:CD1	2.29	0.62
35:NH:188:SER:N	66:NH:1300:ATP:O2B	2.33	0.62
16:LH:33:ASN:OD1	16:LH:357:ILE:HD11	1.98	0.62
35:NH:551:GLU:N	35:NH:551:GLU:OE1	2.32	0.62
2:L1:334:G:O6	9:L8:5:ARG:NH2	2.32	0.62
2:L1:991:G:OP2	34:NG:129:LYS:NZ	2.23	0.62
2:L1:1136:U:O2	59:ST:41:ARG:NH1	2.33	0.62
18:LJ:70:THR:HG22	18:LJ:72:GLN:OE1	2.00	0.62
28:LT:430:ILE:HD11	28:LT:445:MET:SD	2.40	0.62
28:LT:592:ASP:OD1	28:LT:593:PHE:N	2.33	0.62
51:SI:952:PHE:HD2	51:SI:958:VAL:HG22	1.64	0.62
49:SG:160:ILE:HD13	49:SG:189:THR:HG22	1.81	0.62
2:L1:444:C:O2'	2:L1:445:A:OP2	2.12	0.62
16:LH:233:ASP:OD2	16:LH:236:ASN:ND2	2.33	0.62
16:LH:574:LEU:HD12	16:LH:583:LYS:O	2.00	0.62
16:LH:577:ASP:O	16:LH:611:VAL:HG21	1.99	0.62
2:L1:1124:A:N7	41:NS:96:ARG:NH2	2.47	0.62
7:L6:58:LYS:NZ	7:L6:104:PRO:O	2.32	0.62
8:L7:16:LEU:O	8:L7:20:VAL:HG23	2.00	0.62
16:LH:697:PHE:CE1	17:LI:430:LEU:HD12	2.35	0.62
25:LQ:171:CYS:HB2	25:LQ:177:LEU:HD13	1.82	0.62
25:LQ:340:SER:OG	25:LQ:356:THR:OG1	2.17	0.62
25:LQ:753:MET:HE1	25:LQ:825:PRO:HD3	1.81	0.62
31:NB:598:ILE:HD12	47:SC:156:MET:HE1	1.82	0.62
38:NM:97:LEU:HB2	38:NM:228:LEU:HD21	1.82	0.62
2:L1:499:U:O4	56:SQ:138:LYS:NZ	2.33	0.62
55:SP:749:LYS:O	55:SP:756:SER:OG	2.16	0.62
62:SW:204:ARG:NH1	62:SW:250:LEU:O	2.32	0.62
2:L1:1502:G:N2	2:L1:1505:A:OP2	2.27	0.62
9:L8:56:ARG:NH1	9:L8:174:GLY:O	2.33	0.61
30:NA:560:ALA:HB3	30:NA:563:ILE:HD11	1.81	0.61
55:SP:268:PRO:O	55:SP:271:SER:OG	2.14	0.61
55:SP:367:ARG:HD2	55:SP:403:LEU:HD12	1.82	0.61
55:SP:1706:LYS:O	55:SP:1760:ASN:ND2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:915:ARG:NH1	26:LR:773:SER:OG	2.32	0.61
11:LC:58:ASP:OD1	11:LC:59:LYS:N	2.33	0.61
16:LH:237:LEU:HD23	16:LH:238:SER:N	2.16	0.61
23:LO:601:ILE:HD11	23:LO:681:VAL:HG21	1.82	0.61
27:LS:453:VAL:O	48:SE:89:ARG:NH1	2.33	0.61
47:SC:311:ARG:O	47:SC:313:HIS:ND1	2.33	0.61
22:LN:144:ILE:HD12	22:LN:158:VAL:CG1	2.30	0.61
29:LZ:79:LEU:HD23	29:LZ:97:LEU:HD11	1.81	0.61
30:NA:486:ASN:OD1	30:NA:487:ALA:N	2.34	0.61
33:NF:88:LEU:HD12	33:NF:122:ILE:HA	1.82	0.61
36:NI:50:SER:O	36:NI:127:LYS:NZ	2.33	0.61
8:L7:129:LEU:HD21	8:L7:172:VAL:HG11	1.81	0.61
1:L0:9:G:O3'	19:LK:487:ARG:NH2	2.33	0.61
2:L1:1223:A:O2'	59:ST:414:LEU:O	2.19	0.61
8:L7:46:ILE:HD11	8:L7:58:LEU:HB3	1.81	0.61
26:LR:316:VAL:O	26:LR:320:LEU:N	2.33	0.61
55:SP:806:THR:OG1	55:SP:820:THR:OG1	2.16	0.61
25:LQ:905:LEU:HB3	26:LR:786:ILE:HD11	1.83	0.61
30:NA:321:GLU:OE2	30:NA:327:LYS:NZ	2.28	0.61
61:SV:83:LYS:O	61:SV:86:LYS:N	2.34	0.61
14:LF:38:ASP:OD1	14:LF:39:GLU:N	2.33	0.61
5:L4:87:MET:HE2	5:L4:123:LEU:HB2	1.81	0.61
22:LN:48:SER:OG	22:LN:102:LEU:HD23	2.00	0.61
22:LN:287:THR:HG23	22:LN:336:ILE:HG23	1.83	0.61
28:LT:207:ASP:OD2	28:LT:227:THR:OG1	2.19	0.61
30:NA:551:ASN:OD1	30:NA:552:ASP:N	2.34	0.61
6:L5:116:HIS:CE1	6:L5:120:ILE:HD11	2.35	0.60
16:LH:313:LEU:HD22	16:LH:344:CYS:HB3	1.83	0.60
20:LL:306:LEU:HD11	20:LL:310:THR:HA	1.83	0.60
21:LM:258:HIS:CE1	21:LM:282:ILE:HG23	2.36	0.60
26:LR:649:GLU:N	26:LR:649:GLU:OE1	2.34	0.60
30:NA:587:ASP:OD2	30:NA:589:THR:OG1	2.18	0.60
16:LH:455:SER:OG	16:LH:493:PRO:O	2.16	0.60
4:L3:119:ILE:HG22	4:L3:120:ARG:NH1	2.17	0.60
41:NS:444:MET:O	41:NS:511:SER:N	2.33	0.60
45:SA:259:MET:HE3	46:SB:141:LEU:HD23	1.83	0.60
55:SP:1625:ASN:OD1	55:SP:1626:ASP:N	2.34	0.60
16:LH:401:GLN:NE2	16:LH:409:LYS:O	2.34	0.60
51:SI:157:ASN:HD21	51:SI:161:HIS:CE1	2.19	0.60
27:LS:376:LEU:CD1	27:LS:409:ILE:HD11	2.31	0.60
37:NL:165:ALA:O	37:NL:180:GLN:NE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:NL:181:MET:SD	37:NL:300:GLN:NE2	2.74	0.60
54:SM:191:PHE:CD2	54:SM:203:VAL:HG13	2.36	0.60
3:L2:245:U:O4	3:L2:246:A:N6	2.35	0.60
20:LL:2:ASP:OD2	27:LS:280:LYS:NZ	2.34	0.60
26:LR:269:LEU:HD11	26:LR:316:VAL:HG13	1.82	0.60
18:LJ:34:GLN:OE1	18:LJ:71:ARG:NH2	2.35	0.60
29:LZ:64:LEU:HD11	30:NA:437:ILE:CD1	2.31	0.60
8:L7:49:ILE:HD11	8:L7:172:VAL:HG22	1.83	0.60
20:LL:185:PRO:O	20:LL:215:TYR:OH	2.12	0.60
35:NH:359:PHE:HD1	35:NH:397:MET:HE1	1.66	0.60
22:LN:148:SER:OG	22:LN:157:SER:OG	2.18	0.60
23:LO:497:ILE:CD1	23:LO:532:VAL:HG11	2.32	0.60
29:LZ:109:ARG:NH1	29:LZ:155:GLU:OE1	2.34	0.60
35:NH:144:LYS:O	35:NH:176:PHE:N	2.35	0.60
2:L1:763:G:N2	2:L1:774:A:N7	2.50	0.59
20:LL:153:ILE:HG22	20:LL:163:LEU:CD2	2.31	0.59
26:LR:104:PRO:O	34:NG:72:LYS:NZ	2.35	0.59
33:NF:86:GLU:N	33:NF:89:TYR:HB3	2.17	0.59
35:NH:707:PHE:O	35:NH:918:ARG:NH1	2.35	0.59
55:SP:1680:THR:HG23	55:SP:1681:LEU:CD1	2.32	0.59
20:LL:445:LEU:HD22	20:LL:483:ARG:NH2	2.17	0.59
37:NL:152:ILE:C	37:NL:153:LEU:HD12	2.27	0.59
55:SP:1680:THR:HG23	55:SP:1681:LEU:HD12	1.84	0.59
2:L1:1555:A:O2'	2:L1:1556:A:O4'	2.19	0.59
16:LH:176:LEU:HD11	16:LH:185:PHE:HB3	1.83	0.59
16:LH:559:LYS:NZ	16:LH:560:ILE:O	2.27	0.59
34:NG:136:ARG:O	62:SW:248:VAL:HG11	2.02	0.59
2:L1:1534:G:O2'	2:L1:1536:G:O6	2.20	0.59
35:NH:785:GLU:N	35:NH:785:GLU:OE1	2.36	0.59
53:SL:66:LEU:HD11	53:SL:151:TYR:HD2	1.67	0.59
55:SP:1807:GLU:OE2	55:SP:1883:HIS:ND1	2.35	0.59
6:L5:113:ILE:O	6:L5:117:THR:HG23	2.03	0.59
18:LJ:209:LEU:HD21	18:LJ:242:ASN:OD1	2.03	0.59
20:LL:231:ASP:O	20:LL:249:GLU:N	2.34	0.59
23:LO:91:HIS:NE2	23:LO:133:PHE:O	2.33	0.59
26:LR:188:GLU:OE1	26:LR:188:GLU:N	2.35	0.59
16:LH:225:ILE:HD11	16:LH:241:LEU:HD13	1.82	0.59
26:LR:147:ILE:HG21	26:LR:150:LEU:HD21	1.85	0.59
26:LR:343:MET:HE1	26:LR:353:LEU:HD22	1.83	0.59
38:NM:99:ASN:ND2	38:NM:224:ASP:O	2.36	0.59
40:NQ:11:THR:O	40:NQ:14:SER:OG	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SG:157:LEU:HD11	49:SG:189:THR:HB	1.85	0.59
2:L1:110:U:OP1	2:L1:753:A:O2'	2.20	0.59
2:L1:1159:C:N4	54:SM:184:GLU:OE2	2.34	0.59
16:LH:519:LEU:HD11	18:LJ:461:ASP:HB3	1.84	0.59
28:LT:646:VAL:HG13	28:LT:647:THR:HG23	1.84	0.59
35:NH:878:LEU:O	35:NH:881:THR:OG1	2.17	0.59
47:SC:294:ARG:NH1	53:SL:131:SER:OG	2.36	0.59
48:SF:54:MET:SD	48:SF:67:LEU:HD12	2.43	0.59
23:LO:847:ARG:NH1	25:LQ:896:ASP:OD1	2.36	0.59
30:NA:560:ALA:HB3	30:NA:563:ILE:CD1	2.33	0.59
35:NH:356:THR:HG22	35:NH:359:PHE:CE2	2.37	0.59
51:SI:246:ALA:HB2	51:SI:271:ILE:HD11	1.84	0.59
55:SP:29:GLU:OE2	55:SP:31:ALA:HB3	2.02	0.59
55:SP:1381:LYS:HD2	55:SP:1387:ALA:HB2	1.85	0.59
2:L1:1126:G:OP2	41:NS:103:HIS:NE2	2.35	0.59
4:L3:28:ILE:O	4:L3:32:LEU:HD23	2.03	0.59
5:L4:141:THR:OG1	5:L4:143:ASP:OD1	2.19	0.59
7:L6:67:VAL:HG21	7:L6:73:ILE:HD11	1.85	0.59
16:LH:368:ASP:HB3	16:LH:389:LEU:HD22	1.84	0.59
2:L1:1179:G:OP2	59:ST:88:LYS:NZ	2.36	0.58
16:LH:265:ASP:OD1	16:LH:266:ASN:N	2.36	0.58
22:LN:767:LYS:NZ	32:ND:213:LYS:O	2.32	0.58
27:LS:425:ALA:O	27:LS:433:TRP:N	2.33	0.58
36:NI:180:LEU:O	36:NI:184:ILE:N	2.32	0.58
37:NL:254:ASN:ND2	37:NL:317:PHE:O	2.36	0.58
47:SC:89:GLU:OE2	47:SC:100:ARG:NE	2.31	0.58
63:SY:169:ASP:OD1	63:SY:170:GLN:N	2.37	0.58
2:L1:1228:G:OP2	43:OH:45:LEU:N	2.37	0.58
4:L3:45:LEU:HD13	39:NP:36:ILE:HG22	1.85	0.58
12:LD:21:ASN:HD22	12:LD:21:ASN:C	2.11	0.58
18:LJ:484:MET:HE1	20:LL:547:LEU:HD21	1.85	0.58
23:LO:497:ILE:HD11	23:LO:532:VAL:HG11	1.84	0.58
28:LT:824:GLY:O	28:LT:828:LYS:N	2.36	0.58
35:NH:1144:ASP:OD2	35:NH:1146:THR:HG22	2.02	0.58
39:NP:64:HIS:CE1	39:NP:79:LEU:HD21	2.38	0.58
51:SI:952:PHE:CD2	51:SI:958:VAL:HG22	2.38	0.58
28:LT:488:ASN:O	28:LT:492:GLY:N	2.37	0.58
2:L1:747:C:O2'	13:LE:124:LYS:NZ	2.36	0.58
20:LL:153:ILE:HG22	20:LL:163:LEU:HD22	1.85	0.58
47:SC:88:ILE:HG21	47:SC:141:TYR:HE2	1.68	0.58
54:SM:243:GLU:OE1	54:SM:243:GLU:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SP:1738:TYR:OH	55:SP:1745:ILE:HD13	2.03	0.58
2:L1:1127:G:OP2	41:NS:107:ARG:NH1	2.37	0.58
2:L1:1227:A:N6	2:L1:1256:A:O2'	2.33	0.58
20:LL:445:LEU:HD22	20:LL:483:ARG:HH21	1.67	0.58
22:LN:632:ASN:OD1	22:LN:633:CYS:N	2.37	0.58
45:SA:81:ILE:O	45:SA:85:ASN:ND2	2.36	0.58
55:SP:1613:ALA:HB2	55:SP:1639:ILE:HD11	1.84	0.58
58:SS:383:MET:HE2	58:SS:383:MET:N	2.19	0.58
7:L6:18:ILE:HG23	7:L6:23:ARG:HD2	1.84	0.58
16:LH:603:ASN:O	17:LI:592:ARG:NH2	2.36	0.58
13:LE:102:VAL:HG22	13:LE:125:ILE:HD11	1.84	0.58
16:LH:666:ASN:ND2	16:LH:668:THR:OG1	2.35	0.58
28:LT:192:ASN:O	28:LT:196:GLY:N	2.36	0.58
46:SB:63:ILE:HG21	47:SD:232:MET:HE3	1.85	0.58
55:SP:1440:LEU:HD21	55:SP:1476:LEU:HD21	1.86	0.58
2:L1:1036:A:O2'	13:LE:9:ASP:OD2	2.17	0.58
45:SA:267:ASP:OD1	46:SB:275:TYR:OH	2.18	0.58
51:SI:5:ASN:HD22	51:SI:5:ASN:C	2.07	0.58
53:SL:61:PRO:HA	53:SL:62:PRO:C	2.27	0.58
13:LE:18:GLU:HB3	13:LE:65:LEU:HD21	1.85	0.58
35:NH:1157:TYR:HE2	35:NH:1219:ILE:HG23	1.68	0.58
20:LL:21:THR:HG21	20:LL:310:THR:HG21	1.86	0.58
28:LT:41:THR:HG22	28:LT:50:ILE:CD1	2.33	0.58
28:LT:354:SER:N	28:LT:369:ALA:O	2.36	0.58
38:NM:108:ASP:OD1	38:NM:109:LYS:N	2.37	0.58
40:NQ:54:VAL:HG22	40:NQ:64:CYS:SG	2.44	0.58
2:L1:23:G:O6	2:L1:603:U:C2	2.57	0.57
21:LM:184:ASN:ND2	21:LM:220:VAL:O	2.37	0.57
28:LT:640:LEU:HD12	28:LT:653:ILE:CG2	2.34	0.57
38:NM:121:ILE:CG2	38:NM:141:ALA:HB3	2.34	0.57
51:SI:274:TYR:OH	51:SI:306:ASP:OD1	2.21	0.57
63:SY:196:LYS:O	63:SY:199:LYS:N	2.36	0.57
2:L1:434:G:N1	51:SI:56:VAL:O	2.37	0.57
18:LJ:153:ASP:OD1	18:LJ:154:ILE:N	2.37	0.57
22:LN:745:ASP:OD1	22:LN:746:LEU:N	2.37	0.57
26:LR:381:VAL:HG13	26:LR:383:ILE:HD11	1.85	0.57
27:LS:326:LEU:HD22	27:LS:331:LEU:HD13	1.85	0.57
35:NH:751:LYS:NZ	38:NM:196:GLU:OE1	2.37	0.57
39:NP:131:ASP:OD1	39:NP:134:ARG:NH2	2.37	0.57
45:SA:152:LEU:HA	47:SC:218:ILE:HD12	1.86	0.57
46:SB:144:ALA:HB2	47:SD:233:LEU:HD21	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:SB:281:LYS:HA	46:SB:288:THR:HG21	1.85	0.57
47:SD:150:LYS:NZ	47:SD:310:GLU:OE2	2.37	0.57
50:SH:337:VAL:N	51:SI:554:TYR:OH	2.37	0.57
22:LN:186:GLN:OE1	22:LN:188:ALA:N	2.35	0.57
25:LQ:597:ILE:HD13	25:LQ:621:VAL:HG21	1.87	0.57
26:LR:111:ASP:OD2	26:LR:113:THR:OG1	2.22	0.57
28:LT:28:ARG:NH1	28:LT:29:ILE:O	2.38	0.57
38:NM:87:ARG:NH2	38:NM:220:GLN:OE1	2.36	0.57
6:L5:136:ALA:O	6:L5:140:THR:HG22	2.04	0.57
16:LH:313:LEU:HD21	16:LH:321:MET:CE	2.35	0.57
46:SB:212:MET:HE1	46:SB:218:ALA:HB2	1.84	0.57
17:LI:674:GLU:O	17:LI:678:LEU:HD23	2.04	0.57
18:LJ:43:THR:O	18:LJ:304:SER:OG	2.23	0.57
20:LL:476:LEU:HD13	20:LL:479:ILE:HD11	1.87	0.57
25:LQ:895:GLU:OE1	26:LR:797:ASP:N	2.36	0.57
27:LS:164:LEU:HD13	28:LT:175:THR:HA	1.86	0.57
30:NA:357:ILE:HG23	30:NA:357:ILE:O	2.05	0.57
38:NM:224:ASP:OD1	38:NM:225:VAL:N	2.37	0.57
55:SP:1416:GLU:O	55:SP:1419:SER:OG	2.14	0.57
30:NA:504:ASP:OD1	30:NA:505:GLY:N	2.37	0.57
35:NH:754:LEU:HD13	35:NH:893:VAL:HG21	1.86	0.57
18:LJ:484:MET:HE1	20:LL:547:LEU:HD11	1.86	0.57
19:LK:505:MET:HE1	20:LL:507:ILE:HG12	1.87	0.57
25:LQ:472:HIS:CE1	25:LQ:492:SER:HG	2.13	0.57
28:LT:888:LEU:HD21	28:LT:896:ILE:HD11	1.86	0.57
51:SI:118:LEU:HD21	51:SI:809:PRO:HB3	1.86	0.57
1:L0:6:A:O2'	1:L0:7:A:OP2	2.23	0.57
2:L1:1800:A:N3	58:SS:381:ARG:NH2	2.52	0.57
16:LH:517:ASN:OD1	16:LH:518:ASP:N	2.38	0.57
28:LT:205:PHE:CE2	28:LT:231:ILE:HG21	2.40	0.57
30:NA:311:ILE:HD12	51:SI:1032:LEU:HD12	1.86	0.57
51:SI:549:ILE:HD12	51:SI:567:TRP:CE2	2.40	0.57
55:SP:1352:LEU:HD21	55:SP:1398:LEU:CD1	2.34	0.57
2:L1:332:U:OP1	9:L8:31:ARG:NH1	2.37	0.57
20:LL:463:ARG:NH2	20:LL:467:ASP:OD1	2.38	0.57
22:LN:401:ILE:O	22:LN:416:LEU:HD12	2.05	0.57
28:LT:652:CYS:SG	28:LT:654:TRP:NE1	2.77	0.57
41:NS:424:VAL:C	41:NS:429:TYR:O	2.47	0.57
46:SB:1:MET:O	46:SB:86:THR:N	2.35	0.57
58:SS:793:GLU:N	58:SS:793:GLU:OE1	2.38	0.57
25:LQ:836:ILE:HG13	25:LQ:857:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SP:1616:LEU:HD23	55:SP:1635:ILE:HD13	1.87	0.57
26:LR:171:MET:HE1	26:LR:173:LYS:HE3	1.86	0.56
33:NF:99:ARG:NH2	33:NF:119:GLU:OE1	2.38	0.56
37:NL:60:VAL:HG21	37:NL:74:ILE:HD11	1.87	0.56
38:NM:90:GLU:HG3	38:NM:225:VAL:HG23	1.87	0.56
47:SC:88:ILE:HG21	47:SC:141:TYR:CE2	2.39	0.56
47:SC:111:MET:HE1	47:SC:190:PRO:HG3	1.86	0.56
2:L1:25:C:O2'	2:L1:26:A:OP2	2.20	0.56
2:L1:38:C:O3'	10:L9:6:ARG:NH2	2.38	0.56
2:L1:476:U:OP2	31:NB:562:ARG:NH2	2.38	0.56
4:L3:46:VAL:HG21	4:L3:73:MET:HE1	1.87	0.56
10:L9:151:ASP:OD1	10:L9:152:SER:N	2.38	0.56
13:LE:113:HIS:NE2	13:LE:114:GLU:OE1	2.38	0.56
16:LH:610:SER:OG	16:LH:658:GLU:OE2	2.18	0.56
22:LN:285:CYS:SG	22:LN:336:ILE:HG22	2.45	0.56
54:SM:123:VAL:HG12	54:SM:125:PRO:HD2	1.86	0.56
2:L1:1595:U:OP1	51:SI:945:THR:OG1	2.15	0.56
2:L1:1619:C:O2'	15:LG:67:ARG:O	2.15	0.56
6:L5:158:GLN:NE2	6:L5:159:ALA:O	2.38	0.56
16:LH:397:LYS:O	16:LH:424:GLN:NE2	2.38	0.56
16:LH:682:ASN:CG	16:LH:689:ILE:HD11	2.30	0.56
18:LJ:197:ASP:HB2	18:LJ:206:ILE:HD11	1.86	0.56
26:LR:561:SER:O	26:LR:565:PHE:N	2.37	0.56
45:SA:197:GLU:OE2	45:SA:201:TRP:NE1	2.39	0.56
45:SA:265:GLU:N	45:SA:265:GLU:OE1	2.38	0.56
51:SI:861:THR:OG1	51:SI:870:ARG:O	2.12	0.56
55:SP:976:TYR:O	55:SP:980:ASN:ND2	2.37	0.56
17:LI:668:ILE:HG21	19:LK:446:TRP:HA	1.86	0.56
18:LJ:495:ILE:O	18:LJ:498:SER:OG	2.20	0.56
27:LS:155:ILE:HG21	27:LS:160:TYR:CD1	2.40	0.56
30:NA:408:SER:O	30:NA:411:GLU:N	2.39	0.56
35:NH:810:ILE:O	35:NH:814:LEU:HD23	2.05	0.56
46:SB:68:VAL:HG21	46:SB:101:LEU:HD11	1.87	0.56
55:SP:523:LEU:HD12	55:SP:561:LEU:HD11	1.87	0.56
7:L6:5:ILE:CG2	7:L6:113:ILE:HD11	2.35	0.56
16:LH:95:ASP:OD2	16:LH:97:THR:OG1	2.23	0.56
16:LH:634:ASP:O	16:LH:638:PHE:N	2.36	0.56
46:SB:144:ALA:CB	47:SD:233:LEU:HD21	2.35	0.56
20:LL:520:MET:O	20:LL:524:SER:OG	2.21	0.56
27:LS:251:ILE:HG21	27:LS:254:LEU:HD21	1.87	0.56
33:NF:129:TYR:O	33:NF:133:ALA:N	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:NI:16:VAL:CG2	36:NI:141:LEU:HD11	2.35	0.56
49:SG:256:ARG:NH1	49:SG:282:GLU:OE1	2.38	0.56
55:SP:311:ILE:HD11	55:SP:343:ILE:HG23	1.88	0.56
55:SP:1147:ILE:HD12	55:SP:1185:LEU:HD22	1.87	0.56
3:L2:315:A:OP1	45:SA:186:LYS:NZ	2.38	0.56
35:NH:439:HIS:NE2	35:NH:458:ILE:HD13	2.20	0.56
47:SC:253:ILE:HD13	47:SC:269:ILE:HD12	1.88	0.56
3:L2:253:G:OP2	48:SF:95:ARG:NH2	2.39	0.56
8:L7:20:VAL:HG12	8:L7:24:PHE:CE2	2.40	0.56
16:LH:372:LEU:HD21	16:LH:374:LEU:HD21	1.87	0.56
18:LJ:467:LEU:HD21	20:LL:547:LEU:HD12	1.87	0.56
21:LM:187:ASP:HB2	28:LT:336:VAL:HG13	1.88	0.56
46:SB:280:MET:HG3	46:SB:288:THR:HG22	1.87	0.56
30:NA:589:THR:O	30:NA:593:LEU:N	2.33	0.56
47:SD:87:VAL:O	47:SD:100:ARG:N	2.35	0.56
51:SI:993:ASP:OD2	63:SY:34:TYR:OH	2.20	0.56
55:SP:897:PHE:CZ	55:SP:901:ILE:HD11	2.41	0.56
2:L1:493:U:O2'	2:L1:494:U:OP1	2.21	0.56
11:LC:45:ARG:O	11:LC:48:VAL:HG12	2.06	0.56
14:LF:57:VAL:N	14:LF:94:TYR:OH	2.36	0.56
26:LR:692:MET:HE1	30:NA:515:MET:HA	1.88	0.56
38:NM:100:PHE:HA	38:NM:223:PHE:CE1	2.40	0.56
41:NS:428:LEU:HA	41:NS:431:ALA:H	1.71	0.56
47:SC:214:ARG:HB2	47:SC:217:ILE:HD12	1.87	0.56
54:SM:255:GLU:OE1	54:SM:255:GLU:N	2.39	0.56
55:SP:1447:GLU:O	55:SP:1453:ASN:ND2	2.39	0.56
2:L1:1499:G:OP1	39:NP:122:ARG:NH1	2.40	0.55
12:LD:9:SER:N	12:LD:10:GLU:OE1	2.39	0.55
26:LR:220:ILE:HD12	26:LR:239:VAL:HG11	1.87	0.55
20:LL:310:THR:O	20:LL:310:THR:HG22	2.07	0.55
20:LL:324:ASN:OD1	20:LL:325:GLU:N	2.39	0.55
23:LO:455:ILE:CD1	23:LO:476:VAL:HG21	2.36	0.55
26:LR:805:ILE:HG23	26:LR:806:LEU:HD22	1.88	0.55
16:LH:260:SER:OG	16:LH:300:VAL:O	2.24	0.55
22:LN:312:ASN:OD1	22:LN:313:LYS:N	2.39	0.55
22:LN:385:ASN:ND2	22:LN:387:GLU:O	2.40	0.55
35:NH:744:MET:CE	35:NH:814:LEU:HD22	2.35	0.55
37:NL:98:VAL:HG13	37:NL:104:GLU:OE1	2.06	0.55
49:SG:160:ILE:HD12	49:SG:188:TYR:O	2.06	0.55
55:SP:374:LEU:O	55:SP:378:HIS:N	2.39	0.55
27:LS:376:LEU:HD22	27:LS:386:ILE:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SP:315:LEU:O	55:SP:319:THR:HG23	2.06	0.55
3:L2:282:U:O2'	3:L2:284:U:O5'	2.24	0.55
8:L7:136:VAL:N	8:L7:153:LEU:O	2.40	0.55
25:LQ:271:PHE:HD2	25:LQ:351:LEU:HD11	1.71	0.55
25:LQ:822:MET:HE2	25:LQ:822:MET:HA	1.89	0.55
31:NB:26:VAL:HG12	54:SM:14:TYR:HD2	1.71	0.55
47:SD:214:ARG:HB2	47:SD:217:ILE:HD12	1.88	0.55
49:SG:327:ASP:OD1	49:SG:328:ILE:N	2.39	0.55
55:SP:1352:LEU:HD21	55:SP:1398:LEU:HD13	1.88	0.55
18:LJ:248:ARG:NH2	18:LJ:289:ASN:O	2.39	0.55
25:LQ:603:ASP:OD1	25:LQ:604:PHE:N	2.40	0.55
33:NF:5:HIS:HB3	33:NF:117:LEU:HD11	1.89	0.55
45:SA:132:ARG:HB3	47:SC:236:MET:HE2	1.89	0.55
18:LJ:238:ASP:O	18:LJ:242:ASN:N	2.37	0.55
21:LM:390:LEU:HD21	21:LM:394:LEU:HD23	1.87	0.55
28:LT:277:ASP:HB2	28:LT:284:ILE:HD11	1.88	0.55
29:LZ:129:LYS:O	29:LZ:133:GLN:N	2.39	0.55
35:NH:1154:ASN:O	35:NH:1158:LYS:N	2.40	0.55
55:SP:100:GLU:HA	55:SP:103:LEU:HD12	1.88	0.55
16:LH:25:LEU:O	16:LH:32:LYS:NZ	2.39	0.55
28:LT:743:ARG:NH1	30:NA:484:MET:O	2.39	0.55
35:NH:404:GLY:N	35:NH:455:SER:OG	2.40	0.55
35:NH:1146:THR:HG21	35:NH:1180:ASN:ND2	2.22	0.55
16:LH:374:LEU:HD23	16:LH:381:SER:HA	1.88	0.55
23:LO:57:ASN:OD1	23:LO:620:ASN:ND2	2.40	0.55
33:NF:87:ASP:H	33:NF:89:TYR:HB2	1.72	0.55
51:SI:157:ASN:HD21	51:SI:161:HIS:HE1	1.55	0.55
16:LH:66:LEU:CD2	16:LH:119:LEU:HD13	2.37	0.55
37:NL:83:ALA:O	37:NL:110:MET:N	2.40	0.55
45:SA:54:ALA:HB2	45:SA:81:ILE:HD13	1.87	0.55
16:LH:501:THR:OG1	16:LH:503:ASP:OD1	2.14	0.54
16:LH:661:THR:OG1	16:LH:673:ALA:HB3	2.07	0.54
25:LQ:439:LEU:HD12	25:LQ:444:LEU:HD12	1.88	0.54
26:LR:618:ASN:ND2	26:LR:638:ASP:OD1	2.38	0.54
27:LS:261:PRO:C	27:LS:262:LEU:HD22	2.32	0.54
35:NH:577:ARG:NH2	35:NH:626:LYS:O	2.37	0.54
38:NM:97:LEU:CB	38:NM:228:LEU:HD21	2.37	0.54
50:SH:205:VAL:HA	50:SH:208:MET:HE2	1.89	0.54
6:L5:207:THR:O	6:L5:212:LYS:NZ	2.40	0.54
8:L7:64:VAL:HG12	8:L7:94:ALA:HB1	1.89	0.54
21:LM:363:LEU:HD13	21:LM:366:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:480:ASP:OD1	25:LQ:481:LEU:N	2.40	0.54
26:LR:343:MET:CE	26:LR:353:LEU:HD22	2.37	0.54
35:NH:655:LEU:HD13	35:NH:665:HIS:CD2	2.43	0.54
35:NH:833:TYR:OH	36:NI:97:GLU:OE2	2.12	0.54
40:NQ:54:VAL:HG23	40:NQ:63:LEU:HB2	1.89	0.54
55:SP:519:VAL:O	55:SP:523:LEU:HD23	2.07	0.54
9:L8:160:PHE:CD1	9:L8:165:LEU:HD21	2.42	0.54
25:LQ:494:ASP:OD2	25:LQ:496:THR:OG1	2.21	0.54
31:NB:27:ASP:OD2	54:SM:10:ARG:NH2	2.33	0.54
33:NF:72:MET:HE1	33:NF:82:PRO:HD2	1.90	0.54
48:SE:52:ILE:HG22	48:SE:54:MET:SD	2.48	0.54
2:L1:863:A:O5'	13:LE:57:ARG:NH1	2.41	0.54
22:LN:571:THR:HG21	22:LN:632:ASN:ND2	2.21	0.54
26:LR:337:HIS:CE1	26:LR:365:ILE:HD11	2.42	0.54
28:LT:608:THR:OG1	28:LT:610:ARG:NH1	2.40	0.54
29:LZ:64:LEU:O	29:LZ:71:ARG:NH1	2.40	0.54
2:L1:619:A:O4'	51:SI:9:ARG:NH1	2.40	0.54
21:LM:1594:PHE:O	21:LM:1598:LEU:N	2.40	0.54
23:LO:459:SER:HB2	23:LO:466:LEU:HD21	1.89	0.54
27:LS:374:ILE:HD12	27:LS:376:LEU:HD21	1.89	0.54
20:LL:129:PHE:HE1	20:LL:136:LEU:HD13	1.71	0.54
22:LN:143:VAL:HG11	32:ND:198:ILE:HG12	1.89	0.54
26:LR:556:THR:HG22	26:LR:572:GLU:OE2	2.06	0.54
30:NA:311:ILE:CD1	51:SI:1032:LEU:HD12	2.38	0.54
33:NF:37:ILE:HD12	33:NF:71:ILE:HD12	1.90	0.54
35:NH:146:LEU:HD23	35:NH:172:THR:HG21	1.90	0.54
63:SY:153:ASN:HB3	63:SY:167:THR:HG23	1.90	0.54
20:LL:169:SER:OG	20:LL:184:PHE:O	2.23	0.54
22:LN:61:THR:HG21	22:LN:681:ILE:HD13	1.90	0.54
23:LO:673:ARG:NH1	30:NA:451:LEU:O	2.41	0.54
26:LR:662:GLN:NE2	26:LR:666:GLU:OE2	2.40	0.54
26:LR:739:LEU:HD22	26:LR:763:ILE:HD11	1.90	0.54
49:SG:454:GLU:OE1	49:SG:454:GLU:N	2.40	0.54
55:SP:968:ALA:HB1	55:SP:1003:ILE:HD11	1.90	0.54
2:L1:1696:G:OP1	35:NH:312:ARG:NH2	2.41	0.54
6:L5:76:ARG:NH2	6:L5:79:ASN:OD1	2.41	0.54
8:L7:8:ILE:HD13	8:L7:13:PRO:HB3	1.88	0.54
16:LH:154:LEU:HD11	16:LH:171:TYR:HB3	1.89	0.54
22:LN:137:TYR:OH	47:SD:251:ARG:NH2	2.41	0.54
25:LQ:271:PHE:CD2	25:LQ:351:LEU:HD11	2.43	0.54
35:NH:559:GLU:HA	35:NH:585:MET:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L9:26:ALA:HB2	53:SL:55:TYR:CE1	2.43	0.54
13:LE:110:ILE:HG23	13:LE:110:ILE:O	2.08	0.54
35:NH:177:ASN:OD1	35:NH:178:TYR:N	2.41	0.54
38:NH:199:ASN:OD1	38:NH:202:LYS:NZ	2.28	0.54
51:SI:129:ILE:CD1	51:SI:158:ILE:HD13	2.37	0.54
53:SL:68:ASP:OD1	53:SL:69:THR:N	2.39	0.54
2:L1:976:G:N1	2:L1:1023:A:O2'	2.36	0.53
17:LI:711:LEU:HD23	17:LI:712:ASP:N	2.22	0.53
18:LJ:449:GLY:O	18:LJ:455:SER:OG	2.26	0.53
20:LL:543:LEU:O	20:LL:547:LEU:N	2.37	0.53
22:LN:487:VAL:HG21	22:LN:536:VAL:HG21	1.90	0.53
30:NA:356:VAL:HG13	59:ST:764:ARG:HH12	1.73	0.53
45:SA:129:ARG:NH1	47:SC:261:LEU:O	2.41	0.53
55:SP:1087:VAL:O	55:SP:1091:ILE:HG23	2.08	0.53
2:L1:207:U:O2	9:L8:178:ARG:NH2	2.41	0.53
2:L1:995:A:O2'	41:NS:132:ARG:NH2	2.41	0.53
7:L6:120:GLU:OE1	7:L6:120:GLU:N	2.41	0.53
2:L1:867:G:H5'	33:NF:4:MET:HE3	1.89	0.53
3:L2:0:M7G:H82	3:L2:1:G:O4'	2.09	0.53
10:L9:110:GLN:NE2	10:L9:122:VAL:HG12	2.23	0.53
16:LH:197:ILE:HD11	16:LH:213:LYS:HG3	1.89	0.53
16:LH:200:ASN:OD1	16:LH:209:ALA:HB3	2.09	0.53
20:LL:281:ILE:HD12	20:LL:291:ILE:HD11	1.90	0.53
20:LL:577:ASP:OD1	20:LL:578:VAL:N	2.41	0.53
22:LN:368:ASN:OD1	22:LN:369:TYR:N	2.41	0.53
25:LQ:862:LYS:HZ1	28:LT:935:PHE:HB2	1.73	0.53
26:LR:693:ARG:O	26:LR:697:VAL:HG22	2.09	0.53
27:LS:455:ILE:HD12	27:LS:484:VAL:CG1	2.34	0.53
28:LT:375:LEU:HD13	28:LT:414:ILE:HD12	1.88	0.53
36:NI:16:VAL:HG22	36:NI:141:LEU:HD11	1.91	0.53
22:LN:202:ILE:HD13	22:LN:253:ILE:HD12	1.91	0.53
33:NF:87:ASP:H	33:NF:89:TYR:CB	2.22	0.53
50:SH:313:ILE:HD11	50:SH:339:LEU:HD11	1.91	0.53
53:SL:129:SER:O	53:SL:144:ARG:NH2	2.42	0.53
55:SP:1459:LEU:HD11	55:SP:1499:ARG:HD3	1.90	0.53
2:L1:868:G:O2'	33:NF:86:GLU:O	2.25	0.53
2:L1:1478:G:OP1	39:NP:43:ASN:ND2	2.41	0.53
4:L3:28:ILE:HD11	4:L3:54:LEU:HA	1.91	0.53
8:L7:147:ASN:OD1	8:L7:148:LYS:N	2.42	0.53
18:LJ:419:GLN:OE1	18:LJ:422:ARG:NH2	2.41	0.53
25:LQ:177:LEU:HB2	25:LQ:191:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:NH:313:ASN:OD1	35:NH:314:CYS:N	2.40	0.53
47:SD:230:TYR:HD1	47:SD:234:ILE:HD13	1.73	0.53
55:SP:1523:TYR:OH	55:SP:1551:LEU:O	2.20	0.53
2:L1:931:C:H1'	38:NH:120:LEU:HD13	1.89	0.53
16:LH:858:ILE:HG21	27:LS:528:GLN:NE2	2.23	0.53
18:LJ:391:ASN:ND2	18:LJ:403:ASN:OD1	2.41	0.53
18:LJ:424:ARG:NH1	18:LJ:424:ARG:HA	2.24	0.53
37:NL:72:VAL:HA	37:NL:75:LEU:HD12	1.90	0.53
40:NQ:33:LEU:HD22	40:NQ:79:PHE:HD2	1.73	0.53
46:SB:91:GLU:OE2	47:SD:231:ARG:NH1	2.41	0.53
47:SD:221:ILE:HG13	47:SD:221:ILE:O	2.09	0.53
50:SH:234:ASN:ND2	59:ST:805:LEU:O	2.42	0.53
51:SI:833:ARG:NH1	57:SR:138:GLU:O	2.40	0.53
53:SL:139:ASP:OD2	53:SL:140:CYS:N	2.41	0.53
2:L1:778:G:O2'	42:NV:721:ARG:NH2	2.41	0.53
2:L1:1789:G:N7	34:NG:132:ARG:NH2	2.56	0.53
28:LT:731:MET:SD	28:LT:732:ASN:N	2.82	0.53
35:NH:721:VAL:HG23	35:NH:722:LEU:HD12	1.91	0.53
5:L4:64:ILE:HG13	14:LF:18:LEU:HD21	1.91	0.53
36:NI:20:LEU:HD21	36:NI:35:HIS:HB2	1.91	0.53
40:NQ:56:CYS:SG	40:NQ:58:SER:OG	2.66	0.53
47:SC:122:ARG:NE	47:SC:140:GLU:OE2	2.37	0.53
55:SP:323:PHE:HB2	55:SP:364:LEU:HD13	1.89	0.53
2:L1:277:U:O2'	2:L1:278:U:OP1	2.26	0.53
18:LJ:460:ALA:HB1	20:LL:543:LEU:HD21	1.91	0.53
25:LQ:202:ALA:O	25:LQ:227:LYS:NZ	2.34	0.53
40:NQ:31:TYR:HE2	40:NQ:33:LEU:HD21	1.73	0.53
55:SP:1720:ILE:O	55:SP:1724:ASN:ND2	2.42	0.53
2:L1:227:U:O4	55:SP:1529:ARG:NH1	2.42	0.53
2:L1:1783:C:OP2	37:NL:201:GLN:NE2	2.41	0.53
5:L4:212:ASP:OD1	5:L4:216:ASN:N	2.42	0.53
25:LQ:271:PHE:CE1	25:LQ:285:ARG:HB2	2.44	0.53
27:LS:262:LEU:HD11	27:LS:285:VAL:HG21	1.91	0.53
28:LT:572:ALA:O	28:LT:575:GLN:NE2	2.42	0.53
31:NB:23:LEU:HD22	31:NB:27:ASP:OD1	2.09	0.53
35:NH:146:LEU:CD2	35:NH:172:THR:HG21	2.39	0.53
49:SG:245:SER:OG	49:SG:247:ASP:OD1	2.24	0.53
50:SH:98:TYR:N	50:SH:127:ASP:OD2	2.42	0.53
54:SM:191:PHE:HD2	54:SM:203:VAL:HG13	1.72	0.53
2:L1:246:G:H22	12:LD:66:ILE:HG13	1.74	0.52
2:L1:1609:U:O2'	6:L5:105:GLY:O	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LL:281:ILE:HD12	20:LL:291:ILE:CD1	2.39	0.52
26:LR:334:ALA:HB2	26:LR:381:VAL:HG11	1.90	0.52
34:NG:92:LYS:O	34:NG:119:THR:HG21	2.09	0.52
2:L1:128:U:O4	55:SP:943:ARG:NH1	2.42	0.52
16:LH:338:ASN:HB3	16:LH:360:MET:HE1	1.91	0.52
16:LH:574:LEU:HD13	16:LH:584:PHE:CE2	2.45	0.52
17:LI:480:PHE:O	17:LI:484:LYS:N	2.42	0.52
21:LM:216:CYS:C	21:LM:220:VAL:HG23	2.33	0.52
30:NA:515:MET:HE3	30:NA:520:LEU:HD11	1.90	0.52
35:NH:655:LEU:HD23	38:NM:244:VAL:HG11	1.91	0.52
38:NM:244:VAL:HG13	38:NM:244:VAL:O	2.09	0.52
50:SH:274:LYS:O	50:SH:278:GLN:N	2.42	0.52
5:L4:98:ASN:ND2	5:L4:116:ASP:OD1	2.40	0.52
8:L7:46:ILE:HD13	8:L7:60:ILE:HG13	1.92	0.52
11:LC:97:VAL:HG12	11:LC:98:ASP:H	1.74	0.52
26:LR:742:ARG:NH1	30:NA:506:GLU:OE2	2.40	0.52
35:NH:315:ILE:HB	35:NH:553:VAL:HG23	1.91	0.52
38:NM:86:LEU:HD23	38:NM:223:PHE:CE2	2.44	0.52
38:NM:98:THR:N	38:NM:228:LEU:HD11	2.24	0.52
55:SP:389:ILE:O	55:SP:393:PHE:N	2.42	0.52
55:SP:474:ASN:OD1	55:SP:716:TYR:OH	2.26	0.52
61:SV:152:SER:O	61:SV:153:THR:OG1	2.23	0.52
4:L3:120:ARG:HE	59:ST:95:ARG:NH2	2.07	0.52
5:L4:181:VAL:HG21	5:L4:225:VAL:HG13	1.92	0.52
7:L6:23:ARG:O	7:L6:26:VAL:HG12	2.08	0.52
16:LH:560:ILE:CD1	16:LH:575:THR:HG22	2.39	0.52
25:LQ:401:ASP:OD1	25:LQ:402:ASP:N	2.41	0.52
28:LT:896:ILE:HG23	28:LT:905:ILE:HD11	1.90	0.52
33:NF:11:ILE:O	33:NF:11:ILE:HG22	2.09	0.52
50:SH:205:VAL:HG21	50:SH:229:VAL:HG22	1.92	0.52
55:SP:802:ASN:ND2	55:SP:805:LYS:O	2.42	0.52
55:SP:1157:ILE:O	55:SP:1167:TYR:OH	2.26	0.52
55:SP:1239:ASP:OD1	55:SP:1240:THR:N	2.42	0.52
62:SW:131:ASN:O	62:SW:135:LYS:N	2.42	0.52
17:LI:662:ILE:HG23	19:LK:496:LEU:HD12	1.92	0.52
18:LJ:427:VAL:HG22	18:LJ:462:TRP:HZ3	1.75	0.52
21:LM:213:THR:O	21:LM:217:PHE:N	2.37	0.52
22:LN:189:ARG:NH2	32:ND:198:ILE:HD11	2.24	0.52
25:LQ:42:ILE:HG13	25:LQ:51:ILE:HD13	1.92	0.52
29:LZ:130:PHE:O	29:LZ:134:GLY:N	2.43	0.52
33:NF:61:THR:HG22	40:NQ:32:PHE:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:608:SER:OG	16:LH:658:GLU:OE2	2.28	0.52
20:LL:306:LEU:HD12	20:LL:311:MET:O	2.09	0.52
21:LM:331:SER:O	21:LM:334:THR:OG1	2.23	0.52
34:NG:37:GLU:OE2	38:NM:46:THR:OG1	2.27	0.52
50:SH:131:GLU:CB	50:SH:244:THR:HG21	2.40	0.52
51:SI:51:GLU:OE1	57:SR:50:LYS:N	2.34	0.52
55:SP:911:GLN:OE1	55:SP:911:GLN:N	2.43	0.52
2:L1:351:C:O2'	12:LD:104:HIS:NE2	2.43	0.52
5:L4:92:LEU:HD23	14:LF:17:LEU:HD11	1.91	0.52
16:LH:91:ILE:HD11	16:LH:107:ILE:HD12	1.91	0.52
16:LH:533:THR:HG22	16:LH:544:LYS:HE3	1.91	0.52
22:LN:473:THR:HG21	22:LN:496:PHE:HZ	1.75	0.52
25:LQ:760:ILE:HD11	25:LQ:835:PHE:HB2	1.92	0.52
47:SD:157:GLY:O	63:SY:162:SER:OG	2.27	0.52
55:SP:1616:LEU:HD12	55:SP:1619:ILE:HD11	1.91	0.52
2:L1:539:G:OP2	2:L1:539:G:N2	2.32	0.52
2:L1:908:U:O5'	26:LR:534:ARG:NH2	2.43	0.52
2:L1:1143:A:O2'	2:L1:1145:U:OP2	2.23	0.52
15:LG:52:ASP:OD2	15:LG:53:ILE:N	2.43	0.52
28:LT:41:THR:HG22	28:LT:50:ILE:HD12	1.92	0.52
28:LT:415:VAL:N	28:LT:433:ALA:O	2.38	0.52
46:SB:195:LEU:HD23	46:SB:205:TYR:CE2	2.45	0.52
53:SL:66:LEU:HD11	53:SL:151:TYR:CD2	2.44	0.52
59:ST:388:LEU:O	59:ST:392:LYS:N	2.42	0.52
13:LE:83:ILE:O	13:LE:86:ILE:HG22	2.09	0.52
14:LF:34:ASN:HD22	14:LF:34:ASN:N	2.08	0.52
16:LH:91:ILE:HD13	16:LH:109:VAL:HG22	1.91	0.52
20:LL:77:ILE:HD11	20:LL:85:ILE:HG21	1.92	0.52
22:LN:82:ARG:NH2	22:LN:685:SER:O	2.43	0.52
23:LO:567:ASP:OD1	23:LO:569:PHE:N	2.42	0.52
33:NF:25:TRP:CD1	40:NQ:82:LYS:HZ1	2.27	0.52
33:NF:90:TYR:O	33:NF:92:ILE:N	2.43	0.52
36:NI:269:GLU:OE2	36:NI:270:ILE:HG23	2.10	0.52
37:NL:85:GLU:HB3	37:NL:91:ALA:HB2	1.92	0.52
45:SA:61:GLU:OE2	45:SA:65:ASN:ND2	2.43	0.52
46:SB:215:ARG:NH1	46:SB:242:SER:OG	2.42	0.52
47:SC:121:LYS:O	47:SC:143:VAL:HG22	2.10	0.52
55:SP:356:ASP:OD1	55:SP:357:LYS:N	2.42	0.52
55:SP:1385:ASN:O	55:SP:1388:SER:OG	2.20	0.52
2:L1:153:G:H21	7:L6:56:ASN:HD21	1.57	0.52
2:L1:934:C:H42	58:SS:399:LYS:HD3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L6:1:MET:HE1	7:L6:109:LEU:HB2	1.92	0.52
7:L6:5:ILE:HG22	7:L6:113:ILE:HD11	1.92	0.52
22:LN:271:THR:HG21	27:LS:443:VAL:HG21	1.91	0.52
26:LR:548:LEU:CD2	26:LR:562:LEU:HD21	2.40	0.52
38:NM:66:VAL:O	38:NM:86:LEU:N	2.42	0.52
38:NM:86:LEU:HD23	38:NM:223:PHE:HE2	1.75	0.52
51:SI:857:LEU:HD21	51:SI:1032:LEU:HD22	1.91	0.52
3:L2:0:M7G:H82	3:L2:1:G:C1'	2.39	0.51
6:L5:144:GLU:OE2	6:L5:225:ARG:NH2	2.40	0.51
26:LR:355:LEU:HD11	26:LR:365:ILE:HD12	1.92	0.51
27:LS:408:CYS:SG	27:LS:409:ILE:N	2.83	0.51
31:NB:603:THR:HG21	47:SC:160:ASP:HA	1.92	0.51
38:NM:103:MET:SD	38:NM:104:ASP:N	2.83	0.51
55:SP:467:THR:HG23	55:SP:467:THR:O	2.09	0.51
55:SP:706:LEU:HD22	55:SP:770:TYR:CE2	2.45	0.51
1:L0:87:C:O2	16:LH:332:GLN:NE2	2.43	0.51
15:LG:58:GLU:OE1	15:LG:58:GLU:N	2.43	0.51
25:LQ:208:TRP:HE1	25:LQ:222:THR:HG22	1.76	0.51
38:NM:86:LEU:HA	38:NM:223:PHE:CE2	2.45	0.51
55:SP:401:LEU:HD12	55:SP:445:LEU:HD22	1.92	0.51
55:SP:1610:MET:CE	55:SP:1654:VAL:HG22	2.39	0.51
2:L1:65:A:O2'	2:L1:67:A:OP1	2.21	0.51
6:L5:97:LEU:O	6:L5:180:ARG:NH2	2.42	0.51
17:LI:508:ASP:OD1	17:LI:536:ARG:NH2	2.44	0.51
18:LJ:219:ILE:HD13	18:LJ:258:LEU:HB3	1.92	0.51
21:LM:279:MET:HE1	21:LM:302:LEU:HB2	1.92	0.51
22:LN:210:ILE:CD1	22:LN:241:VAL:HG11	2.41	0.51
32:ND:177:ARG:HH11	32:ND:177:ARG:HG2	1.76	0.51
48:SE:110:ILE:O	48:SE:110:ILE:HG22	2.09	0.51
2:L1:1638:G:N3	26:LR:751:LYS:NZ	2.58	0.51
17:LI:558:CYS:O	17:LI:585:ARG:NH2	2.37	0.51
21:LM:216:CYS:O	21:LM:220:VAL:HG23	2.11	0.51
27:LS:288:LEU:HD22	27:LS:324:TRP:CZ3	2.46	0.51
39:NP:15:ILE:HD12	39:NP:56:LYS:HE2	1.92	0.51
50:SH:122:THR:HB	50:SH:130:ILE:HD11	1.92	0.51
51:SI:1112:PHE:CG	56:SQ:178:MET:HE1	2.46	0.51
55:SP:1352:LEU:HD22	55:SP:1371:ILE:HD11	1.92	0.51
2:L1:443:C:O2	2:L1:445:A:N6	2.44	0.51
4:L3:31:ALA:O	4:L3:34:THR:HG22	2.11	0.51
6:L5:128:ASN:OD1	6:L5:130:ILE:HG22	2.11	0.51
21:LM:1087:GLY:O	21:LM:1091:LEU:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:NG:48:VAL:HG21	34:NG:53:ASP:HB2	1.93	0.51
34:NG:85:ALA:H	34:NG:119:THR:HG22	1.75	0.51
54:SM:288:ASP:OD1	54:SM:289:TYR:N	2.43	0.51
55:SP:1308:LEU:HD22	55:SP:1327:THR:HG21	1.92	0.51
63:SY:200:GLN:O	63:SY:204:HIS:ND1	2.44	0.51
6:L5:72:HIS:ND1	11:LC:79:TYR:OH	2.44	0.51
25:LQ:822:MET:HE1	25:LQ:863:PHE:CD1	2.45	0.51
26:LR:768:ASN:O	26:LR:772:LEU:HD12	2.11	0.51
29:LZ:75:GLU:HB3	29:LZ:94:ILE:HD11	1.93	0.51
35:NH:801:LYS:HZ3	36:NI:187:HIS:HB3	1.75	0.51
38:NM:138:PHE:O	38:NM:213:ARG:N	2.44	0.51
47:SC:151:LEU:O	47:SC:155:ILE:HD12	2.11	0.51
47:SC:259:MET:HE2	47:SC:259:MET:N	2.26	0.51
49:SG:568:ILE:HG22	49:SG:570:GLN:HE22	1.75	0.51
20:LL:85:ILE:O	20:LL:99:PHE:N	2.43	0.51
25:LQ:130:ASP:OD2	25:LQ:132:THR:OG1	2.28	0.51
27:LS:379:GLY:N	27:LS:383:TRP:O	2.42	0.51
30:NA:587:ASP:CG	30:NA:589:THR:HG1	2.17	0.51
35:NH:901:ASN:ND2	38:NM:131:ASP:OD1	2.44	0.51
37:NL:94:LEU:HD21	37:NL:107:LEU:HD21	1.91	0.51
55:SP:621:SER:O	55:SP:625:ILE:HD12	2.11	0.51
16:LH:551:HIS:HA	16:LH:583:LYS:HZ3	1.76	0.51
18:LJ:89:PHE:CD1	18:LJ:96:LEU:HD13	2.46	0.51
29:LZ:53:ASP:OD1	30:NA:440:LEU:HD12	2.11	0.51
29:LZ:108:ARG:HA	29:LZ:113:VAL:HG11	1.92	0.51
37:NL:115:MET:HA	37:NL:115:MET:HE3	1.93	0.51
37:NL:210:GLU:N	37:NL:210:GLU:OE1	2.44	0.51
57:SR:74:VAL:HG11	57:SR:104:LEU:HD11	1.92	0.51
2:L1:434:G:O6	51:SI:58:MET:N	2.43	0.51
2:L1:896:U:O2	34:NG:41:ARG:NH1	2.38	0.51
21:LM:184:ASN:OD1	21:LM:189:LEU:HD11	2.10	0.51
23:LO:784:ASP:OD1	23:LO:785:PHE:N	2.44	0.51
25:LQ:24:VAL:O	25:LQ:41:LEU:HD12	2.10	0.51
25:LQ:472:HIS:CD2	25:LQ:492:SER:HG	2.21	0.51
28:LT:120:HIS:C	28:LT:121:LEU:HD22	2.36	0.51
45:SA:210:VAL:O	45:SA:210:VAL:HG13	2.11	0.51
50:SH:305:LYS:O	50:SH:307:ASP:N	2.44	0.51
55:SP:215:VAL:HG11	55:SP:232:LEU:CD1	2.40	0.51
7:L6:6:SER:O	7:L6:113:ILE:HD12	2.11	0.51
16:LH:282:ILE:HD11	16:LH:312:LEU:HD22	1.92	0.51
17:LI:669:ALA:HB3	19:LK:493:LEU:CD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:468:ASP:OD1	22:LN:469:LEU:N	2.44	0.51
22:LN:684:GLU:OE1	22:LN:684:GLU:N	2.38	0.51
27:LS:429:TYR:N	27:LS:455:ILE:O	2.43	0.51
27:LS:523:PHE:CE1	27:LS:530:LEU:HD13	2.45	0.51
28:LT:918:LYS:O	28:LT:921:ARG:NH1	2.44	0.51
30:NA:516:SER:O	30:NA:520:LEU:HD23	2.11	0.51
47:SC:171:LEU:N	47:SC:237:VAL:HG11	2.26	0.51
47:SD:232:MET:HE2	47:SD:232:MET:HA	1.93	0.51
49:SG:409:ASP:OD1	49:SG:410:ASP:N	2.44	0.51
2:L1:863:A:O2'	2:L1:865:A:O5'	2.30	0.50
2:L1:1133:A:OP2	2:L1:1134:C:N4	2.44	0.50
2:L1:1597:A:O3'	54:SM:279:ARG:NH1	2.44	0.50
2:L1:1638:G:H2'	26:LR:751:LYS:HZ1	1.75	0.50
19:LK:505:MET:HE3	20:LL:506:LEU:HD22	1.93	0.50
22:LN:481:ILE:HD11	22:LN:487:VAL:CG2	2.39	0.50
27:LS:210:LYS:O	27:LS:213:SER:OG	2.25	0.50
29:LZ:64:LEU:HD11	30:NA:437:ILE:HD11	1.91	0.50
31:NB:60:GLU:OE2	51:SI:1100:VAL:N	2.43	0.50
50:SH:289:VAL:O	50:SH:317:GLN:NE2	2.36	0.50
55:SP:367:ARG:O	55:SP:407:ARG:NH1	2.44	0.50
55:SP:375:THR:HG22	55:SP:411:PHE:HE1	1.76	0.50
55:SP:1151:ILE:HG23	55:SP:1201:LEU:HD13	1.92	0.50
55:SP:1308:LEU:HB3	55:SP:1350:THR:HG21	1.92	0.50
25:LQ:398:ASP:OD1	25:LQ:399:ILE:N	2.43	0.50
27:LS:245:HIS:O	27:LS:275:TYR:OH	2.29	0.50
35:NH:980:VAL:HG11	35:NH:1011:ARG:NE	2.25	0.50
47:SC:198:GLU:O	47:SC:222:GLU:N	2.45	0.50
47:SD:269:ILE:HD13	47:SD:293:LEU:HD21	1.93	0.50
55:SP:319:THR:HG22	55:SP:361:LEU:HB2	1.93	0.50
55:SP:558:TRP:CE3	55:SP:603:LEU:HD11	2.46	0.50
16:LH:741:SER:O	16:LH:742:ARG:NH2	2.44	0.50
23:LO:210:SER:OG	23:LO:212:ASP:OD1	2.29	0.50
51:SI:71:ILE:HD11	51:SI:276:HIS:CE1	2.47	0.50
2:L1:1701:A:OP1	35:NH:223:ARG:NH1	2.44	0.50
7:L6:18:ILE:HG21	7:L6:24:ILE:CD1	2.41	0.50
7:L6:142:ARG:O	7:L6:146:GLY:N	2.44	0.50
16:LH:511:GLU:OE1	16:LH:511:GLU:N	2.44	0.50
18:LJ:427:VAL:HG22	18:LJ:462:TRP:CZ3	2.46	0.50
20:LL:120:ILE:HG23	20:LL:151:LEU:HD22	1.93	0.50
25:LQ:750:GLU:O	25:LQ:754:GLU:N	2.36	0.50
28:LT:604:SER:OG	28:LT:606:ASP:OD1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:NM:86:LEU:HA	38:NM:223:PHE:HE2	1.75	0.50
46:SB:144:ALA:O	46:SB:148:GLY:N	2.43	0.50
49:SG:569:ASP:OD1	49:SG:570:GLN:N	2.44	0.50
55:SP:389:ILE:O	55:SP:389:ILE:HG22	2.12	0.50
2:L1:1124:A:N6	3:L2:0:M7G:H2'	2.27	0.50
21:LM:187:ASP:N	21:LM:187:ASP:OD2	2.43	0.50
23:LO:209:VAL:HG12	23:LO:215:VAL:HG22	1.93	0.50
25:LQ:858:PHE:CE2	26:LR:803:SER:HA	2.47	0.50
26:LR:541:PHE:HA	26:LR:548:LEU:HD13	1.92	0.50
32:ND:195:GLU:OE1	32:ND:198:ILE:N	2.42	0.50
36:NI:254:LYS:HB2	36:NI:257:PHE:CD1	2.47	0.50
46:SB:228:PRO:HD2	46:SB:231:ILE:HD13	1.94	0.50
47:SC:148:ARG:NH1	47:SC:179:THR:HG23	2.25	0.50
55:SP:1763:LEU:N	55:SP:1805:ASP:OD2	2.45	0.50
2:L1:1670:G:O2'	2:L1:1731:A:N6	2.39	0.50
4:L3:106:GLU:HB2	59:ST:744:LEU:HD11	1.94	0.50
10:L9:59:LEU:HD11	10:L9:72:GLU:OE1	2.11	0.50
16:LH:533:THR:HG22	16:LH:544:LYS:CE	2.42	0.50
20:LL:61:THR:N	20:LL:79:GLY:O	2.41	0.50
25:LQ:864:ASN:O	25:LQ:868:LEU:HD23	2.10	0.50
28:LT:298:VAL:HG13	28:LT:298:VAL:O	2.12	0.50
35:NH:656:ARG:NH2	38:NM:241:GLY:O	2.45	0.50
45:SA:71:GLU:OE1	45:SA:71:GLU:N	2.40	0.50
45:SA:206:LEU:HD23	45:SA:216:PHE:CE1	2.46	0.50
46:SB:177:LEU:HD13	46:SB:265:PHE:HB2	1.94	0.50
47:SC:267:VAL:CG2	47:SC:269:ILE:HD11	2.42	0.50
47:SD:210:MET:HE2	47:SD:210:MET:HA	1.94	0.50
2:L1:251:A:H2	5:L4:131:LEU:HD12	1.77	0.50
7:L6:24:ILE:HG22	7:L6:28:PHE:CE1	2.47	0.50
8:L7:77:LEU:HD23	8:L7:92:PHE:CE2	2.47	0.50
16:LH:574:LEU:HD21	16:LH:582:LEU:HD12	1.93	0.50
21:LM:193:THR:OG1	21:LM:241:ILE:HD11	2.12	0.50
22:LN:402:TRP:CE2	22:LN:416:LEU:HD13	2.46	0.50
25:LQ:837:ASP:OD2	25:LQ:882:ARG:NH2	2.44	0.50
27:LS:429:TYR:HA	27:LS:455:ILE:N	2.26	0.50
28:LT:565:LEU:HD22	28:LT:586:ASN:C	2.37	0.50
35:NH:566:ILE:HG21	35:NH:583:ILE:HD13	1.94	0.50
35:NH:860:GLU:OE2	35:NH:861:ILE:HG23	2.11	0.50
46:SB:14:LEU:HD12	46:SB:75:LEU:HG	1.94	0.50
48:SF:54:MET:O	48:SF:81:VAL:N	2.41	0.50
51:SI:298:VAL:HG23	51:SI:791:ILE:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SP:394:LEU:HD22	55:SP:435:PHE:CG	2.47	0.50
22:LN:687:PHE:CZ	22:LN:688:MET:HE3	2.47	0.50
25:LQ:468:ILE:HB	25:LQ:471:ALA:HB2	1.93	0.50
26:LR:495:ASN:N	26:LR:509:ALA:O	2.42	0.50
31:NB:63:VAL:HG21	63:SY:98:LEU:HD11	1.92	0.50
38:NM:35:PRO:HB3	38:NM:231:LEU:HD21	1.94	0.50
51:SI:841:THR:HG21	51:SI:872:LEU:O	2.11	0.50
5:L4:136:VAL:HG13	5:L4:149:TYR:CE2	2.46	0.50
7:L6:23:ARG:HH11	7:L6:41:VAL:HG12	1.77	0.50
29:LZ:156:ASP:OD1	54:SM:4:ARG:NH2	2.44	0.50
31:NB:538:ARG:NH1	51:SI:151:GLU:OE1	2.44	0.50
35:NH:1180:ASN:OD1	35:NH:1181:VAL:N	2.41	0.50
55:SP:215:VAL:HG11	55:SP:232:LEU:HD11	1.94	0.50
2:L1:251:A:C2	5:L4:131:LEU:HD12	2.47	0.49
26:LR:765:MET:HA	26:LR:765:MET:HE3	1.94	0.49
29:LZ:57:LEU:HD22	30:NA:444:LEU:HD12	1.94	0.49
33:NF:88:LEU:HD23	33:NF:88:LEU:C	2.37	0.49
35:NH:655:LEU:O	38:NM:244:VAL:HG12	2.12	0.49
38:NM:67:GLU:OE1	38:NM:67:GLU:N	2.45	0.49
55:SP:974:TYR:OH	55:SP:1020:ASN:O	2.27	0.49
16:LH:682:ASN:O	16:LH:686:GLY:N	2.42	0.49
23:LO:675:MET:SD	30:NA:450:VAL:HG13	2.52	0.49
35:NH:521:LEU:HD21	35:NH:959:LEU:HG	1.94	0.49
35:NH:693:LYS:O	35:NH:695:GLN:NE2	2.45	0.49
36:NI:262:VAL:O	36:NI:266:LYS:N	2.44	0.49
45:SA:223:ILE:HD11	45:SA:237:LEU:HD22	1.94	0.49
47:SC:320:TYR:C	47:SC:321:MET:HE2	2.37	0.49
50:SH:133:ILE:HG21	50:SH:151:LEU:HD12	1.94	0.49
55:SP:201:ARG:NH2	55:SP:238:GLU:O	2.45	0.49
55:SP:1411:GLU:N	55:SP:1411:GLU:OE2	2.45	0.49
55:SP:1678:MET:HA	55:SP:1690:LEU:HD11	1.94	0.49
8:L7:70:PHE:O	8:L7:74:GLN:N	2.45	0.49
22:LN:97:ARG:NE	32:ND:191:PRO:O	2.30	0.49
26:LR:740:MET:HE3	26:LR:778:MET:CE	2.42	0.49
33:NF:89:TYR:CD2	33:NF:129:TYR:OH	2.65	0.49
53:SL:65:VAL:HG21	53:SL:86:MET:SD	2.53	0.49
2:L1:446:A:H5'	5:L4:59:ARG:HH22	1.77	0.49
26:LR:12:LEU:HD11	26:LR:378:PRO:HG2	1.95	0.49
33:NF:48:SER:OG	33:NF:86:GLU:OE2	2.30	0.49
33:NF:129:TYR:O	33:NF:132:VAL:N	2.45	0.49
7:L6:5:ILE:HD13	7:L6:16:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:139:GLU:OE2	16:LH:172:ARG:NH1	2.46	0.49
16:LH:738:ASN:OD1	16:LH:739:TYR:N	2.46	0.49
17:LI:668:ILE:HG23	17:LI:671:ARG:HH21	1.78	0.49
22:LN:61:THR:HG21	22:LN:681:ILE:CD1	2.42	0.49
30:NA:447:LYS:O	30:NA:451:LEU:HD23	2.12	0.49
33:NF:69:ASN:HB2	33:NF:74:ILE:HD11	1.95	0.49
37:NL:169:ASP:O	37:NL:234:LYS:NZ	2.39	0.49
41:NS:57:ASN:ND2	41:NS:59:ASN:OD1	2.44	0.49
47:SC:142:ARG:NH1	47:SC:186:ASP:OD2	2.45	0.49
23:LO:261:ALA:HB1	23:LO:279:PHE:HB3	1.95	0.49
28:LT:175:THR:HG21	28:LT:218:LEU:HD21	1.94	0.49
29:LZ:149:LEU:HD22	30:NA:451:LEU:HB3	1.95	0.49
37:NL:235:ASN:O	37:NL:294:ARG:NE	2.45	0.49
45:SA:26:ASP:OD1	45:SA:27:ILE:N	2.46	0.49
55:SP:912:SER:O	55:SP:914:LYS:NZ	2.43	0.49
2:L1:1169:G:N1	2:L1:1575:G:OP2	2.42	0.49
8:L7:133:THR:HG21	8:L7:162:ILE:HD13	1.95	0.49
13:LE:86:ILE:HD13	13:LE:104:LEU:HD11	1.94	0.49
16:LH:34:ILE:HG23	16:LH:90:LYS:HA	1.94	0.49
19:LK:505:MET:HE1	20:LL:507:ILE:HG13	1.94	0.49
20:LL:343:ARG:HE	20:LL:347:GLY:HA2	1.77	0.49
28:LT:758:PHE:O	62:SW:176:ARG:NE	2.42	0.49
37:NL:180:GLN:O	37:NL:212:LYS:NZ	2.43	0.49
51:SI:5:ASN:O	51:SI:5:ASN:ND2	2.40	0.49
55:SP:1249:LEU:O	55:SP:1253:ASN:ND2	2.45	0.49
21:LM:221:VAL:O	21:LM:221:VAL:HG12	2.11	0.49
33:NF:72:MET:HE1	33:NF:82:PRO:CD	2.43	0.49
51:SI:56:VAL:HG22	57:SR:52:ILE:HG12	1.94	0.49
16:LH:443:ASN:O	16:LH:447:LYS:N	2.40	0.49
17:LI:711:LEU:HD21	22:LN:733:PHE:CZ	2.47	0.49
25:LQ:341:ALA:HB1	25:LQ:353:LEU:HD21	1.94	0.49
28:LT:673:PHE:HA	28:LT:676:MET:HE2	1.95	0.49
38:NM:73:LEU:HD22	38:NM:84:ILE:HD11	1.95	0.49
55:SP:558:TRP:CZ2	55:SP:607:LEU:HD21	2.47	0.49
62:SW:74:ASP:OD1	62:SW:78:LYS:N	2.46	0.49
63:SY:93:MET:SD	63:SY:94:ASP:N	2.86	0.49
2:L1:600:U:O2	51:SI:44:GLN:NE2	2.44	0.49
16:LH:508:ILE:HG22	16:LH:531:PHE:CE1	2.47	0.49
25:LQ:126:LEU:HD21	25:LQ:168:GLY:HA2	1.94	0.49
37:NL:94:LEU:CD2	37:NL:107:LEU:HD21	2.43	0.49
51:SI:5:ASN:C	51:SI:5:ASN:ND2	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SP:1062:LEU:O	55:SP:1065:VAL:HG12	2.13	0.49
1:L0:278:G:N2	27:LS:539:ASP:OD2	2.38	0.48
23:LO:708:ASP:OD1	23:LO:709:THR:N	2.44	0.48
25:LQ:16:VAL:HG13	25:LQ:16:VAL:O	2.11	0.48
25:LQ:94:LEU:HB2	25:LQ:108:LEU:HD11	1.93	0.48
25:LQ:532:ASP:OD2	25:LQ:552:ASP:N	2.46	0.48
26:LR:342:ASP:OD1	26:LR:343:MET:N	2.46	0.48
35:NH:971:LYS:O	35:NH:1028:ARG:NE	2.46	0.48
46:SB:295:VAL:HG23	46:SB:341:LEU:HD23	1.94	0.48
51:SI:269:VAL:HG12	51:SI:796:VAL:HG21	1.93	0.48
55:SP:717:GLN:NE2	55:SP:718:PRO:O	2.45	0.48
7:L6:50:PHE:HB3	7:L6:111:LEU:HD11	1.95	0.48
16:LH:605:ASN:OD1	16:LH:606:HIS:N	2.46	0.48
23:LO:787:ILE:HG23	23:LO:788:GLU:HG2	1.94	0.48
25:LQ:905:LEU:CB	26:LR:786:ILE:HD11	2.43	0.48
26:LR:25:VAL:HG12	26:LR:294:LEU:HD13	1.95	0.48
36:NI:17:PRO:HB2	36:NI:155:LEU:HD23	1.95	0.48
49:SG:179:ASP:OD1	49:SG:180:LYS:N	2.46	0.48
2:L1:1060:U:OP2	35:NH:865:ARG:NH2	2.42	0.48
16:LH:413:SER:OG	16:LH:414:ILE:N	2.46	0.48
20:LL:551:ILE:HG22	20:LL:555:LYS:HE2	1.95	0.48
27:LS:163:ARG:O	27:LS:167:GLN:NE2	2.45	0.48
28:LT:224:GLY:HA3	28:LT:251:ILE:HG21	1.95	0.48
38:NM:32:ILE:HG23	38:NM:43:VAL:HG23	1.95	0.48
40:NQ:25:VAL:HG13	40:NQ:25:VAL:O	2.13	0.48
55:SP:1384:LEU:O	55:SP:1387:ALA:HB3	2.14	0.48
58:SS:454:MET:HE3	58:SS:460:THR:HB	1.94	0.48
7:L6:57:ASP:OD1	7:L6:60:GLY:N	2.46	0.48
8:L7:41:LEU:HB3	8:L7:70:PHE:HE1	1.78	0.48
13:LE:87:GLU:O	13:LE:90:THR:OG1	2.23	0.48
25:LQ:85:LEU:HD22	25:LQ:94:LEU:HD21	1.95	0.48
25:LQ:638:VAL:HG13	25:LQ:654:TYR:CE1	2.48	0.48
26:LR:255:LYS:HE3	26:LR:257:ILE:HD11	1.96	0.48
35:NH:915:LEU:HD21	35:NH:1089:PHE:HZ	1.79	0.48
35:NH:1217:GLU:O	35:NH:1221:HIS:ND1	2.38	0.48
46:SB:319:ILE:HD12	46:SB:326:LEU:HD22	1.96	0.48
2:L1:152:U:O4'	7:L6:13:GLN:NE2	2.46	0.48
8:L7:150:GLN:OE1	8:L7:151:LYS:N	2.46	0.48
23:LO:261:ALA:HB2	23:LO:281:SER:HB3	1.95	0.48
23:LO:740:VAL:HG13	23:LO:774:TYR:CE2	2.49	0.48
25:LQ:410:SER:OG	25:LQ:413:SER:OG	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LT:375:LEU:HD13	28:LT:414:ILE:CD1	2.42	0.48
28:LT:810:ARG:C	28:LT:811:LEU:HD22	2.39	0.48
37:NL:119:LEU:HD13	37:NL:122:PHE:CE1	2.49	0.48
38:NM:65:VAL:HG22	38:NM:87:ARG:HB3	1.95	0.48
47:SC:81:ARG:C	56:SQ:152:ILE:HD11	2.36	0.48
54:SM:1:MET:HA	54:SM:4:ARG:HG2	1.95	0.48
59:ST:42:GLU:OE2	59:ST:46:LYS:NZ	2.47	0.48
2:L1:85:A:N3	2:L1:148:A:O2'	2.44	0.48
22:LN:192:THR:HG23	22:LN:244:VAL:HG22	1.96	0.48
29:LZ:111:LEU:HA	29:LZ:114:ILE:HG22	1.94	0.48
33:NF:85:PRO:C	33:NF:89:TYR:HB3	2.39	0.48
55:SP:819:ILE:HD11	55:SP:822:SER:HB3	1.96	0.48
3:L2:15:U:OP1	58:SS:466:ARG:NH2	2.41	0.48
17:LI:607:VAL:HG21	17:LI:645:ILE:CD1	2.44	0.48
18:LJ:168:THR:OG1	18:LJ:190:ASP:OD1	2.26	0.48
27:LS:365:ASN:O	27:LS:369:ASN:N	2.44	0.48
28:LT:530:ASP:O	28:LT:534:SER:N	2.46	0.48
33:NF:34:ILE:HD12	33:NF:74:ILE:HD12	1.95	0.48
35:NH:655:LEU:HD12	35:NH:664:THR:C	2.39	0.48
35:NH:801:LYS:HE3	36:NI:184:ILE:HA	1.96	0.48
37:NL:201:GLN:N	37:NL:201:GLN:OE1	2.47	0.48
38:NM:7:LYS:NZ	38:NM:8:ARG:O	2.46	0.48
47:SD:218:ILE:O	47:SD:218:ILE:HG23	2.14	0.48
55:SP:371:VAL:O	55:SP:375:THR:HG23	2.13	0.48
9:L8:11:ARG:NH1	9:L8:15:GLY:O	2.46	0.48
18:LJ:140:LEU:HD23	18:LJ:141:ALA:N	2.29	0.48
21:LM:364:ASN:OD1	21:LM:365:ILE:N	2.47	0.48
22:LN:229:MET:SD	22:LN:270:ALA:HB1	2.53	0.48
27:LS:487:GLU:HA	27:LS:517:THR:HA	1.94	0.48
37:NL:84:VAL:HG23	37:NL:110:MET:HG3	1.95	0.48
55:SP:1555:LEU:HD21	55:SP:1586:ILE:HD11	1.94	0.48
55:SP:1650:LEU:O	55:SP:1654:VAL:HG23	2.14	0.48
1:L0:278:G:H22	27:LS:539:ASP:CG	2.21	0.48
2:L1:318:U:OP1	41:NS:33:ARG:NH2	2.46	0.48
16:LH:690:ASN:ND2	16:LH:749:ASP:O	2.44	0.48
17:LI:650:LEU:CD2	17:LI:655:LEU:HD12	2.43	0.48
25:LQ:45:ALA:O	25:LQ:48:ASP:N	2.46	0.48
30:NA:356:VAL:HG22	59:ST:764:ARG:NH1	2.29	0.48
32:ND:185:GLN:OE1	32:ND:185:GLN:N	2.45	0.48
35:NH:498:MET:SD	35:NH:506:GLN:NE2	2.87	0.48
35:NH:801:LYS:HE2	36:NI:188:MET:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SP:1738:TYR:CE2	55:SP:1745:ILE:HG21	2.49	0.48
16:LH:448:ASN:ND2	16:LH:459:ILE:HG22	2.28	0.48
20:LL:472:LEU:HD23	20:LL:473:LYS:O	2.14	0.48
26:LR:692:MET:HE2	30:NA:519:GLU:OE2	2.14	0.48
47:SC:210:MET:HE1	47:SC:217:ILE:HD13	1.96	0.48
2:L1:1755:A:N9	30:NA:532:LEU:HD11	2.28	0.47
3:L2:169:A:OP2	49:SG:180:LYS:NZ	2.30	0.47
6:L5:51:VAL:O	6:L5:65:ARG:NH2	2.47	0.47
10:L9:110:GLN:HE21	10:L9:122:VAL:HG12	1.79	0.47
19:LK:505:MET:HE3	20:LL:506:LEU:CD2	2.43	0.47
21:LM:46:ASP:OD1	21:LM:47:PHE:N	2.45	0.47
23:LO:405:SER:HB3	23:LO:436:LEU:HD12	1.95	0.47
23:LO:415:ASP:O	23:LO:419:TYR:N	2.47	0.47
48:SF:54:MET:HE1	48:SF:68:PRO:HG3	1.96	0.47
49:SG:168:ASN:O	49:SG:172:PHE:N	2.44	0.47
55:SP:1273:LYS:HE2	55:SP:1352:LEU:HB2	1.96	0.47
22:LN:44:ALA:HB3	22:LN:71:ARG:HB3	1.96	0.47
22:LN:139:CYS:SG	22:LN:144:ILE:HD11	2.54	0.47
25:LQ:170:TRP:CE3	25:LQ:178:ILE:HD12	2.49	0.47
26:LR:591:ILE:HG22	26:LR:601:ILE:CD1	2.44	0.47
27:LS:239:LYS:NZ	27:LS:281:THR:O	2.41	0.47
34:NG:33:LEU:C	38:NM:66:VAL:HG23	2.39	0.47
35:NH:856:THR:HG22	35:NH:858:ARG:H	1.78	0.47
37:NL:226:LEU:O	37:NL:230:VAL:HG12	2.14	0.47
38:NM:59:ASP:OD1	38:NM:60:ALA:N	2.47	0.47
45:SA:304:SER:OG	45:SA:305:GLU:OE1	2.32	0.47
7:L6:78:THR:O	7:L6:81:VAL:HG22	2.14	0.47
23:LO:436:LEU:HD23	23:LO:437:ALA:N	2.29	0.47
26:LR:370:LEU:HD13	26:LR:645:LYS:NZ	2.30	0.47
27:LS:450:GLN:HE22	27:LS:506:THR:HG22	1.80	0.47
33:NF:91:LEU:O	33:NF:94:LYS:N	2.46	0.47
35:NH:469:ASP:O	35:NH:473:LYS:N	2.44	0.47
37:NL:139:PHE:O	37:NL:143:ASN:ND2	2.48	0.47
39:NP:100:ILE:O	39:NP:104:VAL:HG23	2.13	0.47
45:SA:67:ASN:O	45:SA:70:SER:N	2.47	0.47
51:SI:1116:VAL:HG22	56:SQ:187:PHE:HE1	1.78	0.47
55:SP:1440:LEU:CD2	55:SP:1476:LEU:HD21	2.45	0.47
26:LR:393:SER:OG	26:LR:394:LEU:N	2.47	0.47
27:LS:240:ASP:OD2	27:LS:585:LYS:NZ	2.47	0.47
27:LS:544:VAL:HG22	27:LS:551:VAL:HG22	1.96	0.47
35:NH:264:LEU:HD11	35:NH:556:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SD:238:ASP:OD1	47:SD:262:LYS:NZ	2.43	0.47
2:L1:581:U:O2	2:L1:583:C:N4	2.47	0.47
2:L1:1082:C:HO2'	2:L1:1083:G:P	2.37	0.47
2:L1:1663:G:O4'	41:NS:251:ARG:NH1	2.48	0.47
5:L4:95:THR:O	5:L4:95:THR:HG22	2.14	0.47
5:L4:95:THR:HG21	5:L4:97:GLU:OE2	2.14	0.47
17:LI:541:LEU:HD11	17:LI:566:LEU:HD23	1.95	0.47
21:LM:68:ILE:HG23	21:LM:71:ARG:HH21	1.79	0.47
28:LT:627:ASN:OD1	28:LT:647:THR:OG1	2.33	0.47
41:NS:662:MET:N	41:NS:737:LEU:O	2.40	0.47
50:SH:216:LEU:HD12	50:SH:216:LEU:O	2.13	0.47
57:SR:27:ASN:OD1	57:SR:28:ASN:N	2.47	0.47
2:L1:1755:A:N3	30:NA:500:LYS:NZ	2.63	0.47
6:L5:200:ASN:ND2	6:L5:207:THR:OG1	2.48	0.47
15:LG:39:THR:OG1	25:LQ:867:GLU:OE1	2.30	0.47
18:LJ:137:ASN:OD1	18:LJ:138:LYS:N	2.48	0.47
18:LJ:177:ILE:HD13	18:LJ:239:LEU:HD11	1.96	0.47
24:LP:303:GLU:O	24:LP:306:LYS:N	2.47	0.47
25:LQ:262:ILE:HD12	25:LQ:343:TRP:HB3	1.96	0.47
25:LQ:746:LEU:O	25:LQ:751:ARG:NH2	2.47	0.47
30:NA:558:SER:HA	30:NA:575:VAL:HG21	1.96	0.47
35:NH:855:LEU:HD23	35:NH:856:THR:N	2.29	0.47
46:SB:125:PRO:HA	46:SB:131:MET:HE1	1.96	0.47
49:SG:488:ILE:HD12	49:SG:498:VAL:HG22	1.96	0.47
51:SI:247:ASP:N	51:SI:272:TYR:O	2.41	0.47
51:SI:958:VAL:HG11	51:SI:987:TYR:HB3	1.96	0.47
55:SP:370:ASP:OD1	55:SP:370:ASP:N	2.47	0.47
55:SP:782:MET:HE3	55:SP:789:ALA:HB1	1.95	0.47
3:L2:17:G:H21	58:SS:474:ARG:NH2	2.13	0.47
8:L7:123:ASP:O	8:L7:127:GLU:OE1	2.33	0.47
13:LE:103:ILE:O	13:LE:125:ILE:HD12	2.14	0.47
16:LH:246:SER:OG	16:LH:248:GLN:OE1	2.32	0.47
16:LH:561:LEU:HB2	16:LH:613:LEU:HD23	1.95	0.47
18:LJ:89:PHE:CE1	18:LJ:96:LEU:HD13	2.49	0.47
25:LQ:9:GLU:O	25:LQ:685:GLU:N	2.43	0.47
25:LQ:220:THR:CG2	25:LQ:259:ILE:HD11	2.45	0.47
26:LR:65:THR:OG1	26:LR:79:VAL:HG23	2.14	0.47
28:LT:442:THR:O	28:LT:451:GLY:N	2.40	0.47
28:LT:894:ASP:OD1	28:LT:895:VAL:N	2.48	0.47
29:LZ:88:LEU:HD11	29:LZ:97:LEU:HD21	1.95	0.47
36:NI:211:GLY:C	40:NQ:80:ARG:HE	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:NL:68:GLY:HA2	37:NL:71:THR:HG22	1.96	0.47
47:SD:230:TYR:CD1	47:SD:234:ILE:HD13	2.49	0.47
49:SG:159:CYS:SG	49:SG:160:ILE:N	2.88	0.47
49:SG:184:ARG:NH2	49:SG:200:ASP:OD2	2.47	0.47
49:SG:233:GLU:O	49:SG:261:ILE:HD13	2.15	0.47
51:SI:124:ASP:OD2	51:SI:127:ALA:N	2.41	0.47
62:SW:113:TRP:HD1	62:SW:116:ILE:HB	1.79	0.47
2:L1:23:G:C6	2:L1:603:U:O2	2.66	0.47
6:L5:93:LEU:HA	6:L5:172:ILE:HD11	1.97	0.47
11:LC:94:GLN:HB2	11:LC:102:LYS:HD3	1.97	0.47
13:LE:106:THR:HG22	13:LE:109:GLY:O	2.15	0.47
16:LH:318:GLU:OE1	16:LH:484:VAL:HG11	2.15	0.47
16:LH:627:ASP:OD1	16:LH:628:ASP:N	2.48	0.47
25:LQ:561:ASP:OD1	25:LQ:562:SER:N	2.48	0.47
30:NA:304:GLN:O	30:NA:308:ARG:N	2.43	0.47
45:SA:311:ILE:HG23	45:SA:342:LEU:HD12	1.96	0.47
46:SB:61:ASN:O	46:SB:64:ILE:N	2.48	0.47
46:SB:118:ARG:NH2	47:SD:261:LEU:O	2.43	0.47
48:SE:38:ASN:O	48:SE:41:THR:OG1	2.27	0.47
2:L1:1190:C:N4	2:L1:1197:C:O2	2.48	0.47
22:LN:522:SER:HA	22:LN:528:ILE:HD11	1.95	0.47
27:LS:311:ASN:OD1	27:LS:312:ILE:N	2.47	0.47
30:NA:412:ILE:HB	62:SW:221:ARG:NH2	2.30	0.47
30:NA:413:TYR:CD1	62:SW:221:ARG:NH2	2.82	0.47
38:NM:99:ASN:C	38:NM:223:PHE:CD1	2.93	0.47
47:SC:321:MET:HE2	47:SC:321:MET:HA	1.97	0.47
48:SF:48:ILE:O	48:SF:48:ILE:HG22	2.14	0.47
50:SH:280:LEU:HD12	51:SI:631:ILE:HD13	1.95	0.47
55:SP:913:ILE:HD13	55:SP:921:VAL:HG11	1.97	0.47
8:L7:114:ARG:O	8:L7:118:LEU:HD23	2.14	0.47
17:LI:479:PHE:CE1	17:LI:522:THR:HG23	2.50	0.47
17:LI:567:LEU:O	17:LI:571:PHE:N	2.44	0.47
27:LS:277:ILE:HG23	27:LS:277:ILE:O	2.15	0.47
28:LT:95:GLU:OE2	28:LT:97:LYS:NZ	2.47	0.47
35:NH:551:GLU:O	35:NH:555:PHE:N	2.43	0.47
35:NH:565:LYS:O	35:NH:569:VAL:HG22	2.15	0.47
35:NH:1141:GLU:OE2	35:NH:1141:GLU:N	2.46	0.47
47:SD:263:ASP:OD2	47:SD:264:GLN:NE2	2.48	0.47
49:SG:397:PHE:CE2	49:SG:442:ILE:HD11	2.50	0.47
51:SI:864:ASP:O	51:SI:865:SER:OG	2.33	0.47
55:SP:711:GLN:OE1	55:SP:768:THR:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:1682:U:O2	2:L1:1720:G:N2	2.47	0.46
2:L1:1739:C:OP1	25:LQ:333:ARG:NH2	2.44	0.46
6:L5:15:GLU:OE2	28:LT:499:LYS:NZ	2.47	0.46
21:LM:345:ASP:N	21:LM:345:ASP:OD1	2.47	0.46
28:LT:734:LEU:HD23	28:LT:883:THR:CG2	2.46	0.46
6:L5:117:THR:HG21	6:L5:194:LEU:HD23	1.98	0.46
17:LI:456:HIS:ND1	17:LI:456:HIS:O	2.48	0.46
22:LN:161:ASP:OD1	22:LN:162:ASN:N	2.48	0.46
25:LQ:806:MET:HE2	25:LQ:845:LEU:HD22	1.96	0.46
28:LT:62:ASP:O	28:LT:66:LEU:N	2.47	0.46
28:LT:284:ILE:HG23	28:LT:337:VAL:CG1	2.44	0.46
38:NM:29:TRP:CH2	38:NM:47:LEU:HD23	2.50	0.46
47:SD:162:LEU:HD21	47:SD:164:ILE:HB	1.98	0.46
47:SD:214:ARG:CB	47:SD:217:ILE:HD12	2.45	0.46
57:SR:117:ILE:HG23	57:SR:117:ILE:O	2.16	0.46
2:L1:51:A:N1	51:SI:225:ARG:NH1	2.63	0.46
16:LH:357:ILE:HD12	16:LH:371:PHE:CD1	2.50	0.46
18:LJ:418:LEU:HD23	18:LJ:462:TRP:CD1	2.50	0.46
22:LN:95:LYS:O	22:LN:97:ARG:NH1	2.48	0.46
26:LR:89:HIS:O	26:LR:93:GLY:N	2.49	0.46
28:LT:721:LEU:HD21	28:LT:919:GLU:OE2	2.16	0.46
30:NA:344:GLU:C	30:NA:345:LEU:HD22	2.40	0.46
33:NF:83:GLU:CB	33:NF:84:ILE:HD12	2.46	0.46
35:NH:1157:TYR:CE2	35:NH:1219:ILE:HG23	2.48	0.46
62:SW:182:ILE:HG12	62:SW:234:LEU:HD13	1.96	0.46
63:SY:247:GLN:OE1	63:SY:248:ARG:N	2.47	0.46
3:L2:253:G:N7	48:SF:95:ARG:NH1	2.64	0.46
12:LD:132:SER:OG	12:LD:133:LYS:N	2.41	0.46
20:LL:248:THR:OG1	20:LL:250:ASP:OD1	2.23	0.46
21:LM:238:LEU:HD23	21:LM:241:ILE:HD12	1.97	0.46
25:LQ:577:LEU:N	25:LQ:591:SER:O	2.49	0.46
26:LR:26:SER:OG	26:LR:28:ASN:OD1	2.18	0.46
30:NA:322:LYS:O	30:NA:327:LYS:NZ	2.48	0.46
30:NA:374:GLN:OE1	54:SM:245:VAL:HG23	2.15	0.46
37:NL:64:GLY:N	37:NL:84:VAL:O	2.42	0.46
37:NL:177:ALA:HB3	37:NL:227:LEU:HD11	1.98	0.46
37:NL:310:PHE:HA	37:NL:313:VAL:HG12	1.96	0.46
46:SB:12:TYR:CE1	46:SB:63:ILE:HD11	2.51	0.46
55:SP:1454:VAL:HG21	55:SP:1488:MET:HE1	1.98	0.46
8:L7:75:THR:HG23	8:L7:76:LYS:N	2.30	0.46
11:LC:38:LEU:HD22	39:NP:10:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:366:ASN:OD1	16:LH:367:SER:N	2.49	0.46
16:LH:682:ASN:ND2	16:LH:689:ILE:HD11	2.30	0.46
33:NF:84:ILE:HG22	33:NF:89:TYR:HA	1.97	0.46
35:NH:138:ILE:O	35:NH:180:LYS:NZ	2.49	0.46
35:NH:1204:VAL:HG21	35:NH:1212:VAL:HG21	1.97	0.46
55:SP:208:LEU:O	55:SP:212:VAL:HG23	2.16	0.46
55:SP:402:ARG:NH1	55:SP:742:THR:HG21	2.31	0.46
7:L6:57:ASP:OD1	7:L6:61:PHE:N	2.49	0.46
7:L6:76:LEU:N	41:NS:61:GLU:OE1	2.46	0.46
18:LJ:427:VAL:HG13	18:LJ:462:TRP:CZ3	2.51	0.46
26:LR:296:ILE:HG22	26:LR:297:LEU:HD12	1.98	0.46
35:NH:174:TYR:HH	35:NH:226:HIS:HD1	1.62	0.46
2:L1:60:U:OP2	55:SP:12:LYS:NZ	2.41	0.46
18:LJ:262:GLU:OE1	18:LJ:263:ASN:ND2	2.48	0.46
25:LQ:159:LEU:HD13	25:LQ:189:TRP:CD2	2.51	0.46
29:LZ:124:ILE:HD11	31:NB:20:PRO:HG3	1.98	0.46
39:NP:131:ASP:O	39:NP:135:ILE:HD12	2.16	0.46
41:NS:114:ILE:O	41:NS:118:GLN:NE2	2.48	0.46
47:SD:117:VAL:HG23	47:SD:118:TYR:HD1	1.79	0.46
49:SG:158:THR:HG21	49:SG:240:LEU:HA	1.97	0.46
55:SP:642:ILE:HD12	55:SP:669:LEU:CD1	2.45	0.46
55:SP:806:THR:HG1	55:SP:820:THR:HG1	1.52	0.46
55:SP:1173:LEU:O	55:SP:1177:SER:OG	2.16	0.46
13:LE:106:THR:HG23	13:LE:108:ALA:H	1.80	0.46
22:LN:125:GLU:O	22:LN:134:LEU:N	2.49	0.46
25:LQ:224:SER:OG	25:LQ:249:GLU:OE1	2.34	0.46
27:LS:467:THR:HG21	27:LS:522:GLN:CD	2.40	0.46
35:NH:822:ARG:NH1	35:NH:1134:GLU:O	2.49	0.46
40:NQ:56:CYS:O	40:NQ:60:SER:N	2.46	0.46
59:ST:785:VAL:O	59:ST:789:ASN:ND2	2.49	0.46
7:L6:3:LEU:HD23	7:L6:5:ILE:HD11	1.97	0.46
8:L7:67:LEU:CD2	8:L7:94:ALA:HB2	2.32	0.46
16:LH:91:ILE:HD12	16:LH:108:THR:O	2.16	0.46
16:LH:107:ILE:HD11	16:LH:119:LEU:HD11	1.97	0.46
23:LO:33:VAL:HG23	23:LO:33:VAL:O	2.16	0.46
23:LO:721:VAL:O	28:LT:579:ARG:NH2	2.46	0.46
25:LQ:52:TRP:CE2	25:LQ:59:LEU:HD13	2.51	0.46
26:LR:548:LEU:HD21	26:LR:562:LEU:HD21	1.98	0.46
36:NI:162:THR:HB	36:NI:163:PRO:HD3	1.96	0.46
46:SB:3:TYR:CE1	46:SB:16:LYS:HB2	2.50	0.46
55:SP:470:ILE:HD12	55:SP:504:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:577:G:OP1	30:NA:322:LYS:NZ	2.47	0.46
9:L8:159:GLN:HB3	9:L8:165:LEU:HD23	1.97	0.46
20:LL:77:ILE:HD11	20:LL:117:LEU:HD21	1.98	0.46
20:LL:235:LEU:HG	20:LL:246:VAL:HG12	1.99	0.46
21:LM:355:ILE:HG23	21:LM:362:LYS:HB2	1.98	0.46
21:LM:374:ARG:NH1	21:LM:375:LEU:O	2.49	0.46
23:LO:739:LEU:HA	23:LO:754:VAL:HG11	1.98	0.46
27:LS:174:ARG:CZ	27:LS:178:VAL:HG21	2.46	0.46
33:NF:48:SER:HG	33:NF:86:GLU:CD	2.23	0.46
35:NH:543:LEU:HD11	35:NH:691:SER:HB3	1.97	0.46
47:SC:253:ILE:CD1	47:SC:269:ILE:HD12	2.46	0.46
51:SI:130:ASP:OD2	51:SI:131:ILE:N	2.49	0.46
55:SP:581:LEU:HD22	55:SP:607:LEU:HD13	1.98	0.46
55:SP:1175:CYS:O	55:SP:1179:LEU:HD23	2.16	0.46
55:SP:1635:ILE:HG23	55:SP:1636:LEU:HD22	1.97	0.46
2:L1:654:C:O2	2:L1:681:U:N3	2.49	0.45
5:L4:111:VAL:O	5:L4:111:VAL:HG13	2.16	0.45
14:LF:86:GLU:HB2	14:LF:91:LEU:HD21	1.97	0.45
18:LJ:42:VAL:HG23	18:LJ:42:VAL:O	2.15	0.45
25:LQ:474:ALA:HB1	25:LQ:493:ALA:HB3	1.98	0.45
30:NA:553:VAL:O	30:NA:557:LEU:HD12	2.15	0.45
35:NH:356:THR:HG22	35:NH:359:PHE:CZ	2.51	0.45
36:NI:165:PHE:O	36:NI:169:VAL:N	2.41	0.45
37:NL:65:PRO:HG3	37:NL:83:ALA:HB1	1.97	0.45
47:SC:97:TYR:HB2	47:SC:107:VAL:HG23	1.98	0.45
51:SI:763:GLU:OE2	51:SI:767:ILE:HD11	2.16	0.45
55:SP:334:ASN:O	55:SP:337:THR:OG1	2.25	0.45
55:SP:1137:ILE:HG23	55:SP:1185:LEU:HD11	1.97	0.45
13:LE:17:ALA:CB	13:LE:25:VAL:HG22	2.46	0.45
16:LH:34:ILE:HD12	16:LH:89:VAL:O	2.17	0.45
16:LH:667:ASP:OD1	16:LH:668:THR:N	2.49	0.45
21:LM:258:HIS:HE1	21:LM:282:ILE:HG23	1.80	0.45
22:LN:250:THR:HG23	22:LN:252:GLN:HB2	1.98	0.45
23:LO:492:SER:OG	23:LO:493:TRP:N	2.49	0.45
25:LQ:363:GLU:HG2	25:LQ:384:THR:HG22	1.97	0.45
26:LR:370:LEU:HD13	26:LR:645:LYS:HZ1	1.81	0.45
27:LS:554:ASN:OD1	27:LS:555:TRP:N	2.49	0.45
48:SE:15:ALA:O	48:SE:19:GLN:NE2	2.50	0.45
51:SI:77:PRO:HD2	51:SI:80:THR:HG21	1.96	0.45
55:SP:831:PHE:O	55:SP:834:THR:OG1	2.24	0.45
13:LE:62:VAL:HG11	40:NQ:8:LEU:CD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:91:ILE:CD1	16:LH:109:VAL:HG22	2.46	0.45
16:LH:94:GLY:N	16:LH:106:LEU:O	2.49	0.45
21:LM:258:HIS:HB3	21:LM:298:THR:HG21	1.97	0.45
21:LM:1464:GLU:O	21:LM:1468:SER:N	2.49	0.45
22:LN:529:ASN:O	22:LN:545:ARG:NH1	2.50	0.45
30:NA:311:ILE:HG23	30:NA:312:GLU:N	2.32	0.45
55:SP:886:ASP:OD1	55:SP:887:ASN:N	2.48	0.45
20:LL:83:GLY:O	20:LL:101:THR:HG22	2.17	0.45
25:LQ:176:TRP:HZ3	25:LQ:197:ILE:HD13	1.82	0.45
28:LT:175:THR:HG21	28:LT:218:LEU:CD2	2.46	0.45
35:NH:744:MET:HE2	35:NH:814:LEU:HD22	1.97	0.45
38:NM:30:PHE:N	38:NM:46:THR:O	2.37	0.45
38:NM:164:ILE:HG13	38:NM:204:ILE:HG21	1.98	0.45
47:SC:234:ILE:HG22	47:SC:235:GLY:O	2.15	0.45
51:SI:269:VAL:CG1	51:SI:796:VAL:HG21	2.47	0.45
53:SL:135:THR:O	53:SL:135:THR:HG22	2.16	0.45
11:LC:90:VAL:HG21	29:LZ:180:PHE:HE1	1.82	0.45
23:LO:543:ASN:O	23:LO:547:ALA:N	2.49	0.45
25:LQ:415:LYS:HG2	25:LQ:427:THR:HG23	1.99	0.45
27:LS:221:THR:OG1	27:LS:224:ASN:ND2	2.50	0.45
28:LT:640:LEU:HD12	28:LT:653:ILE:HG22	1.98	0.45
33:NF:62:GLN:HB3	33:NF:65:VAL:HG12	1.97	0.45
55:SP:260:HIS:O	55:SP:264:THR:OG1	2.28	0.45
55:SP:1134:MET:HA	55:SP:1134:MET:HE3	1.99	0.45
3:L2:256:G:OP1	45:SA:382:LYS:NZ	2.48	0.45
20:LL:22:VAL:HG13	27:LS:278:ASP:HB2	1.98	0.45
21:LM:185:ASP:O	21:LM:189:LEU:N	2.42	0.45
27:LS:517:THR:HG23	27:LS:517:THR:O	2.16	0.45
27:LS:524:SER:OG	27:LS:527:GLY:N	2.49	0.45
28:LT:287:LEU:HD23	28:LT:290:ILE:HG21	1.98	0.45
28:LT:486:ILE:HD12	28:LT:496:LYS:HB2	1.99	0.45
9:L8:96:LEU:HD21	9:L8:179:CYS:SG	2.56	0.45
25:LQ:338:ILE:HG12	25:LQ:355:LEU:HD13	1.97	0.45
26:LR:251:ASP:OD1	26:LR:252:GLY:N	2.46	0.45
35:NH:1233:ASN:OD1	35:NH:1234:PHE:N	2.49	0.45
51:SI:972:ILE:HD11	63:SY:34:TYR:CZ	2.52	0.45
55:SP:417:LEU:O	55:SP:421:LEU:HD23	2.17	0.45
23:LO:200:SER:OG	23:LO:202:ASP:OD1	2.28	0.45
23:LO:331:GLU:O	23:LO:335:GLU:N	2.50	0.45
33:NF:88:LEU:HD13	33:NF:126:ALA:N	2.32	0.45
35:NH:520:ASN:OD1	35:NH:521:LEU:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SC:196:ALA:O	47:SC:220:ILE:N	2.42	0.45
47:SC:214:ARG:CB	47:SC:217:ILE:HD12	2.47	0.45
55:SP:1571:THR:OG1	55:SP:1572:LEU:N	2.49	0.45
2:L1:78:A:O2'	7:L6:173:PRO:O	2.34	0.45
2:L1:1653:C:O3'	25:LQ:339:LYS:NZ	2.50	0.45
6:L5:119:ASP:O	6:L5:123:VAL:HG23	2.16	0.45
16:LH:769:ASN:OD1	16:LH:770:TYR:N	2.50	0.45
20:LL:470:PHE:HA	20:LL:508:ILE:HG21	1.97	0.45
26:LR:77:THR:HG21	26:LR:117:LEU:HD22	1.99	0.45
31:NB:60:GLU:OE2	51:SI:1100:VAL:HG12	2.16	0.45
35:NH:107:ILE:HD13	35:NH:507:PHE:HE1	1.82	0.45
45:SA:226:LYS:NZ	45:SA:260:GLY:O	2.50	0.45
54:SM:119:ARG:NH2	54:SM:124:MET:SD	2.90	0.45
55:SP:414:LEU:HD12	55:SP:451:VAL:HG21	1.99	0.45
55:SP:538:LEU:HD22	55:SP:574:LEU:HD23	1.98	0.45
55:SP:871:ASP:OD1	55:SP:889:LYS:NZ	2.50	0.45
12:LD:21:ASN:ND2	12:LD:21:ASN:C	2.75	0.45
18:LJ:463:VAL:O	18:LJ:467:LEU:HD13	2.15	0.45
23:LO:146:PHE:N	23:LO:167:ASP:OD2	2.49	0.45
25:LQ:826:PHE:HE1	25:LQ:868:LEU:HD22	1.81	0.45
26:LR:257:ILE:HD12	26:LR:278:LEU:HD11	1.99	0.45
28:LT:118:VAL:HG11	28:LT:121:LEU:HD21	1.99	0.45
28:LT:174:ALA:C	28:LT:175:THR:HG1	2.14	0.45
30:NA:347:PHE:O	30:NA:349:ARG:NH1	2.49	0.45
30:NA:414:GLU:OE2	62:SW:176:ARG:NH2	2.49	0.45
35:NH:930:THR:HG23	35:NH:933:LEU:H	1.82	0.45
38:NM:99:ASN:C	38:NM:223:PHE:HD1	2.25	0.45
45:SA:160:ARG:HG2	47:SC:208:ILE:HD13	1.99	0.45
47:SC:236:MET:HB3	47:SC:262:LYS:HG3	1.98	0.45
49:SG:146:LYS:NZ	49:SG:205:SER:O	2.50	0.45
59:ST:16:ARG:HB2	59:ST:18:LEU:HD23	1.99	0.45
8:L7:139:ARG:HG3	13:LE:51:GLU:OE2	2.17	0.44
16:LH:778:ASP:O	16:LH:781:SER:N	2.50	0.44
18:LJ:504:ILE:HD13	20:LL:499:ASN:HD21	1.81	0.44
20:LL:210:ARG:NH1	20:LL:228:ALA:O	2.50	0.44
21:LM:159:PRO:O	46:SB:412:VAL:HG13	2.16	0.44
25:LQ:109:MET:HE2	25:LQ:109:MET:HA	1.99	0.44
26:LR:779:VAL:O	26:LR:783:ASP:N	2.48	0.44
35:NH:795:GLU:OE1	35:NH:797:THR:N	2.50	0.44
39:NP:22:LEU:CD2	39:NP:28:LEU:HD22	2.46	0.44
41:NS:428:LEU:HA	41:NS:431:ALA:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:SA:199:TYR:CD1	45:SA:220:VAL:HG22	2.52	0.44
50:SH:314:ASN:OD1	50:SH:315:LYS:N	2.49	0.44
51:SI:1121:LYS:HE2	51:SI:1121:LYS:HA	1.99	0.44
55:SP:1501:ARG:NH1	55:SP:1505:ASN:OD1	2.50	0.44
2:L1:560:U:OP2	54:SM:282:ARG:NH2	2.50	0.44
2:L1:1464:G:O3'	54:SM:99:ARG:NH1	2.46	0.44
16:LH:656:ASP:OD1	16:LH:657:SER:N	2.50	0.44
30:NA:347:PHE:CD2	51:SI:964:ALA:HB2	2.52	0.44
34:NG:18:ARG:N	34:NG:29:HIS:O	2.47	0.44
35:NH:345:TYR:HE1	35:NH:472:THR:HG21	1.81	0.44
39:NP:41:SER:OG	39:NP:94:ILE:HG21	2.17	0.44
41:NS:427:PHE:H	41:NS:429:TYR:C	2.24	0.44
50:SH:19:LEU:O	50:SH:23:LEU:HD23	2.16	0.44
2:L1:405:C:O2'	7:L6:92:ARG:O	2.24	0.44
2:L1:1227:A:H61	2:L1:1256:A:C2'	2.30	0.44
10:L9:41:GLU:OE2	10:L9:108:ARG:NE	2.50	0.44
12:LD:76:VAL:HG11	12:LD:87:ARG:HB2	1.99	0.44
16:LH:560:ILE:HD13	16:LH:575:THR:HG22	1.99	0.44
16:LH:693:ASP:O	17:LI:430:LEU:HD11	2.18	0.44
21:LM:216:CYS:O	21:LM:219:ASN:N	2.50	0.44
23:LO:103:LYS:HB3	23:LO:152:LEU:HD11	1.99	0.44
25:LQ:402:ASP:OD2	25:LQ:403:ASN:N	2.50	0.44
55:SP:183:HIS:CD2	55:SP:188:LEU:HD12	2.53	0.44
55:SP:710:ASN:HD22	55:SP:710:ASN:C	2.15	0.44
55:SP:1576:PRO:O	55:SP:1576:PRO:HD2	2.18	0.44
16:LH:667:ASP:O	16:LH:683:LEU:HD21	2.18	0.44
16:LH:683:LEU:HD12	16:LH:684:LEU:N	2.31	0.44
16:LH:884:MET:HE1	21:LM:255:ILE:HG13	1.99	0.44
18:LJ:217:ASN:CG	18:LJ:219:ILE:HD11	2.43	0.44
25:LQ:95:ALA:HB2	25:LQ:129:PHE:CZ	2.51	0.44
25:LQ:291:GLU:O	25:LQ:295:GLY:N	2.47	0.44
26:LR:748:THR:HG23	26:LR:788:TYR:CZ	2.53	0.44
35:NH:146:LEU:HA	35:NH:149:VAL:HG22	1.98	0.44
45:SA:74:VAL:HG12	45:SA:79:LYS:HG3	2.00	0.44
55:SP:323:PHE:CZ	55:SP:739:THR:HG21	2.52	0.44
55:SP:414:LEU:HD11	55:SP:448:VAL:HG22	1.99	0.44
58:SS:388:PHE:O	58:SS:391:GLU:N	2.50	0.44
8:L7:75:THR:HG23	8:L7:76:LYS:H	1.82	0.44
16:LH:289:GLN:OE1	16:LH:290:ILE:N	2.44	0.44
17:LI:607:VAL:HG21	17:LI:645:ILE:HD11	1.99	0.44
22:LN:481:ILE:CD1	22:LN:487:VAL:HG23	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:83:THR:HG21	25:LQ:123:ALA:HB1	1.99	0.44
25:LQ:577:LEU:HD13	25:LQ:619:MET:HE3	1.99	0.44
26:LR:30:LYS:O	26:LR:45:LEU:N	2.46	0.44
35:NH:195:ILE:HG21	35:NH:364:VAL:CG2	2.48	0.44
37:NL:194:ASN:OD1	37:NL:195:ASN:N	2.50	0.44
53:SL:137:ALA:O	53:SL:141:LEU:HD23	2.17	0.44
54:SM:124:MET:HE2	54:SM:266:LEU:CD1	2.48	0.44
55:SP:1352:LEU:HA	55:SP:1355:ILE:HG22	1.99	0.44
9:L8:180:ASP:OD2	9:L8:181:GLY:N	2.51	0.44
12:LD:22:ASN:ND2	12:LD:25:VAL:HG23	2.33	0.44
15:LG:12:VAL:HG22	15:LG:30:VAL:HG12	1.98	0.44
16:LH:313:LEU:HD21	16:LH:321:MET:HE1	1.99	0.44
18:LJ:484:MET:SD	20:LL:547:LEU:HD11	2.57	0.44
23:LO:306:ASN:N	23:LO:320:GLY:O	2.48	0.44
25:LQ:287:ARG:HE	25:LQ:327:HIS:HB2	1.83	0.44
31:NB:221:ALA:HB3	31:NB:222:PRO:HD3	1.99	0.44
38:NM:71:ALA:O	38:NM:75:GLY:N	2.51	0.44
39:NP:124:ILE:O	39:NP:124:ILE:HG23	2.17	0.44
50:SH:340:LYS:HZ1	51:SI:772:MET:HE3	1.83	0.44
54:SM:199:GLY:O	54:SM:203:VAL:HG23	2.17	0.44
55:SP:1147:ILE:O	55:SP:1151:ILE:HD12	2.18	0.44
55:SP:1182:LEU:HD23	55:SP:1223:SER:CB	2.47	0.44
1:L0:65:U:OP2	16:LH:418:ASN:ND2	2.48	0.44
2:L1:130:C:H4'	55:SP:1050:MET:HE1	2.00	0.44
8:L7:77:LEU:HD23	8:L7:92:PHE:HE2	1.83	0.44
16:LH:508:ILE:HD12	16:LH:560:ILE:HG21	1.99	0.44
18:LJ:385:MET:HE1	18:LJ:393:ASN:ND2	2.33	0.44
18:LJ:431:LEU:HD13	18:LJ:466:VAL:CG1	2.48	0.44
23:LO:42:LEU:HD12	23:LO:338:ILE:HG22	1.99	0.44
25:LQ:303:LEU:HG	25:LQ:308:LEU:HD12	1.99	0.44
25:LQ:435:THR:HG21	25:LQ:479:LEU:HB2	1.98	0.44
28:LT:258:THR:OG1	28:LT:306:GLY:N	2.39	0.44
35:NH:260:ASP:OD2	35:NH:479:LYS:NZ	2.49	0.44
47:SC:253:ILE:HD13	47:SC:269:ILE:CD1	2.48	0.44
49:SG:411:PHE:HA	49:SG:427:LEU:HD13	2.00	0.44
51:SI:140:LEU:HD11	51:SI:156:LEU:HD21	1.99	0.44
51:SI:241:HIS:C	51:SI:278:THR:HG22	2.42	0.44
51:SI:871:MET:HE3	51:SI:1009:VAL:HG11	1.98	0.44
51:SI:958:VAL:HB	51:SI:979:ALA:HB2	1.99	0.44
55:SP:625:ILE:HD12	55:SP:625:ILE:H	1.83	0.44
10:L9:101:VAL:O	10:L9:105:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:114:GLY:O	16:LH:134:ILE:HG22	2.17	0.44
35:NH:519:ASP:OD1	35:NH:520:ASN:N	2.50	0.44
35:NH:756:VAL:O	35:NH:756:VAL:HG12	2.18	0.44
35:NH:909:TYR:O	35:NH:913:VAL:HG12	2.17	0.44
48:SE:13:ASP:O	48:SE:17:THR:HG23	2.18	0.44
51:SI:85:LEU:O	51:SI:89:LEU:HD23	2.18	0.44
55:SP:561:LEU:O	55:SP:564:ASN:N	2.50	0.44
58:SS:391:GLU:OE2	58:SS:395:ARG:NH2	2.49	0.44
2:L1:1057:U:O4	35:NH:791:LYS:NZ	2.37	0.44
9:L8:26:LYS:O	9:L8:29:LEU:HD22	2.17	0.44
20:LL:225:VAL:HG23	20:LL:225:VAL:O	2.18	0.44
21:LM:217:PHE:HA	21:LM:220:VAL:HB	2.00	0.44
22:LN:554:ASP:O	22:LN:558:ARG:N	2.46	0.44
25:LQ:99:ALA:HA	25:LQ:123:ALA:HB2	2.00	0.44
25:LQ:468:ILE:CG2	25:LQ:471:ALA:HB2	2.48	0.44
35:NH:548:GLY:O	35:NH:552:ARG:NE	2.51	0.44
35:NH:755:PRO:HB2	35:NH:760:PHE:CD2	2.53	0.44
47:SC:301:LEU:HD23	47:SC:301:LEU:O	2.18	0.44
50:SH:340:LYS:HE3	50:SH:353:THR:HG21	1.99	0.44
54:SM:241:THR:HG1	54:SM:244:GLY:C	2.25	0.44
55:SP:897:PHE:CE1	55:SP:901:ILE:HD11	2.53	0.44
63:SY:196:LYS:HD3	63:SY:196:LYS:N	2.32	0.44
2:L1:96:G:H21	2:L1:426:G:H5'	1.83	0.43
2:L1:886:U:OP2	38:NM:216:LYS:NZ	2.42	0.43
11:LC:97:VAL:HG12	11:LC:98:ASP:N	2.32	0.43
12:LD:10:GLU:OE1	12:LD:10:GLU:N	2.50	0.43
16:LH:89:VAL:HG22	16:LH:110:PHE:O	2.18	0.43
18:LJ:432:TYR:O	18:LJ:470:TYR:OH	2.35	0.43
19:LK:449:GLU:OE1	19:LK:449:GLU:N	2.50	0.43
20:LL:27:GLN:OE1	20:LL:60:VAL:HG22	2.18	0.43
23:LO:760:ILE:HD12	23:LO:760:ILE:H	1.83	0.43
25:LQ:529:GLU:C	25:LQ:530:LEU:HD12	2.42	0.43
26:LR:395:ASP:OD2	26:LR:442:LEU:N	2.46	0.43
27:LS:224:ASN:OD1	27:LS:225:SER:N	2.51	0.43
29:LZ:88:LEU:HD11	29:LZ:97:LEU:CD2	2.48	0.43
32:ND:198:ILE:HG23	32:ND:199:ILE:HG23	1.99	0.43
47:SC:282:ALA:HB2	47:SC:312:ASP:OD1	2.18	0.43
48:SF:40:ALA:O	48:SF:44:LEU:HD23	2.17	0.43
55:SP:399:PHE:O	55:SP:403:LEU:HD23	2.18	0.43
2:L1:545:A:O4'	2:L1:594:A:N6	2.51	0.43
2:L1:575:C:OP1	51:SI:933:LYS:NZ	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L2:327:G:N7	48:SE:42:LYS:NZ	2.66	0.43
11:LC:35:PRO:HD2	11:LC:38:LEU:HD12	1.99	0.43
22:LN:99:ILE:HG21	22:LN:102:LEU:HD21	2.00	0.43
35:NH:477:LEU:HD13	35:NH:480:MET:HE2	1.99	0.43
46:SB:230:GLU:HG2	46:SB:231:ILE:HD12	2.00	0.43
51:SI:799:GLU:OE1	51:SI:799:GLU:N	2.48	0.43
55:SP:105:PRO:O	55:SP:109:LEU:HD23	2.18	0.43
2:L1:194:U:O2'	2:L1:195:G:O5'	2.25	0.43
2:L1:619:A:C4	58:SS:459:MET:HE3	2.54	0.43
16:LH:612:SER:HB2	16:LH:662:VAL:HG12	2.01	0.43
16:LH:887:PHE:O	16:LH:891:VAL:HG23	2.18	0.43
17:LI:539:ASN:O	17:LI:542:SER:OG	2.25	0.43
17:LI:608:GLN:OE1	17:LI:654:LEU:HD12	2.18	0.43
23:LO:421:ASN:ND2	23:LO:423:ARG:O	2.49	0.43
23:LO:710:ILE:O	28:LT:598:ARG:NH2	2.51	0.43
23:LO:814:LYS:NZ	28:LT:936:VAL:O	2.51	0.43
25:LQ:803:GLN:OE1	25:LQ:845:LEU:HD21	2.18	0.43
38:NM:120:LEU:N	38:NM:120:LEU:HD12	2.33	0.43
46:SB:177:LEU:HD13	46:SB:265:PHE:CB	2.48	0.43
55:SP:394:LEU:HD11	55:SP:432:ILE:HA	1.99	0.43
2:L1:68:A:OP1	7:L6:160:ARG:NH2	2.43	0.43
2:L1:609:U:O2'	57:SR:19:ARG:NH2	2.51	0.43
25:LQ:208:TRP:CE2	25:LQ:255:ARG:HD2	2.53	0.43
25:LQ:454:LEU:HD23	25:LQ:455:GLN:N	2.34	0.43
35:NH:162:PHE:O	35:NH:597:ARG:NH2	2.51	0.43
55:SP:917:ASP:O	55:SP:921:VAL:HG12	2.19	0.43
2:L1:888:U:O2	2:L1:988:A:O2'	2.37	0.43
13:LE:62:VAL:HG11	40:NQ:8:LEU:HD22	2.01	0.43
14:LF:73:GLY:C	14:LF:74:LEU:HD22	2.44	0.43
18:LJ:375:HIS:CE1	27:LS:339:ILE:HD11	2.54	0.43
25:LQ:574:LEU:O	25:LQ:592:SER:OG	2.33	0.43
25:LQ:836:ILE:HG13	25:LQ:857:LEU:HD11	1.99	0.43
26:LR:36:VAL:O	26:LR:36:VAL:HG13	2.18	0.43
26:LR:102:SER:OG	26:LR:123:ASP:OD2	2.34	0.43
29:LZ:99:ASN:OD1	29:LZ:100:LYS:N	2.52	0.43
35:NH:270:ILE:CD1	35:NH:294:LEU:HD23	2.48	0.43
45:SA:210:VAL:HG11	45:SA:219:LEU:HD12	1.99	0.43
47:SC:169:LYS:HD2	47:SC:193:VAL:HG22	2.00	0.43
48:SE:54:MET:HE2	48:SE:80:PHE:HE2	1.82	0.43
63:SY:101:THR:O	63:SY:101:THR:HG22	2.18	0.43
2:L1:593:U:P	10:L9:39:LYS:HZ3	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LI:711:LEU:HB2	22:LN:33:VAL:HG21	2.00	0.43
18:LJ:83:VAL:CG2	18:LJ:101:ALA:HB2	2.48	0.43
18:LJ:108:TYR:CE2	18:LJ:116:ILE:HD13	2.53	0.43
18:LJ:504:ILE:HG13	18:LJ:507:MET:HE2	2.00	0.43
22:LN:40:ASP:OD1	22:LN:40:ASP:N	2.52	0.43
26:LR:737:ILE:HG22	26:LR:741:LYS:NZ	2.32	0.43
36:NI:43:GLN:OE1	36:NI:43:GLN:N	2.52	0.43
47:SC:123:ILE:HB	47:SC:141:TYR:HB2	2.01	0.43
55:SP:701:LEU:HD21	55:SP:795:ASP:HB3	2.01	0.43
7:L6:23:ARG:NH1	7:L6:41:VAL:HG12	2.33	0.43
16:LH:448:ASN:HD21	16:LH:468:VAL:HG11	1.84	0.43
23:LO:73:ILE:HD12	23:LO:99:CYS:HB3	1.99	0.43
25:LQ:613:ALA:O	25:LQ:640:LYS:NZ	2.41	0.43
35:NH:203:ILE:HD11	35:NH:290:PHE:CD2	2.54	0.43
37:NL:306:LEU:HD23	37:NL:306:LEU:O	2.18	0.43
38:NM:90:GLU:OE2	38:NM:92:GLN:HG3	2.18	0.43
53:SL:72:ILE:O	53:SL:75:SER:OG	2.31	0.43
55:SP:1221:ILE:HD12	55:SP:1264:LEU:HD12	2.00	0.43
2:L1:755:A:OP1	2:L1:793:A:N6	2.43	0.43
6:L5:34:GLN:O	6:L5:37:GLN:HB3	2.19	0.43
14:LF:22:GLN:HG2	14:LF:74:LEU:HD11	2.00	0.43
16:LH:148:GLU:HG2	16:LH:148:GLU:O	2.19	0.43
18:LJ:417:VAL:HG13	18:LJ:418:LEU:HD12	2.01	0.43
19:LK:420:ILE:HD12	19:LK:424:ILE:HG13	2.01	0.43
23:LO:429:GLU:HG2	23:LO:431:ILE:HD11	1.99	0.43
23:LO:775:LEU:O	23:LO:779:LEU:HD23	2.19	0.43
25:LQ:857:LEU:O	25:LQ:860:ILE:HG22	2.17	0.43
26:LR:454:LEU:N	26:LR:466:TRP:O	2.52	0.43
27:LS:130:ASP:OD1	28:LT:179:LYS:NZ	2.52	0.43
28:LT:32:ASN:ND2	28:LT:649:ASN:OD1	2.52	0.43
30:NA:356:VAL:HG13	59:ST:764:ARG:HH22	1.83	0.43
37:NL:155:PHE:O	37:NL:205:SER:N	2.49	0.43
37:NL:290:LEU:HD13	37:NL:302:ASP:HB3	1.99	0.43
51:SI:1112:PHE:CD2	56:SQ:178:MET:HE1	2.54	0.43
52:SK:70:CYS:N	52:SK:87:ALA:O	2.51	0.43
55:SP:1681:LEU:HD23	55:SP:1686:GLN:O	2.19	0.43
2:L1:494:U:HO2'	2:L1:495:C:P	2.41	0.43
2:L1:556:A:H61	63:SY:19:LEU:HD11	1.83	0.43
7:L6:1:MET:HG3	7:L6:24:ILE:HD12	2.00	0.43
29:LZ:111:LEU:O	29:LZ:115:MET:HE2	2.18	0.43
31:NB:66:MET:HE3	31:NB:66:MET:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:NL:144:GLN:NE2	37:NL:145:PRO:O	2.52	0.43
51:SI:857:LEU:HD21	51:SI:1032:LEU:CD2	2.49	0.43
2:L1:188:A:OP2	2:L1:189:C:N4	2.51	0.43
16:LH:197:ILE:HD11	16:LH:213:LYS:CG	2.49	0.43
17:LI:546:ASP:OD1	17:LI:546:ASP:N	2.52	0.43
21:LM:218:ILE:HD12	21:LM:263:VAL:CG2	2.46	0.43
26:LR:153:TYR:CZ	26:LR:209:LEU:HD11	2.54	0.43
28:LT:229:GLU:CD	28:LT:231:ILE:HD11	2.44	0.43
28:LT:426:GLU:OE1	28:LT:426:GLU:N	2.51	0.43
28:LT:721:LEU:HD11	28:LT:919:GLU:CD	2.44	0.43
41:NS:104:GLN:O	41:NS:107:ARG:N	2.43	0.43
16:LH:317:TRP:HA	16:LH:340:ILE:HG23	2.01	0.42
17:LI:571:PHE:HA	17:LI:610:PHE:CZ	2.54	0.42
21:LM:220:VAL:O	21:LM:220:VAL:HG12	2.18	0.42
22:LN:687:PHE:CE2	22:LN:688:MET:HE3	2.53	0.42
23:LO:810:ILE:HG21	23:LO:821:MET:HE3	2.01	0.42
27:LS:430:GLY:H	27:LS:455:ILE:HB	1.84	0.42
28:LT:326:PRO:O	28:LT:326:PRO:HD2	2.19	0.42
28:LT:734:LEU:HD23	28:LT:883:THR:HG23	2.00	0.42
47:SD:180:SER:O	47:SD:184:VAL:HG23	2.18	0.42
9:L8:6:ASP:OD1	9:L8:7:SER:N	2.52	0.42
18:LJ:105:VAL:CG1	18:LJ:127:THR:HG21	2.49	0.42
20:LL:116:GLN:OE1	20:LL:128:GLN:NE2	2.52	0.42
20:LL:222:THR:HG23	20:LL:222:THR:O	2.19	0.42
20:LL:369:PHE:O	20:LL:524:SER:OG	2.36	0.42
26:LR:12:LEU:HD11	26:LR:378:PRO:CG	2.49	0.42
27:LS:529:ILE:CG2	27:LS:543:LEU:HD12	2.49	0.42
33:NF:89:TYR:CG	33:NF:129:TYR:OH	2.72	0.42
45:SA:13:THR:HG21	45:SA:144:SER:O	2.18	0.42
45:SA:169:LYS:NZ	45:SA:391:ASN:O	2.51	0.42
46:SB:121:LYS:HB2	47:SD:236:MET:HE1	2.01	0.42
49:SG:259:LYS:HE2	49:SG:261:ILE:HD11	2.01	0.42
16:LH:269:GLN:N	16:LH:269:GLN:OE1	2.50	0.42
16:LH:531:PHE:HB2	16:LH:545:THR:OG1	2.19	0.42
27:LS:178:VAL:HG11	28:LT:217:VAL:HG11	2.01	0.42
33:NF:85:PRO:HB2	33:NF:89:TYR:CD2	2.54	0.42
36:NI:176:ASP:O	36:NI:180:LEU:HD23	2.19	0.42
37:NL:68:GLY:CA	37:NL:71:THR:HG22	2.48	0.42
55:SP:1095:SER:HA	55:SP:1136:THR:HG22	2.01	0.42
56:SQ:110:ASP:OD1	56:SQ:111:ASP:N	2.52	0.42
2:L1:1533:C:H5"	4:L3:27:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L7:123:ASP:OD1	8:L7:124:LYS:N	2.51	0.42
10:L9:127:VAL:O	10:L9:131:GLN:HB2	2.19	0.42
11:LC:89:LEU:HD23	11:LC:93:HIS:CD2	2.53	0.42
16:LH:44:TYR:HD2	16:LH:46:ILE:HD11	1.84	0.42
18:LJ:138:LYS:CD	18:LJ:154:ILE:HD11	2.48	0.42
37:NL:178:ASN:HB2	37:NL:227:LEU:HD21	2.01	0.42
39:NP:75:LYS:NZ	39:NP:79:LEU:HD22	2.34	0.42
45:SA:257:ILE:HG13	45:SA:257:ILE:O	2.19	0.42
48:SF:74:LYS:HE2	48:SF:74:LYS:HA	2.01	0.42
49:SG:308:SER:O	49:SG:312:PHE:N	2.53	0.42
63:SY:64:TYR:O	63:SY:67:MET:HB2	2.19	0.42
9:L8:72:ILE:HG22	9:L8:73:SER:N	2.34	0.42
10:L9:61:THR:HG23	53:SL:84:ARG:HH22	1.85	0.42
22:LN:189:ARG:HH22	32:ND:198:ILE:HD11	1.85	0.42
22:LN:363:SER:O	22:LN:367:GLY:N	2.48	0.42
23:LO:523:MET:HE2	23:LO:523:MET:HA	2.01	0.42
25:LQ:634:SER:OG	25:LQ:635:LYS:N	2.53	0.42
26:LR:571:LEU:HD12	26:LR:602:TRP:CD2	2.54	0.42
29:LZ:153:ASN:OD1	29:LZ:154:MET:N	2.52	0.42
33:NF:118:ILE:HG22	33:NF:122:ILE:CD1	2.45	0.42
41:NS:888:ALA:HB1	41:NS:899:GLY:CA	2.50	0.42
49:SG:140:LEU:HD23	49:SG:570:GLN:HE21	1.84	0.42
50:SH:107:ALA:HA	50:SH:114:PHE:CE1	2.54	0.42
51:SI:158:ILE:HD11	51:SI:913:ILE:HD11	2.00	0.42
2:L1:1700:C:H2'	2:L1:1701:A:C8	2.54	0.42
10:L9:136:VAL:HG13	10:L9:136:VAL:O	2.19	0.42
11:LC:52:LEU:HD23	11:LC:60:PHE:CE1	2.55	0.42
16:LH:356:LEU:O	16:LH:357:ILE:HD13	2.20	0.42
16:LH:689:ILE:HD12	16:LH:689:ILE:H	1.84	0.42
17:LI:504:ASN:OD1	17:LI:536:ARG:NH2	2.52	0.42
28:LT:21:SER:O	28:LT:657:ARG:NH1	2.52	0.42
35:NH:550:MET:HA	35:NH:550:MET:HE3	2.01	0.42
35:NH:638:MET:HE2	35:NH:638:MET:HA	2.01	0.42
36:NI:16:VAL:HG12	36:NI:18:PHE:HE1	1.84	0.42
38:NM:20:VAL:HG23	38:NM:21:VAL:HG23	2.02	0.42
45:SA:21:LYS:HZ1	45:SA:49:GLU:N	2.18	0.42
45:SA:180:LEU:HD23	45:SA:184:LEU:HD13	2.00	0.42
55:SP:523:LEU:HD11	55:SP:541:ILE:HG21	2.01	0.42
55:SP:1777:LEU:HD21	55:SP:1789:LEU:CD2	2.50	0.42
57:SR:48:HIS:HB3	57:SR:103:LEU:HD11	2.01	0.42
6:L5:179:ALA:CB	6:L5:194:LEU:HD12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L8:38:ILE:HD11	9:L8:78:ILE:HG21	2.01	0.42
16:LH:473:LEU:HD12	16:LH:474:THR:HG23	2.02	0.42
16:LH:627:ASP:O	16:LH:659:ILE:HD12	2.20	0.42
22:LN:101:GLY:O	22:LN:102:LEU:HD22	2.20	0.42
23:LO:788:GLU:O	28:LT:728:ARG:NH2	2.50	0.42
25:LQ:425:ILE:HG22	25:LQ:426:ARG:HD2	2.01	0.42
27:LS:301:TYR:N	27:LS:311:ASN:O	2.53	0.42
31:NB:19:ASN:HD22	31:NB:23:LEU:HD23	1.85	0.42
35:NH:524:ASP:C	35:NH:525:LEU:HD22	2.45	0.42
47:SD:151:LEU:HD21	47:SD:162:LEU:HD11	2.02	0.42
55:SP:135:LEU:O	55:SP:139:ALA:N	2.49	0.42
55:SP:1069:VAL:O	55:SP:1069:VAL:HG22	2.20	0.42
56:SQ:197:LYS:HE2	56:SQ:197:LYS:HA	2.01	0.42
2:L1:562:G:C5	54:SM:281:ILE:HG23	2.55	0.42
2:L1:934:C:H42	58:SS:399:LYS:CD	2.33	0.42
4:L3:106:GLU:CB	59:ST:744:LEU:HD11	2.50	0.42
5:L4:19:LEU:HD11	5:L4:108:ARG:NE	2.35	0.42
5:L4:175:PHE:CE2	5:L4:222:LEU:HD11	2.54	0.42
16:LH:876:PHE:O	16:LH:879:ILE:HG22	2.19	0.42
20:LL:51:LEU:HD12	20:LL:88:TYR:CE1	2.55	0.42
28:LT:170:LEU:HD22	28:LT:180:LEU:HD21	2.00	0.42
35:NH:820:THR:HG23	35:NH:821:TYR:CD1	2.55	0.42
36:NI:137:CYS:O	36:NI:141:LEU:N	2.46	0.42
40:NQ:47:PHE:O	40:NQ:50:ALA:HB2	2.20	0.42
45:SA:74:VAL:HG13	45:SA:78:LEU:HD23	2.01	0.42
55:SP:625:ILE:HG21	55:SP:642:ILE:HD11	2.01	0.42
55:SP:1181:ILE:O	55:SP:1181:ILE:HG22	2.20	0.42
64:SZ:242:TRP:O	64:SZ:246:ILE:N	2.44	0.42
2:L1:528:U:H4'	51:SI:180:GLN:HG3	2.02	0.42
2:L1:1142:A:H61	59:ST:21:GLN:NE2	2.18	0.42
3:L2:108:A:OP2	3:L2:109:G:N1	2.49	0.42
8:L7:45:SER:OG	8:L7:46:ILE:N	2.53	0.42
13:LE:55:ASP:OD1	13:LE:57:ARG:HB2	2.20	0.42
14:LF:89:TYR:O	14:LF:93:ARG:HG3	2.20	0.42
16:LH:237:LEU:HD23	16:LH:238:SER:H	1.85	0.42
16:LH:297:ILE:HG21	16:LH:484:VAL:HG21	2.02	0.42
23:LO:497:ILE:HD13	23:LO:532:VAL:HG11	2.02	0.42
25:LQ:85:LEU:CD2	25:LQ:94:LEU:HD21	2.50	0.42
26:LR:67:LEU:HD11	26:LR:76:LEU:HD11	2.01	0.42
27:LS:514:LEU:HB3	27:LS:532:MET:HE2	2.02	0.42
33:NF:88:LEU:H	33:NF:89:TYR:HD1	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:NH:519:ASP:O	35:NH:523:TYR:N	2.53	0.42
35:NH:678:ILE:HA	35:NH:681:ILE:HG22	2.02	0.42
38:NM:193:ILE:CD1	38:NM:212:VAL:HG21	2.50	0.42
51:SI:90:VAL:O	51:SI:94:THR:OG1	2.34	0.42
53:SL:84:ARG:O	53:SL:87:MET:N	2.52	0.42
55:SP:523:LEU:CD1	55:SP:561:LEU:HD11	2.49	0.42
62:SW:174:LEU:HD21	62:SW:234:LEU:HD11	2.02	0.42
62:SW:221:ARG:O	62:SW:221:ARG:HD3	2.20	0.42
2:L1:871:G:H2'	2:L1:872:G:C8	2.55	0.42
2:L1:1778:G:OP2	37:NL:162:ARG:NH2	2.49	0.42
5:L4:95:THR:HG23	55:SP:59:LEU:HD12	2.01	0.42
19:LK:492:ILE:CG2	19:LK:496:LEU:HD23	2.50	0.42
20:LL:51:LEU:C	20:LL:51:LEU:HD23	2.45	0.42
25:LQ:159:LEU:HD13	25:LQ:189:TRP:CE3	2.55	0.42
25:LQ:553:ASN:ND2	25:LQ:573:LYS:O	2.53	0.42
26:LR:755:ILE:O	26:LR:759:THR:HG23	2.20	0.42
32:ND:190:LEU:HD12	32:ND:191:PRO:HD2	2.02	0.42
50:SH:115:SER:OG	50:SH:167:HIS:NE2	2.43	0.42
55:SP:360:PHE:CZ	55:SP:364:LEU:HD11	2.55	0.42
55:SP:394:LEU:HD22	55:SP:435:PHE:CD2	2.55	0.42
55:SP:1685:SER:CB	55:SP:1745:ILE:HD11	2.49	0.42
2:L1:123:G:H21	5:L4:146:THR:HG21	1.84	0.41
2:L1:1653:C:OP1	25:LQ:255:ARG:NH2	2.51	0.41
16:LH:693:ASP:OD2	17:LI:495:ARG:NH1	2.53	0.41
16:LH:895:LEU:HD22	21:LM:266:THR:HG21	2.02	0.41
20:LL:539:ARG:HA	20:LL:539:ARG:NE	2.34	0.41
23:LO:131:ARG:NH1	28:LT:639:ASP:OD2	2.53	0.41
26:LR:67:LEU:HD12	26:LR:78:TYR:HB3	2.02	0.41
26:LR:686:MET:HE2	26:LR:735:GLN:HB3	2.02	0.41
34:NG:128:LYS:HE2	62:SW:192:THR:HG23	2.01	0.41
35:NH:118:GLN:N	35:NH:118:GLN:OE1	2.53	0.41
35:NH:1157:TYR:CD2	35:NH:1161:LEU:HD12	2.55	0.41
45:SA:182:ASP:OD1	45:SA:183:GLN:N	2.53	0.41
47:SD:220:ILE:HG12	47:SD:233:LEU:HD23	2.01	0.41
47:SD:234:ILE:HG22	47:SD:235:GLY:O	2.20	0.41
55:SP:10:SER:O	55:SP:15:ARG:NH2	2.48	0.41
2:L1:419:G:O5'	7:L6:72:ARG:NH2	2.53	0.41
2:L1:445:A:N3	2:L1:445:A:H2'	2.35	0.41
16:LH:68:PHE:O	16:LH:75:SER:OG	2.38	0.41
20:LL:232:ILE:HG21	20:LL:235:LEU:HD11	2.02	0.41
22:LN:593:GLU:O	22:LN:611:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LO:852:THR:CG2	26:LR:769:ILE:HD13	2.49	0.41
25:LQ:273:TYR:OH	25:LQ:341:ALA:O	2.32	0.41
27:LS:376:LEU:HD12	27:LS:409:ILE:HD11	2.02	0.41
28:LT:737:LEU:HD23	28:LT:846:ASP:OD2	2.20	0.41
37:NL:168:GLY:O	37:NL:297:LYS:NZ	2.45	0.41
37:NL:227:LEU:HD12	37:NL:231:PHE:CD1	2.55	0.41
46:SB:23:TYR:HB3	46:SB:113:THR:HG22	2.01	0.41
54:SM:176:ILE:HD12	59:ST:57:PRO:HB2	2.00	0.41
55:SP:233:LEU:O	55:SP:237:THR:HG22	2.20	0.41
55:SP:402:ARG:HH12	55:SP:742:THR:HG21	1.85	0.41
5:L4:103:TYR:O	5:L4:182:TYR:OH	2.38	0.41
5:L4:146:THR:O	5:L4:146:THR:HG23	2.21	0.41
18:LJ:263:ASN:O	18:LJ:310:SER:OG	2.38	0.41
23:LO:272:THR:OG1	23:LO:274:LEU:HD23	2.20	0.41
25:LQ:395:ARG:HH22	30:NA:593:LEU:HD13	1.85	0.41
26:LR:345:TYR:OH	26:LR:633:VAL:HG23	2.19	0.41
28:LT:737:LEU:HD23	28:LT:846:ASP:CB	2.50	0.41
30:NA:515:MET:CE	30:NA:520:LEU:HD11	2.50	0.41
31:NB:557:ASP:OD1	31:NB:558:ASN:N	2.53	0.41
35:NH:756:VAL:HG11	35:NH:892:SER:HB2	2.02	0.41
47:SC:297:ARG:NH1	47:SC:322:ARG:O	2.42	0.41
47:SD:195:TYR:CD2	47:SD:234:ILE:HG23	2.55	0.41
48:SE:31:ARG:HD3	48:SE:31:ARG:N	2.34	0.41
49:SG:443:LEU:HD21	49:SG:492:TRP:CZ2	2.55	0.41
51:SI:219:GLU:HA	51:SI:219:GLU:OE1	2.20	0.41
55:SP:725:ASN:OD1	55:SP:726:LYS:N	2.53	0.41
2:L1:628:G:P	33:NF:5:HIS:HE2	2.43	0.41
2:L1:1568:C:O2'	2:L1:1569:A:P	2.78	0.41
4:L3:68:ARG:NE	4:L3:68:ARG:HA	2.35	0.41
8:L7:34:LEU:HD23	8:L7:37:GLU:OE2	2.20	0.41
8:L7:129:LEU:HD21	8:L7:172:VAL:CG1	2.49	0.41
10:L9:112:GLN:O	10:L9:116:LEU:HD23	2.21	0.41
16:LH:699:ASN:C	16:LH:699:ASN:HD22	2.28	0.41
28:LT:274:ILE:HG13	28:LT:286:VAL:HG23	2.03	0.41
33:NF:88:LEU:CD1	33:NF:122:ILE:HA	2.49	0.41
35:NH:1095:ASP:OD1	35:NH:1096:TYR:N	2.53	0.41
39:NP:38:LYS:NZ	39:NP:43:ASN:O	2.37	0.41
45:SA:314:ARG:O	45:SA:318:HIS:N	2.48	0.41
46:SB:140:SER:OG	47:SD:233:LEU:HD12	2.20	0.41
50:SH:125:HIS:HE2	50:SH:263:ASP:CG	2.27	0.41
50:SH:131:GLU:HB3	50:SH:244:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SH:180:MET:HE2	50:SH:180:MET:HA	2.01	0.41
50:SH:216:LEU:HG	50:SH:223:VAL:HG21	2.02	0.41
51:SI:610:LYS:NZ	51:SI:612:VAL:O	2.51	0.41
51:SI:1098:ARG:HA	63:SY:101:THR:HG21	2.01	0.41
55:SP:397:PHE:O	55:SP:401:LEU:HD23	2.20	0.41
55:SP:1357:ASN:ND2	55:SP:1359:GLU:OE2	2.52	0.41
57:SR:141:GLU:N	57:SR:141:GLU:OE2	2.53	0.41
2:L1:335:U:O3'	12:LD:129:ARG:NH1	2.53	0.41
2:L1:381:C:O2'	2:L1:755:A:N1	2.52	0.41
11:LC:89:LEU:HD21	11:LC:105:LEU:CD1	2.50	0.41
18:LJ:443:LEU:HG	18:LJ:483:LEU:HD21	2.02	0.41
21:LM:167:PHE:CE2	21:LM:178:THR:HG21	2.55	0.41
21:LM:1008:PHE:O	21:LM:1012:SER:N	2.41	0.41
25:LQ:6:GLN:NE2	25:LQ:686:GLU:OE2	2.37	0.41
25:LQ:379:PRO:C	25:LQ:380:LEU:HD22	2.45	0.41
25:LQ:418:ASN:HB2	25:LQ:425:ILE:HD11	2.02	0.41
26:LR:127:ILE:HG23	26:LR:136:ILE:CD1	2.50	0.41
31:NB:608:PHE:CD2	53:SL:147:GLN:NE2	2.82	0.41
35:NH:282:ASP:OD1	35:NH:283:TYR:N	2.53	0.41
41:NS:9:ASN:O	41:NS:9:ASN:OD1	2.39	0.41
46:SB:63:ILE:HD13	47:SD:232:MET:SD	2.61	0.41
53:SL:122:ASP:OD2	53:SL:124:ARG:NH2	2.53	0.41
54:SM:162:THR:OG1	54:SM:264:GLY:O	2.30	0.41
2:L1:612:U:OP2	2:L1:613:G:O2'	2.25	0.41
2:L1:992:A:OP2	2:L1:1011:G:N1	2.46	0.41
16:LH:248:GLN:O	16:LH:252:LEU:HD13	2.21	0.41
16:LH:383:LEU:HD11	16:LH:385:ILE:HD11	2.01	0.41
16:LH:555:VAL:HG13	16:LH:555:VAL:O	2.19	0.41
18:LJ:404:ALA:O	18:LJ:409:MET:HE3	2.21	0.41
18:LJ:440:GLU:HG3	18:LJ:441:PRO:HD3	2.03	0.41
21:LM:1500:PHE:O	21:LM:1504:LEU:N	2.48	0.41
23:LO:351:LEU:HD11	23:LO:685:GLN:HB2	2.01	0.41
25:LQ:464:LEU:HD11	25:LQ:467:THR:OG1	2.21	0.41
26:LR:343:MET:HG2	26:LR:355:LEU:HD23	2.02	0.41
27:LS:248:HIS:N	27:LS:269:ASP:OD2	2.53	0.41
28:LT:586:ASN:OD1	28:LT:605:LEU:HB2	2.20	0.41
32:ND:183:THR:OG1	32:ND:185:GLN:OE1	2.34	0.41
35:NH:393:PHE:CE1	35:NH:425:VAL:HG21	2.56	0.41
35:NH:801:LYS:NZ	36:NI:184:ILE:O	2.52	0.41
36:NI:217:GLY:N	40:NQ:75:GLU:OE1	2.50	0.41
38:NM:193:ILE:HD12	38:NM:212:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SC:258:HIS:C	47:SC:259:MET:HE2	2.46	0.41
51:SI:296:PHE:CE2	51:SI:796:VAL:HG22	2.55	0.41
55:SP:1685:SER:O	55:SP:1689:VAL:HG23	2.20	0.41
2:L1:1134:C:O2	50:SH:201:SER:OG	2.32	0.41
5:L4:64:ILE:CG1	14:LF:18:LEU:HD21	2.51	0.41
6:L5:123:VAL:CG1	18:LJ:95:LEU:HD11	2.50	0.41
7:L6:3:LEU:HD11	7:L6:111:LEU:HD22	2.02	0.41
17:LI:668:ILE:HG23	17:LI:671:ARG:NH2	2.35	0.41
17:LI:675:LEU:HD13	19:LK:456:LEU:HD23	2.03	0.41
20:LL:306:LEU:HD11	20:LL:310:THR:CA	2.48	0.41
21:LM:270:LEU:HD21	21:LM:274:ILE:HG21	2.02	0.41
22:LN:425:ASP:OD1	22:LN:426:GLN:N	2.53	0.41
29:LZ:120:MET:HE1	63:SY:61:ASP:C	2.46	0.41
35:NH:715:SER:O	35:NH:719:THR:HG23	2.21	0.41
50:SH:275:VAL:HA	50:SH:278:GLN:HB2	2.01	0.41
55:SP:1273:LYS:NZ	55:SP:1352:LEU:HB2	2.36	0.41
2:L1:934:C:H41	58:SS:396:ARG:N	2.19	0.41
14:LF:36:SER:OG	14:LF:38:ASP:OD1	2.24	0.41
16:LH:610:SER:OG	16:LH:610:SER:O	2.38	0.41
20:LL:297:ASN:O	20:LL:298:LYS:HE2	2.21	0.41
23:LO:119:LEU:HD12	23:LO:163:THR:CG2	2.42	0.41
25:LQ:497:VAL:HG23	25:LQ:530:LEU:HD13	2.02	0.41
27:LS:324:TRP:HE1	27:LS:326:LEU:HD21	1.86	0.41
28:LT:743:ARG:NH1	30:NA:481:PRO:O	2.54	0.41
35:NH:427:LYS:O	35:NH:431:THR:HG22	2.20	0.41
36:NI:181:LYS:O	36:NI:185:HIS:N	2.51	0.41
37:NL:30:PHE:O	37:NL:89:ARG:NE	2.44	0.41
41:NS:515:ILE:N	41:NS:556:ILE:O	2.47	0.41
51:SI:260:THR:HG23	51:SI:261:GLN:HG2	2.02	0.41
54:SM:176:ILE:HD13	59:ST:82:GLY:HA2	2.03	0.41
2:L1:225:A:N1	55:SP:1529:ARG:NH1	2.68	0.41
2:L1:501:U:O2'	2:L1:502:U:OP2	2.29	0.41
2:L1:862:A:O2'	2:L1:963:A:N1	2.39	0.41
2:L1:904:G:H4'	62:SW:241:ARG:NH2	2.36	0.41
2:L1:1480:G:O2'	11:LC:40:GLU:OE1	2.38	0.41
2:L1:1638:G:H2'	26:LR:751:LYS:NZ	2.35	0.41
3:L2:0:M7G:H81	3:L2:0:M7G:H5'1	2.02	0.41
6:L5:93:LEU:O	6:L5:97:LEU:HD23	2.20	0.41
7:L6:78:THR:OG1	7:L6:79:LYS:N	2.54	0.41
9:L8:152:ILE:HG22	9:L8:153:GLU:N	2.36	0.41
10:L9:66:ASP:OD2	10:L9:68:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LE:10:ALA:HA	13:LE:27:ILE:HD12	2.02	0.41
14:LF:51:GLU:HA	14:LF:51:GLU:OE2	2.21	0.41
18:LJ:414:THR:O	18:LJ:418:LEU:HD13	2.20	0.41
20:LL:169:SER:OG	20:LL:170:ILE:N	2.54	0.41
20:LL:175:ILE:H	20:LL:175:ILE:HD12	1.86	0.41
20:LL:300:LEU:HD21	20:LL:316:ASN:HB3	2.03	0.41
21:LM:217:PHE:HE2	21:LM:241:ILE:HG21	1.85	0.41
21:LM:241:ILE:O	21:LM:245:LEU:HD23	2.21	0.41
21:LM:615:ASN:O	21:LM:618:ASP:N	2.54	0.41
22:LN:469:LEU:O	22:LN:473:THR:OG1	2.23	0.41
23:LO:60:ALA:HB3	23:LO:73:ILE:HD11	2.03	0.41
23:LO:779:LEU:HD12	23:LO:824:ILE:CD1	2.50	0.41
24:LP:111:ALA:CB	56:SQ:73:ALA:HB2	2.47	0.41
25:LQ:619:MET:N	25:LQ:619:MET:SD	2.94	0.41
25:LQ:762:GLU:OE1	25:LQ:791:ASN:N	2.53	0.41
25:LQ:840:MET:HE3	25:LQ:886:GLU:HB2	2.03	0.41
25:LQ:901:ASN:O	25:LQ:905:LEU:HD13	2.21	0.41
27:LS:171:ILE:HG22	27:LS:172:TYR:CD1	2.56	0.41
28:LT:256:PHE:CE2	28:LT:264:LEU:HD13	2.56	0.41
29:LZ:149:LEU:HD23	29:LZ:149:LEU:H	1.86	0.41
36:NI:92:GLU:O	36:NI:121:ARG:NH2	2.53	0.41
37:NL:175:LEU:HD23	37:NL:175:LEU:C	2.45	0.41
40:NQ:46:VAL:CG1	40:NQ:54:VAL:HG21	2.50	0.41
47:SC:321:MET:HE2	47:SC:321:MET:CA	2.51	0.41
47:SD:126:GLU:OE1	47:SD:126:GLU:N	2.51	0.41
48:SE:52:ILE:N	48:SE:52:ILE:HD12	2.36	0.41
51:SI:99:ASN:OD1	51:SI:100:ASP:N	2.54	0.41
51:SI:287:ARG:HD3	51:SI:820:ILE:HD12	2.02	0.41
51:SI:1067:LEU:HD22	63:SY:47:THR:HG23	2.03	0.41
55:SP:1182:LEU:HD23	55:SP:1223:SER:HB2	2.03	0.41
55:SP:1399:LEU:HD21	55:SP:1424:MET:HE1	2.03	0.41
55:SP:1613:ALA:CB	55:SP:1639:ILE:HD11	2.50	0.41
62:SW:153:GLN:NE2	62:SW:157:ASP:OD2	2.51	0.41
2:L1:25:C:C2	2:L1:26:A:N7	2.88	0.41
2:L1:1533:C:C5'	4:L3:27:LYS:HE3	2.51	0.41
7:L6:148:SER:OG	7:L6:151:ASP:OD1	2.36	0.41
11:LC:55:VAL:HG11	11:LC:105:LEU:CD1	2.50	0.41
16:LH:454:ILE:H	16:LH:454:ILE:HD12	1.86	0.41
18:LJ:83:VAL:HG22	18:LJ:101:ALA:HB2	2.02	0.41
21:LM:140:LEU:HD23	21:LM:183:PHE:HE1	1.86	0.41
21:LM:559:ASN:N	21:LM:597:HIS:O	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LO:10:LEU:HD13	23:LO:702:LEU:HD23	2.02	0.41
23:LO:351:LEU:C	23:LO:351:LEU:HD12	2.46	0.41
27:LS:128:SEP:O3P	27:LS:128:SEP:N	2.48	0.41
29:LZ:177:ILE:O	29:LZ:177:ILE:HG23	2.19	0.41
33:NF:50:ILE:O	33:NF:54:LEU:HD23	2.21	0.41
35:NH:498:MET:HE2	35:NH:498:MET:HA	2.03	0.41
51:SI:624:LYS:HD3	51:SI:625:TRP:CD1	2.56	0.41
53:SL:80:VAL:HG21	53:SL:180:TYR:HE2	1.86	0.41
55:SP:1478:ASP:N	55:SP:1478:ASP:OD1	2.54	0.41
62:SW:117:TYR:N	62:SW:118:PRO:CD	2.84	0.41
16:LH:414:ILE:HD12	16:LH:414:ILE:H	1.86	0.40
16:LH:663:LYS:NZ	16:LH:713:CYS:SG	2.88	0.40
25:LQ:663:LEU:C	25:LQ:663:LEU:HD23	2.47	0.40
26:LR:223:TRP:CE2	26:LR:233:LEU:HD13	2.56	0.40
26:LR:295:PRO:O	26:LR:296:ILE:HD13	2.20	0.40
35:NH:796:ILE:HG23	35:NH:797:THR:N	2.35	0.40
35:NH:1148:GLN:OE1	35:NH:1149:LEU:HD23	2.22	0.40
37:NL:188:ILE:HD11	37:NL:208:ARG:HB3	2.03	0.40
38:NM:99:ASN:O	38:NM:223:PHE:HD1	2.05	0.40
38:NM:150:VAL:O	58:SS:384:ARG:NE	2.48	0.40
45:SA:244:ASP:OD1	45:SA:245:SER:N	2.54	0.40
46:SB:23:TYR:O	46:SB:112:VAL:HG11	2.21	0.40
47:SC:175:ALA:HB1	47:SC:181:VAL:HG21	2.03	0.40
47:SC:301:LEU:N	47:SC:317:VAL:O	2.48	0.40
50:SH:183:ILE:O	50:SH:312:ARG:NH2	2.52	0.40
53:SL:145:VAL:CG2	53:SL:170:ILE:HD12	2.51	0.40
54:SM:124:MET:HE2	54:SM:266:LEU:HD11	2.03	0.40
55:SP:137:ASP:O	55:SP:140:ILE:HG22	2.21	0.40
2:L1:1634:C:OP1	23:LO:418:ARG:NH1	2.54	0.40
2:L1:1681:A:H2'	2:L1:1682:U:O4'	2.21	0.40
16:LH:308:ASP:OD2	16:LH:309:GLY:N	2.54	0.40
19:LK:407:MET:HE2	19:LK:452:LEU:HG	2.03	0.40
19:LK:486:LEU:O	19:LK:489:SER:N	2.50	0.40
22:LN:122:VAL:HG21	32:ND:192:PRO:HG3	2.03	0.40
22:LN:210:ILE:HD11	22:LN:241:VAL:HG11	2.02	0.40
23:LO:514:VAL:HG22	23:LO:515:TYR:N	2.35	0.40
26:LR:760:ILE:HA	26:LR:763:ILE:HD12	2.03	0.40
27:LS:45:ILE:H	27:LS:45:ILE:HD12	1.86	0.40
35:NH:168:ILE:O	35:NH:172:THR:HG22	2.22	0.40
35:NH:426:ILE:HG21	35:NH:499:LEU:HD12	2.02	0.40
35:NH:1010:GLU:OE2	38:NM:128:LYS:NZ	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:NM:127:VAL:HG13	38:NM:176:VAL:HG11	2.02	0.40
46:SB:8:THR:HG22	46:SB:124:LEU:HD11	2.02	0.40
47:SD:175:ALA:HB1	47:SD:181:VAL:HG21	2.03	0.40
48:SE:53:ILE:HD12	48:SE:53:ILE:N	2.36	0.40
48:SF:85:VAL:HG23	49:SG:552:TRP:HB3	2.03	0.40
51:SI:1042:MET:HB2	51:SI:1044:LEU:HD23	2.03	0.40
55:SP:514:PHE:CD2	55:SP:518:MET:HE1	2.56	0.40
55:SP:1814:PHE:O	55:SP:1818:LEU:HD23	2.21	0.40
2:L1:578:U:OP1	51:SI:840:LYS:NZ	2.54	0.40
2:L1:1534:G:N7	18:LJ:79:ARG:NH1	2.70	0.40
2:L1:1657:U:OP2	25:LQ:450:ARG:NH1	2.50	0.40
5:L4:129:VAL:HG22	5:L4:139:VAL:HG12	2.02	0.40
13:LE:36:LYS:CB	13:LE:110:ILE:HG21	2.51	0.40
16:LH:736:THR:HG22	16:LH:737:ILE:N	2.37	0.40
20:LL:460:ARG:HA	20:LL:460:ARG:NE	2.37	0.40
21:LM:135:LEU:HD23	21:LM:135:LEU:C	2.46	0.40
23:LO:359:ARG:NH2	23:LO:419:TYR:OH	2.54	0.40
23:LO:760:ILE:HA	23:LO:763:ILE:HD12	2.04	0.40
25:LQ:6:GLN:HB3	25:LQ:686:GLU:OE2	2.22	0.40
28:LT:880:LEU:O	28:LT:883:THR:HG22	2.22	0.40
29:LZ:87:VAL:HG22	29:LZ:106:ILE:HD13	2.03	0.40
34:NG:82:LYS:HE3	34:NG:118:VAL:HG11	2.03	0.40
45:SA:175:ILE:HG23	45:SA:176:GLN:HE21	1.86	0.40
48:SE:51:PHE:CE1	48:SE:53:ILE:HD11	2.56	0.40
49:SG:343:ASP:OD1	49:SG:344:ARG:N	2.54	0.40
50:SH:323:ILE:HG23	51:SI:553:ILE:HG13	2.04	0.40
55:SP:642:ILE:HD12	55:SP:669:LEU:HD13	2.03	0.40
55:SP:1323:ARG:O	55:SP:1327:THR:OG1	2.32	0.40
55:SP:1341:GLU:OE2	55:SP:1341:GLU:N	2.51	0.40
2:L1:994:G:H5'	37:NL:174:ARG:HH22	1.86	0.40
2:L1:1657:U:OP1	2:L1:1658:G:O2'	2.21	0.40
4:L3:120:ARG:HE	59:ST:95:ARG:CZ	2.34	0.40
5:L4:58:GLY:O	5:L4:61:VAL:N	2.55	0.40
6:L5:94:THR:HG22	6:L5:114:ILE:HD13	1.99	0.40
14:LF:8:ARG:HG2	42:NV:728:ASN:OD1	2.21	0.40
16:LH:544:LYS:N	16:LH:544:LYS:HD3	2.37	0.40
19:LK:424:ILE:HG22	19:LK:430:LEU:CD1	2.51	0.40
21:LM:25:ARG:NH1	21:LM:45:TYR:OH	2.54	0.40
21:LM:186:MET:HE2	21:LM:223:PHE:HD2	1.86	0.40
22:LN:101:GLY:C	22:LN:102:LEU:HD22	2.46	0.40
22:LN:187:GLU:O	61:SV:167:LYS:NZ	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:631:PHE:CE2	25:LQ:672:VAL:HG21	2.57	0.40
27:LS:233:LEU:CD2	27:LS:235:ILE:HB	2.52	0.40
28:LT:567:ILE:HD11	28:LT:588:ILE:HD13	2.03	0.40
29:LZ:116:HIS:NE2	29:LZ:122:GLU:O	2.54	0.40
32:ND:195:GLU:OE2	32:ND:197:SER:OG	2.34	0.40
37:NL:135:SER:HB3	37:NL:136:PRO:HD3	2.03	0.40
45:SA:177:ALA:HB1	45:SA:288:LEU:HD21	2.04	0.40
49:SG:417:SER:OG	49:SG:418:ASP:N	2.54	0.40
54:SM:5:GLN:O	54:SM:9:ARG:HG3	2.21	0.40
54:SM:273:VAL:O	54:SM:273:VAL:HG13	2.20	0.40
55:SP:113:PHE:O	55:SP:117:LEU:HD23	2.21	0.40
2:L1:70:C:P	7:L6:164:LYS:HZ1	2.44	0.40
2:L1:920:U:H4'	38:NM:65:VAL:HG23	2.03	0.40
16:LH:144:VAL:HG22	16:LH:145:PHE:N	2.36	0.40
16:LH:587:PHE:HA	16:LH:594:TRP:HA	2.03	0.40
16:LH:591:GLU:OE2	20:LL:362:ARG:NH2	2.55	0.40
17:LI:650:LEU:HD23	17:LI:655:LEU:HD12	2.04	0.40
18:LJ:90:ARG:NH1	18:LJ:137:ASN:O	2.55	0.40
18:LJ:500:GLU:O	18:LJ:503:ARG:N	2.55	0.40
20:LL:228:ALA:CB	20:LL:232:ILE:HD11	2.51	0.40
20:LL:349:ASP:O	20:LL:352:SER:OG	2.40	0.40
26:LR:805:ILE:HG23	26:LR:806:LEU:CD2	2.50	0.40
27:LS:41:ASN:O	27:LS:45:ILE:HD12	2.22	0.40
27:LS:432:VAL:HG12	27:LS:433:TRP:N	2.36	0.40
36:NI:269:GLU:CD	36:NI:270:ILE:HG23	2.47	0.40
47:SC:320:TYR:O	47:SC:321:MET:HE2	2.21	0.40
54:SM:281:ILE:HG22	54:SM:283:THR:H	1.86	0.40
55:SP:315:LEU:HD21	55:SP:343:ILE:HG21	2.02	0.40
55:SP:641:ARG:O	55:SP:645:VAL:HG22	2.22	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%)	100 (98%)	2 (2%)	0	100	100
5	L4	242/261 (93%)	235 (97%)	7 (3%)	0	100	100
6	L5	202/225 (90%)	198 (98%)	4 (2%)	0	100	100
7	L6	214/236 (91%)	208 (97%)	6 (3%)	0	100	100
8	L7	174/190 (92%)	171 (98%)	3 (2%)	0	100	100
9	L8	166/200 (83%)	165 (99%)	1 (1%)	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%)	130 (96%)	5 (4%)	0	100	100
13	LE	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
14	LF	128/135 (95%)	126 (98%)	2 (2%)	0	100	100
15	LG	60/67 (90%)	60 (100%)	0	0	100	100
16	LH	788/896 (88%)	769 (98%)	19 (2%)	0	100	100
17	LI	582/713 (82%)	570 (98%)	12 (2%)	0	100	100
18	LJ	470/513 (92%)	460 (98%)	10 (2%)	0	100	100
19	LK	130/575 (23%)	129 (99%)	1 (1%)	0	100	100
20	LL	475/643 (74%)	461 (97%)	14 (3%)	0	100	100
21	LM	1583/1769 (90%)	1552 (98%)	31 (2%)	0	100	100
22	LN	649/776 (84%)	639 (98%)	10 (2%)	0	100	100
23	LO	786/923 (85%)	776 (99%)	10 (1%)	0	100	100
24	LP	375/440 (85%)	373 (100%)	2 (0%)	0	100	100
25	LQ	806/943 (86%)	795 (99%)	11 (1%)	0	100	100
26	LR	785/817 (96%)	767 (98%)	18 (2%)	0	100	100
27	LS	452/594 (76%)	437 (97%)	15 (3%)	0	100	100
28	LT	861/939 (92%)	845 (98%)	16 (2%)	0	100	100
29	LZ	140/183 (76%)	140 (100%)	0	0	100	100
30	NA	312/593 (53%)	312 (100%)	0	0	100	100
31	NB	248/610 (41%)	247 (100%)	1 (0%)	0	100	100
32	ND	70/214 (33%)	69 (99%)	1 (1%)	0	100	100
33	NF	139/151 (92%)	131 (94%)	6 (4%)	2 (1%)	9	40
34	NG	125/137 (91%)	121 (97%)	4 (3%)	0	100	100
35	NH	1063/1237 (86%)	1047 (98%)	16 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	NI	232/297 (78%)	227 (98%)	5 (2%)	0	100	100
37	NL	279/318 (88%)	278 (100%)	1 (0%)	0	100	100
38	NM	231/255 (91%)	221 (96%)	9 (4%)	1 (0%)	30	67
39	NP	130/144 (90%)	125 (96%)	5 (4%)	0	100	100
40	NQ	77/82 (94%)	75 (97%)	2 (3%)	0	100	100
41	NS	917/1267 (72%)	894 (98%)	22 (2%)	1 (0%)	48	82
42	NV	17/733 (2%)	17 (100%)	0	0	100	100
43	OH	118/143 (82%)	117 (99%)	1 (1%)	0	100	100
44	OU	54/152 (36%)	54 (100%)	0	0	100	100
45	SA	390/504 (77%)	386 (99%)	4 (1%)	0	100	100
46	SB	420/511 (82%)	409 (97%)	11 (3%)	0	100	100
47	SC	237/327 (72%)	233 (98%)	4 (2%)	0	100	100
47	SD	234/327 (72%)	233 (100%)	1 (0%)	0	100	100
48	SE	119/126 (94%)	118 (99%)	1 (1%)	0	100	100
48	SF	119/126 (94%)	117 (98%)	2 (2%)	0	100	100
49	SG	453/573 (79%)	448 (99%)	5 (1%)	0	100	100
50	SH	358/367 (98%)	351 (98%)	7 (2%)	0	100	100
51	SI	744/1183 (63%)	732 (98%)	12 (2%)	0	100	100
52	SJ	207/252 (82%)	204 (99%)	3 (1%)	0	100	100
52	SK	225/252 (89%)	223 (99%)	2 (1%)	0	100	100
53	SL	146/189 (77%)	142 (97%)	4 (3%)	0	100	100
54	SM	243/290 (84%)	238 (98%)	5 (2%)	0	100	100
55	SP	1832/2493 (74%)	1809 (99%)	23 (1%)	0	100	100
56	SQ	103/217 (48%)	102 (99%)	1 (1%)	0	100	100
57	SR	130/145 (90%)	130 (100%)	0	0	100	100
58	SS	86/899 (10%)	86 (100%)	0	0	100	100
59	ST	573/810 (71%)	568 (99%)	5 (1%)	0	100	100
60	SU	524/552 (95%)	521 (99%)	3 (1%)	0	100	100
61	SV	151/206 (73%)	149 (99%)	2 (1%)	0	100	100
62	SW	205/274 (75%)	202 (98%)	3 (2%)	0	100	100
63	SY	193/250 (77%)	189 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	SZ	255/483 (53%)	252 (99%)	3 (1%)	0	100	100
All	All	22696/30499 (74%)	22306 (98%)	386 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	NF	89	TYR
41	NS	431	ALA
38	NM	100	PHE
33	NF	85	PRO

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%)	96 (100%)	0	100	100
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%)	108 (99%)	1 (1%)	75	83
15	LG	55/60 (92%)	55 (100%)	0	100	100
16	LH	743/826 (90%)	743 (100%)	0	100	100
17	LI	244/657 (37%)	244 (100%)	0	100	100
18	LJ	421/454 (93%)	421 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	LK	124/533 (23%)	124 (100%)	0	100	100
20	LL	438/574 (76%)	438 (100%)	0	100	100
21	LM	406/1633 (25%)	406 (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	LP	8/414 (2%)	8 (100%)	0	100	100
25	LQ	723/832 (87%)	723 (100%)	0	100	100
26	LR	698/719 (97%)	697 (100%)	1 (0%)	92	94
27	LS	406/528 (77%)	406 (100%)	0	100	100
28	LT	740/819 (90%)	740 (100%)	0	100	100
29	LZ	132/172 (77%)	132 (100%)	0	100	100
30	NA	235/535 (44%)	235 (100%)	0	100	100
31	NB	99/538 (18%)	99 (100%)	0	100	100
32	ND	57/196 (29%)	57 (100%)	0	100	100
33	NF	121/128 (94%)	121 (100%)	0	100	100
34	NG	96/105 (91%)	96 (100%)	0	100	100
35	NH	982/1125 (87%)	982 (100%)	0	100	100
36	NI	220/274 (80%)	220 (100%)	0	100	100
37	NL	257/283 (91%)	256 (100%)	1 (0%)	89	91
38	NM	210/224 (94%)	210 (100%)	0	100	100
39	NP	107/116 (92%)	107 (100%)	0	100	100
40	NQ	68/71 (96%)	68 (100%)	0	100	100
41	NS	135/1140 (12%)	135 (100%)	0	100	100
42	NV	14/671 (2%)	14 (100%)	0	100	100
43	OH	2/119 (2%)	2 (100%)	0	100	100
44	OU	1/135 (1%)	1 (100%)	0	100	100
45	SA	328/435 (75%)	328 (100%)	0	100	100
46	SB	352/433 (81%)	352 (100%)	0	100	100
47	SC	200/240 (83%)	200 (100%)	0	100	100
47	SD	198/240 (82%)	198 (100%)	0	100	100
48	SE	100/104 (96%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	SF	100/104 (96%)	100 (100%)	0	100	100
49	SG	399/503 (79%)	399 (100%)	0	100	100
50	SH	307/312 (98%)	307 (100%)	0	100	100
51	SI	668/1039 (64%)	667 (100%)	1 (0%)	92	94
52	SJ	9/222 (4%)	9 (100%)	0	100	100
52	SK	12/222 (5%)	12 (100%)	0	100	100
53	SL	131/169 (78%)	131 (100%)	0	100	100
54	SM	220/258 (85%)	220 (100%)	0	100	100
55	SP	1725/2307 (75%)	1723 (100%)	2 (0%)	92	94
56	SQ	91/200 (46%)	91 (100%)	0	100	100
57	SR	113/120 (94%)	113 (100%)	0	100	100
58	SS	81/808 (10%)	81 (100%)	0	100	100
59	ST	136/732 (19%)	136 (100%)	0	100	100
60	SU	27/506 (5%)	27 (100%)	0	100	100
61	SV	20/192 (10%)	20 (100%)	0	100	100
62	SW	183/238 (77%)	183 (100%)	0	100	100
63	SY	191/234 (82%)	191 (100%)	0	100	100
64	SZ	14/424 (3%)	14 (100%)	0	100	100
All	All	16214/27168 (60%)	16207 (100%)	7 (0%)	100	100

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	LD	21	ASN
14	LF	34	ASN
26	LR	802	GLN
37	NL	213	ASN
51	SI	5	ASN
55	SP	710	ASN
55	SP	1014	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

Mol	Chain	Res	Type
4	L3	55	HIS

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Mol	Chain	Res	Type
4	L3	71	GLN
5	L4	69	HIS
6	L5	200	ASN
9	L8	159	GLN
12	LD	14	GLN
12	LD	21	ASN
13	LE	42	GLN
13	LE	92	ASN
14	LF	22	GLN
14	LF	29	HIS
15	LG	27	GLN
16	LH	115	HIS
16	LH	325	GLN
16	LH	453	HIS
16	LH	593	ASN
17	LI	597	GLN
18	LJ	39	HIS
18	LJ	128	HIS
18	LJ	135	GLN
18	LJ	263	ASN
18	LJ	376	ASN
18	LJ	393	ASN
18	LJ	496	HIS
19	LK	450	ASN
20	LL	49	ASN
20	LL	302	ASN
20	LL	308	ASN
20	LL	316	ASN
20	LL	458	ASN
20	LL	499	ASN
21	LM	258	HIS
22	LN	227	HIS
22	LN	309	GLN
22	LN	385	ASN
22	LN	452	HIS
22	LN	532	ASN
22	LN	533	HIS
22	LN	574	HIS
23	LO	203	GLN
23	LO	254	HIS
23	LO	259	ASN
23	LO	342	GLN

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Mol	Chain	Res	Type
23	LO	752	ASN
23	LO	791	HIS
25	LQ	411	ASN
25	LQ	677	HIS
26	LR	58	ASN
26	LR	83	GLN
26	LR	299	ASN
26	LR	488	HIS
26	LR	587	GLN
26	LR	757	GLN
27	LS	34	GLN
27	LS	167	GLN
27	LS	217	ASN
27	LS	224	ASN
27	LS	283	HIS
27	LS	310	GLN
27	LS	388	HIS
27	LS	450	GLN
27	LS	472	GLN
27	LS	522	GLN
28	LT	32	ASN
28	LT	120	HIS
28	LT	552	HIS
28	LT	645	HIS
28	LT	910	GLN
29	LZ	48	ASN
29	LZ	74	HIS
31	NB	558	ASN
33	NF	78	ASN
33	NF	105	ASN
35	NH	173	ASN
35	NH	344	ASN
35	NH	582	GLN
35	NH	665	HIS
35	NH	1073	ASN
35	NH	1078	HIS
36	NI	83	HIS
36	NI	96	HIS
36	NI	135	ASN
36	NI	148	HIS
37	NL	144	GLN
37	NL	213	ASN

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Mol	Chain	Res	Type
38	NM	16	GLN
38	NM	99	ASN
39	NP	25	GLN
39	NP	129	GLN
41	NS	247	ASN
45	SA	85	ASN
45	SA	183	GLN
45	SA	334	GLN
46	SB	104	ASN
46	SB	145	HIS
46	SB	302	HIS
46	SB	334	HIS
47	SD	216	ASN
48	SE	25	GLN
48	SE	29	ASN
49	SG	181	ASN
49	SG	235	HIS
49	SG	322	HIS
49	SG	532	HIS
49	SG	547	HIS
49	SG	570	GLN
50	SH	152	HIS
50	SH	234	ASN
51	SI	3	GLN
51	SI	5	ASN
51	SI	157	ASN
51	SI	161	HIS
51	SI	162	HIS
51	SI	276	HIS
51	SI	754	GLN
51	SI	882	ASN
51	SI	925	ASN
51	SI	986	HIS
51	SI	1063	HIS
54	SM	113	ASN
54	SM	169	ASN
54	SM	181	ASN
54	SM	211	ASN
54	SM	235	GLN
55	SP	46	HIS
55	SP	115	HIS
55	SP	183	HIS

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Mol	Chain	Res	Type
55	SP	207	ASN
55	SP	379	GLN
55	SP	383	ASN
55	SP	446	GLN
55	SP	710	ASN
55	SP	840	ASN
55	SP	1002	ASN
55	SP	1093	HIS
55	SP	1100	GLN
55	SP	1114	HIS
55	SP	1453	ASN
55	SP	1502	ASN
55	SP	1786	GLN
55	SP	1860	ASN
59	ST	23	ASN
59	ST	743	GLN
62	SW	197	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L0	63/700 (9%)	10 (15%)	0
2	L1	1431/1803 (79%)	292 (20%)	10 (0%)
3	L2	198/334 (59%)	25 (12%)	1 (0%)
All	All	1692/2837 (59%)	327 (19%)	11 (0%)

All (327) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L0	7	A
1	L0	63	G
1	L0	64	U
1	L0	83	U
1	L0	85	G
1	L0	86	C
1	L0	279	A
1	L0	280	A
1	L0	281	G
1	L0	283	A
2	L1	2	A
2	L1	9	U

Continued on next page...

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Mol	Chain	Res	Type
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	42	G
2	L1	46	A
2	L1	47	A
2	L1	60	U
2	L1	65	A
2	L1	68	A
2	L1	74	U
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	144	U
2	L1	145	A
2	L1	153	G
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	201	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	290	G
2	L1	299	A
2	L1	304	U
2	L1	314	C
2	L1	316	A
2	L1	322	G
2	L1	333	A
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	445	A
2	L1	446	A
2	L1	453	U
2	L1	460	A
2	L1	467	G
2	L1	477	A
2	L1	487	G
2	L1	493	U
2	L1	494	U

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Mol	Chain	Res	Type
2	L1	495	C
2	L1	496	G
2	L1	501	U
2	L1	502	U
2	L1	505	A
2	L1	506	A
2	L1	511	A
2	L1	515	A
2	L1	519	C
2	L1	520	A
2	L1	527	A
2	L1	532	U
2	L1	534	A
2	L1	540	G
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	575	C
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	610	G
2	L1	611	U
2	L1	619	A
2	L1	621	A
2	L1	622	A
2	L1	623	A
2	L1	624	G
2	L1	629	U
2	L1	634	G
2	L1	652	G
2	L1	654	C
2	L1	687	G
2	L1	688	G
2	L1	765	G

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Mol	Chain	Res	Type
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
2	L1	803	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	960	U
2	L1	962	C
2	L1	966	A
2	L1	969	C
2	L1	992	A
2	L1	1003	A
2	L1	1005	A
2	L1	1011	G
2	L1	1026	A
2	L1	1028	C
2	L1	1029	U
2	L1	1032	G

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Mol	Chain	Res	Type
2	L1	1054	U
2	L1	1059	U
2	L1	1060	U
2	L1	1063	U
2	L1	1072	C
2	L1	1076	A
2	L1	1081	A
2	L1	1082	C
2	L1	1083	G
2	L1	1092	A
2	L1	1093	A
2	L1	1096	C
2	L1	1098	U
2	L1	1099	U
2	L1	1100	G
2	L1	1110	G
2	L1	1119	G
2	L1	1136	U
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

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Mol	Chain	Res	Type
2	L1	1275	A
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	1464	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	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	1584	G
2	L1	1590	G
2	L1	1594	G
2	L1	1598	U
2	L1	1599	C
2	L1	1600	A
2	L1	1601	G
2	L1	1618	C
2	L1	1619	C
2	L1	1624	C
2	L1	1628	U
2	L1	1629	G
2	L1	1630	U

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Mol	Chain	Res	Type
2	L1	1631	A
2	L1	1639	C
2	L1	1651	A
2	L1	1653	C
2	L1	1655	A
2	L1	1657	U
2	L1	1658	G
2	L1	1662	G
2	L1	1663	G
2	L1	1664	C
2	L1	1680	G
2	L1	1683	C
2	L1	1697	G
2	L1	1700	C
2	L1	1701	A
2	L1	1702	A
2	L1	1703	C
2	L1	1715	G
2	L1	1716	C
2	L1	1721	A
2	L1	1742	U
2	L1	1744	A
2	L1	1747	G
2	L1	1755	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

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Mol	Chain	Res	Type
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	140	C
3	L2	145	U
3	L2	155	U
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	252	C
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	494	U
2	L1	585	A
2	L1	793	A
2	L1	811	A
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 ⓘ

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	$\# Z > 2$
27	SEP	LS	128	27	8,9,10	1.61	1 (12%)	7,12,14	1.33	1 (14%)

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
27	SEP	LS	128	27	-	6/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	LS	128	SEP	P-O1P	3.54	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	LS	128	SEP	OG-CB-CA	2.67	110.74	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	LS	128	SEP	C-CA-CB-OG
27	LS	128	SEP	CA-CB-OG-P
27	LS	128	SEP	CB-OG-P-O2P
27	LS	128	SEP	CB-OG-P-O3P
27	LS	128	SEP	CB-OG-P-O1P
27	LS	128	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	LS	128	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 40 are monoatomic - leaving 3 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	$\# Z > 2$
66	ATP	NH	1300	65	28,33,33	0.64	0	34,52,52	0.91	1 (2%)
69	GTP	SI	2001	65	29,34,34	0.88	0	35,54,54	0.69	0
68	ADP	NS	1301	65	24,29,29	0.94	1 (4%)	29,45,45	1.24	2 (6%)

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
66	ATP	NH	1300	65	-	2/18/38/38	0/3/3/3
69	GTP	SI	2001	65	-	0/18/38/38	0/3/3/3
68	ADP	NS	1301	65	-	4/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	NS	1301	ADP	O4'-C1'	2.14	1.43	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	NS	1301	ADP	N3-C2-N1	-4.25	122.90	128.67
68	NS	1301	ADP	C4-C5-N7	-2.71	106.48	109.34
66	NH	1300	ATP	C5-C6-N6	2.34	123.87	120.31

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
68	NS	1301	ADP	PA-O3A-PB-O3B
68	NS	1301	ADP	C5'-O5'-PA-O2A
68	NS	1301	ADP	C5'-O5'-PA-O3A
68	NS	1301	ADP	PA-O3A-PB-O1B
66	NH	1300	ATP	PA-O3A-PB-O2B
66	NH	1300	ATP	O4'-C4'-C5'-O5'

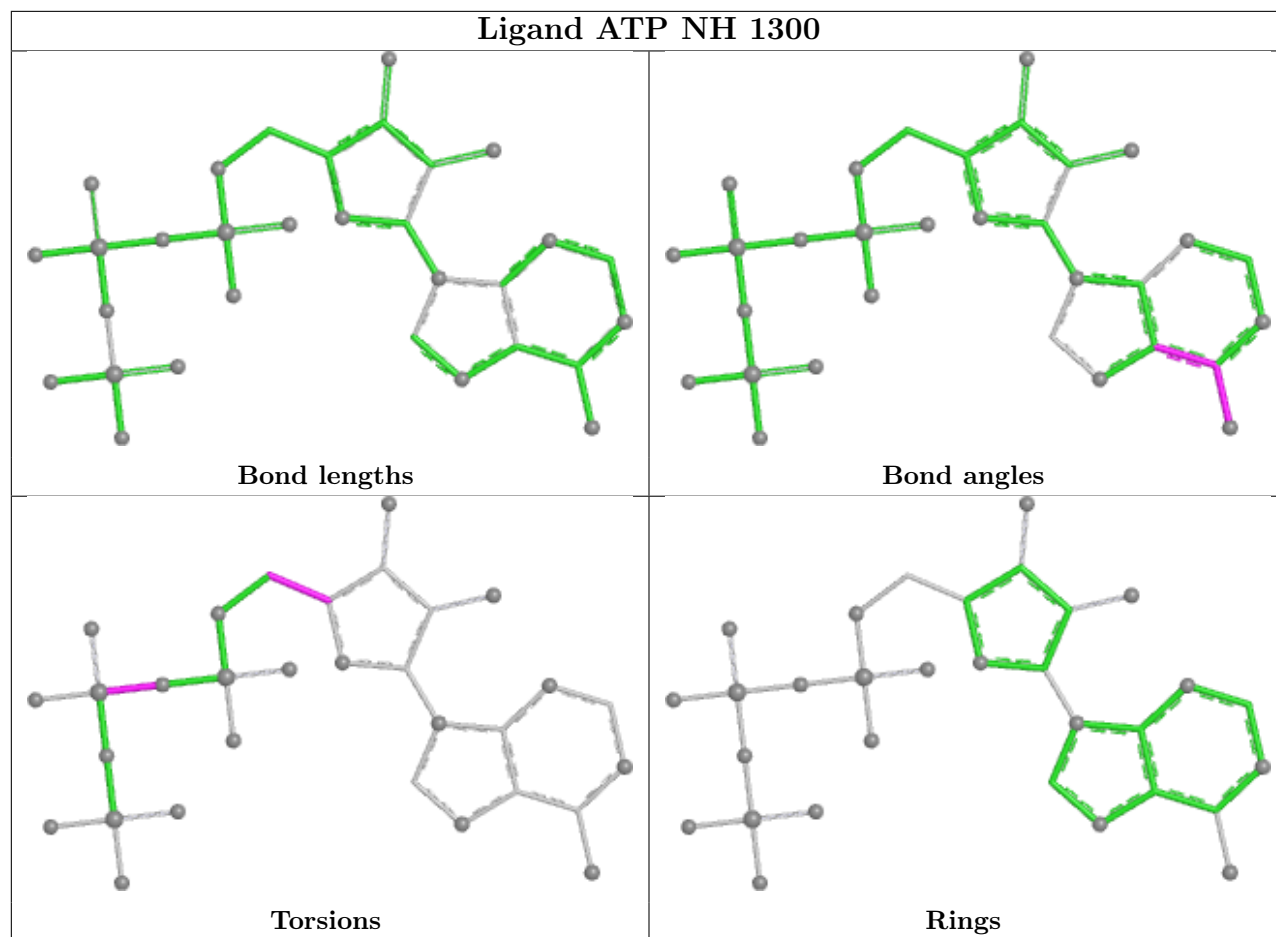
There are no ring outliers.

1 monomer is involved in 1 short contact:

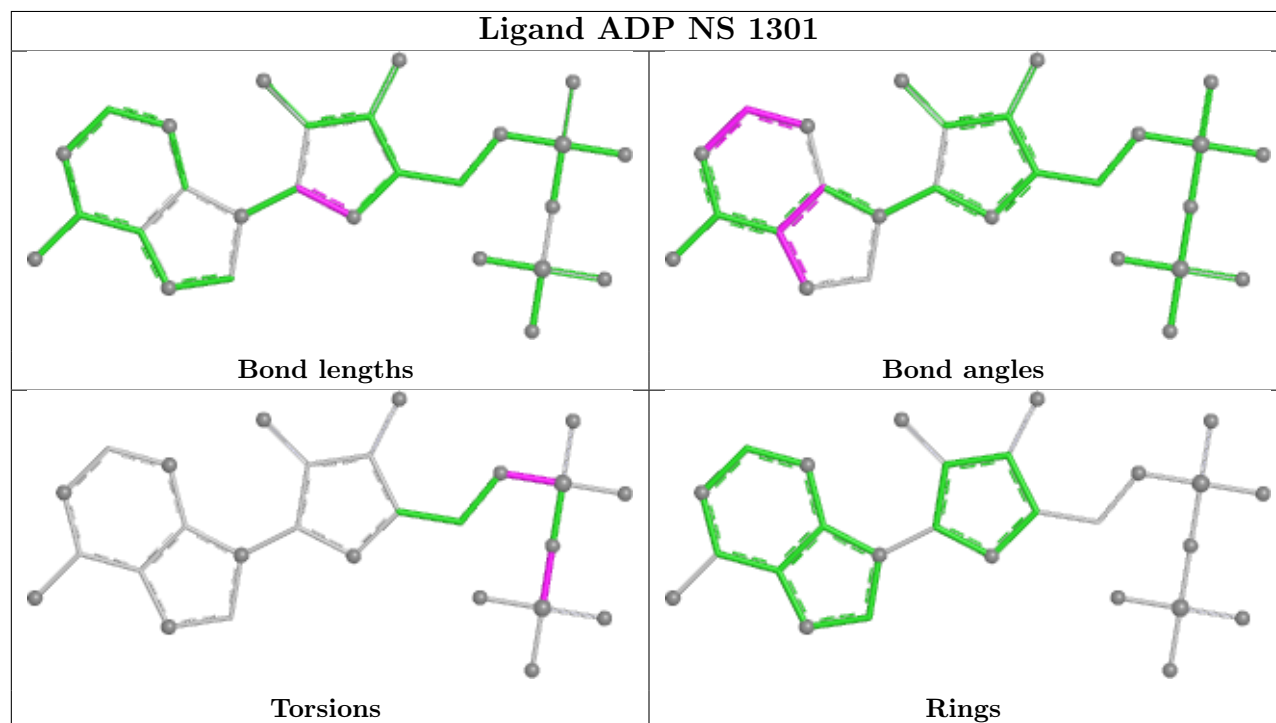
Mol	Chain	Res	Type	Clashes	Symm-Clashes
66	NH	1300	ATP	1	0

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.

Ligand ATP NH 1300



Ligand ADP NS 1301



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.

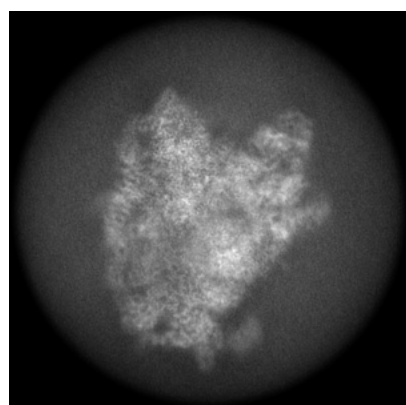
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49086. These allow visual inspection of the internal detail of the map and identification of artifacts.

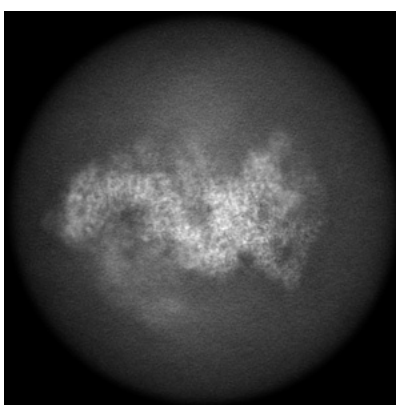
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

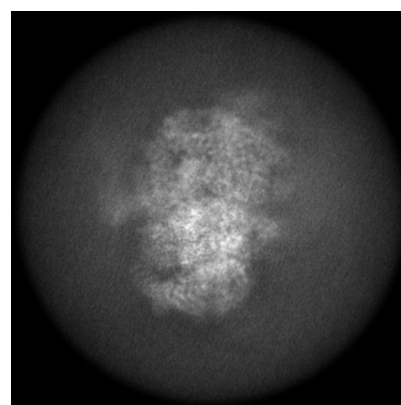
6.1.1 Primary map



X



Y

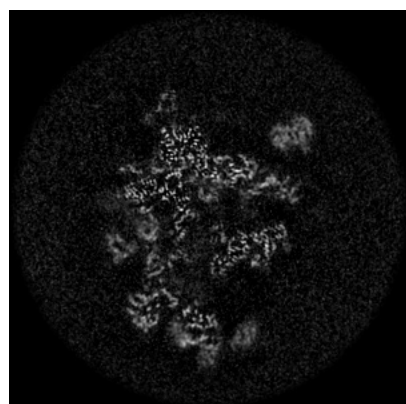


Z

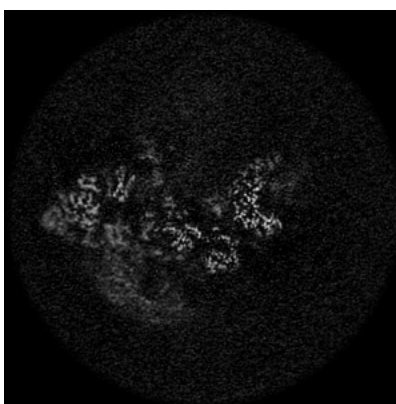
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

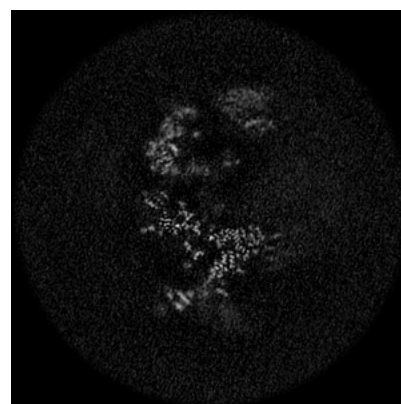
6.2.1 Primary map



X Index: 252



Y Index: 252

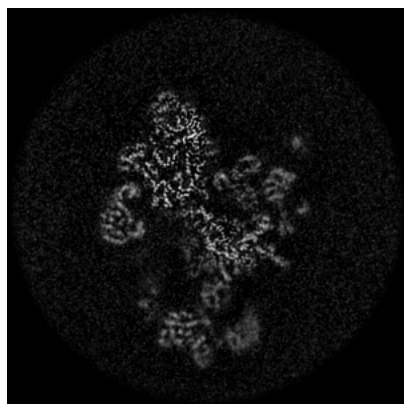


Z Index: 252

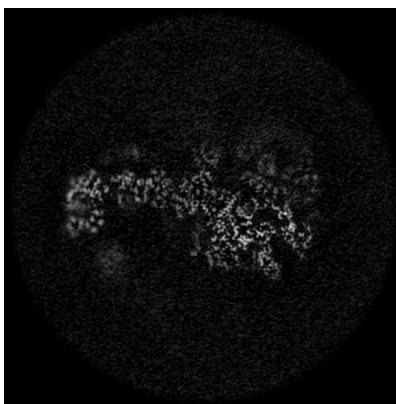
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

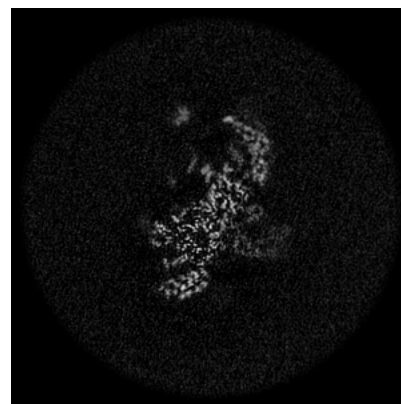
6.3.1 Primary map



X Index: 227



Y Index: 216

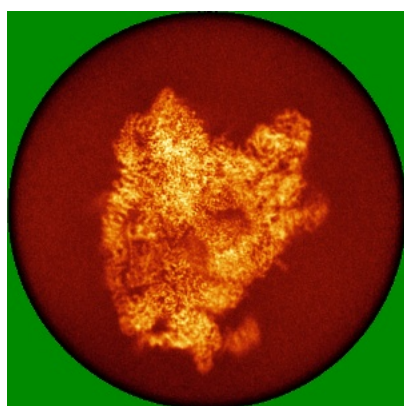


Z Index: 317

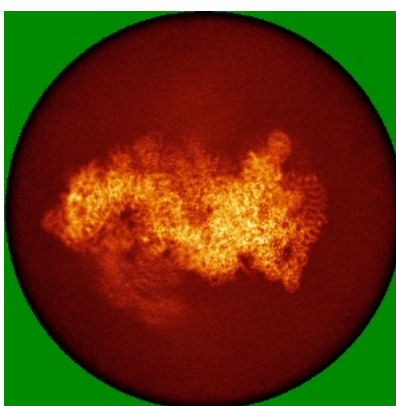
The images above show the largest variance slices of the map in three orthogonal directions.

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

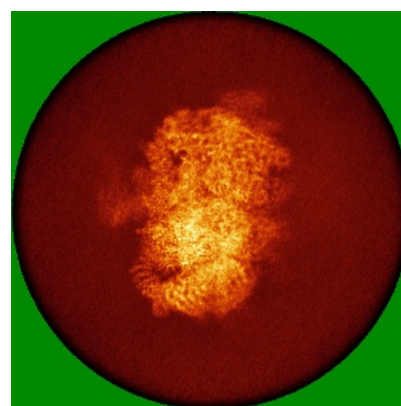
6.4.1 Primary map



X



Y

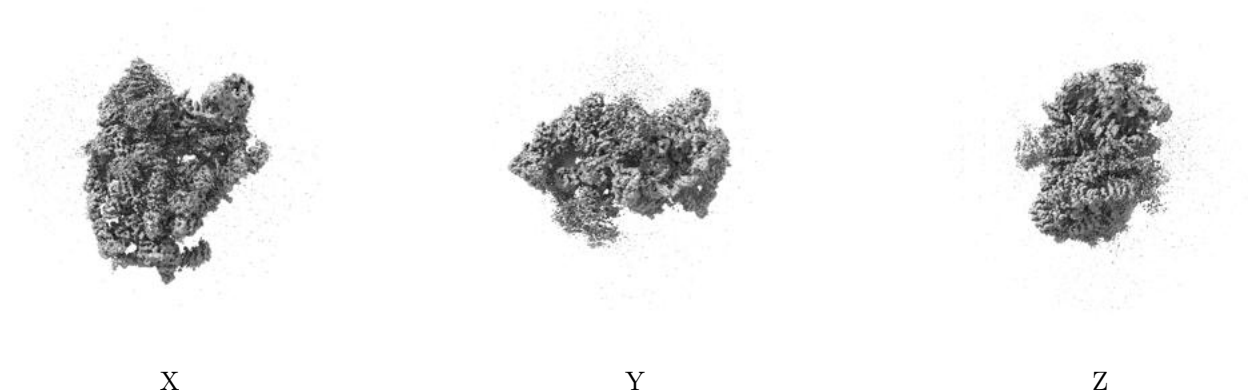


Z

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 0.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

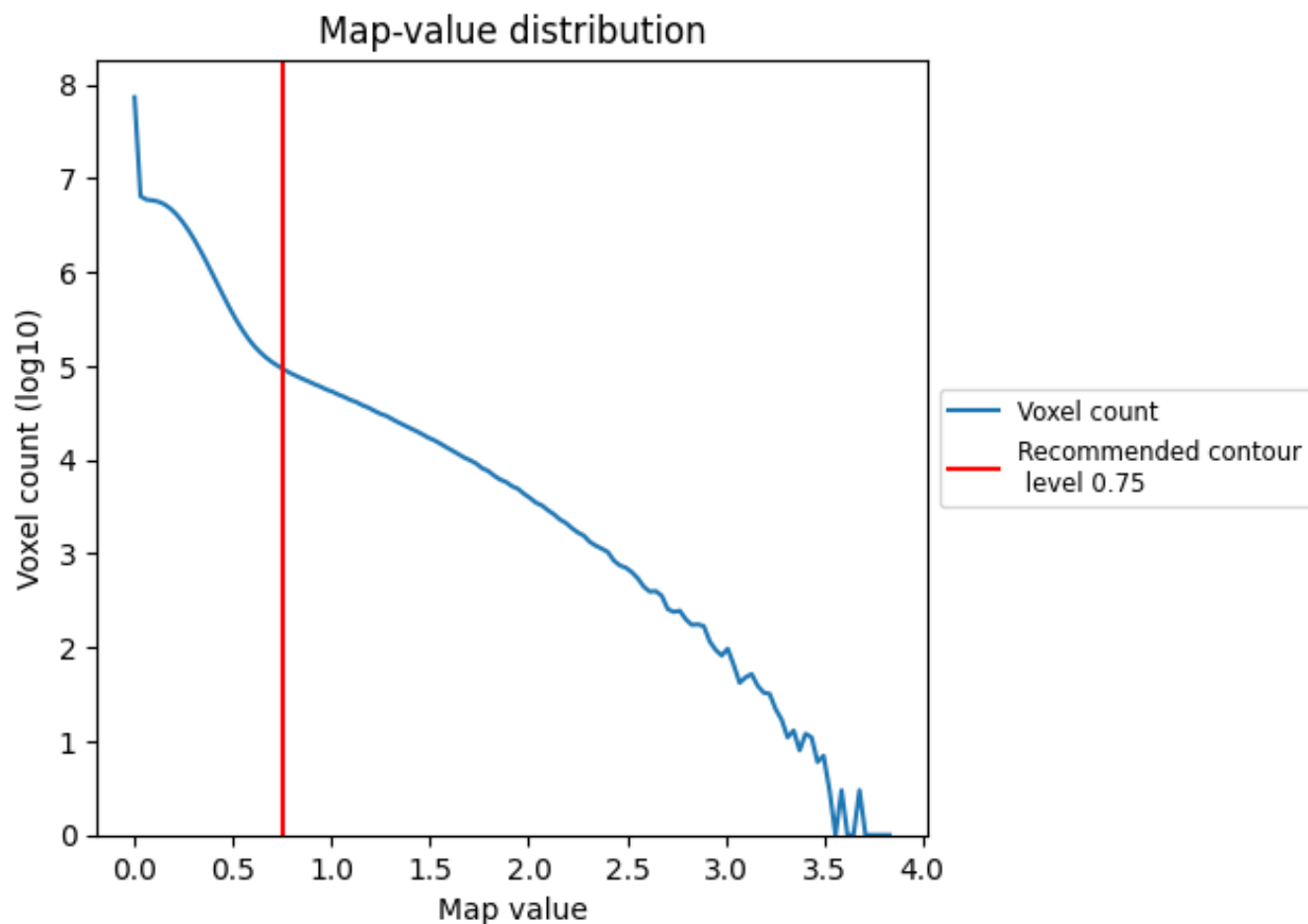
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

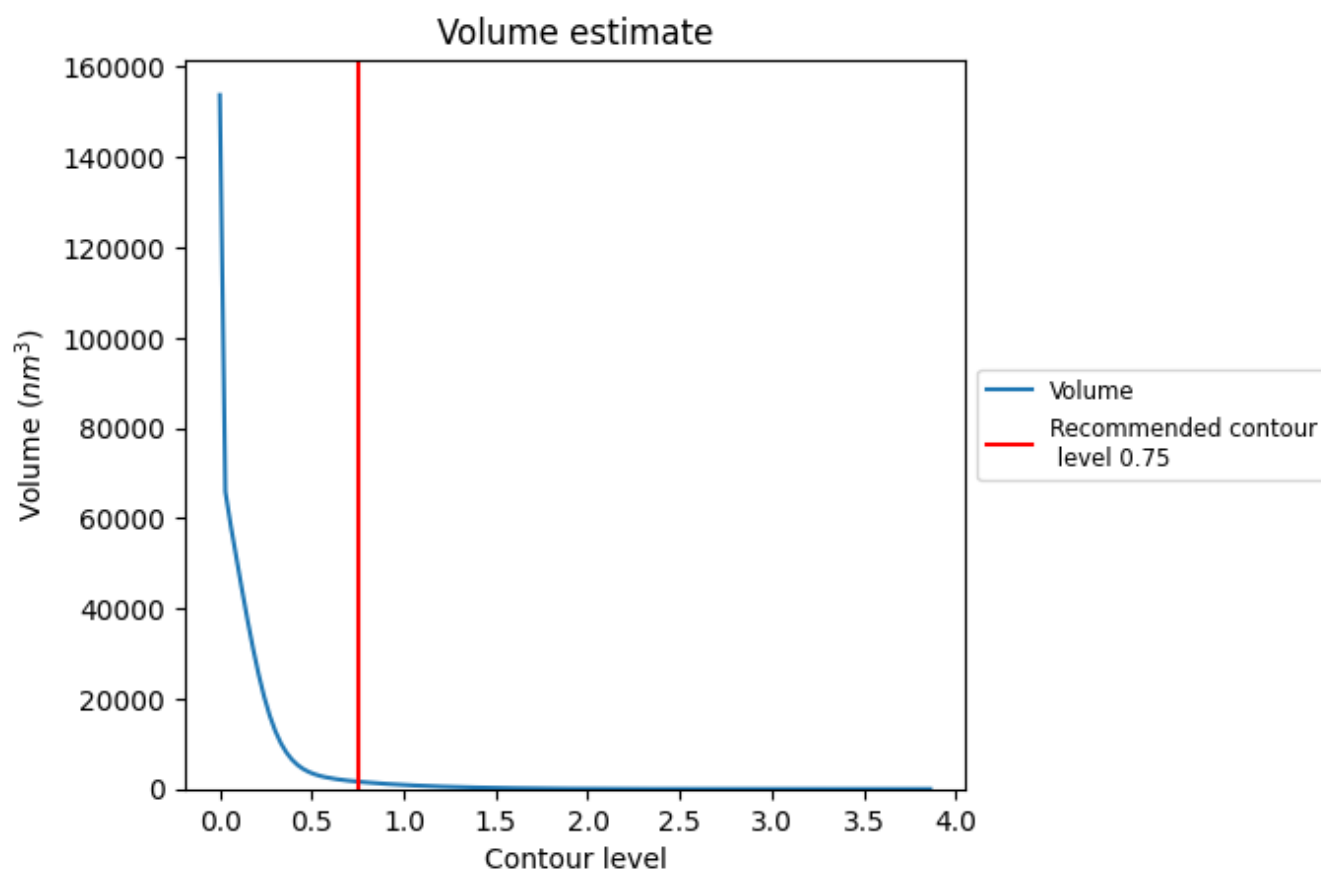
This section contains the results of statistical analysis of the map.

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.

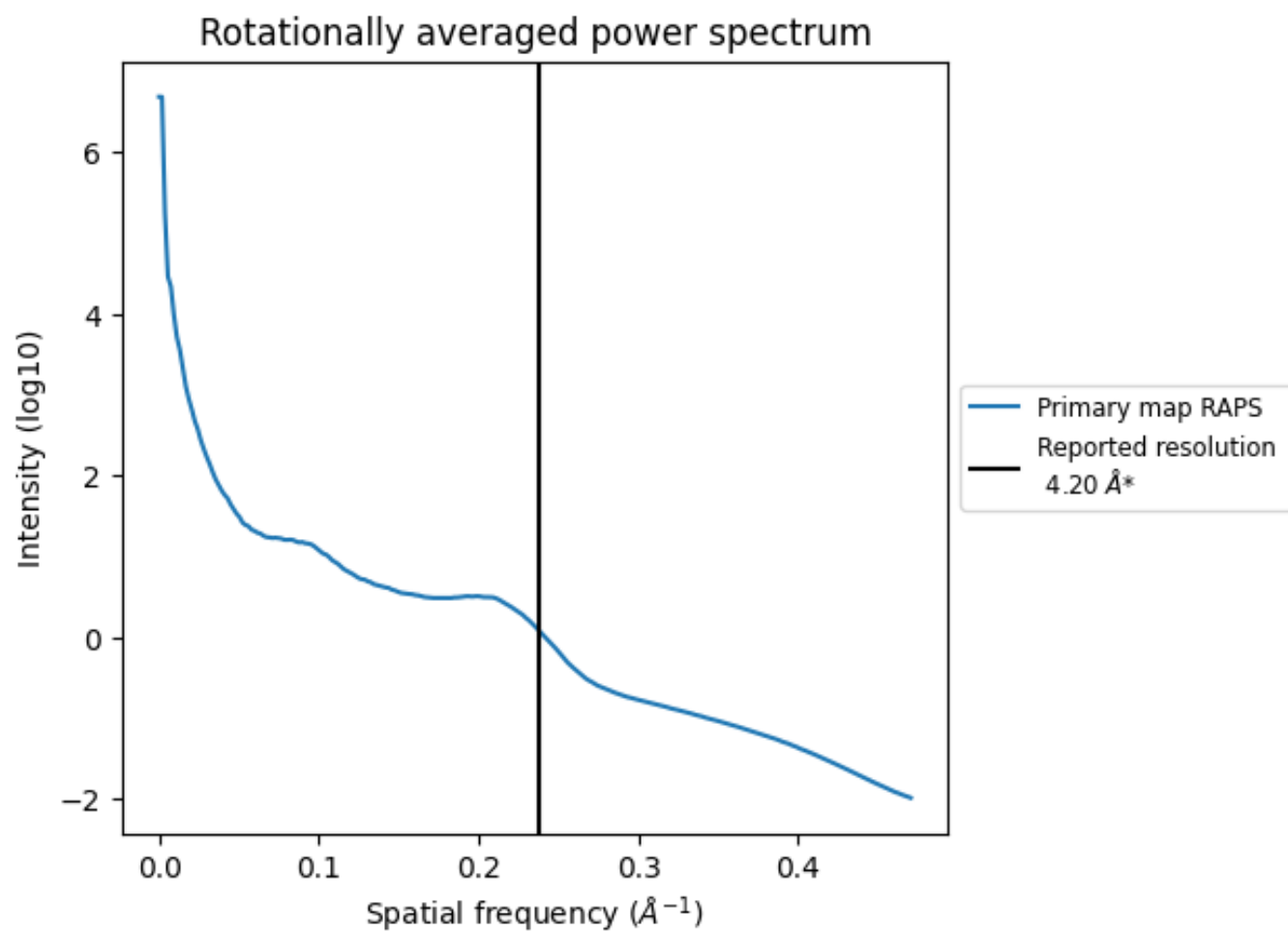
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1623 nm^3 ; this corresponds to an approximate mass of 1466 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 0.238 Å⁻¹

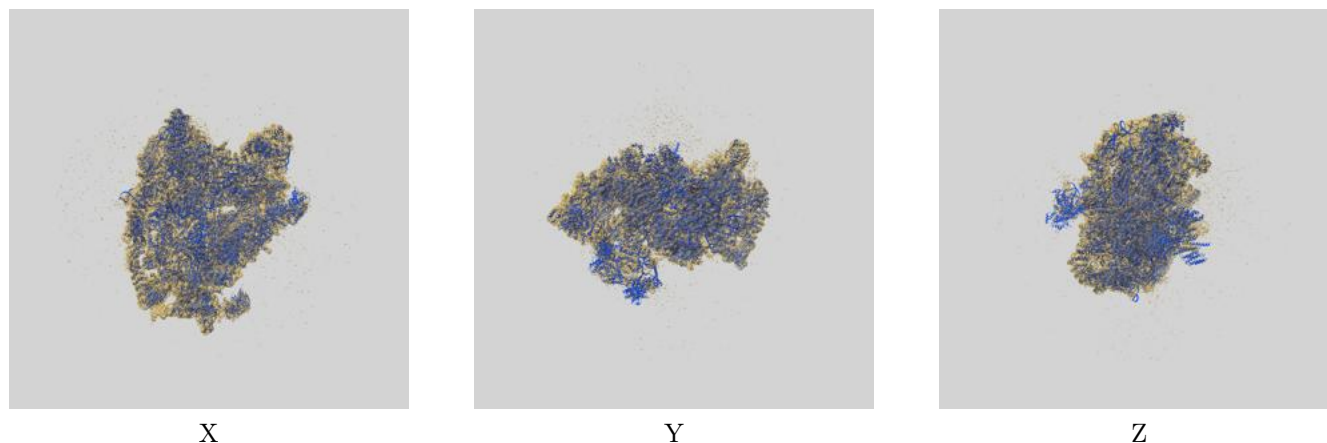
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

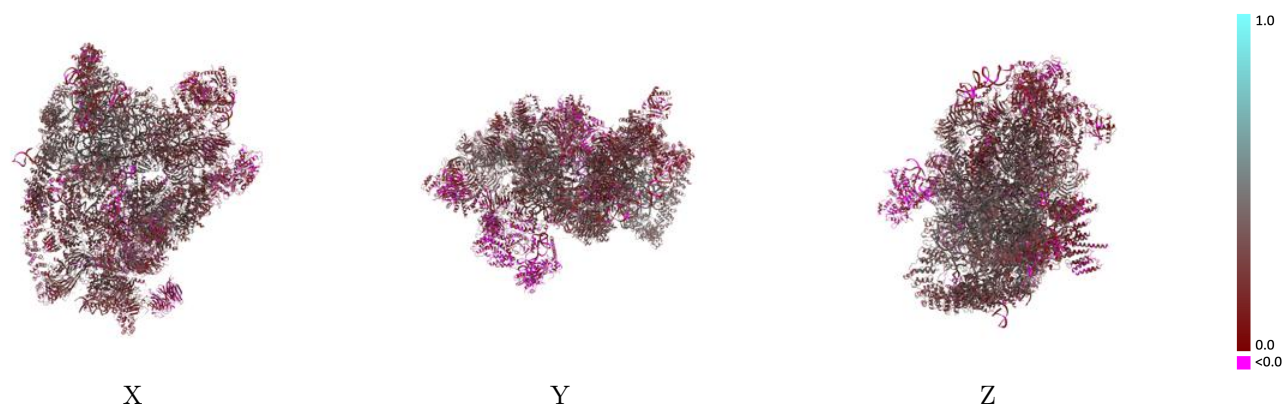
This section contains information regarding the fit between EMDB map EMD-49086 and PDB model 9N76. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



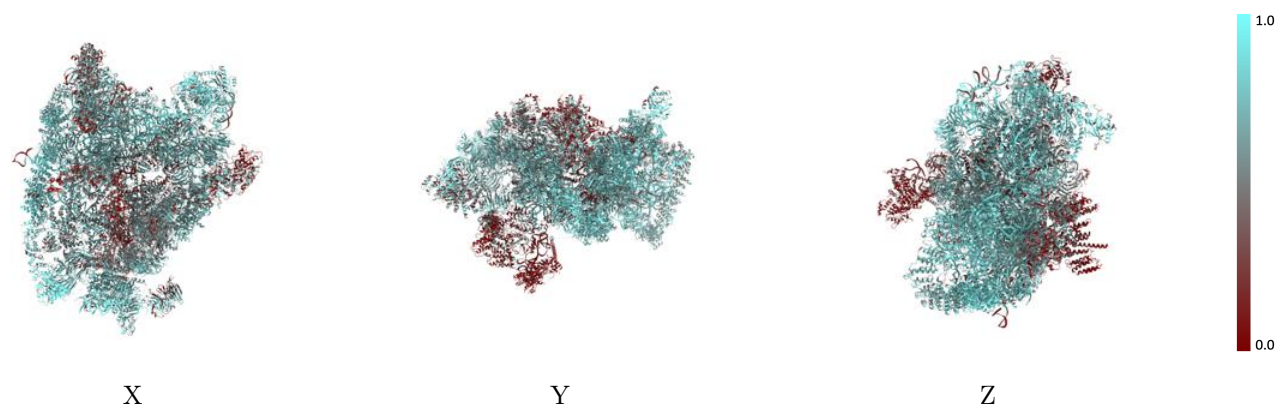
The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



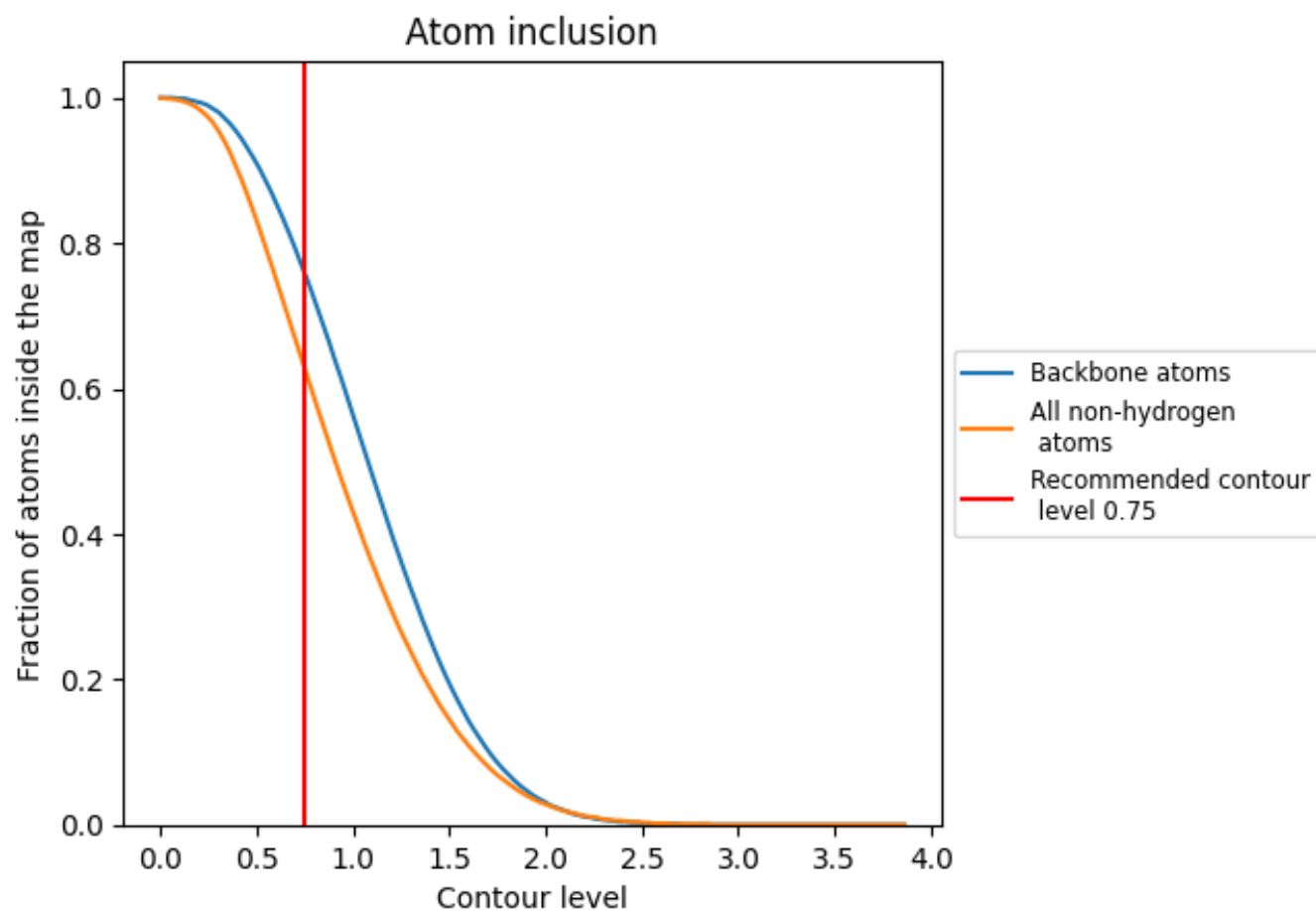
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.75).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 63% 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 (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6260	 0.2730
L0	 0.7610	 0.2410
L1	 0.7540	 0.2990
L2	 0.7320	 0.2630
L3	 0.1260	 0.1370
L4	 0.7400	 0.4150
L5	 0.6590	 0.2880
L6	 0.7440	 0.3900
L7	 0.4150	 0.1970
L8	 0.7670	 0.4040
L9	 0.7460	 0.4050
LC	 0.6470	 0.3570
LD	 0.7550	 0.4030
LE	 0.6750	 0.3930
LF	 0.7530	 0.3680
LG	 0.6660	 0.3920
LH	 0.7000	 0.2670
LI	 0.5720	 0.1340
LJ	 0.6390	 0.1870
LK	 0.6340	 0.1670
LL	 0.6380	 0.2270
LM	 0.6610	 0.2400
LN	 0.7540	 0.3010
LO	 0.6010	 0.3320
LP	 0.1570	 0.1780
LQ	 0.7580	 0.2910
LR	 0.7060	 0.2360
LS	 0.5870	 0.2800
LT	 0.5580	 0.2910
LZ	 0.5220	 0.2850
NA	 0.5620	 0.2810
NB	 0.5220	 0.2560
ND	 0.5120	 0.2250
NF	 0.6470	 0.3350
NG	 0.6950	 0.2930



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Chain	Atom inclusion	Q-score
NH	 0.7350	 0.2010
NI	 0.6540	 0.1920
NL	 0.4630	 0.2150
NM	 0.5590	 0.2620
NP	 0.1180	 0.2200
NQ	 0.6290	 0.3320
NS	 0.3680	 0.1770
NV	 0.3500	 0.2930
OH	 0.0100	 -0.0030
OU	 0.0070	 0.0040
SA	 0.5870	 0.2830
SB	 0.5540	 0.2600
SC	 0.6650	 0.3790
SD	 0.5380	 0.2640
SE	 0.7010	 0.2880
SF	 0.7000	 0.3920
SG	 0.7210	 0.3690
SH	 0.7270	 0.3700
SI	 0.7240	 0.3880
SJ	 0.2800	 0.1200
SK	 0.4200	 0.1460
SL	 0.6850	 0.4040
SM	 0.6270	 0.3610
SP	 0.5730	 0.2910
SQ	 0.5760	 0.3640
SR	 0.7140	 0.4110
SS	 0.3750	 0.2110
ST	 0.2210	 0.1300
SU	 0.2030	 0.0830
SV	 0.7920	 0.2830
SW	 0.6420	 0.2580
SY	 0.5530	 0.2880
SZ	 0.0560	 0.0190