



Full wwPDB EM Validation Report ⓘ

Nov 3, 2025 – 04:46 PM EST

PDB ID : 9N75 / pdb_00009n75
EMDB ID : EMD-49085
Title : SSU processome maturation and disassembly, State I
Authors : Buzovetsky, O.; Klinge, S.
Deposited on : 2025-02-05
Resolution : 3.01 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

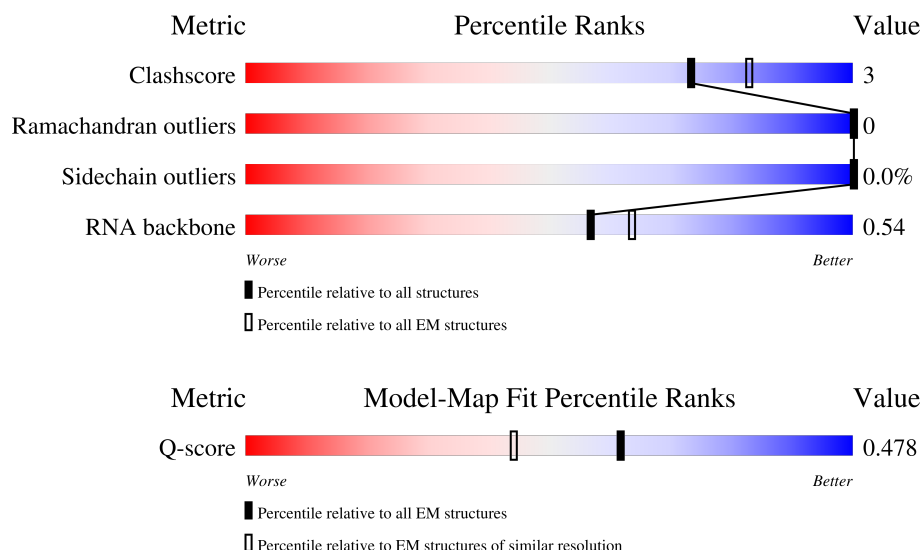
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.01 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	13882 (2.51 - 3.51)

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	1802	
3	L2	334	

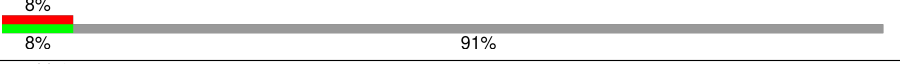

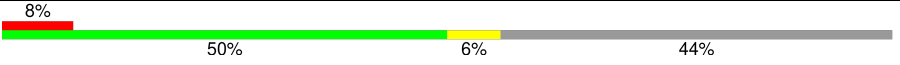
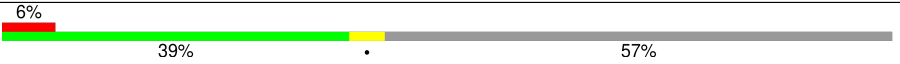
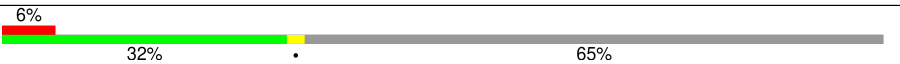
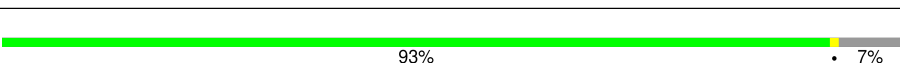
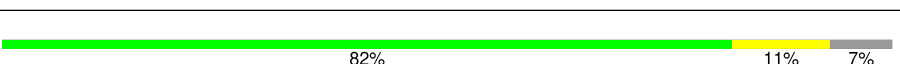
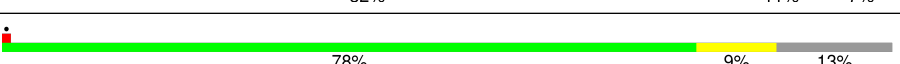
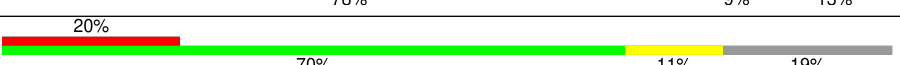
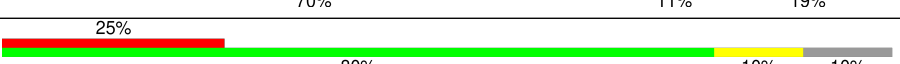
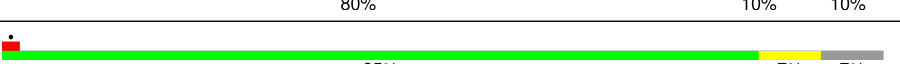
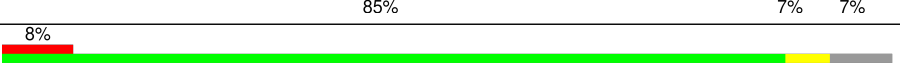

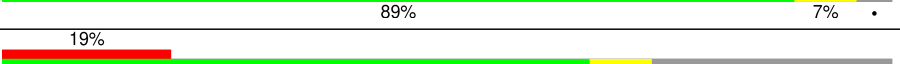

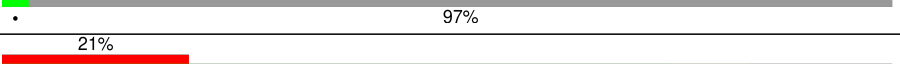



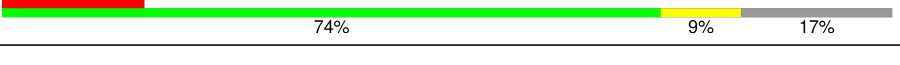
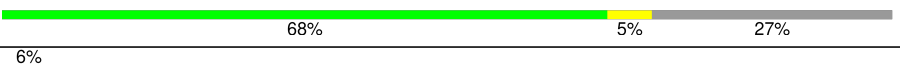

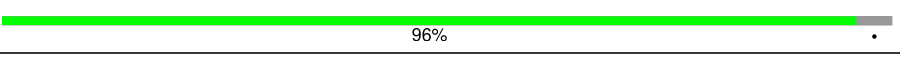
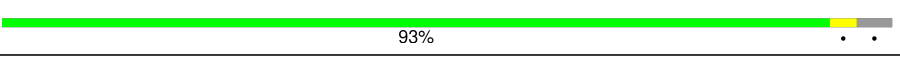

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Mol	Chain	Length	Quality of chain
4	L3	146	
5	L4	261	
6	L5	225	
7	L6	236	
8	L7	190	
9	L8	200	
10	L9	197	
11	LC	143	
12	LD	156	
13	LE	130	
14	LF	135	
15	LG	67	
16	LH	896	
17	LI	713	
18	LJ	513	
19	LK	575	
20	LL	643	
21	LM	1769	
22	LN	776	
23	LO	923	
24	LP	440	
25	LQ	943	
26	LR	817	
27	LS	594	
28	LT	939	



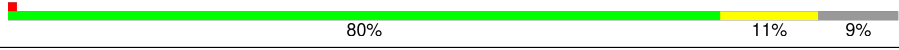



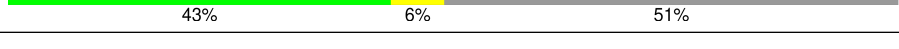
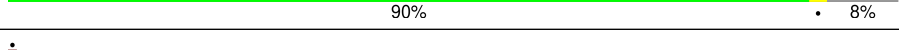
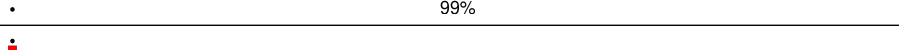
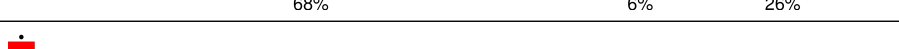




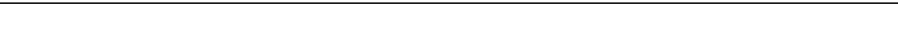
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Mol	Chain	Length	Quality of chain
29	LW	554	
30	LZ	183	
31	NA	593	
32	NB	610	
33	ND	214	
34	NF	151	
35	NG	137	
36	NH	1237	
37	NI	297	
38	NL	318	
39	NM	255	
40	NP	144	
41	NQ	82	
42	NS	1267	
43	NV	733	
44	OH	143	
45	OU	152	
46	SA	504	
47	SB	511	
48	SC	327	
48	SD	327	
49	SE	126	
49	SF	126	
50	SG	573	
51	SH	367	

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Mol	Chain	Length	Quality of chain
52	SI	1183	
53	SJ	252	
53	SK	252	
54	SL	189	
55	SM	290	
56	SP	2493	
57	SQ	217	
58	SR	145	
59	SS	899	
60	ST	810	
61	SU	552	
62	SV	206	
63	SW	274	
64	SY	250	
65	SZ	483	

2 Entry composition [i](#)

There are 70 unique types of molecules in this entry. The entry contains 220521 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	1443	Total	C	N	O	P	0	0
			30807	13782	5497	10085	1443		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L1	1773	4AC	C	conflict	GB 831416138
L1	1801	A	-	insertion	GB 831416138
L1	1802	A	-	insertion	GB 831416138

- Molecule 3 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L2	202	Total	C	N	O	P	0	0
			4288	1916	740	1429	203		

- 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	S	0	0
			1046	662	204	180			

- 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	0	0
			490	302	98	89	1		

- 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	0	0
			6449	4113	1087	1230	19		

- 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	0	0
			3792	2375	679	733	5		

- 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	0	0
			3773	2376	675	711	11		

- 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	0	0
			1068	681	185	199	3		

- 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	0	0
			3871	2458	662	738	13		

- 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
			12777	8259	2090	2391	37		

- 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	S	0	0
			3214	2078	544	576	16		

- 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
			6875	4359	1189	1304	23			

- Molecule 29 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	LW	48	Total	C	N	O	0	0
			411	253	85	73		

- Molecule 30 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

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

- Molecule 31 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	NA	330	Total	C	N	O	S	0	0
			2635	1644	455	531	5		

- Molecule 32 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	NB	262	Total	C	N	O	S	0	0
			2147	1352	375	413	7		

- Molecule 33 is a protein called Bud site selection protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	ND	74	Total	C	N	O	0	0
			609	380	119	110		

- Molecule 34 is a protein called 40S ribosomal protein S13.

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

- Molecule 35 is a protein called 40S ribosomal protein S14-A.

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

- Molecule 36 is a protein called U3 small nucleolar RNA-associated protein 22.

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

- Molecule 37 is a protein called Ribosomal RNA-processing protein 7.

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

- Molecule 38 is a protein called Dimethyladenosine transferase.

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

- Molecule 39 is a protein called Small ribosomal subunit protein eS1A.

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

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

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

- Molecule 41 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 42 is a protein called Probable ATP-dependent RNA helicase DHR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	NS	931	Total	C	N	O	S	0	0
			7483	4764	1313	1369	37		

- Molecule 43 is a protein called Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	NV	23	Total	C	N	O	0	0
			181	115	38	28		

- Molecule 44 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	OH	120	Total	C	N	O	S	0	0
			902	569	159	172	2		

- Molecule 45 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	OU	56	Total	C	N	O	S	0	0
			436	275	80	77	4		

- Molecule 46 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SA	397	Total	C	N	O	S	1	0
			3141	1992	537	602	10		

- Molecule 47 is a protein called Nucleolar protein 58.

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

- Molecule 48 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

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

- Molecule 49 is a protein called 13 kDa ribonucleoprotein-associated protein.

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

- Molecule 50 is a protein called Ribosomal RNA-processing protein 9.

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

- Molecule 51 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

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

- Molecule 52 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SI	760	Total	C	N	O	S	0	0
			6158	3954	1099	1078	27		

- Molecule 53 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SJ	213	Total	C	N	O	S	0	0
			1678	1069	292	306	11		
53	SK	229	Total	C	N	O	S	0	0
			1793	1141	312	329	11		

- Molecule 54 is a protein called rRNA-processing protein FCF1.

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

- Molecule 55 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

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

- Molecule 56 is a protein called U3 small nucleolar RNA-associated protein 20.

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

- Molecule 57 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SQ	107	Total	C	N	O	S	0	0
			909	572	166	168	3		

- Molecule 58 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 59 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	SS	13	Total	C	N	O	0	0
			109	75	17	17		

- Molecule 60 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	ST	597	Total	C	N	O	S	0	0
			4893	3108	857	911	17		

- Molecule 61 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SU	532	Total	C	N	O	S	0	0
			4357	2837	706	800	14		

- Molecule 62 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SV	155	Total	C	N	O	S	0	0
			1296	806	257	232	1		

- Molecule 63 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SW	219	Total	C	N	O	S	0	0
			1725	1095	309	317	4		

- Molecule 64 is a protein called U3 small nucleolar RNA-associated protein 11.

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

- Molecule 65 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SZ	259	Total	C	N	O	S	0	0
			2113	1378	361	371	3		

- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
66	L1	54	Total	Mg	0
			54	54	
66	L9	1	Total	Mg	0
			1	1	
66	NH	1	Total	Mg	0
			1	1	
66	NP	1	Total	Mg	0
			1	1	
66	NS	1	Total	Mg	0
			1	1	
66	SI	1	Total	Mg	0
			1	1	

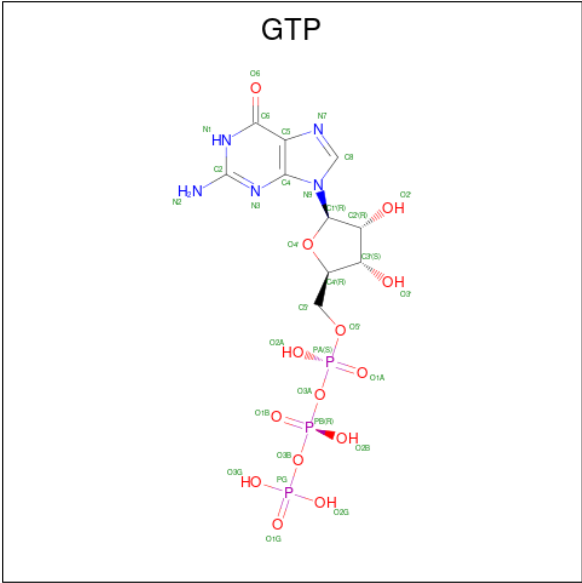
- # ATP





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

- Molecule 70 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

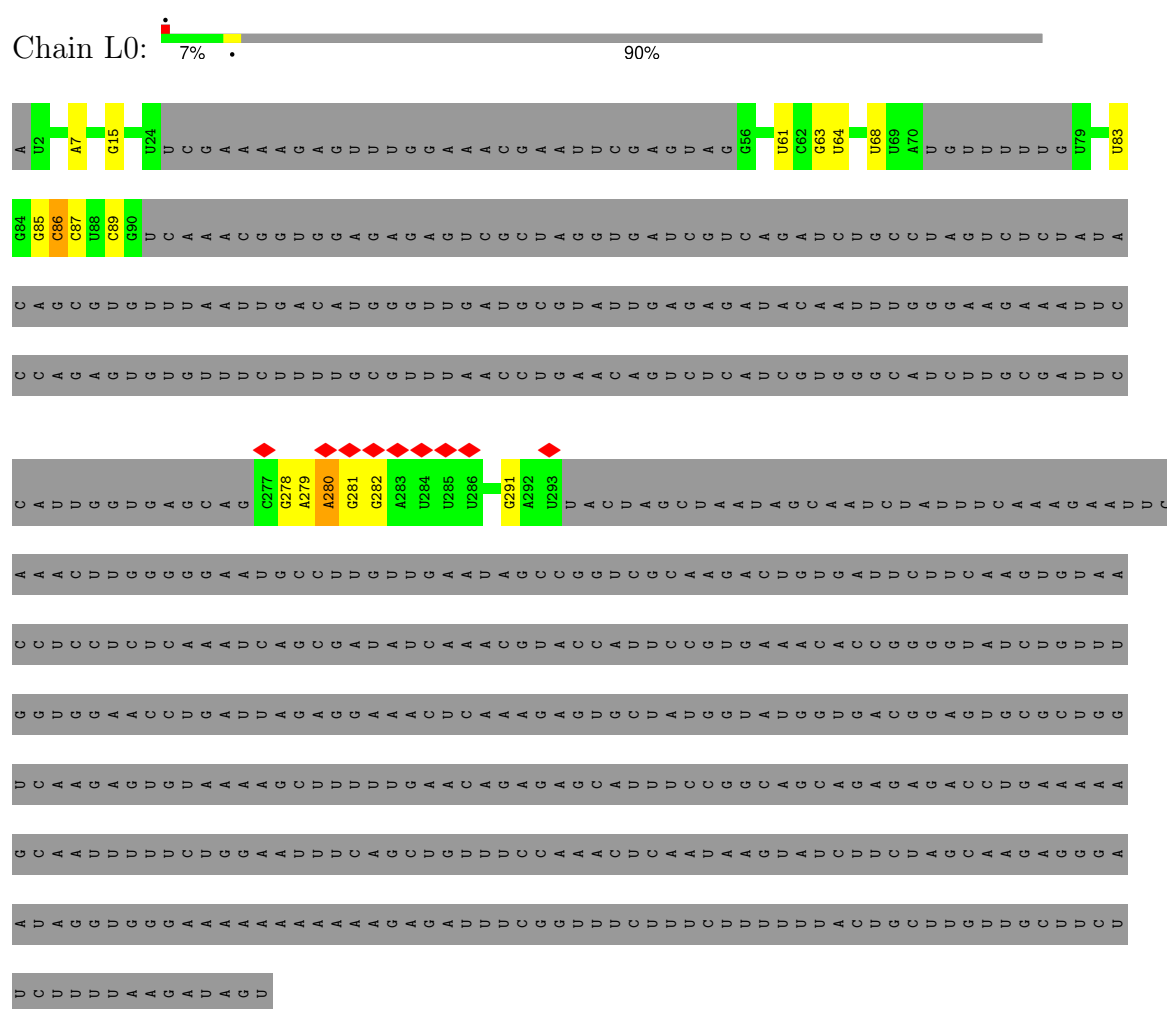


Mol	Chain	Residues	Atoms					AltConf
70	SI	1	Total	C	N	O	P	0
			32	10	5	14	3	

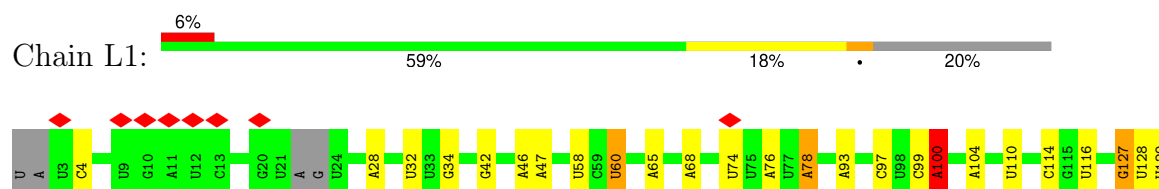
3 Residue-property plots [i](#)

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

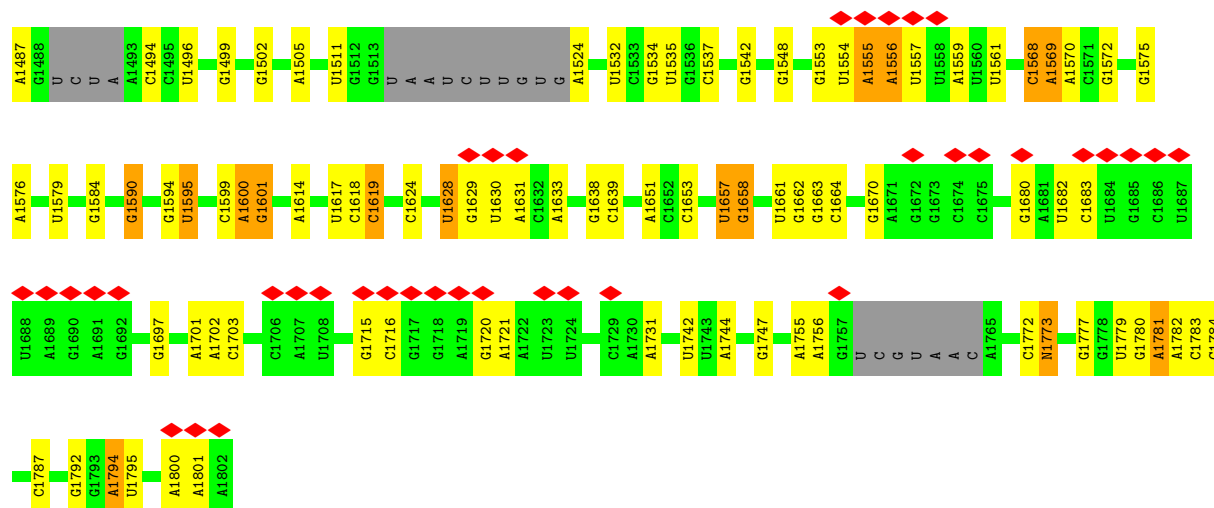
• Molecule 1: 5'ETS rRNA



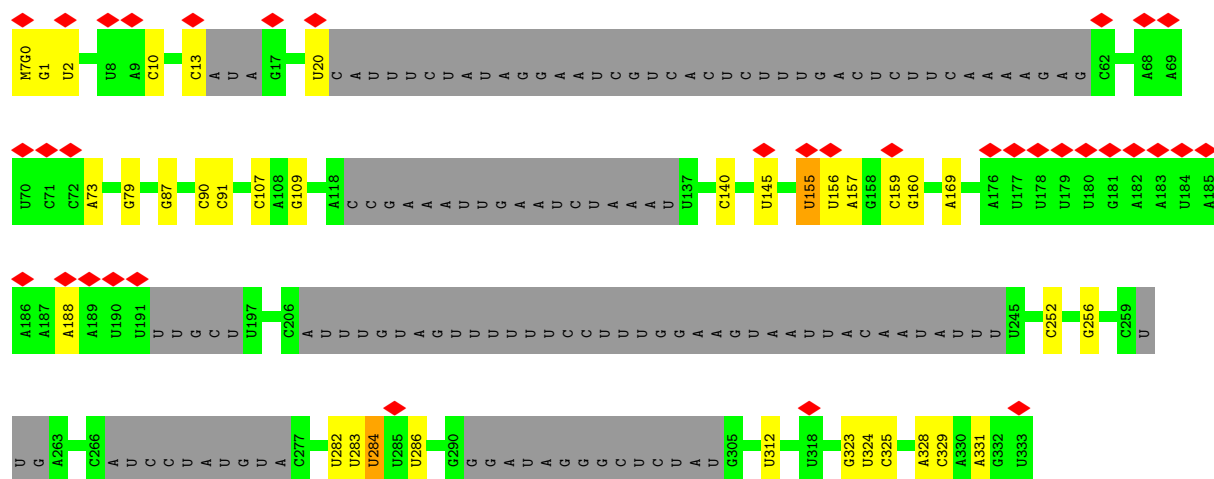
• Molecule 2: 18S rRNA



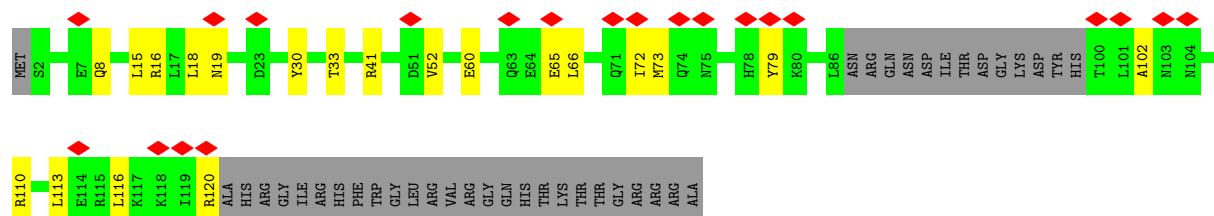




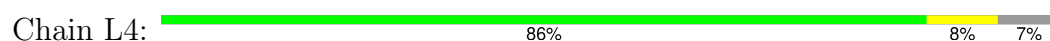
• Molecule 3: U3 snoRNA



• Molecule 4: 40S ribosomal protein S18-A



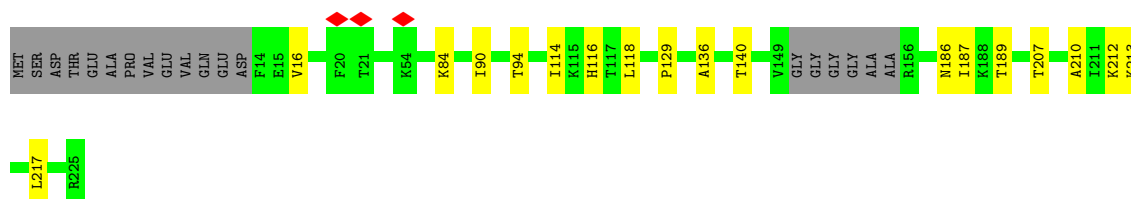
• Molecule 5: 40S ribosomal protein S4-A





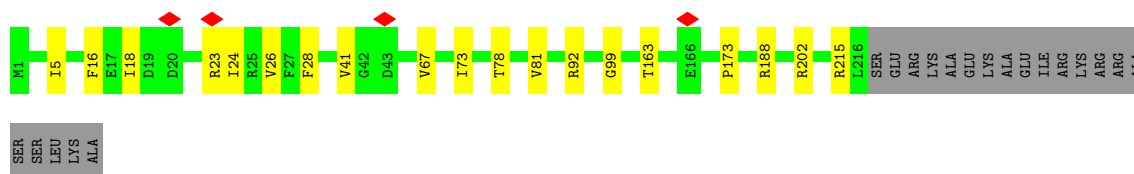
- Molecule 6: 40S ribosomal protein S5

Chain L5: 84% 8% 8%



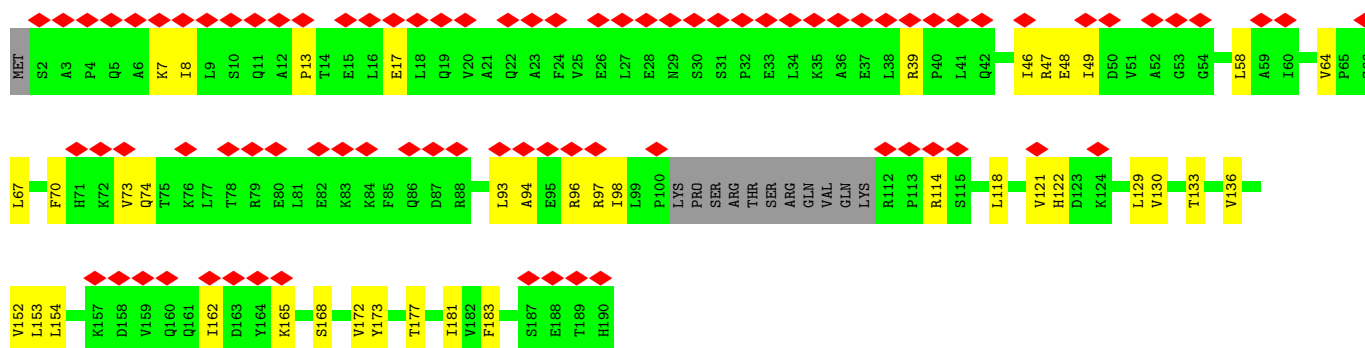
- Molecule 7: 40S ribosomal protein S6-A

Chain L6: 83% 8% 8%



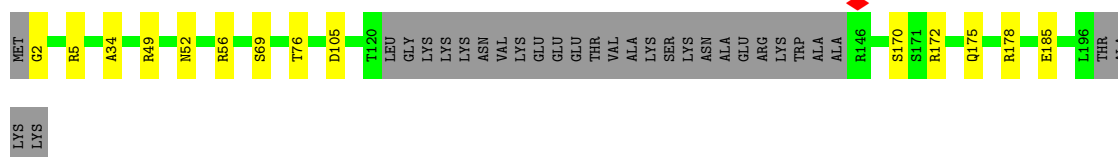
- Molecule 8: 40S ribosomal protein S7-A

Chain L7: 44% 73% 21% 6%

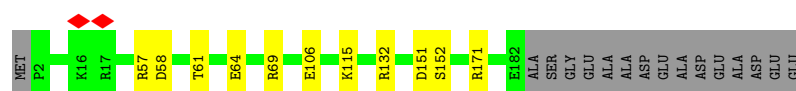
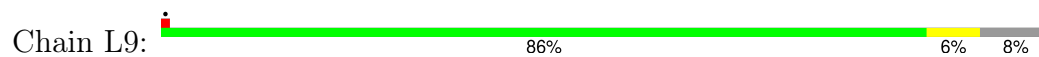


- Molecule 9: 40S ribosomal protein S8-A

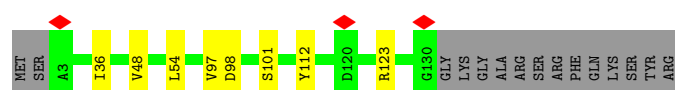
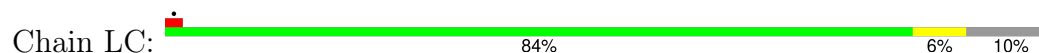
Chain L8: 78% 7% 15%



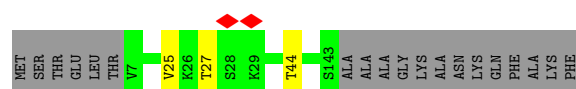
- Molecule 10: 40S ribosomal protein S9-A



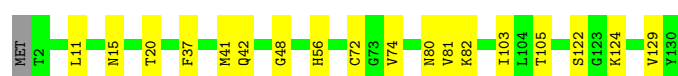
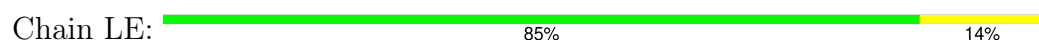
- Molecule 11: 40S ribosomal protein S16-A



- Molecule 12: 40S ribosomal protein S11-A



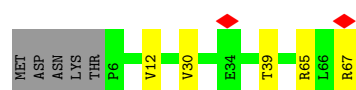
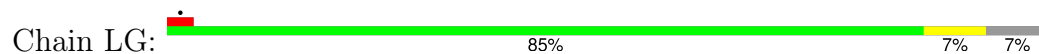
- Molecule 13: 40S ribosomal protein S22-A



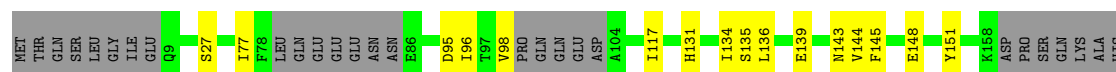
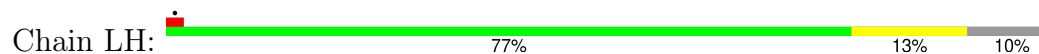
- Molecule 14: 40S ribosomal protein S24-A

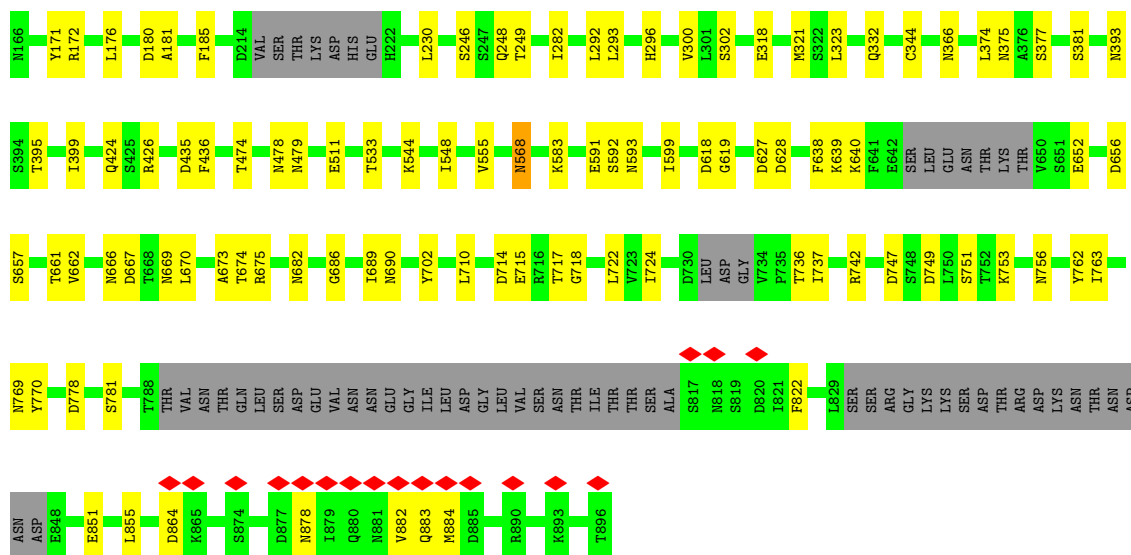


- Molecule 15: 40S ribosomal protein S28-A

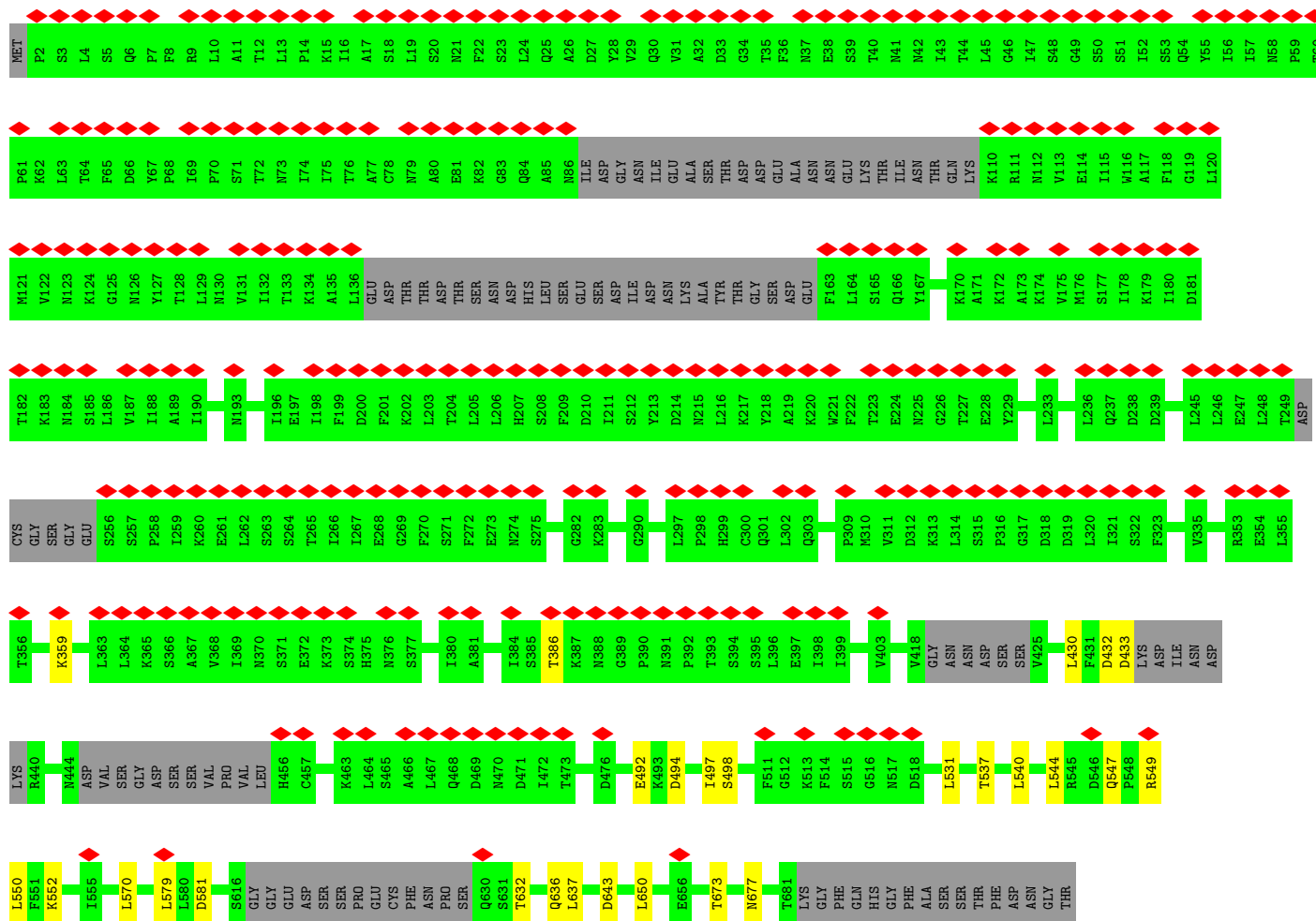
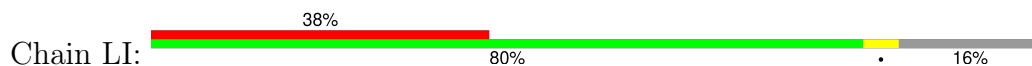


- Molecule 16: NET1-associated nuclear protein 1

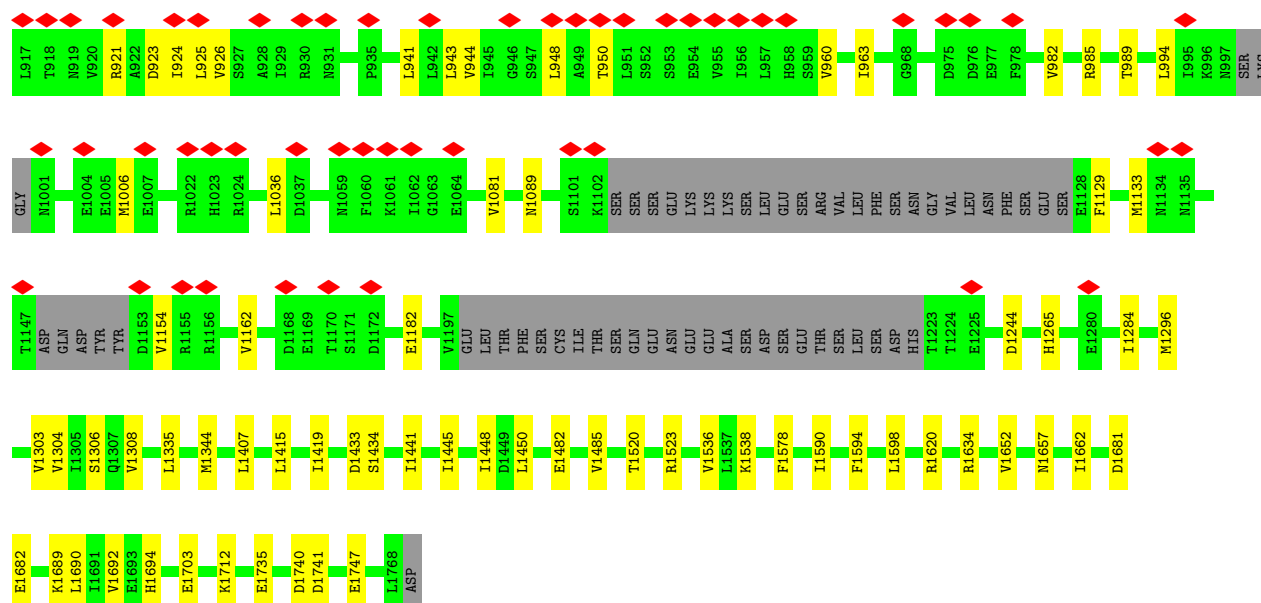




• Molecule 17: U3 small nucleolar RNA-associated protein 8

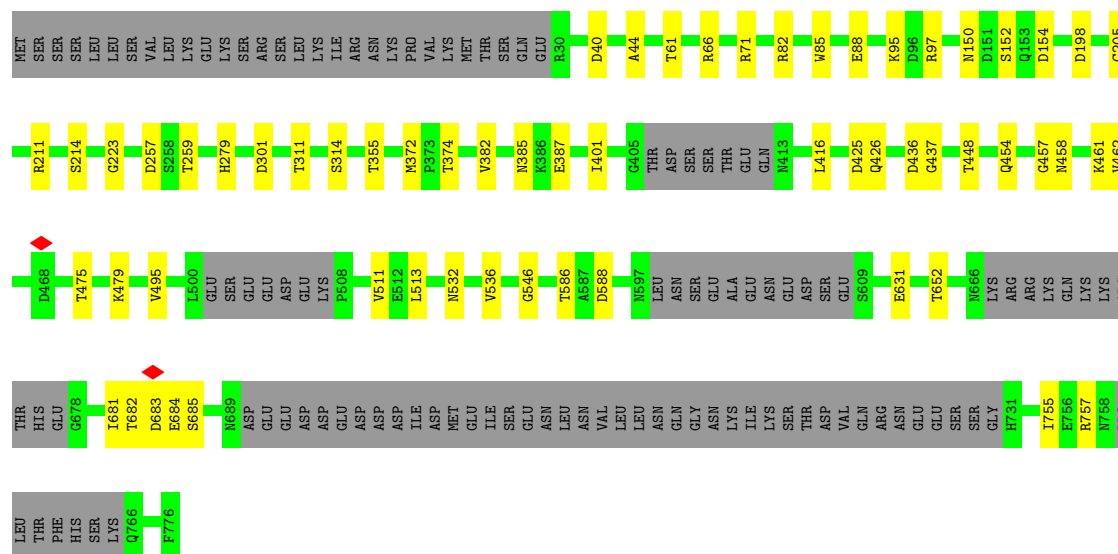






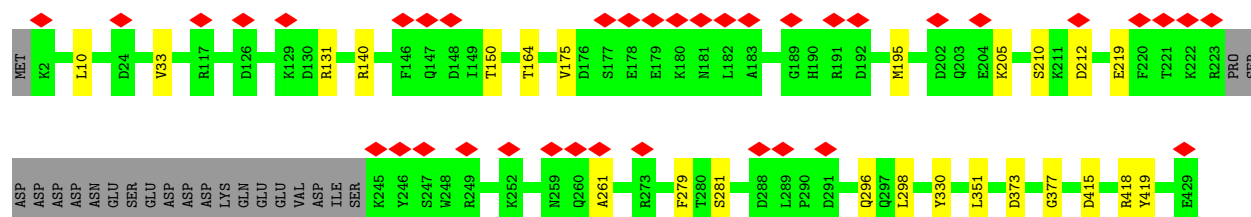
- Molecule 22: U3 small nucleolar RNA-associated protein 4

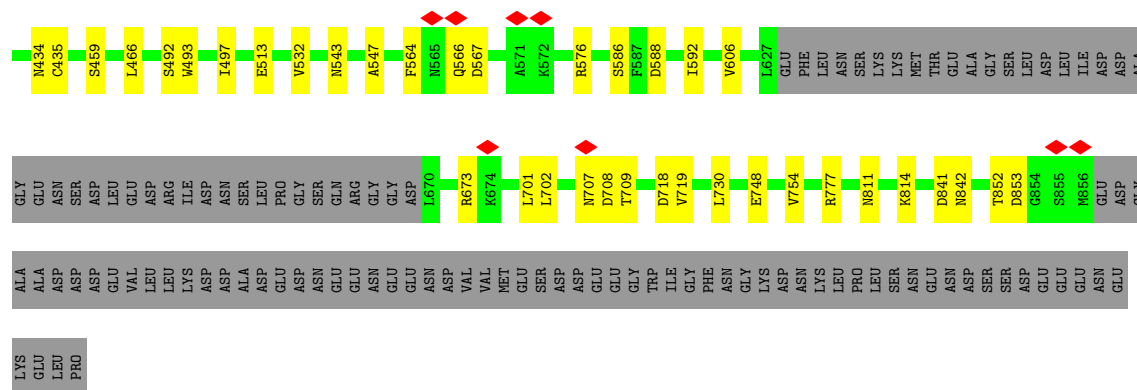
Chain LN: 78% 8% 15%



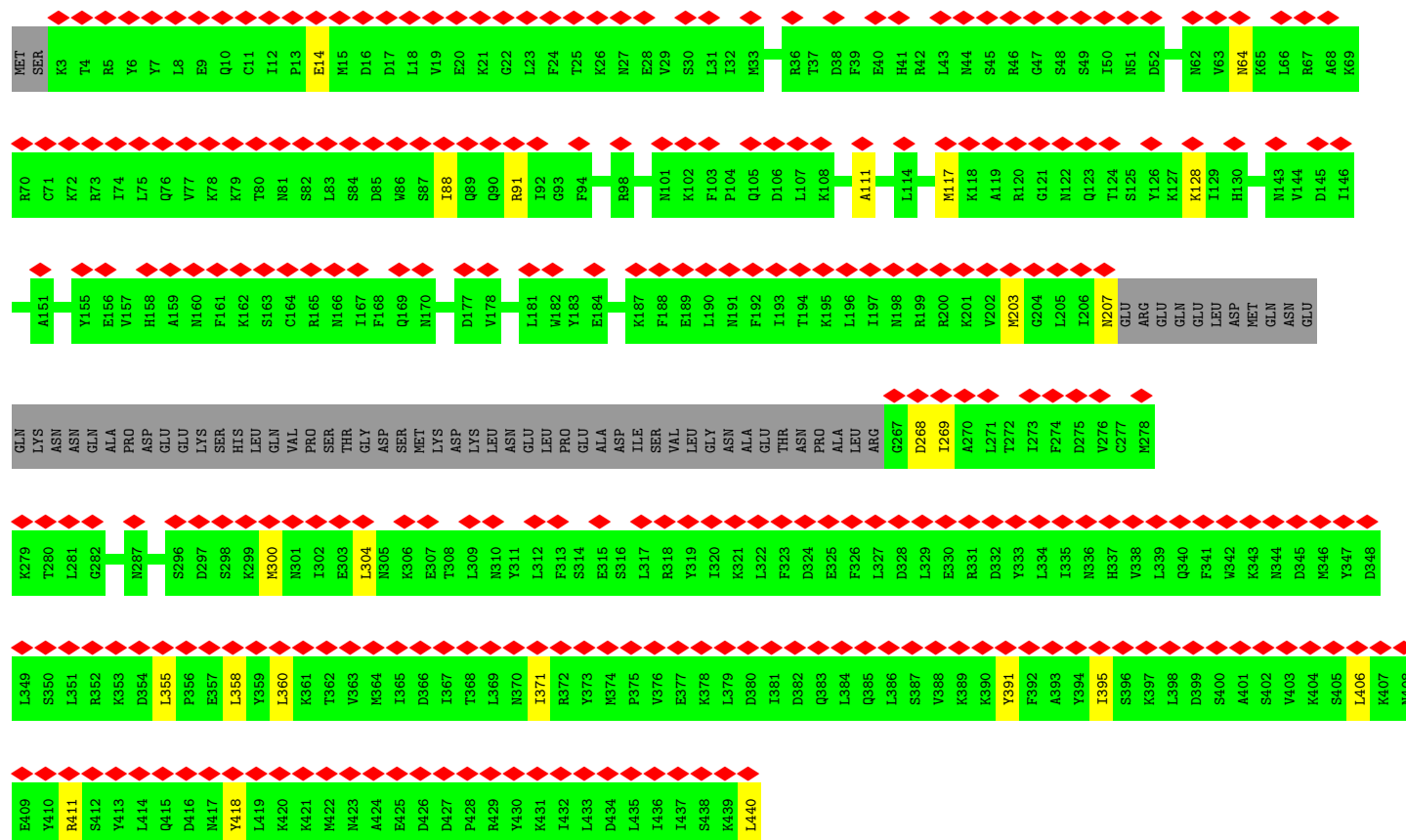
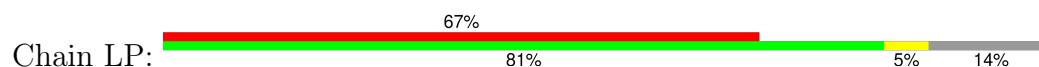
- Molecule 23: Periodic tryptophan protein 2

Chain LO: 5% 79% 7% 14%

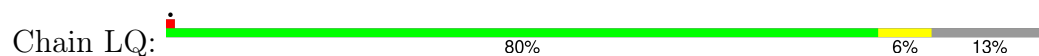


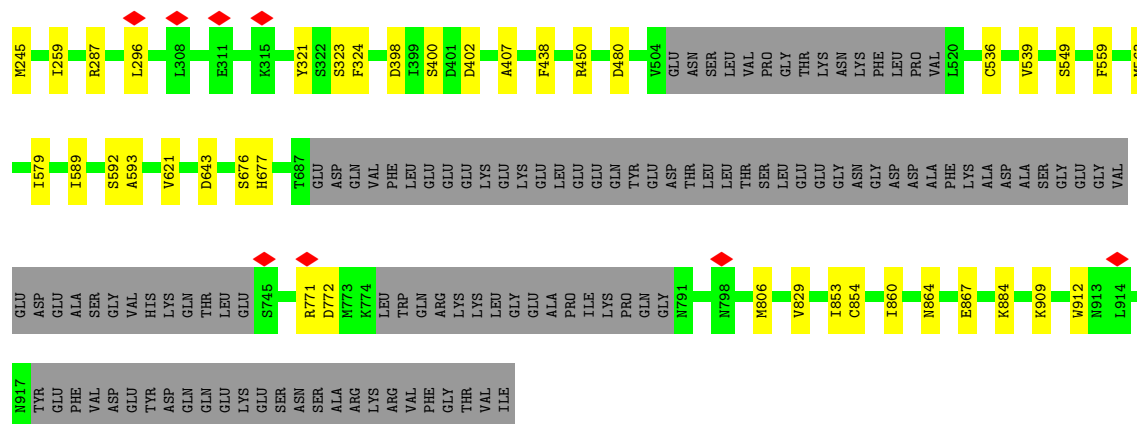


• Molecule 24: U3 small nucleolar RNA-associated protein 6

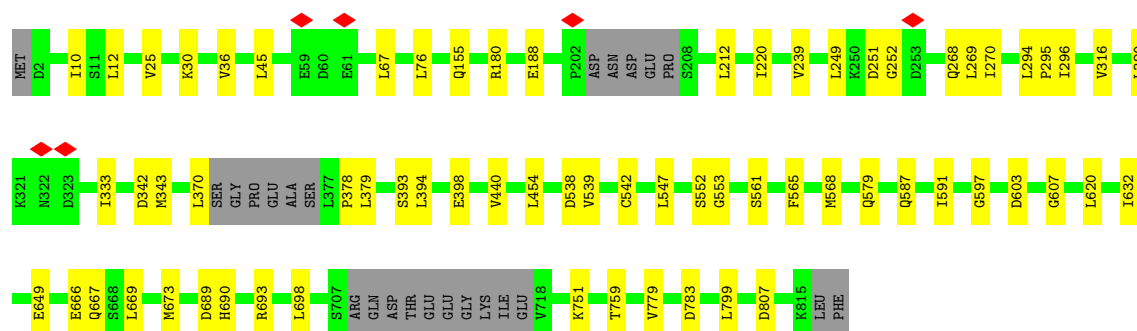
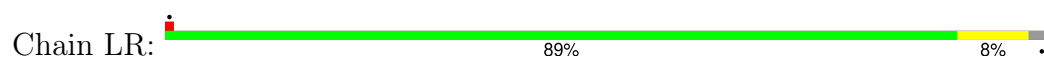


• Molecule 25: U3 small nucleolar RNA-associated protein 12

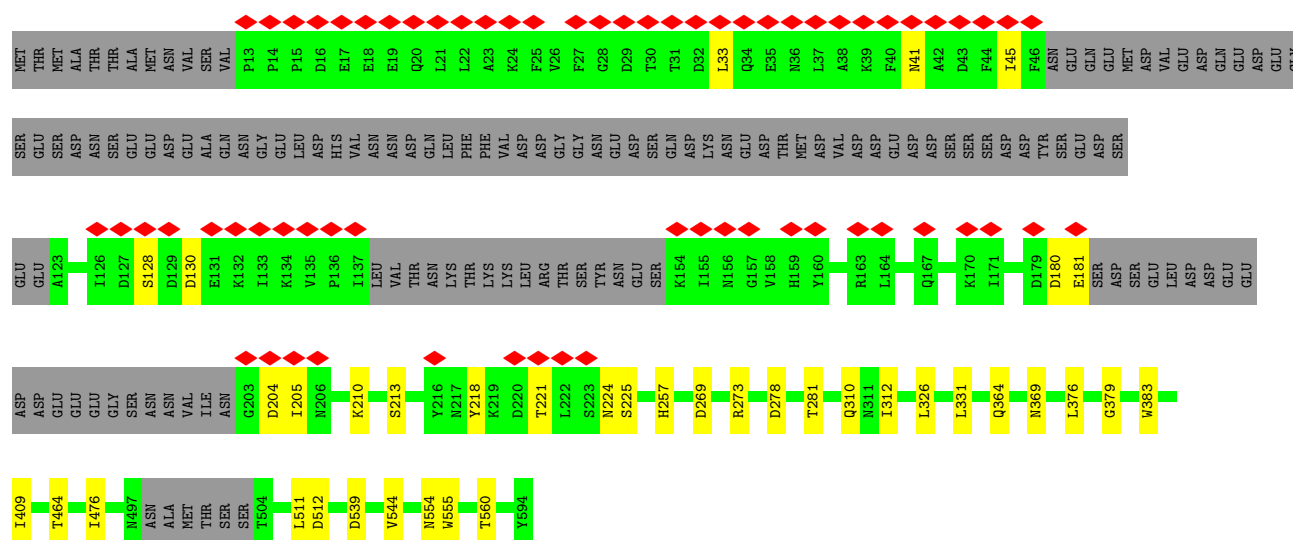




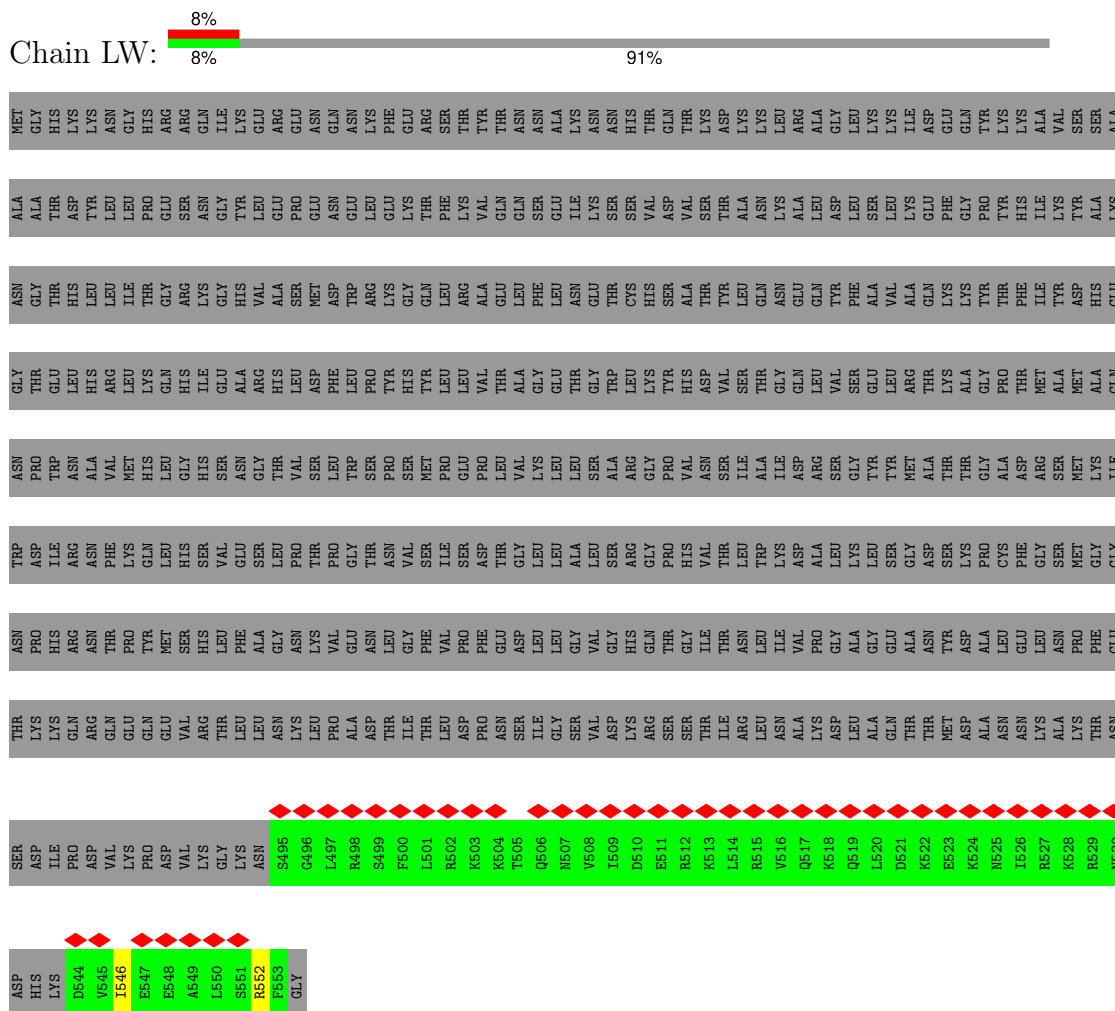
• Molecule 26: U3 small nucleolar RNA-associated protein 13



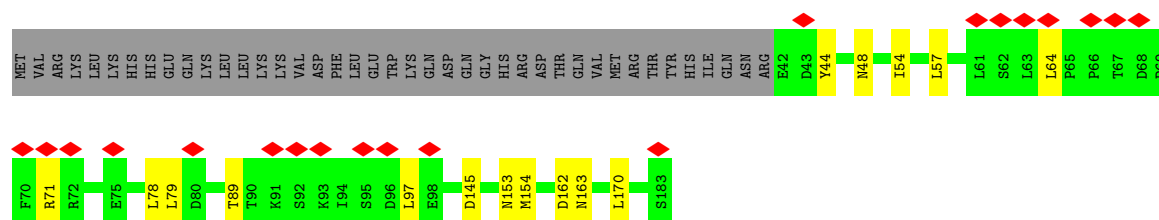
• Molecule 27: U3 small nucleolar RNA-associated protein 18



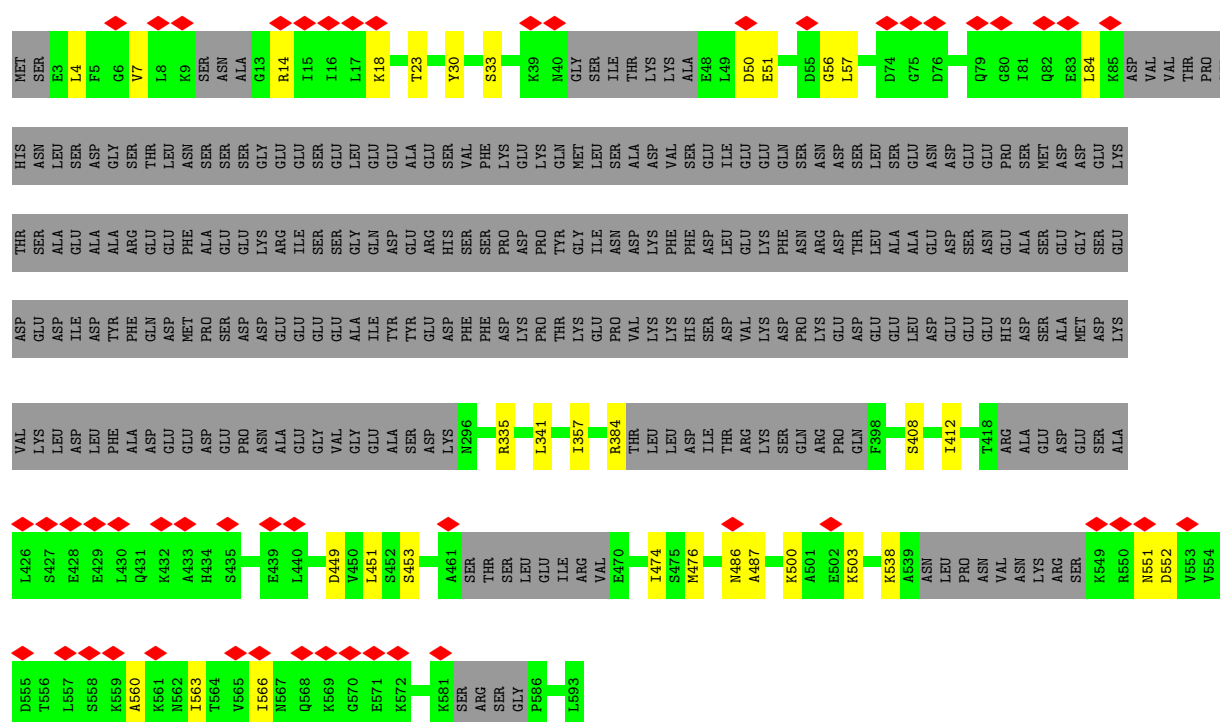
• Molecule 28: U3 small nucleolar RNA-associated protein 21



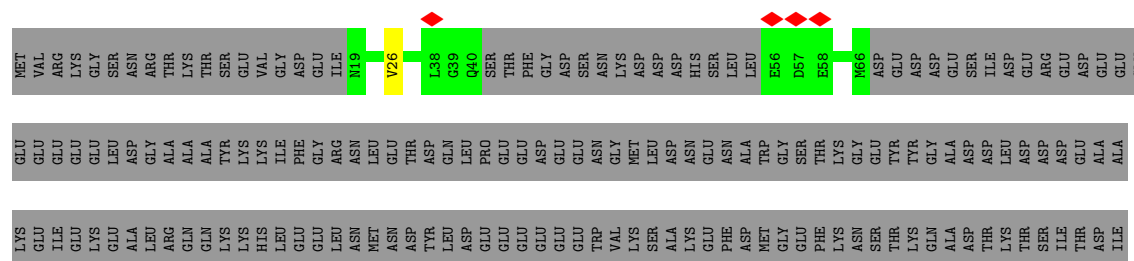
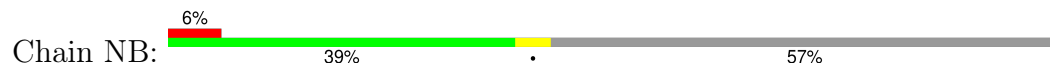
- Molecule 30: U3 small nucleolar ribonucleoprotein protein IMP3

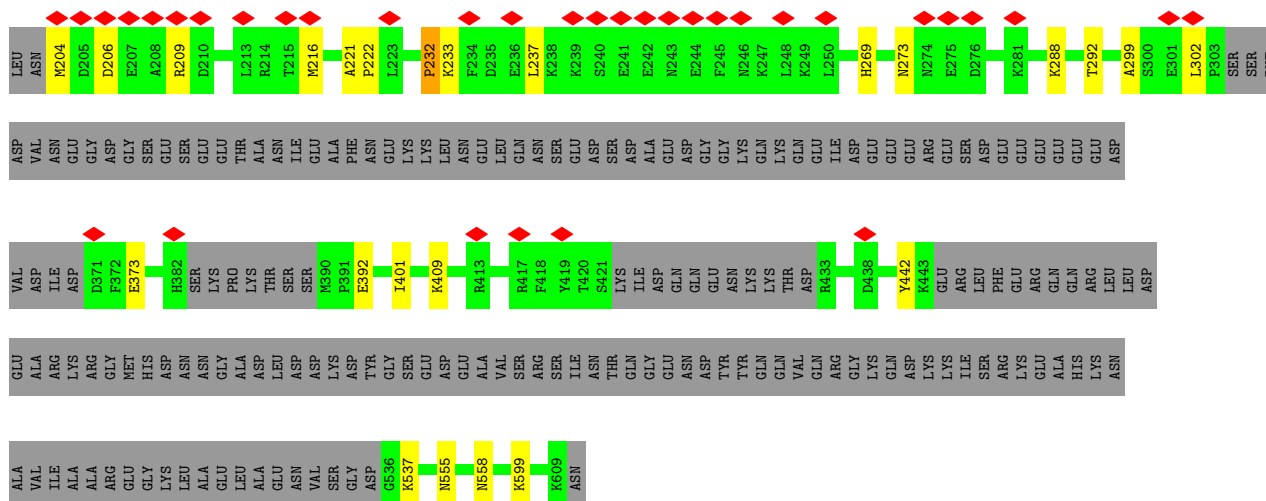


- Molecule 31: U3 small nucleolar RNA-associated protein MPP10

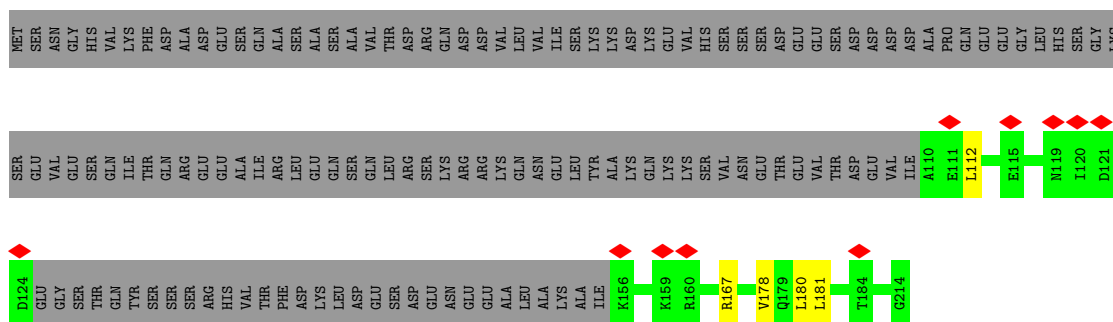


- Molecule 32: Something about silencing protein 10

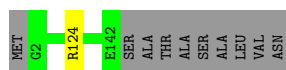




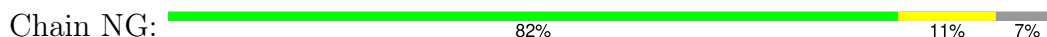
- Molecule 33: Bud site selection protein 21



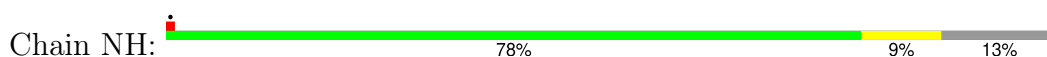
- Molecule 34: 40S ribosomal protein S13

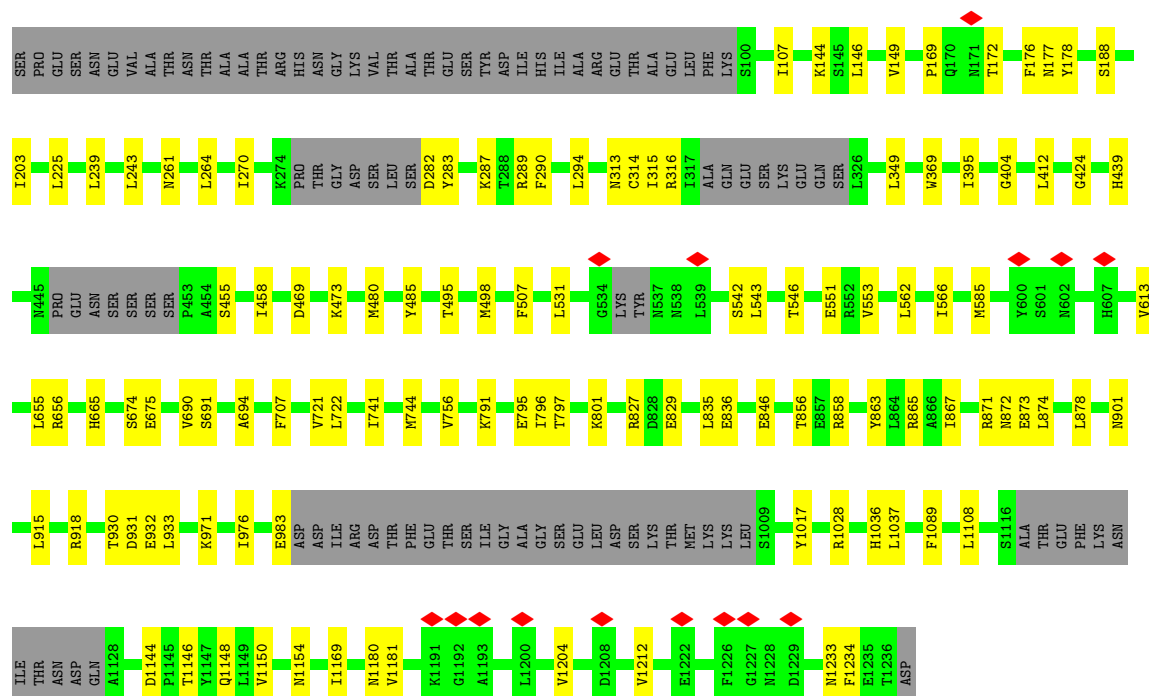


- Molecule 35: 40S ribosomal protein S14-A

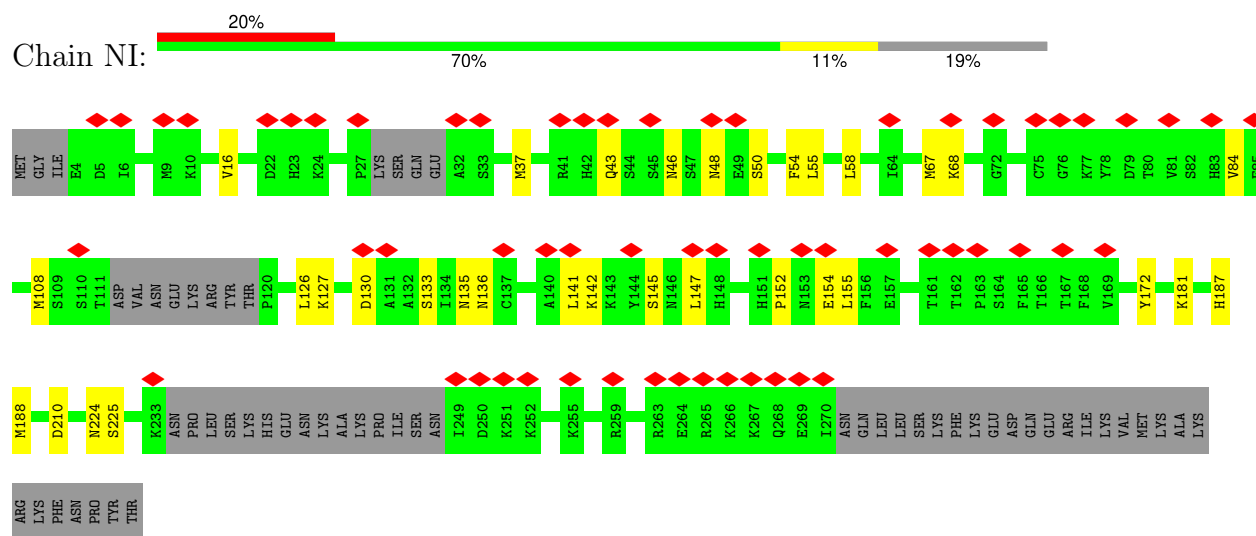


- Molecule 36: U3 small nucleolar RNA-associated protein 22

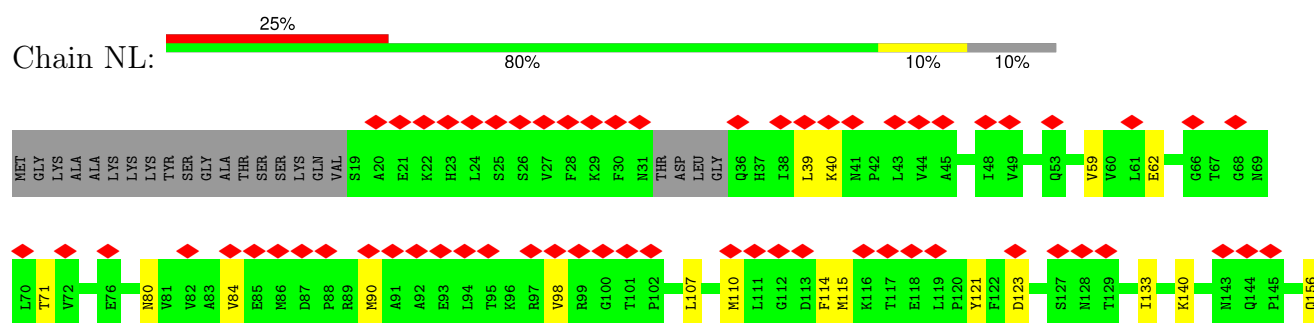


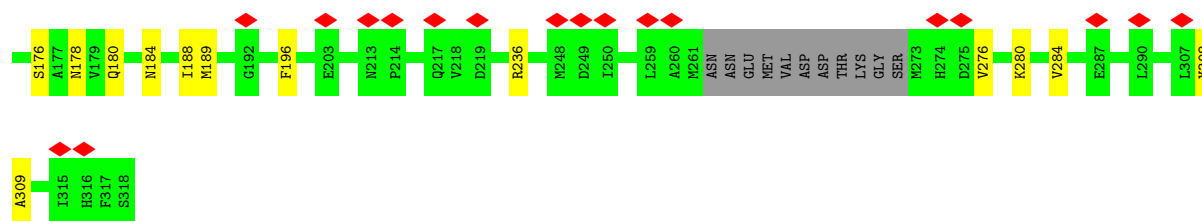


• Molecule 37: Ribosomal RNA-processing protein 7



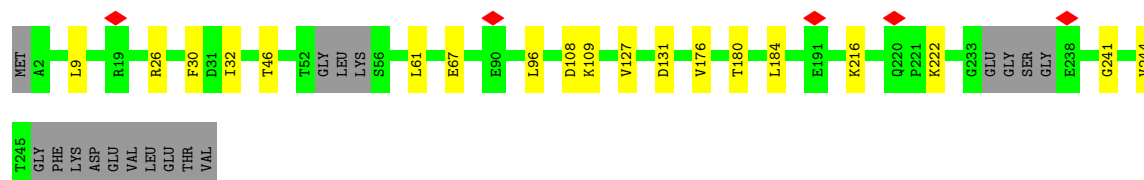
• Molecule 38: Dimethyladenosine transferase





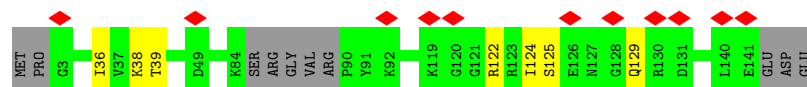
- Molecule 39: Small ribosomal subunit protein eS1A

Chain NM: 85% 7% 7%



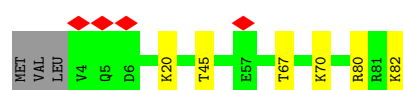
- Molecule 40: 40S ribosomal protein S19-A

Chain NP: 8% 88% 5% 7%



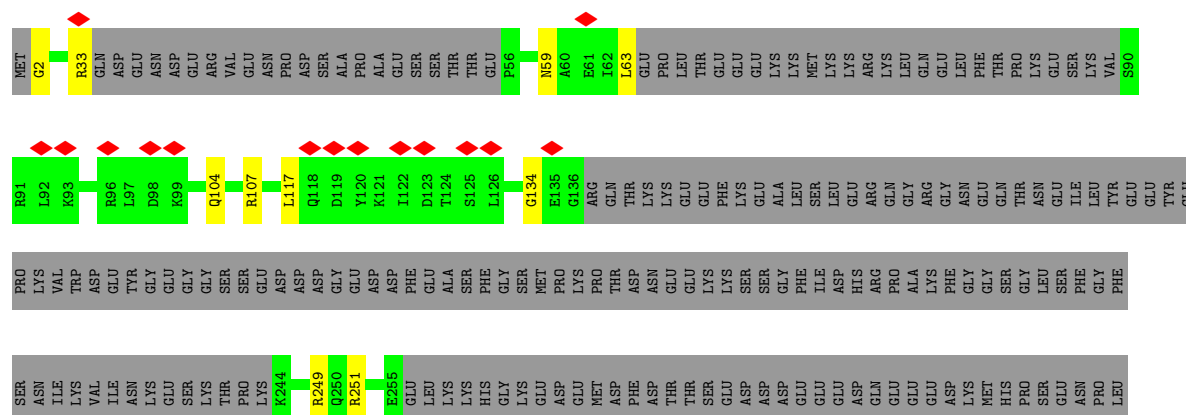
- Molecule 41: 40S ribosomal protein S27-A

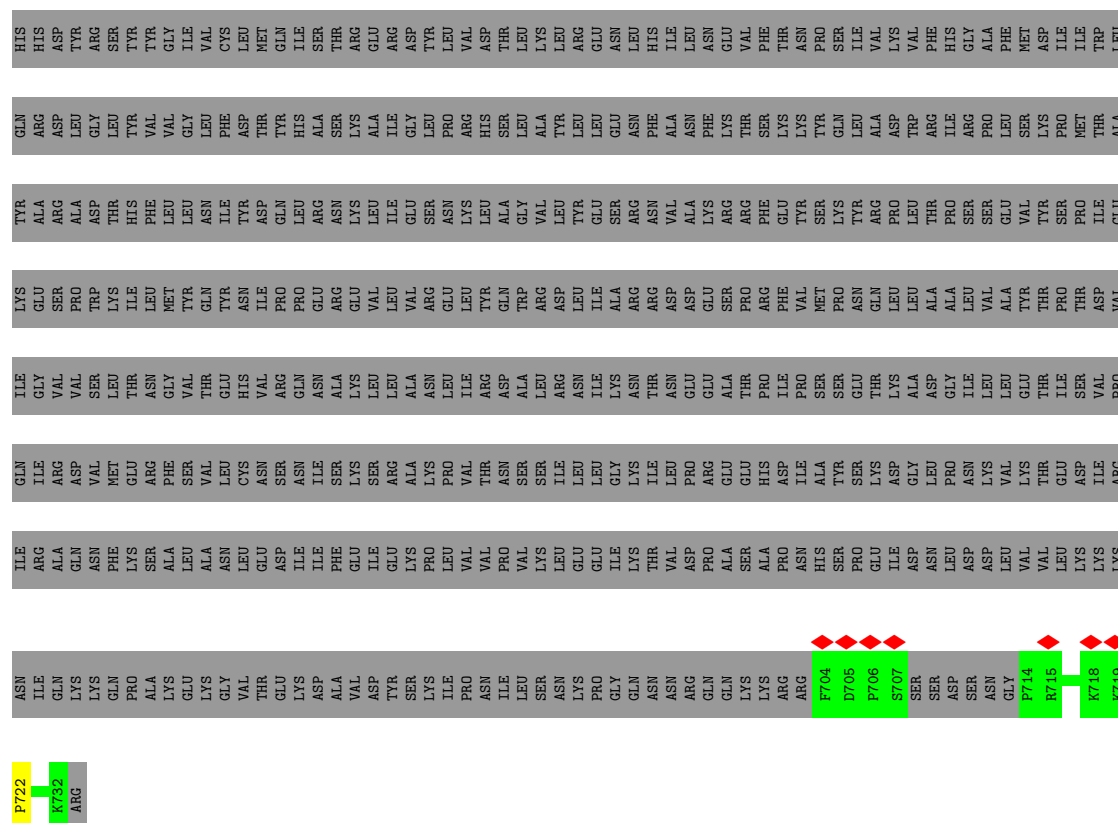
Chain NQ: 5% 89% 7% 7%



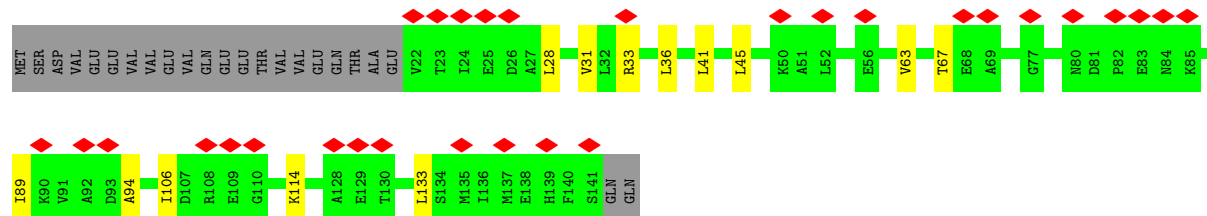
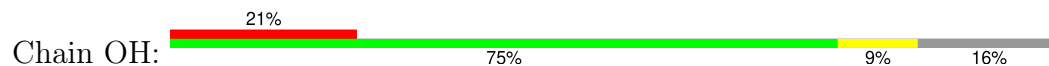
- Molecule 42: Probable ATP-dependent RNA helicase DHR1

Chain NS: 19% 66% 7% 27%

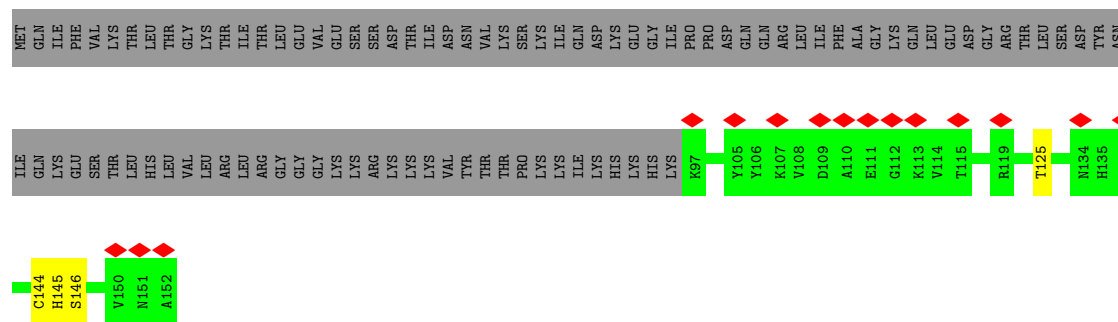




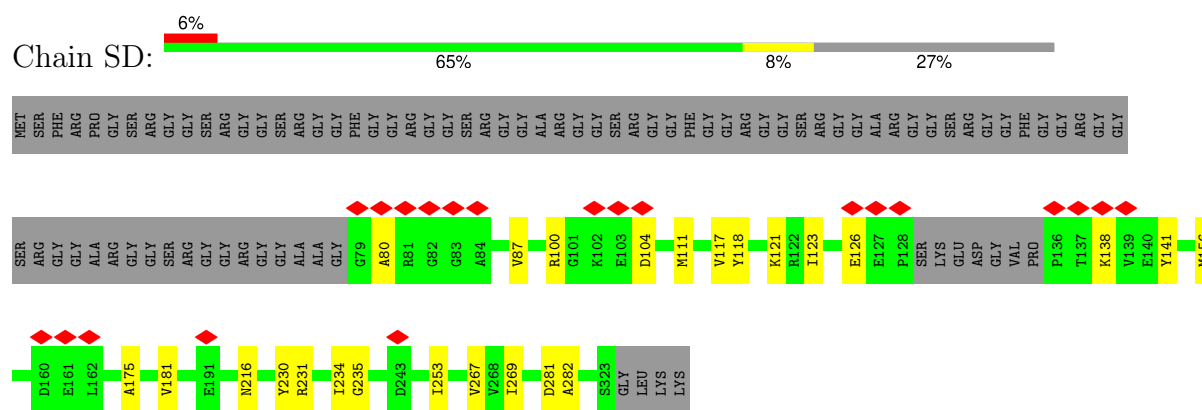
- Molecule 44: 40S ribosomal protein S12



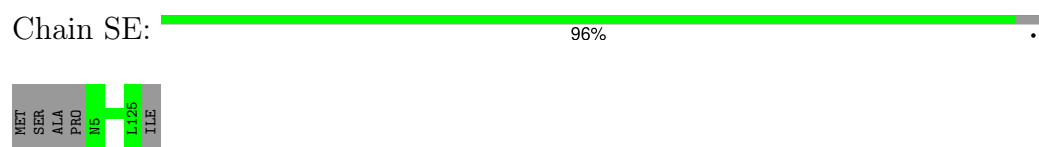
- Molecule 45: Ubiquitin-40S ribosomal protein S31



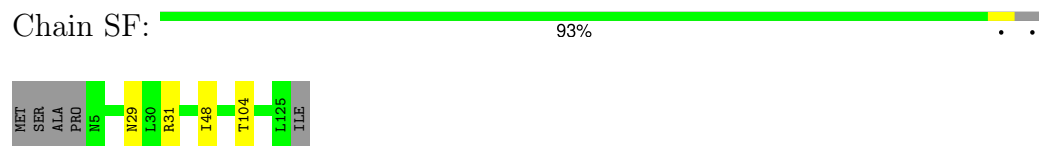
- Molecule 46: Nucleolar protein 56



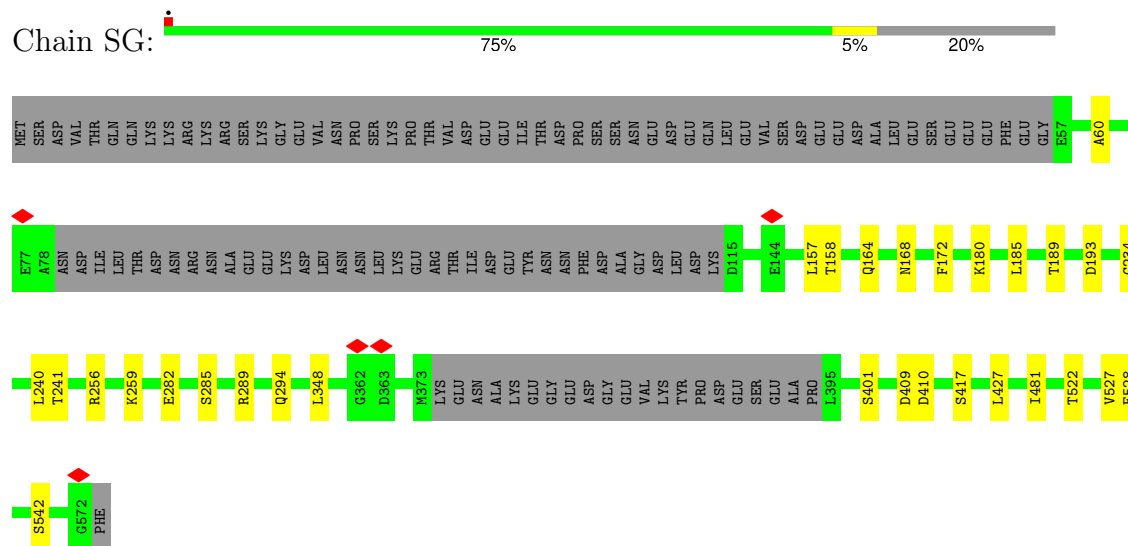
- Molecule 49: 13 kDa ribonucleoprotein-associated protein



- Molecule 49: 13 kDa ribonucleoprotein-associated protein




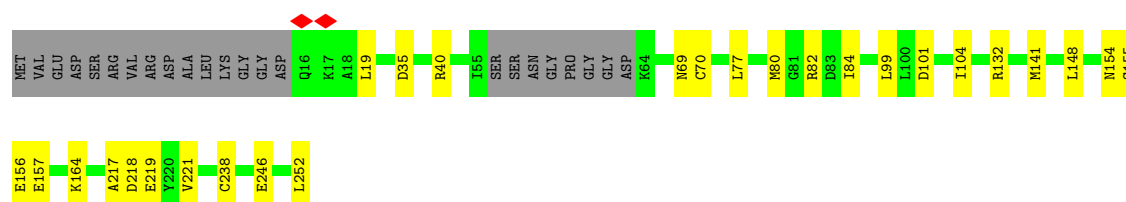
- Molecule 50: Ribosomal RNA-processing protein 9



- Molecule 51: RNA 3'-terminal phosphate cyclase-like protein

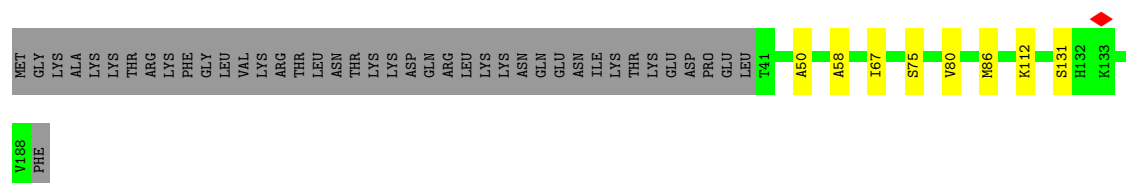


Chain SK: 




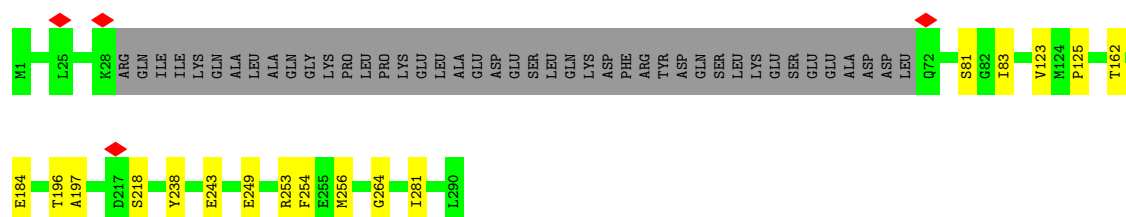
- Molecule 54: rRNA-processing protein FCF1

Chain SL: 



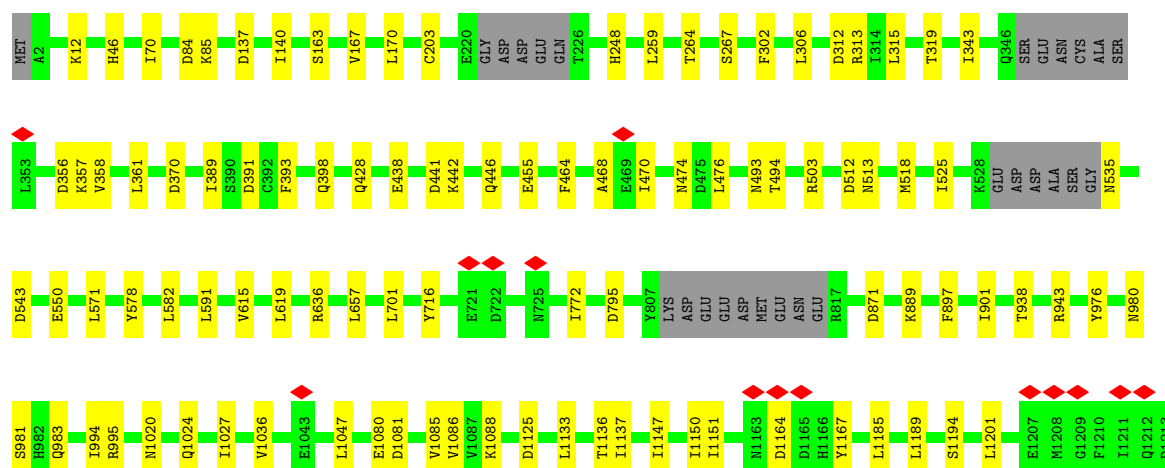
- Molecule 55: U3 small nucleolar ribonucleoprotein protein IMP4

Chain SM: 

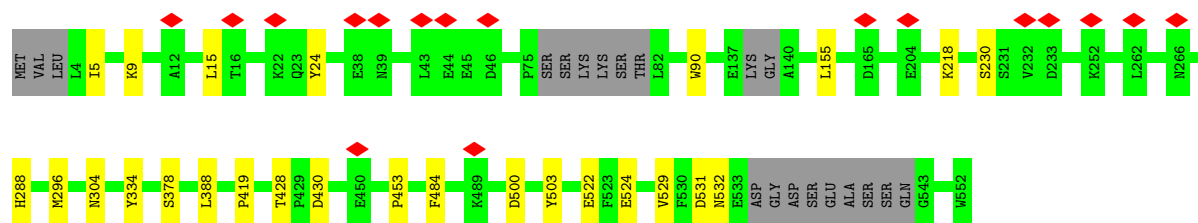


- Molecule 56: U3 small nucleolar RNA-associated protein 20

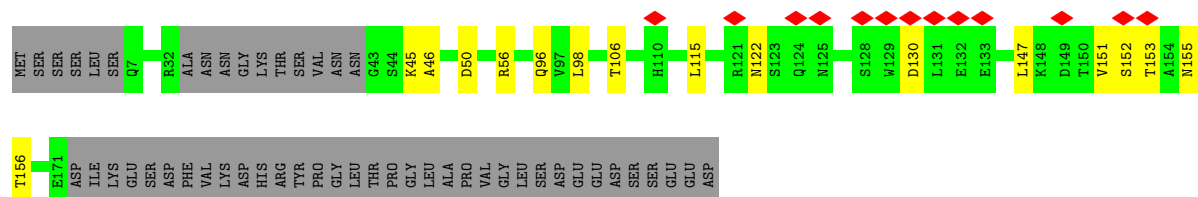
Chain SP: 



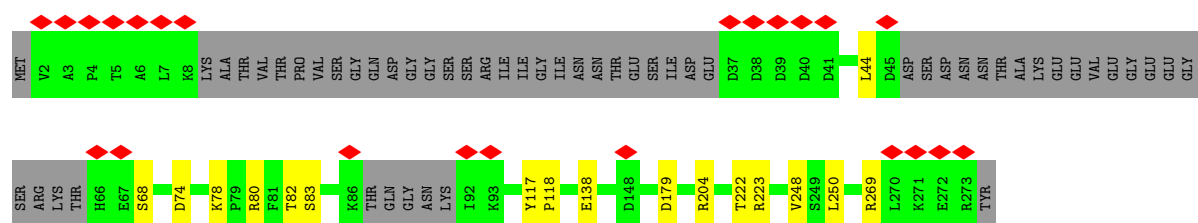
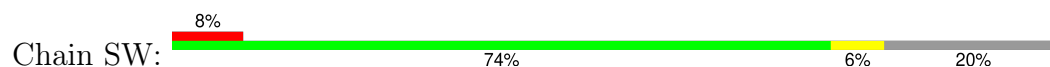




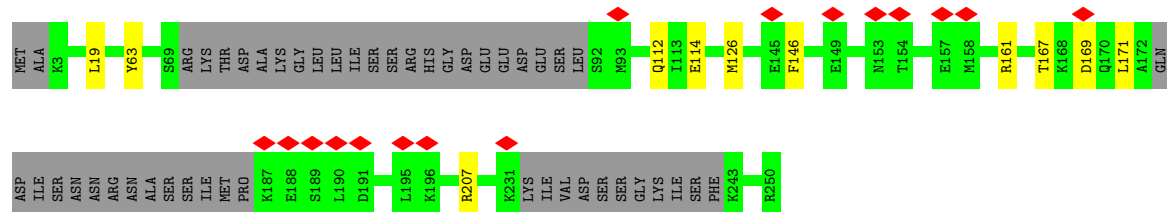
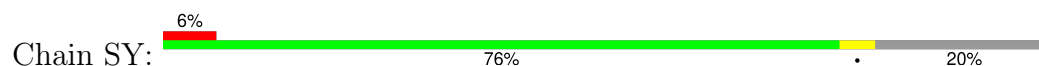
• Molecule 62: Regulator of rDNA transcription protein 14



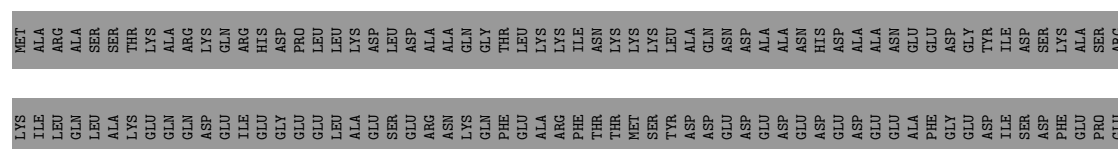
• Molecule 63: Pre-rRNA-processing protein PNO1

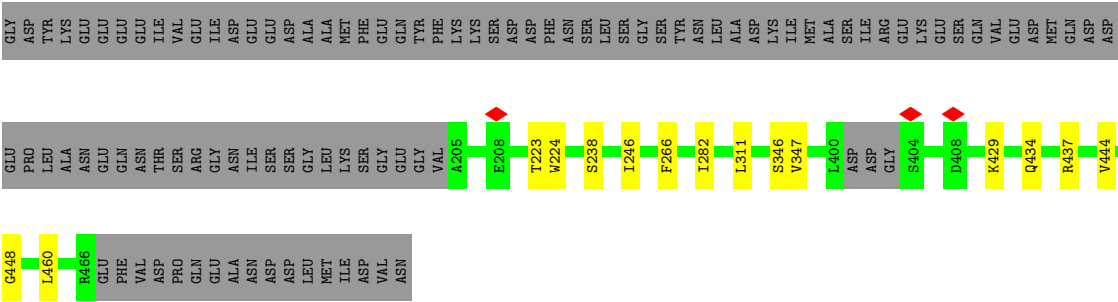


• Molecule 64: U3 small nucleolar RNA-associated protein 11



• Molecule 65: Essential nuclear protein 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95512	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	7.684	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.103	Depositor
Map value standard deviation	0.165	Depositor
Recommended contour level	0.6	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: M7G, MG, ATP, SEP, 4AC, GTP, ZN, A2M, OMG, OMC, OMU, ADP

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	0.12	0/1605	0.22	0/2494
2	L1	0.19	0/33992	0.28	0/52928
3	L2	0.12	0/4748	0.23	0/7372
4	L3	0.15	0/872	0.32	0/1173
5	L4	0.19	0/1977	0.34	0/2664
6	L5	0.14	0/1655	0.30	0/2237
7	L6	0.17	0/1764	0.30	0/2359
8	L7	0.16	0/1451	0.37	0/1956
9	L8	0.20	0/1371	0.30	0/1833
10	L9	0.17	0/1495	0.30	0/2003
11	LC	0.17	0/1015	0.35	0/1367
12	LD	0.20	0/1138	0.35	0/1533
13	LE	0.18	0/1039	0.36	0/1395
14	LF	0.16	0/1060	0.30	0/1412
15	LG	0.14	0/492	0.32	0/659
16	LH	0.18	0/6576	0.38	0/8902
17	LI	0.13	0/3835	0.32	0/5263
18	LJ	0.14	0/3851	0.33	0/5221
19	LK	0.13	0/1085	0.29	0/1463
20	LL	0.14	0/3939	0.31	0/5341
21	LM	0.12	0/12984	0.29	0/17571
22	LN	0.18	0/5359	0.30	0/7255
23	LO	0.14	0/6463	0.29	0/8748
24	LP	0.10	0/3282	0.24	0/4411
25	LQ	0.15	0/6620	0.30	0/8936
26	LR	0.14	0/6313	0.29	0/8551
27	LS	0.18	0/3735	0.28	0/5064
28	LT	0.13	0/7011	0.29	0/9471
29	LW	0.09	0/412	0.22	0/542
30	LZ	0.13	0/1194	0.31	0/1610
31	NA	0.12	0/2657	0.27	0/3559
32	NB	0.18	0/2179	0.39	1/2905 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	ND	0.14	0/613	0.30	0/811
34	NF	0.13	0/1158	0.28	0/1559
35	NG	0.15	0/952	0.28	0/1279
36	NH	0.13	0/8899	0.29	0/12035
37	NI	0.13	0/1994	0.31	0/2684
38	NL	0.15	0/2329	0.35	0/3144
39	NM	0.14	0/1915	0.29	0/2563
40	NP	0.12	0/1056	0.29	0/1416
41	NQ	0.12	0/605	0.28	0/817
42	NS	0.13	0/7623	0.30	0/10256
43	NV	0.19	0/184	0.41	0/240
44	OH	0.11	0/910	0.25	0/1231
45	OU	0.12	0/443	0.30	0/592
46	SA	0.13	0/3188	0.27	0/4293
47	SB	0.14	0/3293	0.29	0/4436
48	SC	0.15	0/1903	0.30	0/2567
48	SD	0.13	0/1885	0.31	0/2543
49	SE	0.18	0/928	0.29	0/1262
49	SF	0.15	0/928	0.30	0/1262
50	SG	0.15	0/3744	0.30	0/5040
51	SH	0.15	0/2832	0.30	0/3825
52	SI	0.16	0/6295	0.31	0/8476
53	SJ	0.13	0/1703	0.32	0/2295
53	SK	0.16	0/1822	0.32	0/2462
54	SL	0.16	0/1193	0.30	0/1611
55	SM	0.16	0/2046	0.31	0/2759
56	SP	0.13	0/15404	0.29	0/20833
57	SQ	0.14	0/926	0.31	0/1237
58	SR	0.16	0/1069	0.32	0/1427
59	SS	0.18	0/115	0.30	0/159
60	ST	0.13	0/4963	0.28	0/6635
61	SU	0.12	0/4466	0.27	0/6054
62	SV	0.11	0/1308	0.28	0/1736
63	SW	0.16	0/1752	0.30	0/2359
64	SY	0.15	0/1736	0.29	0/2292
65	SZ	0.14	0/2167	0.29	0/2940
All	All	0.15	0/227516	0.30	1/315328 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	NB	232	PRO	CA-N-CD	-9.33	98.94	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L0	1437	0	722	8	0
2	L1	30807	0	15545	134	0
3	L2	4288	0	2176	16	0
4	L3	862	0	900	16	0
5	L4	1936	0	2019	13	0
6	L5	1635	0	1697	12	0
7	L6	1740	0	1835	16	0
8	L7	1427	0	1499	28	0
9	L8	1348	0	1366	10	0
10	L9	1470	0	1554	7	0
11	LC	997	0	1054	6	0
12	LD	1112	0	1179	2	0
13	LE	1022	0	1060	11	0
14	LF	1046	0	1114	2	0
15	LG	490	0	529	4	0
16	LH	6449	0	6398	79	0
17	LI	3792	0	2859	22	0
18	LJ	3773	0	3761	33	0
19	LK	1068	0	1120	12	0
20	LL	3871	0	3876	27	0
21	LM	12777	0	13277	91	0
22	LN	5263	0	5270	34	0
23	LO	6321	0	6235	38	0
24	LP	3214	0	3267	15	0
25	LQ	6494	0	6544	41	0
26	LR	6207	0	6247	47	0
27	LS	3662	0	3639	28	0
28	LT	6875	0	6840	48	0
29	LW	411	0	436	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	LZ	1173	0	1208	11	0
31	NA	2635	0	2683	27	0
32	NB	2147	0	2140	20	0
33	ND	609	0	671	5	0
34	NF	1135	0	1197	1	0
35	NG	941	0	979	10	0
36	NH	8693	0	8806	74	0
37	NI	1953	0	1933	23	0
38	NL	2285	0	2359	26	0
39	NM	1891	0	1995	15	0
40	NP	1040	0	1057	7	0
41	NQ	595	0	609	4	0
42	NS	7483	0	7675	65	0
43	NV	181	0	196	1	0
44	OH	902	0	948	11	0
45	OU	436	0	449	3	0
46	SA	3141	0	3156	31	0
47	SB	3255	0	3379	30	0
48	SC	1865	0	1908	12	0
48	SD	1850	0	1889	17	0
49	SE	916	0	964	0	0
49	SF	916	0	964	2	0
50	SG	3672	0	3690	17	0
51	SH	2781	0	2878	12	0
52	SI	6158	0	6342	44	0
53	SJ	1678	0	1756	21	0
53	SK	1793	0	1874	19	0
54	SL	1171	0	1229	5	0
55	SM	2009	0	2027	13	0
56	SP	15102	0	15321	101	0
57	SQ	909	0	906	12	0
58	SR	1052	0	1120	3	0
59	SS	109	0	94	1	0
60	ST	4893	0	5028	43	0
61	SU	4357	0	4348	22	0
62	SV	1296	0	1390	12	0
63	SW	1725	0	1796	13	0
64	SY	1715	0	1789	11	0
65	SZ	2113	0	2160	12	0
66	L1	54	0	0	0	0
66	L9	1	0	0	0	0
66	NH	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	NP	1	0	0	0	0
66	NS	1	0	0	0	0
66	SI	1	0	0	0	0
67	NH	31	0	12	1	0
68	NQ	1	0	0	0	0
68	OU	1	0	0	0	0
68	SL	1	0	0	0	0
69	NS	27	0	12	0	0
70	SI	32	0	12	0	0
All	All	220521	0	204967	1324	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 3.

All (1324) 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	1.42	1.01
20:LL:153:ILE:HG22	20:LL:163:LEU:HD22	1.52	0.90
20:LL:448:ASN:OD1	20:LL:483:ARG:NH2	2.09	0.85
60:ST:232:MET:HE1	65:SZ:223:THR:HG23	1.59	0.85
2:L1:133:U:OP2	56:SP:995:ARG:NH1	2.10	0.84
53:SK:80:MET:SD	53:SK:82:ARG:NH2	2.51	0.84
21:LM:516:PHE:O	21:LM:522:ARG:NH1	2.11	0.83
29:LW:552:ARG:NH2	36:NH:791:LYS:O	2.12	0.83
25:LQ:5:TYR:OH	25:LQ:643:ASP:OD2	1.97	0.82
11:LC:98:ASP:OD2	28:LT:488:ASN:ND2	2.13	0.82
42:NS:476:GLN:NE2	42:NS:481:SER:O	2.13	0.81
1:L0:282:G:O3'	28:LT:395:LYS:NZ	2.14	0.81
19:LK:438:SER:OG	19:LK:478:ASN:ND2	2.14	0.80
2:L1:1003:A:OP1	63:SW:269:ARG:NH2	2.14	0.80
2:L1:1499:G:OP1	40:NP:122:ARG:NH1	2.14	0.80
28:LT:805:PHE:O	42:NS:1212:TYR:OH	1.98	0.80
21:LM:82:ASP:O	21:LM:86:GLN:NE2	2.16	0.79
2:L1:1441:C:OP1	53:SJ:118:ARG:NH2	2.16	0.79
1:L0:86:C:N4	16:LH:318:GLU:OE1	2.16	0.79
21:LM:1523:ARG:NE	62:SV:50:ASP:OD1	2.15	0.79
25:LQ:909:LYS:NZ	26:LR:783:ASP:OD2	2.16	0.78
56:SP:1523:TYR:OH	56:SP:1551:LEU:O	2.01	0.77
23:LO:140:ARG:NH2	23:LO:175:VAL:O	2.17	0.77
2:L1:127:G:N7	7:L6:202:ARG:NH2	2.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:NS:918:SER:HA	42:NS:1083:MET:HE2	1.67	0.77
2:L1:154:G:O6	14:LF:128:LYS:NZ	2.17	0.77
16:LH:145:PHE:CZ	16:LH:230:LEU:HD13	2.19	0.77
2:L1:110:U:OP1	2:L1:753:A:O2'	2.03	0.76
48:SD:80:ALA:O	48:SD:121:LYS:NZ	2.19	0.76
18:LJ:258:LEU:HD21	18:LJ:272:LEU:HD11	1.65	0.76
37:NI:50:SER:O	37:NI:127:LYS:NZ	2.18	0.76
16:LH:139:GLU:OE2	16:LH:172:ARG:NH1	2.19	0.76
18:LJ:238:ASP:OD2	18:LJ:240:THR:OG1	2.03	0.76
62:SV:122:ASN:ND2	64:SY:171:LEU:O	2.19	0.76
8:L7:47:ARG:NH1	8:L7:48:GLU:O	2.20	0.75
17:LI:540:LEU:HD23	17:LI:544:LEU:HD13	1.68	0.75
36:NH:1180:ASN:OD1	36:NH:1181:VAL:N	2.20	0.75
48:SD:100:ARG:NH1	48:SD:104:ASP:OD1	2.20	0.74
2:L1:1638:G:OP2	26:LR:751:LYS:NZ	2.21	0.74
57:SQ:127:ARG:HA	57:SQ:130:LEU:HD13	1.70	0.74
56:SP:264:THR:O	56:SP:313:ARG:NH1	2.20	0.74
2:L1:578:OMU:OP2	52:SI:874:TYR:OH	2.04	0.74
8:L7:122:HIS:ND1	8:L7:177:THR:HG22	2.02	0.74
26:LR:542:CYS:SG	26:LR:587:GLN:NE2	2.61	0.74
2:L1:1011:G:O2'	42:NS:134:GLY:O	2.05	0.73
8:L7:173:TYR:O	8:L7:177:THR:OG1	2.03	0.73
16:LH:393:ASN:ND2	16:LH:435:ASP:OD2	2.20	0.73
42:NS:1030:LEU:HD22	42:NS:1035:MET:HE2	1.69	0.73
3:L2:155:U:OP1	21:LM:1634:ARG:NH2	2.21	0.73
47:SB:7:GLU:OE1	48:SD:231:ARG:NH2	2.22	0.73
16:LH:134:ILE:HG23	16:LH:136:LEU:HD13	1.70	0.73
25:LQ:230:LYS:NZ	25:LQ:245:MET:SD	2.56	0.73
56:SP:493:ASN:ND2	56:SP:525:ILE:O	2.21	0.73
8:L7:96:ARG:NH1	8:L7:97:ARG:O	2.22	0.73
2:L1:1756:A:N7	31:NA:500:LYS:NZ	2.36	0.72
24:LP:14:GLU:OE1	24:LP:91:ARG:NH1	2.21	0.72
2:L1:227:U:O4	56:SP:1529:ARG:NH1	2.22	0.72
2:L1:530:C:O2	14:LF:61:ARG:NH1	2.23	0.72
2:L1:1619:C:O2'	15:LG:67:ARG:O	2.08	0.72
4:L3:60:GLU:OE2	18:LJ:61:THR:OG1	2.07	0.72
32:NB:299:ALA:HA	32:NB:302:LEU:HD13	1.72	0.72
58:SR:57:LEU:HD13	60:ST:788:ILE:HD11	1.72	0.72
24:LP:203:MET:SD	24:LP:207:ASN:ND2	2.62	0.72
25:LQ:287:ARG:NH1	25:LQ:323:SER:O	2.22	0.72
35:NG:31:THR:OG1	35:NG:37:GLU:O	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:NS:1209:ARG:NH1	42:NS:1211:CYS:SG	2.62	0.72
22:LN:682:THR:OG1	22:LN:684:GLU:OE1	2.07	0.71
32:NB:537:LYS:NZ	52:SI:149:GLU:OE2	2.23	0.71
47:SB:14:LEU:HD13	47:SB:79:ILE:HD12	1.72	0.71
21:LM:926:VAL:HG12	21:LM:963:ILE:HD11	1.72	0.71
28:LT:375:LEU:HD22	28:LT:389:MET:HG3	1.72	0.71
38:NL:188:ILE:O	38:NL:189:MET:HE2	1.91	0.71
18:LJ:43:THR:O	18:LJ:304:SER:OG	2.07	0.71
50:SG:401:SER:O	50:SG:417:SER:OG	2.07	0.71
56:SP:1689:VAL:HG22	56:SP:1744:GLU:OE1	1.89	0.71
25:LQ:589:ILE:HG21	25:LQ:621:VAL:HG11	1.73	0.71
32:NB:555:ASN:OD1	32:NB:558:ASN:ND2	2.24	0.71
2:L1:1576:A:OP2	53:SK:164:LYS:NZ	2.22	0.71
30:LZ:162:ASP:OD1	30:LZ:163:ASN:N	2.24	0.71
10:L9:58:ASP:O	10:L9:61:THR:OG1	2.09	0.70
21:LM:923:ASP:OD1	21:LM:924:ILE:N	2.24	0.70
35:NG:82:LYS:NZ	39:NM:67:GLU:OE2	2.24	0.70
60:ST:555:ARG:NH2	61:SU:522:GLU:OE2	2.24	0.70
21:LM:1129:PHE:CZ	21:LM:1133:MET:HE3	2.27	0.70
2:L1:1060:U:OP2	36:NH:865:ARG:NH2	2.24	0.70
20:LL:227:VAL:HG11	28:LT:563:ASP:OD1	1.91	0.70
42:NS:514:ILE:CG2	42:NS:558:MET:HE2	2.22	0.70
56:SP:474:ASN:OD1	56:SP:716:TYR:OH	2.09	0.69
10:L9:106:GLU:OE1	10:L9:115:LYS:NZ	2.25	0.69
40:NP:38:LYS:O	40:NP:39:THR:OG1	2.07	0.69
61:SU:304:ASN:OD1	61:SU:334:TYR:OH	2.09	0.69
36:NH:707:PHE:O	36:NH:918:ARG:NH1	2.26	0.69
20:LL:520:MET:O	20:LL:524:SER:OG	2.10	0.69
21:LM:413:ASP:OD2	21:LM:417:LYS:NZ	2.26	0.69
37:NI:224:ASN:OD1	37:NI:225:SER:N	2.26	0.69
50:SG:185:LEU:HD13	50:SG:527:VAL:HG11	1.75	0.69
50:SG:164:GLN:NE2	50:SG:528:GLU:O	2.26	0.69
60:ST:679:GLU:OE1	60:ST:683:ASN:ND2	2.26	0.69
21:LM:362:LYS:O	21:LM:365:ILE:HG22	1.93	0.68
27:LS:269:ASP:OD2	27:LS:273:ARG:NH1	2.26	0.68
56:SP:358:VAL:HG12	56:SP:389:ILE:HD11	1.73	0.68
16:LH:675:ARG:NH1	17:LI:492:GLU:OE2	2.25	0.68
37:NI:37:MET:HE1	37:NI:58:LEU:HD23	1.73	0.68
45:OU:144:CYS:SG	45:OU:146:SER:OG	2.44	0.68
23:LO:567:ASP:OD1	23:LO:576:ARG:NH2	2.27	0.68
28:LT:207:ASP:OD2	28:LT:227:THR:OG1	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SI:1106:GLU:OE2	57:SQ:119:ARG:NH2	2.26	0.68
4:L3:72:ILE:HD13	4:L3:79:TYR:CD2	2.29	0.68
36:NH:585:MET:SD	36:NH:613:VAL:HG12	2.34	0.68
26:LR:220:ILE:HD12	26:LR:239:VAL:HG11	1.76	0.68
50:SG:234:GLY:O	50:SG:259:LYS:NZ	2.26	0.68
31:NA:341:LEU:O	52:SI:960:ARG:NH1	2.28	0.67
1:L0:68:U:OP2	16:LH:426:ARG:NH2	2.27	0.67
5:L4:141:THR:OG1	5:L4:143:ASP:OD1	2.09	0.67
2:L1:330:G:OP2	9:L8:172:ARG:NH1	2.27	0.67
4:L3:41:ARG:NH2	40:NP:36:ILE:O	2.27	0.67
60:ST:660:ILE:HD13	61:SU:388:LEU:HD13	1.77	0.67
2:L1:1555:A:O2'	2:L1:1556:A:O5'	2.13	0.67
3:L2:79:G:O2'	3:L2:328:A:N1	2.24	0.67
16:LH:77:ILE:HD13	16:LH:117:ILE:HD11	1.76	0.67
36:NH:983:GLU:O	39:NM:222:LYS:NZ	2.28	0.67
15:LG:39:THR:OG1	25:LQ:867:GLU:OE1	2.13	0.67
48:SD:126:GLU:OE1	48:SD:138:LYS:NZ	2.23	0.67
53:SJ:219:GLU:OE2	53:SJ:219:GLU:N	2.25	0.67
2:L1:494:U:OP2	52:SI:1138:ARG:NH1	2.28	0.66
21:LM:1485:VAL:O	21:LM:1538:LYS:NZ	2.28	0.66
28:LT:93:ALA:HB1	28:LT:118:VAL:HG11	1.78	0.66
27:LS:278:ASP:OD2	27:LS:281:THR:OG1	2.12	0.66
47:SB:134:ASN:OD1	47:SB:138:LYS:NZ	2.28	0.66
21:LM:1712:LYS:NZ	21:LM:1747:GLU:OE2	2.27	0.66
42:NS:1057:ASN:OD1	63:SW:80:ARG:NH2	2.28	0.66
2:L1:93:A:O4'	5:L4:3:ARG:NH1	2.29	0.66
16:LH:246:SER:O	16:LH:249:THR:OG1	2.12	0.66
29:LW:546:ILE:HD11	37:NI:181:LYS:NZ	2.10	0.66
37:NI:68:LYS:NZ	37:NI:84:VAL:O	2.19	0.66
56:SP:476:LEU:HD22	56:SP:518:MET:HE1	1.76	0.66
3:L2:312:U:O2'	46:SA:339:GLU:OE2	2.12	0.66
47:SB:161:VAL:HG23	47:SB:162:MET:HE3	1.78	0.66
55:SM:249:GLU:OE1	55:SM:253:ARG:NH1	2.29	0.66
30:LZ:64:LEU:HD23	30:LZ:71:ARG:HB3	1.78	0.65
20:LL:583:GLU:OE1	33:ND:167:ARG:NH1	2.28	0.65
56:SP:1020:ASN:ND2	56:SP:1024:GLN:OE1	2.30	0.65
13:LE:80:ASN:OD1	13:LE:124:LYS:NZ	2.30	0.65
22:LN:681:ILE:HG22	22:LN:683:ASP:H	1.60	0.65
25:LQ:400:SER:OG	25:LQ:402:ASP:OD1	2.10	0.65
35:NG:12:GLN:OE1	35:NG:77:THR:OG1	2.07	0.65
17:LI:632:THR:O	17:LI:636:GLN:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:NL:84:VAL:HG12	38:NL:110:MET:HE3	1.78	0.65
42:NS:377:GLU:N	42:NS:377:GLU:OE1	2.30	0.65
42:NS:1114:ASN:OD1	42:NS:1164:LYS:NZ	2.29	0.65
2:L1:207:U:O2	9:L8:178:ARG:NH2	2.29	0.65
42:NS:884:GLN:NE2	42:NS:893:GLU:OE2	2.30	0.65
56:SP:163:SER:O	56:SP:167:VAL:HG23	1.96	0.65
2:L1:1532:U:OP2	18:LJ:114:ARG:NH1	2.30	0.64
36:NH:656:ARG:NH2	39:NH:241:GLY:O	2.30	0.64
56:SP:1466:ILE:HG23	56:SP:1489:ILE:HD11	1.80	0.64
46:SA:30:ARG:NH1	46:SA:122:GLU:OE2	2.30	0.64
26:LR:649:GLU:OE1	26:LR:649:GLU:N	2.29	0.64
26:LR:188:GLU:OE1	26:LR:188:GLU:N	2.31	0.64
36:NH:188:SER:N	67:NH:1300:ATP:O2B	2.31	0.64
36:NH:871:ARG:NH2	36:NH:873:GLU:OE2	2.29	0.64
48:SD:281:ASP:OD2	48:SD:282:ALA:N	2.31	0.64
9:L8:69:SER:OG	9:L8:185:GLU:OE2	2.09	0.63
24:LP:111:ALA:HB1	57:SQ:73:ALA:HB2	1.80	0.63
25:LQ:161:SER:OG	25:LQ:187:LYS:NZ	2.26	0.63
26:LR:398:GLU:OE2	42:NS:249:ARG:NH2	2.29	0.63
42:NS:609:LYS:NZ	42:NS:712:GLU:OE2	2.24	0.63
20:LL:302:ASN:ND2	20:LL:316:ASN:OD1	2.32	0.63
23:LO:351:LEU:HD22	23:LO:701:LEU:HD11	1.80	0.63
8:L7:93:LEU:HD21	8:L7:129:LEU:HD23	1.81	0.63
18:LJ:197:ASP:HB2	18:LJ:206:ILE:HD11	1.81	0.63
38:NL:115:MET:HG3	38:NL:133:ILE:HD11	1.81	0.63
28:LT:592:ASP:OD1	28:LT:593:PHE:N	2.31	0.63
46:SA:129:ARG:NH1	48:SC:261:LEU:O	2.32	0.63
16:LH:591:GLU:O	16:LH:592:SER:OG	2.15	0.63
32:NB:409:LYS:NZ	61:SU:500:ASP:OD2	2.31	0.63
7:L6:24:ILE:HG22	7:L6:28:PHE:CE1	2.34	0.62
7:L6:67:VAL:HG21	7:L6:73:ILE:HD11	1.81	0.62
6:L5:94:THR:HG22	6:L5:114:ILE:HG13	1.82	0.62
17:LI:643:ASP:OD1	19:LK:502:ARG:NH1	2.32	0.62
28:LT:608:THR:OG1	28:LT:610:ARG:NH1	2.33	0.62
28:LT:646:VAL:HG13	28:LT:647:THR:HG23	1.81	0.62
47:SB:249:GLN:NE2	47:SB:253:ASP:OD1	2.32	0.62
2:L1:1568:C:O2'	2:L1:1569:A:O5'	2.18	0.62
4:L3:18:LEU:HD22	4:L3:73:MET:HE1	1.79	0.62
21:LM:778:SER:O	21:LM:782:VAL:N	2.33	0.62
25:LQ:829:VAL:HG21	25:LQ:864:ASN:HD21	1.64	0.62
2:L1:1779:U:O4	38:NL:178:ASN:ND2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:1781:A:N3	38:NL:156:GLN:NE2	2.47	0.62
8:L7:152:VAL:CG2	8:L7:181:ILE:HD11	2.30	0.62
20:LL:185:PRO:O	20:LL:215:TYR:OH	2.16	0.62
32:NB:599:LYS:NZ	57:SQ:138:LYS:O	2.32	0.62
56:SP:1151:ILE:HG23	56:SP:1201:LEU:HD22	1.81	0.62
25:LQ:181:SER:OG	25:LQ:183:ASP:OD1	2.18	0.62
63:SW:204:ARG:NH1	63:SW:250:LEU:O	2.32	0.62
8:L7:17:GLU:HG2	8:L7:46:ILE:HG22	1.81	0.62
55:SM:123:VAL:HG12	55:SM:125:PRO:HD2	1.81	0.62
60:ST:703:GLN:NE2	61:SU:484:PHE:O	2.33	0.62
32:NB:442:TYR:HH	53:SJ:70:CYS:HG	1.48	0.62
52:SI:1113:ILE:HD11	57:SQ:174:LEU:HD12	1.82	0.62
2:L1:1670:G:O2'	2:L1:1731:A:N6	2.31	0.62
16:LH:778:ASP:O	16:LH:781:SER:N	2.32	0.61
33:ND:112:LEU:HD21	61:SU:90:TRP:CG	2.34	0.61
18:LJ:287:LEU:HD23	18:LJ:287:LEU:O	2.00	0.61
48:SC:294:ARG:NH1	54:SL:131:SER:OG	2.34	0.61
60:ST:263:LYS:O	60:ST:268:LYS:NZ	2.33	0.61
60:ST:280:ASP:OD1	60:ST:281:LYS:N	2.34	0.61
2:L1:1473:U:OP2	6:L5:189:THR:OG1	2.17	0.61
2:L1:1524:A:N3	2:L1:1590:G:O2'	2.28	0.61
8:L7:8:ILE:HD13	8:L7:13:PRO:HB3	1.81	0.61
36:NH:863:TYR:O	36:NH:867:ILE:HD12	2.00	0.61
51:SH:281:GLU:OE1	52:SI:624:LYS:NZ	2.26	0.61
13:LE:42:GLN:NE2	13:LE:48:GLY:O	2.34	0.61
36:NH:531:LEU:HD21	36:NH:562:LEU:HD11	1.81	0.61
56:SP:1416:GLU:O	56:SP:1419:SER:OG	2.13	0.61
60:ST:525:MET:HE3	60:ST:550:VAL:HG12	1.81	0.61
55:SM:243:GLU:OE1	55:SM:243:GLU:N	2.34	0.61
2:L1:128:U:O4	56:SP:943:ARG:NH1	2.33	0.61
36:NH:439:HIS:NE2	36:NH:458:ILE:HD13	2.16	0.61
31:NA:335:ARG:NH2	52:SI:957:GLU:OE1	2.34	0.61
51:SH:301:MET:HE2	51:SH:354:ILE:HD13	1.83	0.61
56:SP:1085:VAL:HG23	56:SP:1086:VAL:HG23	1.83	0.61
2:L1:60:U:OP2	56:SP:12:LYS:NZ	2.32	0.60
2:L1:1204:A:C6	60:ST:211:MET:HE1	2.34	0.60
21:LM:1244:ASP:OD1	21:LM:1284:ILE:HD11	2.01	0.60
23:LO:296:GLN:OE1	23:LO:330:TYR:OH	2.19	0.60
2:L1:99:C:OP2	2:L1:378:A:O2'	2.14	0.60
5:L4:151:ASP:OD2	7:L6:215:ARG:NH2	2.34	0.60
17:LI:632:THR:HG22	19:LK:492:ILE:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LT:174:ALA:O	28:LT:175:THR:OG1	2.15	0.60
26:LR:689:ASP:OD2	31:NA:503:LYS:NZ	2.29	0.60
18:LJ:474:LEU:HD11	18:LJ:484:MET:SD	2.41	0.60
13:LE:81:VAL:O	13:LE:122:SER:OG	2.20	0.60
42:NS:1005:ARG:NH2	42:NS:1140:ILE:HD13	2.17	0.60
56:SP:897:PHE:CZ	56:SP:901:ILE:HD11	2.36	0.60
4:L3:110:ARG:NH2	4:L3:113:LEU:HD22	2.17	0.60
8:L7:168:SER:O	8:L7:172:VAL:HG23	2.02	0.60
36:NH:542:SER:O	36:NH:546:THR:HG23	2.02	0.60
42:NS:1125:THR:OG1	42:NS:1127:ASN:O	2.16	0.60
2:L1:1628:U:OP1	31:NA:538:LYS:NZ	2.28	0.60
20:LL:18:CYS:SG	20:LL:65:TRP:NE1	2.75	0.60
59:SS:661:ASN:OD1	59:SS:664:LEU:N	2.34	0.60
60:ST:605:ASP:OD2	60:ST:607:THR:OG1	2.19	0.60
21:LM:1594:PHE:O	21:LM:1598:LEU:N	2.35	0.59
27:LS:376:LEU:CD1	27:LS:409:ILE:HD11	2.33	0.59
37:NI:54:PHE:O	37:NI:55:LEU:HD22	2.02	0.59
46:SA:49:GLU:OE2	46:SA:140:LYS:NZ	2.34	0.59
50:SG:157:LEU:HD11	50:SG:189:THR:HB	1.84	0.59
21:LM:910:LYS:NZ	21:LM:950:THR:OG1	2.35	0.59
42:NS:1056:GLU:OE1	63:SW:83:SER:OG	2.18	0.59
2:L1:1107:G:OP2	52:SI:18:LYS:NZ	2.35	0.59
19:LK:428:ASP:OD1	19:LK:429:HIS:N	2.35	0.59
31:NA:449:ASP:OD1	31:NA:453:SER:OG	2.20	0.59
27:LS:210:LYS:O	27:LS:213:SER:OG	2.21	0.59
50:SG:522:THR:OG1	50:SG:542:SER:OG	2.20	0.59
27:LS:379:GLY:N	27:LS:383:TRP:O	2.36	0.59
52:SI:831:ARG:NH1	52:SI:835:HIS:O	2.36	0.59
28:LT:520:CYS:SG	28:LT:549:MET:HE3	2.43	0.59
31:NA:384:ARG:HH12	55:SM:83:ILE:HD11	1.67	0.59
36:NH:721:VAL:HG23	36:NH:722:LEU:HD12	1.84	0.59
5:L4:129:VAL:HG22	5:L4:139:VAL:HG12	1.84	0.59
7:L6:18:ILE:HG23	7:L6:23:ARG:HD2	1.84	0.59
16:LH:714:ASP:OD1	16:LH:715:GLU:N	2.36	0.59
23:LO:298:LEU:HD13	31:NA:474:ILE:HD11	1.85	0.59
2:L1:561:G:O2'	2:L1:562:OMG:H5'	2.03	0.58
25:LQ:220:THR:HG23	25:LQ:259:ILE:HD11	1.84	0.58
4:L3:18:LEU:HD22	4:L3:73:MET:CE	2.33	0.58
25:LQ:398:ASP:OD1	25:LQ:438:PHE:N	2.36	0.58
2:L1:1657:U:OP2	25:LQ:450:ARG:NH2	2.36	0.58
42:NS:742:GLU:N	42:NS:742:GLU:OE1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:NI:37:MET:CE	37:NI:58:LEU:HD23	2.32	0.58
51:SH:289:VAL:O	51:SH:317:GLN:NE2	2.35	0.58
51:SH:340:LYS:NZ	52:SI:768:GLU:OE1	2.28	0.58
52:SI:124:ASP:OD1	52:SI:126:ASN:N	2.37	0.58
36:NH:872:ASN:OD1	36:NH:873:GLU:N	2.37	0.58
56:SP:315:LEU:O	56:SP:319:THR:HG23	2.04	0.58
16:LH:682:ASN:CG	16:LH:689:ILE:HD11	2.28	0.58
32:NB:373:GLU:OE2	61:SU:9:LYS:NZ	2.37	0.58
36:NH:313:ASN:OD1	36:NH:314:CYS:N	2.36	0.58
2:L1:277:U:O2'	2:L1:278:U:OP1	2.21	0.58
17:LI:632:THR:HG23	19:LK:492:ILE:HG12	1.85	0.58
17:LI:650:LEU:HD13	19:LK:506:LEU:HD13	1.85	0.58
28:LT:62:ASP:O	28:LT:66:LEU:N	2.36	0.58
36:NH:177:ASN:OD1	36:NH:178:TYR:N	2.36	0.58
46:SA:302:ASN:ND2	46:SA:397:SER:O	2.36	0.58
56:SP:1137:ILE:HD11	56:SP:1150:ILE:HG21	1.86	0.58
16:LH:592:SER:O	16:LH:593:ASN:ND2	2.35	0.57
23:LO:131:ARG:HB2	28:LT:655:THR:HG21	1.86	0.57
36:NH:1204:VAL:HG21	36:NH:1212:VAL:HG21	1.85	0.57
39:NM:244:VAL:O	39:NM:244:VAL:HG13	2.04	0.57
2:L1:1561:U:OP1	52:SI:982:LYS:NZ	2.37	0.57
56:SP:772:ILE:HD12	56:SP:772:ILE:H	1.68	0.57
56:SP:871:ASP:OD1	56:SP:889:LYS:NZ	2.36	0.57
20:LL:253:LEU:CD2	20:LL:301:LEU:HD21	2.34	0.57
62:SV:130:ASP:OD2	64:SY:161:ARG:NH1	2.37	0.57
21:LM:926:VAL:CG1	21:LM:963:ILE:HD11	2.33	0.57
36:NH:203:ILE:HD11	36:NH:290:PHE:CE1	2.39	0.57
56:SP:312:ASP:OD1	56:SP:313:ARG:N	2.37	0.57
37:NI:142:LYS:O	37:NI:145:SER:OG	2.18	0.57
54:SL:50:ALA:HB1	54:SL:58:ALA:HB2	1.87	0.57
56:SP:543:ASP:OD1	56:SP:578:TYR:OH	2.22	0.57
1:L0:278:G:N2	27:LS:539:ASP:OD2	2.33	0.57
2:L1:1638:G:OP2	2:L1:1638:G:N2	2.29	0.57
21:LM:562:THR:HG22	21:LM:613:MET:HE3	1.86	0.57
27:LS:376:LEU:HD13	27:LS:409:ILE:HD11	1.87	0.57
56:SP:1137:ILE:HD11	56:SP:1150:ILE:CG2	2.35	0.57
2:L1:1157:A:O2'	2:L1:1159:C:OP1	2.15	0.57
36:NH:1233:ASN:OD1	36:NH:1234:PHE:N	2.38	0.57
2:L1:472:U:O2'	2:L1:769:A:N3	2.33	0.57
42:NS:923:CYS:HB2	42:NS:1083:MET:HE1	1.87	0.57
56:SP:267:SER:O	56:SP:313:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LR:295:PRO:O	26:LR:296:ILE:HD13	2.04	0.56
35:NG:90:ARG:O	35:NG:92:LYS:NZ	2.37	0.56
36:NH:674:SER:OG	36:NH:675:GLU:OE2	2.18	0.56
63:SW:68:SER:HG	63:SW:82:THR:HG1	1.51	0.56
2:L1:861:U:O2'	13:LE:56:HIS:O	2.24	0.56
16:LH:722:LEU:HD11	16:LH:763:ILE:HG21	1.87	0.56
22:LN:205:CYS:SG	22:LN:211:ARG:NH1	2.77	0.56
16:LH:77:ILE:HD11	16:LH:131:HIS:CD2	2.40	0.56
28:LT:604:SER:OG	28:LT:606:ASP:OD1	2.19	0.56
52:SI:952:PHE:CD2	52:SI:958:VAL:HG22	2.39	0.56
56:SP:1763:LEU:HD22	56:SP:1811:ILE:HD13	1.88	0.56
11:LC:123:ARG:NH2	23:LO:513:GLU:OE1	2.38	0.56
56:SP:512:ASP:OD2	56:SP:513:ASN:N	2.35	0.56
8:L7:96:ARG:HD2	8:L7:121:VAL:HG12	1.87	0.56
56:SP:398:GLN:NE2	56:SP:438:GLU:OE1	2.39	0.56
2:L1:896:U:OP1	39:NM:26:ARG:NH2	2.38	0.56
21:LM:730:GLN:N	21:LM:730:GLN:OE1	2.38	0.56
25:LQ:398:ASP:OD2	25:LQ:407:ALA:HB3	2.05	0.56
30:LZ:54:ILE:CG2	30:LZ:97:LEU:HD21	2.36	0.56
23:LO:195:MET:HE3	23:LO:195:MET:HA	1.87	0.56
23:LO:586:SER:OG	23:LO:588:ASP:OD1	2.09	0.56
24:LP:371:ILE:O	24:LP:418:TYR:OH	2.23	0.56
25:LQ:107:ASP:O	25:LQ:111:LYS:N	2.39	0.56
16:LH:657:SER:OG	16:LH:674:THR:OG1	2.24	0.56
30:LZ:44:TYR:O	30:LZ:48:ASN:ND2	2.33	0.56
2:L1:1555:A:O2'	2:L1:1556:A:O4'	2.23	0.56
21:LM:517:THR:O	21:LM:522:ARG:NH2	2.39	0.56
2:L1:194:U:O2'	2:L1:195:G:O5'	2.17	0.56
36:NH:1108:LEU:HD22	36:NH:1169:ILE:HD11	1.87	0.56
52:SI:219:GLU:N	52:SI:219:GLU:OE1	2.39	0.56
46:SA:223:ILE:HG23	46:SA:223:ILE:O	2.05	0.55
56:SP:1449:ASP:O	56:SP:1453:ASN:ND2	2.36	0.55
17:LI:632:THR:CG2	19:LK:492:ILE:HG23	2.37	0.55
21:LM:311:ASN:OD1	21:LM:312:VAL:N	2.38	0.55
31:NA:486:ASN:OD1	31:NA:487:ALA:N	2.39	0.55
32:NB:392:GLU:N	32:NB:392:GLU:OE1	2.35	0.55
36:NH:480:MET:HE2	36:NH:485:TYR:HA	1.88	0.55
46:SA:265:GLU:OE1	46:SA:265:GLU:N	2.39	0.55
56:SP:319:THR:HG22	56:SP:361:LEU:HB2	1.86	0.55
27:LS:511:LEU:HD13	27:LS:544:VAL:HG21	1.88	0.55
32:NB:401:ILE:H	32:NB:401:ILE:HD12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:SD:117:VAL:HG23	48:SD:118:TYR:HD2	1.70	0.55
5:L4:212:ASP:OD1	5:L4:216:ASN:N	2.39	0.55
6:L5:207:THR:O	6:L5:212:LYS:NZ	2.39	0.55
8:L7:130:VAL:O	8:L7:133:THR:OG1	2.21	0.55
16:LH:682:ASN:O	16:LH:686:GLY:N	2.38	0.55
21:LM:802:PHE:O	21:LM:806:LEU:HD23	2.06	0.55
21:LM:895:GLN:O	21:LM:899:ILE:HD12	2.06	0.55
22:LN:95:LYS:O	22:LN:97:ARG:NH1	2.40	0.55
37:NI:16:VAL:HG21	37:NI:141:LEU:HD11	1.89	0.55
21:LM:1296:MET:HG2	21:LM:1335:LEU:HD21	1.89	0.55
42:NS:1163:ASN:OD1	42:NS:1164:LYS:N	2.40	0.55
53:SJ:51:GLU:HB3	53:SJ:68:LEU:HD12	1.89	0.55
56:SP:1027:ILE:HG23	56:SP:1085:VAL:HG21	1.88	0.55
28:LT:530:ASP:O	28:LT:534:SER:N	2.40	0.55
35:NG:136:ARG:O	63:SW:248:VAL:HG11	2.06	0.55
36:NH:551:GLU:OE1	36:NH:551:GLU:N	2.38	0.55
47:SB:319:ILE:HD12	47:SB:326:LEU:HD22	1.88	0.55
52:SI:3:GLN:NE2	52:SI:5:ASN:OD1	2.39	0.55
2:L1:1502:G:N2	2:L1:1505:A:OP2	2.37	0.55
31:NA:408:SER:O	31:NA:412:ILE:HD12	2.06	0.55
42:NS:486:ASP:OD1	42:NS:487:THR:N	2.40	0.55
2:L1:1223:A:O2'	60:ST:414:LEU:O	2.24	0.55
20:LL:78:LEU:HB3	20:LL:80:MET:HE2	1.89	0.55
44:OH:33:ARG:HE	44:OH:36:LEU:HD12	1.70	0.55
36:NH:543:LEU:HD21	36:NH:691:SER:HB3	1.88	0.55
53:SJ:179:THR:HG22	53:SJ:205:PHE:HB2	1.89	0.55
16:LH:478:ASN:OD1	16:LH:479:ASN:N	2.40	0.55
17:LI:432:ASP:OD1	17:LI:433:ASP:N	2.40	0.55
28:LT:362:GLN:O	28:LT:363:SER:OG	2.22	0.54
18:LJ:259:ASP:OD1	18:LJ:260:TYR:N	2.39	0.54
23:LO:564:PHE:N	23:LO:567:ASP:OD2	2.40	0.54
31:NA:84:LEU:HD23	32:NB:302:LEU:HD23	1.89	0.54
39:NM:180:THR:O	39:NM:184:LEU:N	2.36	0.54
56:SP:1221:ILE:HG23	56:SP:1264:LEU:HD13	1.90	0.54
56:SP:1490:GLU:OE1	56:SP:1529:ARG:NH2	2.40	0.54
61:SU:230:SER:OG	61:SU:288:HIS:ND1	2.40	0.54
36:NH:146:LEU:HD13	36:NH:172:THR:HG21	1.87	0.54
56:SP:1081:ASP:O	56:SP:1085:VAL:HG22	2.07	0.54
28:LT:571:ASP:OD1	28:LT:574:THR:OG1	2.26	0.54
60:ST:660:ILE:HD11	61:SU:388:LEU:HD22	1.88	0.54
16:LH:583:LYS:HE2	16:LH:599:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L9:64:GLU:OE1	10:L9:69:ARG:NH2	2.41	0.54
18:LJ:500:GLU:O	18:LJ:504:ILE:HD12	2.08	0.54
23:LO:841:ASP:OD2	23:LO:842:ASN:N	2.40	0.54
2:L1:392:G:N2	42:NS:59:ASN:OD1	2.28	0.54
17:LI:540:LEU:HD23	17:LI:544:LEU:CD1	2.36	0.54
42:NS:1082:GLN:OE1	63:SW:44:LEU:N	2.41	0.54
46:SA:267:ASP:OD1	47:SB:275:TYR:OH	2.17	0.54
25:LQ:854:CYS:HB3	26:LR:799:LEU:HD12	1.90	0.54
48:SD:87:VAL:O	48:SD:100:ARG:N	2.39	0.54
8:L7:152:VAL:HG21	8:L7:181:ILE:HD11	1.89	0.54
21:LM:725:SER:N	21:LM:728:GLU:OE1	2.40	0.54
28:LT:767:VAL:HG12	28:LT:767:VAL:O	2.08	0.54
42:NS:422:THR:OG1	42:NS:423:GLN:NE2	2.41	0.54
53:SJ:218:ASP:OD1	53:SJ:219:GLU:N	2.41	0.54
16:LH:769:ASN:OD1	16:LH:770:TYR:N	2.39	0.53
42:NS:915:LEU:HD22	42:NS:1049:ILE:HD11	1.90	0.53
47:SB:2:ALA:HB3	47:SB:17:ALA:HB3	1.89	0.53
2:L1:1595:U:OP1	52:SI:945:THR:OG1	2.25	0.53
17:LI:544:LEU:HD23	17:LI:550:LEU:HB3	1.90	0.53
42:NS:1162:ASN:OD1	42:NS:1163:ASN:N	2.41	0.53
44:OH:36:LEU:HG	44:OH:41:LEU:HD12	1.89	0.53
56:SP:1706:LYS:O	56:SP:1760:ASN:ND2	2.40	0.53
2:L1:334:G:O6	9:L8:5:ARG:NH2	2.40	0.53
2:L1:1228:G:N2	44:OH:67:THR:OG1	2.41	0.53
16:LH:724:ILE:HG21	16:LH:762:TYR:CD2	2.44	0.53
17:LI:570:LEU:HD12	17:LI:579:LEU:HD12	1.91	0.53
36:NH:404:GLY:N	36:NH:455:SER:OG	2.41	0.53
42:NS:497:LEU:HD22	42:NS:528:LEU:HD11	1.91	0.53
61:SU:428:THR:OG1	61:SU:430:ASP:OD2	2.24	0.53
23:LO:261:ALA:HB1	23:LO:279:PHE:HB3	1.90	0.53
24:LP:391:TYR:CE2	24:LP:395:ILE:HD11	2.43	0.53
39:NM:61:LEU:HD13	39:NM:96:LEU:CD2	2.39	0.53
60:ST:563:GLU:OE2	61:SU:503:TYR:OH	2.26	0.53
22:LN:586:THR:OG1	22:LN:588:ASP:OD1	2.13	0.53
36:NH:1148:GLN:OE1	37:NI:172:TYR:OH	2.23	0.53
52:SI:142:ILE:HG21	52:SI:190:LEU:HD11	1.90	0.53
52:SI:558:ILE:HD11	52:SI:566:ARG:HH12	1.73	0.53
26:LR:666:GLU:OE2	26:LR:690:HIS:NE2	2.36	0.53
39:NM:61:LEU:HD13	39:NM:96:LEU:HD21	1.91	0.53
56:SP:1600:THR:O	56:SP:1609:ARG:NH2	2.41	0.53
56:SP:1738:TYR:CE2	56:SP:1745:ILE:HG21	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SP:1811:ILE:HG21	56:SP:1879:VAL:HG21	1.90	0.53
2:L1:1269:OMU:HM22	2:L1:1270:G:P	2.49	0.53
21:LM:1482:GLU:OE2	62:SV:56:ARG:NH2	2.40	0.53
36:NH:315:ILE:HB	36:NH:553:VAL:HG23	1.91	0.53
21:LM:281:THR:HG22	27:LS:205:ILE:O	2.09	0.53
42:NS:1227:ILE:O	42:NS:1227:ILE:HG23	2.08	0.53
65:SZ:437:ARG:NH1	65:SZ:460:LEU:O	2.41	0.53
10:L9:151:ASP:OD1	10:L9:152:SER:N	2.42	0.52
26:LR:12:LEU:HD11	26:LR:378:PRO:CG	2.40	0.52
3:L2:169:A:OP2	50:SG:180:LYS:NZ	2.29	0.52
23:LO:673:ARG:NH1	31:NA:451:LEU:O	2.42	0.52
42:NS:915:LEU:HD22	42:NS:1049:ILE:CD1	2.39	0.52
56:SP:1655:ARG:NH1	56:SP:1744:GLU:OE2	2.42	0.52
57:SQ:167:LYS:O	57:SQ:170:LYS:NZ	2.42	0.52
60:ST:555:ARG:NH2	61:SU:524:GLU:OE1	2.41	0.52
21:LM:1081:VAL:HG21	21:LM:1162:VAL:HG22	1.91	0.52
23:LO:673:ARG:NE	30:LZ:145:ASP:OD2	2.36	0.52
38:NL:115:MET:HA	38:NL:115:MET:HE2	1.92	0.52
3:L2:87:G:OP2	47:SB:338:LYS:NZ	2.42	0.52
7:L6:5:ILE:HD12	7:L6:16:PHE:CD2	2.45	0.52
22:LN:66:ARG:NE	22:LN:88:GLU:OE1	2.42	0.52
30:LZ:89:THR:HG21	32:NB:26:VAL:HG23	1.91	0.52
26:LR:249:LEU:HD21	26:LR:316:VAL:HG11	1.91	0.52
31:NA:14:ARG:NH2	32:NB:206:ASP:OD2	2.42	0.52
32:NB:216:MET:HA	32:NB:216:MET:HE3	1.92	0.52
56:SP:356:ASP:OD1	56:SP:357:LYS:N	2.43	0.52
2:L1:1195:C:N3	53:SJ:136:ARG:NH2	2.56	0.52
11:LC:36:ILE:HD11	11:LC:48:VAL:HG12	1.91	0.52
16:LH:702:TYR:CE2	16:LH:710:LEU:HD11	2.45	0.52
22:LN:425:ASP:OD1	22:LN:426:GLN:N	2.43	0.52
23:LO:205:LYS:NZ	23:LO:219:GLU:OE2	2.43	0.52
53:SJ:242:CYS:O	53:SJ:245:ALA:N	2.43	0.52
24:LP:64:ASN:HB2	24:LP:88:ILE:HG21	1.92	0.52
33:ND:180:LEU:HD23	33:ND:181:LEU:N	2.25	0.52
36:NH:1036:HIS:C	36:NH:1037:LEU:HD12	2.34	0.52
51:SH:316:GLU:OE2	52:SI:568:ARG:NH2	2.43	0.52
42:NS:1000:PHE:CE1	42:NS:1144:LEU:HD21	2.45	0.52
42:NS:1214:VAL:HG13	42:NS:1214:VAL:O	2.10	0.52
56:SP:994:ILE:HD12	56:SP:1047:LEU:HD11	1.91	0.52
36:NH:827:ARG:NH1	36:NH:835:LEU:O	2.43	0.52
36:NH:915:LEU:HD21	36:NH:1089:PHE:HZ	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:NH:1144:ASP:OD2	36:NH:1146:THR:HG22	2.09	0.52
42:NS:473:VAL:HG12	42:NS:489:VAL:HB	1.92	0.52
47:SB:240:GLU:HG3	47:SB:241:VAL:HG13	1.92	0.52
52:SI:269:VAL:HG22	52:SI:796:VAL:HG21	1.92	0.52
36:NH:495:THR:HA	36:NH:498:MET:HE2	1.91	0.52
46:SA:54:ALA:HB2	46:SA:81:ILE:HD13	1.92	0.52
2:L1:1148:C:O3'	60:ST:14:LYS:NZ	2.43	0.51
18:LJ:312:ALA:HB3	18:LJ:316:ARG:HH11	1.75	0.51
48:SD:156:MET:HE1	64:SY:126:MET:CE	2.39	0.51
63:SW:74:ASP:OD1	63:SW:78:LYS:N	2.43	0.51
2:L1:748:U:OP1	13:LE:82:LYS:NZ	2.43	0.51
26:LR:393:SER:OG	26:LR:394:LEU:N	2.43	0.51
52:SI:819:GLU:OE1	52:SI:819:GLU:N	2.43	0.51
10:L9:57:ARG:O	10:L9:61:THR:HG23	2.11	0.51
13:LE:11:LEU:HD12	13:LE:74:VAL:HG13	1.93	0.51
21:LM:1089:ASN:ND2	21:LM:1182:GLU:OE1	2.43	0.51
36:NH:239:LEU:O	36:NH:243:LEU:HD23	2.10	0.51
24:LP:268:ASP:OD2	24:LP:269:ILE:N	2.43	0.51
26:LR:673:MET:HE1	26:LR:693:ARG:HG2	1.92	0.51
31:NA:84:LEU:HD23	32:NB:302:LEU:CD2	2.39	0.51
62:SV:155:ASN:OD1	62:SV:156:THR:N	2.43	0.51
2:L1:1057:U:O4	36:NH:791:LYS:NZ	2.43	0.51
17:LI:537:THR:HA	17:LI:540:LEU:HD12	1.90	0.51
38:NL:110:MET:HE1	38:NL:114:PHE:HB3	1.93	0.51
57:SQ:120:ASP:O	57:SQ:124:ILE:HD12	2.11	0.51
62:SV:147:LEU:O	62:SV:151:VAL:HG22	2.09	0.51
1:L0:87:C:O2	16:LH:332:GLN:NE2	2.43	0.51
9:L8:49:ARG:O	9:L8:52:ASN:ND2	2.43	0.51
16:LH:753:LYS:NZ	17:LI:430:LEU:O	2.35	0.51
20:LL:253:LEU:HD21	20:LL:301:LEU:HD21	1.91	0.51
20:LL:458:ASN:OD1	20:LL:460:ARG:NH1	2.44	0.51
21:LM:1445:ILE:HG23	21:LM:1450:LEU:HD11	1.93	0.51
26:LR:12:LEU:HD11	26:LR:378:PRO:HG2	1.92	0.51
53:SJ:71:ASP:OD1	53:SJ:72:ASP:N	2.43	0.51
2:L1:420:A2M:HM'2	2:L1:421:A:O4'	2.09	0.51
7:L6:78:THR:HG22	7:L6:92:ARG:HD2	1.92	0.51
21:LM:235:VAL:HG11	27:LS:218:TYR:CG	2.46	0.51
44:OH:106:ILE:HD12	60:ST:278:GLN:O	2.11	0.51
7:L6:23:ARG:O	7:L6:26:VAL:HG12	2.10	0.51
2:L1:1271:OMG:H2'	2:L1:1272:U:C6	2.46	0.51
18:LJ:304:SER:O	18:LJ:321:GLY:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:LP:355:LEU:HD13	24:LP:358:LEU:HD12	1.92	0.51
36:NH:829:GLU:N	36:NH:829:GLU:OE1	2.44	0.51
56:SP:259:LEU:HD11	56:SP:302:PHE:HE2	1.76	0.51
56:SP:1652:ASP:OD1	56:SP:1655:ARG:NH2	2.43	0.51
16:LH:302:SER:OG	16:LH:344:CYS:N	2.43	0.51
32:NB:269:HIS:O	32:NB:273:ASN:ND2	2.41	0.51
47:SB:230:GLU:HG2	47:SB:231:ILE:HD12	1.92	0.51
2:L1:556:A:H61	64:SY:19:LEU:HD11	1.76	0.50
20:LL:458:ASN:O	20:LL:460:ARG:NH1	2.38	0.50
24:LP:117:MET:HE1	24:LP:128:LYS:HG3	1.92	0.50
60:ST:289:THR:HG23	65:SZ:429:LYS:NZ	2.26	0.50
3:L2:312:U:OP1	57:SQ:163:ARG:NH2	2.44	0.50
31:NA:384:ARG:NH1	55:SM:83:ILE:HD11	2.25	0.50
36:NH:931:ASP:OD1	36:NH:932:GLU:N	2.43	0.50
37:NI:84:VAL:HG11	37:NI:126:LEU:HD21	1.91	0.50
47:SB:221:THR:O	47:SB:236:LYS:NZ	2.43	0.50
56:SP:1382:PRO:O	56:SP:1430:TYR:OH	2.26	0.50
33:ND:112:LEU:HD21	61:SU:90:TRP:CB	2.40	0.50
42:NS:675:ASP:OD1	42:NS:736:SER:OG	2.26	0.50
48:SD:253:ILE:HD13	48:SD:269:ILE:HD12	1.92	0.50
56:SP:1137:ILE:CG2	56:SP:1185:LEU:HD11	2.41	0.50
21:LM:1689:LYS:O	21:LM:1692:VAL:HG22	2.10	0.50
47:SB:110:ASP:OD1	47:SB:113:THR:HG23	2.12	0.50
3:L2:331:A:O2'	47:SB:404:ARG:NH1	2.42	0.50
19:LK:438:SER:O	19:LK:442:THR:HG23	2.12	0.50
28:LT:192:ASN:O	28:LT:196:GLY:N	2.42	0.50
3:L2:0:M7G:H82	3:L2:1:G:O4'	2.11	0.50
25:LQ:53:ASP:OD2	25:LQ:56:THR:OG1	2.30	0.50
36:NH:144:LYS:O	36:NH:176:PHE:N	2.42	0.50
38:NL:90:MET:HE3	38:NL:90:MET:HA	1.93	0.50
53:SK:141:MET:HE2	53:SK:141:MET:HA	1.94	0.50
64:SY:114:GLU:OE2	64:SY:207:ARG:NH2	2.44	0.50
38:NL:308:TYR:HD1	42:NS:117:LEU:HD23	1.75	0.50
8:L7:49:ILE:HD11	8:L7:172:VAL:HG22	1.93	0.50
2:L1:763:G:N2	2:L1:774:A:N7	2.60	0.50
23:LO:459:SER:HB2	23:LO:466:LEU:HD21	1.94	0.50
28:LT:367:LEU:HD21	28:LT:445:MET:SD	2.52	0.50
30:LZ:153:ASN:OD1	30:LZ:154:MET:N	2.45	0.50
56:SP:976:TYR:O	56:SP:980:ASN:ND2	2.44	0.50
21:LM:647:GLU:OE1	21:LM:647:GLU:N	2.40	0.49
21:LM:1681:ASP:OD1	21:LM:1682:GLU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LO:708:ASP:OD1	23:LO:709:THR:N	2.43	0.49
26:LR:547:LEU:HD22	26:LR:568:MET:CE	2.42	0.49
28:LT:626:ASP:OD1	28:LT:627:ASN:N	2.45	0.49
36:NH:1146:THR:HG21	36:NH:1180:ASN:ND2	2.27	0.49
48:SC:175:ALA:HB1	48:SC:181:VAL:HG21	1.93	0.49
56:SP:170:LEU:HD22	56:SP:203:CYS:SG	2.52	0.49
56:SP:1685:SER:O	56:SP:1689:VAL:HG23	2.12	0.49
2:L1:251:A:C2	5:L4:131:LEU:HD12	2.46	0.49
2:L1:558:U:OP1	52:SI:931:LYS:NZ	2.45	0.49
8:L7:70:PHE:O	8:L7:74:GLN:N	2.46	0.49
21:LM:1265:HIS:HB3	46:SA:432:MET:HE1	1.94	0.49
30:LZ:79:LEU:HD23	30:LZ:97:LEU:HD12	1.94	0.49
52:SI:838:ILE:HD12	52:SI:874:TYR:HB3	1.94	0.49
56:SP:1720:ILE:O	56:SP:1724:ASN:ND2	2.45	0.49
5:L4:173:ILE:HD13	5:L4:229:GLY:HA2	1.94	0.49
18:LJ:53:HIS:NE2	18:LJ:311:THR:O	2.45	0.49
18:LJ:209:LEU:HD21	18:LJ:242:ASN:OD1	2.10	0.49
25:LQ:480:ASP:OD2	25:LQ:539:VAL:N	2.44	0.49
41:NQ:67:THR:OG1	41:NQ:70:LYS:O	2.29	0.49
36:NH:655:LEU:HD13	36:NH:665:HIS:CD2	2.48	0.49
42:NS:1003:VAL:HG11	42:NS:1084:ILE:HD13	1.95	0.49
60:ST:388:LEU:O	60:ST:392:LYS:N	2.45	0.49
16:LH:568:ASN:O	16:LH:568:ASN:ND2	2.37	0.49
16:LH:822:PHE:HD1	20:LL:91:LEU:HD21	1.78	0.49
16:LH:883:GLN:OE1	16:LH:884:MET:N	2.45	0.49
25:LQ:676:SER:OG	25:LQ:677:HIS:N	2.45	0.49
39:NM:32:ILE:HG12	39:NM:96:LEU:HD12	1.94	0.49
17:LI:547:GLN:OE1	17:LI:549:ARG:N	2.45	0.49
21:LM:1441:ILE:O	21:LM:1445:ILE:HD12	2.12	0.49
47:SB:163:ILE:HD11	47:SB:283:ILE:HD12	1.94	0.49
2:L1:1794:A:N6	52:SI:2:GLU:OE2	2.46	0.49
28:LT:794:LYS:HE3	42:NS:1204:LEU:HD11	1.93	0.49
47:SB:3:TYR:N	47:SB:86:THR:O	2.42	0.49
48:SD:111:MET:HE2	48:SD:216:ASN:HD22	1.78	0.49
60:ST:232:MET:HE3	65:SZ:224:TRP:HA	1.95	0.49
16:LH:366:ASN:HA	16:LH:399:ILE:HD13	1.95	0.49
18:LJ:134:THR:HG23	18:LJ:135:GLN:OE1	2.13	0.49
21:LM:764:ASN:OD1	21:LM:765:ASN:N	2.44	0.49
39:NM:108:ASP:OD1	39:NM:109:LYS:N	2.45	0.49
46:SA:26:ASP:OD1	46:SA:27:ILE:N	2.46	0.49
53:SJ:74:GLN:N	53:SJ:74:GLN:OE1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SP:615:VAL:HG13	56:SP:619:LEU:HD23	1.93	0.49
2:L1:959:U:OP2	41:NQ:20:LYS:NZ	2.46	0.49
2:L1:1614:A:OP2	6:L5:84:LYS:NZ	2.46	0.49
16:LH:96:ILE:HD12	16:LH:151:TYR:CZ	2.48	0.49
21:LM:287:ASP:O	21:LM:292:LYS:NZ	2.46	0.49
25:LQ:829:VAL:HG13	25:LQ:860:ILE:HG21	1.95	0.49
30:LZ:170:LEU:HD21	64:SY:63:TYR:HB2	1.94	0.49
47:SB:215:ARG:NH1	47:SB:242:SER:OG	2.44	0.49
52:SI:91:ARG:O	52:SI:95:LYS:N	2.44	0.49
56:SP:535:ASN:OD1	56:SP:571:LEU:HD21	2.13	0.49
2:L1:318:U:OP1	42:NS:33:ARG:NH2	2.46	0.49
2:L1:524:U:O2'	2:L1:526:A:N7	2.44	0.48
4:L3:110:ARG:NH2	60:ST:747:GLU:OE2	2.46	0.48
18:LJ:366:TYR:OH	18:LJ:371:GLU:OE2	2.22	0.48
20:LL:436:THR:OG1	20:LL:471:ARG:NH2	2.46	0.48
2:L1:1226:A:H61	44:OH:114:LYS:HG2	1.78	0.48
8:L7:133:THR:HG21	8:L7:162:ILE:HD13	1.95	0.48
21:LM:1740:ASP:OD1	21:LM:1741:ASP:N	2.46	0.48
23:LO:33:VAL:HG23	23:LO:33:VAL:O	2.12	0.48
52:SI:555:MET:O	52:SI:558:ILE:HG22	2.14	0.48
20:LL:520:MET:HA	20:LL:520:MET:HE3	1.94	0.48
21:LM:661:ILE:HG21	21:LM:666:ALA:HB3	1.96	0.48
36:NH:801:LYS:NZ	36:NH:836:GLU:OE1	2.33	0.48
42:NS:1005:ARG:HH21	42:NS:1140:ILE:HD13	1.78	0.48
46:SA:219:LEU:O	46:SA:223:ILE:HG22	2.13	0.48
53:SK:77:LEU:HD22	53:SK:84:ILE:HG22	1.96	0.48
16:LH:180:ASP:OD1	16:LH:181:ALA:N	2.46	0.48
22:LN:150:ASN:ND2	22:LN:154:ASP:OD1	2.43	0.48
36:NH:439:HIS:CE1	36:NH:458:ILE:HD13	2.48	0.48
38:NL:284:VAL:HG13	38:NL:309:ALA:CB	2.44	0.48
46:SA:231:ASP:O	46:SA:235:HIS:ND1	2.43	0.48
52:SI:557:ASN:OD1	52:SI:558:ILE:N	2.46	0.48
2:L1:1193:A:O2'	2:L1:1194:A:O4'	2.30	0.48
5:L4:103:TYR:O	5:L4:182:TYR:OH	2.29	0.48
16:LH:656:ASP:OD1	16:LH:657:SER:N	2.46	0.48
21:LM:235:VAL:HG13	21:LM:239:LEU:HD12	1.95	0.48
21:LM:1296:MET:HE1	21:LM:1306:SER:OG	2.13	0.48
21:LM:1590:ILE:O	21:LM:1590:ILE:HG22	2.13	0.48
23:LO:434:ASN:OD1	23:LO:435:CYS:N	2.47	0.48
35:NG:30:VAL:HG11	35:NG:71:CYS:SG	2.53	0.48
60:ST:247:MET:HA	60:ST:247:MET:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:1697:G:OP2	36:NH:316:ARG:NH1	2.46	0.48
4:L3:15:LEU:HD11	4:L3:66:LEU:HD13	1.95	0.48
6:L5:136:ALA:O	6:L5:140:THR:HG22	2.13	0.48
6:L5:186:ASN:OD1	6:L5:187:ILE:N	2.46	0.48
16:LH:662:VAL:HG23	16:LH:670:LEU:HD21	1.96	0.48
23:LO:415:ASP:O	23:LO:419:TYR:N	2.47	0.48
23:LO:748:GLU:OE2	23:LO:777:ARG:NH2	2.47	0.48
26:LR:603:ASP:O	26:LR:607:GLY:N	2.43	0.48
38:NL:98:VAL:HG11	38:NL:107:LEU:HD23	1.94	0.48
46:SA:185:ASP:OD1	46:SA:285:ARG:NE	2.47	0.48
8:L7:7:LYS:NZ	8:L7:39:ARG:O	2.46	0.48
18:LJ:134:THR:HG23	18:LJ:135:GLN:CD	2.39	0.48
21:LM:864:VAL:O	21:LM:864:VAL:HG23	2.13	0.48
27:LS:224:ASN:OD1	27:LS:225:SER:N	2.47	0.48
51:SH:57:GLU:CD	60:ST:112:VAL:HG23	2.39	0.48
55:SM:218:SER:O	55:SM:238:TYR:OH	2.32	0.48
56:SP:137:ASP:O	56:SP:140:ILE:HG22	2.14	0.48
56:SP:1493:VAL:HG11	56:SP:1547:LEU:HD21	1.96	0.48
2:L1:405:C:O2'	7:L6:92:ARG:O	2.21	0.48
2:L1:514:G:N7	10:L9:171:ARG:NH2	2.62	0.48
6:L5:118:LEU:HD22	6:L5:129:PRO:HB2	1.96	0.48
22:LN:382:VAL:HG11	22:LN:755:ILE:HD13	1.96	0.48
56:SP:1501:ARG:NH1	56:SP:1505:ASN:OD1	2.47	0.48
3:L2:0:M7G:H82	3:L2:1:G:C1'	2.44	0.47
3:L2:282:U:O2'	3:L2:284:U:O5'	2.28	0.47
16:LH:640:LYS:HZ3	16:LH:652:GLU:CG	2.27	0.47
36:NH:107:ILE:HD13	36:NH:507:PHE:HE1	1.77	0.47
40:NP:125:SER:O	40:NP:129:GLN:N	2.40	0.47
44:OH:28:LEU:HD21	44:OH:89:ILE:HD13	1.96	0.47
47:SB:91:GLU:OE2	48:SD:231:ARG:NH1	2.47	0.47
53:SJ:51:GLU:OE2	53:SJ:82:ARG:NH2	2.47	0.47
60:ST:453:ASN:OD1	60:ST:454:ALA:N	2.47	0.47
8:L7:73:VAL:HG22	8:L7:73:VAL:O	2.14	0.47
21:LM:1303:VAL:HG22	21:LM:1344:MET:HE3	1.96	0.47
21:LM:1657:ASN:OD1	21:LM:1657:ASN:O	2.32	0.47
22:LN:448:THR:OG1	22:LN:475:THR:OG1	2.12	0.47
46:SA:28:GLY:O	46:SA:34:VAL:HG21	2.14	0.47
53:SJ:246:GLU:HA	53:SJ:251:ILE:HD12	1.96	0.47
65:SZ:246:ILE:HG21	65:SZ:282:ILE:HD11	1.96	0.47
4:L3:102:ALA:CB	60:ST:740:MET:HE1	2.44	0.47
23:LO:707:ASN:OD1	23:LO:708:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:829:VAL:HG21	25:LQ:864:ASN:ND2	2.28	0.47
26:LR:561:SER:O	26:LR:565:PHE:N	2.47	0.47
36:NH:282:ASP:OD1	36:NH:283:TYR:N	2.47	0.47
42:NS:104:GLN:O	42:NS:107:ARG:N	2.46	0.47
42:NS:497:LEU:HD23	42:NS:497:LEU:O	2.15	0.47
56:SP:1088:LYS:NZ	56:SP:1125:ASP:OD1	2.47	0.47
56:SP:1406:LEU:HD22	56:SP:1488:MET:HB3	1.95	0.47
2:L1:562:OMG:HM23	55:SM:281:ILE:CD1	2.44	0.47
2:L1:1657:U:OP1	2:L1:1658:G:O2'	2.28	0.47
18:LJ:168:THR:OG1	18:LJ:190:ASP:OD1	2.30	0.47
23:LO:210:SER:OG	23:LO:212:ASP:OD1	2.32	0.47
61:SU:378:SER:OG	61:SU:453:PRO:O	2.19	0.47
3:L2:107:C:N4	46:SA:334:GLN:OE1	2.48	0.47
11:LC:54:LEU:HD11	11:LC:112:TYR:CD2	2.49	0.47
18:LJ:272:LEU:N	18:LJ:284:PHE:O	2.46	0.47
23:LO:730:LEU:HD21	23:LO:754:VAL:HG13	1.97	0.47
26:LR:597:GLY:HA2	26:LR:620:LEU:HD13	1.97	0.47
28:LT:198:LEU:HD21	28:LT:201:THR:OG1	2.14	0.47
36:NH:1144:ASP:OD1	36:NH:1169:ILE:HD13	2.15	0.47
2:L1:967:A:OP2	34:NF:124:ARG:NH2	2.43	0.47
3:L2:323:G:O2'	64:SY:112:GLN:OE1	2.30	0.47
16:LH:374:LEU:HD23	16:LH:381:SER:HA	1.96	0.47
20:LL:225:VAL:HG23	20:LL:225:VAL:O	2.14	0.47
21:LM:1433:ASP:OD1	21:LM:1434:SER:N	2.46	0.47
25:LQ:56:THR:OG1	25:LQ:58:ASP:OD1	2.29	0.47
28:LT:762:LEU:HD23	28:LT:766:LYS:HD3	1.95	0.47
36:NH:1169:ILE:HG22	36:NH:1180:ASN:HB2	1.96	0.47
38:NL:121:TYR:OH	38:NL:123:ASP:OD1	2.13	0.47
42:NS:529:ILE:HD11	42:NS:557:ILE:HD13	1.96	0.47
46:SA:21:LYS:N	46:SA:47:LEU:O	2.47	0.47
48:SC:234:ILE:HG22	48:SC:235:GLY:O	2.14	0.47
65:SZ:246:ILE:HD11	65:SZ:266:PHE:CZ	2.49	0.47
1:L0:278:G:H22	27:LS:539:ASP:CG	2.21	0.47
6:L5:90:ILE:O	6:L5:94:THR:HG23	2.14	0.47
8:L7:114:ARG:O	8:L7:118:LEU:HD13	2.15	0.47
8:L7:136:VAL:N	8:L7:153:LEU:O	2.48	0.47
28:LT:824:GLY:O	28:LT:828:LYS:N	2.48	0.47
31:NA:560:ALA:HB3	31:NA:563:ILE:HD12	1.97	0.47
42:NS:408:ASP:OD2	42:NS:409:VAL:N	2.48	0.47
42:NS:497:LEU:HD21	42:NS:507:LEU:HD11	1.95	0.47
42:NS:1190:TYR:CE1	42:NS:1247:VAL:HG21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SB:3:TYR:HB2	47:SB:87:LEU:HD12	1.96	0.47
51:SH:153:THR:O	51:SH:153:THR:HG23	2.15	0.47
53:SK:101:ASP:OD2	53:SK:132:ARG:NH2	2.47	0.47
2:L1:1657:U:O4'	25:LQ:450:ARG:NH1	2.48	0.47
16:LH:627:ASP:OD1	16:LH:628:ASP:N	2.48	0.47
21:LM:193:THR:OG1	21:LM:241:ILE:HD11	2.15	0.47
56:SP:994:ILE:HD11	56:SP:1036:VAL:HG21	1.96	0.47
12:LD:25:VAL:HG12	12:LD:27:THR:HG23	1.97	0.47
31:NA:357:ILE:HG21	55:SM:253:ARG:HH21	1.80	0.47
13:LE:37:PHE:CZ	13:LE:103:ILE:HD12	2.51	0.47
18:LJ:238:ASP:O	18:LJ:242:ASN:N	2.46	0.47
25:LQ:829:VAL:HG13	25:LQ:860:ILE:CG2	2.45	0.47
28:LT:900:ASN:OD1	28:LT:901:LYS:N	2.48	0.47
37:NI:188:MET:HA	37:NI:188:MET:HE2	1.97	0.47
45:OU:125:THR:HG21	65:SZ:238:SER:O	2.14	0.47
48:SC:230:TYR:CD1	48:SC:234:ILE:HD12	2.50	0.47
2:L1:565:C:OP1	52:SI:973:ARG:NH2	2.44	0.46
2:L1:1083:G:OP1	54:SL:112:LYS:NZ	2.33	0.46
2:L1:1472:C:O2	2:L1:1534:G:N2	2.48	0.46
2:L1:1594:G:O2'	2:L1:1600:A:N6	2.45	0.46
3:L2:256:G:OP1	46:SA:382:LYS:NZ	2.48	0.46
13:LE:41:MET:HG2	13:LE:129:VAL:HG21	1.96	0.46
32:NB:221:ALA:HB3	32:NB:222:PRO:HD3	1.97	0.46
42:NS:1122:ALA:O	42:NS:1227:ILE:HG22	2.15	0.46
2:L1:498:G:N7	57:SQ:138:LYS:NZ	2.60	0.46
2:L1:886:U:OP2	39:NM:216:LYS:NZ	2.43	0.46
2:L1:1013:A:O2'	38:NL:236:ARG:NH2	2.48	0.46
8:L7:64:VAL:HG12	8:L7:94:ALA:HB1	1.96	0.46
21:LM:944:VAL:HG12	21:LM:948:LEU:CD1	2.45	0.46
23:LO:718:ASP:OD1	23:LO:719:VAL:N	2.48	0.46
26:LR:269:LEU:HD13	26:LR:320:LEU:HD13	1.96	0.46
36:NH:756:VAL:HG12	36:NH:756:VAL:O	2.15	0.46
50:SG:241:THR:HG21	50:SG:285:SER:HA	1.97	0.46
51:SH:243:ILE:HG23	51:SH:275:VAL:HG21	1.97	0.46
52:SI:99:ASN:OD1	52:SI:100:ASP:N	2.48	0.46
2:L1:1575:G:C5	53:SK:148:LEU:HD21	2.50	0.46
21:LM:708:ALA:O	21:LM:710:LYS:NZ	2.48	0.46
36:NH:169:PRO:HA	36:NH:172:THR:HG22	1.97	0.46
26:LR:180:ARG:NH2	63:SW:82:THR:O	2.48	0.46
36:NH:287:LYS:O	36:NH:289:ARG:NH1	2.49	0.46
38:NL:39:LEU:HD13	38:NL:196:PHE:HE1	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SK:19:LEU:HD21	61:SU:419:PRO:HG3	1.98	0.46
2:L1:1220:C:OP2	65:SZ:346:SER:OG	2.30	0.46
2:L1:1682:U:O2	2:L1:1720:G:N2	2.49	0.46
21:LM:560:ILE:HG22	21:LM:560:ILE:O	2.16	0.46
21:LM:925:LEU:HD12	21:LM:941:LEU:CD2	2.46	0.46
26:LR:155:GLN:OE1	26:LR:155:GLN:HA	2.16	0.46
42:NS:451:ARG:NH1	42:NS:762:ASN:OD1	2.45	0.46
50:SG:60:ALA:HB2	56:SP:46:HIS:HE1	1.80	0.46
56:SP:464:PHE:O	56:SP:468:ALA:HB2	2.16	0.46
19:LK:503:LEU:HA	19:LK:506:LEU:HD12	1.97	0.46
28:LT:767:VAL:HG11	63:SW:179:ASP:HB2	1.97	0.46
37:NI:16:VAL:CG2	37:NI:141:LEU:HD11	2.45	0.46
38:NL:115:MET:O	38:NL:140:LYS:NZ	2.48	0.46
47:SB:2:ALA:HB2	47:SB:20:LYS:HA	1.98	0.46
52:SI:795:LYS:HA	52:SI:795:LYS:HE2	1.96	0.46
2:L1:501:U:O2'	2:L1:502:U:OP2	2.26	0.46
26:LR:698:LEU:HD13	26:LR:759:THR:HG21	1.97	0.46
42:NS:494:ASP:OD1	42:NS:495:GLY:N	2.49	0.46
48:SC:225:ARG:NH2	48:SC:246:GLN:OE1	2.49	0.46
56:SP:1556:ARG:HE	56:SP:1621:LEU:HD13	1.79	0.46
2:L1:556:A:N6	64:SY:19:LEU:HD11	2.31	0.46
2:L1:1227:A:N6	2:L1:1256:A:O2'	2.47	0.46
16:LH:722:LEU:HD11	16:LH:763:ILE:CG2	2.45	0.46
36:NH:976:ILE:HD11	36:NH:1017:TYR:CE1	2.50	0.46
50:SG:256:ARG:NH1	50:SG:282:GLU:OE1	2.49	0.46
50:SG:481:ILE:HD12	50:SG:481:ILE:H	1.81	0.46
53:SJ:141:MET:HA	53:SJ:141:MET:HE2	1.96	0.46
56:SP:358:VAL:CG1	56:SP:389:ILE:HD11	2.44	0.46
61:SU:155:LEU:O	61:SU:218:LYS:NZ	2.48	0.46
2:L1:32:U:O2'	2:L1:594:A:N1	2.45	0.46
2:L1:97:C:H1'	2:L1:426:G:H5'	1.98	0.46
3:L2:331:A:O2'	47:SB:404:ARG:NH2	2.47	0.46
16:LH:747:ASP:OD2	16:LH:751:SER:OG	2.34	0.46
17:LI:570:LEU:HD21	17:LI:637:LEU:HD21	1.98	0.46
36:NH:469:ASP:O	36:NH:473:LYS:N	2.46	0.46
37:NI:67:MET:HE2	37:NI:67:MET:HA	1.97	0.46
49:SF:48:ILE:C	49:SF:104:THR:HG23	2.41	0.46
56:SP:550:GLU:OE1	56:SP:591:LEU:HD21	2.15	0.46
56:SP:1080:GLU:OE1	56:SP:1080:GLU:N	2.46	0.46
58:SR:57:LEU:HD12	58:SR:58:GLY:N	2.31	0.46
16:LH:618:ASP:OD1	16:LH:619:GLY:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SG:289:ARG:NH1	50:SG:294:GLN:OE1	2.48	0.45
56:SP:1308:LEU:O	56:SP:1324:ILE:HD13	2.15	0.45
6:L5:140:THR:OG1	6:L5:210:ALA:HB1	2.16	0.45
22:LN:495:VAL:HG21	22:LN:513:LEU:HD21	1.98	0.45
31:NA:384:ARG:NH2	55:SM:81:SER:O	2.50	0.45
60:ST:289:THR:HG23	65:SZ:429:LYS:HZ1	1.81	0.45
2:L1:495:C:OP1	52:SI:1135:ARG:NH1	2.48	0.45
16:LH:135:SER:C	16:LH:136:LEU:HD12	2.42	0.45
21:LM:247:ALA:HA	27:LS:205:ILE:HD11	1.97	0.45
21:LM:1620:ARG:HB2	21:LM:1662:ILE:HD12	1.99	0.45
38:NL:59:VAL:HG23	38:NL:80:ASN:HB3	1.98	0.45
54:SL:67:ILE:CD1	54:SL:86:MET:HE1	2.46	0.45
6:L5:16:VAL:HG11	28:LT:534:SER:HB3	1.98	0.45
18:LJ:432:TYR:O	18:LJ:470:TYR:OH	2.34	0.45
20:LL:472:LEU:HD23	20:LL:473:LYS:O	2.17	0.45
31:NA:476:MET:HA	31:NA:476:MET:HE3	1.98	0.45
46:SA:44:PHE:CE2	46:SA:48:ILE:HD11	2.52	0.45
47:SB:214:ILE:HD11	47:SB:252:LEU:HD22	1.99	0.45
56:SP:1763:LEU:CD2	56:SP:1811:ILE:HD13	2.46	0.45
60:ST:385:ASP:OD1	60:ST:386:ALA:N	2.48	0.45
8:L7:165:LYS:O	8:L7:168:SER:OG	2.24	0.45
18:LJ:375:HIS:NE2	18:LJ:377:ASP:OD2	2.49	0.45
21:LM:1652:VAL:HG11	21:LM:1690:LEU:HB3	1.98	0.45
21:LM:1662:ILE:HG22	21:LM:1662:ILE:O	2.16	0.45
37:NI:43:GLN:OE1	37:NI:43:GLN:N	2.49	0.45
54:SL:75:SER:OG	54:SL:80:VAL:O	2.34	0.45
56:SP:582:LEU:HB3	56:SP:657:LEU:HD11	1.99	0.45
56:SP:1189:LEU:HD22	56:SP:1194:SER:HB3	1.98	0.45
2:L1:407:A:H4'	42:NS:63:LEU:HD13	1.98	0.45
2:L1:532:U:OP1	10:L9:132:ARG:NH2	2.49	0.45
16:LH:145:PHE:HZ	16:LH:230:LEU:HD13	1.78	0.45
17:LI:494:ASP:O	17:LI:497:ILE:HG22	2.17	0.45
17:LI:673:THR:O	17:LI:677:ASN:ND2	2.49	0.45
21:LM:210:LEU:O	21:LM:214:THR:HG23	2.17	0.45
23:LO:811:ASN:OD1	23:LO:814:LYS:NZ	2.42	0.45
25:LQ:536:CYS:N	25:LQ:549:SER:OG	2.50	0.45
28:LT:132:THR:OG1	28:LT:134:ASP:OD1	2.24	0.45
60:ST:659:GLU:OE1	60:ST:659:GLU:N	2.50	0.45
2:L1:1663:G:OP1	42:NS:251:ARG:NE	2.49	0.45
16:LH:27:SER:OG	16:LH:171:TYR:OH	2.24	0.45
18:LJ:42:VAL:HG23	18:LJ:42:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LM:1265:HIS:CB	46:SA:432:MET:HE1	2.46	0.45
22:LN:152:SER:OG	22:LN:198:ASP:OD2	2.35	0.45
22:LN:374:THR:OG1	22:LN:757:ARG:NH1	2.50	0.45
36:NH:412:LEU:HD21	36:NH:424:GLY:HA3	1.99	0.45
53:SK:104:ILE:N	53:SK:246:GLU:OE1	2.50	0.45
56:SP:1027:ILE:CG2	56:SP:1085:VAL:HG21	2.46	0.45
56:SP:1466:ILE:CG2	56:SP:1489:ILE:HD11	2.45	0.45
62:SV:152:SER:OG	62:SV:153:THR:N	2.50	0.45
18:LJ:285:ASP:CG	18:LJ:293:LYS:HZ3	2.25	0.45
21:LM:1419:ILE:HD13	21:LM:1448:ILE:HD13	1.99	0.45
22:LN:279:HIS:HD1	22:LN:301:ASP:CG	2.25	0.45
26:LR:30:LYS:O	26:LR:45:LEU:N	2.44	0.45
28:LT:354:SER:N	28:LT:369:ALA:O	2.44	0.45
51:SH:337:VAL:N	52:SI:554:TYR:OH	2.44	0.45
53:SJ:240:LYS:NZ	53:SK:246:GLU:OE2	2.48	0.45
53:SK:156:GLU:HG2	53:SK:157:GLU:OE1	2.17	0.45
56:SP:1164:ASP:OD1	56:SP:1167:TYR:N	2.44	0.45
2:L1:1478:G:OP1	40:NP:39:THR:OG1	2.35	0.45
26:LR:538:ASP:OD1	26:LR:539:VAL:N	2.50	0.45
27:LS:257:HIS:HE2	27:LS:310:GLN:HG2	1.80	0.45
48:SD:267:VAL:CG1	48:SD:269:ILE:HD11	2.46	0.45
53:SJ:90:ASP:OD1	53:SJ:91:ILE:N	2.49	0.45
16:LH:640:LYS:HZ3	16:LH:652:GLU:HG2	1.82	0.45
16:LH:682:ASN:ND2	16:LH:689:ILE:HD11	2.32	0.45
19:LK:466:GLU:OE1	19:LK:466:GLU:N	2.50	0.45
27:LS:180:ASP:OD2	27:LS:181:GLU:N	2.49	0.45
52:SI:849:LEU:HD23	52:SI:896:PHE:HB3	1.99	0.45
56:SP:389:ILE:O	56:SP:393:PHE:N	2.50	0.45
16:LH:661:THR:OG1	16:LH:673:ALA:HB3	2.17	0.44
17:LI:498:SER:HB2	17:LI:531:LEU:HD12	1.98	0.44
21:LM:1536:VAL:HG21	21:LM:1578:PHE:CE2	2.52	0.44
22:LN:40:ASP:OD1	22:LN:40:ASP:N	2.50	0.44
47:SB:328:ARG:O	47:SB:332:THR:HG22	2.17	0.44
53:SK:69:ASN:OD1	53:SK:70:CYS:N	2.50	0.44
56:SP:1613:ALA:HB1	56:SP:1639:ILE:HD11	1.98	0.44
5:L4:95:THR:O	5:L4:95:THR:HG22	2.17	0.44
16:LH:395:THR:OG1	16:LH:424:GLN:OE1	2.24	0.44
16:LH:474:THR:HG22	16:LH:511:GLU:HG2	1.99	0.44
20:LL:439:VAL:HG21	61:SU:296:MET:HG3	1.98	0.44
24:LP:391:TYR:CZ	24:LP:395:ILE:HD11	2.52	0.44
31:NA:566:ILE:HD12	38:NL:110:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:NL:176:SER:OG	38:NL:180:GLN:NE2	2.50	0.44
53:SJ:229:ASN:OD1	53:SK:252:LEU:HD23	2.17	0.44
60:ST:391:VAL:O	60:ST:391:VAL:HG12	2.16	0.44
2:L1:100:A2M:H1'	2:L1:100:A2M:HM'3	1.67	0.44
2:L1:1007:OMC:HM23	2:L1:1007:OMC:H1'	1.52	0.44
16:LH:134:ILE:HD11	16:LH:176:LEU:HD13	1.99	0.44
20:LL:146:VAL:HG13	20:LL:147:GLN:NE2	2.33	0.44
20:LL:153:ILE:HG22	20:LL:163:LEU:CD2	2.37	0.44
26:LR:333:ILE:HG23	26:LR:379:LEU:HB3	1.99	0.44
28:LT:613:ASP:O	28:LT:617:GLY:N	2.49	0.44
56:SP:370:ASP:OD1	56:SP:370:ASP:N	2.50	0.44
16:LH:690:ASN:ND2	16:LH:749:ASP:O	2.43	0.44
16:LH:717:THR:HG23	16:LH:718:GLY:N	2.32	0.44
25:LQ:171:CYS:HB2	25:LQ:177:LEU:HD13	1.99	0.44
25:LQ:563:MET:HE2	25:LQ:563:MET:HA	2.00	0.44
36:NH:795:GLU:OE1	36:NH:797:THR:N	2.51	0.44
40:NP:36:ILE:O	40:NP:36:ILE:HG22	2.16	0.44
42:NS:1209:ARG:NH2	42:NS:1238:GLN:OE1	2.50	0.44
46:SA:133:LEU:HA	48:SC:236:MET:HG3	2.00	0.44
52:SI:776:GLN:OE1	52:SI:779:ARG:NH2	2.50	0.44
55:SM:254:PHE:HE2	55:SM:256:MET:HE3	1.83	0.44
60:ST:481:MET:HE1	60:ST:501:PHE:CZ	2.51	0.44
21:LM:94:LEU:HD21	21:LM:125:PHE:CD1	2.52	0.44
21:LM:356:ALA:O	21:LM:360:ARG:NH1	2.50	0.44
23:LO:566:GLN:N	23:LO:566:GLN:OE1	2.51	0.44
27:LS:554:ASN:OD1	27:LS:555:TRP:N	2.51	0.44
38:NL:62:GLU:HG2	38:NL:71:THR:HG22	1.98	0.44
48:SD:234:ILE:HG22	48:SD:235:GLY:O	2.17	0.44
56:SP:441:ASP:OD1	56:SP:442:LYS:N	2.50	0.44
56:SP:1137:ILE:HG23	56:SP:1185:LEU:HD11	2.00	0.44
58:SR:57:LEU:HD11	58:SR:71:CYS:HB2	2.00	0.44
2:L1:1600:A:H4'	2:L1:1601:G:O5'	2.17	0.44
16:LH:96:ILE:HD12	16:LH:151:TYR:OH	2.18	0.44
19:LK:433:ILE:HG22	19:LK:437:ILE:HD12	1.99	0.44
25:LQ:549:SER:HB3	25:LQ:579:ILE:HD11	1.99	0.44
25:LQ:806:MET:HE1	25:LQ:853:ILE:HD11	1.99	0.44
27:LS:312:ILE:CD1	27:LS:326:LEU:HD11	2.48	0.44
44:OH:63:VAL:HG21	44:OH:94:ALA:HA	2.00	0.44
11:LC:97:VAL:HG12	11:LC:98:ASP:N	2.32	0.44
16:LH:176:LEU:HD11	16:LH:185:PHE:HB3	2.00	0.44
31:NA:4:LEU:HD13	31:NA:23:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:NA:56:GLY:O	31:NA:57:LEU:HD12	2.18	0.44
37:NI:210:ASP:O	41:NQ:80:ARG:NH1	2.51	0.44
47:SB:45:ALA:HB1	47:SB:79:ILE:HD11	2.00	0.44
52:SI:130:ASP:OD1	52:SI:131:ILE:N	2.50	0.44
53:SJ:217:ALA:O	53:SJ:221:VAL:HG12	2.18	0.44
53:SK:218:ASP:OD1	53:SK:219:GLU:N	2.51	0.44
2:L1:1226:A:H61	44:OH:114:LYS:CG	2.31	0.44
16:LH:669:ASN:OD1	16:LH:670:LEU:N	2.51	0.44
20:LL:5:VAL:HG23	20:LL:306:LEU:HD11	2.00	0.44
21:LM:324:ASP:OD1	21:LM:325:SER:N	2.51	0.44
21:LM:985:ARG:O	21:LM:989:THR:HG22	2.17	0.44
48:SC:100:ARG:NH1	48:SC:104:ASP:OD2	2.51	0.44
55:SM:162:THR:OG1	55:SM:264:GLY:O	2.29	0.44
2:L1:366:A:OP1	2:L1:758:U:O2'	2.32	0.44
8:L7:98:ILE:HG22	8:L7:121:VAL:HG11	1.99	0.44
23:LO:497:ILE:CD1	23:LO:532:VAL:HG11	2.48	0.44
36:NH:846:GLU:N	36:NH:846:GLU:OE1	2.51	0.44
38:NL:188:ILE:HG22	38:NL:189:MET:HG2	1.99	0.44
42:NS:517:GLU:OE2	42:NS:766:THR:OG1	2.31	0.44
2:L1:447:U:O2'	5:L4:27:TYR:O	2.31	0.43
8:L7:154:LEU:HD11	8:L7:183:PHE:HD2	1.83	0.43
16:LH:96:ILE:HD12	16:LH:151:TYR:CE1	2.52	0.43
22:LN:495:VAL:HG23	22:LN:511:VAL:HB	1.98	0.43
22:LN:631:GLU:OE2	22:LN:652:THR:OG1	2.24	0.43
51:SH:314:ASN:OD1	51:SH:315:LYS:N	2.51	0.43
4:L3:16:ARG:NH2	4:L3:19:ASN:OD1	2.51	0.43
9:L8:172:ARG:HE	9:L8:175:GLN:HG3	1.83	0.43
16:LH:878:ASN:O	16:LH:882:VAL:HG11	2.19	0.43
21:LM:1445:ILE:HD12	21:LM:1445:ILE:H	1.83	0.43
26:LR:251:ASP:OD1	26:LR:252:GLY:N	2.47	0.43
27:LS:512:ASP:N	27:LS:512:ASP:OD1	2.51	0.43
28:LT:814:GLU:OE1	28:LT:822:ARG:NH2	2.51	0.43
36:NH:369:TRP:HE1	36:NH:495:THR:HG21	1.82	0.43
42:NS:1201:THR:HG23	42:NS:1201:THR:O	2.18	0.43
51:SH:57:GLU:OE2	60:ST:112:VAL:HG23	2.18	0.43
53:SK:99:LEU:HD21	53:SK:238:CYS:HB2	1.98	0.43
61:SU:5:ILE:HG22	61:SU:9:LYS:HZ1	1.83	0.43
2:L1:1141:G:N7	60:ST:22:THR:OG1	2.51	0.43
16:LH:548:ILE:CD1	20:LL:363:VAL:HG13	2.49	0.43
22:LN:311:THR:OG1	22:LN:314:SER:OG	2.33	0.43
31:NA:412:ILE:HD12	31:NA:412:ILE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:SA:10:GLU:OE1	48:SC:231:ARG:NE	2.46	0.43
56:SP:306:LEU:HD11	56:SP:343:ILE:HD13	2.00	0.43
56:SP:470:ILE:HG13	56:SP:470:ILE:O	2.18	0.43
2:L1:210:A:OP1	9:L8:170:SER:OG	2.32	0.43
16:LH:375:ASN:OD1	16:LH:377:SER:OG	2.36	0.43
21:LM:218:ILE:HD12	21:LM:263:VAL:HG21	1.99	0.43
22:LN:44:ALA:HB3	22:LN:71:ARG:HB3	1.99	0.43
22:LN:61:THR:HG21	22:LN:681:ILE:HD13	1.99	0.43
25:LQ:212:VAL:HG22	25:LQ:217:LEU:HD12	2.00	0.43
36:NH:901:ASN:ND2	39:NM:131:ASP:OD1	2.51	0.43
42:NS:516:ASP:OD1	42:NS:517:GLU:N	2.50	0.43
46:SA:198:TRP:HB3	46:SA:271:VAL:HG22	2.00	0.43
52:SI:558:ILE:HD11	52:SI:566:ARG:NH1	2.32	0.43
56:SP:391:ASP:O	56:SP:428:GLN:NE2	2.51	0.43
56:SP:1224:LEU:HD21	56:SP:1247:LEU:HD12	2.00	0.43
56:SP:1290:GLU:N	56:SP:1290:GLU:OE1	2.50	0.43
60:ST:576:ILE:HG22	60:ST:576:ILE:O	2.17	0.43
62:SV:106:THR:HG22	62:SV:106:THR:O	2.19	0.43
63:SW:138:GLU:OE1	63:SW:138:GLU:N	2.51	0.43
2:L1:1633:A:O3'	23:LO:418:ARG:NH1	2.52	0.43
16:LH:95:ASP:OD2	16:LH:98:VAL:HG23	2.19	0.43
16:LH:638:PHE:O	16:LH:639:LYS:HD3	2.18	0.43
21:LM:921:ARG:NH1	21:LM:923:ASP:OD2	2.48	0.43
22:LN:532:ASN:OD1	22:LN:546:GLY:N	2.51	0.43
23:LO:261:ALA:HB2	23:LO:281:SER:HB3	1.99	0.43
36:NH:203:ILE:HD11	36:NH:290:PHE:CD1	2.53	0.43
42:NS:456:VAL:HG11	42:NS:740:THR:HG23	2.00	0.43
48:SD:230:TYR:CD1	48:SD:234:ILE:HD12	2.53	0.43
1:L0:280:A:OP2	27:LS:560:THR:OG1	2.34	0.43
2:L1:1773:4AC:H5	2:L1:1773:4AC:HM73	2.00	0.43
18:LJ:488:LYS:HA	18:LJ:491:VAL:HG12	2.01	0.43
21:LM:784:SER:O	47:SB:84:LYS:NZ	2.39	0.43
23:LO:150:THR:N	23:LO:164:THR:O	2.51	0.43
36:NH:867:ILE:HD12	36:NH:867:ILE:H	1.81	0.43
50:SG:158:THR:HG21	50:SG:240:LEU:HA	2.00	0.43
52:SI:838:ILE:HD12	52:SI:874:TYR:CB	2.48	0.43
57:SQ:180:ASP:O	57:SQ:184:ASN:ND2	2.51	0.43
5:L4:86:PHE:CE2	5:L4:87:MET:HE2	2.53	0.43
6:L5:213:LYS:O	6:L5:217:LEU:HD13	2.19	0.43
7:L6:163:THR:HG23	7:L6:163:THR:O	2.18	0.43
17:LI:540:LEU:O	17:LI:544:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LM:925:LEU:HD12	21:LM:941:LEU:HD23	2.01	0.43
25:LQ:912:TRP:CG	26:LR:779:VAL:HG21	2.54	0.43
26:LR:10:ILE:HD12	26:LR:370:LEU:HD22	2.01	0.43
38:NL:276:VAL:HG12	38:NL:280:LYS:HD2	2.00	0.43
39:NM:127:VAL:HG13	39:NM:176:VAL:HG11	2.01	0.43
44:OH:31:VAL:HG13	44:OH:133:LEU:HD21	2.01	0.43
50:SG:168:ASN:O	50:SG:172:PHE:N	2.48	0.43
60:ST:660:ILE:CD1	61:SU:388:LEU:HD22	2.48	0.43
8:L7:152:VAL:HG23	8:L7:181:ILE:HD11	1.98	0.43
8:L7:173:TYR:CE1	8:L7:177:THR:HG21	2.54	0.43
15:LG:12:VAL:HG22	15:LG:30:VAL:HG12	2.01	0.43
21:LM:1694:HIS:ND1	21:LM:1703:GLU:OE2	2.51	0.43
22:LN:454:GLN:O	22:LN:461:LYS:N	2.47	0.43
23:LO:592:ILE:HD12	23:LO:606:VAL:HG22	2.01	0.43
25:LQ:115:LEU:HD22	25:LQ:153:GLU:CG	2.48	0.43
27:LS:221:THR:OG1	27:LS:224:ASN:ND2	2.51	0.43
28:LT:894:ASP:OD1	28:LT:895:VAL:N	2.51	0.43
29:LW:546:ILE:HD11	37:NI:181:LYS:HZ2	1.83	0.43
30:LZ:57:LEU:HD22	30:LZ:78:LEU:HD22	2.01	0.43
37:NI:147:LEU:HD23	37:NI:154:GLU:HG3	2.01	0.43
38:NL:39:LEU:HD12	38:NL:40:LYS:H	1.84	0.43
42:NS:941:ILE:O	42:NS:991:ARG:NH2	2.52	0.43
56:SP:446:GLN:O	56:SP:446:GLN:NE2	2.49	0.43
60:ST:384:HIS:HA	60:ST:428:VAL:HG13	2.00	0.43
4:L3:110:ARG:HH22	4:L3:113:LEU:HD22	1.83	0.43
5:L4:19:LEU:HD11	5:L4:108:ARG:NE	2.33	0.43
12:LD:44:THR:O	12:LD:44:THR:HG23	2.19	0.43
13:LE:15:ASN:ND2	13:LE:72:CYS:O	2.43	0.43
16:LH:321:MET:HE3	16:LH:323:LEU:CD1	2.49	0.43
18:LJ:129:VAL:HB	18:LJ:143:ALA:HB3	2.00	0.43
22:LN:479:LYS:HB3	22:LN:536:VAL:HG22	2.01	0.43
26:LR:547:LEU:HD22	26:LR:568:MET:HE2	2.00	0.43
16:LH:292:LEU:C	16:LH:293:LEU:HD12	2.43	0.43
19:LK:394:HIS:ND1	19:LK:405:ASP:OD2	2.52	0.43
21:LM:943:LEU:HD21	21:LM:982:VAL:HG12	2.00	0.43
23:LO:492:SER:OG	23:LO:493:TRP:N	2.52	0.43
25:LQ:196:CYS:O	26:LR:667:GLN:NE2	2.52	0.43
26:LR:36:VAL:O	26:LR:36:VAL:HG13	2.18	0.43
26:LR:666:GLU:CD	26:LR:690:HIS:HE2	2.24	0.43
27:LS:45:ILE:H	27:LS:45:ILE:HD12	1.84	0.43
28:LT:219:ASP:O	28:LT:235:MET:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:NM:30:PHE:N	39:NM:46:THR:O	2.48	0.43
42:NS:905:PHE:HE2	42:NS:916:LEU:HD21	1.83	0.43
56:SP:981:SER:O	56:SP:983:GLN:NE2	2.49	0.43
2:L1:1227:A:H61	2:L1:1256:A:C2'	2.32	0.42
4:L3:30:TYR:O	4:L3:33:THR:OG1	2.37	0.42
21:LM:475:LEU:HD23	21:LM:497:LEU:HD12	2.00	0.42
21:LM:1154:VAL:HG11	62:SV:96:GLN:NE2	2.34	0.42
24:LP:411:ARG:NH1	24:LP:440:LEU:OXT	2.52	0.42
26:LR:25:VAL:CG1	26:LR:296:ILE:HD11	2.49	0.42
27:LS:130:ASP:OD1	28:LT:179:LYS:NZ	2.51	0.42
31:NA:30:TYR:O	31:NA:33:SER:OG	2.31	0.42
42:NS:1236:VAL:CG2	42:NS:1247:VAL:HG13	2.49	0.42
2:L1:393:C:OP1	9:L8:2:GLY:N	2.52	0.42
2:L1:1228:G:OP2	44:OH:45:LEU:N	2.52	0.42
8:L7:17:GLU:CG	8:L7:46:ILE:HG22	2.49	0.42
16:LH:555:VAL:O	16:LH:555:VAL:HG13	2.19	0.42
16:LH:742:ARG:NH2	16:LH:756:ASN:OD1	2.52	0.42
42:NS:1219:SER:OG	42:NS:1228:GLY:N	2.52	0.42
56:SP:468:ALA:O	56:SP:503:ARG:NH1	2.47	0.42
21:LM:68:ILE:O	21:LM:71:ARG:HG2	2.19	0.42
22:LN:214:SER:O	22:LN:223:GLY:N	2.47	0.42
22:LN:385:ASN:ND2	22:LN:387:GLU:O	2.53	0.42
28:LT:463:VAL:HG13	28:LT:477:ILE:HG23	2.00	0.42
32:NB:204:MET:O	32:NB:209:ARG:NH1	2.52	0.42
36:NH:349:LEU:HD21	36:NH:395:ILE:HD13	2.01	0.42
36:NH:874:LEU:HG	36:NH:878:LEU:HD23	2.01	0.42
36:NH:930:THR:HG23	36:NH:933:LEU:H	1.82	0.42
37:NI:135:ASN:OD1	37:NI:136:ASN:N	2.51	0.42
46:SA:159:SER:OG	48:SC:219:PRO:O	2.37	0.42
48:SD:156:MET:HE1	64:SY:126:MET:HE2	2.00	0.42
2:L1:1190:C:N4	2:L1:1197:C:O2	2.53	0.42
13:LE:20:THR:HG22	13:LE:20:THR:O	2.19	0.42
20:LL:580:TYR:CD2	22:LN:462:VAL:HG11	2.55	0.42
23:LO:543:ASN:O	23:LO:547:ALA:N	2.51	0.42
31:NA:7:VAL:HG21	31:NA:18:LYS:NZ	2.34	0.42
52:SI:157:ASN:O	52:SI:161:HIS:ND1	2.52	0.42
56:SP:84:ASP:OD1	56:SP:85:LYS:N	2.52	0.42
56:SP:1738:TYR:OH	56:SP:1745:ILE:HD13	2.18	0.42
57:SQ:124:ILE:HD12	57:SQ:124:ILE:H	1.85	0.42
60:ST:433:ILE:O	60:ST:452:GLN:NE2	2.50	0.42
65:SZ:444:VAL:O	65:SZ:448:GLY:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:8:GLN:N	4:L3:8:GLN:OE1	2.53	0.42
7:L6:78:THR:O	7:L6:81:VAL:HG22	2.20	0.42
21:LM:1407:LEU:CD1	21:LM:1415:LEU:HD22	2.49	0.42
23:LO:10:LEU:HD13	23:LO:702:LEU:HD23	2.01	0.42
26:LR:440:VAL:CG2	26:LR:454:LEU:HD11	2.49	0.42
28:LT:144:ASP:OD2	28:LT:146:GLN:N	2.51	0.42
31:NA:50:ASP:OD1	31:NA:51:GLU:N	2.52	0.42
36:NH:856:THR:HG22	36:NH:858:ARG:H	1.84	0.42
42:NS:1133:VAL:HG11	42:NS:1157:LEU:CD2	2.50	0.42
47:SB:313:PRO:HG2	47:SB:316:THR:HG23	2.01	0.42
49:SF:29:ASN:O	49:SF:31:ARG:NH1	2.53	0.42
50:SG:409:ASP:OD1	50:SG:410:ASP:N	2.53	0.42
52:SI:126:ASN:OD1	52:SI:1020:SER:OG	2.33	0.42
53:SK:154:ASN:O	53:SK:155:SER:OG	2.33	0.42
2:L1:100:A2M:H8	2:L1:100:A2M:C5'	2.50	0.42
2:L1:1159:C:N4	55:SM:184:GLU:OE2	2.49	0.42
16:LH:246:SER:OG	16:LH:248:GLN:OE1	2.38	0.42
28:LT:738:ASP:OD1	28:LT:738:ASP:N	2.52	0.42
30:LZ:154:MET:HE3	30:LZ:154:MET:HA	2.01	0.42
36:NH:225:LEU:HD12	36:NH:264:LEU:O	2.19	0.42
46:SA:159:SER:HB3	48:SC:208:ILE:HD11	2.01	0.42
4:L3:116:LEU:HD21	4:L3:120:ARG:NH1	2.34	0.42
16:LH:296:HIS:CG	16:LH:300:VAL:HG12	2.55	0.42
16:LH:435:ASP:OD1	16:LH:436:PHE:N	2.50	0.42
18:LJ:100:ASP:OD1	18:LJ:101:ALA:N	2.53	0.42
20:LL:296:ILE:HG23	20:LL:296:ILE:O	2.20	0.42
21:LM:652:MET:HE3	21:LM:652:MET:HA	2.01	0.42
26:LR:25:VAL:HG11	26:LR:296:ILE:HD11	2.01	0.42
36:NH:146:LEU:HA	36:NH:149:VAL:HG12	2.01	0.42
37:NI:130:ASP:O	37:NI:133:SER:OG	2.37	0.42
40:NP:124:ILE:O	40:NP:124:ILE:HG23	2.20	0.42
44:OH:106:ILE:HD13	60:ST:279:LEU:O	2.19	0.42
46:SA:52:SER:OG	46:SA:81:ILE:HD11	2.20	0.42
50:SG:348:LEU:HD13	50:SG:427:LEU:HD11	2.01	0.42
53:SK:35:ASP:O	53:SK:40:ARG:NH2	2.52	0.42
56:SP:1133:LEU:O	56:SP:1136:THR:OG1	2.30	0.42
63:SW:222:THR:O	63:SW:223:ARG:NH1	2.47	0.42
2:L1:896:U:O2	35:NG:41:ARG:NH1	2.46	0.42
17:LI:359:LYS:N	17:LI:386:THR:O	2.47	0.42
21:LM:235:VAL:HG22	21:LM:264:PHE:CE1	2.55	0.42
21:LM:298:THR:O	21:LM:302:LEU:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LR:342:ASP:OD1	26:LR:343:MET:N	2.52	0.42
36:NH:971:LYS:O	36:NH:1028:ARG:NE	2.53	0.42
46:SA:182:ASP:OD1	46:SA:183:GLN:N	2.52	0.42
46:SA:208:LYS:HE2	46:SA:208:LYS:HA	2.02	0.42
56:SP:938:THR:HG22	56:SP:938:THR:O	2.20	0.42
56:SP:1761:ILE:HG22	56:SP:1762:SER:O	2.20	0.42
22:LN:85:TRP:HB2	22:LN:372:MET:HE1	2.02	0.42
42:NS:499:ARG:HG3	42:NS:502:MET:HE2	2.02	0.42
53:SJ:68:LEU:HD13	53:SJ:77:LEU:CD1	2.50	0.42
61:SU:531:ASP:OD1	61:SU:532:ASN:N	2.52	0.42
64:SY:167:THR:HG22	64:SY:169:ASP:H	1.85	0.42
13:LE:105:THR:HG23	13:LE:105:THR:O	2.19	0.42
26:LR:67:LEU:HD11	26:LR:76:LEU:HD11	2.02	0.42
27:LS:364:GLN:NE2	27:LS:369:ASN:OD1	2.53	0.42
31:NA:551:ASN:OD1	31:NA:552:ASP:N	2.53	0.42
51:SH:305:LYS:O	51:SH:307:ASP:N	2.51	0.42
56:SP:455:GLU:OE1	56:SP:455:GLU:N	2.52	0.42
56:SP:701:LEU:HD21	56:SP:795:ASP:HB3	2.01	0.42
65:SZ:311:LEU:HD21	65:SZ:347:VAL:HG22	2.02	0.42
4:L3:120:ARG:NH1	60:ST:754:GLU:OE2	2.42	0.41
7:L6:5:ILE:HD12	7:L6:16:PHE:HD2	1.85	0.41
9:L8:34:ALA:HB2	9:L8:56:ARG:CD	2.50	0.41
28:LT:717:ASP:HB3	28:LT:720:LEU:HD23	2.02	0.41
42:NS:900:LYS:O	42:NS:903:SER:OG	2.32	0.41
43:NV:721:ARG:HD3	43:NV:722:PRO:HD2	2.01	0.41
53:SK:141:MET:HE2	53:SK:141:MET:CA	2.50	0.41
60:ST:383:THR:OG1	60:ST:385:ASP:OD1	2.32	0.41
4:L3:52:VAL:HG12	4:L3:65:GLU:OE1	2.20	0.41
16:LH:134:ILE:CD1	16:LH:176:LEU:HD13	2.50	0.41
16:LH:143:ASN:OD1	16:LH:144:VAL:N	2.53	0.41
16:LH:568:ASN:HD22	16:LH:568:ASN:C	2.26	0.41
21:LM:72:THR:O	27:LS:33:LEU:HD11	2.19	0.41
22:LN:355:THR:OG1	22:LN:372:MET:O	2.36	0.41
27:LS:464:THR:HG21	27:LS:476:ILE:HA	2.02	0.41
32:NB:232:PRO:HD2	32:NB:233:LYS:N	2.35	0.41
50:SG:193:ASP:OD1	50:SG:193:ASP:O	2.38	0.41
52:SI:773:THR:O	52:SI:777:ARG:N	2.45	0.41
52:SI:1058:GLU:N	52:SI:1058:GLU:OE1	2.53	0.41
56:SP:1594:LEU:HB2	56:SP:1616:LEU:HD21	2.01	0.41
2:L1:381:C:O2'	2:L1:755:A:N1	2.50	0.41
16:LH:666:ASN:OD1	16:LH:667:ASP:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LJ:85:TYR:O	18:LJ:86:SER:OG	2.34	0.41
21:LM:1520:THR:HG21	62:SV:45:LYS:HB2	2.02	0.41
26:LR:669:LEU:CD2	26:LR:673:MET:HE2	2.51	0.41
36:NH:741:ILE:HA	36:NH:744:MET:HE2	2.02	0.41
46:SA:217:ALA:O	46:SA:221:LEU:HD23	2.21	0.41
56:SP:1147:ILE:O	56:SP:1151:ILE:HD12	2.20	0.41
65:SZ:434:GLN:OE1	65:SZ:434:GLN:HA	2.20	0.41
1:L0:291:G:OP1	28:LT:67:HIS:NE2	2.33	0.41
2:L1:1204:A:C5	60:ST:211:MET:HE1	2.55	0.41
2:L1:1568:C:HO2'	2:L1:1569:A:P	2.43	0.41
7:L6:23:ARG:NE	7:L6:41:VAL:O	2.54	0.41
16:LH:533:THR:HG22	16:LH:544:LYS:HG2	2.02	0.41
21:LM:1407:LEU:HD12	21:LM:1415:LEU:HD22	2.02	0.41
24:LP:300:MET:O	24:LP:304:LEU:HD23	2.21	0.41
25:LQ:592:SER:OG	25:LQ:593:ALA:N	2.52	0.41
25:LQ:884:LYS:NZ	26:LR:807:ASP:OD1	2.39	0.41
26:LR:25:VAL:HG12	26:LR:294:LEU:HD13	2.01	0.41
28:LT:367:LEU:HD22	28:LT:375:LEU:HD21	2.02	0.41
28:LT:549:MET:HE2	28:LT:560:LEU:HD21	2.02	0.41
33:ND:178:VAL:HG11	64:SY:146:PHE:CD2	2.55	0.41
35:NG:48:VAL:HG21	35:NG:53:ASP:HB2	2.02	0.41
36:NH:270:ILE:CD1	36:NH:294:LEU:HD23	2.51	0.41
42:NS:939:PRO:O	42:NS:1030:LEU:HD23	2.19	0.41
52:SI:777:ARG:NE	52:SI:781:GLU:OE2	2.54	0.41
56:SP:493:ASN:OD1	56:SP:494:THR:N	2.53	0.41
61:SU:15:LEU:HD11	61:SU:24:TYR:CD1	2.55	0.41
2:L1:493:U:O2'	2:L1:494:U:OP1	2.32	0.41
2:L1:585:A:O2'	2:L1:586:G:OP1	2.36	0.41
2:L1:1787:C:OP1	35:NG:127:ARG:NH2	2.53	0.41
5:L4:173:ILE:HD11	5:L4:235:TYR:CD2	2.55	0.41
20:LL:261:VAL:O	20:LL:273:LYS:NZ	2.41	0.41
21:LM:899:ILE:HD12	21:LM:899:ILE:H	1.86	0.41
21:LM:963:ILE:HD12	21:LM:963:ILE:H	1.84	0.41
21:LM:1006:MET:HG3	21:LM:1036:LEU:HD22	2.02	0.41
21:LM:1304:VAL:O	21:LM:1308:VAL:HG23	2.20	0.41
24:LP:111:ALA:HB2	57:SQ:69:PHE:CE2	2.55	0.41
27:LS:204:ASP:OD2	27:LS:210:LYS:NZ	2.26	0.41
36:NH:691:SER:OG	36:NH:694:ALA:HB2	2.20	0.41
37:NI:108:MET:HE2	37:NI:187:HIS:CE1	2.55	0.41
6:L5:116:HIS:HE1	18:LJ:115:THR:HG21	1.85	0.41
25:LQ:115:LEU:HD22	25:LQ:153:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:NS:421:THR:HG21	42:NS:458:MET:HG3	2.01	0.41
42:NS:423:GLN:OE1	42:NS:426:GLN:NE2	2.54	0.41
53:SJ:125:ASN:O	53:SJ:128:VAL:HG12	2.20	0.41
60:ST:433:ILE:HD12	60:ST:459:LEU:HD22	2.02	0.41
11:LC:98:ASP:OD1	11:LC:101:SER:OG	2.36	0.41
16:LH:736:THR:HG22	16:LH:737:ILE:N	2.35	0.41
26:LR:579:GLN:HE21	39:NM:9:LEU:HD22	1.86	0.41
27:LS:41:ASN:O	27:LS:45:ILE:HD12	2.21	0.41
53:SK:156:GLU:OE1	53:SK:156:GLU:N	2.54	0.41
2:L1:78:A:O2'	7:L6:173:PRO:O	2.32	0.41
18:LJ:404:ALA:HB2	18:LJ:417:VAL:HG11	2.02	0.41
23:LO:351:LEU:CD2	23:LO:701:LEU:HD11	2.48	0.41
23:LO:373:ASP:O	23:LO:377:GLY:N	2.47	0.41
23:LO:852:THR:HG22	23:LO:853:ASP:N	2.36	0.41
28:LT:107:GLU:N	28:LT:107:GLU:OE1	2.54	0.41
55:SM:196:THR:HG22	55:SM:197:ALA:N	2.36	0.41
2:L1:284:G:N7	7:L6:188:ARG:NH1	2.67	0.41
2:L1:358:U:OP2	42:NS:2:GLY:N	2.53	0.41
2:L1:888:U:O2	2:L1:988:A:O2'	2.39	0.41
2:L1:974:A2M:HM'3	2:L1:974:A2M:H1'	1.89	0.41
16:LH:722:LEU:C	16:LH:722:LEU:HD23	2.45	0.41
18:LJ:504:ILE:HD12	18:LJ:504:ILE:H	1.85	0.41
24:LP:117:MET:HE1	24:LP:128:LYS:CG	2.51	0.41
24:LP:360:LEU:HD22	24:LP:406:LEU:HB2	2.02	0.41
25:LQ:245:MET:HB3	25:LQ:321:TYR:CE1	2.56	0.41
26:LR:212:LEU:HD11	26:LR:220:ILE:HG21	2.02	0.41
26:LR:268:GLN:HG3	26:LR:270:ILE:HD11	2.02	0.41
28:LT:226:VAL:O	28:LT:226:VAL:HG22	2.20	0.41
28:LT:550:VAL:HG12	28:LT:591:PHE:CE2	2.56	0.41
38:NL:84:VAL:CG1	38:NL:110:MET:HE3	2.48	0.41
38:NL:284:VAL:HG13	38:NL:309:ALA:HB1	2.03	0.41
46:SA:244:ASP:OD1	46:SA:245:SER:N	2.54	0.41
47:SB:67:LYS:HA	47:SB:67:LYS:HE3	2.03	0.41
48:SD:175:ALA:HB1	48:SD:181:VAL:HG21	2.03	0.41
53:SJ:218:ASP:HA	53:SJ:221:VAL:HG12	2.02	0.41
56:SP:772:ILE:HD12	56:SP:772:ILE:N	2.35	0.41
60:ST:456:ILE:HD13	61:SU:529:VAL:HG21	2.03	0.41
2:L1:58:U:OP1	2:L1:456:A:O2'	2.34	0.41
2:L1:632:U:O2'	2:L1:1103:U:OP1	2.34	0.41
2:L1:992:A:OP2	2:L1:1011:G:N1	2.44	0.41
9:L8:76:THR:HG21	9:L8:105:ASP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:282:ILE:CD1	16:LH:293:LEU:HD13	2.51	0.41
18:LJ:129:VAL:HG11	18:LJ:174:LEU:HB2	2.03	0.41
21:LM:498:PHE:CD2	21:LM:539:LEU:HD11	2.56	0.41
22:LN:257:ASP:OD1	22:LN:259:THR:OG1	2.28	0.41
22:LN:436:ASP:OD1	22:LN:437:GLY:N	2.54	0.41
26:LR:552:SER:OG	26:LR:553:GLY:N	2.53	0.41
28:LT:32:ASN:HB3	28:LT:54:VAL:HG13	2.02	0.41
36:NH:1150:VAL:HG12	36:NH:1154:ASN:OD1	2.20	0.41
62:SV:98:LEU:HD21	62:SV:115:LEU:HD21	2.03	0.41
2:L1:188:A:OP2	2:L1:189:C:N4	2.52	0.40
2:L1:1124:A:H61	3:L2:0:M7G:H2'	1.85	0.40
16:LH:864:ASP:OD1	16:LH:864:ASP:N	2.53	0.40
21:LM:960:VAL:HG11	21:LM:994:LEU:HD21	2.02	0.40
25:LQ:126:LEU:HD23	25:LQ:169:PHE:CD2	2.56	0.40
36:NH:796:ILE:HG23	36:NH:797:THR:N	2.36	0.40
37:NI:46:ASN:ND2	37:NI:48:ASN:OD1	2.54	0.40
46:SA:44:PHE:HD2	46:SA:138:LEU:HD21	1.86	0.40
48:SC:117:VAL:HG23	48:SC:118:TYR:HD1	1.87	0.40
48:SD:123:ILE:O	48:SD:141:TYR:N	2.52	0.40
53:SJ:246:GLU:O	53:SJ:250:ASN:N	2.54	0.40
2:L1:1480:G:H2'	2:L1:1481:C:O4'	2.21	0.40
3:L2:0:M7G:H5'1	3:L2:0:M7G:H81	2.04	0.40
7:L6:67:VAL:HG13	7:L6:99:GLY:HA2	2.02	0.40
8:L7:46:ILE:HD11	8:L7:58:LEU:HG	2.02	0.40
16:LH:148:GLU:O	16:LH:148:GLU:HG3	2.21	0.40
20:LL:95:VAL:HG13	20:LL:95:VAL:O	2.20	0.40
21:LM:905:THR:O	21:LM:909:LEU:HD23	2.20	0.40
21:LM:1520:THR:HG22	62:SV:46:ALA:N	2.37	0.40
26:LR:591:ILE:HD13	26:LR:632:ILE:HD13	2.04	0.40
28:LT:515:ARG:O	28:LT:531:PHE:N	2.49	0.40
32:NB:233:LYS:O	32:NB:237:LEU:HD23	2.21	0.40
35:NG:18:ARG:HE	35:NG:31:THR:HG21	1.86	0.40
36:NH:566:ILE:HD13	36:NH:690:VAL:HG21	2.03	0.40
37:NI:152:PRO:HA	37:NI:155:LEU:HD23	2.03	0.40
47:SB:3:TYR:O	47:SB:88:ILE:N	2.42	0.40
52:SI:841:THR:HG23	52:SI:859:ILE:HA	2.02	0.40
56:SP:70:ILE:HG13	56:SP:70:ILE:O	2.22	0.40
56:SP:1151:ILE:HD12	56:SP:1151:ILE:H	1.85	0.40
2:L1:1204:A:C2	60:ST:211:MET:HE1	2.56	0.40
18:LJ:285:ASP:OD1	18:LJ:285:ASP:N	2.54	0.40
21:LM:79:ILE:O	21:LM:124:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:684:GLU:OE1	22:LN:684:GLU:N	2.41	0.40
25:LQ:296:LEU:HD23	25:LQ:324:PHE:CZ	2.55	0.40
45:OU:140:TYR:OH	45:OU:145:HIS:ND1	2.43	0.40
56:SP:1534:LEU:HD21	56:SP:1597:ILE:HG21	2.03	0.40
63:SW:117:TYR:N	63:SW:118:PRO:CD	2.84	0.40
2:L1:165:G:O3'	56:SP:636:ARG:NH2	2.55	0.40
2:L1:256:A:H2'	2:L1:257:A:O4'	2.21	0.40
2:L1:1124:A:O2'	38:NL:184:ASN:OD1	2.40	0.40
15:LG:65:ARG:O	15:LG:67:ARG:NH1	2.54	0.40
21:LM:756:LEU:HA	21:LM:759:ILE:HG22	2.04	0.40
21:LM:1735:GLU:OE1	56:SP:248:HIS:NE2	2.55	0.40
22:LN:457:GLY:O	22:LN:458:ASN:OD1	2.39	0.40
25:LQ:771:ARG:NH1	25:LQ:772:ASP:OD1	2.54	0.40
41:NQ:45:THR:OG1	41:NQ:82:LYS:NZ	2.54	0.40
47:SB:46:ALA:HB3	47:SB:75:LEU:HD11	2.04	0.40
47:SB:79:ILE:O	47:SB:79:ILE:HG22	2.20	0.40
53:SK:217:ALA:O	53:SK:221:VAL:HG12	2.21	0.40
16:LH:749:ASP:OD1	16:LH:749:ASP:C	2.65	0.40
16:LH:851:GLU:O	16:LH:855:LEU:HD23	2.22	0.40
17:LI:552:LYS:NZ	17:LI:581:ASP:OD2	2.48	0.40
22:LN:82:ARG:NH2	22:LN:685:SER:O	2.55	0.40
22:LN:401:ILE:O	22:LN:416:LEU:HD12	2.21	0.40
25:LQ:559:PHE:O	25:LQ:563:MET:N	2.47	0.40
27:LS:326:LEU:HD13	27:LS:331:LEU:HD13	2.03	0.40
32:NB:288:LYS:O	32:NB:292:THR:HG22	2.21	0.40
36:NH:261:ASN:ND2	36:NH:261:ASN:O	2.54	0.40
38:NL:98:VAL:O	38:NL:98:VAL:HG22	2.21	0.40
42:NS:1213:VAL:HG21	42:NS:1238:GLN:NE2	2.36	0.40
56:SP:1268:ILE:CG2	56:SP:1284:LEU:HD11	2.51	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%)	101 (99%)	1 (1%)	0	100	100
5	L4	242/261 (93%)	241 (100%)	1 (0%)	0	100	100
6	L5	202/225 (90%)	199 (98%)	3 (2%)	0	100	100
7	L6	214/236 (91%)	212 (99%)	2 (1%)	0	100	100
8	L7	174/190 (92%)	170 (98%)	4 (2%)	0	100	100
9	L8	166/200 (83%)	165 (99%)	1 (1%)	0	100	100
10	L9	179/197 (91%)	177 (99%)	2 (1%)	0	100	100
11	LC	126/143 (88%)	123 (98%)	3 (2%)	0	100	100
12	LD	135/156 (86%)	132 (98%)	3 (2%)	0	100	100
13	LE	127/130 (98%)	126 (99%)	1 (1%)	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%)	770 (98%)	18 (2%)	0	100	100
17	LI	582/713 (82%)	573 (98%)	9 (2%)	0	100	100
18	LJ	470/513 (92%)	464 (99%)	6 (1%)	0	100	100
19	LK	130/575 (23%)	130 (100%)	0	0	100	100
20	LL	475/643 (74%)	462 (97%)	13 (3%)	0	100	100
21	LM	1583/1769 (90%)	1563 (99%)	20 (1%)	0	100	100
22	LN	649/776 (84%)	636 (98%)	13 (2%)	0	100	100
23	LO	786/923 (85%)	776 (99%)	10 (1%)	0	100	100
24	LP	375/440 (85%)	374 (100%)	1 (0%)	0	100	100
25	LQ	806/943 (86%)	788 (98%)	18 (2%)	0	100	100
26	LR	785/817 (96%)	769 (98%)	16 (2%)	0	100	100
27	LS	452/594 (76%)	446 (99%)	6 (1%)	0	100	100
28	LT	861/939 (92%)	849 (99%)	12 (1%)	0	100	100
29	LW	44/554 (8%)	44 (100%)	0	0	100	100
30	LZ	140/183 (76%)	140 (100%)	0	0	100	100
31	NA	312/593 (53%)	312 (100%)	0	0	100	100
32	NB	248/610 (41%)	246 (99%)	2 (1%)	0	100	100
33	ND	70/214 (33%)	69 (99%)	1 (1%)	0	100	100
34	NF	139/151 (92%)	138 (99%)	1 (1%)	0	100	100
35	NG	125/137 (91%)	121 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	NH	1063/1237 (86%)	1053 (99%)	10 (1%)	0	100	100
37	NI	232/297 (78%)	224 (97%)	8 (3%)	0	100	100
38	NL	279/318 (88%)	275 (99%)	4 (1%)	0	100	100
39	NM	231/255 (91%)	228 (99%)	3 (1%)	0	100	100
40	NP	130/144 (90%)	128 (98%)	2 (2%)	0	100	100
41	NQ	77/82 (94%)	76 (99%)	1 (1%)	0	100	100
42	NS	917/1267 (72%)	909 (99%)	8 (1%)	0	100	100
43	NV	19/733 (3%)	19 (100%)	0	0	100	100
44	OH	118/143 (82%)	117 (99%)	1 (1%)	0	100	100
45	OU	54/152 (36%)	54 (100%)	0	0	100	100
46	SA	390/504 (77%)	386 (99%)	4 (1%)	0	100	100
47	SB	420/511 (82%)	414 (99%)	6 (1%)	0	100	100
48	SC	237/327 (72%)	235 (99%)	2 (1%)	0	100	100
48	SD	234/327 (72%)	231 (99%)	3 (1%)	0	100	100
49	SE	119/126 (94%)	117 (98%)	2 (2%)	0	100	100
49	SF	119/126 (94%)	116 (98%)	3 (2%)	0	100	100
50	SG	453/573 (79%)	444 (98%)	9 (2%)	0	100	100
51	SH	358/367 (98%)	352 (98%)	6 (2%)	0	100	100
52	SI	746/1183 (63%)	733 (98%)	13 (2%)	0	100	100
53	SJ	207/252 (82%)	205 (99%)	2 (1%)	0	100	100
53	SK	225/252 (89%)	221 (98%)	4 (2%)	0	100	100
54	SL	146/189 (77%)	139 (95%)	7 (5%)	0	100	100
55	SM	243/290 (84%)	241 (99%)	2 (1%)	0	100	100
56	SP	1832/2493 (74%)	1808 (99%)	24 (1%)	0	100	100
57	SQ	103/217 (48%)	101 (98%)	2 (2%)	0	100	100
58	SR	130/145 (90%)	129 (99%)	1 (1%)	0	100	100
59	SS	9/899 (1%)	9 (100%)	0	0	100	100
60	ST	573/810 (71%)	570 (100%)	3 (0%)	0	100	100
61	SU	524/552 (95%)	522 (100%)	2 (0%)	0	100	100
62	SV	151/206 (73%)	149 (99%)	2 (1%)	0	100	100
63	SW	211/274 (77%)	209 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	SY	193/250 (77%)	189 (98%)	4 (2%)	0	100	100
65	SZ	255/483 (53%)	250 (98%)	5 (2%)	0	100	100
All	All	22673/31053 (73%)	22355 (99%)	318 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L3	96/129 (74%)	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%)	124 (100%)	0	100	100
13	LE	110/111 (99%)	110 (100%)	0	100	100
14	LF	109/113 (96%)	109 (100%)	0	100	100
15	LG	55/60 (92%)	55 (100%)	0	100	100
16	LH	743/826 (90%)	742 (100%)	1 (0%)	92	97
17	LI	244/657 (37%)	244 (100%)	0	100	100
18	LJ	421/454 (93%)	421 (100%)	0	100	100
19	LK	124/533 (23%)	124 (100%)	0	100	100
20	LL	438/574 (76%)	438 (100%)	0	100	100
21	LM	1477/1633 (90%)	1477 (100%)	0	100	100
22	LN	603/713 (85%)	603 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	LO	695/812 (86%)	695 (100%)	0	100	100
24	LP	359/414 (87%)	359 (100%)	0	100	100
25	LQ	723/832 (87%)	723 (100%)	0	100	100
26	LR	698/719 (97%)	698 (100%)	0	100	100
27	LS	406/528 (77%)	406 (100%)	0	100	100
28	LT	762/819 (93%)	762 (100%)	0	100	100
29	LW	46/480 (10%)	46 (100%)	0	100	100
30	LZ	132/172 (77%)	132 (100%)	0	100	100
31	NA	299/535 (56%)	299 (100%)	0	100	100
32	NB	233/538 (43%)	233 (100%)	0	100	100
33	ND	70/196 (36%)	70 (100%)	0	100	100
34	NF	121/128 (94%)	121 (100%)	0	100	100
35	NG	96/105 (91%)	96 (100%)	0	100	100
36	NH	982/1125 (87%)	982 (100%)	0	100	100
37	NI	220/274 (80%)	220 (100%)	0	100	100
38	NL	257/283 (91%)	257 (100%)	0	100	100
39	NM	210/224 (94%)	210 (100%)	0	100	100
40	NP	107/116 (92%)	107 (100%)	0	100	100
41	NQ	68/71 (96%)	68 (100%)	0	100	100
42	NS	836/1140 (73%)	836 (100%)	0	100	100
43	NV	18/671 (3%)	18 (100%)	0	100	100
44	OH	97/119 (82%)	97 (100%)	0	100	100
45	OU	47/135 (35%)	47 (100%)	0	100	100
46	SA	339/435 (78%)	339 (100%)	0	100	100
47	SB	352/433 (81%)	352 (100%)	0	100	100
48	SC	200/240 (83%)	200 (100%)	0	100	100
48	SD	198/240 (82%)	198 (100%)	0	100	100
49	SE	100/104 (96%)	100 (100%)	0	100	100
49	SF	100/104 (96%)	100 (100%)	0	100	100
50	SG	399/503 (79%)	399 (100%)	0	100	100
51	SH	307/312 (98%)	307 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	SI	669/1039 (64%)	669 (100%)	0	100	100
53	SJ	192/222 (86%)	192 (100%)	0	100	100
53	SK	205/222 (92%)	205 (100%)	0	100	100
54	SL	131/169 (78%)	131 (100%)	0	100	100
55	SM	220/258 (85%)	220 (100%)	0	100	100
56	SP	1725/2307 (75%)	1725 (100%)	0	100	100
57	SQ	98/200 (49%)	98 (100%)	0	100	100
58	SR	113/120 (94%)	113 (100%)	0	100	100
59	SS	10/808 (1%)	10 (100%)	0	100	100
60	ST	544/732 (74%)	544 (100%)	0	100	100
61	SU	489/506 (97%)	489 (100%)	0	100	100
62	SV	147/192 (77%)	147 (100%)	0	100	100
63	SW	192/238 (81%)	192 (100%)	0	100	100
64	SY	191/234 (82%)	191 (100%)	0	100	100
65	SZ	232/424 (55%)	232 (100%)	0	100	100
All	All	20309/27648 (74%)	20308 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	LH	568	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (168) such sidechains are listed below:

Mol	Chain	Res	Type
4	L3	75	ASN
5	L4	67	GLN
5	L4	98	ASN
5	L4	142	HIS
6	L5	37	GLN
6	L5	116	HIS
7	L6	80	ASN
9	L8	111	GLN
9	L8	116	HIS
11	LC	74	HIS
12	LD	14	GLN

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Mol	Chain	Res	Type
12	LD	92	HIS
12	LD	104	HIS
12	LD	110	HIS
14	LF	29	HIS
16	LH	150	ASN
16	LH	190	GLN
16	LH	491	GLN
16	LH	579	ASN
16	LH	593	ASN
16	LH	759	HIS
16	LH	878	ASN
17	LI	504	ASN
17	LI	553	GLN
17	LI	597	GLN
18	LJ	51	HIS
18	LJ	112	ASN
18	LJ	121	ASN
18	LJ	291	GLN
18	LJ	391	ASN
18	LJ	403	ASN
19	LK	478	ASN
20	LL	240	GLN
21	LM	747	GLN
21	LM	774	ASN
21	LM	958	HIS
21	LM	1487	ASN
21	LM	1585	ASN
21	LM	1728	GLN
22	LN	268	GLN
22	LN	385	ASN
22	LN	533	HIS
22	LN	574	HIS
23	LO	66	GLN
23	LO	156	GLN
23	LO	203	GLN
23	LO	452	ASN
23	LO	552	ASN
24	LP	89	GLN
25	LQ	203	HIS
25	LQ	383	HIS
25	LQ	422	HIS
25	LQ	451	ASN

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Mol	Chain	Res	Type
25	LQ	608	HIS
25	LQ	620	ASN
25	LQ	871	GLN
26	LR	54	HIS
26	LR	157	ASN
26	LR	420	ASN
26	LR	488	HIS
26	LR	587	GLN
26	LR	735	GLN
27	LS	34	GLN
27	LS	167	GLN
27	LS	362	HIS
27	LS	388	HIS
27	LS	412	GLN
27	LS	472	GLN
28	LT	88	HIS
28	LT	120	HIS
28	LT	736	HIS
28	LT	793	GLN
30	LZ	116	HIS
31	NA	40	ASN
31	NA	568	GLN
32	NB	246	ASN
34	NF	5	HIS
34	NF	105	ASN
36	NH	197	GLN
36	NH	238	HIS
36	NH	261	ASN
36	NH	582	GLN
36	NH	606	ASN
36	NH	1078	HIS
37	NI	148	HIS
37	NI	197	GLN
38	NL	180	GLN
38	NL	201	GLN
38	NL	213	ASN
39	NM	74	GLN
39	NM	149	GLN
39	NM	211	HIS
41	NQ	19	HIS
42	NS	405	HIS
42	NS	406	HIS

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Mol	Chain	Res	Type
42	NS	881	GLN
42	NS	884	GLN
42	NS	1158	HIS
44	OH	80	ASN
46	SA	95	ASN
46	SA	125	GLN
46	SA	407	GLN
47	SB	334	HIS
47	SB	344	HIS
48	SC	93	HIS
48	SD	216	ASN
49	SF	5	ASN
50	SG	321	HIS
50	SG	547	HIS
51	SH	12	GLN
51	SH	126	ASN
51	SH	152	HIS
51	SH	176	GLN
51	SH	234	ASN
52	SI	3	GLN
52	SI	8	HIS
52	SI	22	HIS
52	SI	26	HIS
52	SI	112	HIS
52	SI	200	GLN
52	SI	241	HIS
52	SI	314	GLN
52	SI	754	GLN
52	SI	878	HIS
52	SI	904	ASN
52	SI	925	ASN
52	SI	986	HIS
52	SI	1037	GLN
53	SJ	250	ASN
53	SK	250	ASN
54	SL	148	HIS
55	SM	24	GLN
55	SM	169	ASN
56	SP	46	HIS
56	SP	183	HIS
56	SP	398	GLN
56	SP	426	GLN

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Mol	Chain	Res	Type
56	SP	428	GLN
56	SP	840	ASN
56	SP	982	HIS
56	SP	983	GLN
56	SP	1002	ASN
56	SP	1014	ASN
56	SP	1020	ASN
56	SP	1114	HIS
56	SP	1241	GLN
56	SP	1458	GLN
56	SP	1475	GLN
56	SP	1491	HIS
56	SP	1508	GLN
56	SP	1625	ASN
56	SP	1707	HIS
56	SP	1737	ASN
56	SP	1816	HIS
57	SQ	184	ASN
60	ST	527	GLN
60	ST	617	HIS
60	ST	713	HIS
61	SU	86	GLN
61	SU	260	ASN
61	SU	343	GLN
61	SU	472	HIS
61	SU	474	HIS
64	SY	45	GLN
64	SY	65	HIS
64	SY	68	HIS
64	SY	200	GLN
65	SZ	351	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L0	63/700 (9%)	12 (19%)	0
2	L1	1423/1802 (78%)	267 (18%)	8 (0%)
3	L2	192/334 (57%)	23 (11%)	1 (0%)
All	All	1678/2836 (59%)	302 (17%)	9 (0%)

All (302) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L0	7	A
1	L0	15	G
1	L0	61	U
1	L0	63	G
1	L0	64	U
1	L0	83	U
1	L0	85	G
1	L0	86	C
1	L0	89	C
1	L0	279	A
1	L0	280	A
1	L0	281	G
2	L1	4	C
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	78	A
2	L1	100	A2M
2	L1	104	A
2	L1	114	C
2	L1	116	U
2	L1	127	G
2	L1	129	U
2	L1	134	U
2	L1	136	C
2	L1	137	U
2	L1	140	A
2	L1	142	G
2	L1	144	U
2	L1	145	A
2	L1	159	U
2	L1	166	C
2	L1	186	C
2	L1	187	G
2	L1	189	C
2	L1	190	C
2	L1	193	U

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Mol	Chain	Res	Type
2	L1	194	U
2	L1	195	G
2	L1	201	G
2	L1	204	G
2	L1	226	A
2	L1	233	C
2	L1	234	G
2	L1	241	U
2	L1	242	U
2	L1	260	U
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	314	C
2	L1	316	A
2	L1	322	G
2	L1	337	G
2	L1	338	C
2	L1	344	A
2	L1	352	A
2	L1	359	A
2	L1	360	A
2	L1	361	C
2	L1	400	A
2	L1	401	A
2	L1	402	C
2	L1	404	G
2	L1	417	A
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

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Mol	Chain	Res	Type
2	L1	448	C
2	L1	460	A
2	L1	467	G
2	L1	477	A
2	L1	487	G
2	L1	494	U
2	L1	495	C
2	L1	496	G
2	L1	501	U
2	L1	502	U
2	L1	505	A
2	L1	506	A
2	L1	515	A
2	L1	519	C
2	L1	520	A
2	L1	532	U
2	L1	534	A
2	L1	540	G
2	L1	542	A
2	L1	545	A
2	L1	548	G
2	L1	563	U
2	L1	564	G
2	L1	565	C
2	L1	570	A
2	L1	575	C
2	L1	578	OMU
2	L1	580	A
2	L1	583	C
2	L1	585	A
2	L1	586	G
2	L1	594	A
2	L1	595	G
2	L1	611	U
2	L1	619	A2M
2	L1	622	A
2	L1	624	G
2	L1	629	U
2	L1	647	G
2	L1	652	G
2	L1	654	C
2	L1	688	G

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Mol	Chain	Res	Type
2	L1	691	C
2	L1	752	A
2	L1	765	G
2	L1	766	U
2	L1	774	A
2	L1	775	G
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	914	G
2	L1	921	U
2	L1	926	A
2	L1	933	A
2	L1	934	C
2	L1	935	U
2	L1	951	A
2	L1	960	U
2	L1	966	A
2	L1	969	C
2	L1	992	A
2	L1	1005	A
2	L1	1011	G
2	L1	1026	A
2	L1	1028	C

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Mol	Chain	Res	Type
2	L1	1029	U
2	L1	1032	G
2	L1	1039	A
2	L1	1054	U
2	L1	1059	U
2	L1	1060	U
2	L1	1063	U
2	L1	1076	A
2	L1	1081	A
2	L1	1082	C
2	L1	1092	A
2	L1	1096	C
2	L1	1098	U
2	L1	1099	U
2	L1	1100	G
2	L1	1119	G
2	L1	1139	A
2	L1	1158	C
2	L1	1159	C
2	L1	1189	A
2	L1	1191	U
2	L1	1192	C
2	L1	1193	A
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	1267	G
2	L1	1268	G
2	L1	1269	OMU
2	L1	1270	G
2	L1	1273	G
2	L1	1275	A
2	L1	1276	U
2	L1	1436	A
2	L1	1437	U
2	L1	1440	C

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Mol	Chain	Res	Type
2	L1	1451	C
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	1511	U
2	L1	1535	U
2	L1	1537	C
2	L1	1542	G
2	L1	1548	G
2	L1	1553	G
2	L1	1554	U
2	L1	1555	A
2	L1	1556	A
2	L1	1557	U
2	L1	1559	A
2	L1	1569	A
2	L1	1570	A
2	L1	1579	U
2	L1	1584	G
2	L1	1590	G
2	L1	1595	U
2	L1	1599	C
2	L1	1600	A
2	L1	1601	G
2	L1	1617	U
2	L1	1618	C
2	L1	1619	C
2	L1	1624	C
2	L1	1628	U
2	L1	1629	G
2	L1	1630	U
2	L1	1631	A
2	L1	1639	OMC
2	L1	1651	A
2	L1	1653	C
2	L1	1657	U
2	L1	1658	G
2	L1	1661	U

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Mol	Chain	Res	Type
2	L1	1662	G
2	L1	1664	C
2	L1	1680	G
2	L1	1683	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
3	L2	2	U
3	L2	10	C
3	L2	13	C
3	L2	20	U
3	L2	73	A
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

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Mol	Chain	Res	Type
3	L2	252	C
3	L2	283	U
3	L2	284	U
3	L2	286	U
3	L2	324	U
3	L2	325	C
3	L2	329	C

All (9) RNA pucker outliers are listed below:

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	OMG	L1	1271	2	19,26,27	1.15	2 (10%)	21,38,41	0.78	1 (4%)
2	OMC	L1	1639	2	19,22,23	0.50	0	25,31,34	0.64	0
2	A2M	L1	28	2	18,25,26	0.76	0	20,36,39	1.01	1 (5%)
2	4AC	L1	1773	2	21,24,25	0.69	0	28,34,37	0.84	1 (3%)
2	A2M	L1	796	2	18,25,26	0.72	0	20,36,39	1.05	2 (10%)
2	A2M	L1	541	2	18,25,26	0.72	0	20,36,39	1.17	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	L1	562	2	19,26,27	1.20	2 (10%)	21,38,41	0.95	1 (4%)
2	OMU	L1	1269	2	19,22,23	2.06	6 (31%)	25,31,34	1.84	5 (20%)
27	SEP	LS	128	27	8,9,10	1.61	1 (12%)	7,12,14	1.32	1 (14%)
2	A2M	L1	974	2	18,25,26	0.71	0	20,36,39	0.91	1 (5%)
2	A2M	L1	100	2,66	18,25,26	0.73	0	20,36,39	0.99	3 (15%)
2	A2M	L1	619	2	18,25,26	0.69	0	20,36,39	1.14	3 (15%)
2	A2M	L1	436	2	18,25,26	0.72	0	20,36,39	1.13	1 (5%)
2	OMG	L1	1572	2	19,26,27	1.12	2 (10%)	21,38,41	0.87	1 (4%)
2	A2M	L1	420	2	18,25,26	0.71	0	20,36,39	1.06	2 (10%)
2	OMG	L1	1126	2	19,26,27	1.13	2 (10%)	21,38,41	0.82	1 (4%)
2	OMC	L1	414	2	19,22,23	0.55	0	25,31,34	0.68	0
2	OMU	L1	578	2	19,22,23	2.01	6 (31%)	25,31,34	1.87	5 (20%)
2	OMC	L1	1007	2	19,22,23	0.52	0	25,31,34	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	L1	1271	2	-	2/5/27/28	0/3/3/3
2	OMC	L1	1639	2	-	1/9/27/28	0/2/2/2
2	A2M	L1	28	2	-	1/5/27/28	0/3/3/3
2	4AC	L1	1773	2	-	5/11/29/30	0/2/2/2
2	A2M	L1	796	2	-	0/5/27/28	0/3/3/3
2	A2M	L1	541	2	-	0/5/27/28	0/3/3/3
2	OMG	L1	562	2	-	1/5/27/28	0/3/3/3
2	OMU	L1	1269	2	-	6/9/27/28	0/2/2/2
27	SEP	LS	128	27	-	3/6/8/10	-
2	A2M	L1	974	2	-	1/5/27/28	0/3/3/3
2	A2M	L1	100	2,66	-	3/5/27/28	0/3/3/3
2	A2M	L1	619	2	-	5/5/27/28	0/3/3/3
2	A2M	L1	436	2	-	1/5/27/28	0/3/3/3
2	OMG	L1	1572	2	-	1/5/27/28	0/3/3/3
2	A2M	L1	420	2	-	0/5/27/28	0/3/3/3
2	OMG	L1	1126	2	-	0/5/27/28	0/3/3/3
2	OMC	L1	414	2	-	0/9/27/28	0/2/2/2
2	OMU	L1	578	2	-	2/9/27/28	0/2/2/2
2	OMC	L1	1007	2	-	1/9/27/28	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L1	1269	OMU	C6-N1	4.72	1.49	1.38
2	L1	578	OMU	C6-N1	4.60	1.49	1.38
2	L1	1269	OMU	C2-N1	4.14	1.44	1.38
2	L1	1269	OMU	C5-C4	4.10	1.52	1.43
2	L1	578	OMU	C2-N1	4.00	1.44	1.38
2	L1	578	OMU	C5-C4	3.94	1.52	1.43
27	LS	128	SEP	P-O1P	3.52	1.61	1.50
2	L1	562	OMG	C8-N7	-3.05	1.30	1.34
2	L1	1271	OMG	C8-N7	-3.00	1.30	1.34
2	L1	1126	OMG	C8-N7	-2.87	1.30	1.34
2	L1	578	OMU	O4-C4	-2.81	1.19	1.24
2	L1	1269	OMU	O4-C4	-2.73	1.19	1.24
2	L1	1572	OMG	C8-N7	-2.72	1.30	1.34
2	L1	562	OMG	C5-C6	-2.55	1.42	1.47
2	L1	578	OMU	C2-N3	2.50	1.42	1.38
2	L1	1269	OMU	C2-N3	2.47	1.42	1.38
2	L1	1271	OMG	C5-C6	-2.43	1.42	1.47
2	L1	1126	OMG	C5-C6	-2.40	1.42	1.47
2	L1	1572	OMG	C5-C6	-2.34	1.42	1.47
2	L1	578	OMU	O2-C2	-2.26	1.19	1.23
2	L1	1269	OMU	O2-C2	-2.19	1.19	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L1	578	OMU	C4-N3-C2	-5.63	119.62	126.61
2	L1	1269	OMU	C4-N3-C2	-5.39	119.92	126.61
2	L1	1269	OMU	N3-C2-N1	4.13	120.27	114.89
2	L1	578	OMU	N3-C2-N1	4.05	120.17	114.89
2	L1	578	OMU	C5-C4-N3	3.82	120.16	114.80
2	L1	1269	OMU	C5-C4-N3	3.62	119.87	114.80
2	L1	578	OMU	O4-C4-C5	-3.12	119.77	125.16
2	L1	1269	OMU	O4-C4-C5	-2.93	120.10	125.16
27	LS	128	SEP	OG-CB-CA	2.73	110.80	108.14
2	L1	619	A2M	C4'-O4'-C1'	2.66	112.36	109.92
2	L1	578	OMU	O2-C2-N1	-2.44	119.62	122.80
2	L1	541	A2M	C4'-O4'-C1'	-2.43	107.70	109.92
2	L1	796	A2M	N3-C2-N1	-2.42	125.39	128.67
2	L1	28	A2M	N3-C2-N1	-2.39	125.43	128.67
2	L1	562	OMG	O6-C6-C5	2.35	128.98	124.32
2	L1	1126	OMG	O6-C6-C5	2.33	128.93	124.32
2	L1	1572	OMG	O6-C6-C5	2.30	128.88	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L1	541	A2M	N3-C2-N1	-2.29	125.56	128.67
2	L1	619	A2M	N3-C2-N1	-2.29	125.57	128.67
2	L1	436	A2M	N3-C2-N1	-2.28	125.58	128.67
2	L1	541	A2M	C4-C5-N7	-2.25	106.95	109.34
2	L1	420	A2M	N3-C2-N1	-2.24	125.63	128.67
2	L1	974	A2M	N3-C2-N1	-2.24	125.63	128.67
2	L1	619	A2M	C4-C5-N7	-2.24	106.97	109.34
2	L1	100	A2M	C4'-O4'-C1'	2.23	111.97	109.92
2	L1	1269	OMU	O2-C2-N1	-2.23	119.89	122.80
2	L1	100	A2M	N3-C2-N1	-2.19	125.70	128.67
2	L1	1773	4AC	CM7-C7-N4	2.16	118.75	115.27
2	L1	1271	OMG	O6-C6-C5	2.12	128.52	124.32
2	L1	796	A2M	C4-C5-N7	-2.08	107.14	109.34
2	L1	420	A2M	C4-C5-N7	-2.05	107.17	109.34
2	L1	100	A2M	C4-C5-N7	-2.02	107.20	109.34

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L1	28	A2M	C1'-C2'-O2'-CM'
2	L1	100	A2M	C1'-C2'-O2'-CM'
2	L1	436	A2M	C1'-C2'-O2'-CM'
2	L1	974	A2M	C1'-C2'-O2'-CM'
2	L1	1007	OMC	C1'-C2'-O2'-CM2
27	LS	128	SEP	C-CA-CB-OG
27	LS	128	SEP	CA-CB-OG-P
2	L1	1773	4AC	N3-C4-N4-C7
2	L1	1773	4AC	C5-C4-N4-C7
2	L1	1269	OMU	C2'-C1'-N1-C6
2	L1	100	A2M	C3'-C4'-C5'-O5'
2	L1	578	OMU	O4'-C4'-C5'-O5'
2	L1	100	A2M	O4'-C4'-C5'-O5'
2	L1	578	OMU	C3'-C4'-C5'-O5'
2	L1	619	A2M	O4'-C4'-C5'-O5'
2	L1	1271	OMG	O4'-C4'-C5'-O5'
2	L1	1271	OMG	C3'-C4'-C5'-O5'
2	L1	1269	OMU	C2'-C1'-N1-C2
2	L1	619	A2M	C3'-C4'-C5'-O5'
2	L1	1269	OMU	O4'-C4'-C5'-O5'
2	L1	1773	4AC	O7-C7-N4-C4
2	L1	1773	4AC	CM7-C7-N4-C4

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Mol	Chain	Res	Type	Atoms
2	L1	619	A2M	C4'-C5'-O5'-P
2	L1	1269	OMU	O4'-C1'-N1-C2
2	L1	1269	OMU	O4'-C1'-N1-C6
2	L1	619	A2M	C3'-C2'-O2'-CM'
2	L1	1572	OMG	O4'-C4'-C5'-O5'
2	L1	619	A2M	C1'-C2'-O2'-CM'
2	L1	1639	OMC	C4'-C5'-O5'-P
2	L1	562	OMG	O4'-C4'-C5'-O5'
27	LS	128	SEP	CB-OG-P-O3P
2	L1	1269	OMU	C3'-C4'-C5'-O5'
2	L1	1773	4AC	C3'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L1	1271	OMG	1	0
2	L1	1773	4AC	1	0
2	L1	562	OMG	2	0
2	L1	1269	OMU	1	0
2	L1	974	A2M	1	0
2	L1	100	A2M	2	0
2	L1	420	A2M	1	0
2	L1	578	OMU	1	0
2	L1	1007	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 65 ligands modelled in this entry, 62 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
69	ADP	NS	1301	66	24,29,29	0.93	1 (4%)	29,45,45	1.31	3 (10%)
70	GTP	SI	2001	66	29,34,34	0.93	1 (3%)	35,54,54	0.70	0
67	ATP	NH	1300	66	28,33,33	0.67	0	34,52,52	0.91	1 (2%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	NS	1301	ADP	O4'-C1'	2.08	1.43	1.40
70	SI	2001	GTP	PA-O2A	-2.01	1.46	1.55

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	NS	1301	ADP	N3-C2-N1	-4.36	122.75	128.67
69	NS	1301	ADP	C4-C5-N7	-2.64	106.55	109.34
67	NH	1300	ATP	C5-C6-N6	2.32	123.84	120.31
69	NS	1301	ADP	O4'-C1'-N9	2.26	111.74	108.75

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	SI	2001	GTP	PB-O3B-PG-O2G
70	SI	2001	GTP	PB-O3B-PG-O3G
69	NS	1301	ADP	O4'-C4'-C5'-O5'
69	NS	1301	ADP	C3'-C4'-C5'-O5'
70	SI	2001	GTP	PA-O3A-PB-O1B
69	NS	1301	ADP	PB-O3A-PA-O1A
67	NH	1300	ATP	PA-O3A-PB-O3B
69	NS	1301	ADP	PB-O3A-PA-O2A

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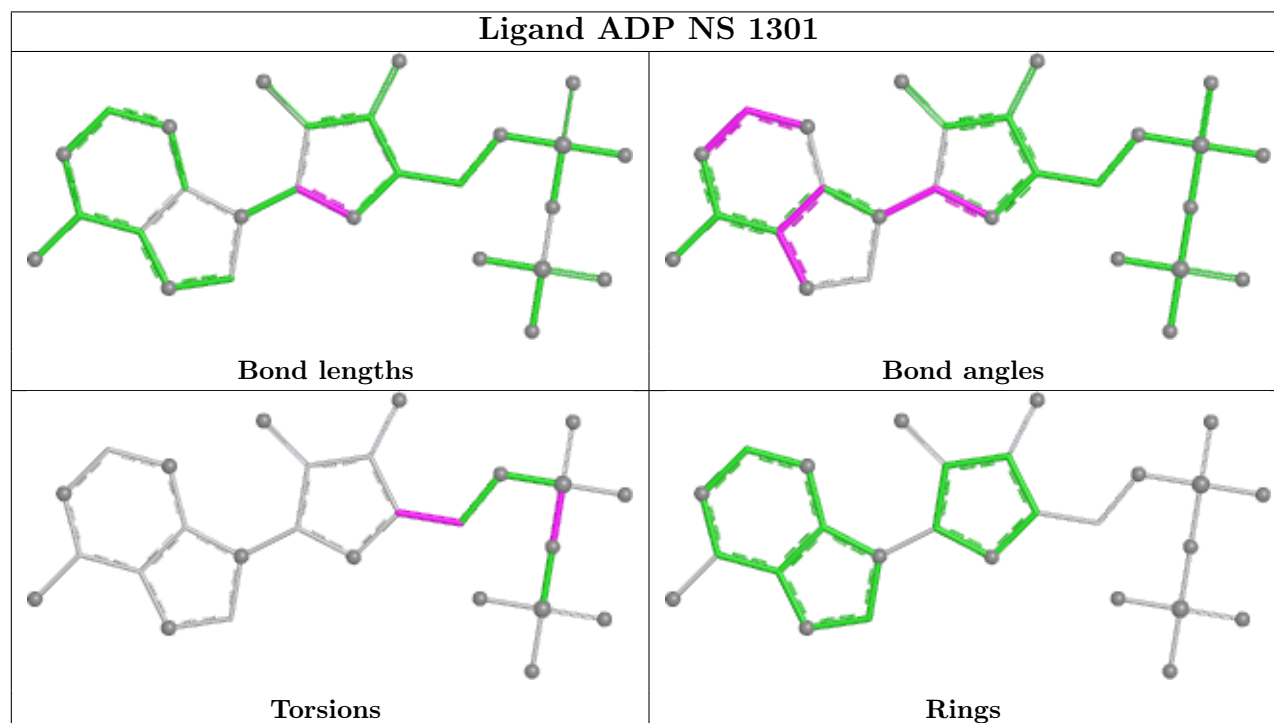
Mol	Chain	Res	Type	Atoms
67	NH	1300	ATP	PA-O3A-PB-O1B
67	NH	1300	ATP	PA-O3A-PB-O2B

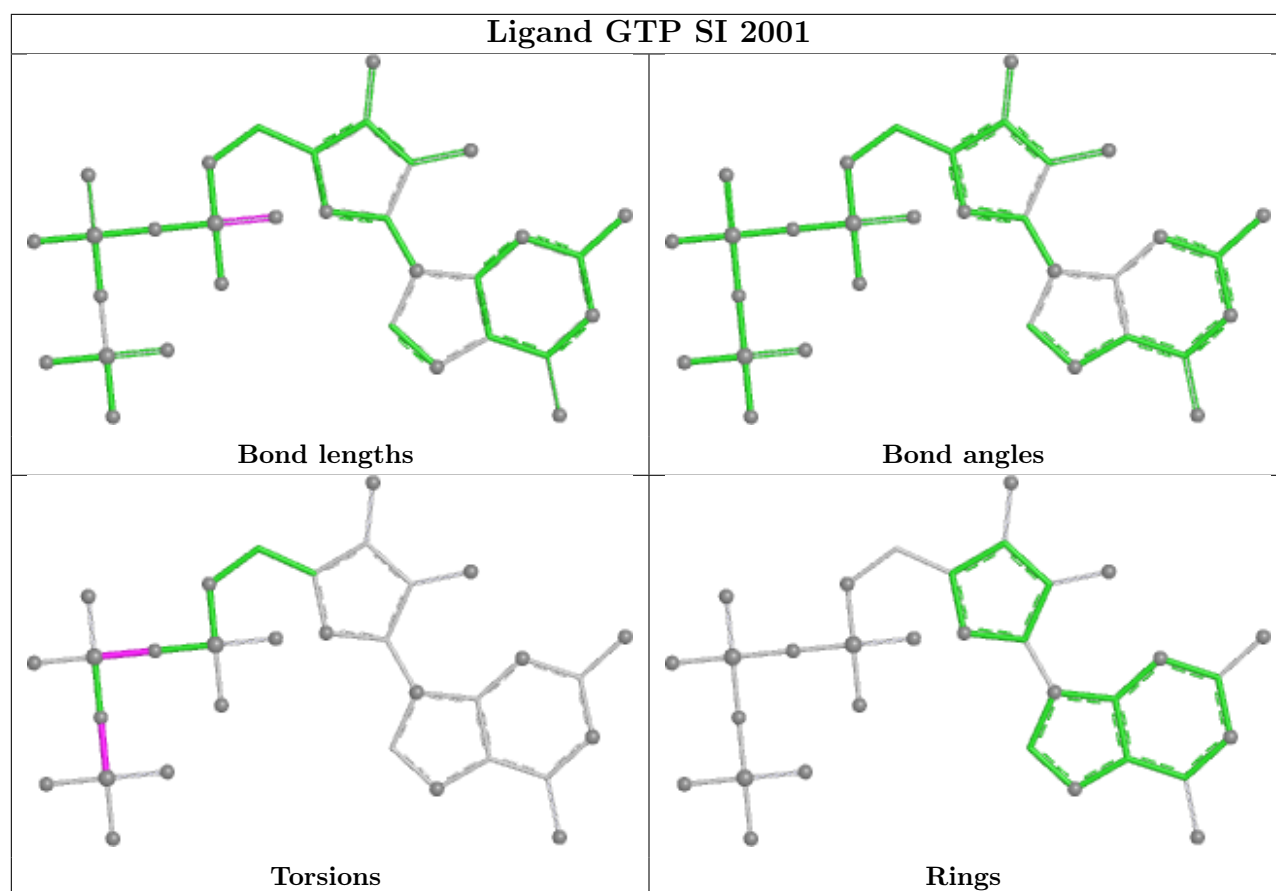
There are no ring outliers.

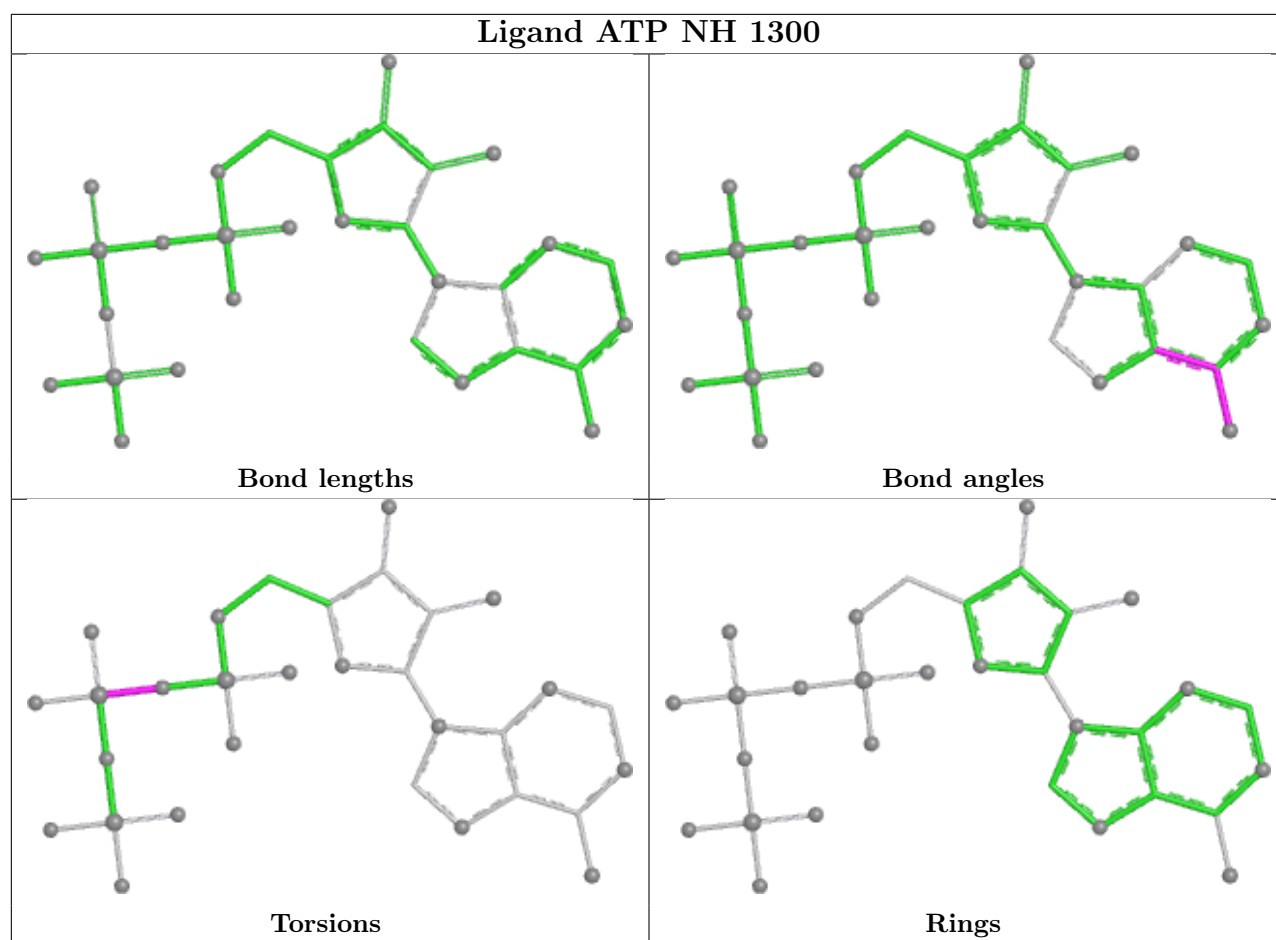
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

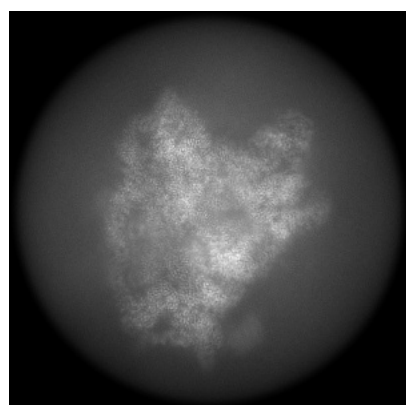
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49085. These allow visual inspection of the internal detail of the map and identification of artifacts.

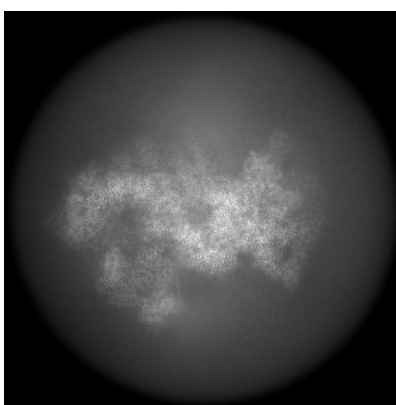
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

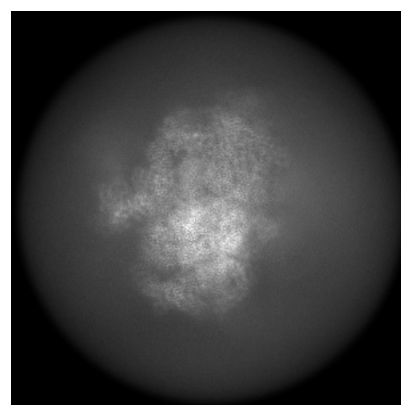
6.1.1 Primary map



X



Y

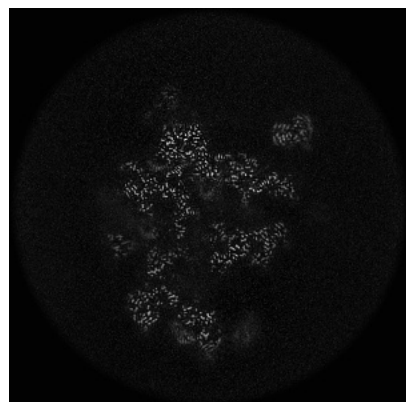


Z

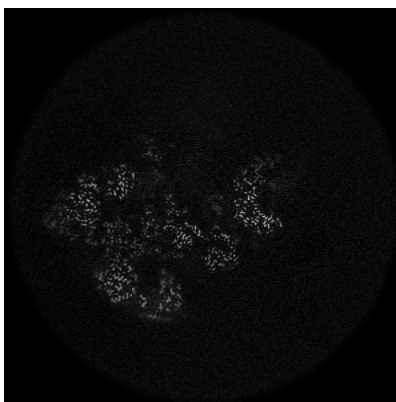
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

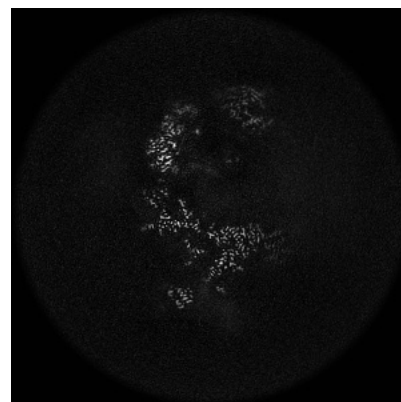
6.2.1 Primary map



X Index: 252



Y Index: 252

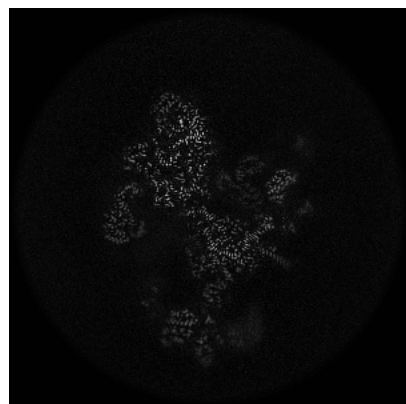


Z Index: 252

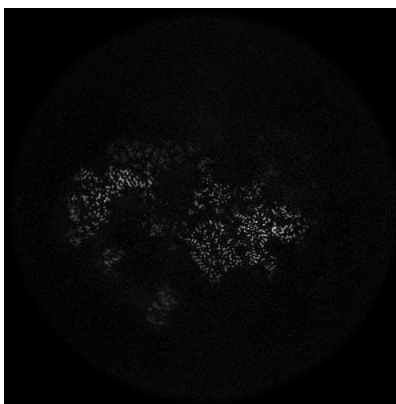
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

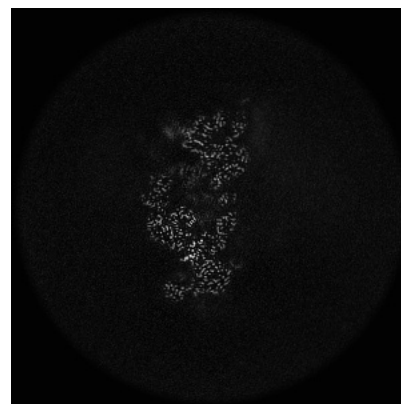
6.3.1 Primary map



X Index: 227



Y Index: 228

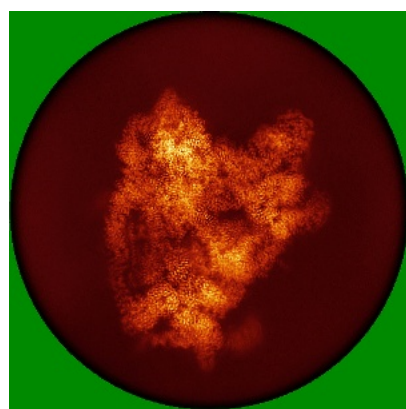


Z Index: 280

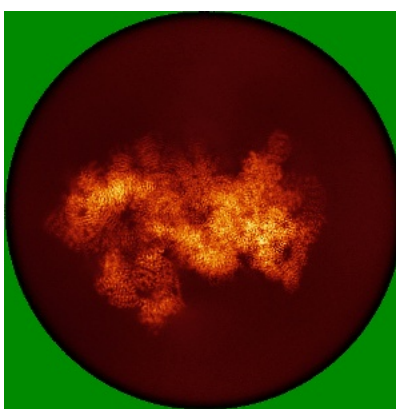
The images above show the largest variance slices of the map in three orthogonal directions.

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

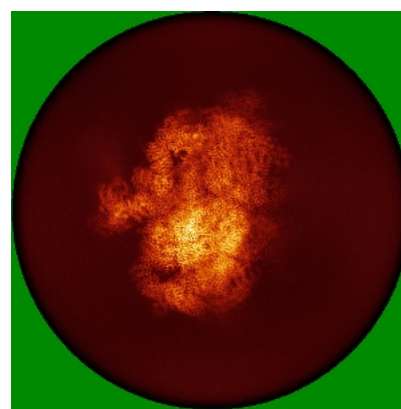
6.4.1 Primary map



X



Y

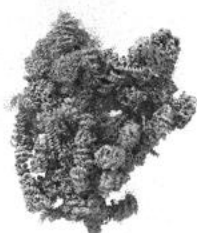


Z

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

6.5 Orthogonal surface views [i](#)

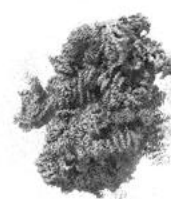
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

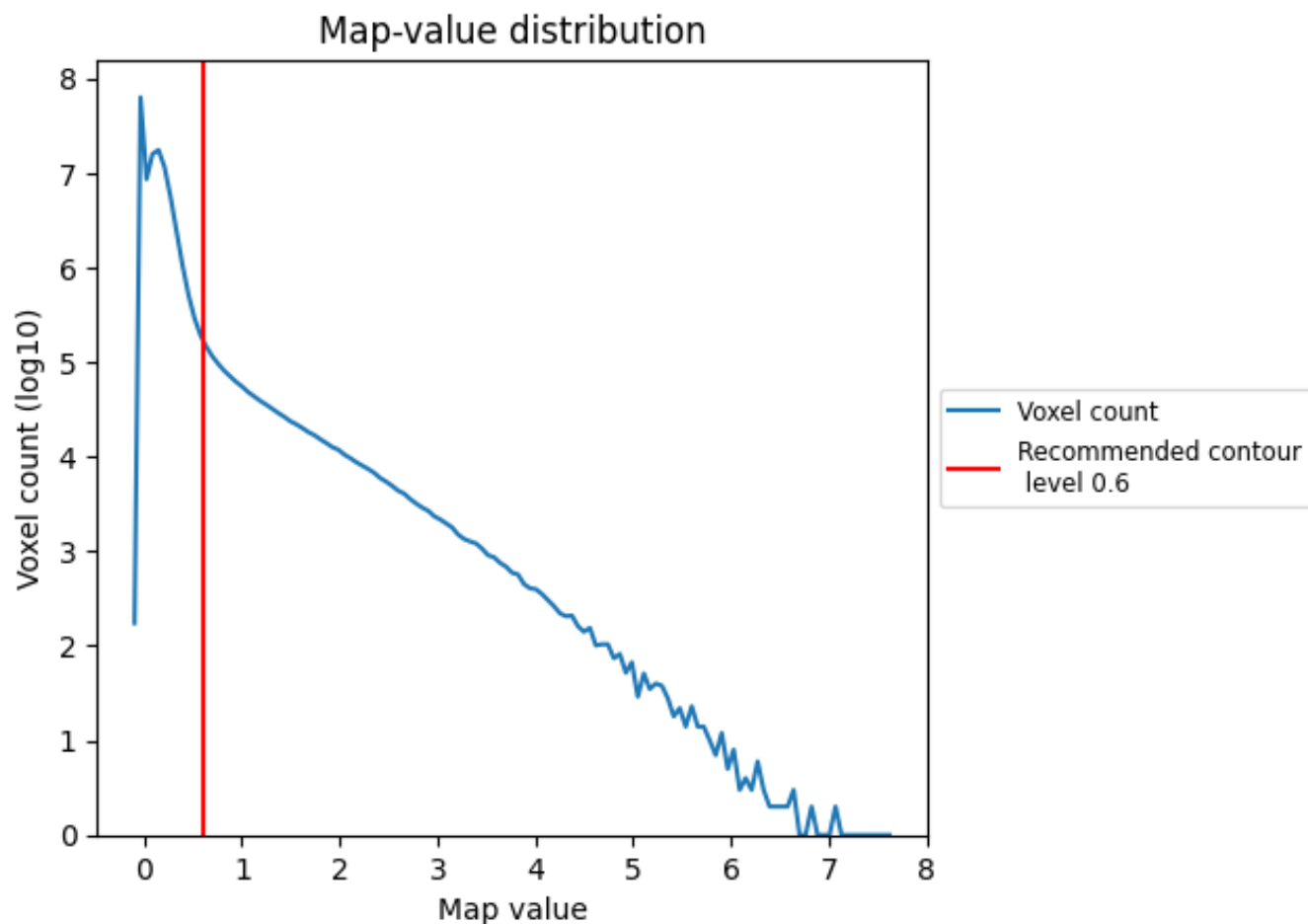
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

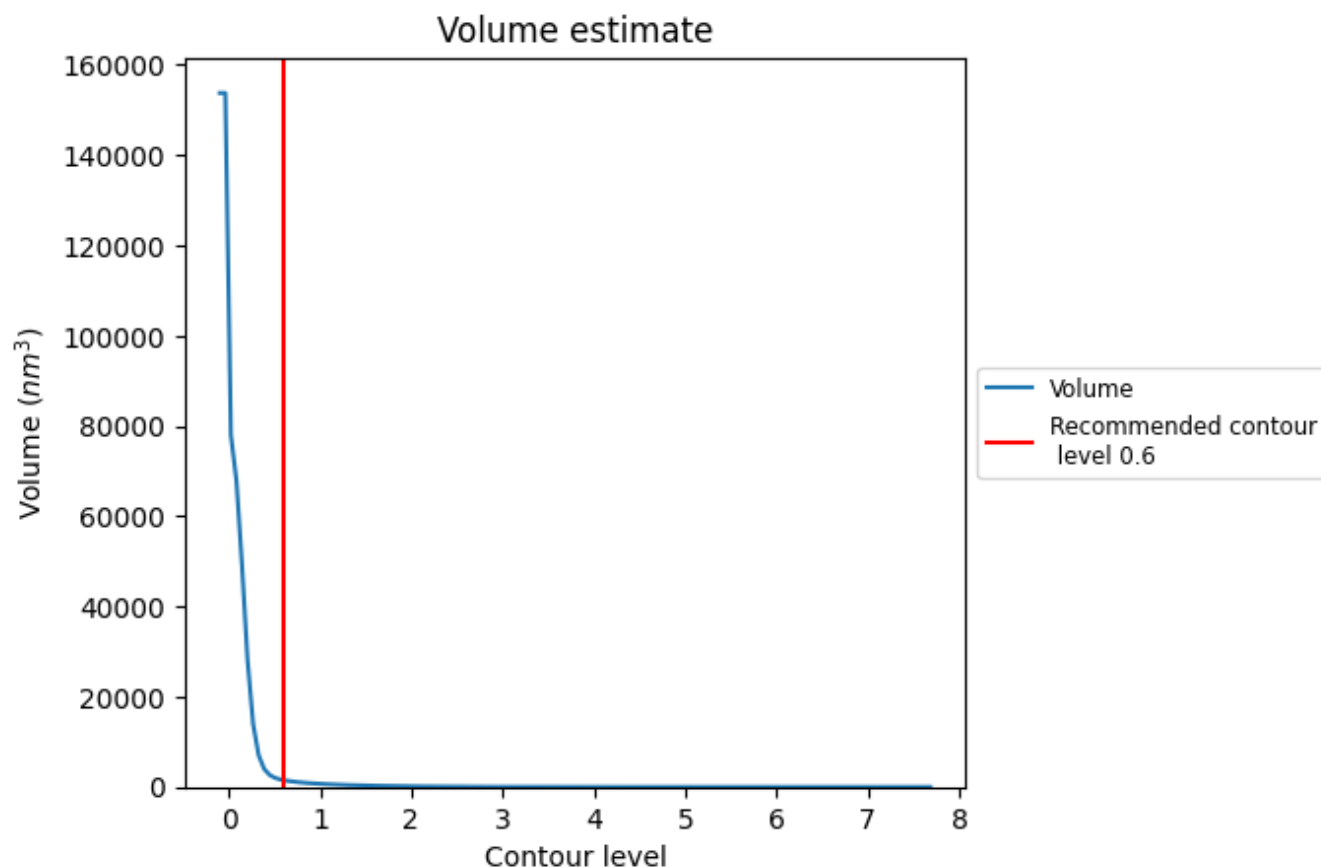
This section contains the results of statistical analysis of the map.

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.

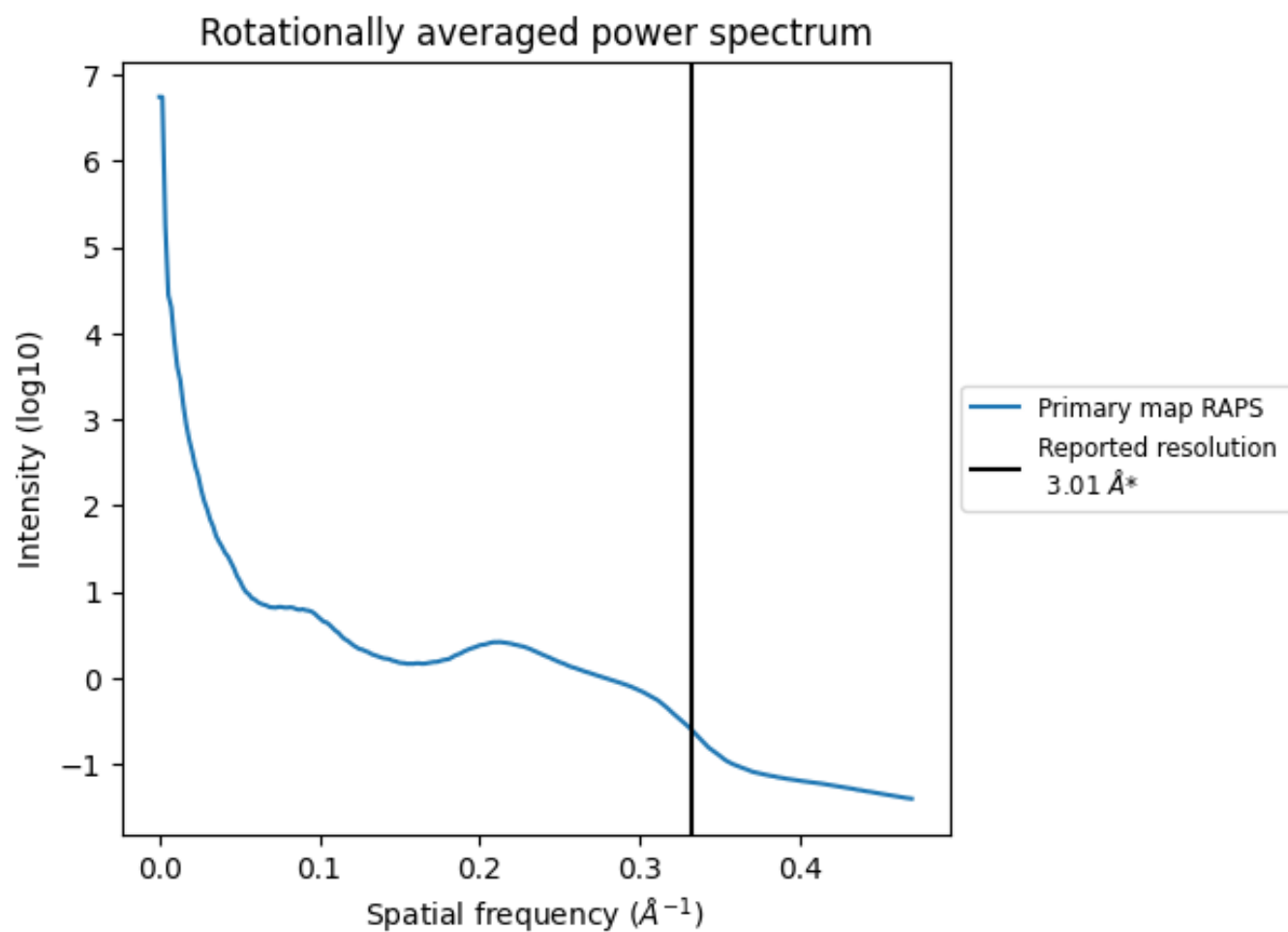
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1520 nm^3 ; this corresponds to an approximate mass of 1373 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 0.332 \AA^{-1}

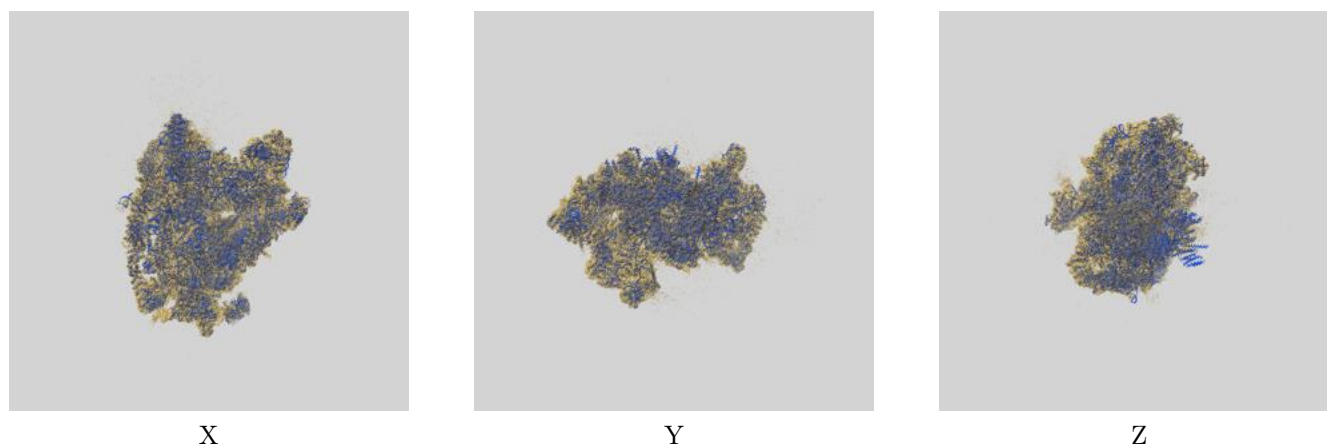
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

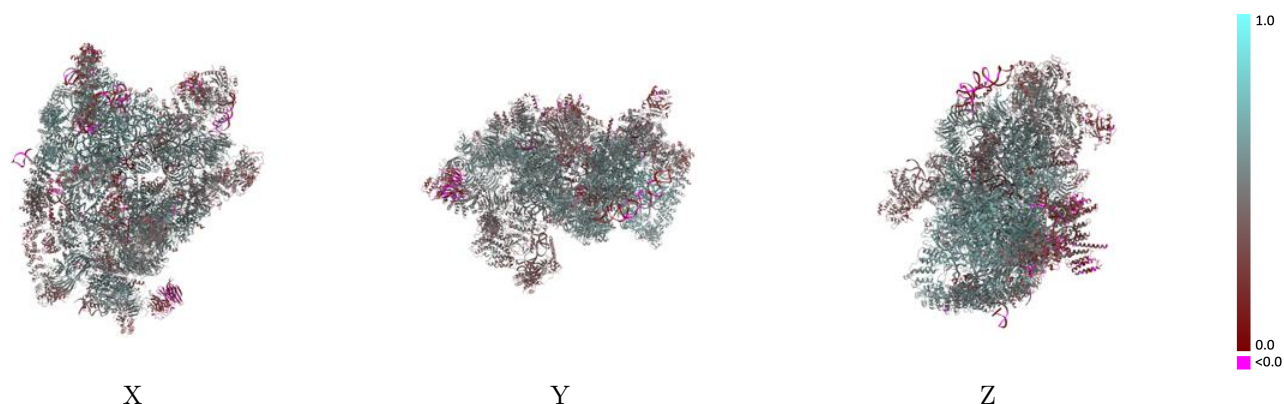
This section contains information regarding the fit between EMDB map EMD-49085 and PDB model 9N75. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



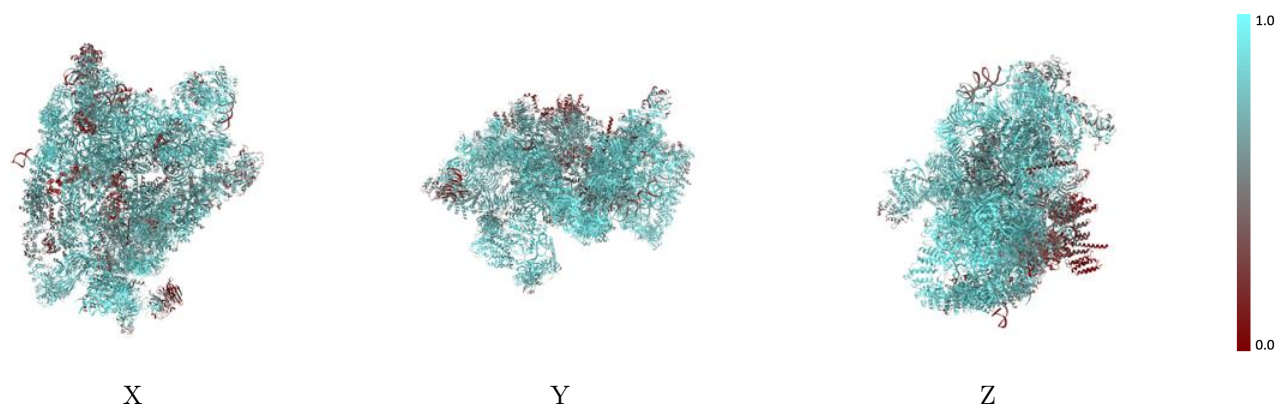
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



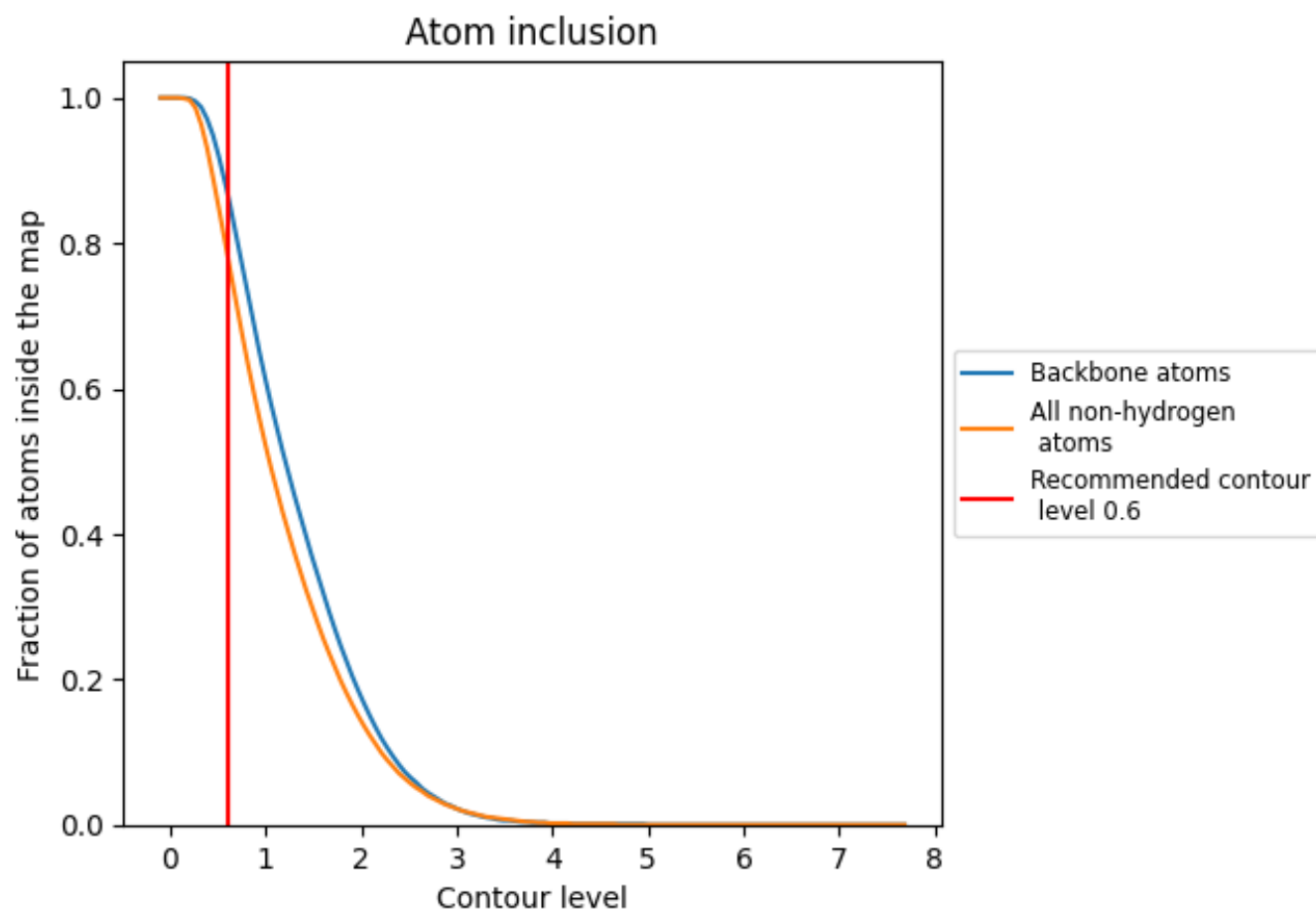
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 79% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7860	 0.4780
L0	 0.8120	 0.4130
L1	 0.8800	 0.5110
L2	 0.7570	 0.4260
L3	 0.5930	 0.4360
L4	 0.9700	 0.6350
L5	 0.8070	 0.5200
L6	 0.9110	 0.5800
L7	 0.4580	 0.2730
L8	 0.9650	 0.6280
L9	 0.9230	 0.5970
LC	 0.8710	 0.5580
LD	 0.9570	 0.6270
LE	 0.9300	 0.6060
LF	 0.9290	 0.6080
LG	 0.8490	 0.5660
LH	 0.8710	 0.5100
LI	 0.5210	 0.2540
LJ	 0.7850	 0.4660
LK	 0.6840	 0.3520
LL	 0.8150	 0.4810
LM	 0.6580	 0.4030
LN	 0.9140	 0.5510
LO	 0.7950	 0.5140
LP	 0.2290	 0.2920
LQ	 0.9120	 0.5170
LR	 0.8800	 0.5320
LS	 0.7990	 0.5030
LT	 0.7430	 0.4810
LW	 0.1360	 0.2560
LZ	 0.7120	 0.4800
NA	 0.6920	 0.4620
NB	 0.6890	 0.4360
ND	 0.6780	 0.3890
NF	 0.8760	 0.5710



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Chain	Atom inclusion	Q-score
NG	 0.9280	 0.5650
NH	 0.8330	 0.4300
NI	 0.6030	 0.2960
NL	 0.5520	 0.3760
NM	 0.7940	 0.5150
NP	 0.7130	 0.5000
NQ	 0.8310	 0.5270
NS	 0.5760	 0.3950
NV	 0.5710	 0.4270
OH	 0.5470	 0.2940
OU	 0.5460	 0.2800
SA	 0.7030	 0.4560
SB	 0.6460	 0.4480
SC	 0.9180	 0.5920
SD	 0.7660	 0.4870
SE	 0.9320	 0.5670
SF	 0.9370	 0.5990
SG	 0.8980	 0.5770
SH	 0.9070	 0.5870
SI	 0.8980	 0.5870
SJ	 0.8390	 0.3980
SK	 0.8740	 0.4520
SL	 0.9210	 0.5940
SM	 0.8840	 0.5720
SP	 0.7280	 0.4790
SQ	 0.8000	 0.5530
SR	 0.9490	 0.6100
SS	 0.2640	 0.3230
ST	 0.8080	 0.4290
SU	 0.7720	 0.3790
SV	 0.6650	 0.4110
SW	 0.8090	 0.5110
SY	 0.7630	 0.4940
SZ	 0.8810	 0.3870