



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:33 PM UTC

PDB ID : 9N74 / pdb_00009n74
EMDB ID : EMD-49084
Title : SSU processome maturation and disassembly, State H
Authors : Buzovetsky, O.; Klinge, S.
Deposited on : 2025-02-05
Resolution : 2.65 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

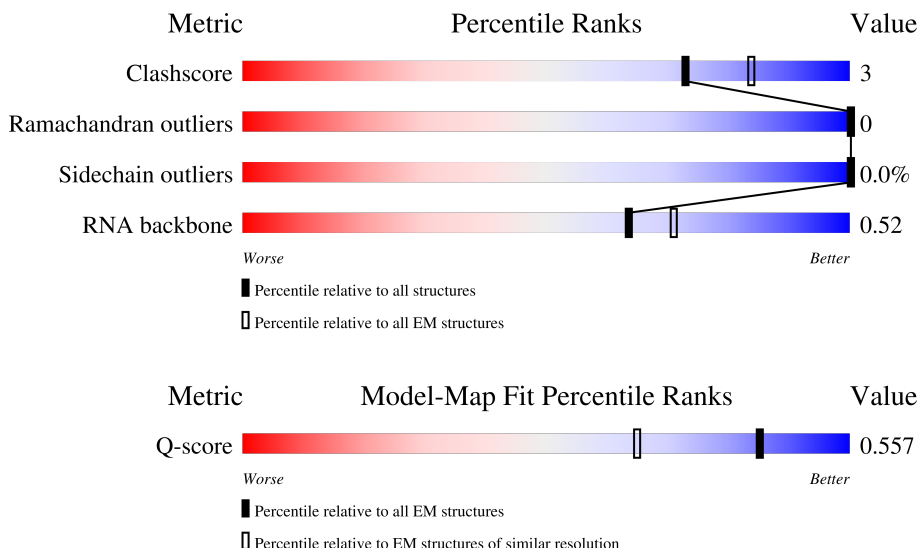
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9050 (2.15 - 3.15)

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.

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2	L1	1802	
3	L2	334	

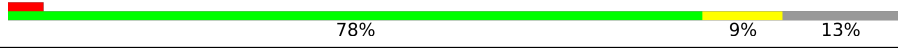
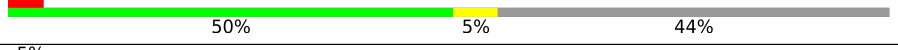
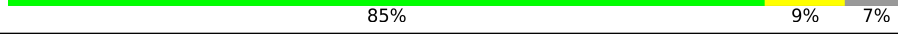
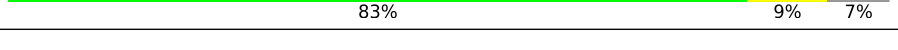
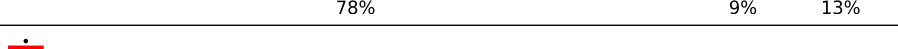
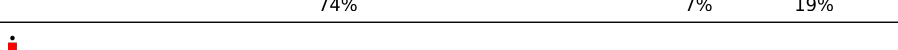
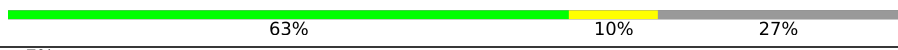
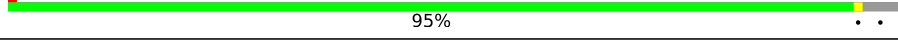
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Mol	Chain	Length	Quality of chain
4	L3	146	
5	L4	261	
6	L5	225	
7	L6	236	
8	L7	190	
9	L8	200	
10	L9	197	
11	LC	143	
12	LD	156	
13	LE	130	
14	LF	135	
15	LG	67	
16	LH	896	
17	LI	713	
18	LJ	513	
19	LK	575	
20	LL	643	
21	LM	1769	
22	LN	776	
23	LO	923	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

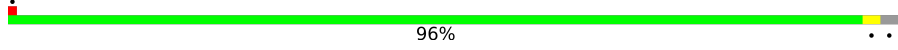
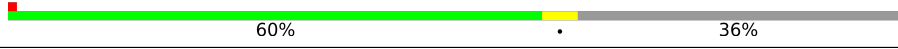
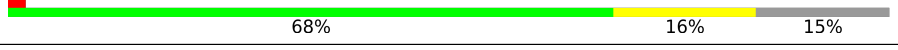
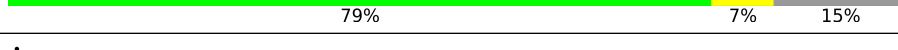
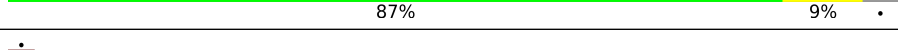
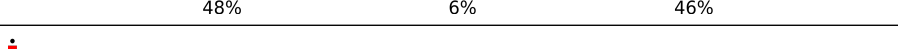
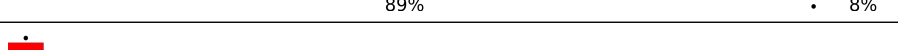
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Mol	Chain	Length	Quality of chain
29	LU	489	
30	LW	554	
31	LZ	183	
32	NA	593	
33	NB	610	
34	ND	214	
35	NF	151	
36	NG	137	
37	NH	1237	
38	NI	297	
39	NL	318	
40	NM	255	
41	NP	144	
42	NQ	82	
43	NS	1267	
44	NV	733	
45	OA	1729	
46	OH	143	
47	OU	152	
48	SA	504	
49	SB	511	
50	SC	327	
50	SD	327	
51	SE	126	
51	SF	126	

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Mol	Chain	Length	Quality of chain
52	SG	573	
53	SH	367	
54	SI	1183	
55	SJ	252	
55	SK	252	
56	SL	189	
57	SM	290	
58	SP	2493	
59	SQ	217	
60	SR	145	
61	SS	899	
62	ST	810	
63	SU	552	
64	SV	206	
65	SW	274	
66	SX	30	
67	SY	250	
68	SZ	483	

2 Entry composition

There are 73 unique types of molecules in this entry. The entry contains 238225 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	64	Total	C	N	O	P	0	0
			1370	612	247	447	64		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L1	1485	Total	C	N	O	P	0	0
			31696	14179	5647	10385	1485		

- Molecule 3 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L2	214	Total	C	N	O	P	0	0
			4543	2030	783	1515	215		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LH	806	Total	C	N	O	S		
			6449	4113	1087	1230	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LI	600	Total	C	N	O	S		
			4209	2671	725	804	9	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LM	1618	Total	C	N	O	S	0	0
			12908	8337	2113	2421	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 Protein SOF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LU	454	Total	C	N	O	S	0	0
			3707	2318	677	696	16		

- Molecule 30 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LW	459	Total	C	N	O	S	0	0
			3627	2288	645	683	11		

- Molecule 31 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LZ	160	Total	C	N	O	S	0	0
			1332	848	245	233	6		

- Molecule 32 is a protein called U3 small nucleolar RNA-associated protein MPP10.

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

- Molecule 33 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	NB	264	Total	C	N	O	S	0	0
			2164	1364	378	415	7		

- Molecule 34 is a protein called Bud site selection protein 21.

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

- Molecule 35 is a protein called 40S ribosomal protein S13.

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

- Molecule 36 is a protein called 40S ribosomal protein S14-A.

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

- Molecule 37 is a protein called U3 small nucleolar RNA-associated protein 22.

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

- Molecule 38 is a protein called Ribosomal RNA-processing protein 7.

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

- Molecule 39 is a protein called Dimethyladenosine transferase.

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

- Molecule 40 is a protein called Small ribosomal subunit protein eS1A.

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

- Molecule 41 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 42 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 43 is a protein called Probable ATP-dependent RNA helicase DHR1.

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

- Molecule 44 is a protein called Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	NV	47	Total	C	N	O	0	0
			373	239	70	64		

- Molecule 45 is a protein called rRNA biogenesis protein RRP5.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	OA	279	Total	C	N	O	0	0
			1428	863	280	285		

- Molecule 46 is a protein called 40S ribosomal protein S12.

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

- Molecule 47 is a protein called Ubiquitin-40S ribosomal protein S31.

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

- Molecule 48 is a protein called Nucleolar protein 56.

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

- Molecule 49 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SB	433	Total	C	N	O	S	0	0
			3338	2104	570	654	10		

- Molecule 50 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

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

- Molecule 51 is a protein called 13 kDa ribonucleoprotein-associated protein.

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

- Molecule 52 is a protein called Ribosomal RNA-processing protein 9.

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

- Molecule 53 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

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

- Molecule 54 is a protein called Ribosome biogenesis protein BMS1.

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

- Molecule 55 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SJ	213	Total	C	N	O	S	0	0
			1678	1069	292	306	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
55	SK	229	Total	C	N	O	S	0	0
			1793	1141	312	329	11		

- Molecule 56 is a protein called rRNA-processing protein FCF1.

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

- Molecule 57 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

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

- Molecule 58 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SP	2405	Total	C	N	O	S	0	0
			19588	12604	3275	3644	65		

- Molecule 59 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SQ	117	Total	C	N	O	S	0	0
			991	626	180	182	3		

- Molecule 60 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 61 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	SS	329	Total	C	N	O	P	S	1	0
			2679	1664	487	517	1	10		

- Molecule 62 is a protein called Nucleolar complex protein 14.

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

- Molecule 63 is a protein called Nucleolar complex protein 4.

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

- Molecule 64 is a protein called Regulator of rDNA transcription protein 14.

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

- Molecule 65 is a protein called Pre-rRNA-processing protein PNO1.

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

- Molecule 66 is a protein called Unassigned peptides.

Mol	Chain	Residues	Atoms				AltConf	Trace
66	SX	30	Total	C	N	O	0	0
			159	98	31	30		

- Molecule 67 is a protein called U3 small nucleolar RNA-associated protein 11.

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

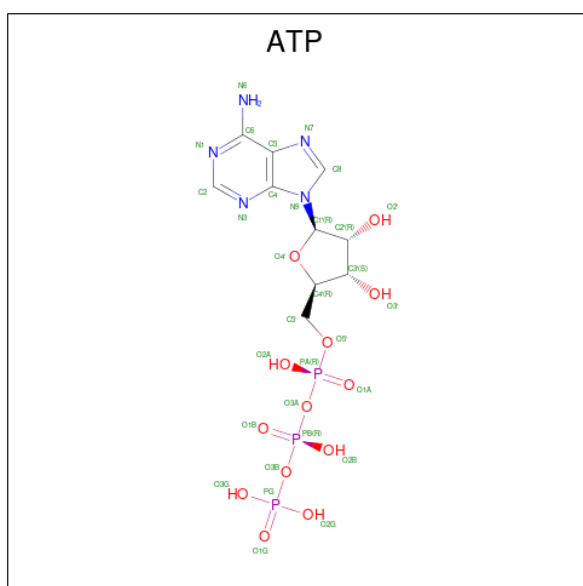
- Molecule 68 is a protein called Essential nuclear protein 1.

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

- Molecule 69 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
69	L1	36	Total	Mg	0
			36	36	
69	NH	1	Total	Mg	0
			1	1	
69	NS	1	Total	Mg	0
			1	1	
69	SI	1	Total	Mg	0
			1	1	

- Molecule 70 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

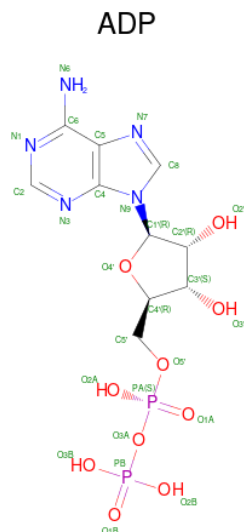


Mol	Chain	Residues	Atoms					AltConf
70	NH	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 71 is ZINC ION (CCD ID: ZN) (formula: Zn).

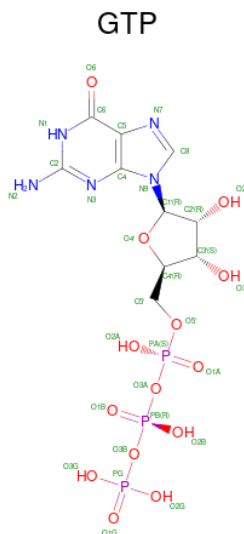
Mol	Chain	Residues	Atoms		AltConf
71	NQ	1	Total	Zn	0
			1	1	
71	OU	1	Total	Zn	0
			1	1	
71	SL	1	Total	Zn	0
			1	1	

- Molecule 72 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 73 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

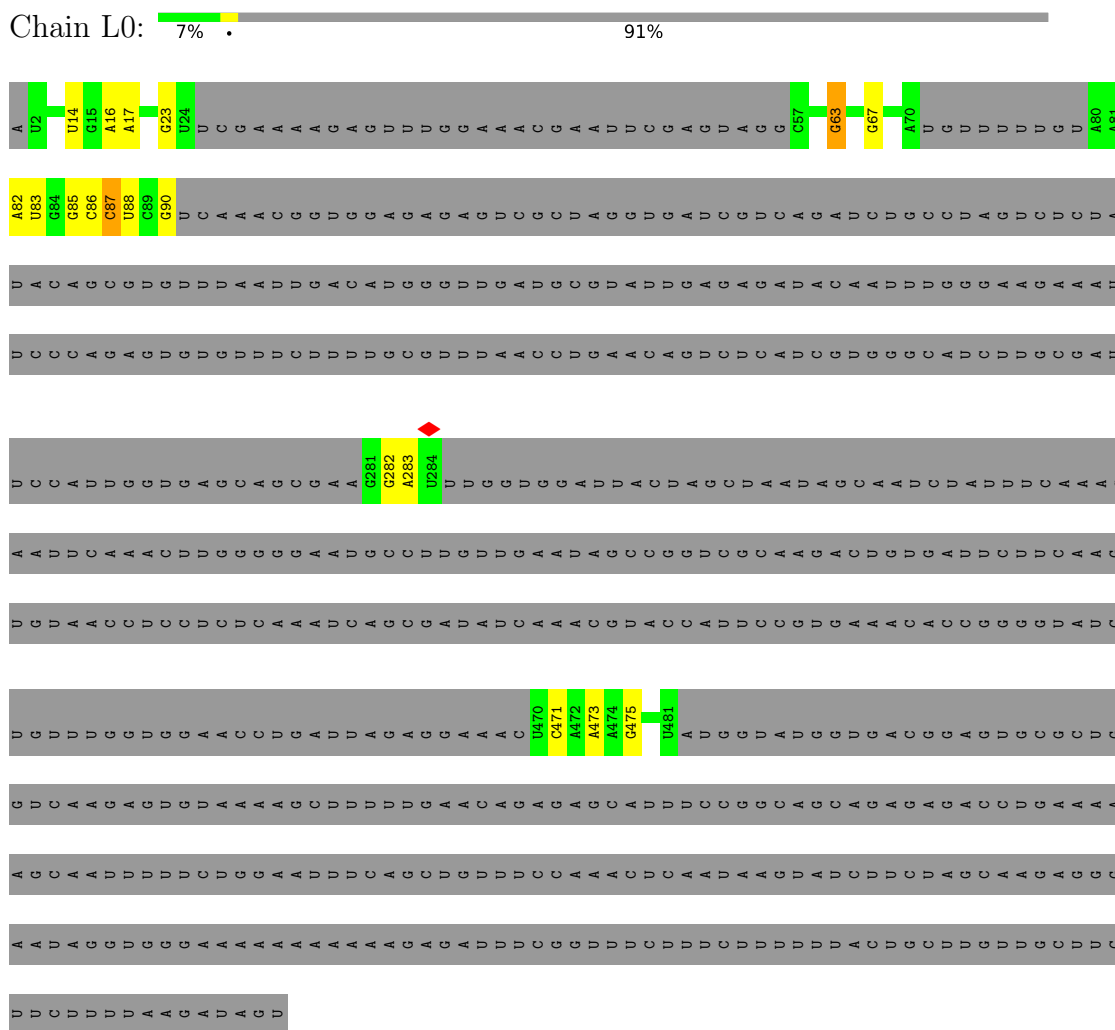


Mol	Chain	Residues	Atoms					AltConf
73	SI	1	Total	C	N	O	P	0
			32	10	5	14	3	

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.

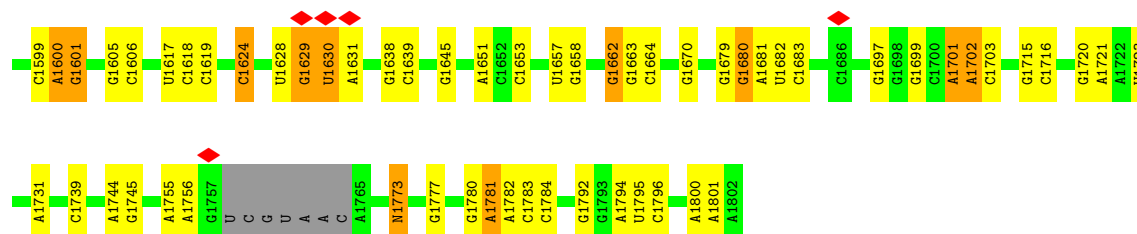
• Molecule 1: 5'ETS rRNA



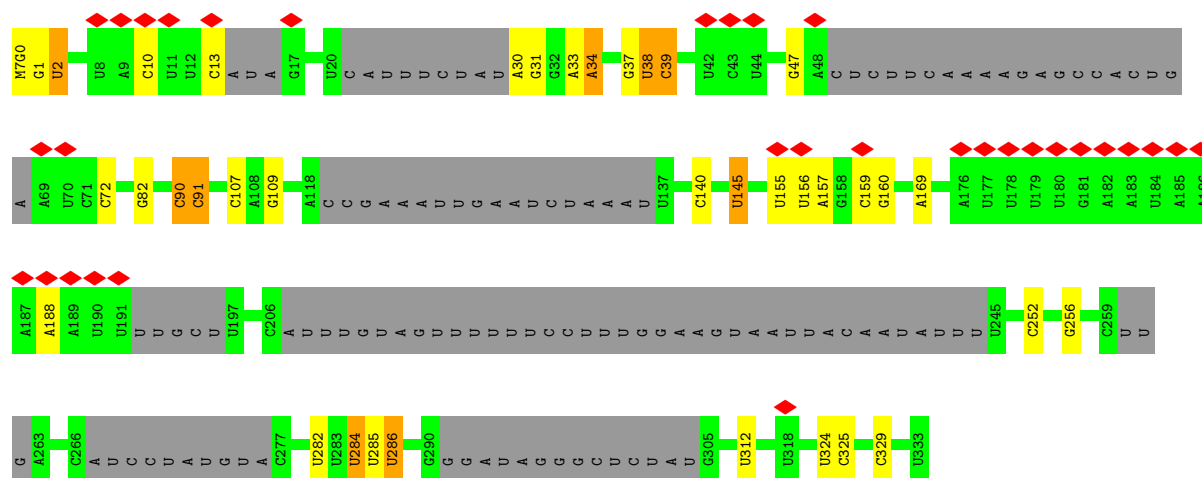
• Molecule 2: 18S rRNA



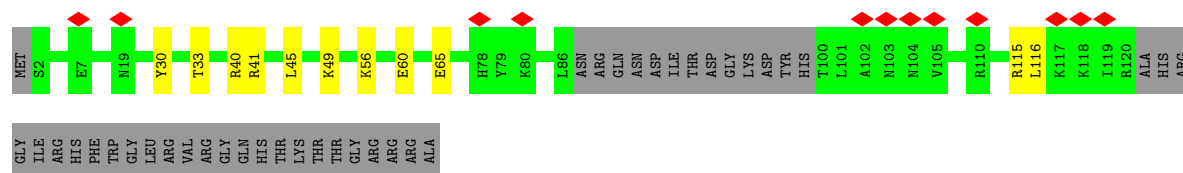




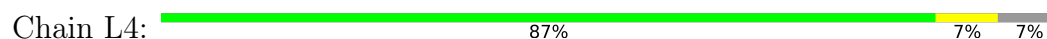
• Molecule 3: U3 snoRNA



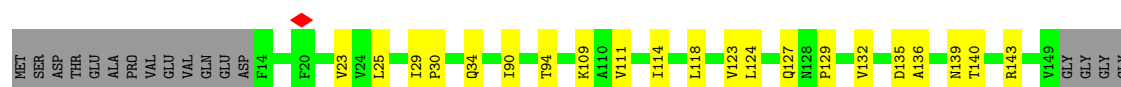
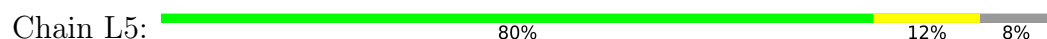
• Molecule 4: 40S ribosomal protein S18-A



• Molecule 5: 40S ribosomal protein S4-A

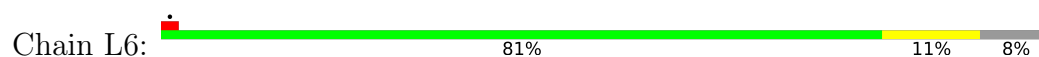


• Molecule 6: 40S ribosomal protein S5

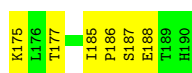
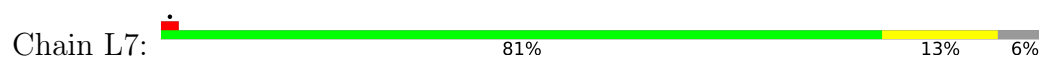




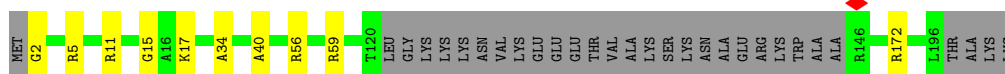
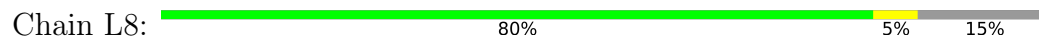
- Molecule 7: 40S ribosomal protein S6-A



- Molecule 8: 40S ribosomal protein S7-A



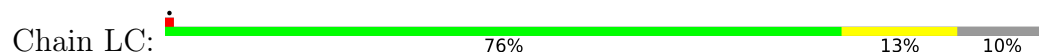
- Molecule 9: 40S ribosomal protein S8-A



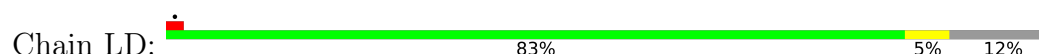
- Molecule 10: 40S ribosomal protein S9-A



- Molecule 11: 40S ribosomal protein S16-A

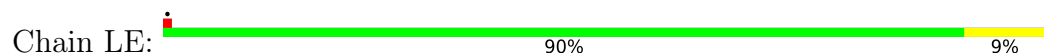


- Molecule 12: 40S ribosomal protein S11-A





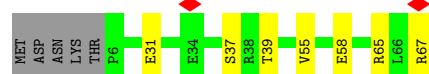
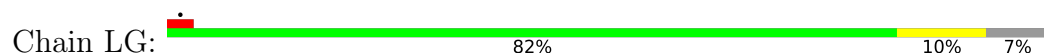
- Molecule 13: 40S ribosomal protein S22-A



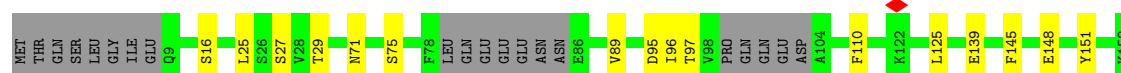
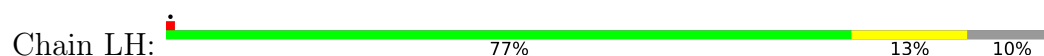
- Molecule 14: 40S ribosomal protein S24-A



- Molecule 15: 40S ribosomal protein S28-A

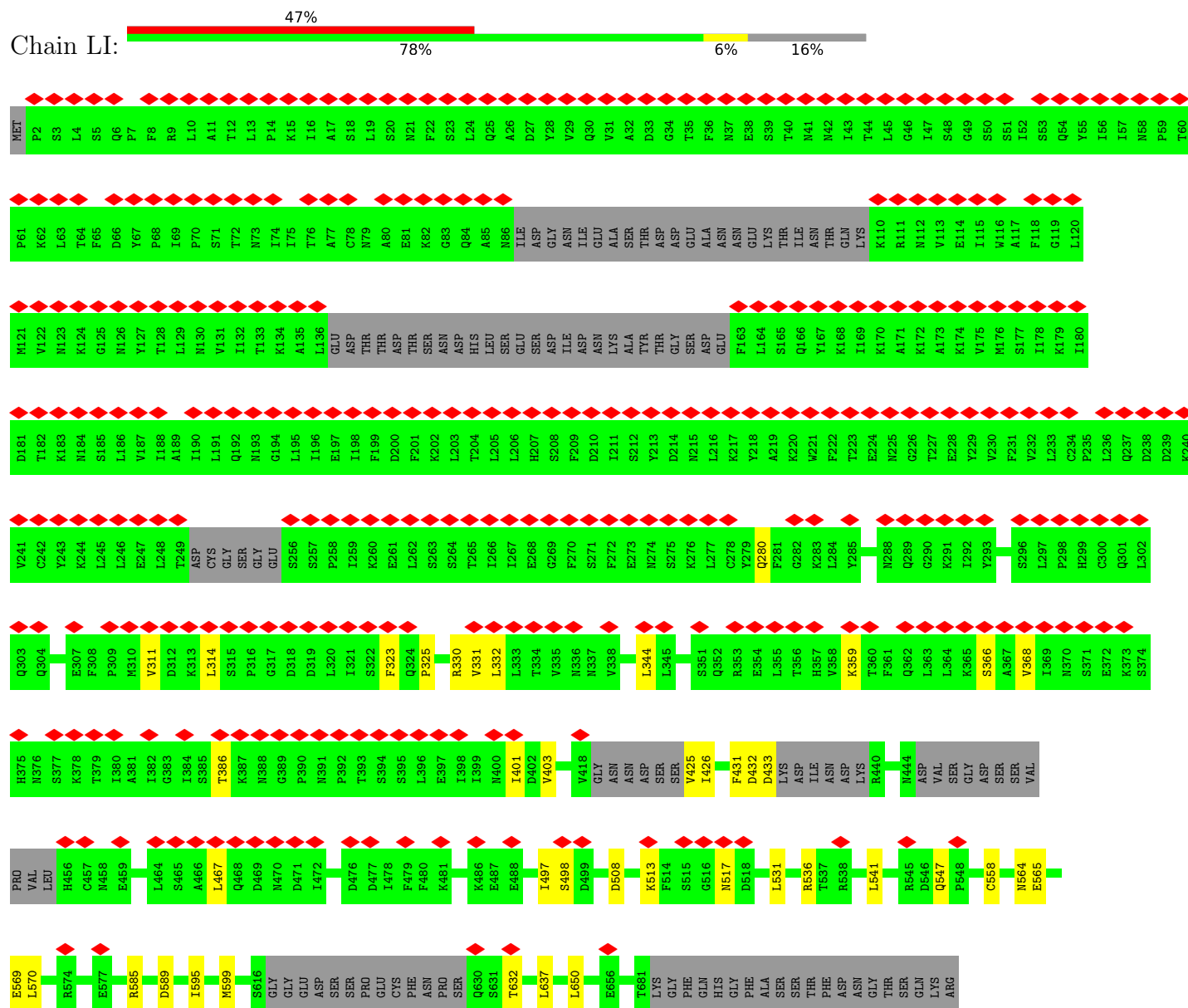


- Molecule 16: NET1-associated nuclear protein 1



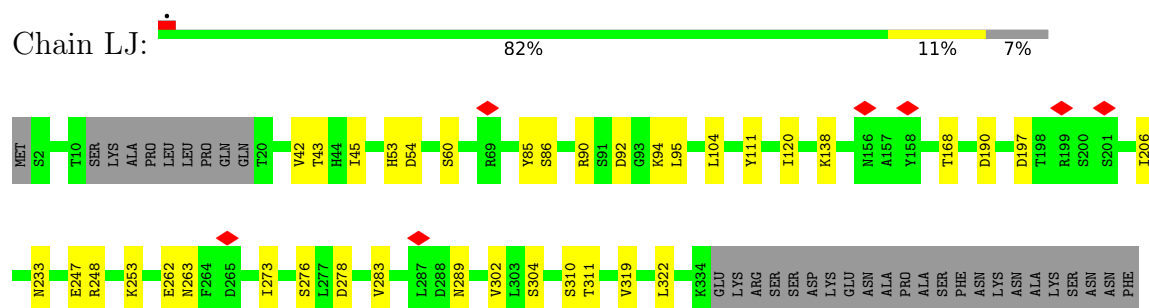
• Molecule 17: U3 small nucleolar RNA-associated protein 8

Chain LI:



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

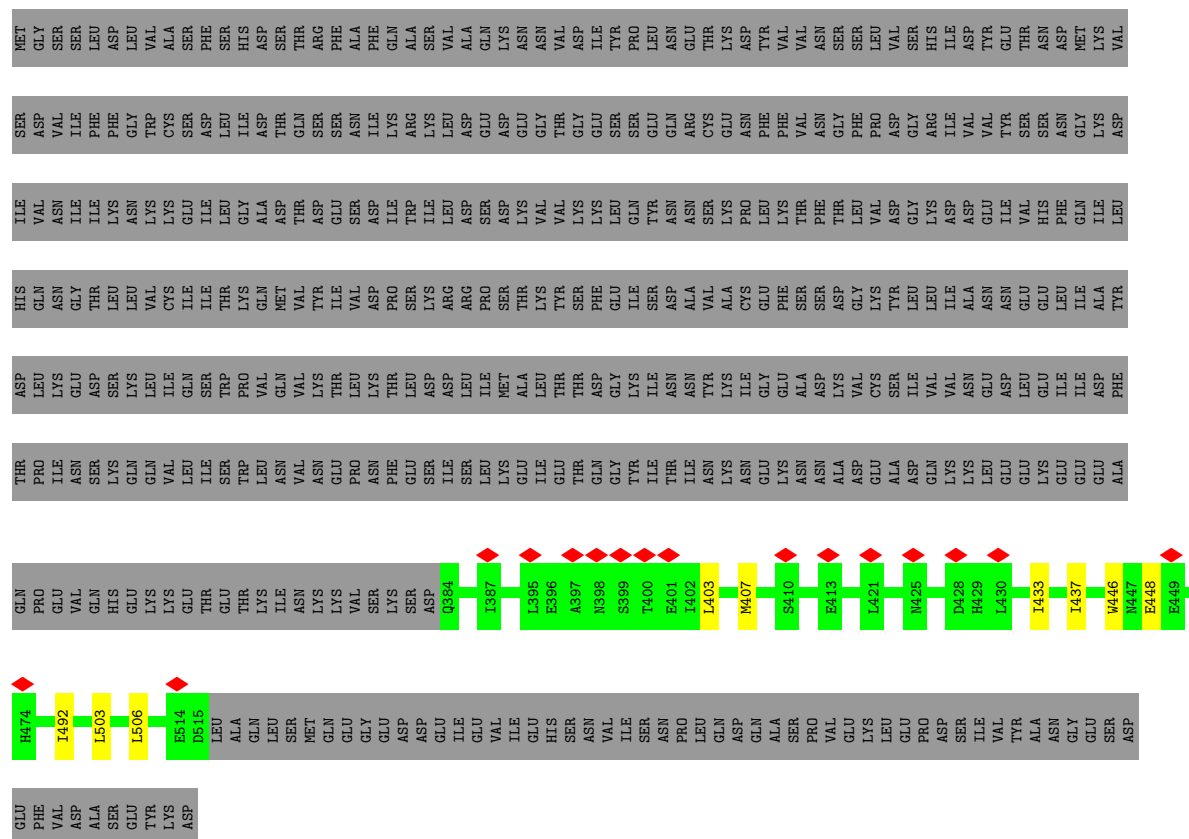
Chain LJ:





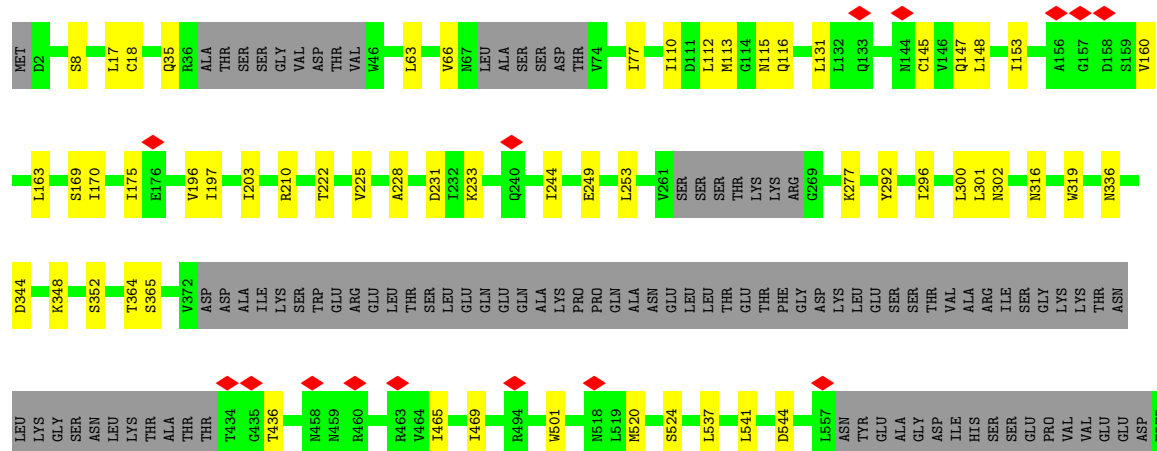
• Molecule 19: U3 small nucleolar RNA-associated protein 9

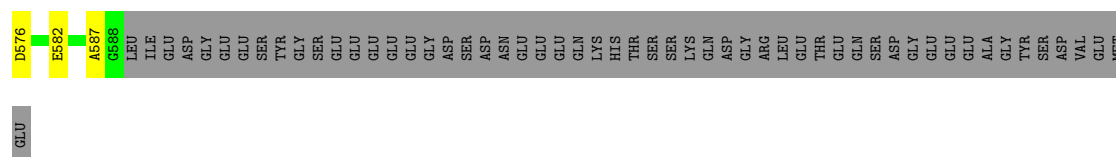
Chain LK: 21% 77%



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

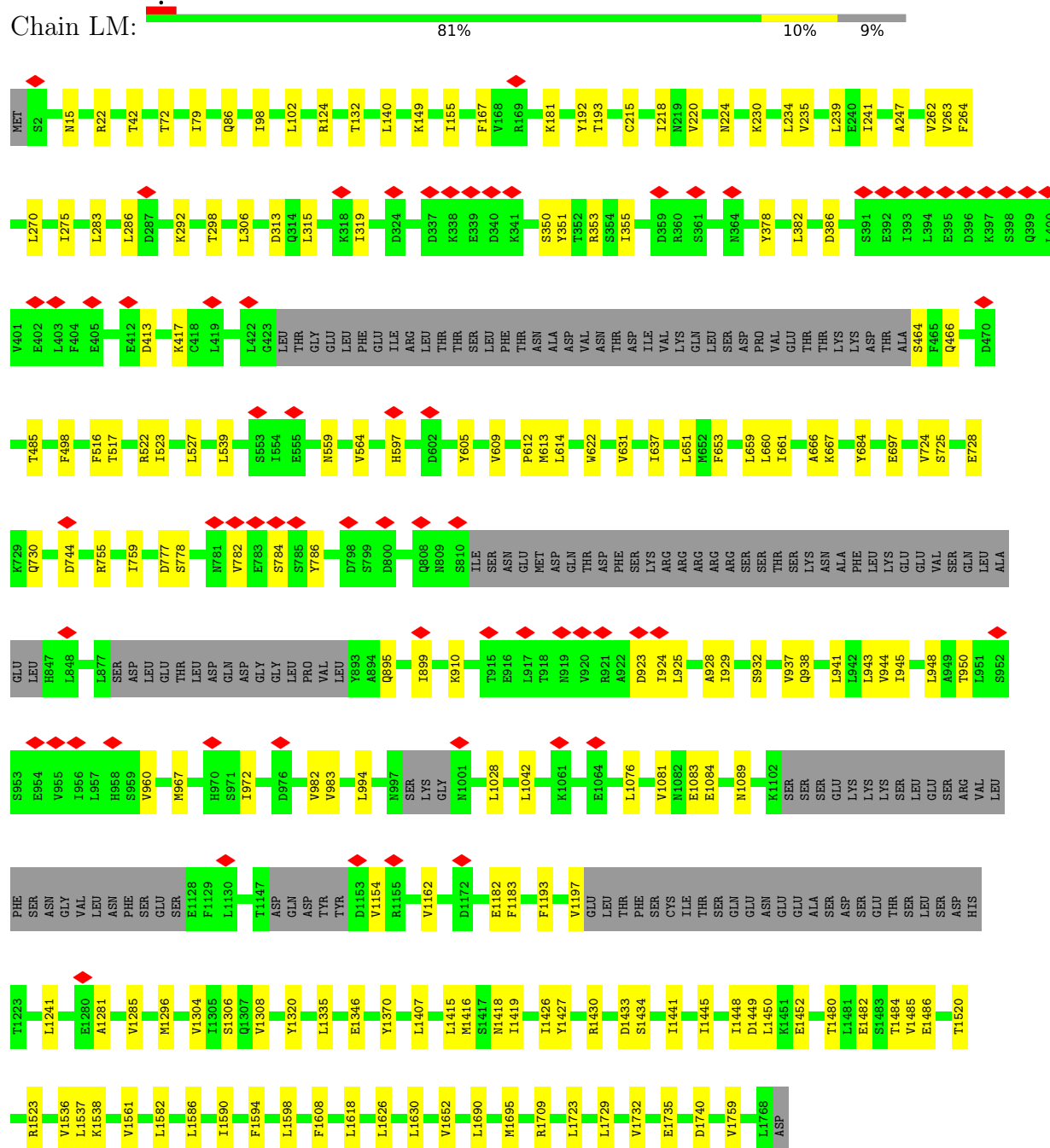
Chain LL: 66% 9% 24%





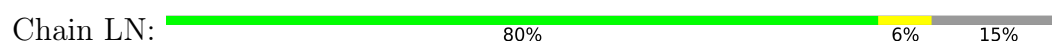
• Molecule 21: U3 small nucleolar RNA-associated protein 10

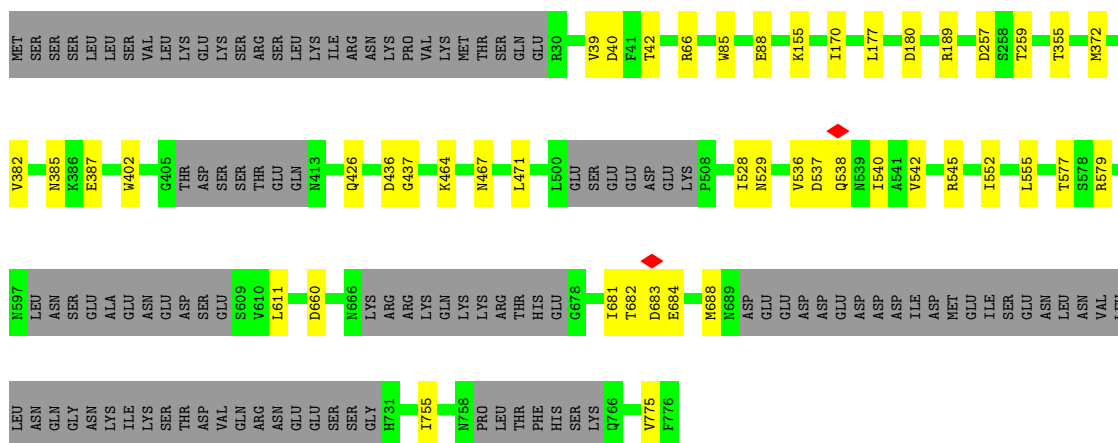
Chain LM:



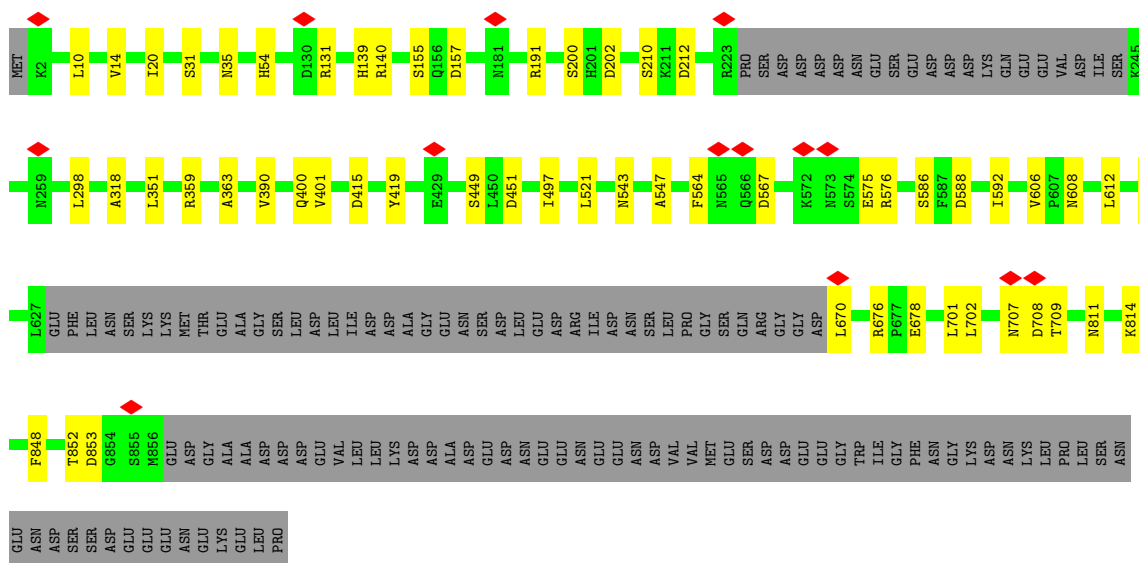
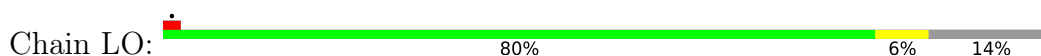
• Molecule 22: U3 small nucleolar RNA-associated protein 4

Chain LN:

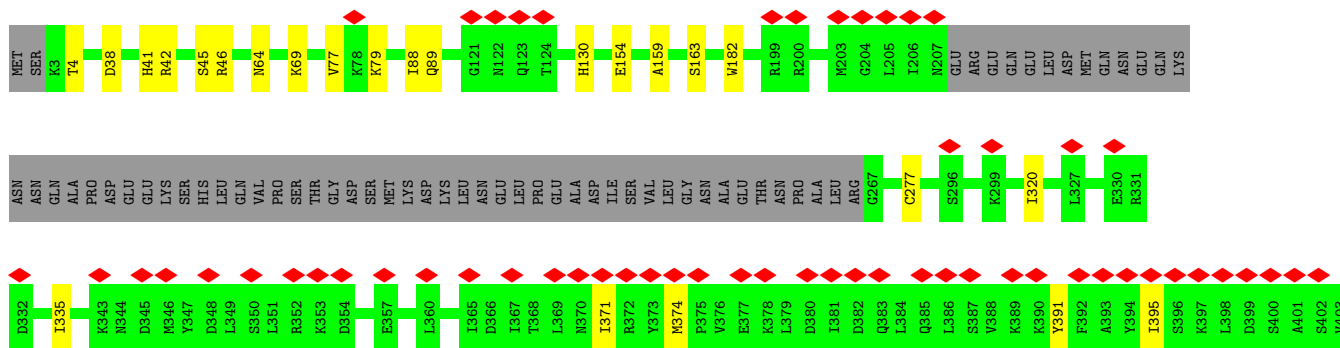
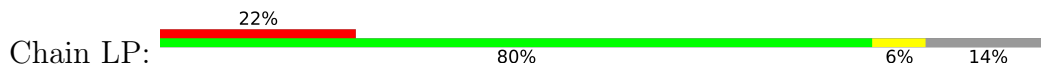




• Molecule 23: Periodic tryptophan protein 2



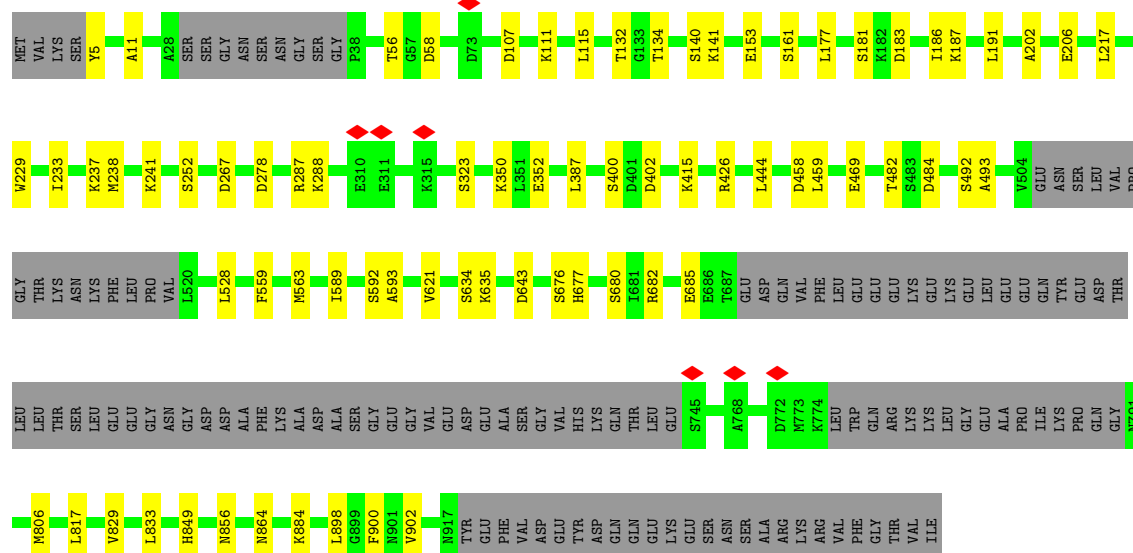
• Molecule 24: U3 small nucleolar RNA-associated protein 6





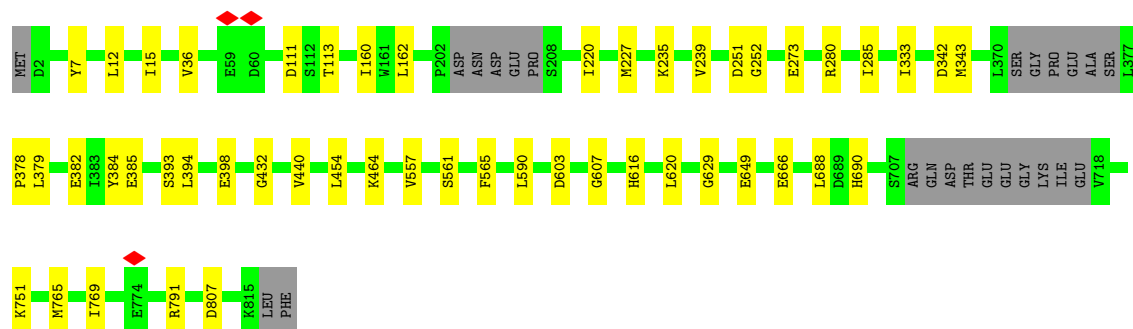
• Molecule 25: U3 small nucleolar RNA-associated protein 12

Chain LQ: 79% 8% 13%



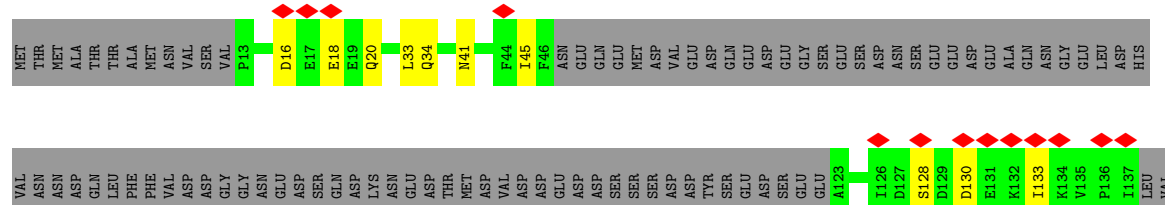
• Molecule 26: U3 small nucleolar RNA-associated protein 13

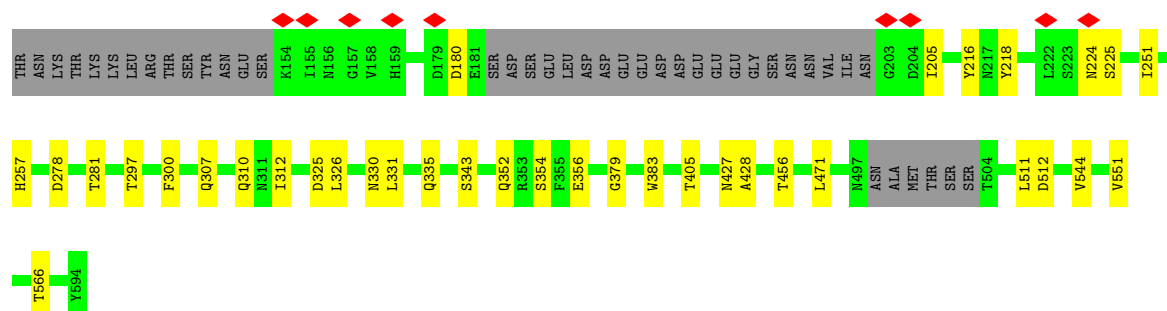
Chain LR: 91% 6% 3%



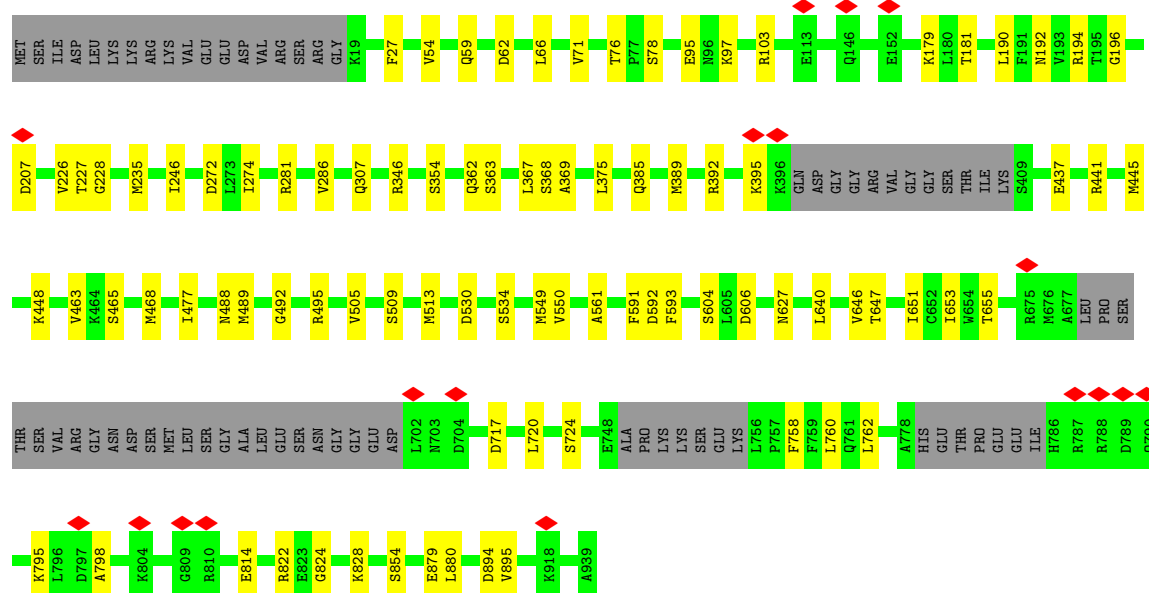
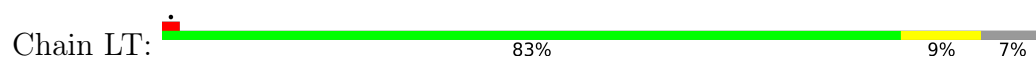
• Molecule 27: U3 small nucleolar RNA-associated protein 18

Chain LS: 70% 8% 22%

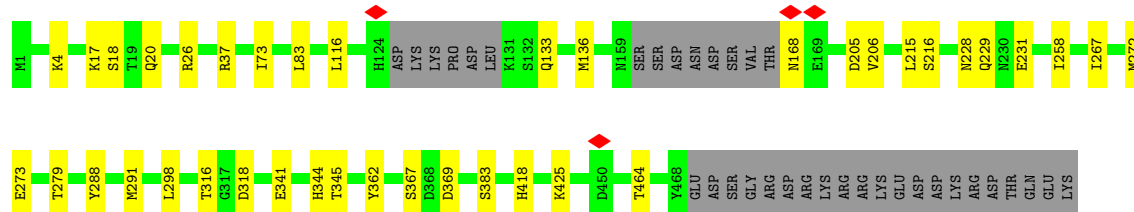
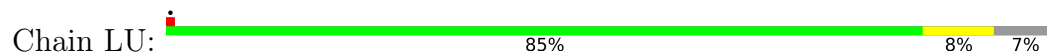




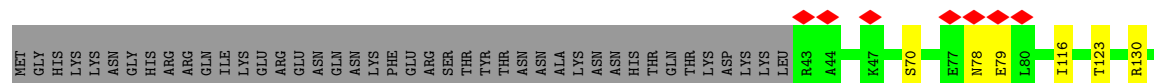
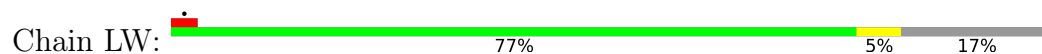
- Molecule 28: U3 small nucleolar RNA-associated protein 21



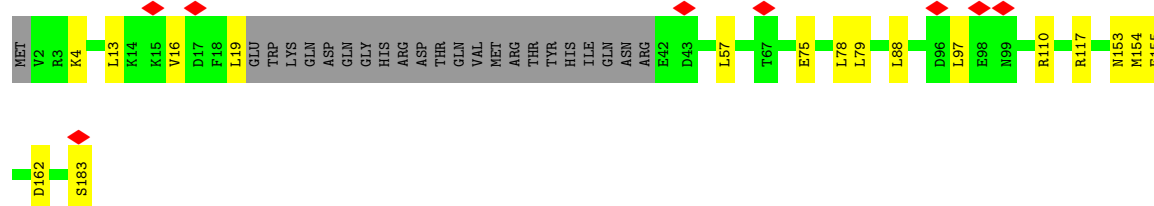
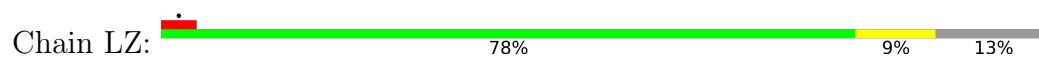
- Molecule 29: Protein SOF1



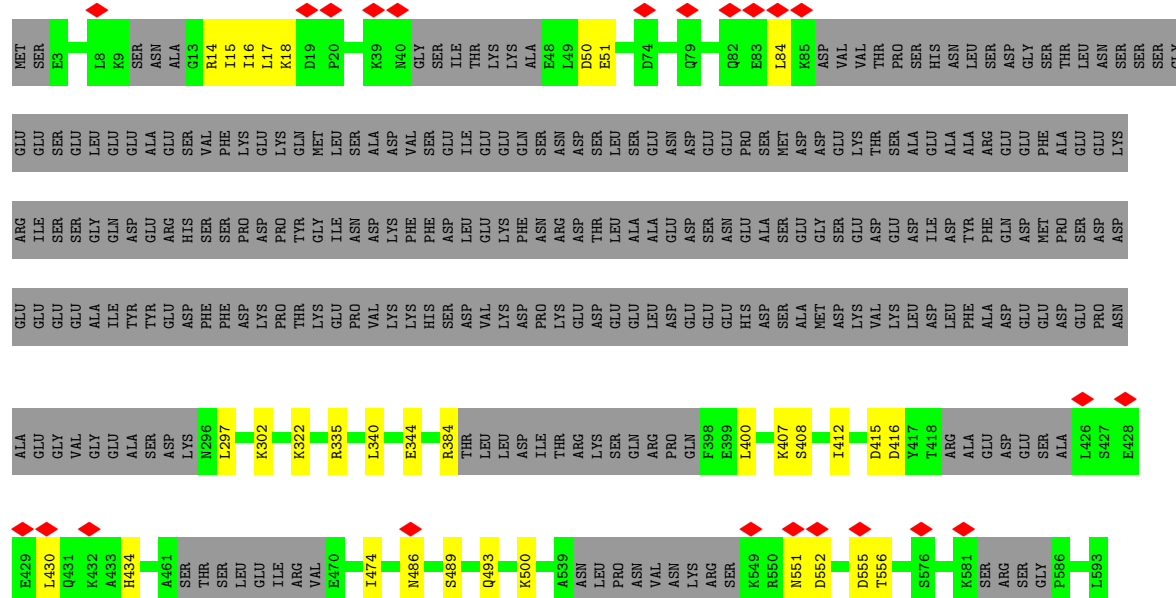
- Molecule 30: U3 small nucleolar RNA-associated protein 7



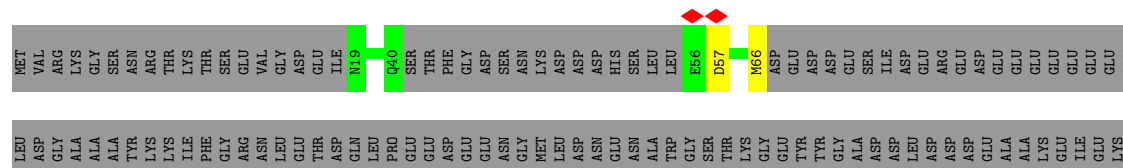
- Molecule 31: U3 small nucleolar ribonucleoprotein protein IMP3

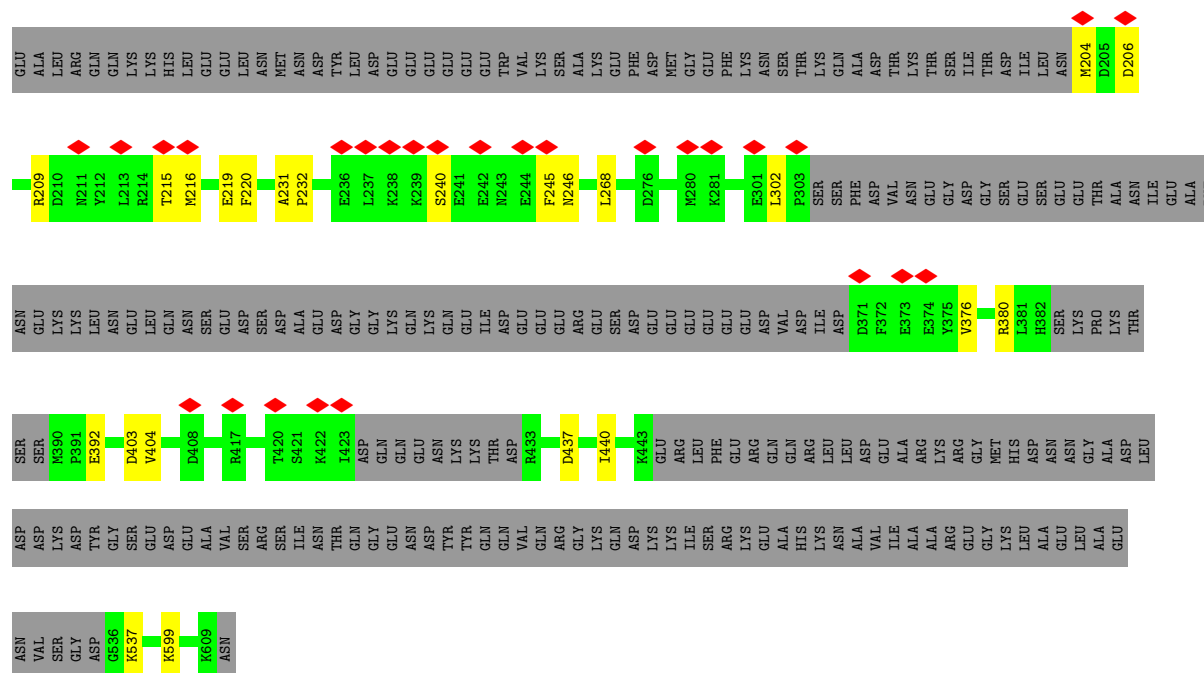


- Molecule 32: U3 small nucleolar RNA-associated protein MPP10

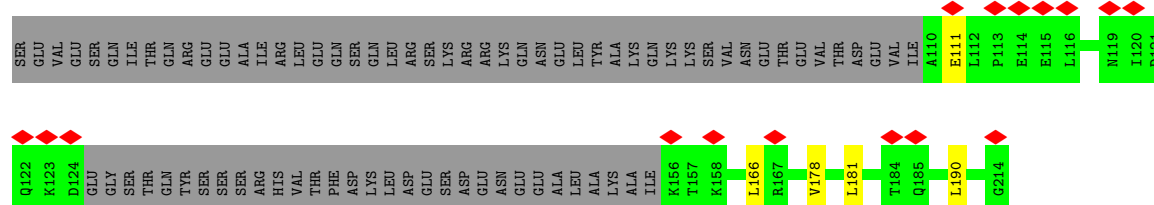
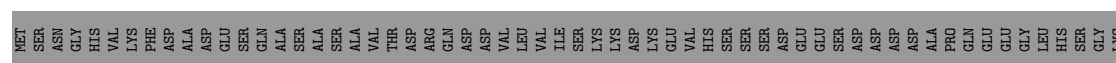


- Molecule 33: Something about silencing protein 10

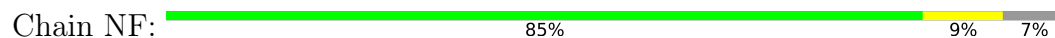




- Molecule 34: Bud site selection protein 21



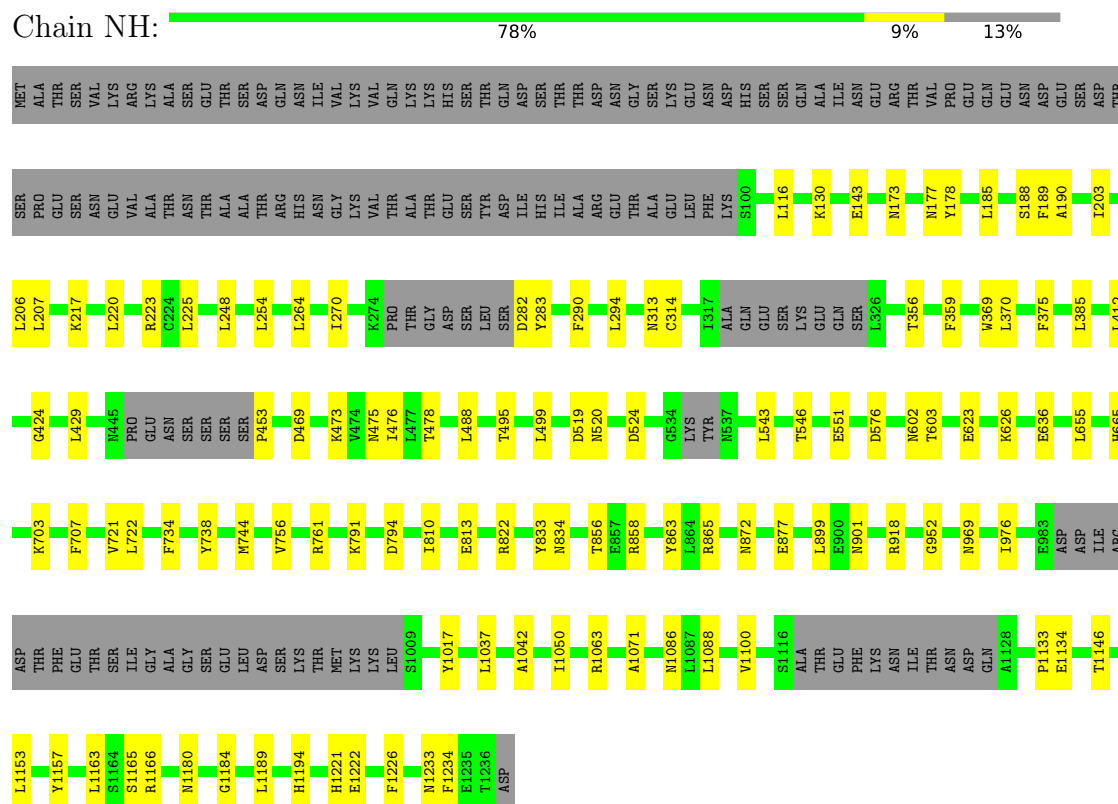
- Molecule 35: 40S ribosomal protein S13



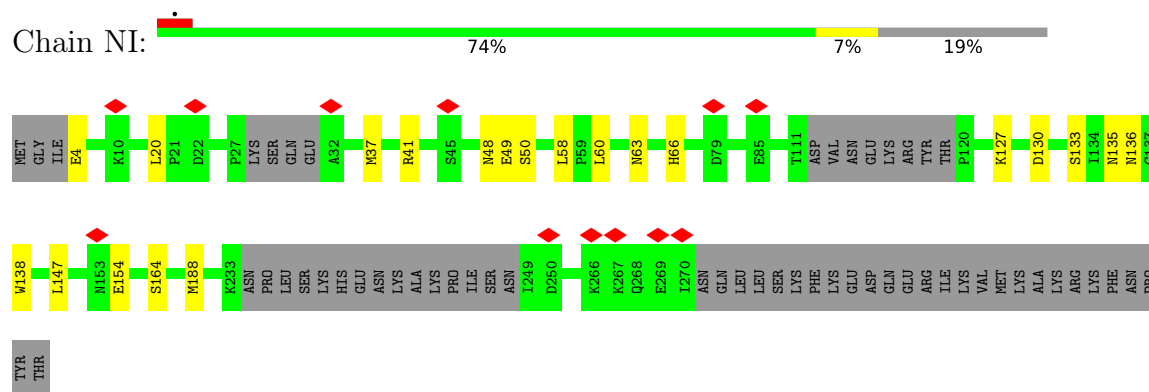
- Molecule 36: 40S ribosomal protein S14-A



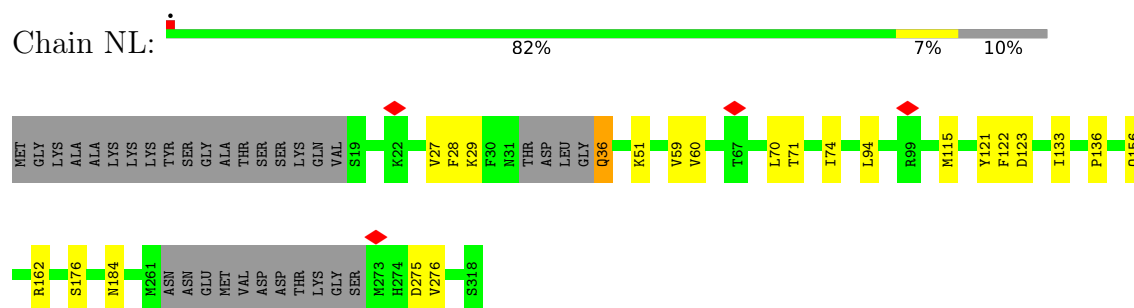
- Molecule 37: U3 small nucleolar RNA-associated protein 22



- Molecule 38: Ribosomal RNA-processing protein 7

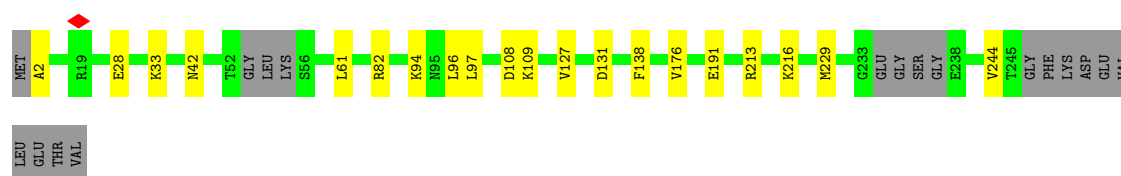


- Molecule 39: Dimethyladenosine transferase



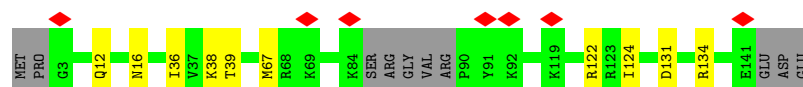
- Molecule 40: Small ribosomal subunit protein eS1A

Chain NM:  85% 8% 7%



- Molecule 41: 40S ribosomal protein S19-A

Chain NP:  5% 86% 7% 7%



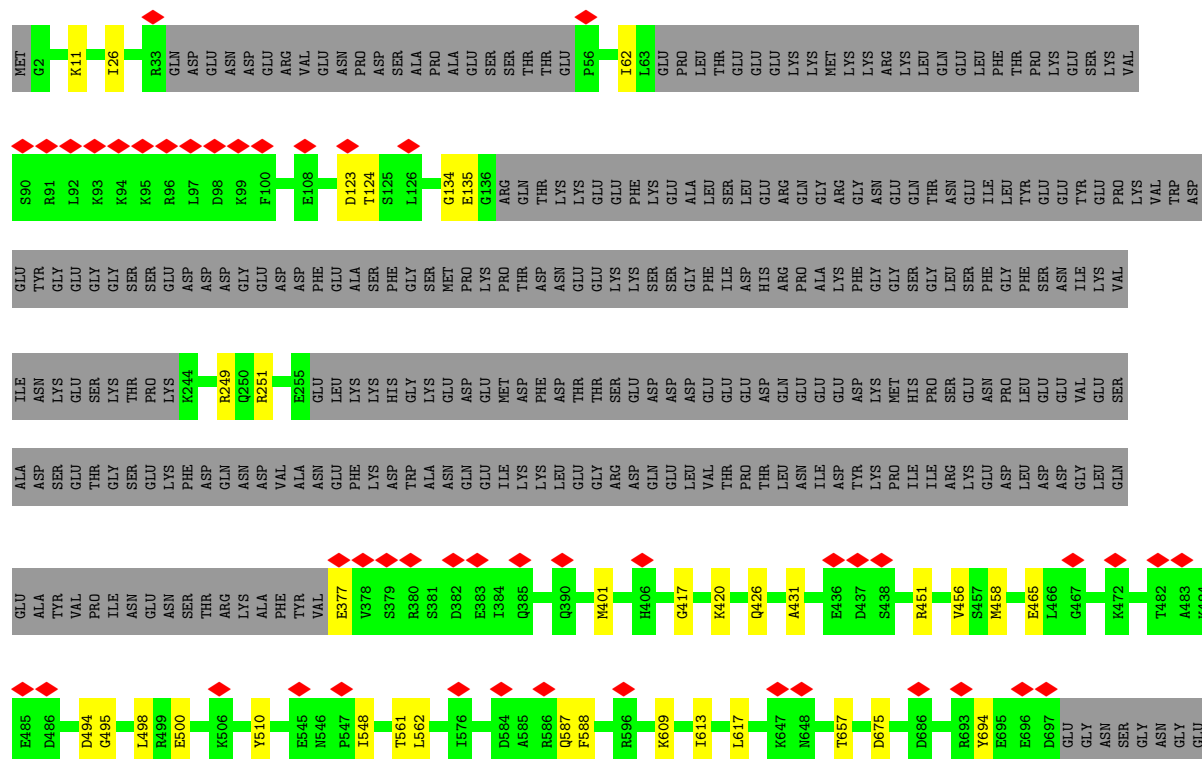
- Molecule 42: 40S ribosomal protein S27-A

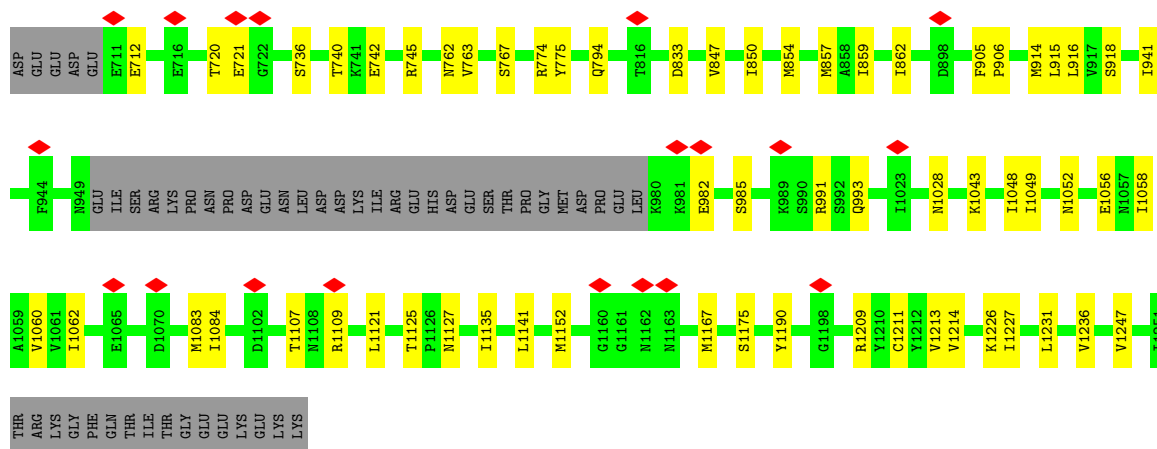
Chain NQ:  90% 6% .



- Molecule 43: Probable ATP-dependent RNA helicase DHR1

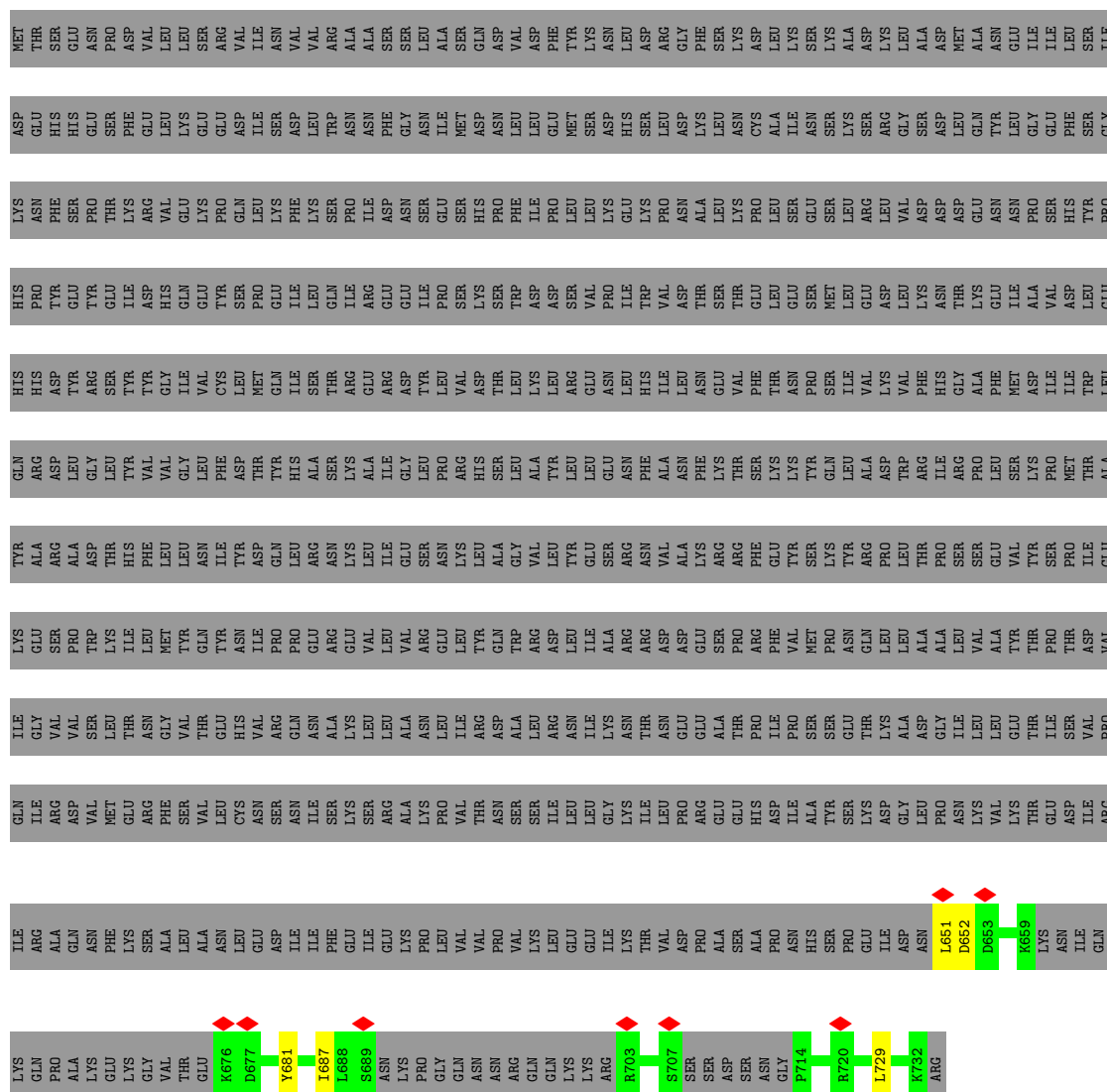
Chain NS:  5% 66% 8% 27%



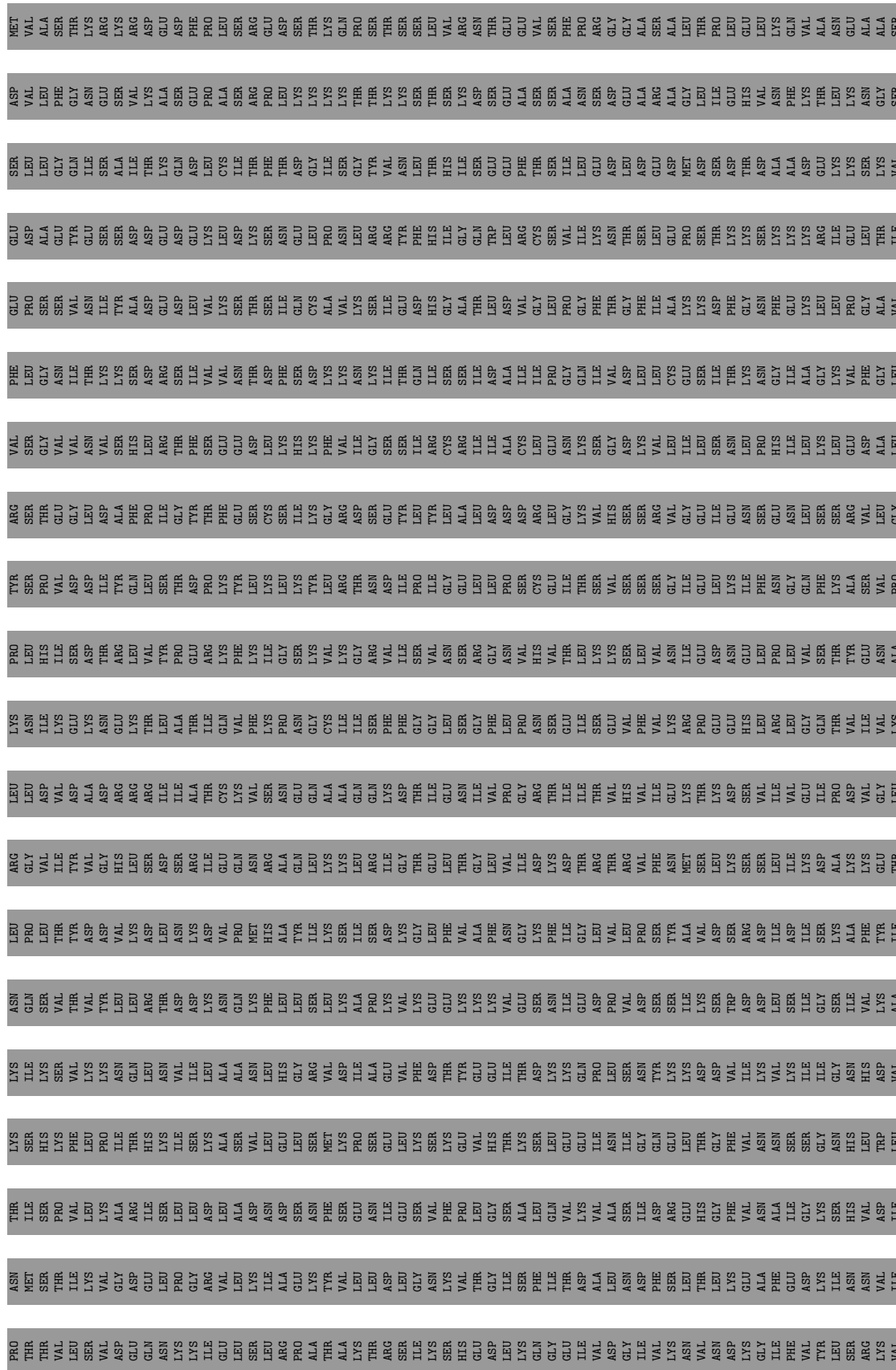


• Molecule 44: Exosome complex exonuclease RRP6

Chain NV: 6% . 94%

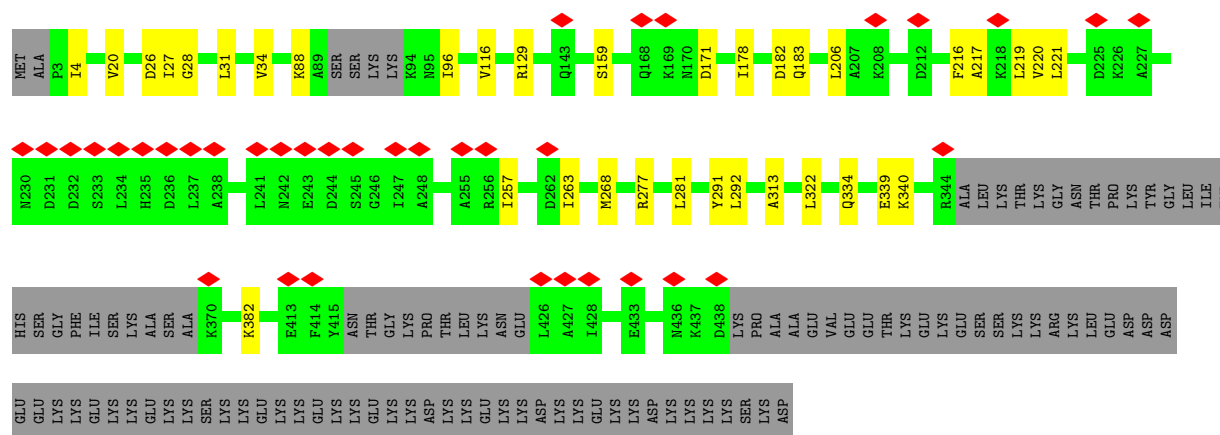
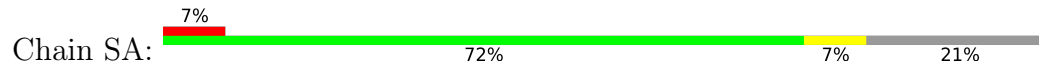


• Molecule 45: rRNA biogenesis protein RRP5

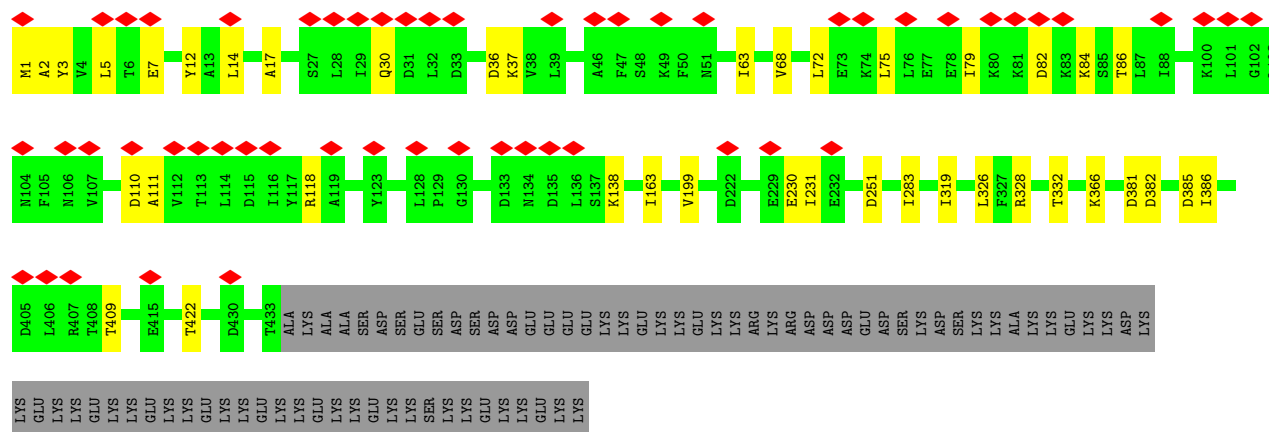
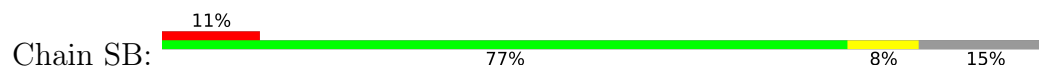




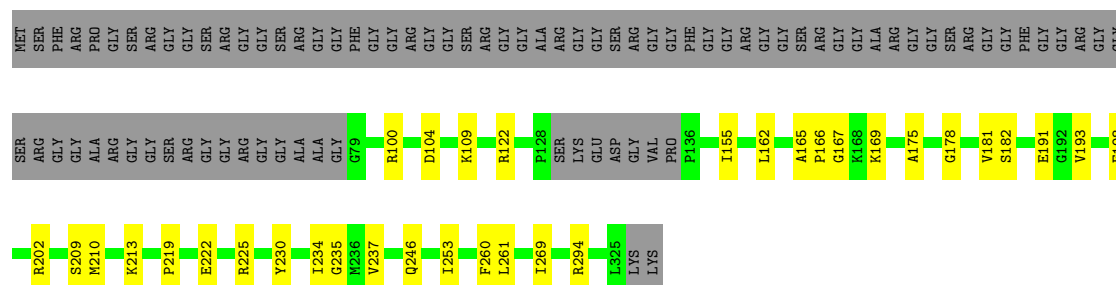
- Molecule 48: Nucleolar protein 56



- Molecule 49: Nucleolar protein 58



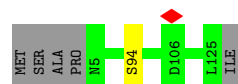
- Molecule 50: rRNA 2'-O-methyltransferase fibrillar



- Molecule 50: rRNA 2'-O-methyltransferase fibrillar



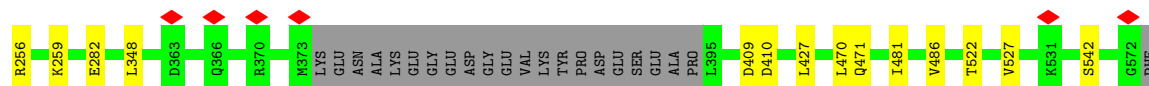
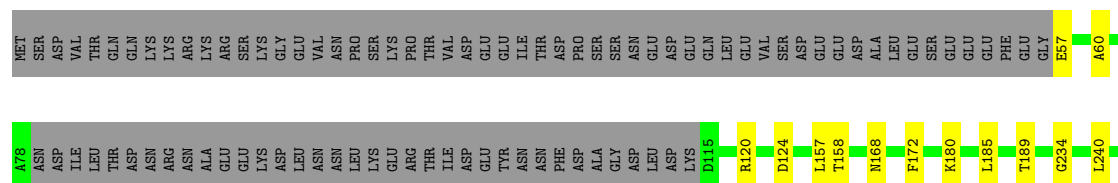
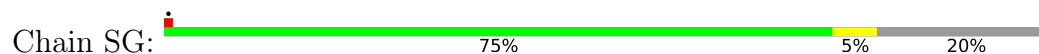
- Molecule 51: 13 kDa ribonucleoprotein-associated protein



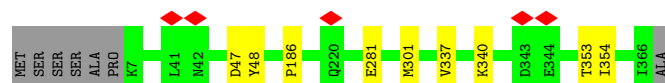
- Molecule 51: 13 kDa ribonucleoprotein-associated protein



- Molecule 52: Ribosomal RNA-processing protein 9

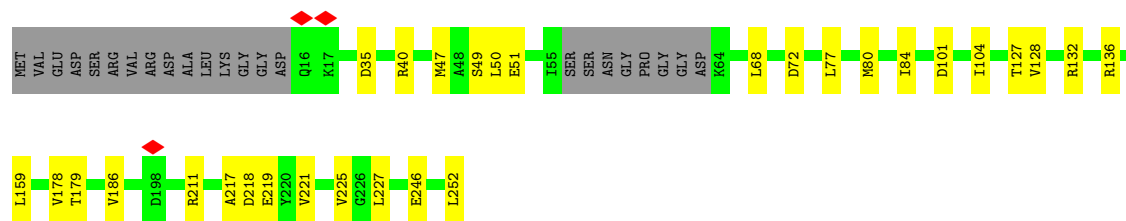


- Molecule 53: RNA 3'-terminal phosphate cyclase-like protein



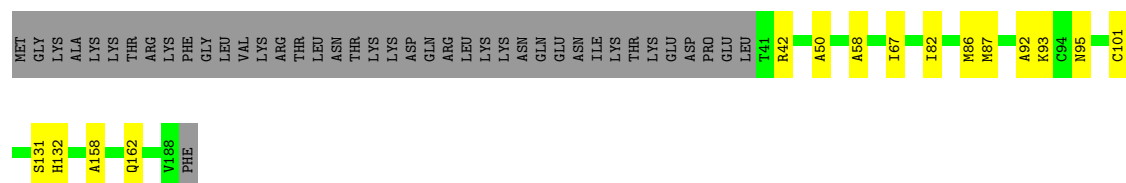
- Molecule 54: Ribosome biogenesis protein BMS1





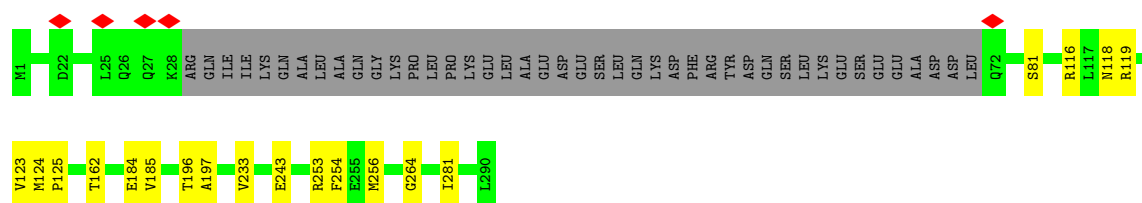
- Molecule 56: rRNA-processing protein FCF1

Chain SL: 70% 8% 22%



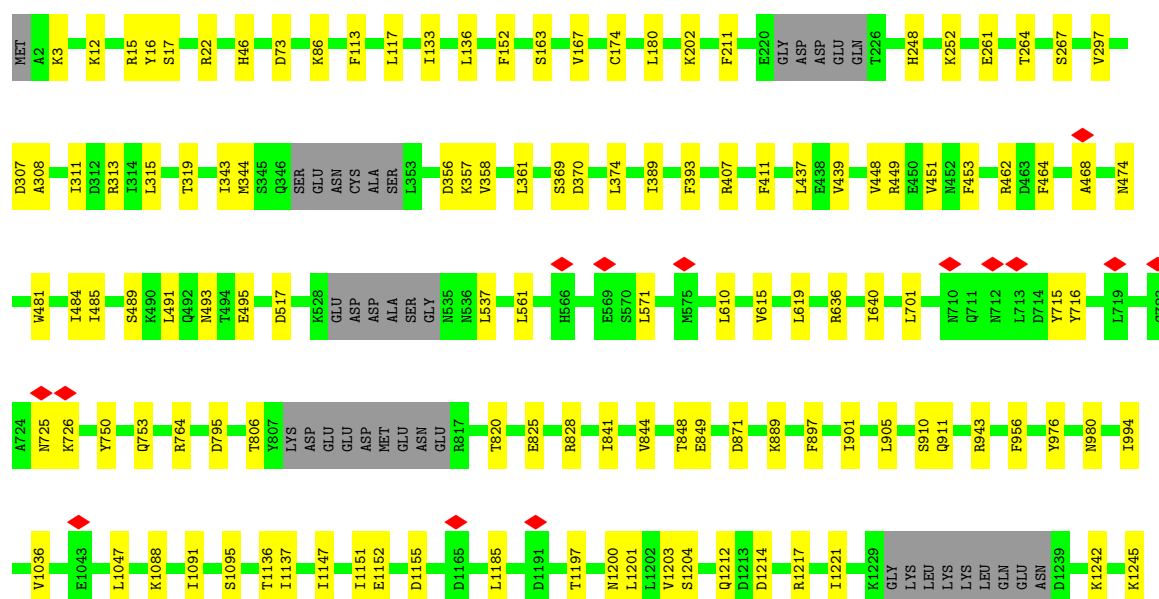
- Molecule 57: U3 small nucleolar ribonucleoprotein protein IMP4

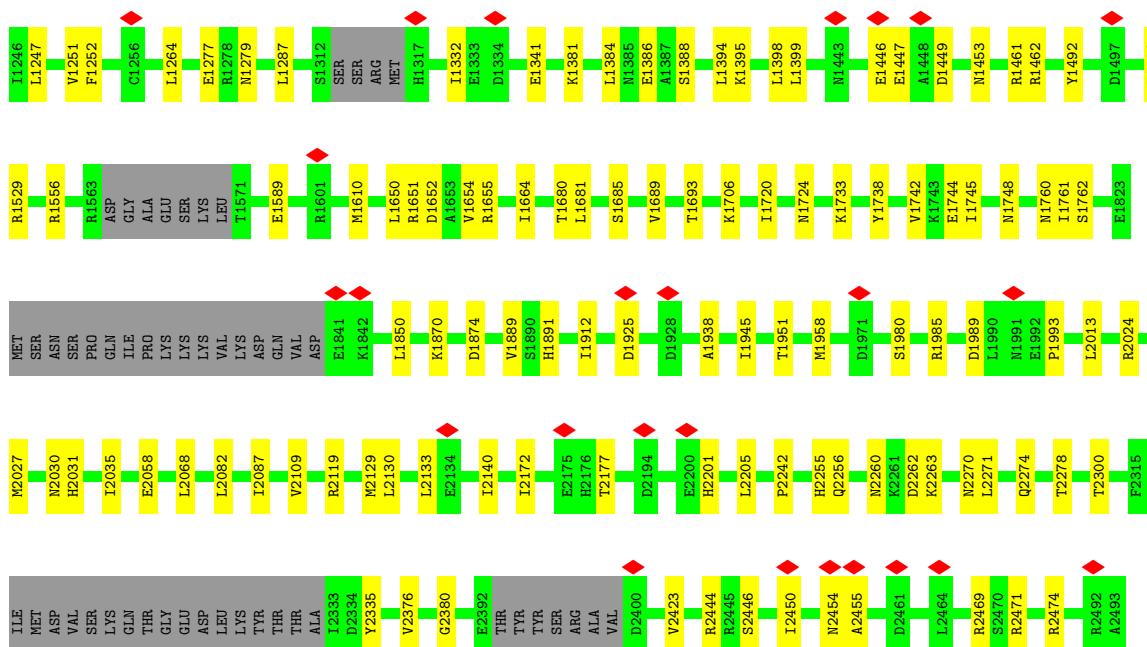
Chain SM: 79% 7% 15%



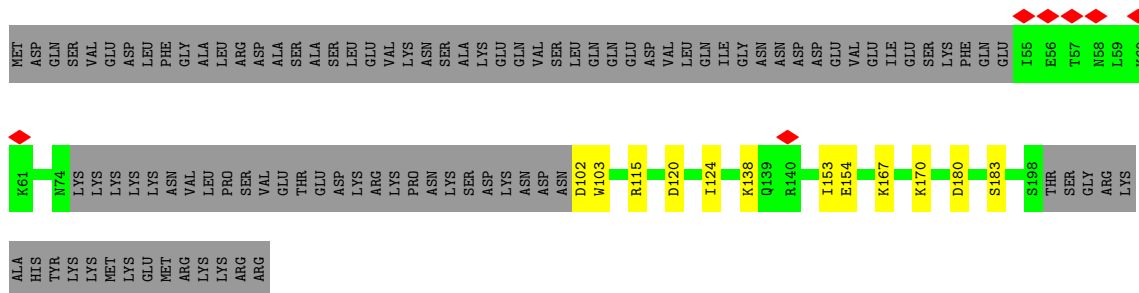
- Molecule 58: U3 small nucleolar RNA-associated protein 20

Chain SP: 87% 9% 4%

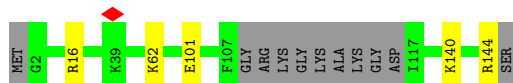




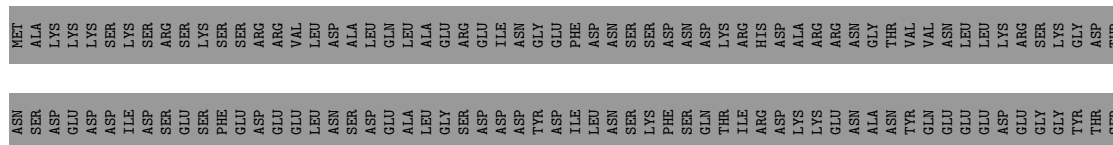
- Molecule 59: rRNA-processing protein FCF2

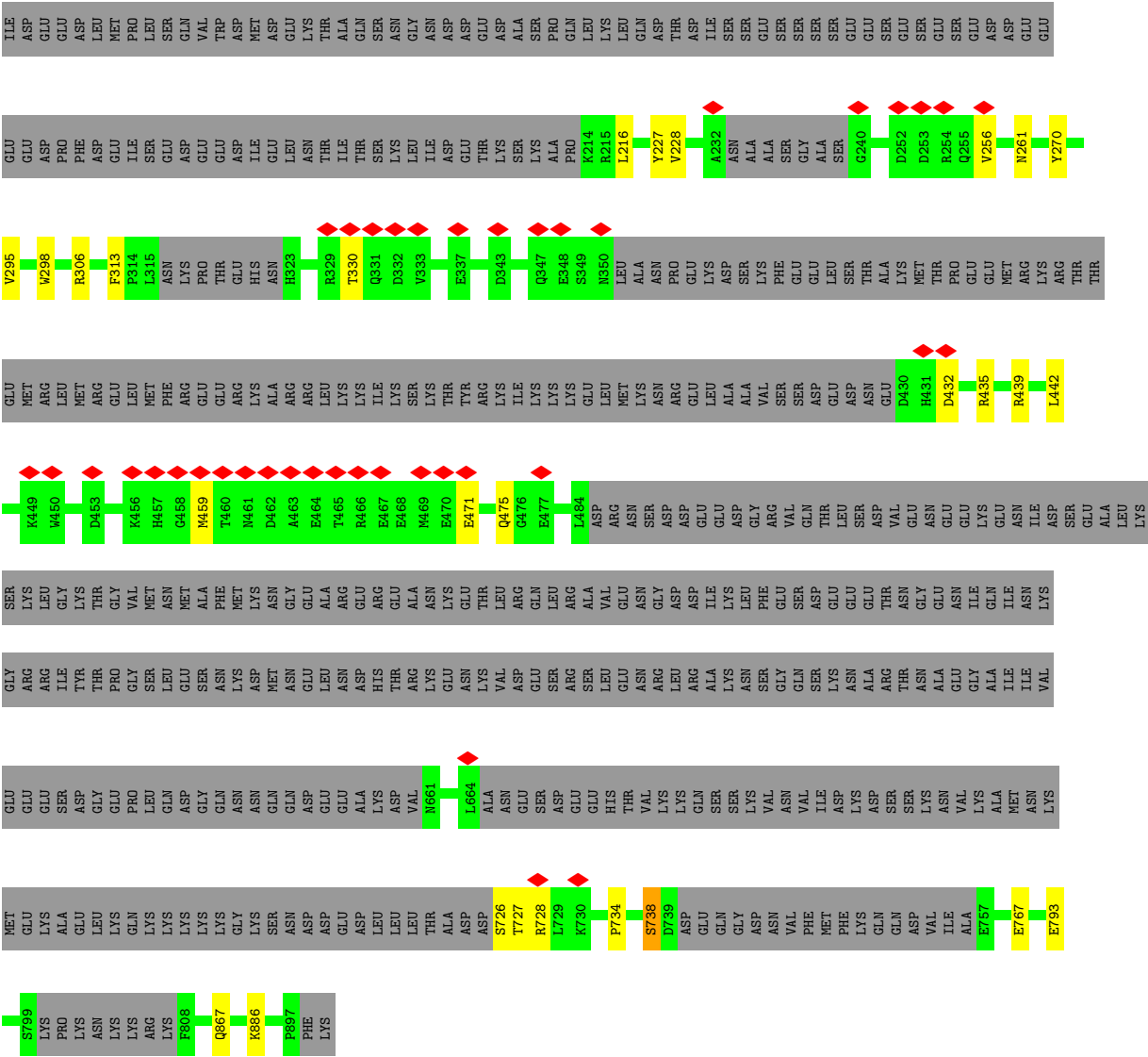


- Molecule 60: 40S ribosomal protein S23-A



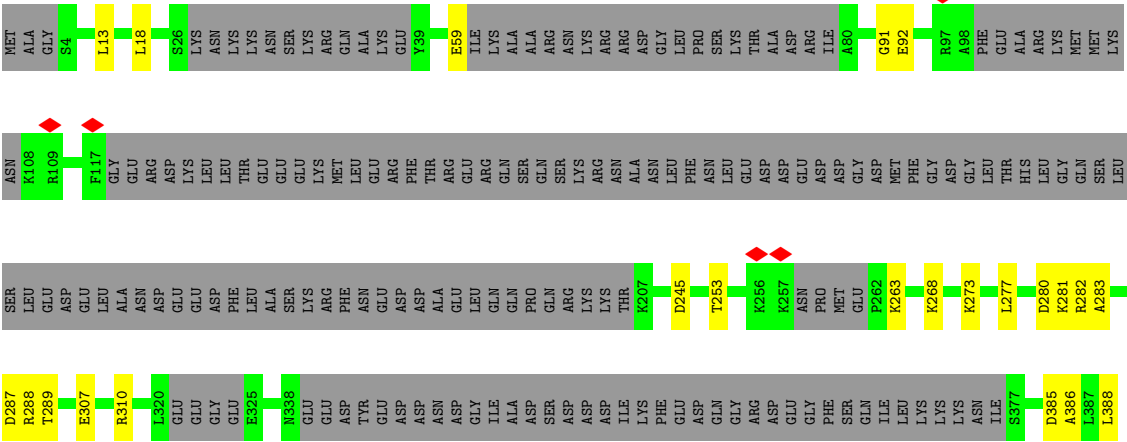
- Molecule 61: U3 small nucleolar RNA-associated protein 14

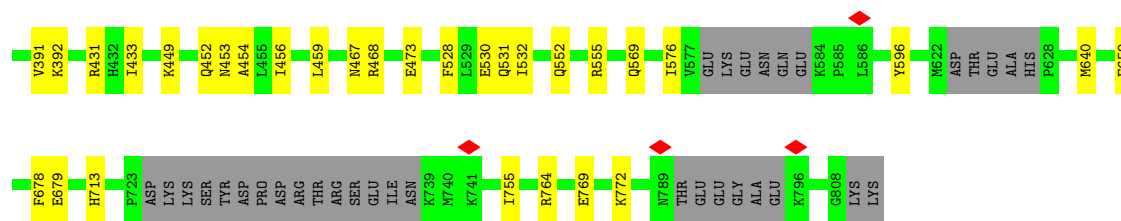




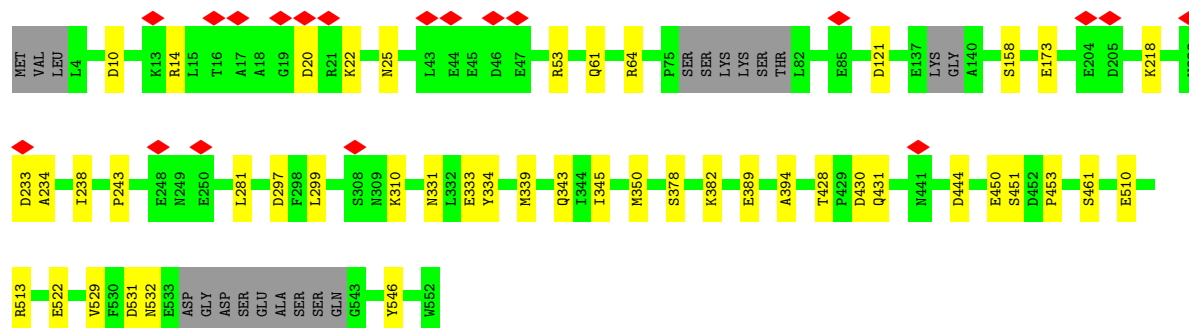
• Molecule 62: Nucleolar complex protein 14

Chain ST: 67% 7% 26%

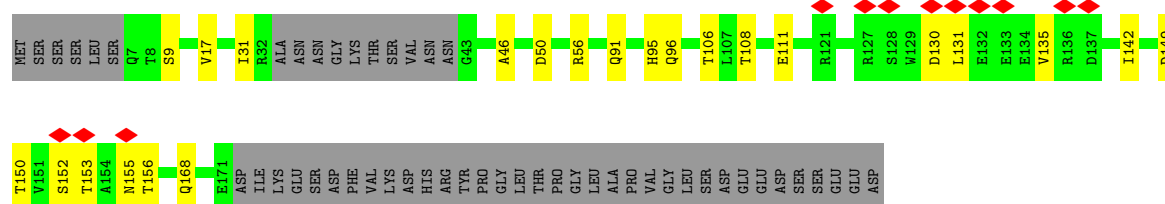




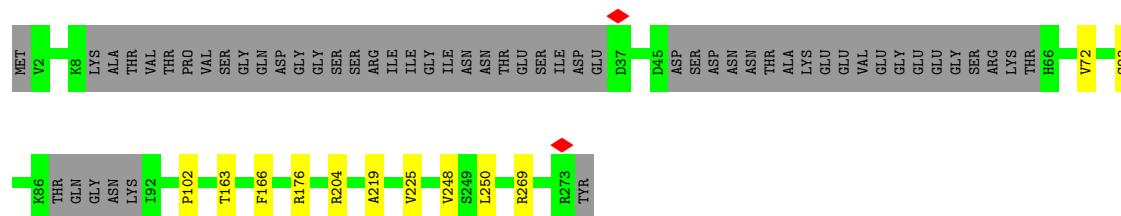
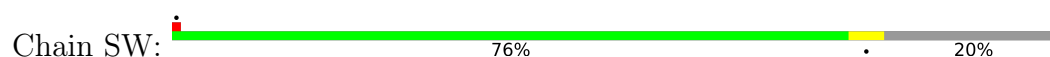
• Molecule 63: Nucleolar complex protein 4



• Molecule 64: Regulator of rDNA transcription protein 14

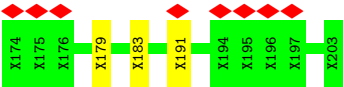


• Molecule 65: Pre-rRNA-processing protein PNO1

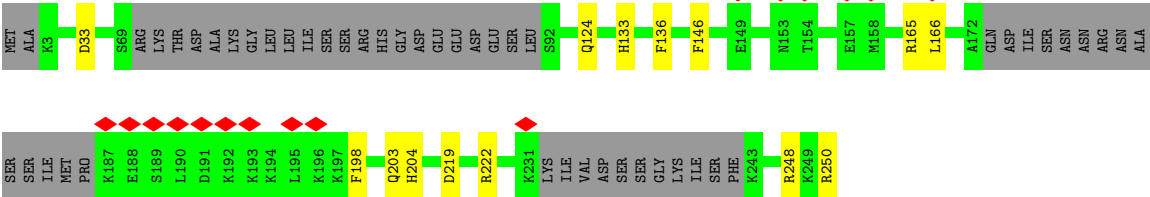
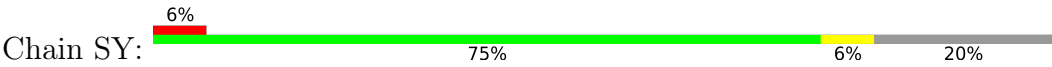


• Molecule 66: Unassigned peptides

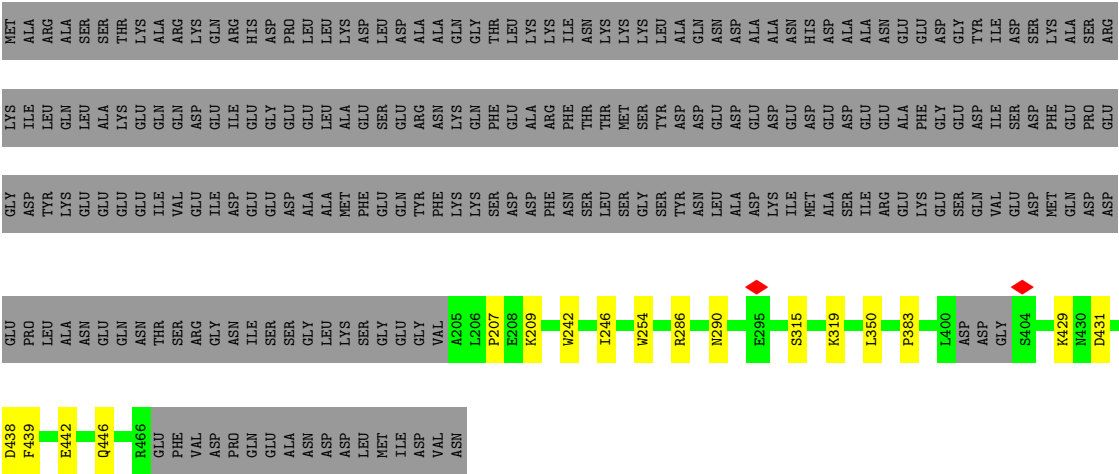




- Molecule 67: U3 small nucleolar RNA-associated protein 11



- Molecule 68: 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	328554	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	9.372	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.123	Depositor
Map value standard deviation	0.203	Depositor
Recommended contour level	0.6	Depositor
Map size ($\text{\AA}$)	535.75195, 535.75195, 535.75195	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: OMC, A2M, ATP, 4AC, M7G, OMU, GTP, ZN, SEP, ADP, OMG, MG

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	0.14	0/1529	0.27	0/2372
2	L1	0.22	1/34982 (0.0%)	0.31	0/54465
3	L2	0.14	0/5032	0.25	0/7812
4	L3	0.14	0/872	0.34	0/1173
5	L4	0.21	0/1977	0.36	0/2664
6	L5	0.16	0/1655	0.32	0/2237
7	L6	0.19	0/1764	0.38	0/2359
8	L7	0.16	0/1451	0.38	0/1956
9	L8	0.21	0/1371	0.34	0/1833
10	L9	0.18	0/1495	0.34	0/2003
11	LC	0.32	1/1015 (0.1%)	0.51	2/1367 (0.1%)
12	LD	0.22	0/1138	0.38	0/1533
13	LE	0.20	0/1039	0.38	0/1395
14	LF	0.19	0/1060	0.35	0/1412
15	LG	0.16	0/492	0.34	0/659
16	LH	0.20	0/6576	0.39	0/8902
17	LI	0.12	0/4267	0.30	0/5815
18	LJ	0.15	0/3851	0.34	0/5221
19	LK	0.11	0/1085	0.26	0/1463
20	LL	0.16	0/3939	0.32	0/5341
21	LM	0.15	0/13115	0.30	0/17751
22	LN	0.19	0/5359	0.32	0/7255
23	LO	0.17	0/6463	0.33	0/8748
24	LP	0.12	0/3282	0.26	0/4411
25	LQ	0.25	0/6620	0.36	0/8936
26	LR	0.19	0/6313	0.33	0/8551
27	LS	0.22	0/3735	0.32	0/5064
28	LT	0.14	0/7011	0.30	0/9471
29	LU	0.18	0/3784	0.33	0/5092
30	LW	0.16	0/3705	0.31	0/5008
31	LZ	0.14	0/1355	0.36	0/1821
32	NA	0.13	0/2657	0.28	0/3559

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	NB	0.16	0/2196	0.33	0/2927
34	ND	0.13	0/613	0.27	0/811
35	NF	0.16	0/1158	0.31	0/1559
36	NG	0.24	0/952	0.38	0/1279
37	NH	0.22	0/8899	0.34	1/12035 (0.0%)
38	NI	0.17	0/1994	0.34	0/2684
39	NL	0.13	0/2329	0.29	0/3144
40	NM	0.16	0/1915	0.32	0/2563
41	NP	0.14	0/1056	0.32	0/1416
42	NQ	0.16	0/605	0.33	0/817
43	NS	0.15	0/7623	0.33	0/10256
44	NV	0.14	0/376	0.30	0/496
45	OA	0.10	0/1434	0.26	0/1999
46	OH	0.12	0/910	0.26	0/1231
47	OU	0.11	0/443	0.26	0/592
48	SA	0.13	0/3188	0.28	0/4293
49	SB	0.12	0/3377	0.28	0/4551
50	SC	0.17	0/1903	0.32	0/2567
50	SD	0.16	0/1885	0.34	0/2543
51	SE	0.19	0/928	0.32	0/1262
51	SF	0.16	0/928	0.30	0/1262
52	SG	0.15	0/3744	0.30	0/5040
53	SH	0.17	0/2832	0.30	0/3825
54	SI	0.17	0/6295	0.33	0/8476
55	SJ	0.18	0/1703	0.37	0/2295
55	SK	0.21	0/1822	0.36	0/2462
56	SL	0.19	0/1193	0.34	0/1611
57	SM	0.17	0/2046	0.32	0/2759
58	SP	0.14	0/19965	0.30	0/26982
59	SQ	0.14	0/1009	0.30	0/1348
60	SR	0.18	0/1069	0.37	0/1427
61	SS	0.15	0/2712	0.34	0/3637
62	ST	0.15	0/4963	0.30	0/6635
63	SU	0.14	0/4466	0.28	0/6054
64	SV	0.14	0/1308	0.30	0/1736
65	SW	0.19	0/1752	0.34	0/2359
66	SX	0.30	0/15	0.14	0/20
67	SY	0.16	0/1736	0.34	0/2292
68	SZ	0.17	0/2167	0.32	0/2940
All	All	0.18	2/245498 (0.0%)	0.32	3/339834 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	LC	126	PRO	CG-CD	-7.75	1.24	1.50
2	L1	1269	OMU	O3'-P	5.09	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	LC	126	PRO	N-CD-CG	-9.47	89.00	103.20
37	NH	453	PRO	CA-N-CD	-8.17	100.56	112.00
11	LC	126	PRO	CA-N-CD	-5.95	103.67	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	1370	0	692	6	0
2	L1	31696	0	15995	126	0
3	L2	4543	0	2304	17	0
4	L3	862	0	900	12	0
5	L4	1936	0	2019	11	0
6	L5	1635	0	1697	20	0
7	L6	1740	0	1835	23	0
8	L7	1427	0	1499	16	0
9	L8	1348	0	1366	8	0
10	L9	1470	0	1554	7	0
11	LC	997	0	1054	13	0
12	LD	1112	0	1179	6	0
13	LE	1022	0	1060	9	0
14	LF	1046	0	1114	3	0
15	LG	490	0	529	5	0
16	LH	6449	0	6398	77	0
17	LI	4209	0	3724	30	0
18	LJ	3773	0	3761	38	0
19	LK	1068	0	1120	9	0
20	LL	3871	0	3876	43	0
21	LM	12908	0	13407	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	LN	5263	0	5270	28	0
23	LO	6321	0	6235	40	0
24	LP	3214	0	3267	18	0
25	LQ	6494	0	6544	46	0
26	LR	6207	0	6247	35	0
27	LS	3662	0	3639	31	0
28	LT	6875	0	6840	59	0
29	LU	3707	0	3655	30	0
30	LW	3627	0	3612	23	0
31	LZ	1332	0	1388	13	0
32	NA	2635	0	2683	26	0
33	NB	2164	0	2164	24	0
34	ND	609	0	671	5	0
35	NF	1135	0	1197	10	0
36	NG	941	0	979	10	0
37	NH	8693	0	8806	77	0
38	NI	1953	0	1933	14	0
39	NL	2285	0	2359	19	0
40	NM	1891	0	1995	13	0
41	NP	1040	0	1057	11	0
42	NQ	595	0	610	3	0
43	NS	7483	0	7675	64	0
44	NV	373	0	405	4	0
45	OA	1428	0	741	3	0
46	OH	902	0	948	11	0
47	OU	436	0	446	7	0
48	SA	3141	0	3156	26	0
49	SB	3338	0	3448	28	0
50	SC	1865	0	1908	24	0
50	SD	1850	0	1889	20	0
51	SE	916	0	964	1	0
51	SF	916	0	964	10	0
52	SG	3672	0	3690	17	0
53	SH	2781	0	2878	6	0
54	SI	6158	0	6342	38	0
55	SJ	1678	0	1756	28	0
55	SK	1793	0	1874	28	0
56	SL	1171	0	1229	12	0
57	SM	2009	0	2027	17	0
58	SP	19588	0	19914	146	0
59	SQ	991	0	1004	11	0
60	SR	1052	0	1120	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	SS	2679	0	2658	24	0
62	ST	4893	0	5028	42	0
63	SU	4357	0	4348	30	0
64	SV	1296	0	1390	19	0
65	SW	1725	0	1796	11	0
66	SX	159	0	42	2	0
67	SY	1715	0	1789	14	0
68	SZ	2113	0	2160	14	0
69	L1	36	0	0	0	0
69	NH	1	0	0	0	0
69	NS	1	0	0	0	0
69	SI	1	0	0	0	0
70	NH	31	0	12	1	0
71	NQ	1	0	0	0	0
71	OU	1	0	0	0	0
71	SL	1	0	0	0	0
72	NS	27	0	12	2	0
73	SI	32	0	12	0	0
All	All	238225	0	221859	1517	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 (1517) 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)
2:L1:127:G:N7	7:L6:202:ARG:NH2	2.21	0.87
18:LJ:262:GLU:OE1	18:LJ:263:ASN:ND2	2.08	0.87
2:L1:849:C:OP2	58:SP:2474:ARG:NH2	2.09	0.86
3:L2:312:U:O2'	48:SA:339:GLU:OE2	1.94	0.85
25:LQ:233:ILE:O	25:LQ:241:LYS:NZ	2.10	0.85
21:LM:516:PHE:O	21:LM:522:ARG:NH1	2.10	0.85
54:SI:1110:ARG:O	54:SI:1114:GLN:NE2	2.11	0.83
16:LH:393:ASN:ND2	16:LH:435:ASP:OD2	2.11	0.83
40:NM:28:GLU:OE2	40:NM:94:LYS:NZ	2.11	0.83
29:LU:367:SER:OG	29:LU:369:ASP:OD1	1.96	0.83
13:LE:97:ARG:NH2	58:SP:1850:LEU:O	2.13	0.82
25:LQ:287:ARG:NH1	25:LQ:323:SER:O	2.11	0.82
49:SB:68:VAL:HG13	49:SB:72:LEU:HD22	1.60	0.82
25:LQ:161:SER:OG	25:LQ:187:LYS:NZ	2.10	0.82
64:SV:108:THR:OG1	64:SV:111:GLU:OE1	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LJ:276:SER:OG	18:LJ:278:ASP:OD1	1.96	0.82
57:SM:233:VAL:HG21	57:SM:256:MET:HE3	1.61	0.81
58:SP:1610:MET:HE2	58:SP:1654:VAL:HG22	1.61	0.81
21:LM:1523:ARG:NE	64:SV:50:ASP:OD1	2.13	0.81
56:SL:158:ALA:O	56:SL:162:GLN:NE2	2.13	0.81
43:NS:609:LYS:NZ	43:NS:712:GLU:OE2	2.14	0.81
58:SP:1651:ARG:NH1	58:SP:1744:GLU:OE1	2.14	0.80
25:LQ:5:TYR:OH	25:LQ:643:ASP:OD2	1.99	0.80
12:LD:80:MET:SD	12:LD:83:THR:OG1	2.41	0.79
20:LL:436:THR:OG1	63:SU:297:ASP:OD2	1.99	0.79
28:LT:103:ARG:NH1	61:SS:734:PRO:O	2.14	0.79
62:ST:555:ARG:NH2	63:SU:522:GLU:OE2	2.15	0.79
4:L3:41:ARG:NH2	41:NP:36:ILE:O	2.16	0.78
29:LU:26:ARG:NH2	61:SS:867:GLN:O	2.16	0.78
2:L1:1200:G:N2	55:SK:72:ASP:OD1	2.16	0.78
22:LN:66:ARG:NE	22:LN:88:GLU:OE1	2.17	0.78
1:L0:282:G:O2'	28:LT:395:LYS:NZ	2.15	0.78
38:NI:63:ASN:OD1	38:NI:66:HIS:ND1	2.17	0.77
33:NB:57:ASP:OD1	59:SQ:115:ARG:NH2	2.16	0.77
24:LP:69:LYS:NZ	27:LS:18:GLU:OE2	2.14	0.77
58:SP:2024:ARG:NH1	61:SS:270:TYR:OH	2.18	0.77
25:LQ:181:SER:OG	25:LQ:183:ASP:OD1	2.03	0.77
39:NL:36:GLN:N	39:NL:36:GLN:HE21	1.82	0.77
24:LP:38:ASP:OD1	24:LP:42:ARG:NH2	2.18	0.76
37:NH:369:TRP:HE1	37:NH:495:THR:HG21	1.49	0.76
21:LM:1485:VAL:O	21:LM:1538:LYS:NZ	2.19	0.76
30:LW:130:ARG:NH2	30:LW:379:GLU:OE2	2.17	0.76
62:ST:449:LYS:NZ	63:SU:532:ASN:OD1	2.15	0.76
40:NM:82:ARG:NH1	40:NM:191:GLU:OE2	2.19	0.76
16:LH:720:ILE:HG12	16:LH:745:ILE:HD13	1.68	0.76
27:LS:307:GLN:NE2	27:LS:471:LEU:O	2.19	0.76
23:LO:586:SER:OG	23:LO:588:ASP:OD1	2.00	0.76
49:SB:14:LEU:HD13	49:SB:79:ILE:HD12	1.68	0.75
2:L1:1080:U:O2'	29:LU:425:LYS:NZ	2.15	0.75
16:LH:29:THR:O	16:LH:200:ASN:ND2	2.20	0.75
34:ND:111:GLU:OE2	63:SU:25:ASN:ND2	2.19	0.75
21:LM:609:VAL:HG11	21:LM:660:LEU:HD11	1.68	0.75
62:ST:307:GLU:OE1	62:ST:310:ARG:NH2	2.20	0.75
33:NB:599:LYS:NZ	59:SQ:138:LYS:O	2.20	0.75
28:LT:207:ASP:OD2	28:LT:227:THR:OG1	2.05	0.74
33:NB:437:ASP:O	55:SJ:88:ARG:NH1	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:NS:763:VAL:O	43:NS:767:SER:OG	2.05	0.74
2:L1:1000:C:OP2	39:NL:29:LYS:NZ	2.17	0.74
28:LT:307:GLN:NE2	49:SB:422:THR:O	2.20	0.74
43:NS:1209:ARG:NH1	43:NS:1211:CYS:SG	2.60	0.74
21:LM:725:SER:N	21:LM:728:GLU:OE1	2.21	0.74
27:LS:325:ASP:O	27:LS:330:ASN:ND2	2.20	0.74
21:LM:313:ASP:O	21:LM:350:SER:OG	2.03	0.74
52:SG:120:ARG:NH1	52:SG:124:ASP:OD1	2.20	0.74
3:L2:107:C:N4	48:SA:334:GLN:OE1	2.21	0.73
54:SI:831:ARG:NH1	54:SI:835:HIS:O	2.21	0.73
37:NH:969:ASN:HA	45:OA:1414:LEU:HD11	1.71	0.72
48:SA:291:TYR:OH	49:SB:251:ASP:OD1	2.06	0.72
11:LC:50:GLU:OE2	11:LC:82:ARG:NH2	2.22	0.72
52:SG:234:GLY:O	52:SG:259:LYS:NZ	2.22	0.72
53:SH:186:PRO:O	54:SI:634:ARG:NH1	2.23	0.71
58:SP:15:ARG:NH1	58:SP:16:TYR:O	2.22	0.71
18:LJ:263:ASN:O	18:LJ:310:SER:OG	2.08	0.71
22:LN:682:THR:OG1	22:LN:684:GLU:OE1	2.08	0.71
1:L0:283:A:OP2	28:LT:392:ARG:NH2	2.22	0.71
29:LU:291:MET:HE1	61:SS:295:VAL:HG11	1.72	0.71
58:SP:750:TYR:O	58:SP:753:GLN:NE2	2.24	0.71
20:LL:302:ASN:ND2	20:LL:316:ASN:OD1	2.23	0.71
3:L2:169:A:OP2	52:SG:180:LYS:NZ	2.18	0.71
2:L1:530:C:O2	14:LF:61:ARG:NH1	2.24	0.70
41:NP:38:LYS:O	41:NP:39:THR:OG1	2.09	0.70
49:SB:3:TYR:OH	49:SB:82:ASP:OD2	2.09	0.70
58:SP:358:VAL:HG12	58:SP:389:ILE:HD11	1.73	0.70
25:LQ:350:LYS:NZ	25:LQ:352:GLU:OE2	2.24	0.70
33:NB:537:LYS:NZ	54:SI:149:GLU:OE2	2.25	0.70
62:ST:530:GLU:OE1	62:ST:531:GLN:NE2	2.24	0.70
2:L1:763:G:OP1	10:L9:78:ARG:NH2	2.25	0.70
43:NS:1125:THR:OG1	43:NS:1127:ASN:O	2.10	0.70
18:LJ:54:ASP:OD2	18:LJ:111:TYR:OH	2.06	0.70
32:NA:407:LYS:NZ	32:NA:415:ASP:OD2	2.25	0.70
39:NL:162:ARG:O	39:NL:176:SER:OG	2.08	0.69
25:LQ:482:THR:OG1	25:LQ:484:ASP:OD1	2.06	0.69
50:SC:294:ARG:NH1	56:SL:131:SER:OG	2.25	0.69
7:L6:24:ILE:HG22	7:L6:28:PHE:CE2	2.28	0.69
21:LM:413:ASP:OD2	21:LM:417:LYS:NZ	2.24	0.69
40:NM:33:LYS:NZ	40:NM:42:ASN:OD1	2.23	0.69
27:LS:257:HIS:NE2	27:LS:310:GLN:OE1	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SP:1938:ALA:HB3	61:SS:459:MET:HE1	1.74	0.69
21:LM:485:THR:OG1	21:LM:605:TYR:O	2.09	0.69
63:SU:339:MET:O	63:SU:343:GLN:NE2	2.25	0.69
23:LO:449:SER:OG	23:LO:451:ASP:OD1	2.10	0.69
25:LQ:186:ILE:HG12	25:LQ:202:ALA:HB2	1.75	0.68
43:NS:1056:GLU:OE2	65:SW:83:SER:OG	2.07	0.68
24:LP:130:HIS:NE2	24:LP:154:GLU:OE2	2.26	0.68
23:LO:35:ASN:ND2	23:LO:54:HIS:O	2.25	0.68
28:LT:95:GLU:OE2	28:LT:97:LYS:NZ	2.26	0.68
38:NI:63:ASN:ND2	38:NI:164:SER:OG	2.26	0.68
63:SU:20:ASP:OD2	63:SU:22:LYS:NZ	2.27	0.68
26:LR:285:ILE:HD12	26:LR:385:GLU:HG3	1.76	0.68
2:L1:643:G:OP1	8:L7:175:LYS:NZ	2.27	0.68
2:L1:1228:G:OP2	46:OH:45:LEU:N	2.26	0.68
42:NQ:67:THR:OG1	42:NQ:70:LYS:O	2.11	0.68
52:SG:157:LEU:HD11	52:SG:189:THR:HB	1.76	0.68
64:SV:155:ASN:OD1	64:SV:156:THR:N	2.27	0.68
17:LI:595:ILE:HG22	17:LI:599:MET:HE3	1.76	0.67
58:SP:1341:GLU:OE2	58:SP:1381:LYS:NZ	2.26	0.67
64:SV:149:ASP:OD1	64:SV:150:THR:N	2.27	0.67
2:L1:93:A:O4'	5:L4:3:ARG:NH1	2.27	0.67
15:LG:31:GLU:HG2	15:LG:39:THR:HG22	1.76	0.67
40:NM:97:LEU:HD12	40:NM:229:MET:HE1	1.76	0.67
43:NS:982:GLU:O	43:NS:985:SER:OG	2.12	0.67
17:LI:325:PRO:O	17:LI:366:SER:OG	2.12	0.67
20:LL:520:MET:O	20:LL:524:SER:OG	2.12	0.67
2:L1:885:G:N2	36:NG:124:ASP:OD2	2.28	0.67
31:LZ:162:ASP:O	31:LZ:183:SER:OG	2.08	0.67
31:LZ:117:ARG:NH2	31:LZ:155:GLU:OE2	2.28	0.67
43:NS:915:LEU:HD22	43:NS:1049:ILE:HD11	1.75	0.67
22:LN:529:ASN:O	22:LN:545:ARG:NH1	2.27	0.66
2:L1:127:G:O2'	2:L1:129:U:OP1	2.14	0.66
2:L1:1499:G:OP1	41:NP:122:ARG:NH1	2.27	0.66
43:NS:1056:GLU:O	43:NS:1060:VAL:HG13	1.96	0.66
2:L1:1555:A:O2'	2:L1:1556:A:O5'	2.14	0.66
23:LO:811:ASN:OD1	23:LO:814:LYS:NZ	2.28	0.66
49:SB:30:GLN:O	49:SB:37:LYS:NZ	2.28	0.66
63:SU:510:GLU:OE1	63:SU:513:ARG:NH1	2.29	0.66
50:SD:80:ALA:O	67:SY:124:GLN:NE2	2.28	0.66
2:L1:1003:A:OP1	65:SW:269:ARG:NH2	2.28	0.66
28:LT:468:MET:HE3	28:LT:489:MET:HE2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LM:784:SER:O	49:SB:84:LYS:NZ	2.22	0.66
21:LM:937:VAL:O	21:LM:941:LEU:HD12	1.96	0.66
37:NH:543:LEU:O	37:NH:546:THR:OG1	2.13	0.66
30:LW:434:LEU:HD23	31:LZ:13:LEU:HD23	1.78	0.65
26:LR:649:GLU:OE1	26:LR:649:GLU:N	2.29	0.65
58:SP:1528:ARG:NH1	58:SP:1589:GLU:OE2	2.29	0.65
58:SP:825:GLU:OE2	58:SP:828:ARG:NH1	2.28	0.65
2:L1:828:U:OP2	58:SP:2444:ARG:NH2	2.30	0.65
18:LJ:43:THR:O	18:LJ:304:SER:OG	2.14	0.65
20:LL:153:ILE:HG22	20:LL:163:LEU:HG	1.77	0.65
68:SZ:315:SER:OG	68:SZ:319:LYS:NZ	2.30	0.65
2:L1:1781:A:N3	39:NL:156:GLN:NE2	2.44	0.65
43:NS:1048:ILE:O	43:NS:1052:ASN:ND2	2.29	0.65
46:OH:53:THR:HG21	47:OU:106:TYR:OH	1.97	0.65
58:SP:2242:PRO:O	61:SS:216:LEU:HD12	1.97	0.64
52:SG:185:LEU:HD13	52:SG:527:VAL:HG11	1.79	0.64
2:L1:284:G:N7	7:L6:188:ARG:NH1	2.45	0.64
13:LE:81:VAL:O	13:LE:122:SER:OG	2.14	0.64
30:LW:295:ASP:OD1	30:LW:297:SER:OG	2.13	0.64
2:L1:494:U:OP2	54:SI:1138:ARG:NH1	2.31	0.64
18:LJ:92:ASP:OD2	18:LJ:94:LYS:NZ	2.26	0.64
25:LQ:267:ASP:OD1	25:LQ:288:LYS:NZ	2.23	0.64
33:NB:403:ASP:OD1	33:NB:404:VAL:N	2.31	0.64
58:SP:1655:ARG:HE	58:SP:1693:THR:HG22	1.63	0.64
57:SM:123:VAL:HG12	57:SM:125:PRO:HD2	1.78	0.64
58:SP:2130:LEU:HB3	58:SP:2172:ILE:HD11	1.78	0.64
17:LI:585:ARG:NE	17:LI:589:ASP:OD2	2.28	0.64
21:LM:967:MET:HE2	21:LM:983:VAL:HG23	1.78	0.64
22:LN:681:ILE:HG22	22:LN:683:ASP:H	1.63	0.64
50:SD:251:ARG:NH2	50:SD:296:GLU:OE2	2.31	0.64
6:L5:94:THR:HG22	6:L5:114:ILE:HG13	1.80	0.63
11:LC:8:GLN:OE1	11:LC:21:HIS:NE2	2.31	0.63
25:LQ:177:LEU:HB3	25:LQ:191:LEU:HD21	1.80	0.63
58:SP:315:LEU:O	58:SP:319:THR:HG23	1.97	0.63
42:NQ:55:THR:HG22	42:NQ:62:ILE:HD13	1.79	0.63
16:LH:139:GLU:OE2	16:LH:172:ARG:NH1	2.32	0.63
16:LH:435:ASP:O	16:LH:762:TYR:OH	2.08	0.63
21:LM:517:THR:O	21:LM:522:ARG:NH2	2.31	0.63
40:NM:61:LEU:HD13	40:NM:96:LEU:HD21	1.80	0.63
56:SL:93:LYS:NZ	56:SL:95:ASN:OD1	2.32	0.63
58:SP:495:GLU:OE1	58:SP:495:GLU:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:1223:A:OP2	46:OH:113:ARG:NH1	2.32	0.63
62:ST:263:LYS:O	62:ST:268:LYS:NZ	2.32	0.63
2:L1:1179:G:OP1	62:ST:91:GLY:N	2.31	0.63
2:L1:1638:G:OP2	26:LR:751:LYS:NZ	2.20	0.63
37:NH:1037:LEU:HD22	37:NH:1050:ILE:HG22	1.81	0.63
63:SU:428:THR:OG1	63:SU:430:ASP:OD1	2.16	0.63
2:L1:1189:A:N1	2:L1:1192:C:N4	2.46	0.63
51:SF:23:VAL:HG21	51:SF:117:VAL:HG21	1.81	0.63
37:NH:834:ASN:ND2	37:NH:863:TYR:OH	2.32	0.63
55:SK:68:LEU:HD11	55:SK:80:MET:HE1	1.81	0.63
32:NA:18:LYS:O	33:NB:268:LEU:HD11	1.97	0.62
20:LL:277:LYS:NZ	20:LL:319:TRP:O	2.30	0.62
21:LM:79:ILE:O	21:LM:124:ARG:NH1	2.32	0.62
21:LM:1081:VAL:HG21	21:LM:1162:VAL:HG22	1.80	0.62
29:LU:272:MET:HE3	61:SS:313:PHE:HE2	1.63	0.62
48:SA:129:ARG:NH2	50:SC:261:LEU:O	2.30	0.62
50:SC:202:ARG:NH2	51:SF:72:GLU:OE2	2.33	0.62
1:L0:88:U:O2'	27:LS:343:SER:O	2.16	0.62
2:L1:846:G:OP2	58:SP:2469:ARG:NH2	2.32	0.62
16:LH:714:ASP:OD1	16:LH:715:GLU:N	2.33	0.62
50:SD:103:GLU:OE1	50:SD:103:GLU:N	2.32	0.62
29:LU:362:TYR:HH	29:LU:383:SER:HG	1.48	0.62
30:LW:116:ILE:CG2	30:LW:398:ILE:HD12	2.30	0.62
10:L9:53:ARG:NH2	56:SL:92:ALA:HB2	2.14	0.62
28:LT:437:GLU:OE2	28:LT:441:ARG:NH2	2.33	0.62
37:NH:177:ASN:OD1	37:NH:178:TYR:N	2.33	0.62
43:NS:941:ILE:O	43:NS:991:ARG:NH2	2.33	0.62
2:L1:862:A:OP1	35:NF:20:ARG:NH1	2.32	0.62
22:LN:170:ILE:HG22	22:LN:177:LEU:HD23	1.82	0.62
27:LS:427:ASN:OD1	27:LS:428:ALA:N	2.33	0.62
58:SP:264:THR:O	58:SP:313:ARG:NH1	2.32	0.62
23:LO:567:ASP:OD1	23:LO:576:ARG:NH2	2.32	0.62
2:L1:561:G:O2'	2:L1:562:OMG:H5'	1.99	0.61
2:L1:1096:C:H42	13:LE:18:GLU:HG2	1.65	0.61
17:LI:570:LEU:HD21	17:LI:637:LEU:HD21	1.82	0.61
58:SP:1212:GLN:OE1	58:SP:1212:GLN:N	2.31	0.61
2:L1:1555:A:O2'	2:L1:1556:A:O4'	2.19	0.61
58:SP:2274:GLN:O	58:SP:2278:THR:HG23	2.01	0.61
20:LL:147:GLN:O	20:LL:148:LEU:HD22	2.01	0.61
33:NB:240:SER:OG	33:NB:246:ASN:ND2	2.31	0.61
32:NA:50:ASP:OD2	32:NA:51:GLU:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:NH:794:ASP:OD1	37:NH:858:ARG:NH2	2.32	0.61
18:LJ:273:ILE:CD1	18:LJ:283:VAL:HG22	2.30	0.61
29:LU:273:GLU:OE1	61:SS:306:ARG:NH2	2.33	0.61
20:LL:115:ASN:OD1	20:LL:131:LEU:N	2.33	0.61
37:NH:721:VAL:HG23	37:NH:722:LEU:HD12	1.83	0.61
40:NM:127:VAL:HG13	40:NM:176:VAL:HG11	1.82	0.61
58:SP:1650:LEU:O	58:SP:1654:VAL:HG23	2.00	0.61
2:L1:1191:U:OP1	55:SK:211:ARG:NH2	2.34	0.61
2:L1:1629:G:O2'	2:L1:1630:U:O4'	2.13	0.61
29:LU:133:GLN:NE2	29:LU:168:ASN:O	2.33	0.61
38:NI:135:ASN:OD1	38:NI:136:ASN:N	2.34	0.61
29:LU:316:THR:OG1	29:LU:318:ASP:OD2	2.18	0.60
18:LJ:248:ARG:NH2	18:LJ:289:ASN:O	2.34	0.60
21:LM:464:SER:OG	21:LM:466:GLN:OE1	2.19	0.60
21:LM:1089:ASN:ND2	21:LM:1182:GLU:OE1	2.34	0.60
37:NH:1157:TYR:OH	37:NH:1222:GLU:OE1	2.18	0.60
21:LM:910:LYS:NZ	21:LM:950:THR:OG1	2.33	0.60
55:SJ:73:HIS:O	55:SJ:77:LEU:HD13	2.01	0.60
27:LS:278:ASP:OD2	27:LS:281:THR:OG1	2.19	0.60
50:SC:169:LYS:HG2	50:SC:193:VAL:HG22	1.83	0.60
58:SP:1394:LEU:HD12	58:SP:1398:LEU:HD12	1.82	0.60
2:L1:110:U:OP1	2:L1:753:A:O2'	2.20	0.60
27:LS:512:ASP:O	67:SY:250:ARG:NH1	2.35	0.60
58:SP:1652:ASP:OD1	58:SP:1655:ARG:NH1	2.35	0.60
2:L1:814:A:O2'	35:NF:73:ARG:NH2	2.35	0.60
28:LT:192:ASN:O	28:LT:196:GLY:N	2.34	0.60
29:LU:73:ILE:HG23	29:LU:83:LEU:HD11	1.84	0.60
57:SM:116:ARG:NH1	57:SM:118:ASN:OD1	2.35	0.60
58:SP:453:PHE:CE1	58:SP:485:ILE:HG23	2.37	0.60
61:SS:471:GLU:OE2	61:SS:475:GLN:NE2	2.35	0.60
21:LM:351:TYR:CE1	21:LM:355:ILE:HD11	2.36	0.60
37:NH:856:THR:HG22	37:NH:858:ARG:H	1.66	0.60
58:SP:1251:VAL:HG23	58:SP:1252:PHE:HD1	1.67	0.60
58:SP:1447:GLU:OE1	58:SP:1447:GLU:N	2.35	0.60
68:SZ:442:GLU:OE2	68:SZ:446:GLN:NE2	2.34	0.60
2:L1:495:C:OP1	54:SI:1135:ARG:NH1	2.35	0.59
21:LM:777:ASP:OD2	21:LM:778:SER:N	2.35	0.59
25:LQ:829:VAL:HG21	25:LQ:864:ASN:HD21	1.66	0.59
57:SM:243:GLU:OE1	57:SM:243:GLU:N	2.35	0.59
36:NG:136:ARG:O	65:SW:248:VAL:HG11	2.01	0.59
43:NS:613:ILE:CD1	43:NS:617:LEU:HD12	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SI:838:ILE:HD12	54:SI:874:TYR:HB3	1.83	0.59
58:SP:369:SER:O	58:SP:407:ARG:NH2	2.34	0.59
58:SP:489:SER:OG	58:SP:493:ASN:OD1	2.15	0.59
58:SP:2119:ARG:NH1	61:SS:227:TYR:O	2.35	0.59
58:SP:2278:THR:HG22	58:SP:2335:TYR:OH	2.02	0.59
16:LH:145:PHE:CE2	16:LH:230:LEU:HD13	2.37	0.59
26:LR:220:ILE:HD12	26:LR:239:VAL:HG11	1.85	0.59
39:NL:59:VAL:HG13	39:NL:122:PHE:HA	1.84	0.59
64:SV:131:LEU:HD21	64:SV:135:VAL:HG21	1.84	0.59
58:SP:1742:VAL:HB	58:SP:1745:ILE:HD12	1.83	0.59
16:LH:744:ILE:HD11	17:LI:431:PHE:HZ	1.67	0.59
32:NA:408:SER:O	32:NA:412:ILE:HD12	2.02	0.59
2:L1:1096:C:O4'	13:LE:19:LYS:NZ	2.35	0.59
21:LM:1695:MET:HE2	21:LM:1732:VAL:HG11	1.84	0.59
54:SI:918:ILE:HD12	60:SR:144:ARG:HH12	1.66	0.59
21:LM:1482:GLU:OE2	64:SV:56:ARG:NH2	2.36	0.59
67:SY:219:ASP:OD1	67:SY:222:ARG:NH2	2.35	0.59
2:L1:1594:G:O2'	2:L1:1600:A:N6	2.35	0.59
63:SU:233:ASP:OD2	63:SU:234:ALA:N	2.36	0.59
22:LN:355:THR:OG1	22:LN:372:MET:O	2.21	0.59
23:LO:622:ALA:O	23:LO:676:ARG:NH2	2.35	0.59
28:LT:592:ASP:OD1	28:LT:593:PHE:N	2.35	0.59
43:NS:613:ILE:HD12	43:NS:617:LEU:HD12	1.85	0.59
58:SP:311:ILE:HD11	58:SP:343:ILE:HG23	1.85	0.59
68:SZ:438:ASP:OD2	68:SZ:439:PHE:N	2.36	0.59
16:LH:537:ASN:OD1	16:LH:538:GLU:N	2.35	0.59
2:L1:1159:C:N4	57:SM:184:GLU:OE2	2.34	0.58
16:LH:698:VAL:HG11	16:LH:707:MET:HE2	1.85	0.58
21:LM:1486:GLU:OE2	64:SV:56:ARG:NH1	2.36	0.58
28:LT:346:ARG:NH2	28:LT:385:GLN:OE1	2.36	0.58
29:LU:116:LEU:HD11	29:LU:136:MET:CE	2.33	0.58
43:NS:1227:ILE:O	43:NS:1227:ILE:HG23	2.02	0.58
49:SB:118:ARG:NH2	50:SD:261:LEU:O	2.36	0.58
50:SD:283:GLU:OE1	50:SD:283:GLU:N	2.35	0.58
2:L1:967:A:OP2	35:NF:124:ARG:NH2	2.35	0.58
3:L2:256:G:OP1	48:SA:382:LYS:NZ	2.35	0.58
20:LL:35:GLN:OE1	20:LL:316:ASN:ND2	2.36	0.58
63:SU:350:MET:HE3	63:SU:394:ALA:HB1	1.84	0.58
22:LN:684:GLU:OE1	22:LN:684:GLU:N	2.35	0.58
37:NH:369:TRP:HE3	37:NH:370:LEU:HD12	1.68	0.58
62:ST:277:LEU:HD12	68:SZ:383:PRO:HG2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L4:212:ASP:OD1	5:L4:216:ASN:N	2.36	0.58
21:LM:22:ARG:NH2	29:LU:20:GLN:O	2.35	0.58
21:LM:193:THR:OG1	21:LM:241:ILE:HD11	2.03	0.58
23:LO:575:GLU:OE1	23:LO:575:GLU:N	2.37	0.58
21:LM:778:SER:O	21:LM:782:VAL:N	2.37	0.58
2:L1:330:G:OP2	9:L8:172:ARG:NH1	2.37	0.58
16:LH:612:SER:HB3	16:LH:662:VAL:HG12	1.86	0.58
20:LL:336:ASN:ND2	27:LS:335:GLN:OE1	2.37	0.58
58:SP:571:LEU:HD13	58:SP:610:LEU:HD22	1.86	0.58
19:LK:448:GLU:N	19:LK:448:GLU:OE1	2.37	0.58
30:LW:123:THR:HG23	30:LW:140:ARG:HH21	1.69	0.58
25:LQ:680:SER:OG	25:LQ:682:ARG:NH1	2.37	0.58
16:LH:722:LEU:HD11	16:LH:763:ILE:HG21	1.86	0.57
20:LL:112:LEU:HD12	20:LL:116:GLN:O	2.04	0.57
23:LO:608:ASN:ND2	28:LT:513:MET:SD	2.76	0.57
25:LQ:132:THR:HG23	25:LQ:134:THR:HG22	1.85	0.57
53:SH:301:MET:HE2	53:SH:354:ILE:HD13	1.85	0.57
2:L1:577:G:OP1	32:NA:322:LYS:NZ	2.32	0.57
36:NG:31:THR:OG1	36:NG:37:GLU:O	2.03	0.57
55:SK:68:LEU:HD13	55:SK:77:LEU:CD2	2.34	0.57
58:SP:1200:ASN:OD1	58:SP:1242:LYS:NZ	2.34	0.57
7:L6:18:ILE:HG23	7:L6:23:ARG:HD2	1.85	0.57
21:LM:730:GLN:N	21:LM:730:GLN:OE1	2.38	0.57
27:LS:511:LEU:HD13	27:LS:544:VAL:HG21	1.86	0.57
32:NA:555:ASP:OD1	32:NA:556:THR:N	2.37	0.57
16:LH:780:GLU:N	16:LH:780:GLU:OE1	2.37	0.57
18:LJ:492:ARG:NH2	20:LL:544:ASP:OD2	2.38	0.57
2:L1:277:U:O2'	2:L1:278:U:OP1	2.22	0.57
25:LQ:469:GLU:OE2	25:LQ:469:GLU:N	2.37	0.57
2:L1:1034:C:HO2'	13:LE:2:THR:N	2.02	0.57
3:L2:38:U:O2'	3:L2:39:C:OP2	2.21	0.57
50:SC:178:GLY:O	50:SC:182:SER:OG	2.22	0.57
58:SP:1738:TYR:OH	58:SP:1745:ILE:HD13	2.05	0.57
23:LO:131:ARG:HH22	28:LT:640:LEU:HD21	1.70	0.57
20:LL:465:ILE:O	20:LL:469:ILE:HD12	2.05	0.57
23:LO:351:LEU:HD22	23:LO:701:LEU:HD11	1.86	0.57
28:LT:604:SER:OG	28:LT:606:ASP:OD1	2.20	0.57
30:LW:178:ASP:OD1	30:LW:179:HIS:N	2.38	0.57
38:NI:50:SER:O	38:NI:127:LYS:NZ	2.38	0.57
58:SP:517:ASP:OD2	58:SP:715:TYR:OH	2.13	0.57
18:LJ:432:TYR:O	18:LJ:470:TYR:OH	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:NH:707:PHE:O	37:NH:918:ARG:NH1	2.37	0.57
63:SU:430:ASP:OD1	63:SU:431:GLN:N	2.37	0.57
43:NS:500:GLU:OE1	43:NS:510:TYR:OH	2.13	0.56
43:NS:742:GLU:N	43:NS:742:GLU:OE1	2.38	0.56
21:LM:925:LEU:HD23	21:LM:945:ILE:HD11	1.86	0.56
21:LM:923:ASP:OD1	21:LM:924:ILE:N	2.38	0.56
23:LO:35:ASN:OD1	23:LO:54:HIS:N	2.34	0.56
23:LO:707:ASN:OD1	23:LO:708:ASP:N	2.38	0.56
50:SC:202:ARG:NH2	51:SF:78:TYR:OH	2.38	0.56
56:SL:82:ILE:HG23	56:SL:86:MET:HE3	1.86	0.56
31:LZ:153:ASN:OD1	31:LZ:154:MET:N	2.38	0.56
57:SM:162:THR:OG1	57:SM:264:GLY:O	2.17	0.56
2:L1:54:C:O2'	2:L1:459:G:N7	2.35	0.56
20:LL:145:CYS:HB3	20:LL:148:LEU:HD21	1.86	0.56
62:ST:433:ILE:HD12	62:ST:459:LEU:HD22	1.86	0.56
17:LI:595:ILE:CG2	17:LI:599:MET:HE3	2.34	0.56
23:LO:708:ASP:OD1	23:LO:709:THR:N	2.38	0.56
54:SI:1062:ARG:NH2	67:SY:33:ASP:O	2.39	0.56
58:SP:73:ASP:OD2	58:SP:86:LYS:NZ	2.31	0.56
65:SW:204:ARG:NH1	65:SW:250:LEU:O	2.35	0.56
2:L1:334:G:O6	9:L8:5:ARG:NH2	2.37	0.56
2:L1:821:U:OP1	58:SP:2471:ARG:NH2	2.38	0.56
18:LJ:479:VAL:O	18:LJ:483:LEU:HD23	2.05	0.56
27:LS:180:ASP:OD2	28:LT:281:ARG:NH2	2.38	0.56
37:NH:203:ILE:HD11	37:NH:290:PHE:CE2	2.40	0.56
2:L1:578:OMU:OP2	54:SI:874:TYR:OH	2.16	0.56
28:LT:181:THR:HG23	28:LT:235:MET:HE2	1.88	0.56
28:LT:814:GLU:OE1	28:LT:822:ARG:NH1	2.39	0.56
20:LL:582:GLU:OE2	22:LN:464:LYS:NZ	2.27	0.56
21:LM:42:THR:O	29:LU:17:LYS:NZ	2.39	0.56
30:LW:178:ASP:OD1	30:LW:179:HIS:ND1	2.39	0.56
36:NG:12:GLN:OE1	36:NG:77:THR:OG1	2.05	0.56
55:SK:178:VAL:CG2	55:SK:225:VAL:HG22	2.36	0.56
58:SP:1137:ILE:HG23	58:SP:1185:LEU:HD21	1.88	0.56
7:L6:21:GLU:OE1	7:L6:25:ARG:NH2	2.39	0.56
29:LU:116:LEU:HD11	29:LU:136:MET:HE2	1.88	0.56
2:L1:1662:G:O3'	43:NS:251:ARG:NH1	2.32	0.55
11:LC:45:ARG:O	11:LC:48:VAL:HG22	2.06	0.55
39:NL:36:GLN:N	39:NL:36:GLN:NE2	2.52	0.55
55:SK:178:VAL:HG21	55:SK:225:VAL:HG22	1.87	0.55
18:LJ:302:VAL:HG22	18:LJ:322:LEU:CD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LM:15:ASN:ND2	30:LW:140:ARG:O	2.39	0.55
21:LM:1076:LEU:HD12	21:LM:1084:GLU:HG2	1.87	0.55
35:NF:48:SER:OG	35:NF:86:GLU:OE1	2.09	0.55
37:NH:495:THR:O	37:NH:499:LEU:N	2.37	0.55
38:NI:37:MET:SD	38:NI:58:LEU:HD23	2.46	0.55
43:NS:915:LEU:HD22	43:NS:1049:ILE:CD1	2.34	0.55
52:SG:409:ASP:OD1	52:SG:410:ASP:N	2.38	0.55
55:SK:128:VAL:HA	55:SK:159:LEU:HD12	1.88	0.55
21:LM:353:ARG:NH1	21:LM:386:ASP:OD2	2.40	0.55
27:LS:216:TYR:OH	28:LT:272:ASP:OD2	2.23	0.55
28:LT:226:VAL:HG13	28:LT:227:THR:HG23	1.88	0.55
6:L5:30:PRO:O	6:L5:34:GLN:NE2	2.39	0.55
37:NH:1146:THR:HG21	37:NH:1180:ASN:ND2	2.21	0.55
48:SA:28:GLY:O	48:SA:34:VAL:HG21	2.05	0.55
48:SA:257:ILE:O	49:SB:138:LYS:NZ	2.36	0.55
54:SI:838:ILE:HD12	54:SI:874:TYR:CB	2.36	0.55
63:SU:173:GLU:N	63:SU:173:GLU:OE1	2.40	0.55
2:L1:803:A:O2'	13:LE:107:SER:O	2.16	0.55
6:L5:207:THR:O	6:L5:212:LYS:NZ	2.39	0.55
27:LS:16:ASP:O	27:LS:20:GLN:NE2	2.39	0.55
43:NS:498:LEU:HD13	43:NS:857:MET:HE3	1.89	0.55
45:OA:1408:ASP:OD2	45:OA:1412:SER:N	2.39	0.55
53:SH:281:GLU:OE1	54:SI:624:LYS:NZ	2.40	0.55
54:SI:97:THR:OG1	54:SI:214:ARG:NH2	2.39	0.55
21:LM:1695:MET:HE1	21:LM:1729:LEU:HD11	1.89	0.55
37:NH:143:GLU:N	37:NH:143:GLU:OE2	2.40	0.55
65:SW:102:PRO:CD	65:SW:163:THR:HG23	2.36	0.55
2:L1:472:U:O2'	2:L1:769:A:N3	2.39	0.55
4:L3:30:TYR:O	4:L3:33:THR:OG1	2.25	0.55
16:LH:698:VAL:HG11	16:LH:707:MET:CE	2.36	0.55
24:LP:182:TRP:CG	24:LP:277:CYS:HG	2.24	0.55
30:LW:204:LEU:HD21	30:LW:225:VAL:HG21	1.87	0.55
43:NS:1107:THR:HG23	43:NS:1109:ARG:HG2	1.89	0.55
2:L1:1125:A:O2'	2:L1:1126:OMG:H5'	2.07	0.55
7:L6:5:ILE:HD12	7:L6:16:PHE:HD2	1.72	0.55
27:LS:352:GLN:NE2	27:LS:354:SER:O	2.40	0.55
37:NH:744:MET:HE1	37:NH:810:ILE:HA	1.89	0.55
58:SP:1446:GLU:OE1	58:SP:1461:ARG:NH2	2.40	0.55
8:L7:159:VAL:HG21	8:L7:188:GLU:OE1	2.07	0.55
8:L7:159:VAL:HG21	8:L7:188:GLU:CD	2.32	0.55
29:LU:26:ARG:NH1	30:LW:412:ASP:OD2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:NH:313:ASN:OD1	37:NH:314:CYS:N	2.40	0.55
55:SK:68:LEU:HD13	55:SK:77:LEU:HD23	1.89	0.55
58:SP:2376:VAL:O	58:SP:2380:GLY:N	2.40	0.55
21:LM:661:ILE:HG21	21:LM:666:ALA:HB3	1.88	0.54
50:SD:159:LEU:HD11	50:SD:317:VAL:HG21	1.89	0.54
51:SF:51:PHE:CE1	51:SF:53:ILE:HD11	2.42	0.54
58:SP:163:SER:O	58:SP:167:VAL:HG23	2.07	0.54
58:SP:1680:THR:HG23	58:SP:1681:LEU:HG	1.89	0.54
2:L1:1226:A:H61	46:OH:114:LYS:HG2	1.72	0.54
26:LR:280:ARG:NH2	37:NH:636:GLU:OE2	2.39	0.54
49:SB:319:ILE:HD12	49:SB:326:LEU:HD22	1.89	0.54
22:LN:426:GLN:OE1	34:ND:190:LEU:HD13	2.07	0.54
33:NB:204:MET:O	33:NB:209:ARG:NH1	2.40	0.54
43:NS:1043:LYS:NZ	43:NS:1062:ILE:O	2.40	0.54
24:LP:45:SER:OG	24:LP:46:ARG:N	2.41	0.54
26:LR:616:HIS:CG	26:LR:620:LEU:HD21	2.42	0.54
58:SP:841:ILE:O	58:SP:844:VAL:HG22	2.07	0.54
2:L1:97:C:H1'	2:L1:426:G:H5'	1.90	0.54
4:L3:116:LEU:HD21	62:ST:755:ILE:HG12	1.88	0.54
6:L5:123:VAL:CG1	18:LJ:95:LEU:HD11	2.38	0.54
16:LH:71:ASN:HD22	16:LH:125:LEU:HD21	1.72	0.54
47:OU:100:LEU:HD12	47:OU:103:LEU:CD1	2.38	0.54
18:LJ:482:GLU:OE2	18:LJ:483:LEU:HD22	2.08	0.54
25:LQ:898:LEU:O	25:LQ:902:VAL:HG23	2.08	0.54
58:SP:1951:THR:N	58:SP:1989:ASP:OD2	2.38	0.54
16:LH:720:ILE:CG1	16:LH:745:ILE:HD13	2.36	0.54
16:LH:744:ILE:HD11	17:LI:431:PHE:CZ	2.43	0.54
33:NB:66:MET:HE1	67:SY:204:HIS:CD2	2.43	0.54
52:SG:481:ILE:HD13	52:SG:486:VAL:HG13	1.88	0.54
55:SK:104:ILE:N	55:SK:246:GLU:OE2	2.41	0.54
2:L1:1478:G:OP1	41:NP:39:THR:OG1	2.25	0.54
19:LK:503:LEU:HA	19:LK:506:LEU:HD12	1.90	0.54
21:LM:564:VAL:HG11	21:LM:622:TRP:HZ3	1.72	0.54
43:NS:675:ASP:OD1	43:NS:736:SER:OG	2.20	0.54
2:L1:886:U:OP2	40:NM:216:LYS:NZ	2.28	0.54
6:L5:90:ILE:O	6:L5:94:THR:HG23	2.07	0.54
16:LH:474:THR:HG22	16:LH:511:GLU:HG2	1.90	0.54
21:LM:1370:TYR:OH	21:LM:1418:ASN:OD1	2.21	0.54
23:LO:848:PHE:O	23:LO:852:THR:OG1	2.21	0.54
40:NM:244:VAL:O	40:NM:244:VAL:HG13	2.08	0.54
48:SA:178:ILE:HD11	48:SA:313:ALA:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SG:57:GLU:N	52:SG:57:GLU:OE2	2.41	0.54
58:SP:1720:ILE:O	58:SP:1724:ASN:ND2	2.41	0.54
5:L4:141:THR:OG1	5:L4:143:ASP:OD1	2.26	0.54
21:LM:1740:ASP:OD1	58:SP:202:LYS:NZ	2.28	0.54
24:LP:64:ASN:ND2	24:LP:89:GLN:OE1	2.41	0.54
6:L5:25:LEU:HD12	6:L5:29:ILE:HD13	1.90	0.53
21:LM:944:VAL:HG12	21:LM:948:LEU:CD1	2.38	0.53
62:ST:552:GLN:NE2	63:SU:546:TYR:O	2.40	0.53
15:LG:58:GLU:OE1	15:LG:58:GLU:N	2.42	0.53
58:SP:2450:ILE:O	58:SP:2454:ASN:ND2	2.41	0.53
62:ST:388:LEU:O	62:ST:392:LYS:N	2.41	0.53
2:L1:1682:U:O2	2:L1:1720:G:N2	2.41	0.53
21:LM:235:VAL:HG11	27:LS:218:TYR:CG	2.43	0.53
24:LP:391:TYR:CE2	24:LP:395:ILE:HD11	2.43	0.53
55:SJ:41:MET:HE3	55:SJ:241:PHE:CE2	2.43	0.53
64:SV:152:SER:O	64:SV:153:THR:OG1	2.26	0.53
20:LL:18:CYS:SG	20:LL:63:LEU:HD12	2.48	0.53
26:LR:561:SER:O	26:LR:565:PHE:N	2.40	0.53
26:LR:666:GLU:CD	26:LR:690:HIS:HE2	2.17	0.53
32:NA:297:LEU:O	32:NA:302:LYS:NZ	2.41	0.53
50:SC:100:ARG:NH1	50:SC:104:ASP:OD2	2.42	0.53
58:SP:319:THR:HG22	58:SP:361:LEU:HB2	1.90	0.53
5:L4:129:VAL:HG22	5:L4:139:VAL:HG12	1.90	0.53
16:LH:681:ILE:HG13	16:LH:688:VAL:HG12	1.90	0.53
22:LN:385:ASN:ND2	22:LN:387:GLU:O	2.41	0.53
55:SJ:171:LEU:HD22	55:SJ:203:CYS:SG	2.49	0.53
3:L2:145:U:O4	21:LM:1709:ARG:NH2	2.42	0.53
11:LC:69:VAL:HG21	11:LC:81:ILE:CG1	2.39	0.53
17:LI:280:GLN:CD	17:LI:368:VAL:HG11	2.34	0.53
18:LJ:197:ASP:HB2	18:LJ:206:ILE:HD11	1.91	0.53
21:LM:1536:VAL:HG11	21:LM:1582:LEU:HD13	1.90	0.53
21:LM:1652:VAL:HG11	21:LM:1690:LEU:HB3	1.91	0.53
43:NS:1141:LEU:HD11	43:NS:1152:MET:HE2	1.91	0.53
58:SP:464:PHE:O	58:SP:468:ALA:HB2	2.09	0.53
58:SP:615:VAL:HG13	58:SP:619:LEU:HD23	1.90	0.53
23:LO:155:SER:OG	23:LO:157:ASP:OD1	2.24	0.53
26:LR:333:ILE:HG23	26:LR:379:LEU:HB3	1.90	0.53
36:NG:45:GLY:O	40:NM:2:ALA:N	2.42	0.53
50:SC:237:VAL:HG12	50:SC:260:PHE:O	2.09	0.53
55:SK:218:ASP:OD2	55:SK:219:GLU:N	2.41	0.53
58:SP:806:THR:OG1	58:SP:820:THR:OG1	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:1594:G:HO2'	2:L1:1600:A:N6	2.07	0.53
25:LQ:56:THR:OG1	25:LQ:58:ASP:OD1	2.21	0.53
46:OH:56:GLU:OE1	46:OH:124:LYS:NZ	2.40	0.53
2:L1:1194:A:N6	55:SJ:129:ARG:O	2.37	0.53
10:L9:53:ARG:HH21	56:SL:92:ALA:HB2	1.73	0.53
21:LM:1735:GLU:OE1	58:SP:248:HIS:NE2	2.42	0.53
26:LR:382:GLU:OE1	26:LR:384:TYR:OH	2.26	0.53
49:SB:230:GLU:HG2	49:SB:231:ILE:HD12	1.90	0.53
55:SK:101:ASP:OD2	55:SK:132:ARG:NH1	2.40	0.53
61:SS:726:SER:O	61:SS:727:THR:HG22	2.08	0.53
62:ST:596:TYR:OH	63:SU:310:LYS:NZ	2.33	0.53
21:LM:1419:ILE:HD13	21:LM:1448:ILE:HD13	1.91	0.53
50:SC:253:ILE:HD13	50:SC:269:ILE:HG12	1.91	0.53
58:SP:474:ASN:OD1	58:SP:716:TYR:OH	2.17	0.53
62:ST:640:MET:HE1	62:ST:678:PHE:HE2	1.73	0.53
1:L0:475:G:OP1	31:LZ:4:LYS:N	2.40	0.52
2:L1:1594:G:HO2'	2:L1:1600:A:H61	1.57	0.52
16:LH:576:ALA:HB2	16:LH:613:LEU:HD11	1.91	0.52
18:LJ:253:LYS:NZ	63:SU:331:ASN:OD1	2.42	0.52
49:SB:1:MET:O	49:SB:86:THR:N	2.41	0.52
4:L3:56:LYS:NZ	4:L3:65:GLU:OE2	2.42	0.52
7:L6:5:ILE:HD12	7:L6:16:PHE:CD2	2.44	0.52
23:LO:415:ASP:O	23:LO:419:TYR:N	2.42	0.52
33:NB:219:GLU:OE2	66:SX:191:UNK:N	2.43	0.52
2:L1:1193:A:O2'	2:L1:1194:A:O4'	2.25	0.52
21:LM:1407:LEU:HD12	21:LM:1415:LEU:HD22	1.91	0.52
56:SL:67:ILE:CD1	56:SL:86:MET:HE1	2.40	0.52
56:SL:67:ILE:HD11	56:SL:86:MET:HE1	1.90	0.52
43:NS:456:VAL:HG11	43:NS:740:THR:HG23	1.92	0.52
55:SK:77:LEU:HB2	55:SK:84:ILE:HG22	1.90	0.52
21:LM:1427:TYR:O	21:LM:1430:ARG:NH2	2.42	0.52
29:LU:215:LEU:O	29:LU:216:SER:OG	2.21	0.52
58:SP:1214:ASP:OD1	58:SP:1217:ARG:NH2	2.42	0.52
63:SU:281:LEU:CD2	63:SU:299:LEU:HD21	2.40	0.52
2:L1:1568:C:O2'	2:L1:1569:A:O5'	2.28	0.52
5:L4:151:ASP:OD2	7:L6:215:ARG:NH2	2.42	0.52
6:L5:136:ALA:O	6:L5:140:THR:HG22	2.09	0.52
21:LM:1441:ILE:O	21:LM:1445:ILE:HD12	2.10	0.52
23:LO:210:SER:OG	23:LO:212:ASP:OD1	2.26	0.52
27:LS:326:LEU:HD12	27:LS:331:LEU:HD13	1.91	0.52
50:SC:225:ARG:NH1	50:SC:246:GLN:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SP:2446:SER:O	58:SP:2450:ILE:HD12	2.10	0.52
62:ST:245:ASP:OD2	68:SZ:209:LYS:NZ	2.33	0.52
2:L1:1057:U:O4	37:NH:791:LYS:NZ	2.33	0.52
5:L4:87:MET:HE2	5:L4:123:LEU:HB2	1.91	0.52
40:NM:138:PHE:O	40:NM:213:ARG:N	2.42	0.52
55:SJ:196:LEU:HD21	55:SJ:200:GLU:HG2	1.92	0.52
58:SP:439:VAL:O	58:SP:449:ARG:NH1	2.43	0.52
58:SP:491:LEU:HD12	58:SP:491:LEU:O	2.09	0.52
59:SQ:180:ASP:OD2	59:SQ:183:SER:OG	2.26	0.52
63:SU:333:GLU:OE1	63:SU:334:TYR:N	2.43	0.52
2:L1:410:A:O3'	43:NS:11:LYS:NZ	2.43	0.52
12:LD:93:TYR:OH	12:LD:98:ASN:OD1	2.27	0.52
18:LJ:500:GLU:O	18:LJ:504:ILE:HD12	2.09	0.52
20:LL:147:GLN:C	20:LL:148:LEU:HD22	2.34	0.52
41:NP:131:ASP:OD1	41:NP:134:ARG:NH2	2.43	0.52
47:OU:133:ALA:N	47:OU:140:TYR:O	2.38	0.52
54:SI:918:ILE:HD12	60:SR:144:ARG:NH1	2.25	0.52
54:SI:925:ASN:OD1	54:SI:926:ILE:N	2.43	0.52
58:SP:1462:ARG:NH1	58:SP:1492:TYR:OH	2.42	0.52
61:SS:439:ARG:O	61:SS:442:LEU:N	2.43	0.52
21:LM:895:GLN:O	21:LM:899:ILE:HD12	2.10	0.52
30:LW:78:ASN:OD1	30:LW:79:GLU:N	2.43	0.52
48:SA:159:SER:OG	50:SC:219:PRO:O	2.25	0.52
58:SP:1706:LYS:O	58:SP:1760:ASN:ND2	2.43	0.52
7:L6:182:GLN:HE21	7:L6:186:ARG:HG3	1.74	0.52
24:LP:371:ILE:O	24:LP:418:TYR:OH	2.27	0.52
28:LT:27:PHE:HB2	28:LT:655:THR:HG23	1.91	0.52
28:LT:367:LEU:HD22	28:LT:375:LEU:HD21	1.92	0.51
48:SA:88:LYS:NZ	61:SS:330:THR:O	2.30	0.51
54:SI:258:ILE:HD13	54:SI:265:ILE:HD11	1.92	0.51
58:SP:2454:ASN:OD1	58:SP:2455:ALA:N	2.43	0.51
62:ST:280:ASP:OD1	62:ST:281:LYS:N	2.43	0.51
3:L2:33:A:O2'	3:L2:34:A:OP2	2.25	0.51
6:L5:23:VAL:HG11	11:LC:58:ASP:OD1	2.10	0.51
6:L5:25:LEU:HD12	6:L5:29:ILE:CD1	2.39	0.51
20:LL:66:VAL:HG21	20:LL:77:ILE:HG23	1.92	0.51
39:NL:71:THR:HG21	39:NL:94:LEU:HD11	1.92	0.51
20:LL:233:LYS:NZ	20:LL:292:TYR:O	2.44	0.51
21:LM:1081:VAL:CG2	21:LM:1162:VAL:HG22	2.40	0.51
22:LN:257:ASP:OD1	22:LN:259:THR:OG1	2.21	0.51
27:LS:379:GLY:N	27:LS:383:TRP:O	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:OH:71:ILE:HD11	47:OU:100:LEU:HD11	1.92	0.51
16:LH:682:ASN:O	16:LH:686:GLY:N	2.43	0.51
21:LM:943:LEU:HD22	21:LM:982:VAL:HG23	1.91	0.51
2:L1:1271:OMG:H2'	2:L1:1272:U:C6	2.45	0.51
5:L4:181:VAL:HG11	5:L4:195:ILE:HD11	1.91	0.51
15:LG:65:ARG:O	15:LG:67:ARG:NH1	2.43	0.51
16:LH:521:SER:OG	18:LJ:461:ASP:OD2	2.29	0.51
16:LH:642:GLU:N	16:LH:642:GLU:OE1	2.44	0.51
26:LR:393:SER:OG	26:LR:394:LEU:N	2.44	0.51
28:LT:646:VAL:HG23	28:LT:647:THR:HG23	1.93	0.51
32:NA:551:ASN:OD1	32:NA:552:ASP:N	2.43	0.51
3:L2:82:G:OP1	49:SB:366:LYS:NZ	2.39	0.51
8:L7:133:THR:HG21	8:L7:162:ILE:HD13	1.92	0.51
48:SA:171:ASP:OD2	48:SA:322:LEU:N	2.43	0.51
55:SK:51:GLU:HG3	55:SK:68:LEU:HD12	1.93	0.51
58:SP:994:ILE:HD12	58:SP:1047:LEU:HD11	1.92	0.51
2:L1:31:C:OP1	60:SR:140:LYS:NZ	2.42	0.51
21:LM:786:TYR:O	49:SB:84:LYS:NZ	2.39	0.51
26:LR:666:GLU:OE2	26:LR:688:LEU:HD13	2.11	0.51
43:NS:494:ASP:OD1	43:NS:495:GLY:N	2.43	0.51
43:NS:993:GLN:NE2	43:NS:1028:ASN:OD1	2.44	0.51
52:SG:158:THR:HG21	52:SG:240:LEU:HA	1.91	0.51
14:LF:103:ALA:O	14:LF:108:ARG:NH1	2.44	0.51
17:LI:564:ASN:OD1	17:LI:565:GLU:N	2.43	0.51
25:LQ:589:ILE:HG21	25:LQ:621:VAL:HG11	1.92	0.51
39:NL:115:MET:HG3	39:NL:133:ILE:HD11	1.93	0.51
50:SD:178:GLY:CA	50:SD:210:MET:HE2	2.41	0.51
2:L1:498:G:N7	59:SQ:138:LYS:NZ	2.53	0.51
20:LL:8:SER:OG	20:LL:17:LEU:HD11	2.10	0.51
32:NA:16:ILE:HG23	32:NA:17:LEU:HD22	1.92	0.51
39:NL:70:LEU:O	39:NL:74:ILE:HD12	2.11	0.51
43:NS:420:LYS:N	72:NS:1301:ADP:O3B	2.44	0.51
49:SB:163:ILE:HD11	49:SB:283:ILE:HD12	1.93	0.51
55:SK:128:VAL:CA	55:SK:159:LEU:HD12	2.41	0.51
2:L1:493:U:O2'	2:L1:494:U:OP1	2.21	0.50
2:L1:1670:G:O2'	2:L1:1731:A:N6	2.44	0.50
21:LM:786:TYR:C	49:SB:84:LYS:HZ3	2.19	0.50
21:LM:1083:GLU:N	21:LM:1083:GLU:OE1	2.43	0.50
43:NS:587:GLN:NE2	43:NS:588:PHE:O	2.44	0.50
54:SI:241:HIS:C	54:SI:278:THR:HG22	2.36	0.50
2:L1:1471:A:OP1	6:L5:185:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:1606:C:OP1	57:SM:123:VAL:HG13	2.10	0.50
20:LL:469:ILE:HD11	20:LL:501:TRP:CE3	2.46	0.50
21:LM:275:ILE:HG13	21:LM:306:LEU:HD11	1.94	0.50
28:LT:375:LEU:HD22	28:LT:389:MET:SD	2.52	0.50
37:NH:703:LYS:NZ	37:NH:1086:ASN:OD1	2.37	0.50
55:SJ:180:LEU:HD13	55:SJ:237:ALA:HB1	1.92	0.50
4:L3:45:LEU:HD22	41:NP:36:ILE:HD11	1.93	0.50
13:LE:11:LEU:HD12	13:LE:74:VAL:HG13	1.93	0.50
21:LM:378:TYR:O	21:LM:382:LEU:HD23	2.11	0.50
23:LO:191:ARG:NH2	61:SS:767:GLU:OE1	2.44	0.50
37:NH:173:ASN:O	37:NH:173:ASN:ND2	2.44	0.50
37:NH:1226:PHE:CE2	38:NI:60:LEU:HD21	2.46	0.50
43:NS:914:MET:HE3	43:NS:1084:ILE:HA	1.93	0.50
55:SJ:52:THR:HG22	55:SJ:142:VAL:HG12	1.93	0.50
56:SL:101:CYS:SG	56:SL:132:HIS:CE1	3.04	0.50
2:L1:381:C:O2'	2:L1:755:A:N1	2.43	0.50
18:LJ:168:THR:OG1	18:LJ:190:ASP:OD1	2.28	0.50
21:LM:651:LEU:HD21	21:LM:684:TYR:HD2	1.76	0.50
21:LM:1445:ILE:HG23	21:LM:1450:LEU:HD11	1.93	0.50
23:LO:200:SER:OG	23:LO:202:ASP:OD1	2.26	0.50
30:LW:321:ASN:ND2	30:LW:379:GLU:O	2.44	0.50
51:SF:51:PHE:HE1	51:SF:53:ILE:HD11	1.77	0.50
16:LH:210:HIS:NE2	16:LH:226:SER:OG	2.44	0.50
16:LH:769:ASN:OD1	16:LH:770:TYR:N	2.43	0.50
28:LT:354:SER:N	28:LT:369:ALA:O	2.39	0.50
37:NH:1233:ASN:OD1	37:NH:1234:PHE:N	2.44	0.50
43:NS:918:SER:HA	43:NS:1083:MET:HE2	1.94	0.50
2:L1:612:U:OP2	2:L1:613:G:O2'	2.28	0.50
3:L2:30:A:N6	29:LU:341:GLU:OE2	2.44	0.50
22:LN:382:VAL:HG11	22:LN:755:ILE:HD13	1.94	0.50
32:NA:430:LEU:O	32:NA:434:HIS:ND1	2.41	0.50
58:SP:1685:SER:HB2	58:SP:1745:ILE:HD11	1.94	0.50
2:L1:973:A:H2'	2:L1:974:A2M:H8	1.92	0.50
3:L2:90:C:O2'	3:L2:91:C:OP1	2.22	0.50
3:L2:282:U:O2'	3:L2:284:U:O5'	2.28	0.50
16:LH:720:ILE:HD12	16:LH:774:PHE:CD2	2.46	0.50
18:LJ:85:TYR:O	18:LJ:86:SER:OG	2.26	0.50
24:LP:154:GLU:O	24:LP:159:ALA:N	2.44	0.50
34:ND:181:LEU:HD21	67:SY:136:PHE:HB3	1.94	0.50
43:NS:451:ARG:NH2	43:NS:762:ASN:OD1	2.45	0.50
43:NS:1121:LEU:HD22	43:NS:1226:LYS:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SS:793:GLU:OE1	61:SS:793:GLU:N	2.45	0.50
21:LM:1296:MET:HE1	21:LM:1306:SER:OG	2.12	0.50
32:NA:415:ASP:OD1	32:NA:416:ASP:N	2.44	0.50
52:SG:348:LEU:HD13	52:SG:427:LEU:HD11	1.93	0.50
58:SP:725:ASN:OD1	58:SP:726:LYS:N	2.44	0.50
2:L1:1699:G:N2	2:L1:1702:A:OP2	2.45	0.50
27:LS:326:LEU:HD12	27:LS:331:LEU:CD1	2.42	0.50
44:NV:651:LEU:HD12	44:NV:652:ASP:HB2	1.94	0.50
58:SP:1738:TYR:CE2	58:SP:1745:ILE:HG21	2.47	0.50
58:SP:1889:VAL:HG22	58:SP:1925:ASP:O	2.12	0.50
58:SP:2027:MET:HE1	58:SP:2082:LEU:HD22	1.92	0.50
2:L1:1124:A:O2'	39:NL:184:ASN:ND2	2.44	0.49
16:LH:95:ASP:OD2	16:LH:97:THR:OG1	2.30	0.49
17:LI:650:LEU:HD12	19:LK:506:LEU:HD13	1.94	0.49
32:NA:84:LEU:HD13	33:NB:302:LEU:HD13	1.94	0.49
48:SA:339:GLU:OE1	48:SA:340:LYS:NZ	2.30	0.49
59:SQ:102:ASP:OD2	59:SQ:103:TRP:N	2.45	0.49
16:LH:778:ASP:O	16:LH:781:SER:N	2.45	0.49
21:LM:1154:VAL:HG21	64:SV:96:GLN:CD	2.37	0.49
25:LQ:829:VAL:HG21	25:LQ:864:ASN:ND2	2.27	0.49
26:LR:15:ILE:HD13	26:LR:379:LEU:HD22	1.94	0.49
37:NH:1063:ARG:NH1	45:OA:1405:ALA:O	2.44	0.49
62:ST:92:GLU:OE1	62:ST:764:ARG:NH1	2.45	0.49
17:LI:632:THR:HB	19:LK:492:ILE:HG12	1.94	0.49
21:LM:1426:ILE:HG21	21:LM:1441:ILE:HD11	1.94	0.49
58:SP:344:MET:HE3	58:SP:344:MET:HA	1.94	0.49
3:L2:0:M7G:H82	3:L2:1:G:O4'	2.11	0.49
7:L6:67:VAL:HG21	7:L6:73:ILE:HD11	1.93	0.49
26:LR:557:VAL:HG11	26:LR:590:LEU:HD21	1.95	0.49
55:SJ:38:THR:OG1	55:SJ:40:ARG:NH2	2.45	0.49
55:SK:49:SER:C	55:SK:50:LEU:HD12	2.38	0.49
58:SP:2129:MET:SD	58:SP:2133:LEU:HD11	2.52	0.49
6:L5:124:LEU:O	18:LJ:138:LYS:NZ	2.45	0.49
12:LD:101:GLU:OE1	60:SR:16:ARG:NH2	2.44	0.49
37:NH:756:VAL:HG12	37:NH:756:VAL:O	2.13	0.49
48:SA:178:ILE:CD1	48:SA:292:LEU:HD21	2.43	0.49
50:SC:209:SER:O	50:SC:213:LYS:NZ	2.34	0.49
54:SI:56:VAL:HG23	60:SR:101:GLU:HG3	1.94	0.49
58:SP:1203:VAL:HG13	58:SP:1245:LYS:NZ	2.28	0.49
65:SW:102:PRO:HD2	65:SW:163:THR:HG23	1.94	0.49
2:L1:251:A:C2	5:L4:131:LEU:HD12	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LM:218:ILE:HD12	21:LM:263:VAL:HB	1.93	0.49
21:LM:1626:LEU:O	21:LM:1630:LEU:HD23	2.12	0.49
22:LN:537:ASP:OD2	22:LN:577:THR:HG23	2.13	0.49
25:LQ:177:LEU:CB	25:LQ:191:LEU:HD21	2.43	0.49
29:LU:258:ILE:HG22	29:LU:464:THR:HG22	1.93	0.49
1:L0:63:G:O6	16:LH:259:VAL:N	2.45	0.49
2:L1:1060:U:OP2	37:NH:865:ARG:NH2	2.39	0.49
10:L9:57:ARG:HG2	56:SL:87:MET:HE3	1.94	0.49
39:NL:71:THR:HG21	39:NL:94:LEU:CD1	2.43	0.49
54:SI:207:LEU:HD23	54:SI:219:GLU:HG2	1.94	0.49
57:SM:119:ARG:CZ	57:SM:124:MET:HE2	2.43	0.49
30:LW:176:ILE:HD13	31:LZ:19:LEU:HD12	1.93	0.49
48:SA:26:ASP:OD1	48:SA:27:ILE:N	2.44	0.49
48:SA:178:ILE:HD11	48:SA:313:ALA:CB	2.43	0.49
58:SP:1088:LYS:O	58:SP:1091:ILE:HG22	2.12	0.49
63:SU:158:SER:O	63:SU:218:LYS:NZ	2.46	0.49
8:L7:159:VAL:HG23	8:L7:185:ILE:HD13	1.95	0.49
17:LI:332:LEU:HD11	17:LI:401:ILE:HD13	1.94	0.49
20:LL:348:LYS:NZ	20:LL:352:SER:O	2.36	0.49
24:LP:154:GLU:OE1	24:LP:163:SER:OG	2.17	0.49
37:NH:822:ARG:NH1	37:NH:1133:PRO:O	2.44	0.49
44:NV:681:TYR:OH	58:SP:1891:HIS:O	2.25	0.49
52:SG:470:LEU:O	52:SG:471:GLN:NE2	2.45	0.49
8:L7:168:SER:O	8:L7:172:VAL:HG23	2.13	0.49
23:LO:140:ARG:HD2	61:SS:728:ARG:HH12	1.78	0.49
23:LO:298:LEU:HD13	32:NA:474:ILE:HD11	1.94	0.49
29:LU:73:ILE:CG2	29:LU:83:LEU:HD11	2.42	0.49
37:NH:1037:LEU:CD2	37:NH:1050:ILE:HG22	2.43	0.49
18:LJ:53:HIS:NE2	18:LJ:311:THR:O	2.45	0.48
21:LM:498:PHE:CD2	21:LM:539:LEU:HD11	2.48	0.48
21:LM:697:GLU:OE2	21:LM:697:GLU:N	2.46	0.48
24:LP:320:ILE:HD12	24:LP:335:ILE:HG23	1.95	0.48
26:LR:111:ASP:OD2	26:LR:113:THR:OG1	2.31	0.48
28:LT:894:ASP:OD1	28:LT:895:VAL:N	2.46	0.48
37:NH:203:ILE:HD11	37:NH:290:PHE:CD2	2.48	0.48
58:SP:1394:LEU:CD1	58:SP:1398:LEU:HD12	2.43	0.48
63:SU:378:SER:OG	63:SU:453:PRO:O	2.19	0.48
21:LM:929:ILE:HD12	21:LM:929:ILE:H	1.78	0.48
29:LU:228:ASN:OD1	29:LU:229:GLN:N	2.46	0.48
49:SB:36:ASP:OD1	49:SB:37:LYS:N	2.46	0.48
50:SD:178:GLY:O	50:SD:182:SER:OG	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SI:952:PHE:CD2	54:SI:958:VAL:HG22	2.48	0.48
58:SP:1152:GLU:OE2	58:SP:1197:THR:OG1	2.09	0.48
62:ST:569:GLN:NE2	63:SU:389:GLU:OE2	2.46	0.48
21:LM:1433:ASP:OD1	21:LM:1434:SER:N	2.47	0.48
22:LN:579:ARG:NH1	22:LN:660:ASP:OD1	2.46	0.48
25:LQ:252:SER:OG	25:LQ:278:ASP:OD2	2.24	0.48
26:LR:160:ILE:HG22	26:LR:160:ILE:O	2.14	0.48
26:LR:162:LEU:HD21	26:LR:227:MET:HE1	1.96	0.48
38:NI:188:MET:HA	38:NI:188:MET:HE2	1.95	0.48
57:SM:253:ARG:NH1	62:ST:59:GLU:OE2	2.46	0.48
62:ST:769:GLU:O	62:ST:772:LYS:N	2.46	0.48
4:L3:116:LEU:HD21	62:ST:755:ILE:CG1	2.44	0.48
21:LM:235:VAL:HG13	21:LM:239:LEU:HD12	1.95	0.48
22:LN:467:ASN:O	22:LN:471:LEU:HD23	2.13	0.48
24:LP:391:TYR:CZ	24:LP:395:ILE:HD11	2.49	0.48
37:NH:901:ASN:ND2	40:NM:131:ASP:OD1	2.47	0.48
37:NH:1189:LEU:C	37:NH:1194:HIS:HE2	2.21	0.48
58:SP:307:ASP:OD1	58:SP:308:ALA:N	2.45	0.48
17:LI:632:THR:HB	19:LK:492:ILE:HG23	1.95	0.48
21:LM:181:LYS:HD3	49:SB:409:THR:HG21	1.94	0.48
33:NB:66:MET:HE3	67:SY:203:GLN:HB2	1.95	0.48
43:NS:1214:VAL:HG13	43:NS:1214:VAL:O	2.13	0.48
55:SK:227:LEU:HD23	55:SK:227:LEU:H	1.79	0.48
58:SP:389:ILE:O	58:SP:393:PHE:N	2.47	0.48
11:LC:97:VAL:HG12	11:LC:98:ASP:H	1.78	0.48
21:LM:1285:VAL:HG21	21:LM:1320:TYR:CE1	2.49	0.48
23:LO:670:LEU:HD23	23:LO:670:LEU:O	2.13	0.48
49:SB:385:ASP:OD1	49:SB:386:ILE:N	2.47	0.48
63:SU:345:ILE:O	63:SU:382:LYS:NZ	2.46	0.48
2:L1:1756:A:N7	32:NA:500:LYS:NZ	2.52	0.48
8:L7:186:PRO:O	8:L7:187:SER:OG	2.24	0.48
22:LN:538:GLN:O	22:LN:540:ILE:HD12	2.14	0.48
26:LR:398:GLU:OE2	43:NS:249:ARG:NH2	2.39	0.48
37:NH:551:GLU:OE1	37:NH:551:GLU:N	2.44	0.48
50:SC:234:ILE:HG22	50:SC:235:GLY:O	2.14	0.48
55:SK:179:THR:CG2	55:SK:221:VAL:HG11	2.43	0.48
1:L0:87:C:O2	16:LH:332:GLN:NE2	2.46	0.48
16:LH:145:PHE:CZ	16:LH:230:LEU:HD13	2.48	0.48
18:LJ:90:ARG:HH11	18:LJ:95:LEU:HD13	1.77	0.48
37:NH:282:ASP:OD1	37:NH:283:TYR:N	2.47	0.48
43:NS:401:MET:HE2	43:NS:431:ALA:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:NS:417:GLY:N	72:NS:1301:ADP:O1B	2.46	0.48
58:SP:910:SER:OG	58:SP:911:GLN:OE1	2.32	0.48
64:SV:91:GLN:O	64:SV:95:HIS:ND1	2.40	0.48
25:LQ:528:LEU:HD22	25:LQ:563:MET:CE	2.44	0.48
37:NH:189:PHE:CG	37:NH:203:ILE:HD12	2.49	0.48
24:LP:4:THR:HG21	24:LP:41:HIS:CE1	2.49	0.48
28:LT:62:ASP:O	28:LT:66:LEU:N	2.46	0.48
28:LT:717:ASP:HB3	28:LT:720:LEU:HD23	1.95	0.48
40:NM:108:ASP:OD1	40:NM:109:LYS:N	2.46	0.48
43:NS:850:ILE:HG22	43:NS:854:MET:HE2	1.95	0.48
58:SP:1277:GLU:OE2	58:SP:1279:ASN:ND2	2.42	0.48
2:L1:60:U:OP2	58:SP:12:LYS:NZ	2.40	0.47
6:L5:143:ARG:HD2	15:LG:55:VAL:HG11	1.96	0.47
21:LM:315:LEU:HD12	21:LM:319:ILE:HG21	1.96	0.47
21:LM:972:ILE:HG12	21:LM:1028:LEU:HD22	1.96	0.47
31:LZ:13:LEU:HD13	31:LZ:16:VAL:HG21	1.95	0.47
32:NA:14:ARG:NH2	33:NB:206:ASP:OD2	2.45	0.47
41:NP:67:MET:HA	41:NP:67:MET:HE2	1.95	0.47
43:NS:847:VAL:HA	43:NS:850:ILE:HD12	1.96	0.47
24:LP:64:ASN:HB2	24:LP:88:ILE:HG21	1.95	0.47
28:LT:627:ASN:ND2	28:LT:647:THR:OG1	2.47	0.47
54:SI:819:GLU:OE1	54:SI:819:GLU:N	2.47	0.47
59:SQ:120:ASP:O	59:SQ:124:ILE:HD12	2.14	0.47
2:L1:878:G:O2'	35:NF:108:ASP:OD1	2.31	0.47
2:L1:1107:G:OP2	54:SI:18:LYS:NZ	2.43	0.47
17:LI:650:LEU:CD1	19:LK:506:LEU:HD13	2.45	0.47
49:SB:14:LEU:HD12	49:SB:75:LEU:HG	1.97	0.47
52:SG:522:THR:HG1	52:SG:542:SER:HG	1.61	0.47
55:SJ:51:GLU:OE1	55:SJ:82:ARG:NH1	2.41	0.47
58:SP:537:LEU:HD23	58:SP:561:LEU:HD13	1.95	0.47
37:NH:469:ASP:O	37:NH:473:LYS:N	2.46	0.47
38:NI:4:GLU:OE1	38:NI:4:GLU:N	2.47	0.47
50:SC:230:TYR:CD1	50:SC:234:ILE:HD12	2.49	0.47
58:SP:1151:ILE:HG23	58:SP:1201:LEU:HD22	1.97	0.47
58:SP:2140:ILE:CG2	61:SS:256:VAL:HG13	2.45	0.47
62:ST:287:ASP:OD1	62:ST:288:ARG:N	2.46	0.47
62:ST:528:PHE:HB3	62:ST:532:ILE:HD12	1.97	0.47
8:L7:114:ARG:O	8:L7:118:LEU:HD23	2.13	0.47
21:LM:86:GLN:OE1	27:LS:34:GLN:NE2	2.44	0.47
21:LM:1296:MET:HG2	21:LM:1335:LEU:HD21	1.96	0.47
26:LR:666:GLU:OE2	26:LR:690:HIS:NE2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:NP:12:GLN:O	41:NP:16:ASN:ND2	2.47	0.47
54:SI:929:VAL:HG21	54:SI:1006:TRP:HB3	1.97	0.47
2:L1:498:G:OP1	56:SL:42:ARG:NH2	2.47	0.47
4:L3:60:GLU:OE1	18:LJ:60:SER:OG	2.24	0.47
7:L6:24:ILE:HG22	7:L6:28:PHE:HE2	1.76	0.47
17:LI:323:PHE:CE1	17:LI:331:VAL:HG21	2.49	0.47
20:LL:231:ASP:O	20:LL:249:GLU:N	2.46	0.47
31:LZ:88:LEU:HD11	31:LZ:97:LEU:CD2	2.45	0.47
49:SB:7:GLU:OE1	50:SD:231:ARG:NH2	2.47	0.47
52:SG:256:ARG:NH1	52:SG:282:GLU:OE1	2.47	0.47
8:L7:49:ILE:HD11	8:L7:172:VAL:HG22	1.96	0.47
13:LE:55:ASP:OD1	13:LE:55:ASP:N	2.48	0.47
20:LL:222:THR:O	20:LL:222:THR:HG23	2.14	0.47
21:LM:1441:ILE:CG2	21:LM:1480:THR:HG22	2.45	0.47
23:LO:14:VAL:O	23:LO:31:SER:OG	2.33	0.47
25:LQ:11:ALA:HB2	25:LQ:685:GLU:HB2	1.96	0.47
25:LQ:426:ARG:NE	25:LQ:459:LEU:O	2.47	0.47
37:NH:429:LEU:HD13	37:NH:488:LEU:HD21	1.96	0.47
37:NH:655:LEU:O	40:NM:244:VAL:HG12	2.15	0.47
39:NL:27:VAL:HG23	39:NL:28:PHE:CD2	2.50	0.47
47:OU:100:LEU:HD12	47:OU:103:LEU:HD13	1.97	0.47
51:SF:23:VAL:HG22	51:SF:113:GLN:HG2	1.97	0.47
61:SS:313:PHE:O	61:SS:886:LYS:NZ	2.48	0.47
62:ST:289:THR:HG23	68:SZ:429:LYS:NZ	2.30	0.47
63:SU:10:ASP:O	63:SU:14:ARG:NE	2.48	0.47
2:L1:1189:A:C8	55:SK:84:ILE:HD11	2.50	0.47
7:L6:128:THR:CG2	58:SP:640:ILE:HD13	2.45	0.47
23:LO:852:THR:OG1	26:LR:765:MET:HE1	2.15	0.47
25:LQ:817:LEU:HD21	25:LQ:856:ASN:OD1	2.14	0.47
28:LT:550:VAL:HG12	28:LT:591:PHE:HE2	1.80	0.47
19:LK:446:TRP:HZ2	19:LK:492:ILE:HD12	1.78	0.47
26:LR:432:GLY:O	26:LR:464:LYS:NZ	2.40	0.47
27:LS:224:ASN:OD1	27:LS:225:SER:N	2.48	0.47
28:LT:274:ILE:HG13	28:LT:286:VAL:HG23	1.96	0.47
50:SD:175:ALA:HB1	50:SD:181:VAL:HG21	1.96	0.47
50:SD:234:ILE:HG22	50:SD:235:GLY:O	2.15	0.47
20:LL:197:ILE:HD13	20:LL:244:ILE:HD11	1.97	0.47
39:NL:275:ASP:OD1	39:NL:276:VAL:N	2.48	0.47
50:SD:87:VAL:O	50:SD:100:ARG:N	2.44	0.47
52:SG:60:ALA:HB2	58:SP:46:HIS:HE1	1.78	0.47
58:SP:905:LEU:HD12	58:SP:956:PHE:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:ST:59:GLU:N	62:ST:59:GLU:OE1	2.48	0.47
2:L1:194:U:O2'	2:L1:195:G:O5'	2.23	0.46
2:L1:326:G:OP1	12:LD:57:LYS:NZ	2.46	0.46
2:L1:1605:G:OP1	57:SM:119:ARG:NH1	2.42	0.46
5:L4:230:GLU:OE1	5:L4:233:LYS:NZ	2.36	0.46
28:LT:879:GLU:HG3	28:LT:880:LEU:HD12	1.96	0.46
43:NS:458:MET:HE3	43:NS:458:MET:HA	1.96	0.46
50:SC:175:ALA:HB1	50:SC:181:VAL:HG21	1.97	0.46
55:SJ:252:LEU:HD21	55:SK:186:VAL:HG11	1.95	0.46
2:L1:246:G:N2	12:LD:38:ALA:O	2.45	0.46
28:LT:463:VAL:HG13	28:LT:477:ILE:HG23	1.97	0.46
58:SP:994:ILE:HD11	58:SP:1036:VAL:HG21	1.97	0.46
58:SP:2068:LEU:HG	58:SP:2109:VAL:HG21	1.95	0.46
64:SV:106:THR:HG22	64:SV:106:THR:O	2.15	0.46
2:L1:227:U:O4	58:SP:1529:ARG:NE	2.37	0.46
7:L6:128:THR:HG21	58:SP:640:ILE:HD13	1.98	0.46
20:LL:163:LEU:CD1	20:LL:175:ILE:HD11	2.46	0.46
22:LN:40:ASP:OD1	22:LN:40:ASP:N	2.48	0.46
25:LQ:400:SER:OG	25:LQ:402:ASP:OD1	2.18	0.46
32:NA:84:LEU:HD11	33:NB:245:PHE:HA	1.97	0.46
37:NH:1221:HIS:CD2	38:NI:20:LEU:HD13	2.51	0.46
43:NS:1236:VAL:CG2	43:NS:1247:VAL:HG13	2.45	0.46
48:SA:217:ALA:O	48:SA:221:LEU:HD23	2.16	0.46
2:L1:1169:G:N1	2:L1:1575:G:OP2	2.46	0.46
11:LC:29:ILE:HD13	11:LC:52:LEU:HD21	1.96	0.46
18:LJ:431:LEU:O	18:LJ:470:TYR:OH	2.31	0.46
21:LM:1582:LEU:HD11	21:LM:1586:LEU:HD12	1.97	0.46
25:LQ:107:ASP:O	25:LQ:111:LYS:N	2.46	0.46
30:LW:218:ASP:O	30:LW:222:GLY:N	2.45	0.46
46:OH:97:LEU:HD23	46:OH:118:ALA:O	2.15	0.46
59:SQ:167:LYS:O	59:SQ:170:LYS:NZ	2.48	0.46
16:LH:743:ILE:HD11	16:LH:763:ILE:HD12	1.97	0.46
28:LT:550:VAL:HG12	28:LT:591:PHE:CE2	2.51	0.46
58:SP:1945:ILE:O	58:SP:1985:ARG:NH1	2.47	0.46
8:L7:122:HIS:CD2	8:L7:177:THR:HG22	2.50	0.46
11:LC:98:ASP:OD1	28:LT:495:ARG:NH2	2.41	0.46
17:LI:498:SER:HB3	17:LI:531:LEU:HD12	1.96	0.46
21:LM:1416:MET:HE2	21:LM:1452:GLU:HG3	1.98	0.46
21:LM:1590:ILE:O	21:LM:1590:ILE:HG22	2.14	0.46
23:LO:359:ARG:NH2	23:LO:419:TYR:OH	2.49	0.46
38:NI:130:ASP:O	38:NI:133:SER:OG	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SP:252:LYS:CG	58:SP:297:VAL:HG21	2.46	0.46
62:ST:391:VAL:O	62:ST:391:VAL:HG12	2.16	0.46
7:L6:121:LEU:HD13	7:L6:124:LEU:HD12	1.98	0.46
10:L9:87:SER:OG	10:L9:89:ASP:OD1	2.25	0.46
16:LH:248:GLN:O	16:LH:252:LEU:HD23	2.16	0.46
16:LH:357:ILE:HD12	16:LH:371:PHE:CE1	2.50	0.46
16:LH:401:GLN:NE2	16:LH:409:LYS:O	2.49	0.46
20:LL:169:SER:OG	20:LL:170:ILE:N	2.48	0.46
21:LM:1480:THR:O	21:LM:1484:THR:HG23	2.15	0.46
28:LT:389:MET:HE3	28:LT:448:LYS:HA	1.98	0.46
28:LT:530:ASP:O	28:LT:534:SER:N	2.47	0.46
30:LW:258:LEU:O	30:LW:267:LEU:N	2.45	0.46
31:LZ:88:LEU:HD11	31:LZ:97:LEU:HD21	1.96	0.46
32:NA:335:ARG:CZ	32:NA:340:LEU:HD13	2.46	0.46
58:SP:2256:GLN:O	58:SP:2260:ASN:ND2	2.48	0.46
62:ST:679:GLU:OE1	62:ST:679:GLU:N	2.47	0.46
68:SZ:242:TRP:O	68:SZ:246:ILE:HG22	2.15	0.46
68:SZ:290:ASN:HD22	68:SZ:290:ASN:C	2.21	0.46
2:L1:1254:U:OP1	46:OH:50:LYS:NZ	2.28	0.46
16:LH:864:ASP:N	16:LH:864:ASP:OD1	2.48	0.46
21:LM:1695:MET:HE1	21:LM:1729:LEU:CD1	2.46	0.46
23:LO:852:THR:HG21	26:LR:769:ILE:HG13	1.96	0.46
37:NH:225:LEU:HD12	37:NH:264:LEU:O	2.16	0.46
43:NS:1135:ILE:HD13	43:NS:1167:MET:HE3	1.97	0.46
50:SD:178:GLY:HA3	50:SD:210:MET:HE2	1.98	0.46
54:SI:98:LEU:HD21	54:SI:354:ILE:HD13	1.98	0.46
62:ST:431:ARG:NH1	62:ST:473:GLU:OE2	2.45	0.46
2:L1:68:A:OP1	7:L6:160:ARG:NH2	2.41	0.46
3:L2:285:U:O2'	3:L2:286:U:OP1	2.33	0.46
20:LL:210:ARG:NH1	20:LL:228:ALA:O	2.48	0.46
21:LM:559:ASN:N	21:LM:597:HIS:O	2.49	0.46
28:LT:179:LYS:HB3	28:LT:190:LEU:HD11	1.98	0.46
37:NH:1153:LEU:HD21	37:NH:1226:PHE:CE2	2.51	0.46
43:NS:774:ARG:NH1	43:NS:775:TYR:OH	2.49	0.46
50:SC:167:GLY:HA2	50:SC:191:GLU:HG2	1.98	0.46
51:SF:7:LYS:NZ	51:SF:62:GLU:OE2	2.48	0.46
55:SK:47:MET:HE2	55:SK:47:MET:H	1.80	0.46
62:ST:283:ALA:HB1	68:SZ:431:ASP:OD2	2.15	0.46
68:SZ:246:ILE:HD11	68:SZ:254:TRP:CZ2	2.50	0.46
2:L1:974:A2M:HM'3	2:L1:974:A2M:H1'	1.74	0.46
7:L6:23:ARG:O	7:L6:26:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LI:311:VAL:HG13	17:LI:314:LEU:HD12	1.98	0.46
20:LL:296:ILE:HG23	20:LL:296:ILE:O	2.16	0.46
21:LM:264:PHE:HE2	21:LM:270:LEU:HD21	1.80	0.46
21:LM:1346:GLU:OE2	64:SV:9:SER:OG	2.34	0.46
21:LM:1723:LEU:HD13	21:LM:1759:VAL:HG12	1.98	0.46
22:LN:436:ASP:OD1	22:LN:437:GLY:N	2.49	0.46
23:LO:670:LEU:HD22	31:LZ:110:ARG:HH21	1.80	0.46
37:NH:206:LEU:C	37:NH:207:LEU:HD23	2.41	0.46
58:SP:1993:PRO:HB2	58:SP:2035:ILE:HG21	1.97	0.46
8:L7:8:ILE:HG21	8:L7:13:PRO:HB3	1.97	0.45
16:LH:883:GLN:OE1	16:LH:884:MET:N	2.48	0.45
20:LL:344:ASP:OD1	20:LL:348:LYS:N	2.50	0.45
20:LL:576:ASP:N	20:LL:576:ASP:OD2	2.48	0.45
23:LO:400:GLN:HG3	23:LO:401:VAL:HG23	1.98	0.45
26:LR:36:VAL:O	26:LR:36:VAL:HG13	2.16	0.45
35:NF:132:VAL:HG12	35:NF:132:VAL:O	2.16	0.45
37:NH:1134:GLU:OE2	37:NH:1134:GLU:N	2.47	0.45
43:NS:720:THR:HG22	43:NS:721:GLU:N	2.31	0.45
16:LH:435:ASP:O	16:LH:437:THR:HG23	2.17	0.45
16:LH:724:ILE:HG21	16:LH:762:TYR:CD2	2.52	0.45
16:LH:778:ASP:OD2	16:LH:779:ILE:N	2.49	0.45
16:LH:817:SER:O	16:LH:821:ILE:HD12	2.17	0.45
25:LQ:217:LEU:HB3	25:LQ:229:TRP:HB2	1.98	0.45
27:LS:544:VAL:HG22	27:LS:551:VAL:HG22	1.98	0.45
28:LT:640:LEU:HD22	28:LT:653:ILE:CG2	2.46	0.45
49:SB:5:LEU:HD21	49:SB:72:LEU:HD11	1.99	0.45
58:SP:356:ASP:OD1	58:SP:357:LYS:N	2.49	0.45
4:L3:115:ARG:NH1	32:NA:344:GLU:OE2	2.48	0.45
8:L7:9:LEU:HD21	8:L7:42:GLN:HG3	1.98	0.45
16:LH:321:MET:HE3	16:LH:323:LEU:CD1	2.46	0.45
25:LQ:528:LEU:HD22	25:LQ:563:MET:HE3	1.97	0.45
26:LR:12:LEU:HD21	26:LR:378:PRO:HG3	1.98	0.45
43:NS:794:GLN:NE2	43:NS:906:PRO:O	2.50	0.45
58:SP:994:ILE:HD12	58:SP:1047:LEU:CD1	2.46	0.45
59:SQ:154:GLU:OE1	59:SQ:154:GLU:N	2.43	0.45
17:LI:517:ASN:O	17:LI:547:GLN:NE2	2.49	0.45
21:LM:1183:PHE:CG	21:LM:1241:LEU:HD21	2.51	0.45
24:LP:371:ILE:HA	24:LP:374:MET:HE3	1.97	0.45
27:LS:45:ILE:H	27:LS:45:ILE:HD12	1.81	0.45
28:LT:465:SER:OG	28:LT:505:VAL:O	2.28	0.45
48:SA:182:ASP:OD1	48:SA:183:GLN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SJ:141:MET:N	55:SJ:141:MET:HE2	2.31	0.45
58:SP:1761:ILE:HG22	58:SP:1762:SER:O	2.17	0.45
3:L2:2:U:O4'	39:NL:51:LYS:NZ	2.41	0.45
3:L2:31:G:N7	29:LU:345:THR:HG21	2.32	0.45
9:L8:17:LYS:HD3	43:NS:26:ILE:HG21	1.98	0.45
16:LH:71:ASN:ND2	16:LH:125:LEU:HD21	2.31	0.45
17:LI:467:LEU:O	17:LI:513:LYS:NZ	2.50	0.45
28:LT:362:GLN:O	28:LT:363:SER:OG	2.22	0.45
46:OH:123:VAL:HG11	46:OH:126:TRP:CZ3	2.51	0.45
50:SC:178:GLY:HA2	50:SC:210:MET:HE2	1.99	0.45
58:SP:1733:LYS:NZ	58:SP:1748:ASN:OD1	2.47	0.45
58:SP:2030:ASN:OD1	58:SP:2031:HIS:N	2.50	0.45
62:ST:385:ASP:OD1	62:ST:386:ALA:N	2.49	0.45
2:L1:1011:G:O2'	43:NS:134:GLY:O	2.26	0.45
16:LH:96:ILE:HD12	16:LH:151:TYR:CE1	2.51	0.45
20:LL:225:VAL:HG23	20:LL:225:VAL:O	2.15	0.45
21:LM:1407:LEU:HD13	21:LM:1415:LEU:HD13	1.98	0.45
28:LT:54:VAL:HG23	28:LT:54:VAL:O	2.16	0.45
33:NB:403:ASP:OD1	33:NB:404:VAL:HG23	2.17	0.45
37:NH:524:ASP:OD1	37:NH:952:GLY:N	2.48	0.45
43:NS:694:TYR:OH	43:NS:833:ASP:OD2	2.29	0.45
54:SI:866:ARG:NH2	60:SR:62:LYS:O	2.50	0.45
3:L2:39:C:O2'	29:LU:18:SER:O	2.34	0.45
18:LJ:273:ILE:HD13	18:LJ:283:VAL:HG22	1.98	0.45
19:LK:403:LEU:HG	19:LK:407:MET:HE2	1.99	0.45
29:LU:344:HIS:NE2	29:LU:418:HIS:O	2.47	0.45
32:NA:15:ILE:HD11	33:NB:220:PHE:HE1	1.81	0.45
37:NH:602:ASN:OD1	37:NH:603:THR:N	2.49	0.45
48:SA:277:ARG:O	48:SA:281:LEU:HD13	2.16	0.45
50:SC:122:ARG:O	59:SQ:153:ILE:N	2.44	0.45
50:SD:92:ARG:NE	67:SY:165:ARG:O	2.50	0.45
58:SP:1870:LYS:NZ	58:SP:1874:ASP:OD2	2.50	0.45
58:SP:2262:ASP:OD1	58:SP:2263:LYS:N	2.50	0.45
6:L5:123:VAL:HG13	18:LJ:95:LEU:HD11	1.98	0.45
16:LH:71:ASN:O	16:LH:75:SER:OG	2.35	0.45
16:LH:292:LEU:C	16:LH:293:LEU:HD12	2.41	0.45
23:LO:497:ILE:HD11	23:LO:521:LEU:HD11	1.98	0.45
25:LQ:589:ILE:CG2	25:LQ:621:VAL:HG11	2.47	0.45
35:NF:140:LYS:NZ	35:NF:142:GLU:O	2.49	0.45
58:SP:2255:HIS:HA	58:SP:2300:THR:HG22	1.98	0.45
62:ST:433:ILE:O	62:ST:452:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:331:A:OP1	9:L8:56:ARG:NH1	2.50	0.45
9:L8:34:ALA:HB2	9:L8:56:ARG:HD2	1.99	0.45
20:LL:197:ILE:HD11	20:LL:203:ILE:HB	1.99	0.45
21:LM:220:VAL:O	21:LM:224:ASN:ND2	2.50	0.45
29:LU:4:LYS:NZ	30:LW:70:SER:O	2.50	0.45
37:NH:188:SER:N	70:NH:1300:ATP:O2B	2.50	0.45
50:SC:109:LYS:NZ	59:SQ:103:TRP:O	2.35	0.45
50:SC:155:ILE:HD11	50:SC:162:LEU:HD21	1.99	0.45
58:SP:1095:SER:HA	58:SP:1136:THR:HG22	1.98	0.45
58:SP:2058:GLU:OE1	61:SS:261:ASN:ND2	2.50	0.45
2:L1:128:U:O4	58:SP:943:ARG:NH1	2.50	0.45
5:L4:163:ASP:O	5:L4:167:GLY:N	2.43	0.45
11:LC:69:VAL:HG21	11:LC:81:ILE:HG12	1.98	0.45
28:LT:103:ARG:NH2	61:SS:738:SEP:O1P	2.50	0.45
28:LT:724:SER:HB3	28:LT:880:LEU:HD13	1.97	0.45
54:SI:260:THR:HG23	54:SI:261:GLN:HG3	1.98	0.45
58:SP:2201:HIS:HD2	58:SP:2205:LEU:HD23	1.81	0.45
2:L1:71:A:OP2	7:L6:164:LYS:NZ	2.37	0.44
2:L1:1539:G:H4'	4:L3:40:ARG:NH2	2.32	0.44
5:L4:87:MET:HE1	5:L4:236:ILE:HG21	1.99	0.44
21:LM:928:ALA:HB3	21:LM:941:LEU:HD22	1.99	0.44
23:LO:678:GLU:N	23:LO:678:GLU:OE1	2.50	0.44
30:LW:176:ILE:HD13	31:LZ:19:LEU:CD1	2.47	0.44
32:NA:400:LEU:HD11	65:SW:219:ALA:HB2	1.99	0.44
37:NH:254:LEU:HD22	37:NH:270:ILE:HG13	1.99	0.44
38:NI:147:LEU:HD23	38:NI:154:GLU:HG3	1.98	0.44
55:SJ:197:ASP:OD2	55:SJ:198:ASP:N	2.46	0.44
58:SP:1221:ILE:HG23	58:SP:1264:LEU:HD12	1.97	0.44
62:ST:456:ILE:HD13	63:SU:529:VAL:HG21	1.98	0.44
2:L1:559:C:H5''	54:SI:867:THR:HG21	1.99	0.44
27:LS:130:ASP:OD1	28:LT:179:LYS:NZ	2.50	0.44
37:NH:976:ILE:HG22	37:NH:1042:ALA:HB3	1.99	0.44
55:SJ:204:VAL:HG21	55:SJ:241:PHE:CE2	2.53	0.44
58:SP:1912:ILE:HG23	58:SP:1958:MET:HG3	2.00	0.44
64:SV:142:ILE:HG21	67:SY:198:PHE:HB3	2.00	0.44
68:SZ:254:TRP:O	68:SZ:286:ARG:NH2	2.45	0.44
6:L5:111:VAL:HG12	11:LC:43:ILE:HD11	1.99	0.44
7:L6:73:ILE:HD12	43:NS:62:ILE:HD11	2.00	0.44
11:LC:101:SER:O	11:LC:105:LEU:HD13	2.17	0.44
20:LL:163:LEU:HD12	20:LL:175:ILE:HD11	1.98	0.44
21:LM:631:VAL:HG21	22:LN:611:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:NB:206:ASP:OD1	33:NB:209:ARG:NH2	2.51	0.44
34:ND:178:VAL:HG11	67:SY:146:PHE:CD2	2.53	0.44
4:L3:45:LEU:HD13	41:NP:36:ILE:HD12	1.98	0.44
25:LQ:267:ASP:O	25:LQ:288:LYS:NZ	2.49	0.44
32:NA:15:ILE:HD11	33:NB:220:PHE:CE1	2.52	0.44
35:NF:25:TRP:O	42:NQ:82:LYS:NZ	2.51	0.44
58:SP:136:LEU:HD13	58:SP:152:PHE:CZ	2.53	0.44
58:SP:1395:LYS:HA	58:SP:1399:LEU:HD12	1.98	0.44
18:LJ:104:LEU:HD12	18:LJ:120:ILE:O	2.17	0.44
26:LR:603:ASP:O	26:LR:607:GLY:N	2.38	0.44
30:LW:123:THR:HG23	30:LW:140:ARG:NH2	2.32	0.44
43:NS:548:ILE:HD12	43:NS:548:ILE:H	1.82	0.44
11:LC:113:ASP:OD1	11:LC:115:THR:OG1	2.32	0.44
21:LM:149:LYS:NZ	21:LM:167:PHE:O	2.38	0.44
23:LO:20:ILE:HD12	23:LO:318:ALA:HB1	2.00	0.44
28:LT:509:SER:OG	28:LT:549:MET:SD	2.59	0.44
28:LT:758:PHE:O	65:SW:176:ARG:NE	2.50	0.44
37:NH:475:ASN:O	37:NH:478:THR:HG23	2.18	0.44
39:NL:115:MET:HE2	39:NL:136:PRO:HB2	1.99	0.44
50:SD:304:LEU:HD13	67:SY:133:HIS:HD2	1.82	0.44
52:SG:522:THR:OG1	52:SG:542:SER:OG	2.33	0.44
2:L1:1773:4AC:CM7	2:L1:1773:4AC:H5	2.48	0.44
21:LM:1304:VAL:O	21:LM:1308:VAL:HG23	2.17	0.44
21:LM:1520:THR:HG22	64:SV:46:ALA:N	2.32	0.44
22:LN:42:THR:HG23	22:LN:42:THR:O	2.18	0.44
39:NL:60:VAL:HG11	39:NL:74:ILE:HG21	2.00	0.44
43:NS:135:GLU:OE1	43:NS:135:GLU:N	2.47	0.44
50:SC:178:GLY:CA	50:SC:210:MET:HE2	2.48	0.44
55:SJ:198:ASP:OD1	55:SJ:199:ASP:N	2.50	0.44
58:SP:1689:VAL:O	58:SP:1693:THR:HG23	2.18	0.44
9:L8:11:ARG:NH1	9:L8:15:GLY:O	2.49	0.44
16:LH:461:ASP:O	16:LH:465:ASN:N	2.51	0.44
17:LI:508:ASP:OD1	17:LI:536:ARG:NH1	2.50	0.44
21:LM:485:THR:HG22	21:LM:485:THR:O	2.18	0.44
21:LM:614:LEU:HD11	21:LM:653:PHE:CG	2.52	0.44
25:LQ:140:SER:OG	25:LQ:141:LYS:N	2.51	0.44
28:LT:367:LEU:HD21	28:LT:445:MET:HE1	1.99	0.44
33:NB:215:THR:HG23	33:NB:216:MET:N	2.33	0.44
43:NS:123:ASP:OD1	43:NS:124:THR:N	2.48	0.44
54:SI:142:ILE:HG21	54:SI:190:LEU:HD11	2.00	0.44
55:SJ:68:LEU:HD22	55:SJ:77:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LL:587:ALA:HB2	34:ND:166:LEU:HD21	2.00	0.44
22:LN:528:ILE:HD12	22:LN:688:MET:SD	2.58	0.44
23:LO:852:THR:HG22	23:LO:853:ASP:N	2.33	0.44
33:NB:376:VAL:O	63:SU:53:ARG:NH1	2.51	0.44
37:NH:185:LEU:HD23	37:NH:190:ALA:HB2	2.00	0.44
37:NH:476:ILE:HD12	37:NH:476:ILE:H	1.83	0.44
39:NL:115:MET:HE2	39:NL:136:PRO:CB	2.47	0.44
52:SG:481:ILE:HD12	52:SG:481:ILE:H	1.83	0.44
55:SK:68:LEU:HB3	55:SK:77:LEU:HD21	1.98	0.44
55:SK:217:ALA:O	55:SK:221:VAL:HG22	2.18	0.44
16:LH:89:VAL:HG22	16:LH:110:PHE:O	2.17	0.43
16:LH:545:THR:CG2	16:LH:593:ASN:HB2	2.48	0.43
18:LJ:366:TYR:OH	18:LJ:371:GLU:OE2	2.17	0.43
21:LM:1441:ILE:HG23	21:LM:1480:THR:HG22	1.99	0.43
23:LO:564:PHE:N	23:LO:567:ASP:OD2	2.47	0.43
25:LQ:387:LEU:O	25:LQ:415:LYS:NZ	2.45	0.43
58:SP:1147:ILE:O	58:SP:1151:ILE:HD12	2.17	0.43
6:L5:118:LEU:HD22	6:L5:129:PRO:HB2	2.01	0.43
16:LH:821:ILE:HD12	16:LH:821:ILE:H	1.83	0.43
16:LH:879:ILE:HD12	21:LM:215:CYS:SG	2.58	0.43
17:LI:432:ASP:OD1	17:LI:433:ASP:N	2.51	0.43
21:LM:247:ALA:HA	27:LS:205:ILE:HD11	1.99	0.43
21:LM:960:VAL:HG11	21:LM:994:LEU:HD21	2.00	0.43
25:LQ:676:SER:OG	25:LQ:677:HIS:N	2.51	0.43
54:SI:933:LYS:HD2	54:SI:1002:ILE:HG21	2.00	0.43
58:SP:252:LYS:HG3	58:SP:297:VAL:HG21	1.99	0.43
2:L1:1163:A:O3'	6:L5:166:ARG:NH2	2.49	0.43
2:L1:1681:A:H2'	2:L1:1682:U:O4'	2.18	0.43
21:LM:1608:PHE:HZ	21:LM:1618:LEU:HD22	1.84	0.43
23:LO:139:HIS:CD2	23:LO:140:ARG:HG2	2.54	0.43
25:LQ:900:PHE:HZ	26:LR:765:MET:HE3	1.83	0.43
26:LR:235:LYS:NZ	26:LR:273:GLU:O	2.52	0.43
26:LR:616:HIS:CD2	26:LR:620:LEU:HD21	2.54	0.43
43:NS:1175:SER:OG	43:NS:1231:LEU:HD12	2.18	0.43
50:SC:198:GLU:O	50:SC:222:GLU:N	2.51	0.43
53:SH:337:VAL:N	54:SI:554:TYR:OH	2.49	0.43
2:L1:405:C:O2'	7:L6:92:ARG:O	2.28	0.43
2:L1:1679:G:N2	2:L1:1723:U:O4	2.52	0.43
3:L2:38:U:O2	24:LP:46:ARG:NH2	2.52	0.43
21:LM:264:PHE:CE2	21:LM:270:LEU:HD21	2.53	0.43
21:LM:651:LEU:HD21	21:LM:684:TYR:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LT:488:ASN:O	28:LT:492:GLY:N	2.47	0.43
38:NI:41:ARG:HH12	38:NI:138:TRP:CD1	2.37	0.43
43:NS:561:THR:HG22	43:NS:562:LEU:N	2.34	0.43
55:SJ:217:ALA:O	55:SJ:221:VAL:HG12	2.18	0.43
58:SP:374:LEU:HD23	58:SP:411:PHE:CE2	2.53	0.43
58:SP:374:LEU:HD23	58:SP:411:PHE:CZ	2.53	0.43
58:SP:448:VAL:O	58:SP:451:VAL:HG12	2.18	0.43
58:SP:1384:LEU:O	58:SP:1388:SER:N	2.50	0.43
64:SV:152:SER:OG	64:SV:153:THR:N	2.51	0.43
2:L1:1030:A:H62	54:SI:6:LYS:NZ	2.16	0.43
16:LH:717:THR:HG23	16:LH:718:GLY:N	2.34	0.43
18:LJ:42:VAL:HG23	18:LJ:42:VAL:O	2.18	0.43
28:LT:228:GLY:O	28:LT:246:ILE:N	2.49	0.43
43:NS:657:THR:HG22	43:NS:745:ARG:HH22	1.82	0.43
51:SF:23:VAL:CG2	51:SF:117:VAL:HG21	2.48	0.43
51:SF:57:ASP:O	51:SF:84:ARG:NH1	2.52	0.43
58:SP:17:SER:O	58:SP:22:ARG:NH1	2.51	0.43
2:L1:324:U:OP1	12:LD:133:LYS:NZ	2.38	0.43
16:LH:278:GLY:HA2	16:LH:300:VAL:HG13	2.01	0.43
16:LH:296:HIS:CG	16:LH:300:VAL:HG12	2.53	0.43
18:LJ:233:ASN:ND2	18:LJ:247:GLU:OE2	2.52	0.43
25:LQ:592:SER:OG	25:LQ:593:ALA:N	2.50	0.43
25:LQ:806:MET:HE2	25:LQ:849:HIS:CB	2.48	0.43
41:NP:124:ILE:O	41:NP:124:ILE:HG23	2.19	0.43
53:SH:340:LYS:HE3	53:SH:353:THR:HG21	1.99	0.43
55:SJ:53:HIS:CD2	55:SJ:80:MET:HE2	2.54	0.43
58:SP:370:ASP:OD1	58:SP:370:ASP:N	2.52	0.43
62:ST:253:THR:HG21	68:SZ:207:PRO:HG3	2.00	0.43
62:ST:282:ARG:HH21	68:SZ:350:LEU:HD21	1.83	0.43
62:ST:640:MET:HE1	62:ST:678:PHE:CE2	2.53	0.43
15:LG:37:SER:O	15:LG:39:THR:HG23	2.19	0.43
16:LH:435:ASP:OD1	16:LH:436:PHE:N	2.46	0.43
28:LT:76:THR:OG1	28:LT:78:SER:O	2.26	0.43
38:NI:63:ASN:H	38:NI:66:HIS:HD1	1.67	0.43
57:SM:196:THR:HG22	57:SM:197:ALA:N	2.34	0.43
58:SP:1332:ILE:HD13	58:SP:2423:VAL:HG11	2.00	0.43
6:L5:135:ASP:OD2	6:L5:139:ASN:ND2	2.51	0.43
21:LM:286:LEU:HD22	21:LM:292:LYS:HA	2.01	0.43
28:LT:795:LYS:O	28:LT:798:ALA:HB3	2.19	0.43
37:NH:356:THR:HG23	37:NH:359:PHE:HB2	2.00	0.43
55:SJ:189:VAL:HG13	55:SJ:244:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SJ:192:TYR:OH	55:SJ:223:GLU:OE2	2.35	0.43
58:SP:1556:ARG:NH1	58:SP:1664:ILE:HG23	2.33	0.43
18:LJ:432:TYR:CD2	22:LN:775:VAL:HG21	2.54	0.43
20:LL:77:ILE:HD12	20:LL:110:ILE:HD12	1.99	0.43
21:LM:612:PRO:O	21:LM:613:MET:HE2	2.19	0.43
28:LT:561:ALA:HB2	28:LT:591:PHE:CE1	2.54	0.43
28:LT:824:GLY:O	28:LT:828:LYS:N	2.52	0.43
28:LT:854:SER:HB2	28:LT:895:VAL:HG21	2.01	0.43
33:NB:440:ILE:O	55:SK:136:ARG:NH2	2.50	0.43
54:SI:99:ASN:OD1	54:SI:100:ASP:N	2.52	0.43
58:SP:437:LEU:O	58:SP:764:ARG:NH1	2.49	0.43
22:LN:155:LYS:NZ	22:LN:180:ASP:OD2	2.39	0.43
27:LS:251:ILE:O	27:LS:566:THR:HG23	2.18	0.43
28:LT:368:SER:OG	28:LT:651:ILE:HD11	2.18	0.43
29:LU:37:ARG:NH1	30:LW:449:ILE:O	2.45	0.43
58:SP:2087:ILE:HD12	58:SP:2129:MET:HG3	2.01	0.43
2:L1:435:C:H3'	2:L1:436:A2M:H5'	2.00	0.42
16:LH:357:ILE:HG23	16:LH:371:PHE:CE1	2.54	0.42
16:LH:851:GLU:O	16:LH:855:LEU:HD23	2.19	0.42
21:LM:42:THR:O	21:LM:42:THR:HG22	2.18	0.42
25:LQ:559:PHE:O	25:LQ:563:MET:N	2.49	0.42
38:NI:48:ASN:OD1	38:NI:49:GLU:N	2.52	0.42
50:SD:106:LEU:HD22	50:SD:156:MET:HE3	2.01	0.42
2:L1:632:U:O2'	2:L1:1103:U:OP1	2.31	0.42
8:L7:77:LEU:HD22	8:L7:92:PHE:CZ	2.53	0.42
8:L7:159:VAL:HG21	8:L7:188:GLU:OE2	2.19	0.42
14:LF:43:LYS:HB3	44:NV:729:LEU:HD11	2.01	0.42
16:LH:662:VAL:HG23	16:LH:670:LEU:HD21	2.01	0.42
17:LI:558:CYS:O	17:LI:585:ARG:NH2	2.41	0.42
23:LO:10:LEU:HD13	23:LO:702:LEU:HD23	1.99	0.42
23:LO:592:ILE:HD12	23:LO:606:VAL:HG22	1.99	0.42
32:NA:384:ARG:NH1	57:SM:81:SER:O	2.52	0.42
66:SX:179:UNK:O	66:SX:183:UNK:N	2.51	0.42
2:L1:165:G:O3'	58:SP:636:ARG:NH2	2.52	0.42
18:LJ:435:ASP:H	18:LJ:438:THR:HG22	1.84	0.42
21:LM:72:THR:O	27:LS:33:LEU:HD11	2.19	0.42
21:LM:1561:VAL:HG13	21:LM:1561:VAL:O	2.19	0.42
23:LO:363:ALA:HB1	23:LO:390:VAL:HB	2.01	0.42
25:LQ:444:LEU:HD23	25:LQ:458:ASP:HA	2.01	0.42
37:NH:976:ILE:HD11	37:NH:1017:TYR:CZ	2.53	0.42
48:SA:178:ILE:HD13	48:SA:292:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SS:432:ASP:OD1	61:SS:435:ARG:NH2	2.53	0.42
2:L1:762:A:OP1	10:L9:79:ARG:NH2	2.45	0.42
19:LK:433:ILE:HG22	19:LK:437:ILE:HD12	2.00	0.42
21:LM:609:VAL:CG1	21:LM:660:LEU:HD11	2.43	0.42
23:LO:35:ASN:OD1	23:LO:35:ASN:O	2.38	0.42
37:NH:173:ASN:HD22	37:NH:173:ASN:C	2.21	0.42
37:NH:1100:VAL:HG22	37:NH:1234:PHE:CE2	2.54	0.42
43:NS:905:PHE:HE2	43:NS:916:LEU:HD21	1.85	0.42
50:SD:80:ALA:HB3	67:SY:124:GLN:HE21	1.83	0.42
50:SD:178:GLY:HA2	50:SD:210:MET:HE2	2.01	0.42
54:SI:33:VAL:HG21	54:SI:39:MET:HE2	2.01	0.42
55:SK:49:SER:O	55:SK:50:LEU:HD12	2.20	0.42
64:SV:131:LEU:CD2	64:SV:135:VAL:HG21	2.49	0.42
2:L1:395:U:H2'	2:L1:396:G:O4'	2.19	0.42
2:L1:1699:G:N7	37:NH:217:LYS:NZ	2.60	0.42
17:LI:711:LEU:CD2	17:LI:713:ILE:HG23	2.49	0.42
24:LP:77:VAL:HG12	24:LP:79:LYS:H	1.84	0.42
26:LR:7:TYR:OH	26:LR:629:GLY:O	2.30	0.42
26:LR:251:ASP:OD1	26:LR:252:GLY:N	2.46	0.42
26:LR:342:ASP:OD1	26:LR:343:MET:N	2.51	0.42
29:LU:272:MET:HE3	61:SS:313:PHE:CE2	2.50	0.42
29:LU:288:TYR:O	29:LU:298:LEU:N	2.45	0.42
39:NL:275:ASP:OD1	39:NL:276:VAL:HG23	2.19	0.42
46:OH:63:VAL:HG21	46:OH:94:ALA:HA	2.01	0.42
58:SP:1980:SER:OG	58:SP:2013:LEU:HD12	2.20	0.42
64:SV:130:ASP:O	64:SV:131:LEU:HB3	2.20	0.42
2:L1:562:OMG:HM23	57:SM:281:ILE:CD1	2.49	0.42
4:L3:45:LEU:HD13	41:NP:36:ILE:CD1	2.49	0.42
4:L3:45:LEU:HD11	4:L3:49:LYS:HE3	2.01	0.42
16:LH:849:ASP:OD1	16:LH:852:ASP:N	2.47	0.42
22:LN:536:VAL:HG23	22:LN:555:LEU:HD11	2.01	0.42
26:LR:791:ARG:NH2	32:NA:493:GLN:OE1	2.51	0.42
35:NF:135:LEU:HD21	35:NF:139:TRP:CD2	2.54	0.42
36:NG:18:ARG:HE	36:NG:31:THR:HG21	1.84	0.42
49:SB:110:ASP:OD1	49:SB:111:ALA:N	2.53	0.42
55:SJ:141:MET:HE2	55:SJ:141:MET:HA	2.02	0.42
58:SP:871:ASP:OD1	58:SP:889:LYS:NZ	2.53	0.42
63:SU:450:GLU:OE2	63:SU:451:SER:N	2.52	0.42
2:L1:77:U:OP1	58:SP:3:LYS:NZ	2.49	0.42
17:LI:497:ILE:HG22	17:LI:497:ILE:O	2.20	0.42
23:LO:612:LEU:HD21	28:LT:513:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LS:133:ILE:HD11	28:LT:194:ARG:CZ	2.50	0.42
30:LW:302:ASP:O	30:LW:306:PHE:N	2.52	0.42
37:NH:623:GLU:O	37:NH:626:LYS:NZ	2.44	0.42
37:NH:1165:SER:OG	37:NH:1166:ARG:N	2.52	0.42
53:SH:47:ASP:OD1	53:SH:48:TYR:N	2.53	0.42
55:SK:127:THR:HG21	62:ST:713:HIS:CD2	2.55	0.42
58:SP:1247:LEU:O	58:SP:1251:VAL:HG22	2.20	0.42
65:SW:166:PHE:CE1	65:SW:225:VAL:HG23	2.54	0.42
9:L8:40:ALA:O	9:L8:59:ARG:NE	2.48	0.42
20:LL:300:LEU:HD21	20:LL:316:ASN:HD22	1.85	0.42
22:LN:85:TRP:HB2	22:LN:372:MET:HE1	2.01	0.42
24:LP:422:MET:HE1	24:LP:433:LEU:HD12	2.00	0.42
25:LQ:884:LYS:HD2	26:LR:807:ASP:OD1	2.20	0.42
48:SA:96:ILE:HG23	48:SA:116:VAL:HG23	2.01	0.42
51:SE:94:SER:OG	67:SY:248:ARG:NH1	2.50	0.42
62:ST:273:LYS:O	62:ST:277:LEU:HD23	2.19	0.42
63:SU:61:GLN:OE1	63:SU:64:ARG:NH2	2.52	0.42
17:LI:541:LEU:HD22	17:LI:569:GLU:OE1	2.19	0.42
18:LJ:45:ILE:HD13	18:LJ:319:VAL:HG12	2.01	0.42
18:LJ:449:GLY:O	18:LJ:455:SER:OG	2.37	0.42
21:LM:659:LEU:O	21:LM:667:LYS:NZ	2.53	0.42
21:LM:1416:MET:HE3	21:LM:1449:ASP:HB3	2.02	0.42
37:NH:207:LEU:HD11	37:NH:294:LEU:HD12	2.01	0.42
37:NH:761:ARG:HD2	37:NH:899:LEU:HD23	2.02	0.42
62:ST:277:LEU:HD12	68:SZ:383:PRO:CG	2.50	0.42
2:L1:393:C:OP1	9:L8:2:GLY:N	2.52	0.42
2:L1:1474:G:OP1	6:L5:109:LYS:NZ	2.53	0.42
6:L5:140:THR:HG23	6:L5:171:ALA:HB1	2.02	0.42
16:LH:25:LEU:HD21	16:LH:171:TYR:OH	2.20	0.42
16:LH:870:ASN:HA	16:LH:873:THR:HG23	2.02	0.42
21:LM:230:LYS:O	21:LM:234:LEU:HD13	2.20	0.42
56:SL:50:ALA:HB1	56:SL:58:ALA:HB2	2.01	0.42
2:L1:487:G:OP1	54:SI:1126:LYS:NZ	2.52	0.41
21:LM:1193:PHE:O	21:LM:1197:VAL:HG23	2.20	0.41
21:LM:1281:ALA:O	21:LM:1285:VAL:HG23	2.20	0.41
21:LM:1594:PHE:O	21:LM:1598:LEU:N	2.53	0.41
31:LZ:75:GLU:O	31:LZ:79:LEU:HD23	2.20	0.41
37:NH:744:MET:HE3	37:NH:813:GLU:HB3	2.02	0.41
47:OU:100:LEU:HD12	47:OU:103:LEU:HD11	2.01	0.41
48:SA:257:ILE:O	48:SA:257:ILE:HG13	2.20	0.41
49:SB:381:ASP:OD2	49:SB:382:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SJ:209:MET:HE1	55:SJ:216:PHE:CD2	2.54	0.41
6:L5:127:GLN:NE2	6:L5:132:VAL:HG22	2.35	0.41
7:L6:78:THR:O	7:L6:81:VAL:HG22	2.21	0.41
17:LI:570:LEU:CD2	17:LI:637:LEU:HD21	2.49	0.41
32:NA:335:ARG:NH2	54:SI:957:GLU:OE1	2.44	0.41
36:NG:30:VAL:HG11	36:NG:71:CYS:SG	2.60	0.41
37:NH:1146:THR:HG21	37:NH:1180:ASN:HD22	1.84	0.41
54:SI:157:ASN:O	54:SI:161:HIS:ND1	2.53	0.41
63:SU:444:ASP:OD1	63:SU:461:SER:OG	2.37	0.41
7:L6:206:ALA:O	7:L6:210:GLN:OE1	2.38	0.41
11:LC:97:VAL:HG12	11:LC:98:ASP:N	2.34	0.41
16:LH:25:LEU:HD23	16:LH:27:SER:H	1.84	0.41
16:LH:287:ASP:OD1	16:LH:287:ASP:N	2.53	0.41
16:LH:736:THR:HG22	16:LH:737:ILE:N	2.35	0.41
20:LL:113:MET:HG2	20:LL:153:ILE:HD11	2.00	0.41
21:LM:1407:LEU:CD1	21:LM:1415:LEU:HD13	2.50	0.41
21:LM:1537:LEU:O	21:LM:1538:LYS:CB	2.67	0.41
26:LR:162:LEU:HD11	26:LR:227:MET:HE1	2.01	0.41
30:LW:116:ILE:HG22	30:LW:398:ILE:HD12	1.98	0.41
31:LZ:57:LEU:HD22	31:LZ:78:LEU:HD22	2.01	0.41
37:NH:1163:LEU:HD23	37:NH:1184:GLY:HA2	2.01	0.41
39:NL:121:TYR:OH	39:NL:123:ASP:OD1	2.17	0.41
43:NS:859:ILE:O	43:NS:862:ILE:HD11	2.21	0.41
50:SD:239:CYS:SG	50:SD:240:VAL:N	2.92	0.41
58:SP:897:PHE:CZ	58:SP:901:ILE:HD11	2.55	0.41
2:L1:1600:A:H4'	2:L1:1601:G:O5'	2.20	0.41
16:LH:254:TYR:CD2	16:LH:414:ILE:HD12	2.55	0.41
16:LH:601:LEU:O	16:LH:601:LEU:HD23	2.20	0.41
20:LL:253:LEU:CD2	20:LL:301:LEU:HD21	2.50	0.41
21:LM:932:SER:O	21:LM:938:GLN:NE2	2.53	0.41
26:LR:440:VAL:CG2	26:LR:454:LEU:HD11	2.51	0.41
43:NS:426:GLN:NE2	43:NS:465:GLU:OE1	2.45	0.41
48:SA:31:LEU:O	48:SA:34:VAL:HG22	2.21	0.41
48:SA:206:LEU:HD11	48:SA:219:LEU:HD23	2.03	0.41
48:SA:216:PHE:O	48:SA:220:VAL:HG23	2.19	0.41
54:SI:968:THR:HG22	54:SI:1001:VAL:HG12	2.02	0.41
62:ST:467:ASN:OD1	62:ST:468:ARG:N	2.53	0.41
7:L6:73:ILE:HD12	43:NS:62:ILE:CD1	2.50	0.41
8:L7:136:VAL:N	8:L7:153:LEU:O	2.53	0.41
20:LL:537:LEU:O	20:LL:541:LEU:HD23	2.20	0.41
21:LM:637:ILE:O	21:LM:637:ILE:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LS:300:PHE:CE1	27:LS:312:ILE:HD11	2.56	0.41
37:NH:130:LYS:HZ3	37:NH:248:LEU:HD11	1.85	0.41
51:SF:23:VAL:HG21	51:SF:117:VAL:CG2	2.49	0.41
52:SG:168:ASN:O	52:SG:172:PHE:N	2.49	0.41
55:SJ:228:SER:HA	55:SK:252:LEU:HD23	2.02	0.41
55:SK:35:ASP:O	55:SK:40:ARG:NH2	2.53	0.41
57:SM:254:PHE:HE2	57:SM:256:MET:HE2	1.86	0.41
61:SS:228:VAL:O	61:SS:228:VAL:HG12	2.21	0.41
62:ST:453:ASN:OD1	62:ST:454:ALA:N	2.54	0.41
64:SV:17:VAL:HG11	64:SV:31:ILE:HD12	2.02	0.41
16:LH:583:LYS:HE2	16:LH:599:ILE:HD12	2.03	0.41
16:LH:637:THR:HG23	16:LH:639:LYS:H	1.85	0.41
25:LQ:132:THR:CG2	25:LQ:134:THR:HG22	2.50	0.41
37:NH:576:ASP:OD1	37:NH:626:LYS:NZ	2.47	0.41
44:NV:687:ILE:HD12	44:NV:687:ILE:H	1.85	0.41
55:SJ:196:LEU:HD23	55:SJ:197:ASP:O	2.20	0.41
58:SP:113:PHE:O	58:SP:117:LEU:HD23	2.21	0.41
58:SP:848:THR:OG1	58:SP:849:GLU:OE2	2.38	0.41
17:LI:425:VAL:HG12	17:LI:426:ILE:HG12	2.03	0.41
18:LJ:443:LEU:HD22	18:LJ:484:MET:HE1	2.03	0.41
20:LL:196:VAL:HG13	20:LL:196:VAL:O	2.21	0.41
20:LL:364:THR:OG1	20:LL:365:SER:N	2.54	0.41
21:LM:132:THR:OG1	21:LM:155:ILE:HD11	2.20	0.41
21:LM:1536:VAL:CG1	21:LM:1582:LEU:HD13	2.51	0.41
25:LQ:634:SER:OG	25:LQ:635:LYS:N	2.53	0.41
33:NB:231:ALA:HB3	33:NB:232:PRO:HD3	2.01	0.41
37:NH:217:LYS:HG2	37:NH:220:LEU:HD12	2.03	0.41
58:SP:462:ARG:HD2	58:SP:462:ARG:C	2.46	0.41
58:SP:1155:ASP:OD1	58:SP:1204:SER:OG	2.23	0.41
63:SU:238:ILE:HD13	63:SU:243:PRO:HG3	2.03	0.41
63:SU:531:ASP:OD1	63:SU:532:ASN:N	2.52	0.41
2:L1:1196:A:N3	55:SJ:136:ARG:NH1	2.69	0.41
16:LH:16:SER:HB3	16:LH:783:LEU:HB2	2.02	0.41
16:LH:148:GLU:HG2	16:LH:148:GLU:O	2.21	0.41
16:LH:429:ILE:HD12	16:LH:735:PRO:O	2.21	0.41
17:LI:331:VAL:HG13	17:LI:344:LEU:HD11	2.03	0.41
21:LM:523:ILE:O	21:LM:527:LEU:HD23	2.21	0.41
21:LM:899:ILE:HD12	21:LM:899:ILE:H	1.86	0.41
22:LN:39:VAL:HG22	22:LN:402:TRP:CZ3	2.55	0.41
27:LS:297:THR:HG22	27:LS:356:GLU:O	2.20	0.41
29:LU:267:ILE:HG12	29:LU:279:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LW:287:TYR:CD1	30:LW:304:ARG:HG3	2.56	0.41
37:NH:655:LEU:HD13	37:NH:665:HIS:CD2	2.55	0.41
37:NH:1071:ALA:HB1	37:NH:1088:LEU:HD21	2.03	0.41
2:L1:928:U:C1'	36:NG:124:ASP:OD2	2.69	0.41
2:L1:1126:OMG:H1'	2:L1:1126:OMG:HM23	1.56	0.41
2:L1:1582:U:OP1	57:SM:116:ARG:NH2	2.53	0.41
2:L1:1680:G:H21	2:L1:1681:A:N6	2.19	0.41
7:L6:182:GLN:NE2	7:L6:186:ARG:HG3	2.35	0.41
10:L9:161:THR:O	10:L9:161:THR:HG22	2.21	0.41
18:LJ:504:ILE:HD12	18:LJ:504:ILE:H	1.86	0.41
21:LM:724:VAL:HG12	21:LM:759:ILE:CD1	2.51	0.41
21:LM:755:ARG:O	21:LM:759:ILE:HG22	2.20	0.41
25:LQ:206:GLU:OE1	25:LQ:206:GLU:N	2.54	0.41
25:LQ:492:SER:OG	25:LQ:493:ALA:N	2.54	0.41
29:LU:231:GLU:OE1	61:SS:298:TRP:NE1	2.53	0.41
43:NS:401:MET:HE2	43:NS:431:ALA:HB1	2.01	0.41
43:NS:1058:ILE:CG2	65:SW:72:VAL:HG11	2.50	0.41
43:NS:1058:ILE:HG22	65:SW:72:VAL:HG11	2.02	0.41
49:SB:12:TYR:CE1	49:SB:63:ILE:HD11	2.56	0.41
49:SB:328:ARG:O	49:SB:332:THR:HG22	2.20	0.41
55:SK:77:LEU:CD1	55:SK:84:ILE:HG22	2.50	0.41
58:SP:133:ILE:HG23	58:SP:180:LEU:HD11	2.02	0.41
58:SP:976:TYR:O	58:SP:980:ASN:ND2	2.54	0.41
62:ST:13:LEU:HD23	62:ST:18:LEU:HD12	2.02	0.41
62:ST:576:ILE:HG22	62:ST:576:ILE:O	2.20	0.41
2:L1:1663:G:H5'	43:NS:251:ARG:NH1	2.35	0.41
2:L1:1701:A:OP1	37:NH:223:ARG:NH1	2.52	0.41
16:LH:282:ILE:CD1	16:LH:293:LEU:HD13	2.51	0.41
17:LI:330:ARG:NH1	17:LI:403:VAL:O	2.54	0.41
20:LL:160:VAL:HG23	20:LL:160:VAL:O	2.20	0.41
21:LM:218:ILE:HD12	21:LM:263:VAL:CB	2.51	0.41
21:LM:262:VAL:CG2	21:LM:298:THR:HG23	2.51	0.41
22:LN:189:ARG:NH2	64:SV:168:GLN:OE1	2.54	0.41
22:LN:542:VAL:HG22	22:LN:552:ILE:HD12	2.03	0.41
25:LQ:237:LYS:O	25:LQ:238:MET:HB3	2.21	0.41
28:LT:59:GLN:HG2	28:LT:71:VAL:HG12	2.03	0.41
28:LT:760:LEU:HB3	28:LT:762:LEU:HD13	2.02	0.41
32:NA:412:ILE:HD12	32:NA:412:ILE:H	1.85	0.41
35:NF:87:ASP:OD1	35:NF:87:ASP:N	2.53	0.41
37:NH:375:PHE:CZ	37:NH:385:LEU:HD21	2.56	0.41
37:NH:519:ASP:OD1	37:NH:520:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:SB:199:VAL:HG13	49:SB:199:VAL:O	2.20	0.41
50:SD:268:VAL:HG22	50:SD:317:VAL:HG22	2.03	0.41
2:L1:565:C:OP1	54:SI:973:ARG:NH2	2.53	0.40
2:L1:1624:C:OP1	57:SM:185:VAL:HG13	2.21	0.40
13:LE:23:ARG:NH1	13:LE:65:LEU:O	2.54	0.40
16:LH:265:ASP:OD1	16:LH:266:ASN:N	2.53	0.40
23:LO:543:ASN:O	23:LO:547:ALA:N	2.53	0.40
29:LU:205:ASP:OD1	29:LU:206:VAL:N	2.54	0.40
30:LW:197:ASP:OD1	30:LW:198:PHE:N	2.53	0.40
36:NG:22:SER:OG	36:NG:23:PHE:N	2.53	0.40
46:OH:36:LEU:HG	46:OH:41:LEU:HD12	2.04	0.40
50:SC:230:TYR:HD1	50:SC:234:ILE:HD12	1.85	0.40
55:SJ:141:MET:HE2	55:SJ:141:MET:CA	2.51	0.40
57:SM:233:VAL:CG2	57:SM:256:MET:HE3	2.42	0.40
59:SQ:124:ILE:HD12	59:SQ:124:ILE:H	1.87	0.40
16:LH:282:ILE:HD13	16:LH:293:LEU:HD13	2.03	0.40
17:LI:359:LYS:N	17:LI:386:THR:O	2.50	0.40
20:LL:175:ILE:HD12	20:LL:175:ILE:H	1.87	0.40
21:LM:140:LEU:HD12	21:LM:192:TYR:CE1	2.56	0.40
21:LM:744:ASP:OD1	21:LM:744:ASP:N	2.53	0.40
27:LS:405:THR:HG21	27:LS:456:THR:HA	2.04	0.40
33:NB:392:GLU:OE1	33:NB:392:GLU:N	2.54	0.40
37:NH:116:LEU:HD23	37:NH:116:LEU:H	1.86	0.40
37:NH:412:LEU:HD21	37:NH:424:GLY:HA3	2.03	0.40
43:NS:1190:TYR:HB3	43:NS:1213:VAL:HG11	2.02	0.40
48:SA:263:ILE:HD11	48:SA:268:MET:HE2	2.03	0.40
50:SC:165:ALA:HB1	50:SC:166:PRO:HD2	2.04	0.40
58:SP:174:CYS:HG	58:SP:211:PHE:HE1	1.69	0.40
58:SP:1247:LEU:HB3	58:SP:1287:LEU:HD11	2.02	0.40
58:SP:1386:GLU:OE1	58:SP:1386:GLU:N	2.50	0.40
58:SP:1449:ASP:O	58:SP:1453:ASN:ND2	2.51	0.40
58:SP:2270:ASN:OD1	58:SP:2271:LEU:N	2.54	0.40
67:SY:166:LEU:HD12	67:SY:166:LEU:N	2.36	0.40
2:L1:28:A2M:HM'3	2:L1:28:A2M:H1'	1.88	0.40
16:LH:372:LEU:HD21	16:LH:374:LEU:HD21	2.04	0.40
16:LH:720:ILE:HD12	16:LH:774:PHE:CG	2.56	0.40
21:LM:98:ILE:O	21:LM:102:LEU:HD23	2.21	0.40
21:LM:220:VAL:HG12	21:LM:234:LEU:HD21	2.04	0.40
21:LM:1042:LEU:HD21	21:LM:1076:LEU:HD11	2.03	0.40
36:NG:123:SER:O	36:NG:124:ASP:OD1	2.39	0.40
37:NH:130:LYS:NZ	37:NH:248:LEU:HD11	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:NS:377:GLU:N	43:NS:377:GLU:OE1	2.54	0.40
58:SP:481:TRP:HA	58:SP:484:ILE:HD12	2.03	0.40
58:SP:701:LEU:HD21	58:SP:795:ASP:HB3	2.03	0.40
58:SP:2177:THR:HG23	58:SP:2177:THR:O	2.21	0.40
16:LH:574:LEU:HD21	16:LH:622:ILE:HD13	2.02	0.40
18:LJ:404:ALA:HB2	18:LJ:417:VAL:HG11	2.03	0.40
21:LM:140:LEU:HD12	21:LM:192:TYR:HE1	1.86	0.40
21:LM:283:LEU:HA	21:LM:286:LEU:HD12	2.03	0.40
25:LQ:115:LEU:HD22	25:LQ:153:GLU:CG	2.51	0.40
37:NH:734:PHE:O	37:NH:738:TYR:N	2.50	0.40
37:NH:833:TYR:OH	37:NH:877:GLU:OE2	2.35	0.40
48:SA:4:ILE:HG22	48:SA:20:VAL:HG21	2.04	0.40
49:SB:2:ALA:HB3	49:SB:17:ALA:HB3	2.04	0.40
55:SJ:121:LEU:HD11	55:SJ:167:ILE:HD13	2.03	0.40
62:ST:659:GLU:OE1	62:ST:659:GLU:N	2.55	0.40
2:L1:319:U:H4'	2:L1:323:A:C8	2.57	0.40
8:L7:130:VAL:HG21	8:L7:135:ILE:HG13	2.03	0.40
25:LQ:829:VAL:O	25:LQ:833:LEU:HD23	2.20	0.40
27:LS:41:ASN:O	27:LS:45:ILE:HD12	2.22	0.40
32:NA:486:ASN:O	32:NA:489:SER:OG	2.32	0.40
33:NB:380:ARG:NH2	63:SU:121:ASP:OD2	2.51	0.40
37:NH:872:ASN:HD22	37:NH:872:ASN:C	2.29	0.40
47:OU:99:LYS:HG2	47:OU:100:LEU:HD23	2.03	0.40
55:SJ:144:LEU:HD11	55:SJ:160:LEU:HB3	2.03	0.40
58:SP:261:GLU:O	58:SP:267:SER:OG	2.33	0.40
58:SP:2450:ILE:HD12	58:SP:2450:ILE:H	1.86	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%)	239 (99%)	3 (1%)	0	100	100
6	L5	202/225 (90%)	199 (98%)	3 (2%)	0	100	100
7	L6	214/236 (91%)	211 (99%)	3 (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%)	179 (100%)	0	0	100	100
11	LC	126/143 (88%)	122 (97%)	4 (3%)	0	100	100
12	LD	135/156 (86%)	130 (96%)	5 (4%)	0	100	100
13	LE	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
14	LF	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
15	LG	60/67 (90%)	60 (100%)	0	0	100	100
16	LH	788/896 (88%)	761 (97%)	27 (3%)	0	100	100
17	LI	582/713 (82%)	576 (99%)	6 (1%)	0	100	100
18	LJ	470/513 (92%)	462 (98%)	8 (2%)	0	100	100
19	LK	130/575 (23%)	130 (100%)	0	0	100	100
20	LL	475/643 (74%)	464 (98%)	11 (2%)	0	100	100
21	LM	1602/1769 (91%)	1581 (99%)	21 (1%)	0	100	100
22	LN	649/776 (84%)	640 (99%)	9 (1%)	0	100	100
23	LO	786/923 (85%)	774 (98%)	12 (2%)	0	100	100
24	LP	375/440 (85%)	374 (100%)	1 (0%)	0	100	100
25	LQ	806/943 (86%)	778 (96%)	28 (4%)	0	100	100
26	LR	785/817 (96%)	767 (98%)	18 (2%)	0	100	100
27	LS	452/594 (76%)	446 (99%)	6 (1%)	0	100	100
28	LT	861/939 (92%)	851 (99%)	10 (1%)	0	100	100
29	LU	448/489 (92%)	439 (98%)	9 (2%)	0	100	100
30	LW	453/554 (82%)	443 (98%)	10 (2%)	0	100	100
31	LZ	156/183 (85%)	156 (100%)	0	0	100	100
32	NA	312/593 (53%)	311 (100%)	1 (0%)	0	100	100
33	NB	250/610 (41%)	245 (98%)	5 (2%)	0	100	100
34	ND	70/214 (33%)	70 (100%)	0	0	100	100
35	NF	139/151 (92%)	138 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	NG	125/137 (91%)	122 (98%)	3 (2%)	0	100	100
37	NH	1063/1237 (86%)	1050 (99%)	13 (1%)	0	100	100
38	NI	232/297 (78%)	225 (97%)	7 (3%)	0	100	100
39	NL	279/318 (88%)	276 (99%)	3 (1%)	0	100	100
40	NM	231/255 (91%)	227 (98%)	4 (2%)	0	100	100
41	NP	130/144 (90%)	128 (98%)	2 (2%)	0	100	100
42	NQ	77/82 (94%)	75 (97%)	2 (3%)	0	100	100
43	NS	917/1267 (72%)	899 (98%)	18 (2%)	0	100	100
44	NV	39/733 (5%)	39 (100%)	0	0	100	100
45	OA	275/1729 (16%)	274 (100%)	1 (0%)	0	100	100
46	OH	118/143 (82%)	118 (100%)	0	0	100	100
47	OU	54/152 (36%)	52 (96%)	2 (4%)	0	100	100
48	SA	390/504 (77%)	387 (99%)	3 (1%)	0	100	100
49	SB	431/511 (84%)	427 (99%)	4 (1%)	0	100	100
50	SC	237/327 (72%)	234 (99%)	3 (1%)	0	100	100
50	SD	234/327 (72%)	233 (100%)	1 (0%)	0	100	100
51	SE	119/126 (94%)	118 (99%)	1 (1%)	0	100	100
51	SF	119/126 (94%)	116 (98%)	3 (2%)	0	100	100
52	SG	453/573 (79%)	442 (98%)	11 (2%)	0	100	100
53	SH	358/367 (98%)	348 (97%)	10 (3%)	0	100	100
54	SI	746/1183 (63%)	736 (99%)	10 (1%)	0	100	100
55	SJ	207/252 (82%)	203 (98%)	4 (2%)	0	100	100
55	SK	225/252 (89%)	220 (98%)	5 (2%)	0	100	100
56	SL	146/189 (77%)	140 (96%)	6 (4%)	0	100	100
57	SM	243/290 (84%)	242 (100%)	1 (0%)	0	100	100
58	SP	2383/2493 (96%)	2357 (99%)	26 (1%)	0	100	100
59	SQ	113/217 (52%)	111 (98%)	2 (2%)	0	100	100
60	SR	130/145 (90%)	128 (98%)	2 (2%)	0	100	100
61	SS	313/899 (35%)	308 (98%)	5 (2%)	0	100	100
62	ST	573/810 (71%)	566 (99%)	7 (1%)	0	100	100
63	SU	524/552 (95%)	518 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	SV	151/206 (73%)	149 (99%)	2 (1%)	0	100	100
65	SW	211/274 (77%)	209 (99%)	2 (1%)	0	100	100
66	SX	1/30 (3%)	0	1 (100%)	0	100	100
67	SY	193/250 (77%)	189 (98%)	4 (2%)	0	100	100
68	SZ	255/483 (53%)	252 (99%)	3 (1%)	0	100	100
All	All	24739/33301 (74%)	24353 (98%)	386 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L3	96/129 (74%)	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%)	743 (100%)	0	100	100
17	LI	377/657 (57%)	377 (100%)	0	100	100
18	LJ	421/454 (93%)	421 (100%)	0	100	100
19	LK	124/533 (23%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	LL	438/574 (76%)	438 (100%)	0	100	100
21	LM	1492/1633 (91%)	1492 (100%)	0	100	100
22	LN	603/713 (85%)	603 (100%)	0	100	100
23	LO	695/812 (86%)	695 (100%)	0	100	100
24	LP	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	LU	409/443 (92%)	409 (100%)	0	100	100
30	LW	395/480 (82%)	395 (100%)	0	100	100
31	LZ	150/172 (87%)	150 (100%)	0	100	100
32	NA	299/535 (56%)	299 (100%)	0	100	100
33	NB	235/538 (44%)	235 (100%)	0	100	100
34	ND	70/196 (36%)	70 (100%)	0	100	100
35	NF	121/128 (94%)	121 (100%)	0	100	100
36	NG	96/105 (91%)	96 (100%)	0	100	100
37	NH	982/1125 (87%)	982 (100%)	0	100	100
38	NI	220/274 (80%)	220 (100%)	0	100	100
39	NL	257/283 (91%)	256 (100%)	1 (0%)	84	93
40	NM	210/224 (94%)	210 (100%)	0	100	100
41	NP	107/116 (92%)	107 (100%)	0	100	100
42	NQ	68/71 (96%)	68 (100%)	0	100	100
43	NS	836/1140 (73%)	836 (100%)	0	100	100
44	NV	41/671 (6%)	41 (100%)	0	100	100
45	OA	16/1544 (1%)	16 (100%)	0	100	100
46	OH	97/119 (82%)	97 (100%)	0	100	100
47	OU	47/135 (35%)	47 (100%)	0	100	100
48	SA	339/435 (78%)	339 (100%)	0	100	100
49	SB	359/433 (83%)	359 (100%)	0	100	100
50	SC	200/240 (83%)	200 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	SD	198/240 (82%)	198 (100%)	0	100	100
51	SE	100/104 (96%)	100 (100%)	0	100	100
51	SF	100/104 (96%)	100 (100%)	0	100	100
52	SG	399/503 (79%)	399 (100%)	0	100	100
53	SH	307/312 (98%)	307 (100%)	0	100	100
54	SI	669/1039 (64%)	669 (100%)	0	100	100
55	SJ	192/222 (86%)	192 (100%)	0	100	100
55	SK	205/222 (92%)	205 (100%)	0	100	100
56	SL	131/169 (78%)	131 (100%)	0	100	100
57	SM	220/258 (85%)	220 (100%)	0	100	100
58	SP	2229/2307 (97%)	2229 (100%)	0	100	100
59	SQ	108/200 (54%)	108 (100%)	0	100	100
60	SR	113/120 (94%)	113 (100%)	0	100	100
61	SS	292/807 (36%)	292 (100%)	0	100	100
62	ST	544/732 (74%)	544 (100%)	0	100	100
63	SU	489/506 (97%)	489 (100%)	0	100	100
64	SV	147/192 (77%)	147 (100%)	0	100	100
65	SW	192/238 (81%)	192 (100%)	0	100	100
66	SX	1/1 (100%)	1 (100%)	0	100	100
67	SY	191/234 (82%)	191 (100%)	0	100	100
68	SZ	232/424 (55%)	232 (100%)	0	100	100
All	All	22078/29635 (74%)	22077 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
39	NL	36	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (215) such sidechains are listed below:

Mol	Chain	Res	Type
5	L4	67	GLN
5	L4	69	HIS
5	L4	142	HIS

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Mol	Chain	Res	Type
6	L5	127	GLN
6	L5	224	ASN
7	L6	34	GLN
7	L6	80	ASN
8	L7	122	HIS
8	L7	147	ASN
8	L7	190	HIS
9	L8	84	HIS
10	L9	155	HIS
12	LD	14	GLN
12	LD	92	HIS
12	LD	104	HIS
14	LF	29	HIS
14	LF	133	ASN
16	LH	105	HIS
16	LH	115	HIS
16	LH	146	HIS
16	LH	255	ASN
16	LH	325	GLN
16	LH	478	ASN
16	LH	491	GLN
16	LH	540	ASN
16	LH	542	ASN
16	LH	725	ASN
16	LH	759	HIS
16	LH	870	ASN
16	LH	878	ASN
17	LI	329	ASN
17	LI	375	HIS
17	LI	553	GLN
17	LI	677	ASN
18	LJ	24	GLN
18	LJ	44	HIS
18	LJ	51	HIS
18	LJ	135	GLN
18	LJ	233	ASN
18	LJ	263	ASN
20	LL	35	GLN
20	LL	297	ASN
20	LL	302	ASN
20	LL	316	ASN
21	LM	304	GLN

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Mol	Chain	Res	Type
21	LM	774	ASN
21	LM	847	HIS
21	LM	1307	GLN
21	LM	1585	ASN
22	LN	216	GLN
22	LN	532	ASN
22	LN	574	HIS
23	LO	254	HIS
23	LO	296	GLN
23	LO	452	ASN
23	LO	552	ASN
23	LO	825	GLN
24	LP	41	HIS
24	LP	191	ASN
25	LQ	116	ASN
25	LQ	194	HIS
25	LQ	275	GLN
25	LQ	383	HIS
25	LQ	608	HIS
25	LQ	628	HIS
25	LQ	679	HIS
25	LQ	803	GLN
25	LQ	849	HIS
25	LQ	911	GLN
25	LQ	916	HIS
26	LR	309	GLN
26	LR	315	ASN
26	LR	753	HIS
26	LR	802	GLN
27	LS	20	GLN
27	LS	283	HIS
27	LS	307	GLN
28	LT	88	HIS
28	LT	108	HIS
28	LT	120	HIS
28	LT	172	HIS
28	LT	305	ASN
28	LT	552	HIS
28	LT	627	ASN
28	LT	736	HIS
28	LT	793	GLN
28	LT	816	HIS

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Mol	Chain	Res	Type
28	LT	903	GLN
28	LT	910	GLN
28	LT	911	ASN
28	LT	916	HIS
29	LU	133	GLN
30	LW	155	HIS
30	LW	170	GLN
30	LW	305	ASN
30	LW	424	GLN
31	LZ	74	HIS
32	NA	40	ASN
32	NA	304	GLN
32	NA	382	GLN
32	NA	431	GLN
33	NB	269	HIS
33	NB	407	GLN
35	NF	123	HIS
37	NH	197	GLN
37	NH	582	GLN
37	NH	689	HIS
37	NH	723	ASN
37	NH	834	ASN
37	NH	901	ASN
37	NH	1082	GLN
37	NH	1221	HIS
38	NI	42	HIS
38	NI	90	ASN
38	NI	151	HIS
38	NI	224	ASN
39	NL	184	ASN
39	NL	201	GLN
40	NM	211	HIS
43	NS	103	HIS
43	NS	405	HIS
43	NS	406	HIS
43	NS	522	ASN
43	NS	550	HIS
43	NS	634	HIS
43	NS	860	HIS
43	NS	1158	HIS
48	SA	125	GLN
48	SA	156	HIS

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Mol	Chain	Res	Type
48	SA	391	ASN
49	SB	55	ASN
49	SB	71	GLN
51	SE	25	GLN
52	SG	168	ASN
52	SG	181	ASN
52	SG	226	HIS
52	SG	449	ASN
53	SH	15	GLN
53	SH	152	HIS
54	SI	22	HIS
54	SI	112	HIS
54	SI	200	GLN
54	SI	776	GLN
54	SI	900	GLN
54	SI	986	HIS
54	SI	1037	GLN
55	SJ	69	ASN
55	SK	69	ASN
56	SL	64	GLN
57	SM	164	GLN
57	SM	168	HIS
58	SP	39	HIS
58	SP	46	HIS
58	SP	79	GLN
58	SP	183	HIS
58	SP	207	ASN
58	SP	398	GLN
58	SP	418	GLN
58	SP	446	GLN
58	SP	791	ASN
58	SP	802	ASN
58	SP	851	HIS
58	SP	1014	ASN
58	SP	1046	HIS
58	SP	1093	HIS
58	SP	1100	GLN
58	SP	1114	HIS
58	SP	1241	GLN
58	SP	1458	GLN
58	SP	1460	HIS
58	SP	1483	HIS

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Mol	Chain	Res	Type
58	SP	1491	HIS
58	SP	1502	ASN
58	SP	1505	ASN
58	SP	1508	GLN
58	SP	1516	GLN
58	SP	1540	GLN
58	SP	1688	HIS
58	SP	1707	HIS
58	SP	1737	ASN
58	SP	1786	GLN
58	SP	1802	HIS
58	SP	1991	ASN
58	SP	2045	GLN
58	SP	2060	GLN
58	SP	2108	ASN
58	SP	2176	HIS
58	SP	2201	HIS
58	SP	2362	GLN
59	SQ	135	HIS
61	SS	276	GLN
61	SS	475	GLN
61	SS	825	ASN
61	SS	875	HIS
62	ST	384	HIS
62	ST	452	GLN
62	ST	527	GLN
62	ST	713	HIS
62	ST	743	GLN
63	SU	51	ASN
63	SU	228	HIS
63	SU	260	ASN
63	SU	288	HIS
63	SU	290	HIS
63	SU	370	HIS
63	SU	474	HIS
64	SV	96	GLN
64	SV	101	HIS
67	SY	6	HIS
67	SY	65	HIS
67	SY	124	GLN
67	SY	133	HIS
67	SY	247	GLN

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Mol	Chain	Res	Type
68	SZ	290	ASN
68	SZ	302	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L0	59/700 (8%)	14 (23%)	0
2	L1	1463/1802 (81%)	277 (18%)	7 (0%)
3	L2	203/334 (60%)	26 (12%)	1 (0%)
All	All	1725/2836 (60%)	317 (18%)	8 (0%)

All (317) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L0	14	U
1	L0	16	A
1	L0	17	A
1	L0	23	G
1	L0	63	G
1	L0	67	G
1	L0	82	A
1	L0	83	U
1	L0	85	G
1	L0	86	C
1	L0	87	C
1	L0	90	G
1	L0	471	C
1	L0	473	A
2	L1	4	C
2	L1	9	U
2	L1	26	A
2	L1	34	G
2	L1	42	G
2	L1	46	A
2	L1	47	A
2	L1	60	U
2	L1	65	A
2	L1	68	A
2	L1	74	U
2	L1	76	A
2	L1	78	A

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Mol	Chain	Res	Type
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	189	C
2	L1	190	C
2	L1	193	U
2	L1	195	G
2	L1	204	G
2	L1	205	U
2	L1	226	A
2	L1	233	C
2	L1	234	G
2	L1	241	U
2	L1	242	U
2	L1	260	U
2	L1	261	U
2	L1	265	A
2	L1	275	C
2	L1	276	C
2	L1	278	U
2	L1	279	G
2	L1	280	U
2	L1	290	G
2	L1	299	A
2	L1	304	U
2	L1	314	C
2	L1	316	A
2	L1	322	G
2	L1	337	G

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Mol	Chain	Res	Type
2	L1	338	C
2	L1	344	A
2	L1	352	A
2	L1	359	A
2	L1	360	A
2	L1	361	C
2	L1	400	A
2	L1	401	A
2	L1	402	C
2	L1	404	G
2	L1	423	G
2	L1	424	C
2	L1	425	A
2	L1	426	G
2	L1	436	A2M
2	L1	437	A
2	L1	438	A
2	L1	439	U
2	L1	444	C
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	519	C
2	L1	527	A
2	L1	532	U
2	L1	534	A
2	L1	540	G
2	L1	542	A
2	L1	545	A
2	L1	563	U
2	L1	564	G
2	L1	565	C
2	L1	570	A

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Mol	Chain	Res	Type
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	652	G
2	L1	688	G
2	L1	700	C
2	L1	705	U
2	L1	734	A
2	L1	737	A
2	L1	765	G
2	L1	766	U
2	L1	774	A
2	L1	785	U
2	L1	786	C
2	L1	787	G
2	L1	788	A
2	L1	789	A
2	L1	790	U
2	L1	793	A
2	L1	794	U
2	L1	803	A
2	L1	809	A
2	L1	811	A
2	L1	812	A
2	L1	813	U
2	L1	817	A
2	L1	819	G
2	L1	820	U
2	L1	823	G
2	L1	824	G
2	L1	825	U
2	L1	846	G
2	L1	848	C

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Mol	Chain	Res	Type
2	L1	853	G
2	L1	859	A
2	L1	860	U
2	L1	862	A
2	L1	863	A
2	L1	876	G
2	L1	886	U
2	L1	898	A
2	L1	914	G
2	L1	921	U
2	L1	926	A
2	L1	928	U
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	970	A
2	L1	971	A
2	L1	992	A
2	L1	993	A
2	L1	1002	G
2	L1	1005	A
2	L1	1011	G
2	L1	1026	A
2	L1	1028	C
2	L1	1029	U
2	L1	1032	G
2	L1	1039	A
2	L1	1059	U
2	L1	1060	U
2	L1	1063	U
2	L1	1081	A
2	L1	1082	C
2	L1	1092	A
2	L1	1098	U
2	L1	1099	U
2	L1	1100	G
2	L1	1114	G
2	L1	1119	G
2	L1	1122	G

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Mol	Chain	Res	Type
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	1195	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
2	L1	1451	C
2	L1	1453	G
2	L1	1465	C
2	L1	1471	A
2	L1	1481	C
2	L1	1486	G
2	L1	1487	A
2	L1	1494	C
2	L1	1496	U
2	L1	1511	U
2	L1	1512	G
2	L1	1535	U
2	L1	1537	C
2	L1	1542	G
2	L1	1548	G
2	L1	1553	G

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Mol	Chain	Res	Type
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	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	1645	G
2	L1	1651	A
2	L1	1653	C
2	L1	1657	U
2	L1	1658	G
2	L1	1662	G
2	L1	1664	C
2	L1	1680	G
2	L1	1683	C
2	L1	1697	G
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	1739	C
2	L1	1744	A
2	L1	1745	G
2	L1	1755	A

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Mol	Chain	Res	Type
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	1796	C
2	L1	1800	A
2	L1	1801	A
3	L2	2	U
3	L2	10	C
3	L2	13	C
3	L2	34	A
3	L2	37	G
3	L2	38	U
3	L2	39	C
3	L2	47	G
3	L2	72	C
3	L2	90	C
3	L2	91	C
3	L2	109	G
3	L2	140	C
3	L2	145	U
3	L2	155	U
3	L2	156	U
3	L2	157	A
3	L2	159	C
3	L2	160	G
3	L2	188	A
3	L2	252	C
3	L2	284	U
3	L2	286	U
3	L2	324	U
3	L2	325	C
3	L2	329	C

All (8) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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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	1555	A
2	L1	1568	C
3	L2	156	U

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

20 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	1126	2	23,26,27	0.47	0	32,38,41	0.48	0
2	OMG	L1	1572	2	23,26,27	0.54	0	32,38,41	0.54	0
2	A2M	L1	619	2	22,25,26	0.88	0	30,36,39	1.93	6 (20%)
2	A2M	L1	541	2	22,25,26	0.92	1 (4%)	30,36,39	1.99	8 (26%)
2	A2M	L1	100	69,2	22,25,26	0.87	0	30,36,39	1.92	6 (20%)
2	OMC	L1	1639	2	19,22,23	0.50	0	25,31,34	0.61	0
2	OMU	L1	578	2	19,22,23	2.02	7 (36%)	25,31,34	1.81	5 (20%)
2	OMC	L1	1007	2	19,22,23	0.58	0	25,31,34	0.69	0
61	SEP	SS	738	61	8,9,10	1.57	1 (12%)	7,12,14	1.19	1 (14%)
27	SEP	LS	128	27	8,9,10	1.62	1 (12%)	7,12,14	1.34	1 (14%)
2	A2M	L1	420	2	22,25,26	0.89	0	30,36,39	1.94	8 (26%)
2	4AC	L1	1773	2	21,24,25	0.72	0	28,34,37	0.96	1 (3%)
2	A2M	L1	436	2	22,25,26	0.88	0	30,36,39	1.95	7 (23%)
2	A2M	L1	28	2	22,25,26	0.92	1 (4%)	30,36,39	1.96	8 (26%)
2	OMG	L1	562	2	23,26,27	0.53	0	32,38,41	0.59	0
2	A2M	L1	796	2	22,25,26	0.88	0	30,36,39	2.05	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	L1	974	2	22,25,26	0.92	1 (4%)	30,36,39	1.91	6 (20%)
2	OMC	L1	414	2	19,22,23	0.59	0	25,31,34	0.74	0
2	OMG	L1	1271	2	23,26,27	0.45	0	32,38,41	0.47	0
2	OMU	L1	1269	2	19,22,23	2.05	6 (31%)	25,31,34	1.90	5 (20%)

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	1126	2	-	1/9/27/28	0/3/3/3
2	OMG	L1	1572	2	-	1/9/27/28	0/3/3/3
2	A2M	L1	619	2	-	3/9/27/28	0/3/3/3
2	A2M	L1	541	2	-	0/9/27/28	0/3/3/3
2	A2M	L1	100	69,2	-	3/9/27/28	0/3/3/3
2	OMC	L1	1639	2	-	1/9/27/28	0/2/2/2
2	OMU	L1	578	2	-	2/9/27/28	0/2/2/2
2	OMC	L1	1007	2	-	0/9/27/28	0/2/2/2
61	SEP	SS	738	61	-	0/6/8/10	-
27	SEP	LS	128	27	-	4/6/8/10	-
2	A2M	L1	420	2	-	0/9/27/28	0/3/3/3
2	4AC	L1	1773	2	-	2/11/29/30	0/2/2/2
2	A2M	L1	436	2	-	5/9/27/28	0/3/3/3
2	A2M	L1	28	2	-	1/9/27/28	0/3/3/3
2	OMG	L1	562	2	-	0/9/27/28	0/3/3/3
2	A2M	L1	796	2	-	0/9/27/28	0/3/3/3
2	A2M	L1	974	2	-	1/9/27/28	0/3/3/3
2	OMC	L1	414	2	-	0/9/27/28	0/2/2/2
2	OMG	L1	1271	2	-	2/9/27/28	0/3/3/3
2	OMU	L1	1269	2	-	2/9/27/28	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L1	1269	OMU	C6-N1	4.68	1.49	1.38
2	L1	578	OMU	C6-N1	4.68	1.49	1.38
2	L1	1269	OMU	C2-N1	4.24	1.45	1.38
2	L1	1269	OMU	C5-C4	4.04	1.52	1.43
2	L1	578	OMU	C5-C4	4.03	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L1	578	OMU	C2-N1	3.88	1.44	1.38
27	LS	128	SEP	P-O1P	3.52	1.61	1.50
61	SS	738	SEP	P-O1P	3.46	1.61	1.50
2	L1	578	OMU	O4-C4	-2.82	1.19	1.24
2	L1	1269	OMU	O4-C4	-2.72	1.19	1.24
2	L1	578	OMU	C2-N3	2.49	1.42	1.38
2	L1	1269	OMU	O2-C2	-2.37	1.18	1.23
2	L1	1269	OMU	C2-N3	2.30	1.42	1.38
2	L1	578	OMU	O2-C2	-2.26	1.19	1.23
2	L1	541	A2M	C5-N7	-2.09	1.35	1.39
2	L1	578	OMU	C4-N3	2.08	1.42	1.38
2	L1	974	A2M	C5-N7	-2.06	1.35	1.39
2	L1	28	A2M	C5-N7	-2.01	1.35	1.39

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L1	541	A2M	C5-C4-N3	-6.03	118.41	126.72
2	L1	974	A2M	C5-C4-N3	-5.96	118.52	126.72
2	L1	796	A2M	C5-C4-N3	-5.92	118.56	126.72
2	L1	100	A2M	C5-C4-N3	-5.80	118.72	126.72
2	L1	619	A2M	C5-C4-N3	-5.75	118.80	126.72
2	L1	1269	OMU	C4-N3-C2	-5.70	119.54	126.61
2	L1	436	A2M	C5-C4-N3	-5.54	119.09	126.72
2	L1	420	A2M	C5-C4-N3	-5.51	119.12	126.72
2	L1	578	OMU	C4-N3-C2	-5.48	119.81	126.61
2	L1	28	A2M	C5-C4-N3	-5.43	119.23	126.72
2	L1	974	A2M	N3-C4-N9	4.46	134.75	127.17
2	L1	1269	OMU	N3-C2-N1	4.43	120.65	114.89
2	L1	541	A2M	N3-C4-N9	4.39	134.63	127.17
2	L1	796	A2M	N3-C4-N9	4.37	134.61	127.17
2	L1	100	A2M	N3-C4-N9	4.33	134.53	127.17
2	L1	420	A2M	N3-C4-N9	4.23	134.36	127.17
2	L1	619	A2M	N3-C4-N9	4.21	134.33	127.17
2	L1	436	A2M	N3-C4-N9	4.18	134.28	127.17
2	L1	28	A2M	N3-C4-N9	4.13	134.19	127.17
2	L1	578	OMU	C5-C4-N3	3.91	120.28	114.80
2	L1	578	OMU	N3-C2-N1	3.76	119.78	114.89
2	L1	1269	OMU	C5-C4-N3	3.74	120.04	114.80
2	L1	796	A2M	C5-N7-C8	3.68	109.23	103.45
2	L1	436	A2M	C5-N7-C8	3.65	109.19	103.45
2	L1	100	A2M	C5-N7-C8	3.55	109.03	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L1	619	A2M	C5-N7-C8	3.52	108.99	103.45
2	L1	28	A2M	C5-N7-C8	3.51	108.96	103.45
2	L1	420	A2M	C5-N7-C8	3.43	108.85	103.45
2	L1	974	A2M	C5-N7-C8	3.43	108.84	103.45
2	L1	796	A2M	N9-C8-N7	-3.33	109.21	113.94
2	L1	436	A2M	N9-C8-N7	-3.31	109.23	113.94
2	L1	541	A2M	C5-N7-C8	3.30	108.64	103.45
2	L1	420	A2M	N9-C8-N7	-3.27	109.29	113.94
2	L1	796	A2M	C4-C5-N7	-3.16	106.97	110.58
2	L1	28	A2M	N9-C8-N7	-3.12	109.50	113.94
2	L1	436	A2M	C4-C5-N7	-3.09	107.05	110.58
2	L1	619	A2M	N9-C8-N7	-3.06	109.59	113.94
2	L1	100	A2M	C4-C5-N7	-3.06	107.08	110.58
2	L1	619	A2M	C4-C5-N7	-3.05	107.09	110.58
2	L1	578	OMU	O4-C4-C5	-3.04	119.92	125.16
2	L1	974	A2M	C4-C5-N7	-3.02	107.12	110.58
2	L1	28	A2M	C4-C5-N7	-3.01	107.14	110.58
2	L1	28	A2M	C2'-C1'-N9	-3.00	108.82	113.75
2	L1	100	A2M	N9-C8-N7	-2.98	109.71	113.94
2	L1	1269	OMU	O4-C4-C5	-2.96	120.06	125.16
2	L1	541	A2M	C4-C5-N7	-2.92	107.24	110.58
2	L1	541	A2M	C2-N3-C4	2.87	118.83	111.83
2	L1	420	A2M	C4-C5-N7	-2.85	107.32	110.58
2	L1	974	A2M	N9-C8-N7	-2.81	109.94	113.94
2	L1	796	A2M	C2'-C1'-N9	-2.79	109.15	113.75
2	L1	420	A2M	C2-N3-C4	2.79	118.64	111.83
2	L1	796	A2M	C2-N3-C4	2.77	118.61	111.83
2	L1	974	A2M	C2-N3-C4	2.77	118.60	111.83
2	L1	1773	4AC	CM7-C7-N4	2.76	119.72	115.27
2	L1	619	A2M	C2-N3-C4	2.76	118.57	111.83
2	L1	541	A2M	N9-C8-N7	-2.73	110.06	113.94
2	L1	100	A2M	C2-N3-C4	2.73	118.50	111.83
27	LS	128	SEP	OG-CB-CA	2.72	110.79	108.14
2	L1	28	A2M	C2-N3-C4	2.71	118.44	111.83
2	L1	436	A2M	C2-N3-C4	2.64	118.27	111.83
2	L1	578	OMU	O2-C2-N1	-2.51	119.53	122.80
61	SS	738	SEP	OG-CB-CA	2.46	110.54	108.14
2	L1	541	A2M	C2'-C1'-N9	-2.32	109.94	113.75
2	L1	28	A2M	N3-C2-N1	-2.31	125.09	128.58
2	L1	1269	OMU	O2-C2-N1	-2.29	119.81	122.80
2	L1	420	A2M	C4-N9-C8	2.18	108.03	105.74
2	L1	420	A2M	N3-C2-N1	-2.16	125.32	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L1	541	A2M	N3-C2-N1	-2.12	125.37	128.58
2	L1	436	A2M	C4-N9-C8	2.06	107.90	105.74

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	LS	128	SEP	CA-CB-OG-P
27	LS	128	SEP	CB-OG-P-O2P
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	436	A2M	C2'-C1'-N9-C8
2	L1	974	A2M	C1'-C2'-O2'-CM'
2	L1	1126	OMG	C1'-C2'-O2'-CM2
2	L1	100	A2M	O4'-C4'-C5'-O5'
2	L1	100	A2M	C3'-C4'-C5'-O5'
2	L1	578	OMU	C3'-C4'-C5'-O5'
2	L1	578	OMU	O4'-C4'-C5'-O5'
2	L1	619	A2M	O4'-C4'-C5'-O5'
2	L1	1269	OMU	C3'-C4'-C5'-O5'
2	L1	1269	OMU	O4'-C4'-C5'-O5'
2	L1	436	A2M	C2'-C1'-N9-C4
2	L1	619	A2M	C3'-C4'-C5'-O5'
2	L1	1271	OMG	C3'-C4'-C5'-O5'
2	L1	619	A2M	C4'-C5'-O5'-P
2	L1	1773	4AC	O7-C7-N4-C4
2	L1	1773	4AC	CM7-C7-N4-C4
27	LS	128	SEP	CB-OG-P-O3P
2	L1	436	A2M	C3'-C4'-C5'-O5'
2	L1	1271	OMG	O4'-C4'-C5'-O5'
27	LS	128	SEP	CB-OG-P-O1P
2	L1	436	A2M	O4'-C4'-C5'-O5'
2	L1	1572	OMG	O4'-C4'-C5'-O5'
2	L1	1639	OMC	C4'-C5'-O5'-P

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L1	1126	OMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L1	578	OMU	1	0
61	SS	738	SEP	1	0
2	L1	1773	4AC	1	0
2	L1	436	A2M	1	0
2	L1	28	A2M	1	0
2	L1	562	OMG	2	0
2	L1	974	A2M	2	0
2	L1	1271	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 42 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	$\# Z > 2$
72	ADP	NS	1301	69	28,29,29	1.45	5 (17%)	43,45,45	1.89	11 (25%)
73	GTP	SI	2001	69	33,34,34	1.83	6 (18%)	50,54,54	1.47	7 (14%)
70	ATP	NH	1300	69	32,33,33	0.40	0	48,52,52	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	ADP	NS	1301	69	-	3/16/32/32	0/3/3/3
73	GTP	SI	2001	69	-	0/22/38/38	0/3/3/3
70	ATP	NH	1300	69	-	2/22/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	SI	2001	GTP	C5-N7	6.66	1.52	1.39
72	NS	1301	ADP	C5-C4	4.80	1.47	1.39
73	SI	2001	GTP	C8-N9	-4.26	1.28	1.37
73	SI	2001	GTP	C4-N9	-3.77	1.28	1.38
72	NS	1301	ADP	C5-C6	2.65	1.48	1.41
72	NS	1301	ADP	C8-N7	2.42	1.36	1.31
72	NS	1301	ADP	C5-N7	-2.38	1.34	1.39
72	NS	1301	ADP	PA-O3A	2.30	1.62	1.59
73	SI	2001	GTP	C4-N3	2.25	1.39	1.34
73	SI	2001	GTP	PB-O2B	-2.01	1.46	1.55
73	SI	2001	GTP	PA-O2A	-2.01	1.46	1.55

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	SI	2001	GTP	C8-N9-C4	7.03	119.21	106.03
72	NS	1301	ADP	C5-C4-N3	-5.91	118.58	126.72
72	NS	1301	ADP	N3-C4-N9	4.48	134.79	127.17
72	NS	1301	ADP	C2-N3-C4	3.76	121.02	111.83
72	NS	1301	ADP	C4-C5-N7	-3.72	106.33	110.58
72	NS	1301	ADP	N3-C2-N1	-3.67	123.02	128.58
72	NS	1301	ADP	C5-N7-C8	2.79	107.84	103.45
73	SI	2001	GTP	N9-C4-N3	2.73	131.42	125.95
73	SI	2001	GTP	C6-C5-N7	2.55	134.92	130.29
72	NS	1301	ADP	C2-N1-C6	2.43	122.72	118.73
72	NS	1301	ADP	C4-N9-C8	2.31	108.16	105.74
72	NS	1301	ADP	C3'-C2'-C1'	2.29	105.79	101.46
73	SI	2001	GTP	C1'-N9-C8	-2.18	120.55	126.73
73	SI	2001	GTP	C1'-N9-C4	-2.12	120.24	126.49
73	SI	2001	GTP	C8-N7-C5	-2.08	100.56	104.26
72	NS	1301	ADP	C6-C5-N7	2.07	136.08	132.09
72	NS	1301	ADP	N9-C8-N7	-2.04	111.04	113.94
73	SI	2001	GTP	C5-C4-N9	-2.03	102.02	105.66

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	NH	1300	ATP	O4'-C4'-C5'-O5'
72	NS	1301	ADP	PB-O3A-PA-O1A
72	NS	1301	ADP	O4'-C4'-C5'-O5'

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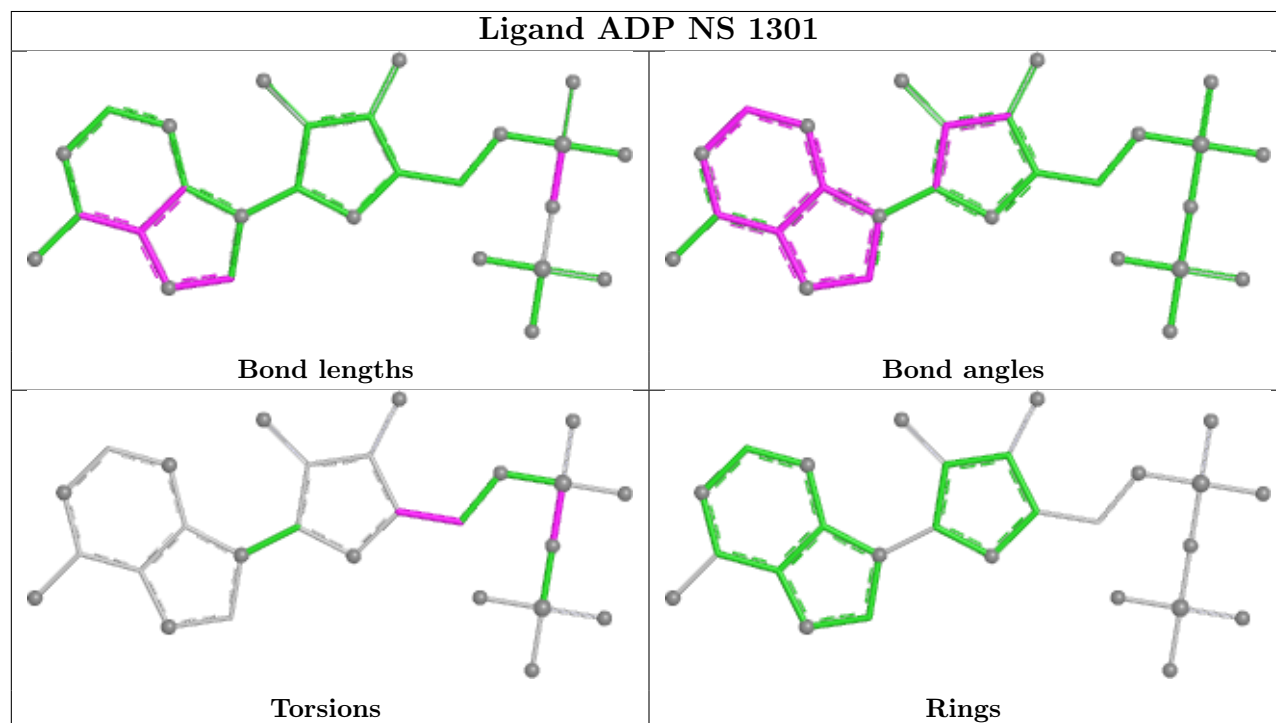
Mol	Chain	Res	Type	Atoms
72	NS	1301	ADP	PB-O3A-PA-O2A
70	NH	1300	ATP	C3'-C4'-C5'-O5'

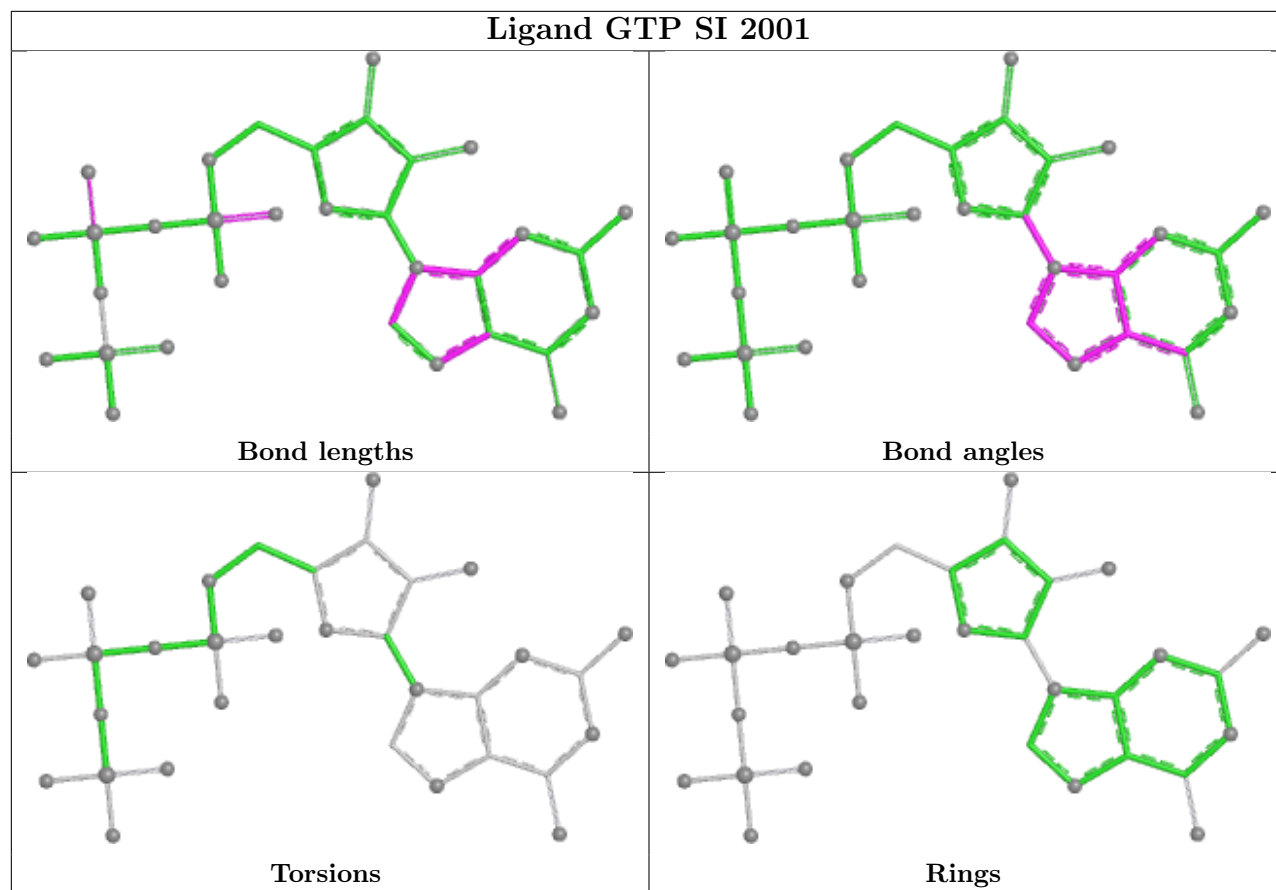
There are no ring outliers.

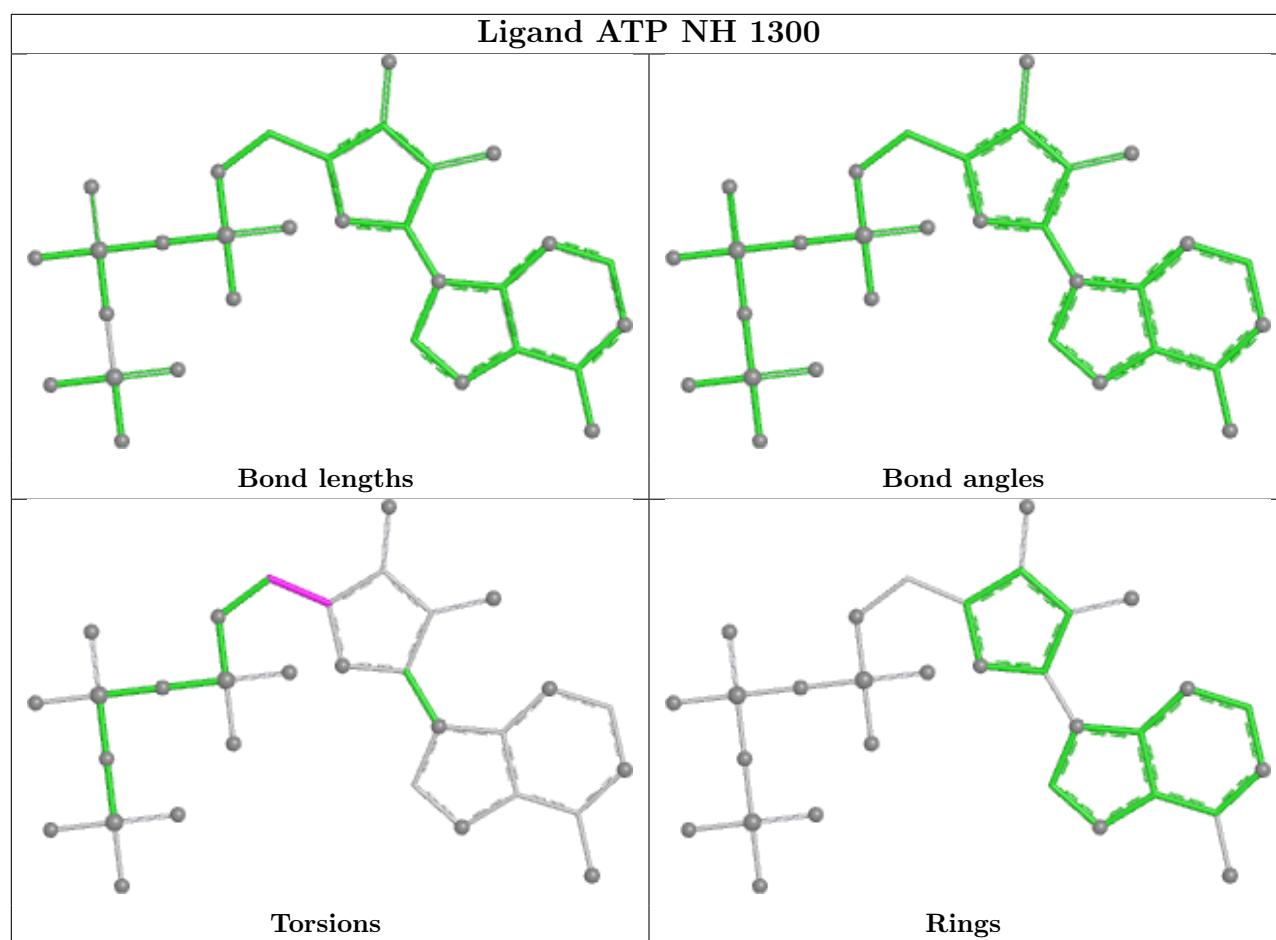
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	NS	1301	ADP	2	0
70	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.

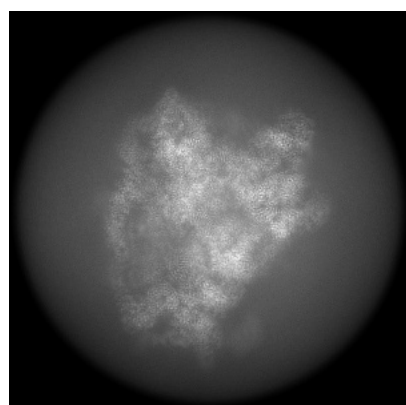
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49084. These allow visual inspection of the internal detail of the map and identification of artifacts.

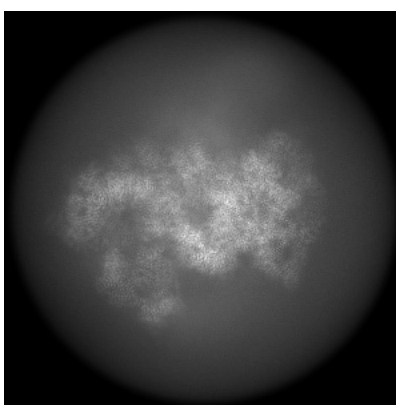
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

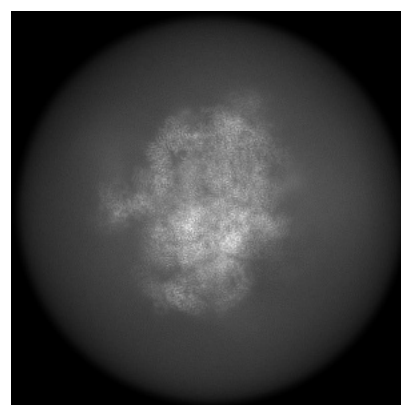
6.1.1 Primary map



X



Y

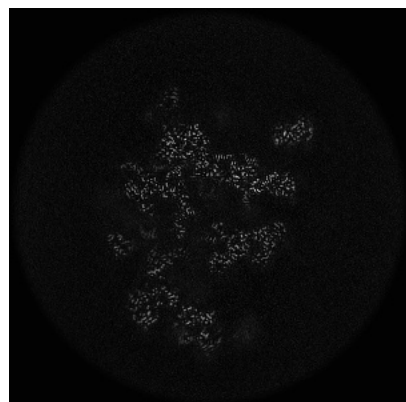


Z

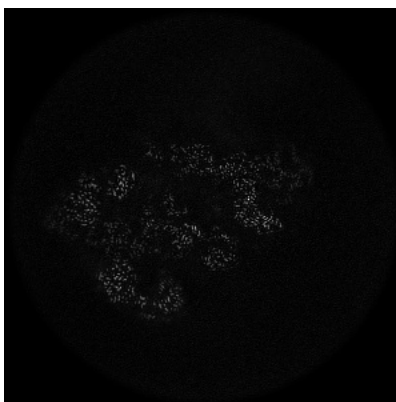
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

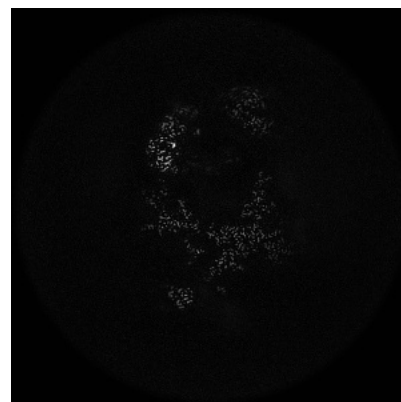
6.2.1 Primary map



X Index: 252



Y Index: 252

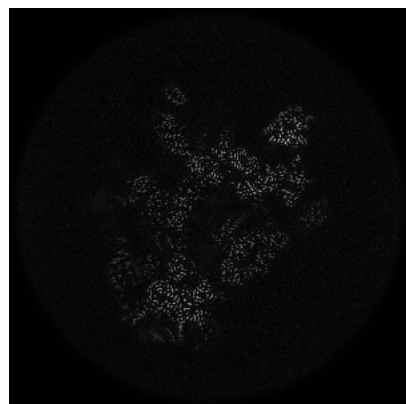


Z Index: 252

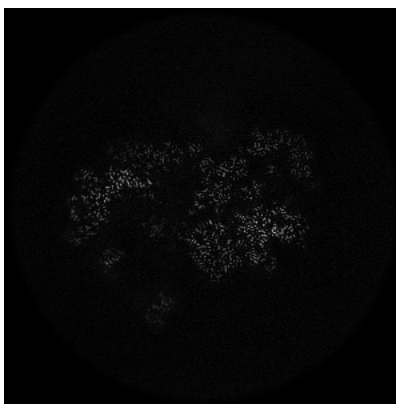
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

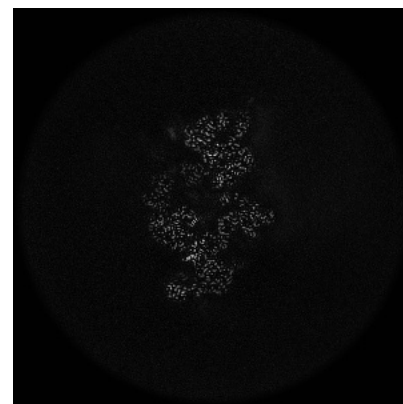
6.3.1 Primary map



X Index: 273



Y Index: 228

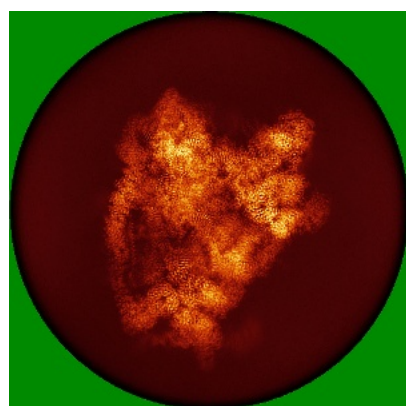


Z Index: 280

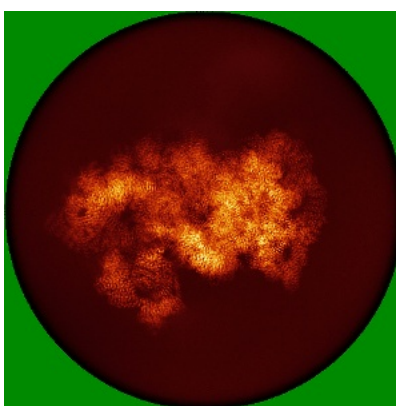
The images above show the largest variance slices of the map in three orthogonal directions.

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

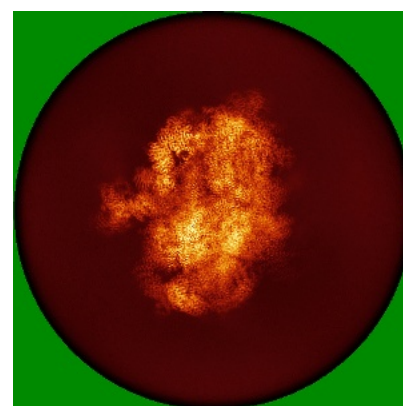
6.4.1 Primary map



X



Y

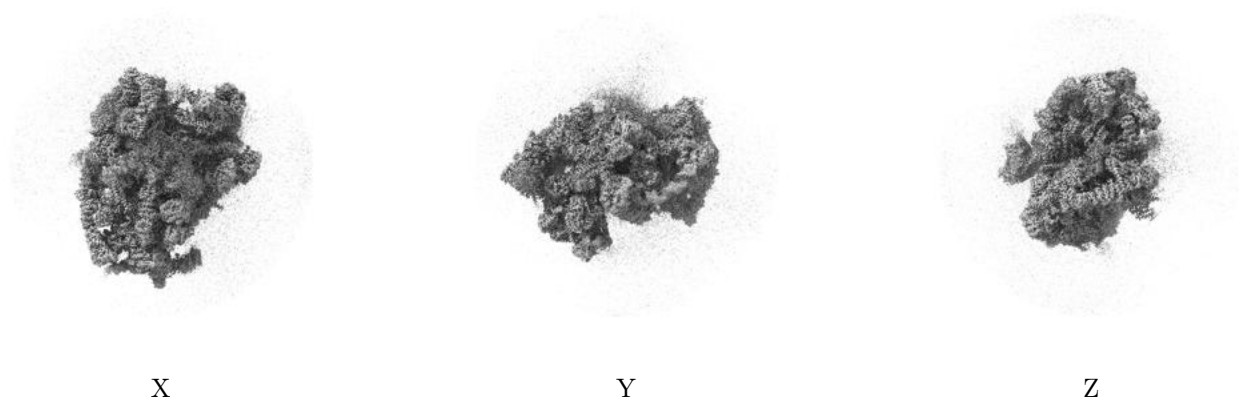


Z

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



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.

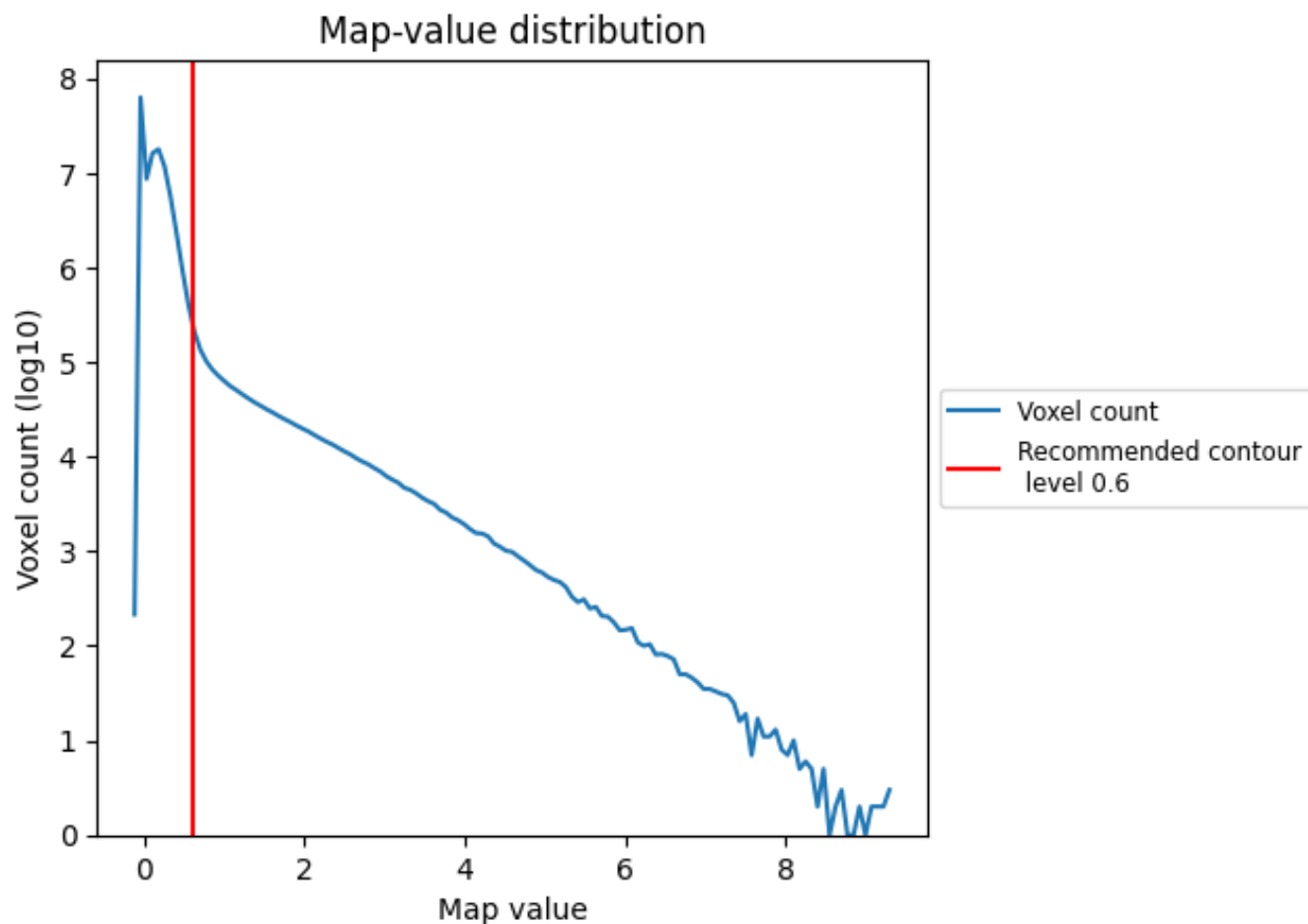
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

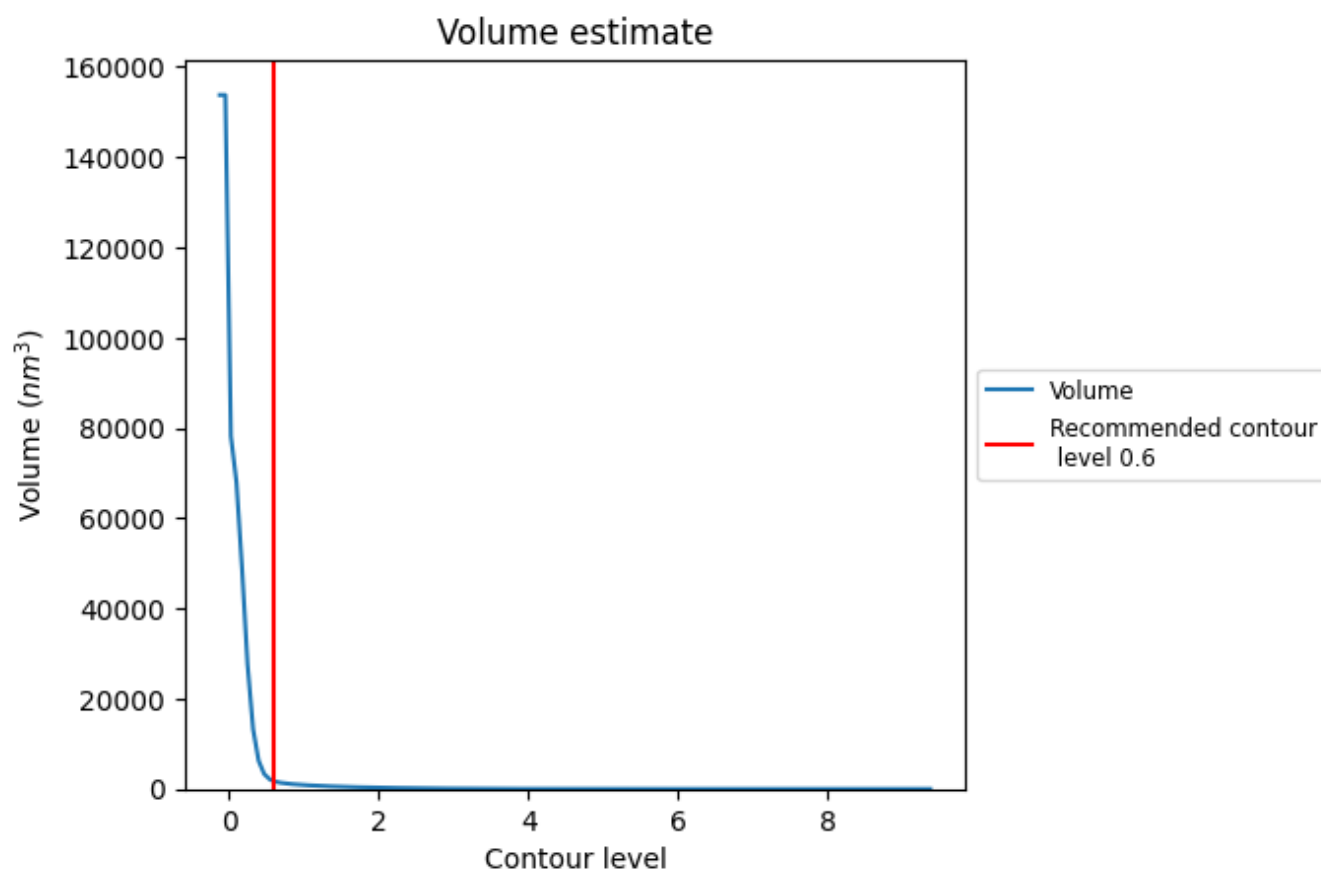
This section contains the results of statistical analysis of the map.

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.

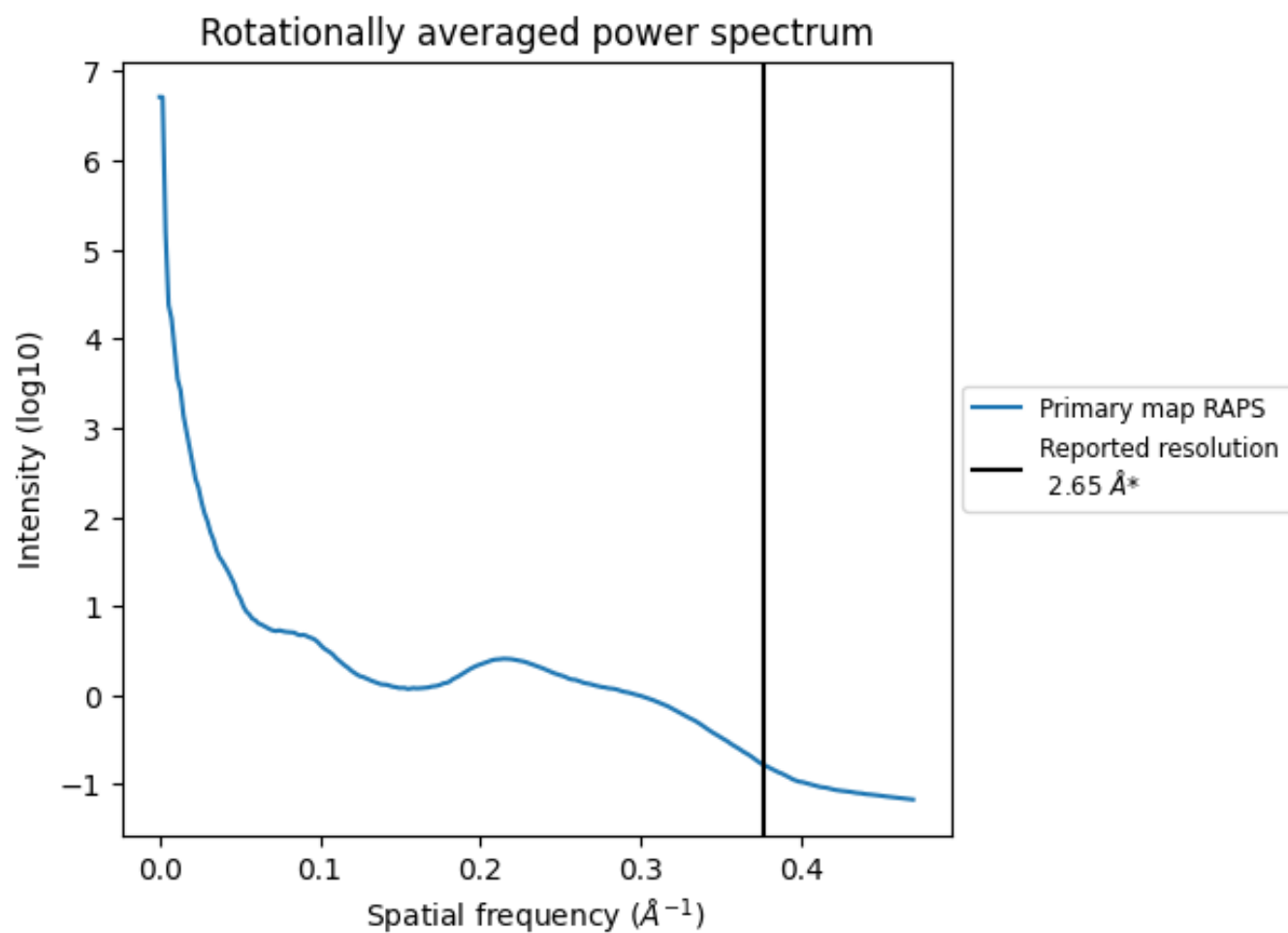
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1771 nm³; this corresponds to an approximate mass of 1600 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 0.377 Å⁻¹

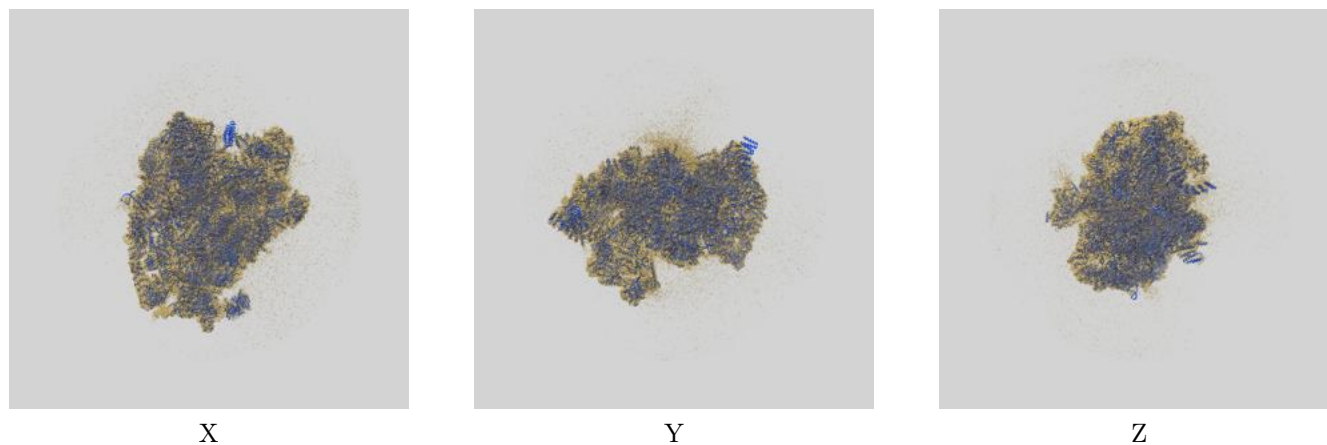
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

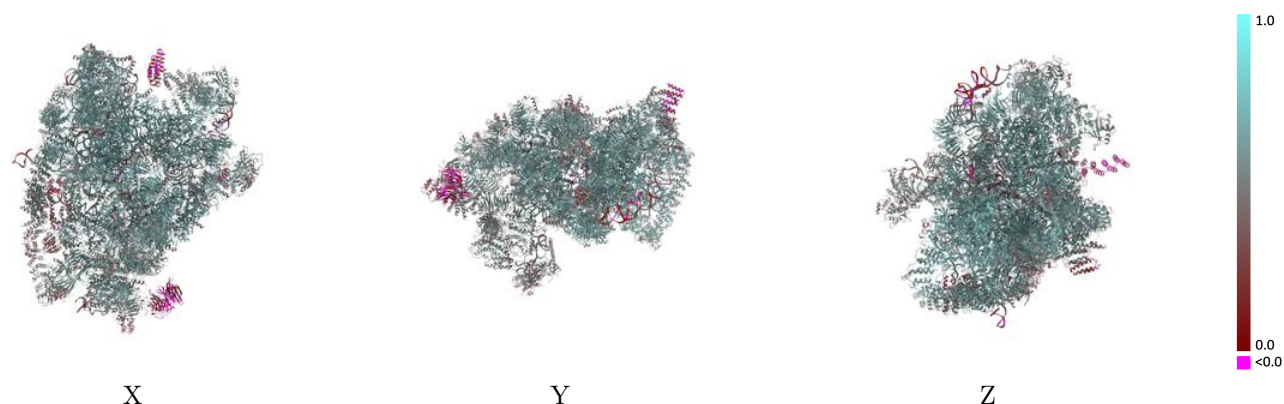
This section contains information regarding the fit between EMDB map EMD-49084 and PDB model 9N74. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



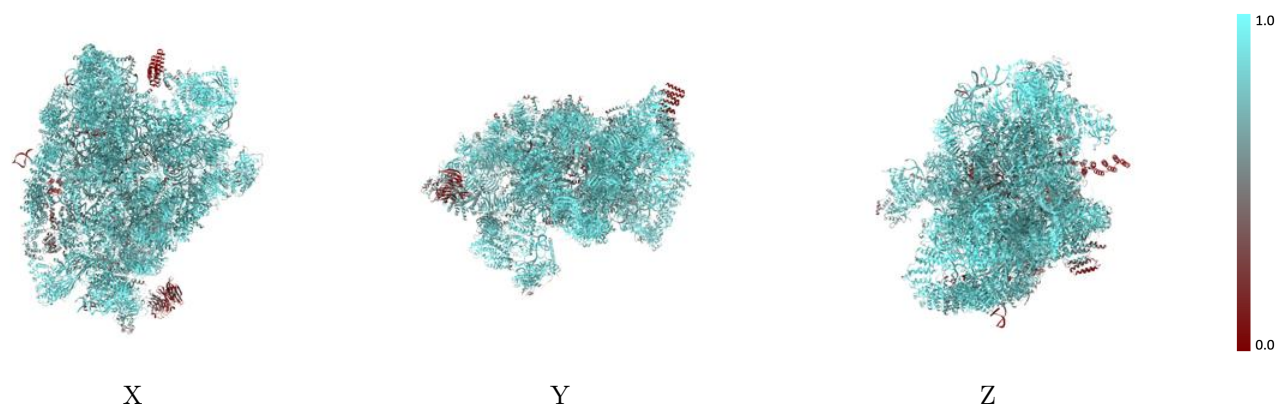
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



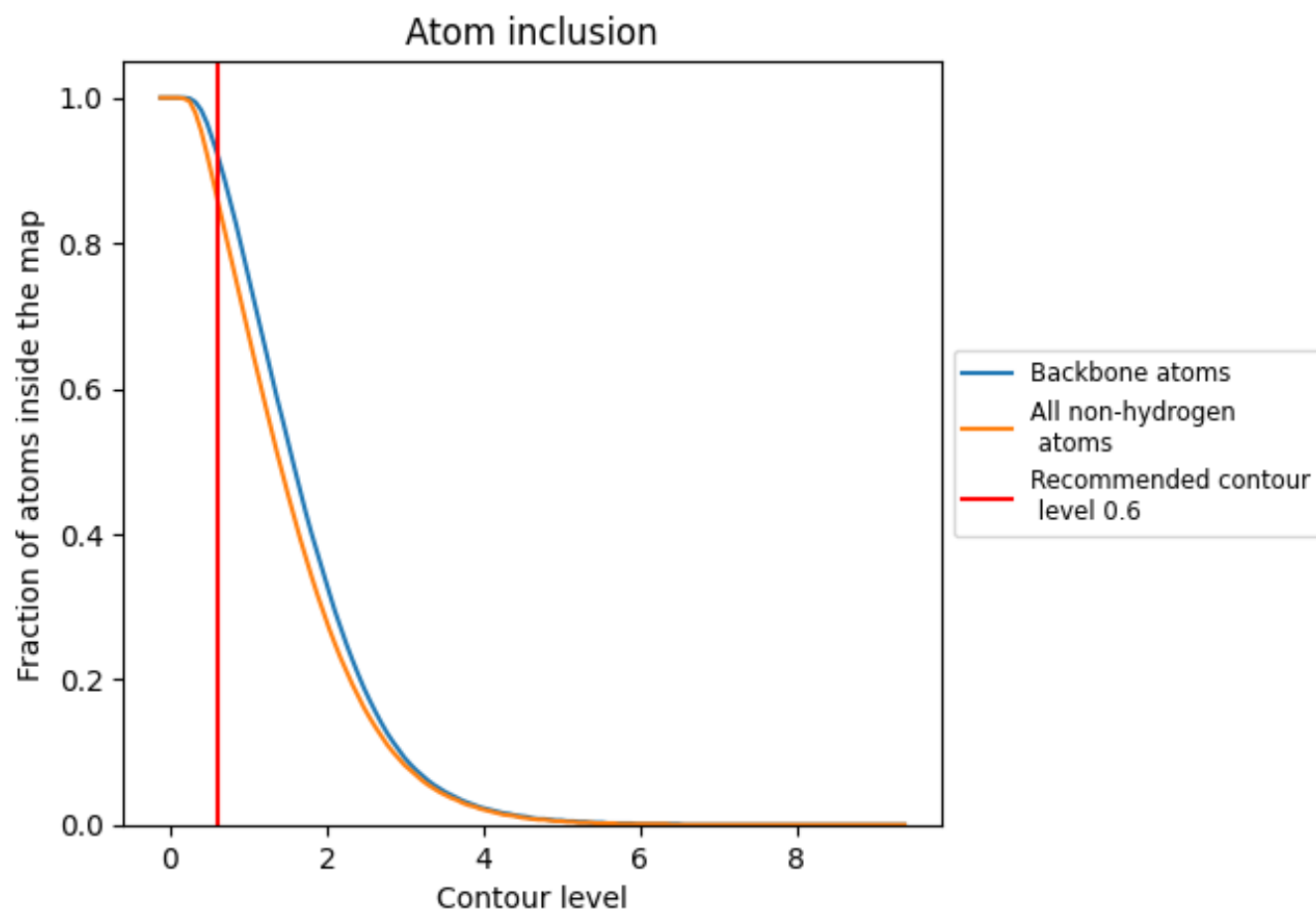
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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	 0.8630	 0.5570
L0	 0.8460	 0.4790
L1	 0.9200	 0.5810
L2	 0.7860	 0.4940
L3	 0.6700	 0.4510
L4	 0.9670	 0.6760
L5	 0.8670	 0.5680
L6	 0.9120	 0.6110
L7	 0.8270	 0.5540
L8	 0.9570	 0.6620
L9	 0.9320	 0.6440
LC	 0.9300	 0.6270
LD	 0.9490	 0.6680
LE	 0.9580	 0.6740
LF	 0.9350	 0.6500
LG	 0.8790	 0.5970
LH	 0.8920	 0.5480
LI	 0.4270	 0.2430
LJ	 0.8400	 0.5200
LK	 0.6520	 0.3760
LL	 0.8400	 0.5140
LM	 0.8300	 0.5020
LN	 0.9290	 0.5830
LO	 0.9150	 0.6230
LP	 0.6530	 0.4760
LQ	 0.9390	 0.5800
LR	 0.9420	 0.6160
LS	 0.8960	 0.5880
LT	 0.8830	 0.5910
LU	 0.9440	 0.6550
LW	 0.8960	 0.6260
LZ	 0.8300	 0.5700
NA	 0.7860	 0.5220
NB	 0.7460	 0.4890
ND	 0.6500	 0.4090



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Chain	Atom inclusion	Q-score
NF	 0.9230	 0.6350
NG	 0.9750	 0.6410
NH	 0.9600	 0.5840
NI	 0.8460	 0.5060
NL	 0.8030	 0.5600
NM	 0.9420	 0.6120
NP	 0.8070	 0.5560
NQ	 0.9470	 0.6360
NS	 0.7990	 0.4960
NV	 0.6680	 0.4980
OA	 0.3550	 0.2710
OH	 0.6340	 0.4010
OU	 0.6740	 0.3970
SA	 0.7820	 0.5300
SB	 0.7290	 0.5040
SC	 0.9460	 0.6520
SD	 0.7760	 0.5070
SE	 0.9490	 0.6050
SF	 0.9560	 0.6650
SG	 0.9050	 0.6200
SH	 0.9320	 0.6390
SI	 0.9110	 0.6300
SJ	 0.8440	 0.4640
SK	 0.9030	 0.5180
SL	 0.9660	 0.6620
SM	 0.9270	 0.6350
SP	 0.8770	 0.5810
SQ	 0.8310	 0.5870
SR	 0.9460	 0.6520
SS	 0.7370	 0.5220
ST	 0.8480	 0.5070
SU	 0.8160	 0.4670
SV	 0.7320	 0.4570
SW	 0.9250	 0.6110
SX	 0.6900	 0.3540
SY	 0.7780	 0.5370
SZ	 0.9140	 0.4930