



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:46 PM UTC

PDB ID : 9N6Y / pdb_00009n6y
EMDB ID : EMD-49078
Title : SSU processome maturation and disassembly, State C
Authors : Buzovetsky, O.; Klinge, S.
Deposited on : 2025-02-05
Resolution : 3.65 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

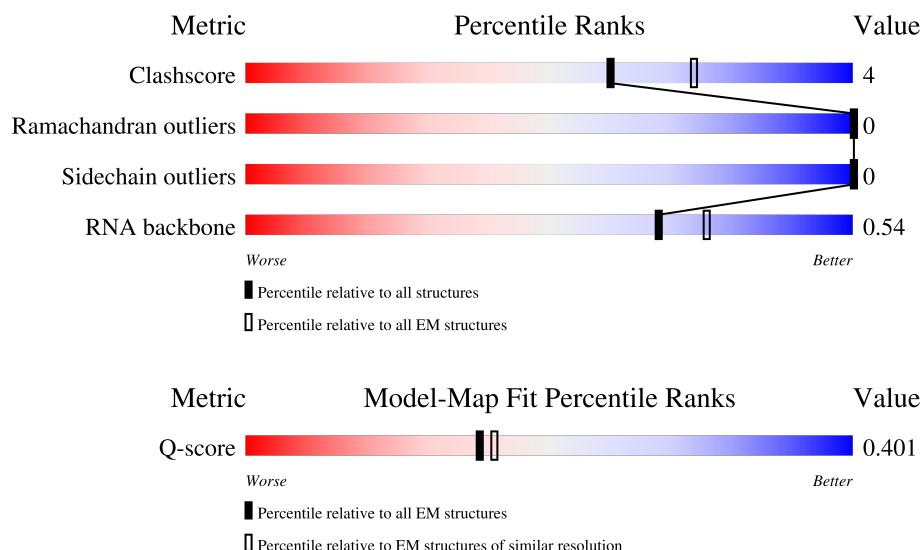
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.65 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	11564 (3.15 - 4.15)

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.

Mol	Chain	Length	Quality of chain
1	L0	700	12% 48% 13% 36%
2	L1	1808	5% 50% 15% 33%
3	L2	333	5% 41% 9% 47%

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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	

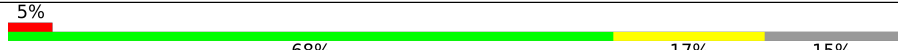
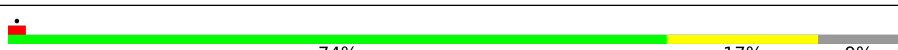
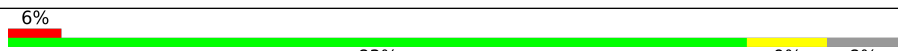
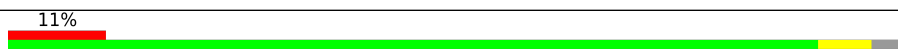
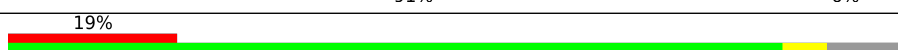
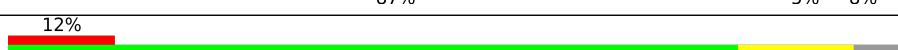
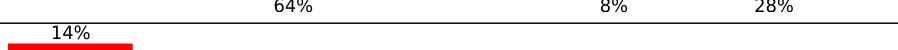
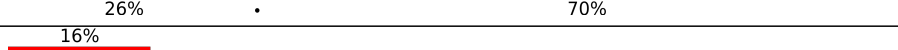
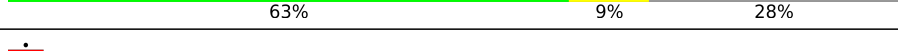
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Mol	Chain	Length	Quality of chain
29	LU	489	
30	LV	707	
31	LW	554	
32	LX	1056	
32	LY	1056	
33	LZ	183	
34	NA	593	
35	NB	610	
36	NC	357	
37	ND	214	
38	NE	346	
39	NF	151	
40	NG	137	
41	NH	1237	
42	NI	297	
43	NK	316	
44	NM	255	
45	NN	534	
46	NQ	82	
47	NV	733	
48	OA	1729	
49	SA	504	
50	SB	511	
51	SC	327	
51	SD	327	

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Mol	Chain	Length	Quality of chain
52	SE	126	
52	SF	126	
53	SG	573	
54	SH	367	
55	SI	1183	
56	SJ	252	
56	SK	252	
57	SL	189	
58	SM	290	
59	SN	274	
60	SP	2493	
61	SQ	217	
62	SR	145	
63	SS	899	
64	ST	810	
65	SU	552	
66	SV	206	
67	SW	274	
68	SY	250	
69	SZ	483	

2 Entry composition

There are 73 unique types of molecules in this entry. The entry contains 245176 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	445	Total	C	N	O	P	0	0
			9483	4239	1674	3125	445		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L1	1205	Total	C	N	O	P	0	0
			25709	11494	4600	8410	1205		

- Molecule 3 is a RNA chain called TPA: *Saccharomyces cerevisiae* U3a gene for small nucleolar RNA U3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L2	175	Total	C	N	O	P	0	0
			3712	1661	649	1227	175		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L3	97	Total	C	N	O	S	0	0
			786	498	144	142	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	206	Total	C	N	O	S	0	0
			1653	1043	315	293	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L7	169	Total	C	N	O	S	0	0
			1347	869	230	248			

- 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	171	Total	C	N	O	S	0	0
			1388	879	268	240	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LC	125	Total	C	N	O	S	0	0
			973	625	174	174			

- 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	0	0
			1046	662	204	180		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LH	808	Total	C	N	O	S	0	0
			6465	4123	1090	1233	19		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LJ	493	Total	C	N	O	S	0	0
			3911	2462	702	735	12		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LL	504	Total	C	N	O	S	0	0
			3982	2522	679	768	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LM	1613	Total	C	N	O	S	0	0
			9380	5798	1748	1822	12		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
23	LO	834	Total	C	N	O	P	S	0	0
			6639	4223	1140	1256	1	19		

- Molecule 24 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LP	380	Total	C	N	O	S	0	0
			3220	2081	545	578	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LQ	841	Total	C	N	O	S	0	0
			6707	4284	1125	1271	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	480	Total	C	N	O	P	S	0	0
			3793	2402	666	715	1	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LT	873	Total	C	N	O	S	0	0
			6876	4363	1188	1303	22		

- Molecule 29 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LU	460	Total	C	N	O	S	0	0
			3756	2349	685	706	16		

- Molecule 30 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LV	405	Total	C	N	O	S	0	0
			3286	2083	567	626	10		

- Molecule 31 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LW	535	Total	C	N	O	S	0	0
			4237	2656	762	807	12		

- Molecule 32 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LX	842	Total	C	N	O	S	0	0
			6720	4301	1155	1238	26		
32	LY	846	Total	C	N	O	S	0	0
			6179	3918	1079	1165	17		

- Molecule 33 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LZ	181	Total	C	N	O	S	0	0
			1524	964	286	267	7		

- Molecule 34 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	NA	286	Total	C	N	O	S	0	0
			2075	1279	378	414	4		

- Molecule 35 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	NB	267	Total	C	N	O	S	0	0
			1873	1156	360	356	1		

- Molecule 36 is a protein called U3 small nucleolar ribonucleoprotein protein LCP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	NC	115	Total	C	N	O	S	0	0
			777	484	145	145	3		

- Molecule 37 is a protein called Bud site selection protein 21.

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

- Molecule 38 is a protein called Protein FAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NE	215	Total	C	N	O	S	0	0
			1649	1021	327	298	3		

- Molecule 39 is a protein called 40S ribosomal protein S13.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	NG	119	Total	C	N	O	S	0	0
			875	541	166	165	3		

- Molecule 41 is a protein called U3 small nucleolar RNA-associated protein 22.

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

- Molecule 42 is a protein called Ribosomal RNA-processing protein 7.

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

- Molecule 43 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	NK	257	Total	C	N	O	S	0	0
			2107	1344	369	381	13		

- Molecule 44 is a protein called Small ribosomal subunit protein eS1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	NM	230	Total	C	N	O	S	0	0
			1838	1163	337	334	4		

- Molecule 45 is a protein called Protein BFR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	NN	267	Total	C	N	O	S	0	0
			1930	1212	343	373	2		

- Molecule 46 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 47 is a protein called Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	NV	8	Total	C	N	O	0	0
			64	42	12	10		

- Molecule 48 is a protein called rRNA biogenesis protein RRP5.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	OA	171	Total	C	N	O	0	0
			888	539	172	177		

- Molecule 49 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SA	385	Total	C	N	O	S	0	0
			3035	1926	521	579	9		

- Molecule 50 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SB	436	Total	C	N	O	S	0	0
			3357	2116	574	657	10		

- Molecule 51 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SC	241	Total	C	N	O	S	0	0
			1871	1185	337	339	10		
51	SD	232	Total	C	N	O	S	0	0
			1817	1153	324	330	10		

- Molecule 52 is a protein called 13 kDa ribonucleoprotein-associated protein.

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

- Molecule 53 is a protein called Ribosomal RNA-processing protein 9.

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

- Molecule 54 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

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

- Molecule 55 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SI	811	Total	C	N	O	S	0	0
			6577	4219	1156	1173	29		

- Molecule 56 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

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

- Molecule 57 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SL	173	Total	C	N	O	S	0	0
			1384	881	254	239	10		

- Molecule 58 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SM	282	Total	C	N	O	S	0	0
			2296	1441	430	418	7		

- Molecule 59 is a protein called Ribosome biogenesis protein UTP30.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SN	253	Total	C	N	O	S	0	0
			2053	1313	364	368	8		

- Molecule 60 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SP	2356	Total	C	N	O	S	0	0
			18367	11791	3084	3434	58		

- Molecule 61 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SQ	151	Total	C	N	O	S	0	0
			1280	807	240	228	5		

- Molecule 62 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SR	104	Total	C	N	O	S	0	0
			792	506	145	139	2		

- Molecule 63 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SS	272	Total	C	N	O	S	0	0
			2267	1415	427	415	10		

- Molecule 64 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	ST	582	Total	C	N	O	S	0	0
			4448	2823	802	811	12		

- Molecule 65 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SU	534	Total	C	N	O	S	0	0
			4370	2845	709	802	14		

- Molecule 66 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SV	147	Total	C	N	O		0	0
			869	529	160	180			

- Molecule 67 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SW	199	Total	C	N	O	S	0	0
			1565	998	284	279	4		

- Molecule 68 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SY	233	Total	C	N	O	S	0	0
			1953	1218	379	349	7		

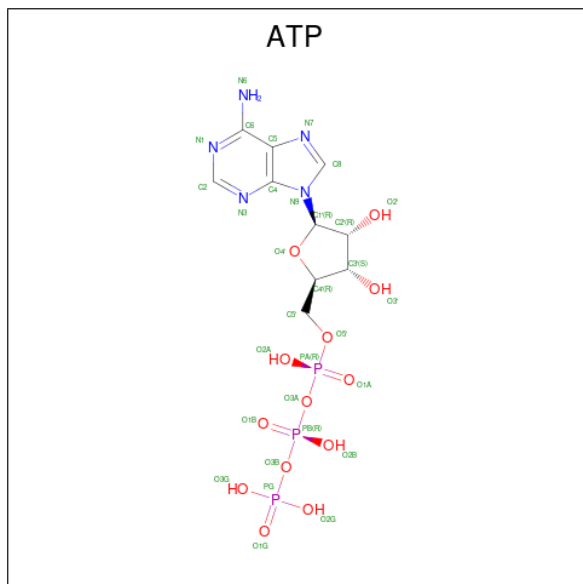
- Molecule 69 is a protein called Essential nuclear protein 1.

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

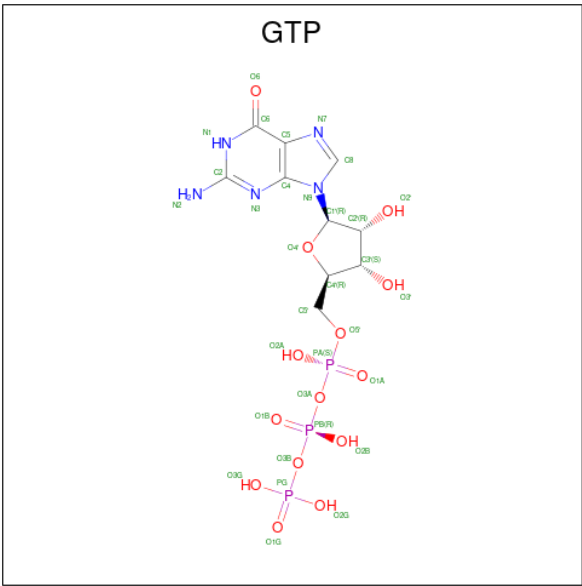
- Molecule 70 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
70	L0	3	Total	Mg	0
			3	3	
70	L1	26	Total	Mg	0
			26	26	
70	L2	2	Total	Mg	0
			2	2	
70	NH	1	Total	Mg	0
			1	1	
70	SI	1	Total	Mg	0
			1	1	
70	SM	1	Total	Mg	0
			1	1	

- Molecule 71 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

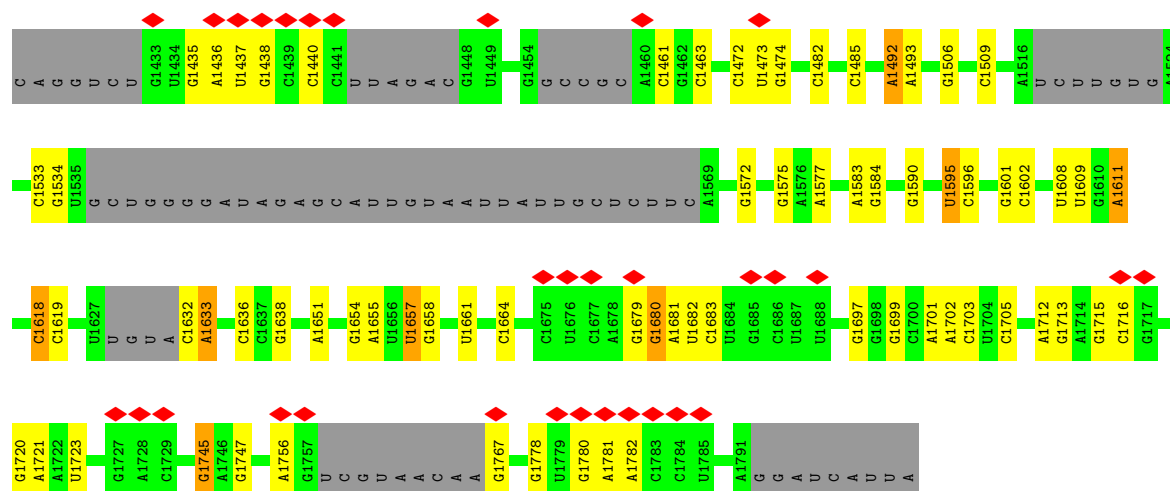


- Molecule 73 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

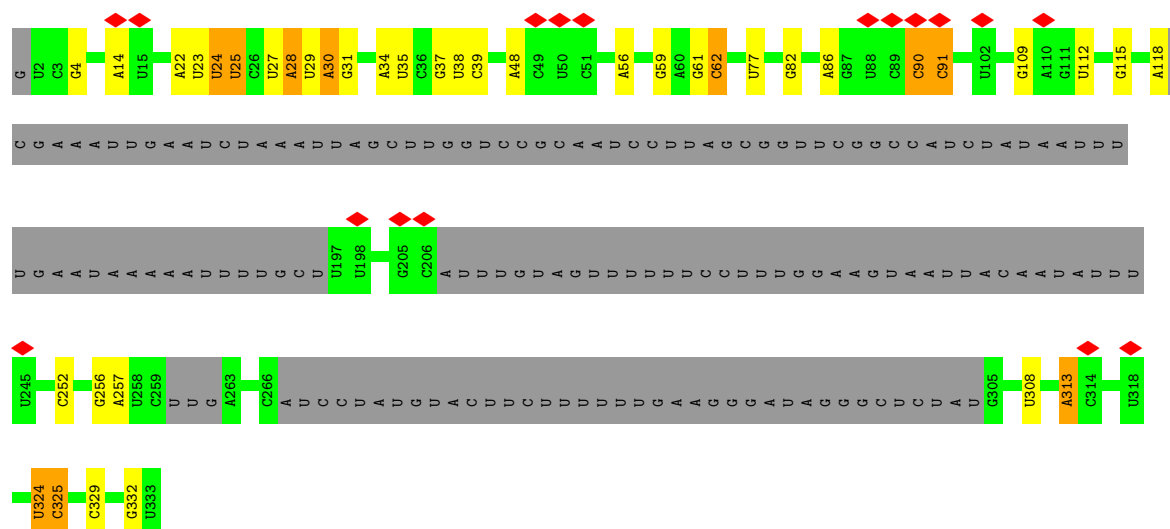


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
73	SI	1	32	10	5	14	3	0

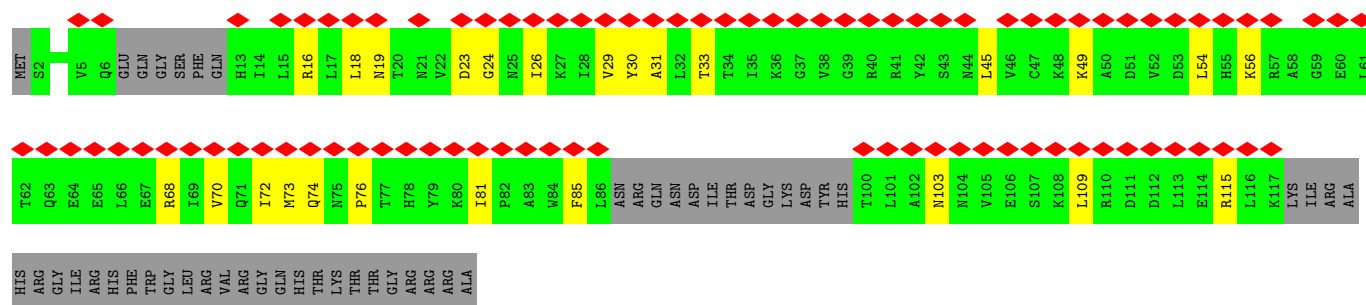




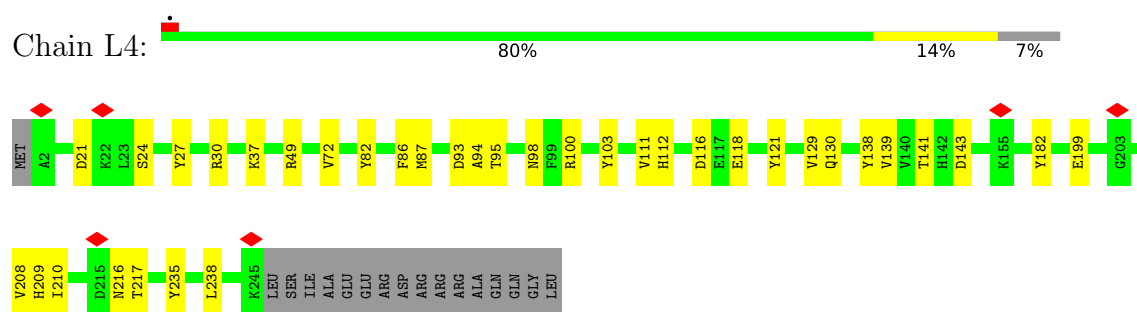
- Molecule 3: TPA: *Saccharomyces cerevisiae* U3a gene for small nucleolar RNA U3a



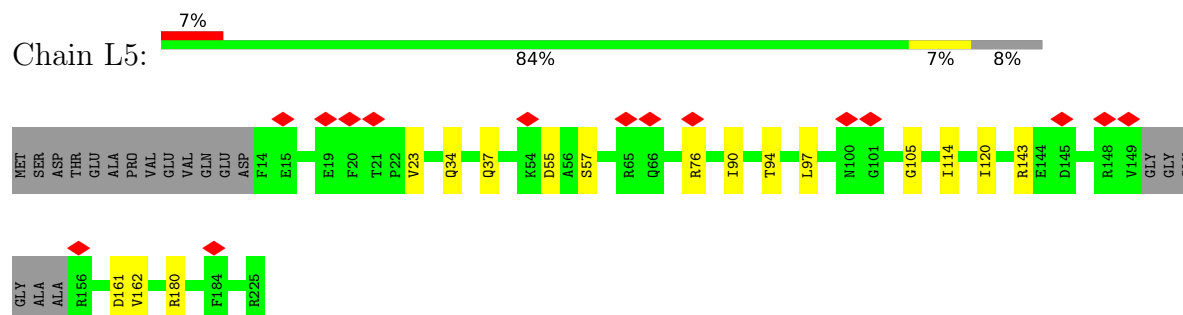
- Molecule 4: 40S ribosomal protein S18-A



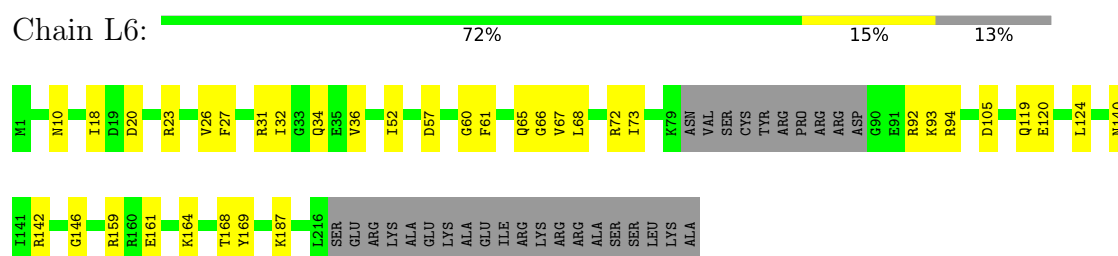
- Molecule 5: 40S ribosomal protein S4-A



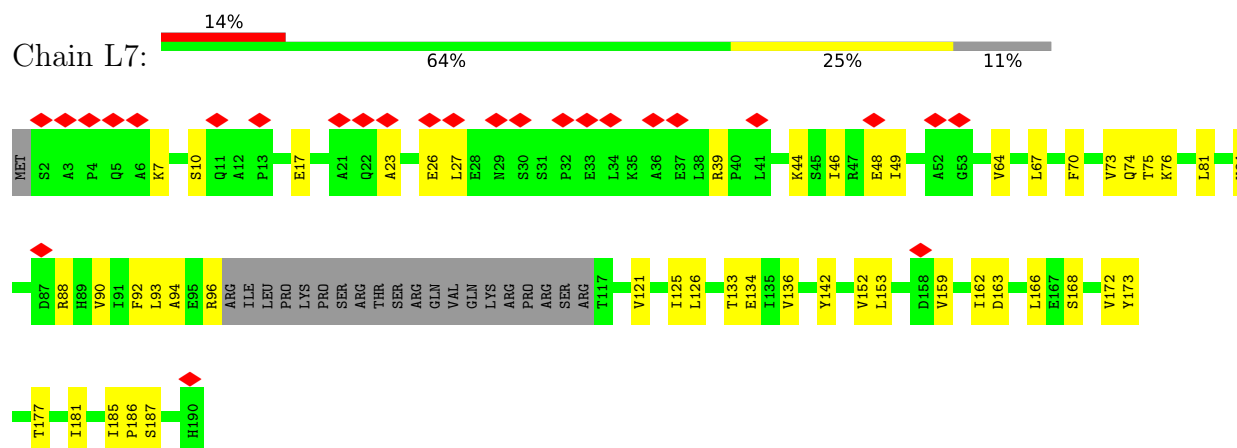
- Molecule 6: 40S ribosomal protein S5



- Molecule 7: 40S ribosomal protein S6-A

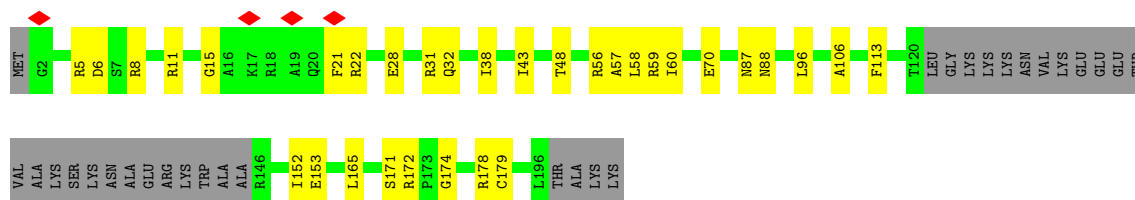


- Molecule 8: 40S ribosomal protein S7-A

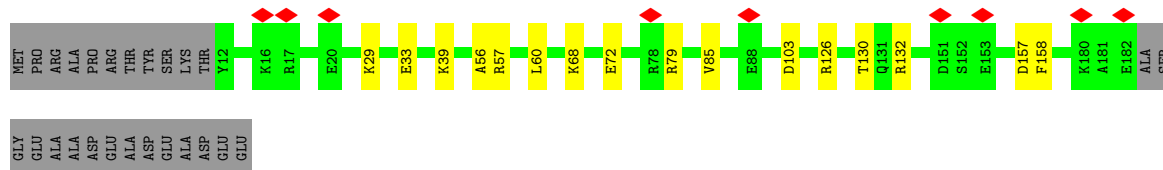
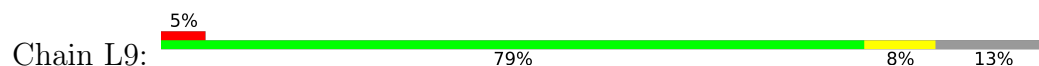


- Molecule 9: 40S ribosomal protein S8-A

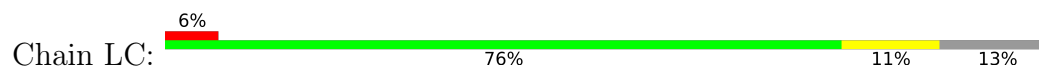




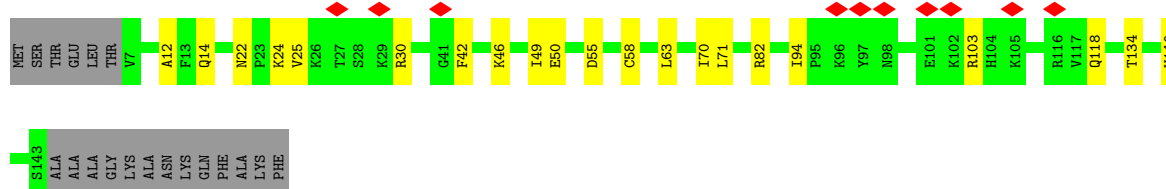
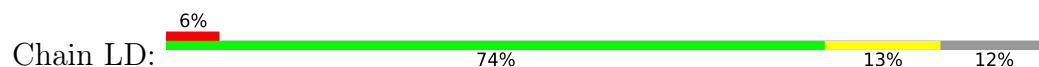
- Molecule 10: 40S ribosomal protein S9-A



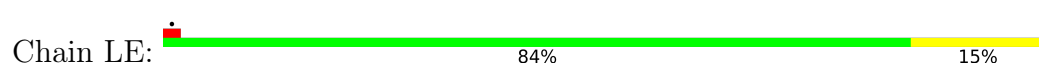
- Molecule 11: 40S ribosomal protein S16-A



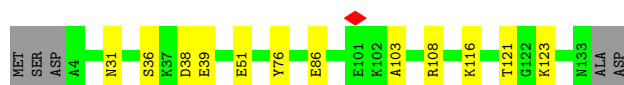
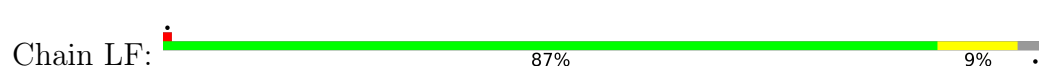
- Molecule 12: 40S ribosomal protein S11-A



- Molecule 13: 40S ribosomal protein S22-A



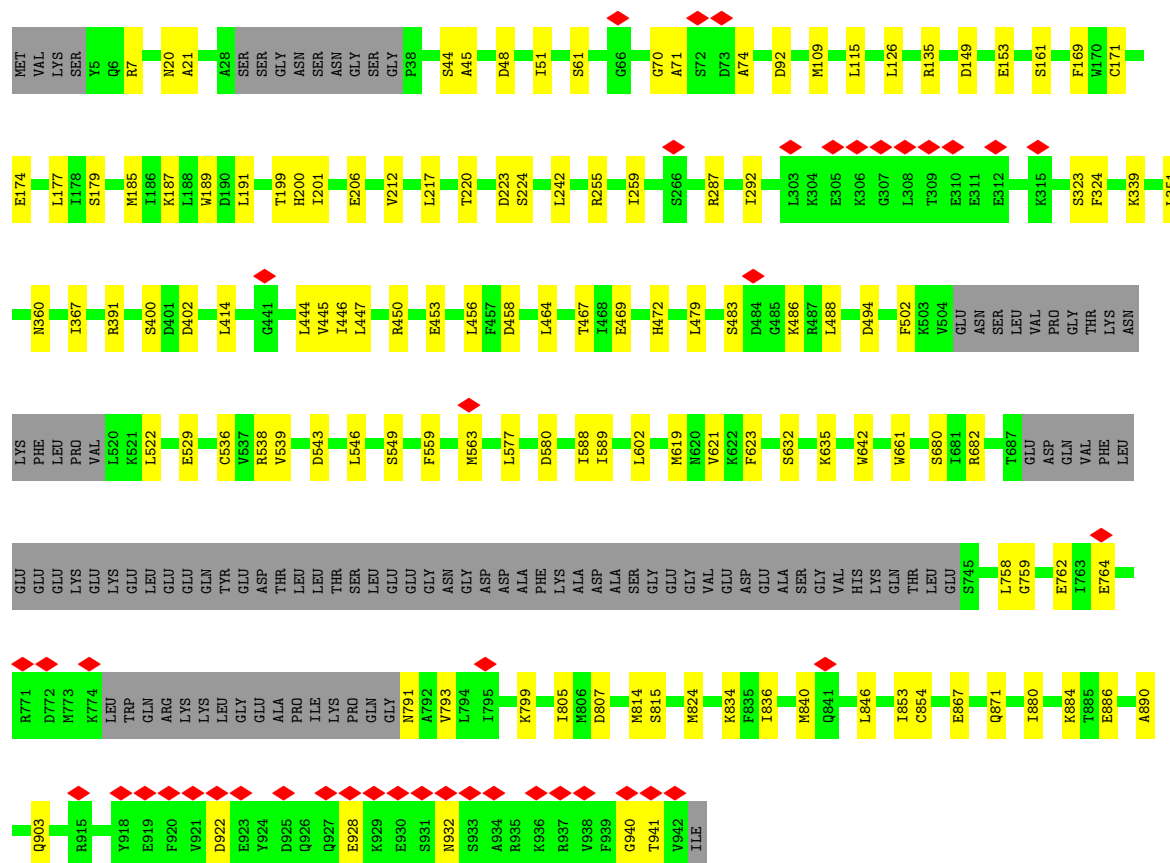
- Molecule 14: 40S ribosomal protein S24-A



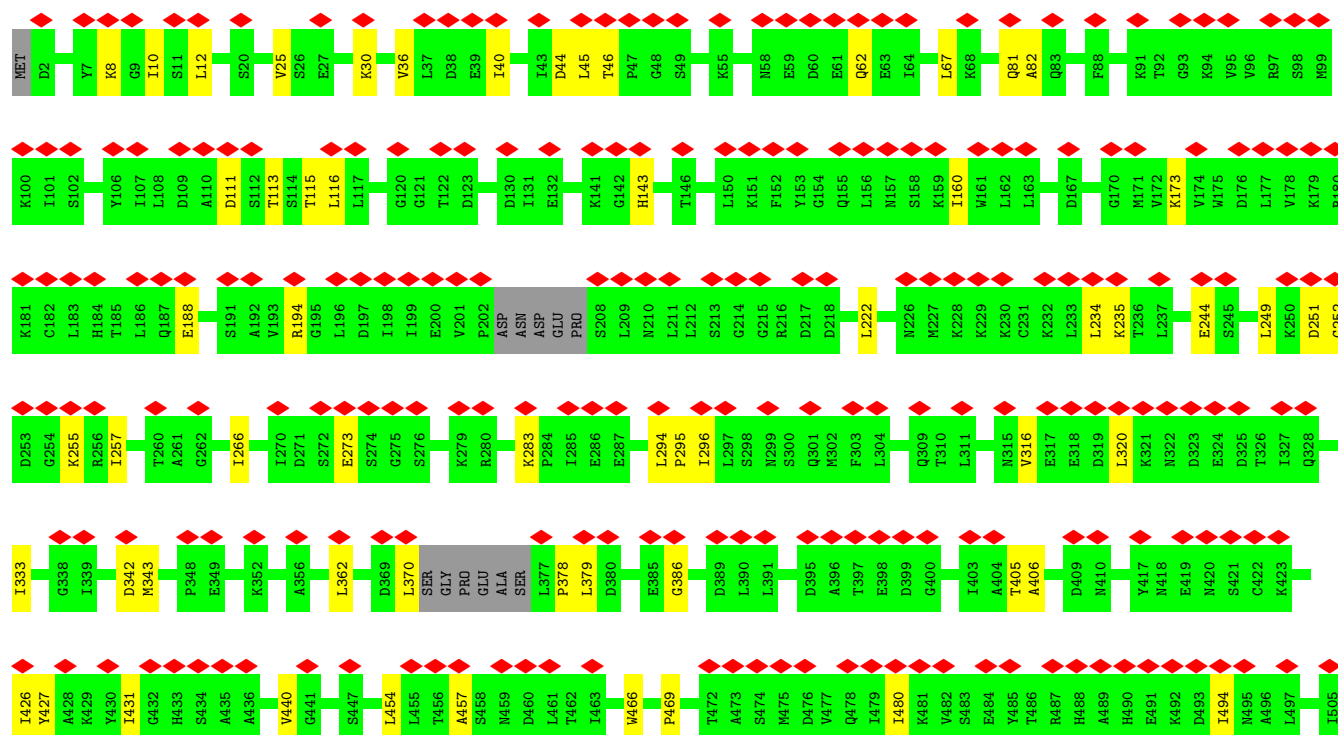
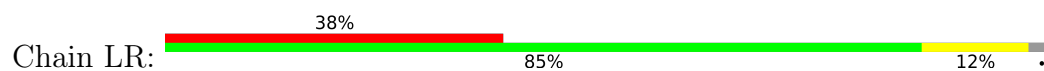
-
- Diagram illustrating the structure of the E3 complex, showing various domains (MET, ASP, ASN, LYS, THR, P6, V12, R29, V30, E34, D35, T36, D52, V55, R64, R65, L66, R67) and their interactions, with red diamonds indicating specific sites of interest.

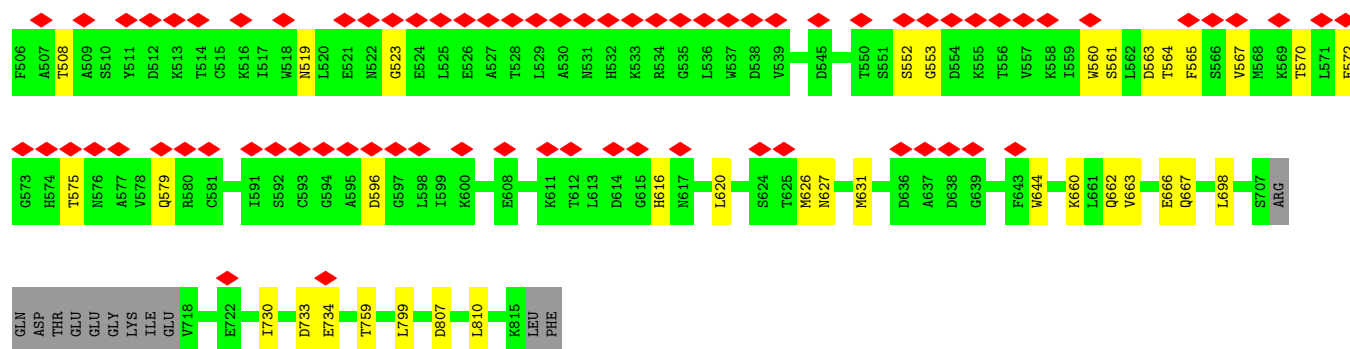
- | | | | | | |
|------|------|------|------|------|------|
| E856 | ASN | I495 | L293 | I153 | MET |
| | THR | T496 | | | THR |
| E861 | GLN | D497 | S302 | K158 | GLN |
| | LEU | L498 | | ASP | SER |
| D864 | SER | | E318 | PRO | LEU |
| | ASP | T509 | K321 | SER | GLY |
| | GLU | Y510 | | GLN | ILE |
| M869 | VAL | | | ALA | GLU |
| | ASN | G686 | Q332 | LYS | Q9 |
| I879 | ASN | F687 | L334 | HIS | |
| Q880 | GLY | V688 | | N166 | S16 |
| N881 | GLU | L689 | | | |
| | ILE | | I341 | Y171 | S27 |
| T896 | LEU | F692 | I342 | R172 | |
| | ASP | | D343 | L173 | S38 |
| | GLY | L574 | C344 | A175 | Q39 |
| | LEU | G581 | I357 | L176 | D40 |
| | VAL | L582 | L358 | T177 | R42 |
| | SER | | | | |
| ASN | ASN | H590 | N366 | A181 | I77 |
| THR | THR | F604 | S367 | E186 | F78 |
| THR | THR | | L372 | I197 | L79 |
| THR | THR | S612 | L373 | | GLN |
| GLY | GLY | L613 | L374 | N200 | GLU |
| ALA | ALA | | | L201 | GLU |
| S817 | | D618 | D378 | K213 | ASN |
| | | | L379 | B214 | N85 |
| D820 | LEU | I622 | T380 | VAL | V69 |
| R821 | ASP | F626 | S381 | THR | T97 |
| F822 | GLY | D627 | S404 | SER | Y98 |
| L826 | GLY | D628 | A405 | LYS | PRO |
| R827 | W734 | | S413 | ASP | GLN |
| K828 | F735 | D634 | I414 | GLN | GLY |
| L829 | T736 | | | HIS | ASP |
| | I737 | | | GLU | ASP |
| SER | | E642 | M418 | H222 | |
| SER | LEU | SER | H419 | | A104 |
| ARG | GLY | GLU | S431 | D233 | F110 |
| GLY | L750 | ASN | A434 | S234 | |
| LYS | | THR | | V235 | I117 |
| SER | K753 | LYS | T437 | N236 | |
| ASP | | THR | T436 | L237 | E127 |
| THR | Y762 | V650 | | | |
| ARG | I763 | | M443 | T244 | F132 |
| ASP | S764 | T654 | | L245 | |
| LYS | | L655 | K447 | T249 | L136 |
| ASN | N769 | D656 | | D265 | A137 |
| THR | Y770 | S657 | V457 | N266 | D138 |
| ASN | | E658 | | | E139 |
| ASP | F774 | I659 | K464 | T282 | V144 |
| ASN | D778 | V662 | M465 | V283 | |
| ASP | I779 | K663 | E466 | Q289 | S147 |
| E848 | | L664 | L473 | L292 | E148 |
| D849 | T788 | I685 | | | R152 |
| E850 | THR | | | | |
| E851 | VAL | I671 | | | |
| D852 | | | | | |

- [illegible]



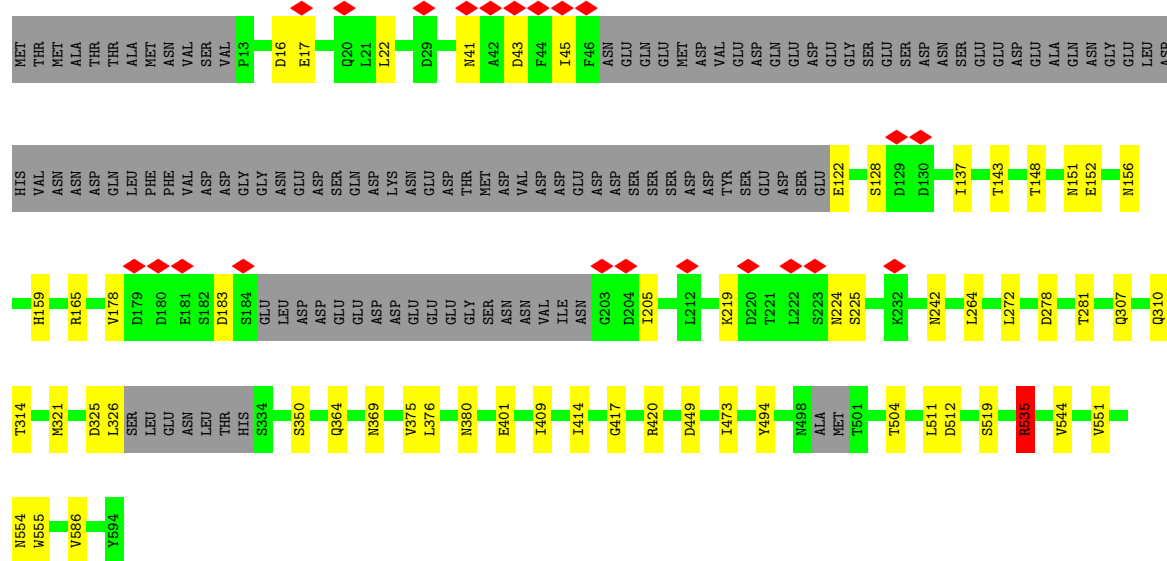
• Molecule 26: U3 small nucleolar RNA-associated protein 13





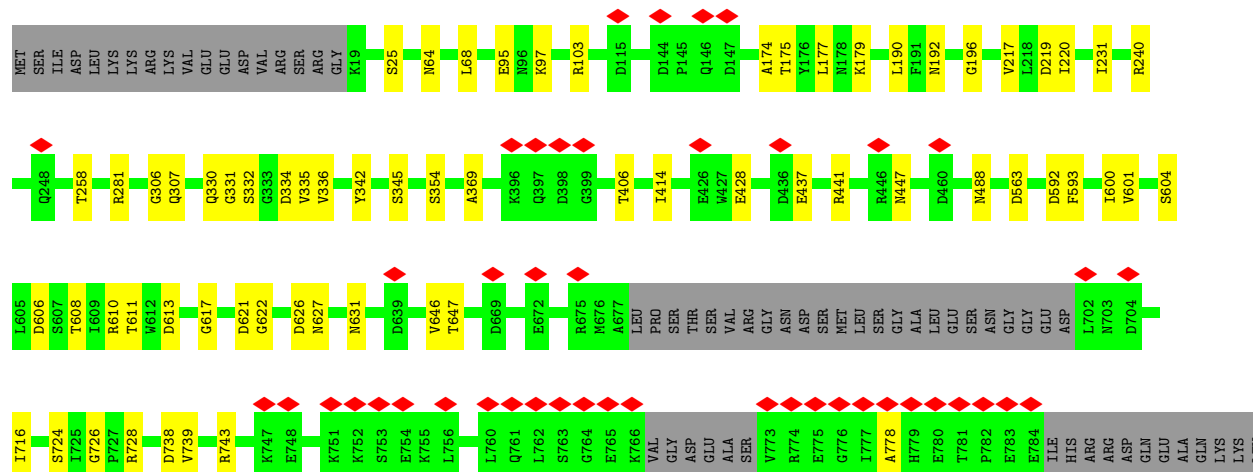
• Molecule 27: U3 small nucleolar RNA-associated protein 18

Chain LS: 71% 9% 19%



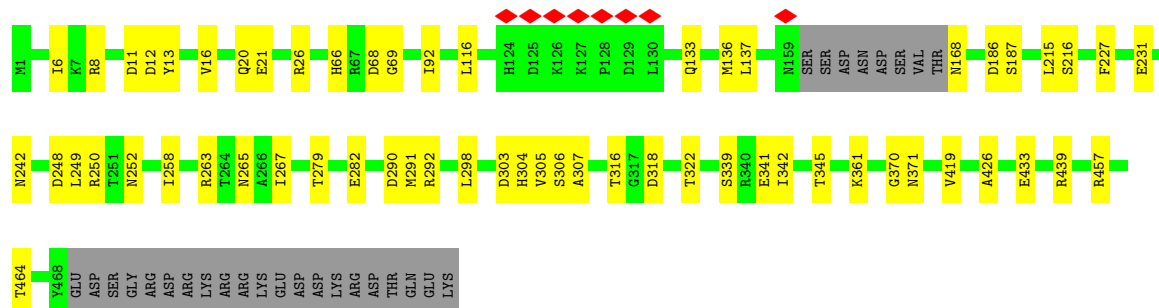
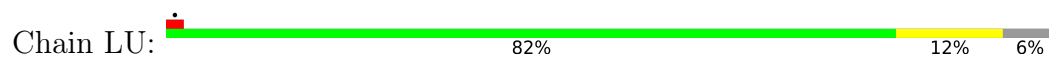
• Molecule 28: U3 small nucleolar RNA-associated protein 21

Chain LT: 84% 9% 7%

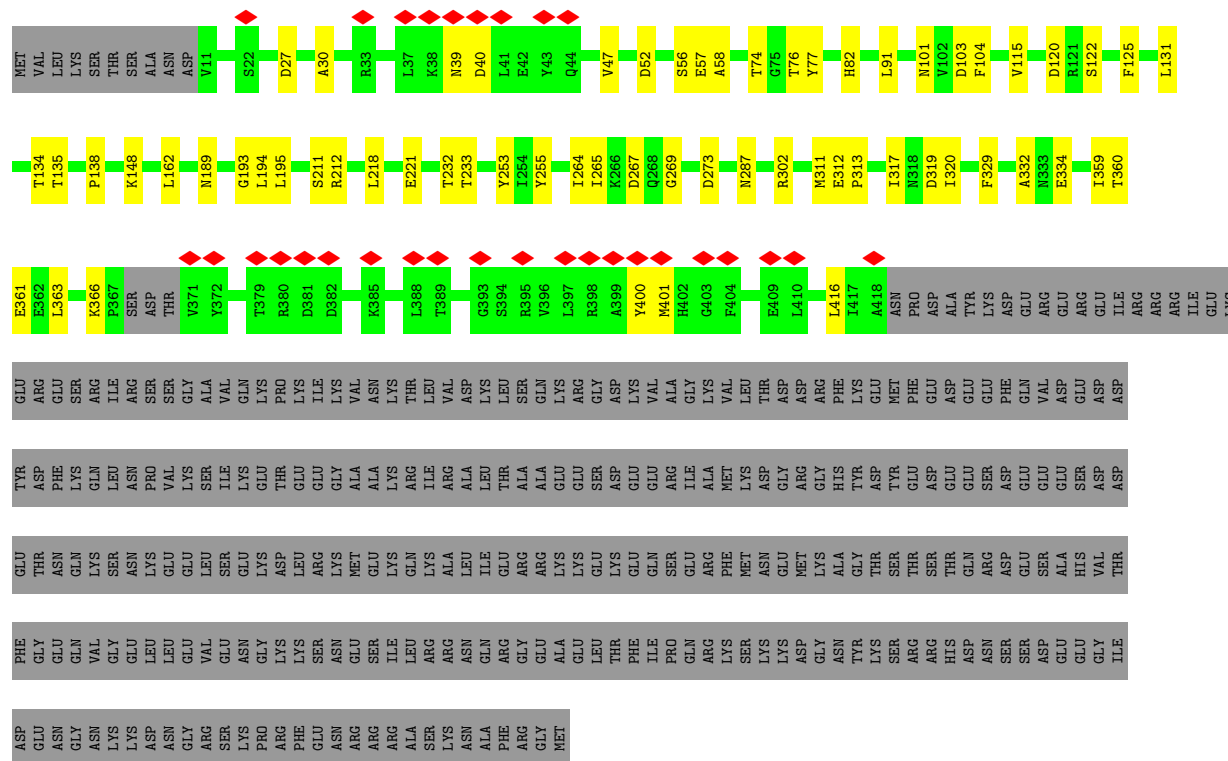




• Molecule 29: Protein SOF1



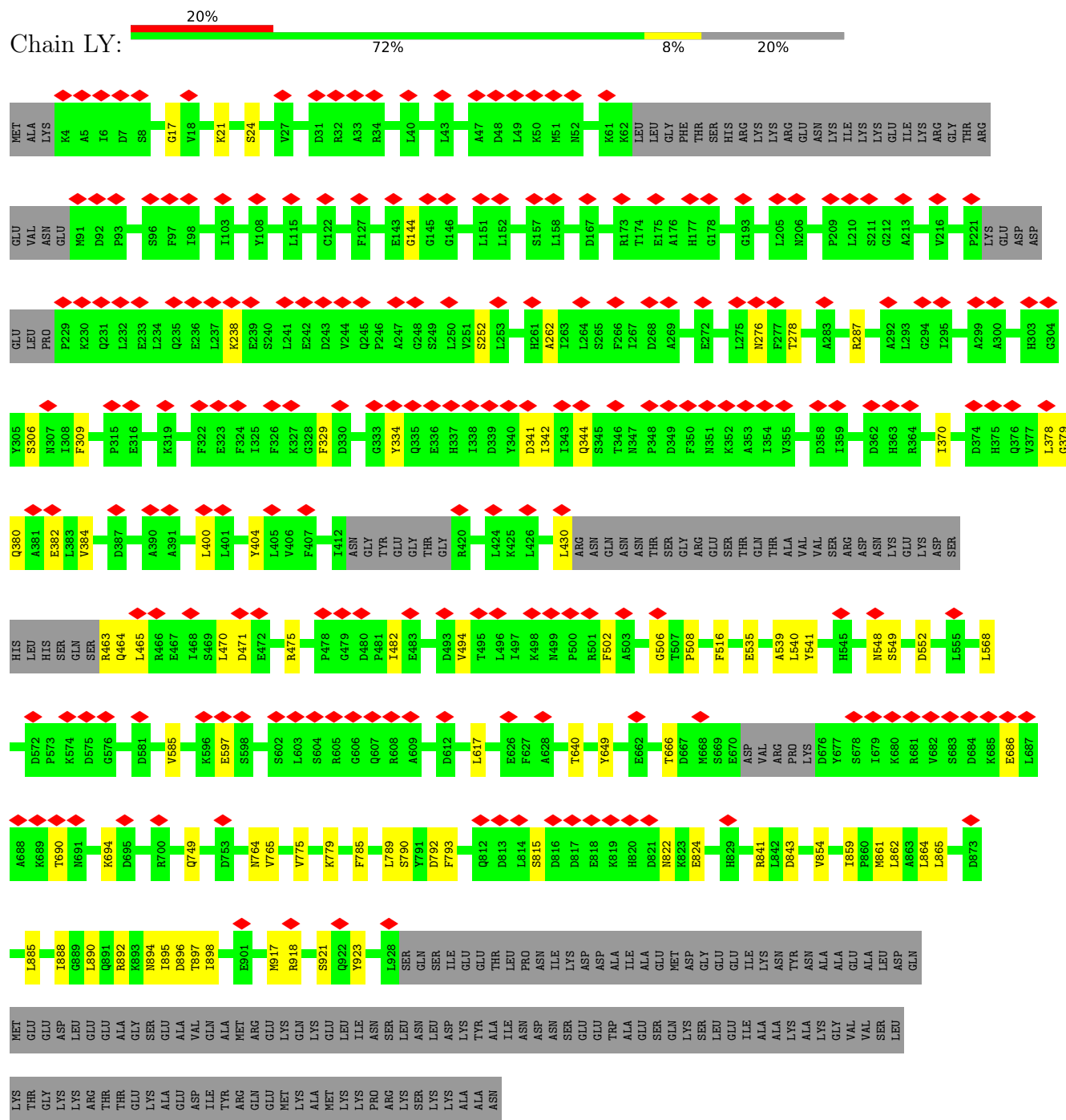
• Molecule 30: Ribosome biogenesis protein ENP2



• Molecule 31: U3 small nucleolar RNA-associated protein 7

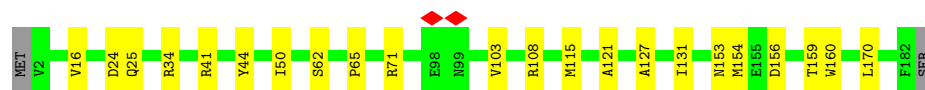


Chain LY:

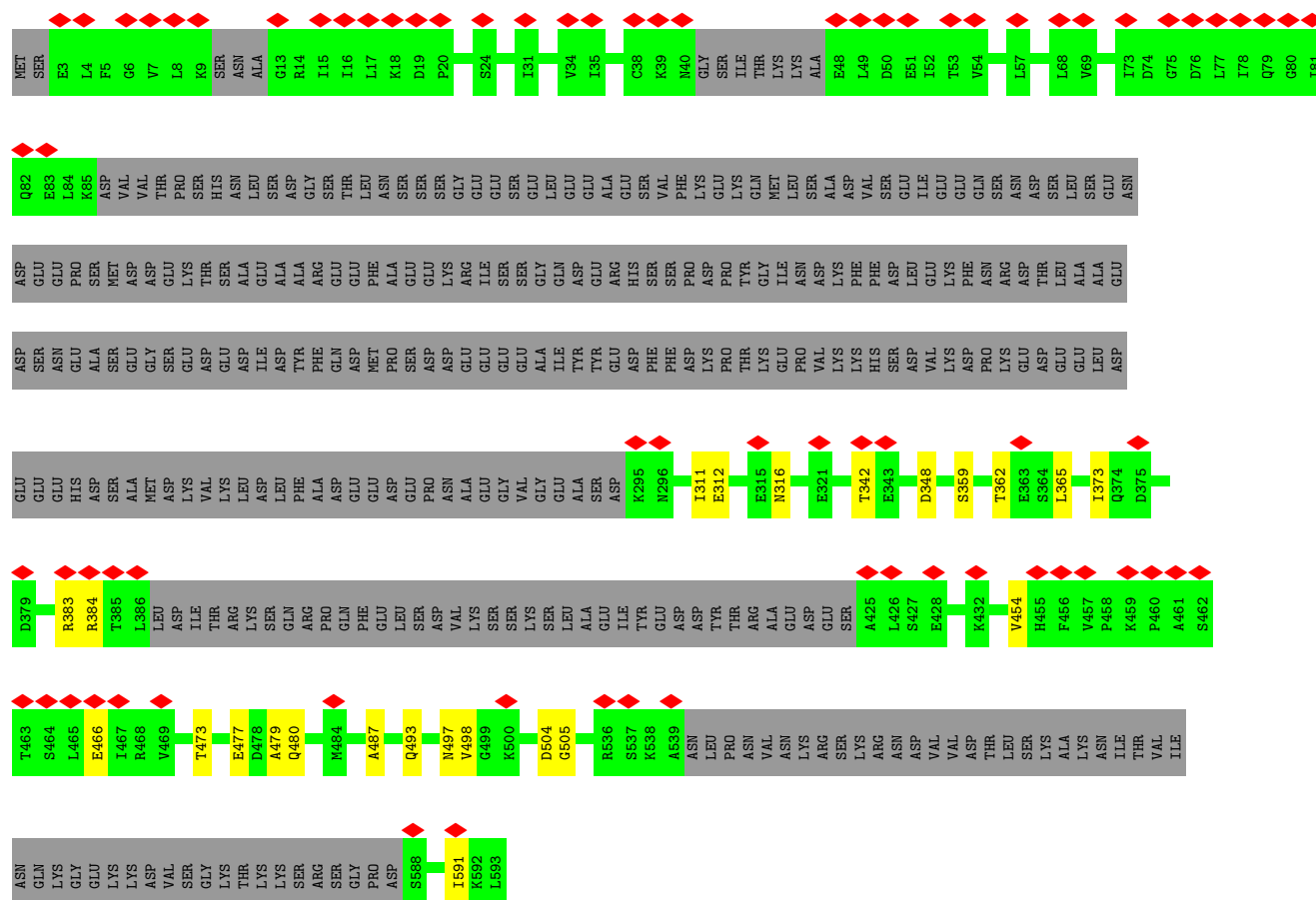


Chain LZ:

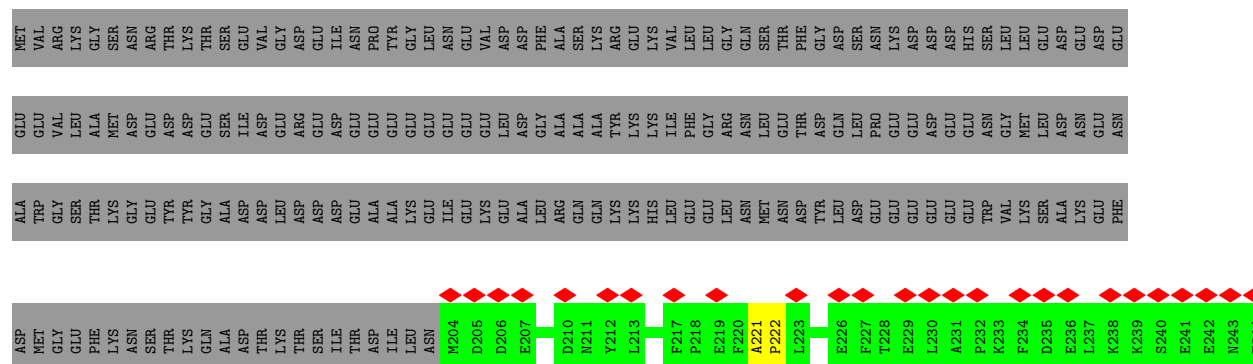
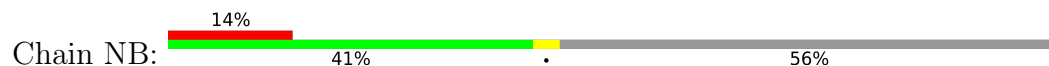


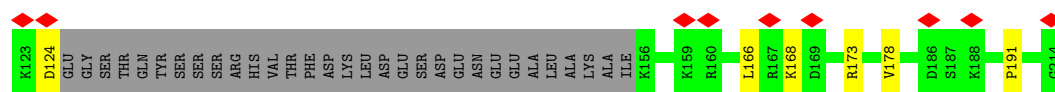


- Molecule 34: U3 small nucleolar RNA-associated protein MPP10

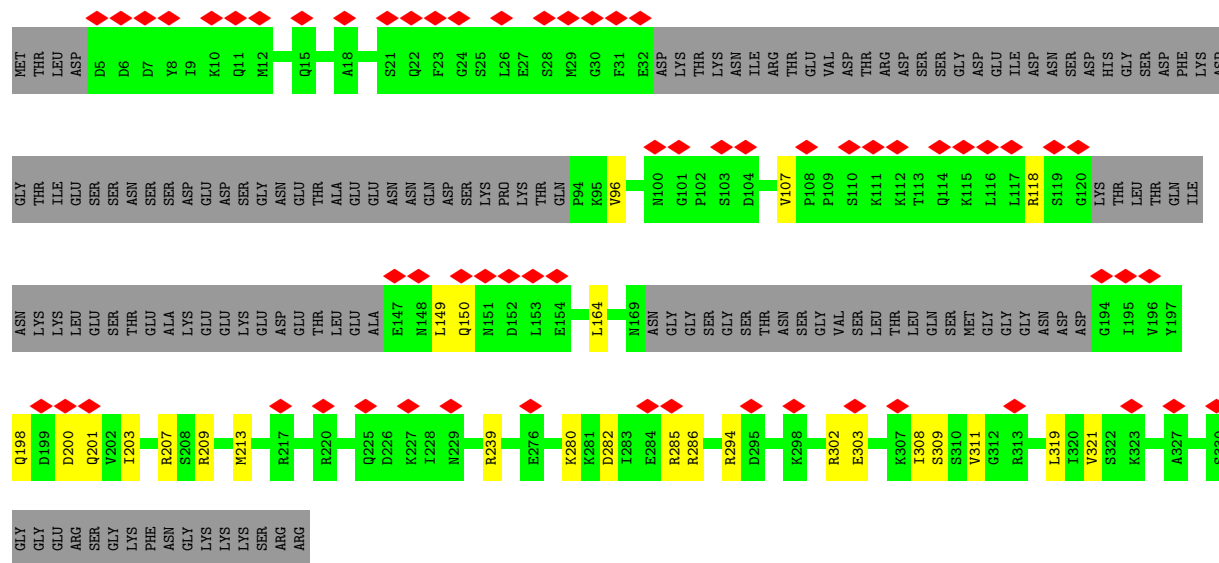


- Molecule 35: Something about silencing protein 10

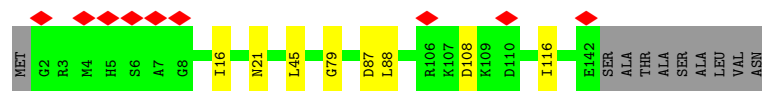
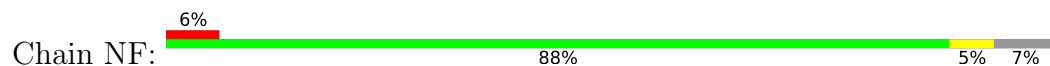




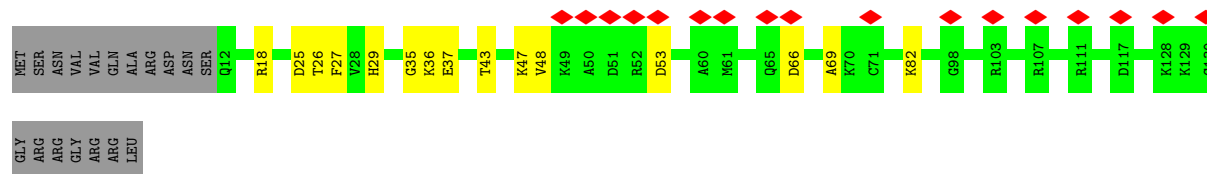
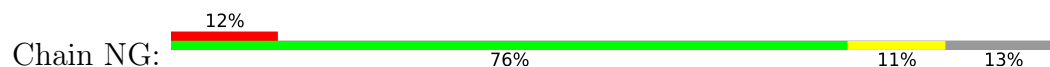
- Molecule 38: Protein FAF1



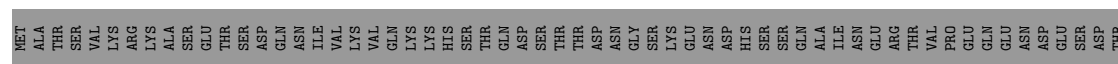
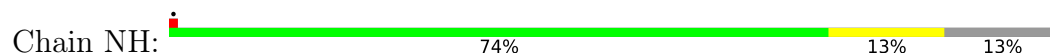
- Molecule 39: 40S ribosomal protein S13

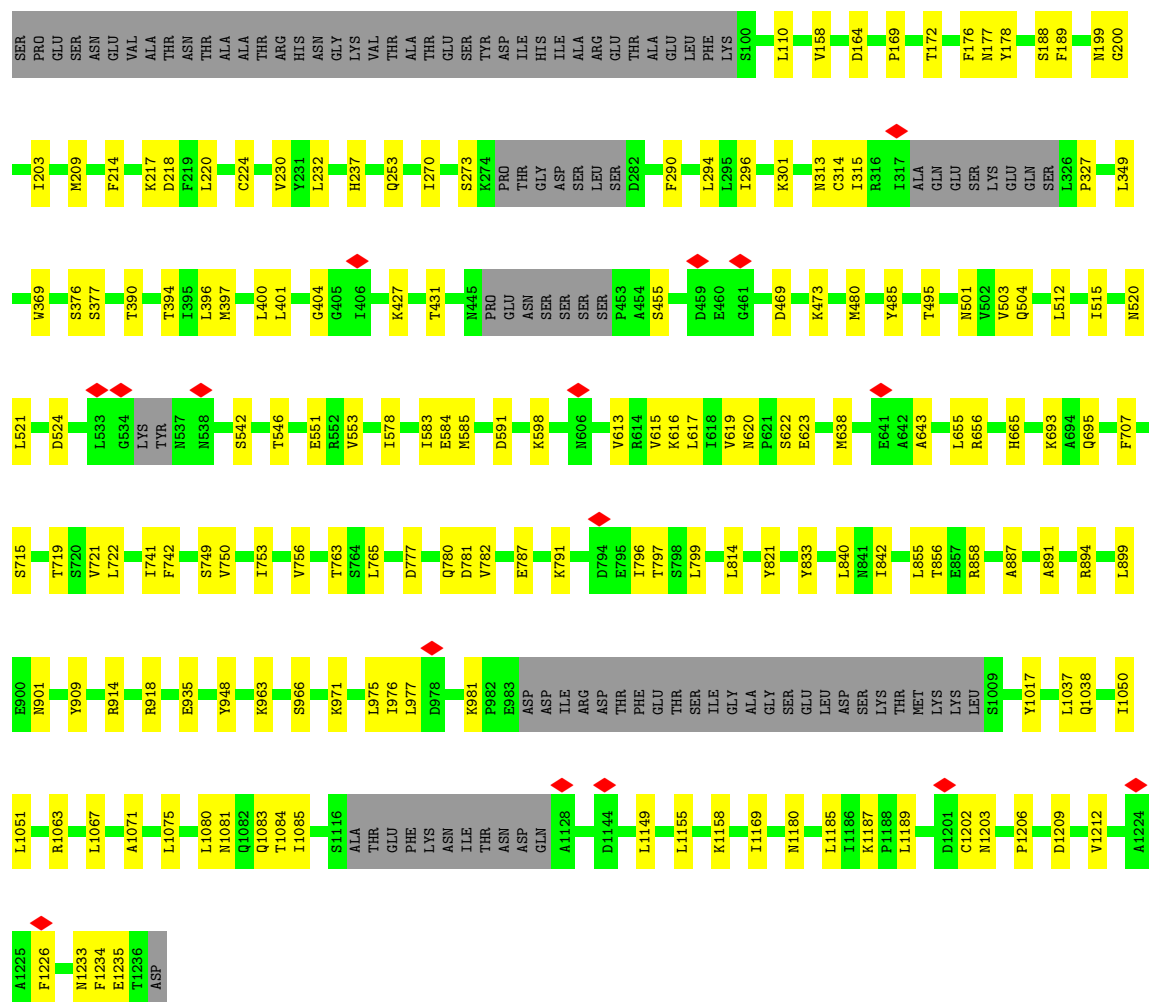


- Molecule 40: 40S ribosomal protein S14-A

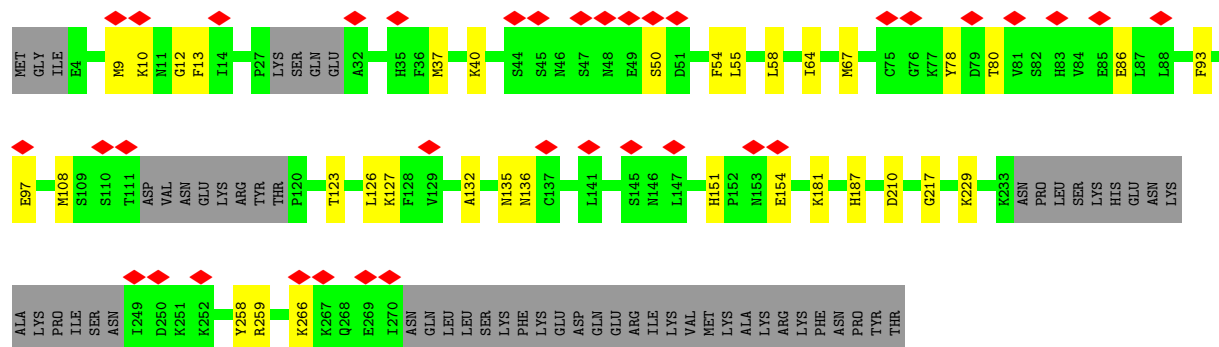
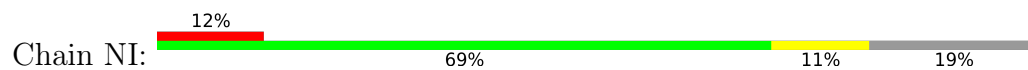


- Molecule 41: U3 small nucleolar RNA-associated protein 22

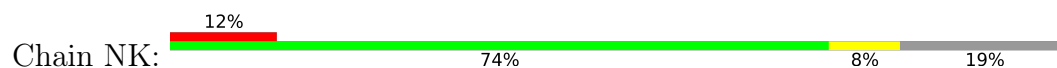


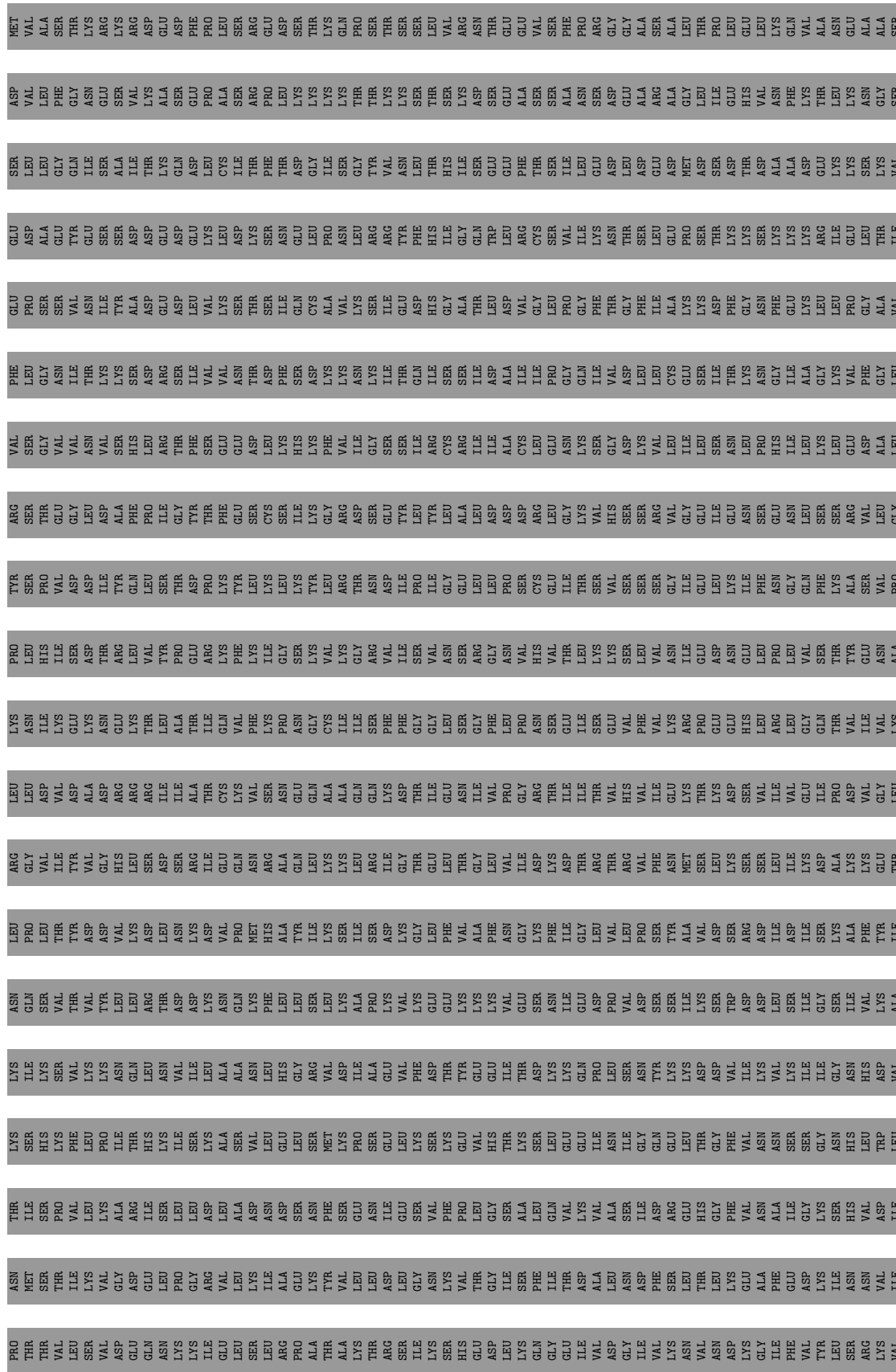


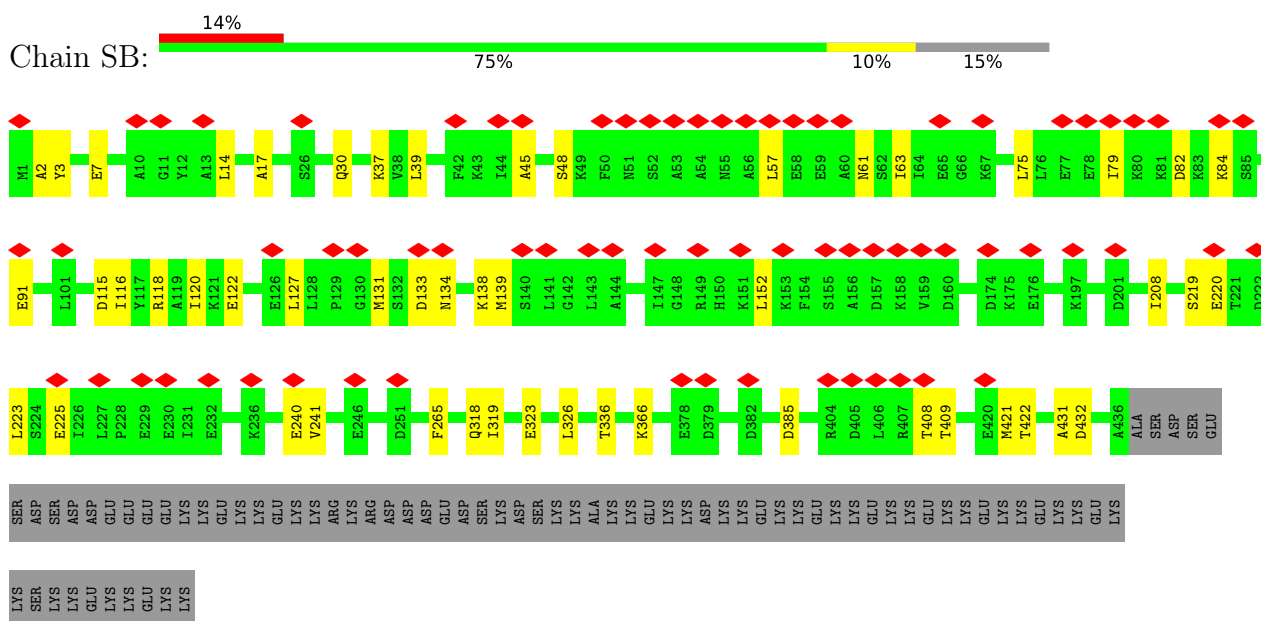
• Molecule 42: Ribosomal RNA-processing protein 7



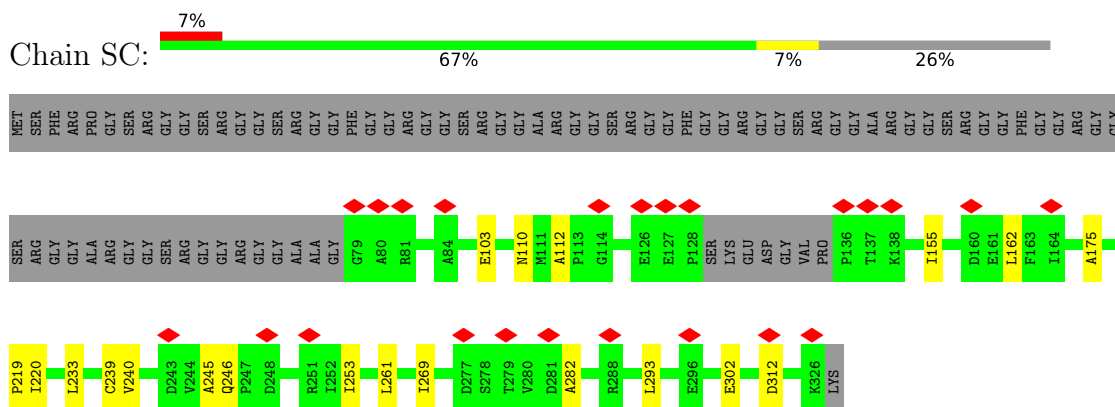
• Molecule 43: KRR1 small subunit processome component



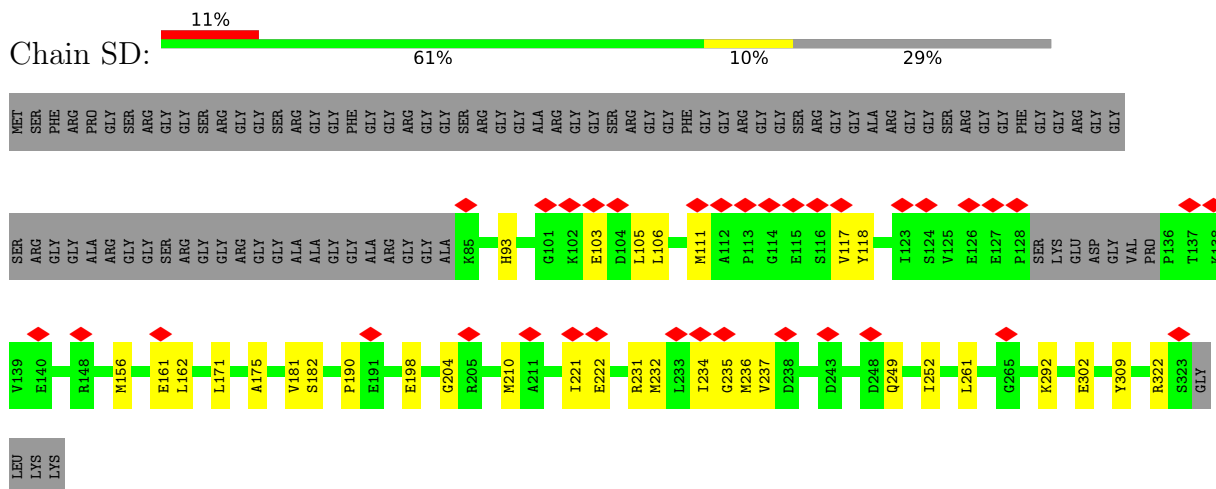




- Molecule 51: rRNA 2'-O-methyltransferase fibrillar

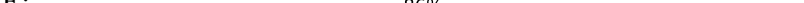


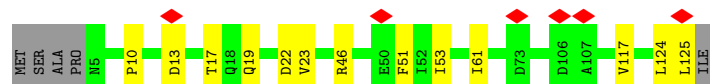
- Molecule 51: rRNA 2'-O-methyltransferase fibrillar

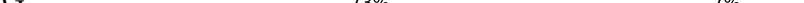


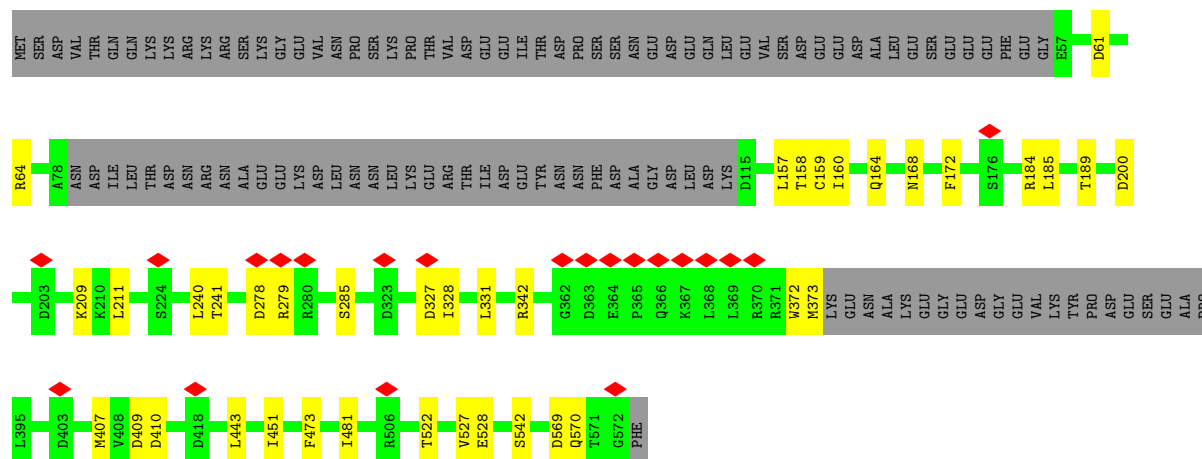
- Molecule 52: 13 kDa ribonucleoprotein-associated protein



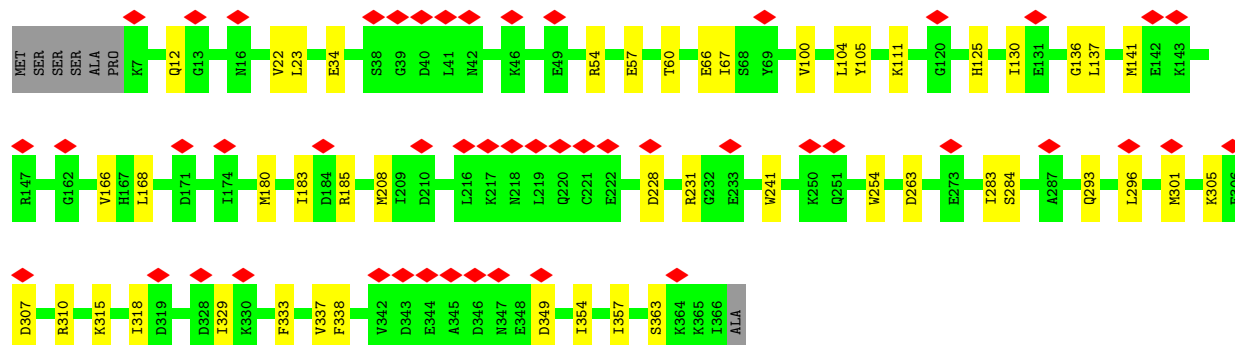
- Chain SF: 

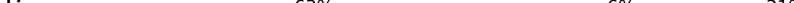


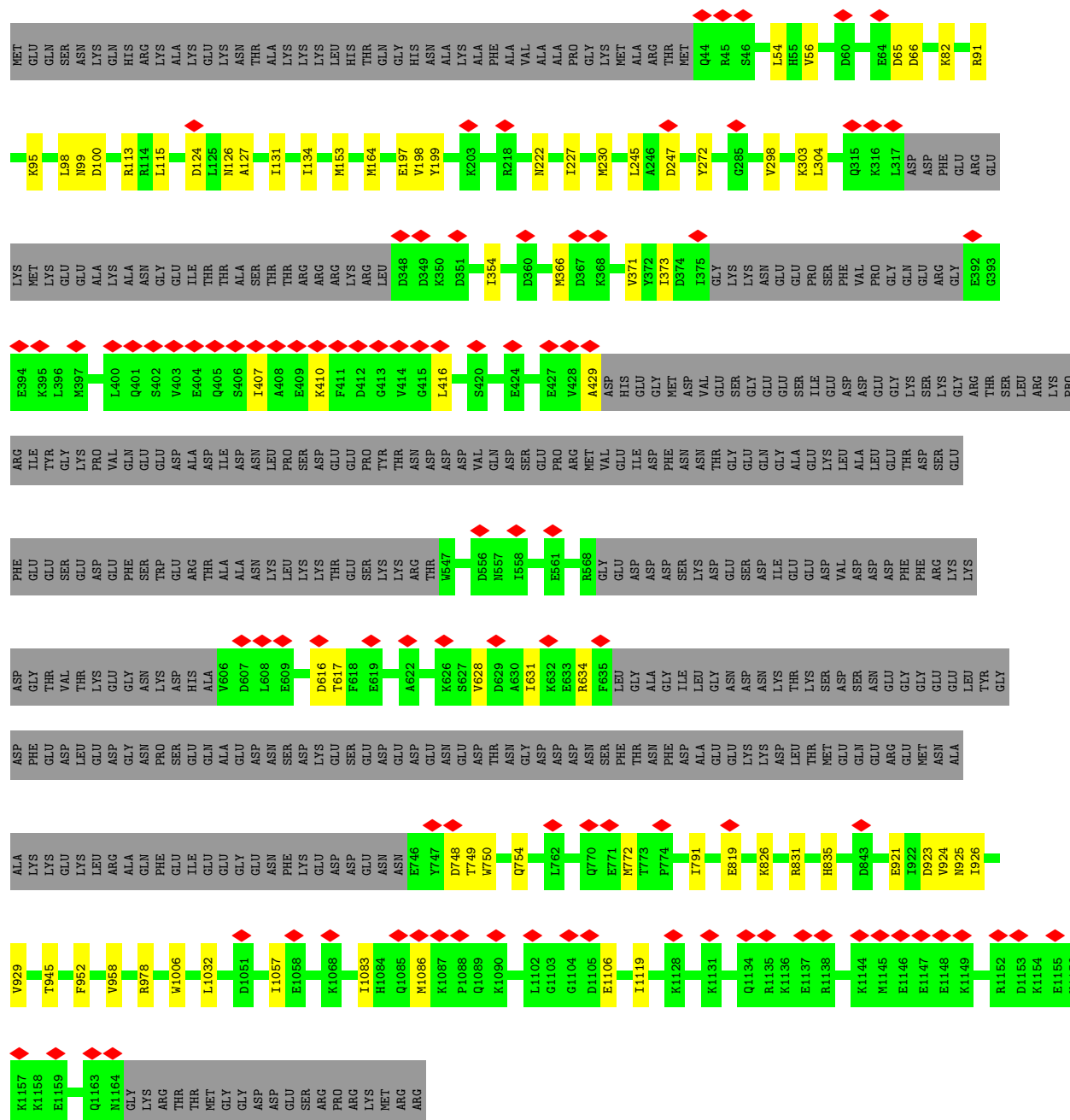
- Chain SG:  73% 7% 20%



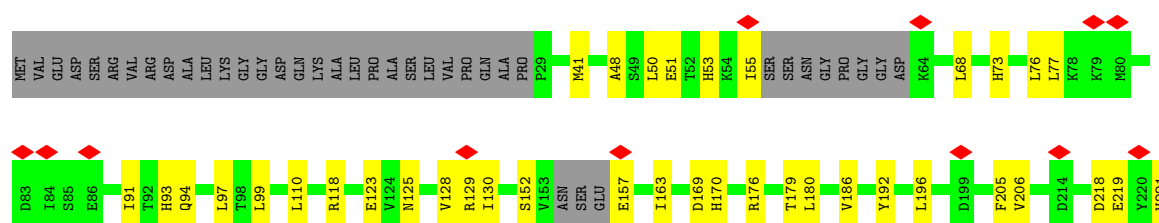
- Chain SH: 

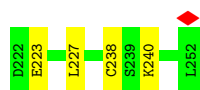


- Chain SI: 



• Molecule 56: Ribosomal RNA small subunit methyltransferase NEP1





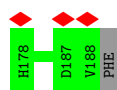
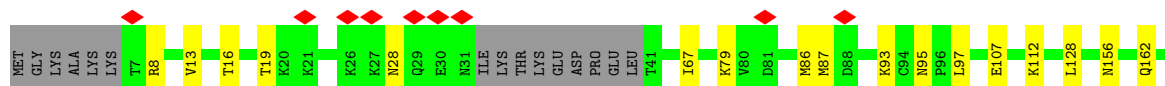
- Molecule 56: Ribosomal RNA small subunit methyltransferase NEP1

Chain SK: 74% 17% 9%



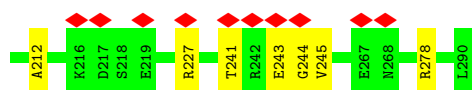
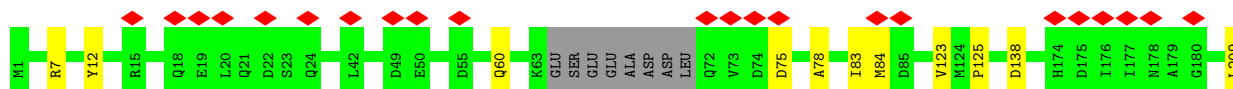
- Molecule 57: rRNA-processing protein FCF1

Chain SL: 6% 83% 9% 8%



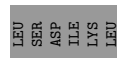
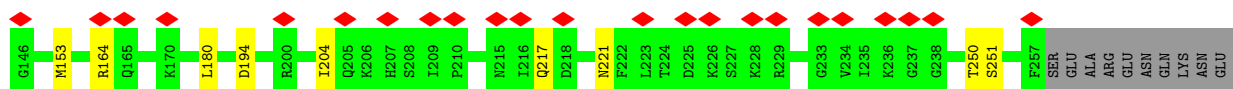
- Molecule 58: U3 small nucleolar ribonucleoprotein protein IMP4

Chain SM: 11% 91% 6% 2%

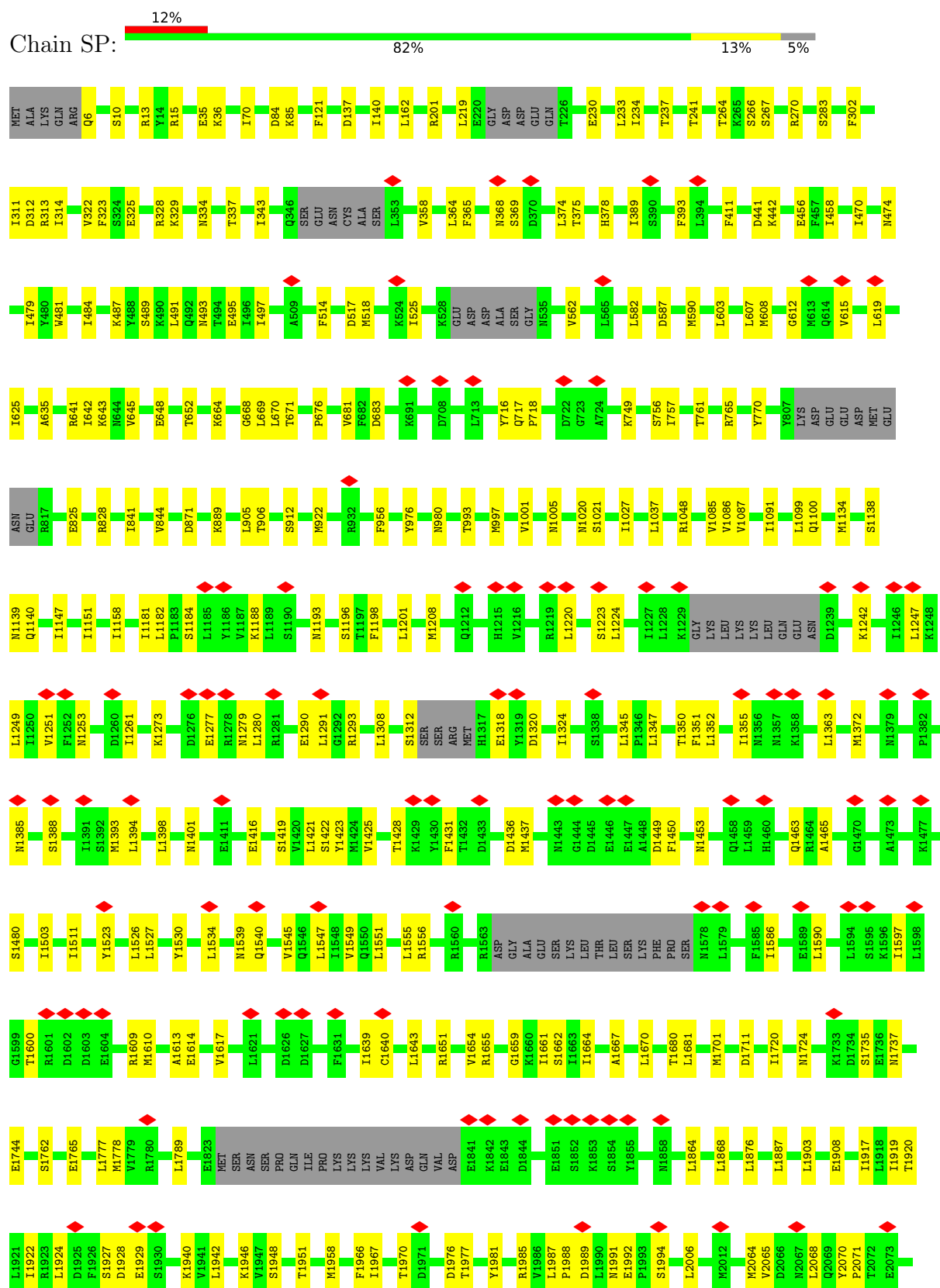


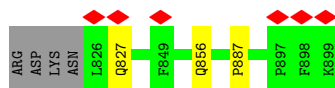
- Molecule 59: Ribosome biogenesis protein UTP30

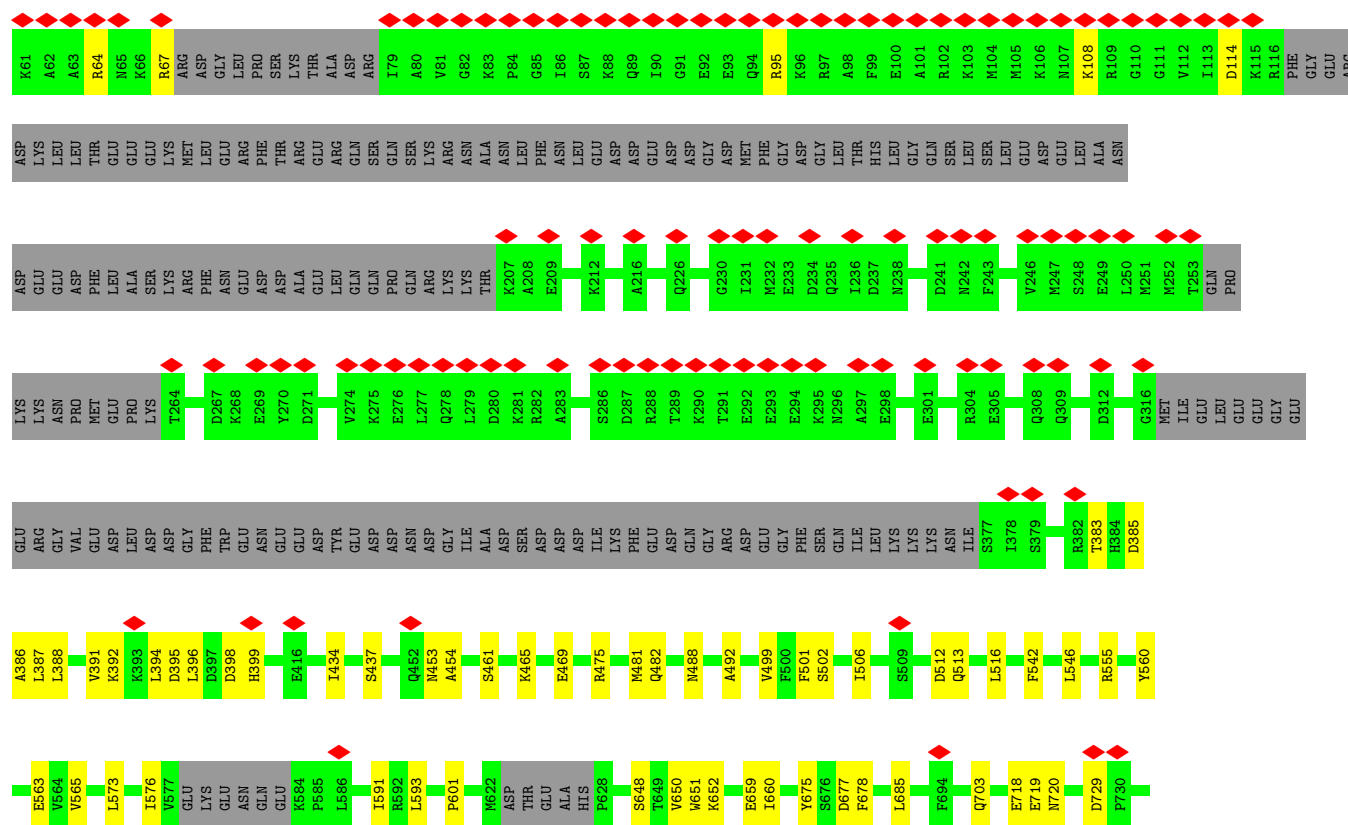
Chain SN: 19% 87% 5% 8%



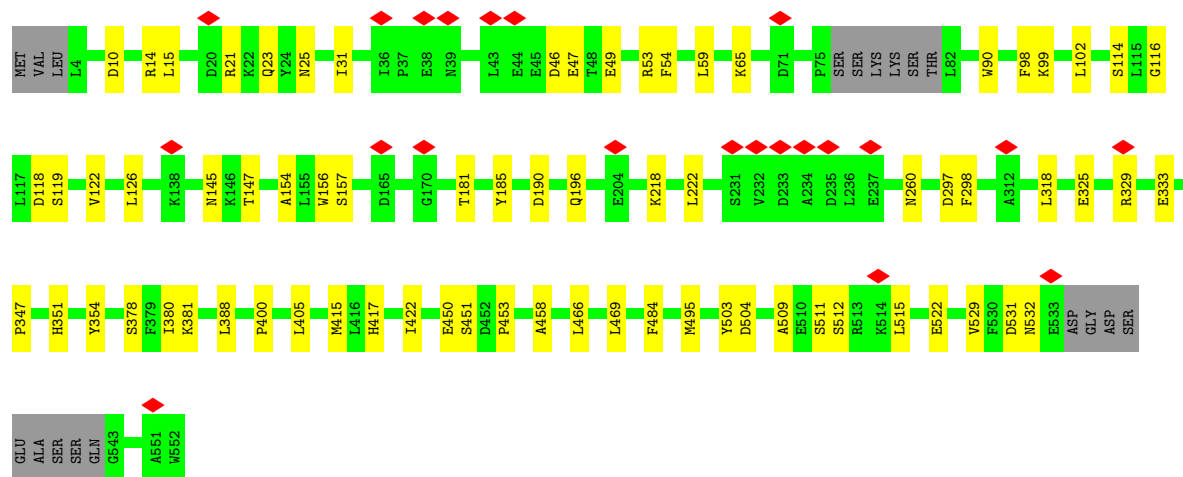
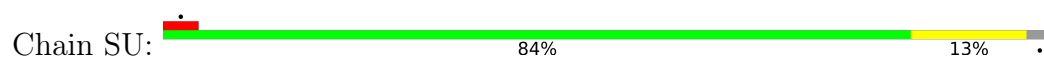
• Molecule 60: U3 small nucleolar RNA-associated protein 20



[illegible]



• Molecule 65: Nucleolar complex protein 4



• Molecule 66: Regulator of rDNA transcription protein 14





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23899	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 ($e^-/\text{\AA}^2$)	60	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	4.462	Depositor
Minimum map value	0.000	Depositor
Average map value	0.110	Depositor
Map value standard deviation	0.179	Depositor
Recommended contour level	0.77	Depositor
Map size (Å)	535.75195, 535.75195, 535.75195	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.063, 1.063, 1.063	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L0	0.12	0/10603	0.25	0/16514
2	L1	0.14	0/28743	0.28	0/44737
3	L2	0.12	0/4143	0.24	0/6440
4	L3	0.17	0/794	0.43	0/1069
5	L4	0.15	0/1977	0.35	0/2664
6	L5	0.15	0/1655	0.33	0/2237
7	L6	0.16	0/1674	0.36	0/2236
8	L7	0.19	0/1369	0.41	0/1846
9	L8	0.16	0/1371	0.37	0/1833
10	L9	0.15	0/1410	0.35	0/1888
11	LC	0.36	1/990 (0.1%)	0.56	3/1335 (0.2%)
12	LD	0.17	0/1138	0.38	0/1533
13	LE	0.17	0/1039	0.37	0/1395
14	LF	0.16	0/1060	0.35	0/1412
15	LG	0.13	0/492	0.31	0/659
16	LH	0.17	0/6592	0.39	0/8924
17	LI	0.14	0/3835	0.35	0/5263
18	LJ	0.16	0/3993	0.34	0/5413
19	LK	0.15	0/1085	0.32	0/1463
20	LL	0.13	0/4052	0.30	0/5501
21	LM	0.13	0/9462	0.32	1/13078 (0.0%)
22	LN	0.15	0/5359	0.31	0/7255
23	LO	0.16	0/6773	0.32	0/9164
24	LP	0.13	0/3288	0.29	0/4419
25	LQ	0.16	1/6837 (0.0%)	0.32	0/9227
26	LR	0.13	0/6313	0.31	0/8551
27	LS	0.16	0/3866	0.30	1/5239 (0.0%)
28	LT	0.15	0/7015	0.32	0/9479
29	LU	0.16	0/3835	0.32	0/5162
30	LV	0.18	0/3360	0.37	0/4549
31	LW	0.15	0/4321	0.32	0/5832
32	LX	0.15	0/6852	0.34	0/9258

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LY	0.14	0/6292	0.33	0/8556
33	LZ	0.14	0/1553	0.31	0/2089
34	NA	0.14	0/2090	0.34	0/2817
35	NB	0.13	0/1891	0.32	0/2541
36	NC	0.14	0/783	0.35	0/1056
37	ND	0.13	0/613	0.33	0/811
38	NE	0.12	0/1662	0.32	0/2212
39	NF	0.13	0/1158	0.32	0/1559
40	NG	0.15	0/886	0.33	0/1194
41	NH	0.15	0/8899	0.32	0/12035
42	NI	0.17	0/1994	0.37	0/2684
43	NK	0.14	0/2144	0.34	0/2880
44	NM	0.14	0/1862	0.31	0/2494
45	NN	0.11	0/1953	0.29	0/2646
46	NQ	0.15	0/605	0.33	0/817
47	NV	0.22	0/64	0.39	0/81
48	OA	0.10	0/892	0.27	0/1241
49	SA	0.12	0/3082	0.28	0/4151
50	SB	0.15	0/3396	0.33	0/4576
51	SC	0.15	0/1906	0.31	0/2570
51	SD	0.18	0/1852	0.37	0/2500
52	SE	0.15	0/928	0.31	0/1262
52	SF	0.14	0/928	0.34	0/1262
53	SG	0.14	0/3744	0.31	0/5040
54	SH	0.15	0/2832	0.36	0/3825
55	SI	0.15	0/6719	0.33	0/9043
56	SJ	0.15	0/1703	0.35	0/2295
56	SK	0.16	0/1822	0.37	0/2462
57	SL	0.15	0/1406	0.33	0/1890
58	SM	0.15	0/2337	0.33	0/3148
59	SN	0.14	0/2088	0.34	0/2808
60	SP	0.13	0/18707	0.31	0/25354
61	SQ	0.14	0/1302	0.31	0/1728
62	SR	0.16	0/804	0.34	0/1074
63	SS	0.16	0/2307	0.43	2/3091 (0.1%)
64	ST	0.14	0/4513	0.31	0/6075
65	SU	0.14	0/4480	0.31	0/6073
66	SV	0.15	0/875	0.36	0/1206
67	SW	0.15	0/1591	0.34	0/2143
68	SY	0.14	0/1978	0.36	0/2616
69	SZ	0.13	0/1326	0.33	0/1859
All	All	0.15	2/253263 (0.0%)	0.32	7/351339 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
27	LS	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	LC	126	PRO	CG-CD	-8.60	1.21	1.50
25	LQ	255	ARG	C-N	6.61	1.36	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	LC	126	PRO	N-CD-CG	-10.40	87.60	103.20
11	LC	126	PRO	CA-N-CD	-9.81	98.26	112.00
21	LM	1021	PRO	CA-N-CD	-9.05	99.33	112.00
11	LC	126	PRO	CA-CB-CG	-5.87	93.35	104.50
63	SS	313	PHE	CA-C-N	-5.45	113.03	119.84
63	SS	313	PHE	C-N-CA	-5.45	113.03	119.84
27	LS	535	ARG	CG-CD-NE	5.14	123.32	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	LS	535	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L0	9483	0	4770	32	0
2	L1	25709	0	12967	140	0
3	L2	3712	0	1882	18	0
4	L3	786	0	823	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L4	1936	0	2019	23	0
6	L5	1635	0	1697	11	0
7	L6	1653	0	1750	26	0
8	L7	1347	0	1406	32	0
9	L8	1348	0	1366	25	0
10	L9	1388	0	1467	11	0
11	LC	973	0	1029	12	0
12	LD	1112	0	1179	16	0
13	LE	1022	0	1060	18	0
14	LF	1046	0	1114	9	0
15	LG	490	0	529	4	0
16	LH	6465	0	6415	97	0
17	LI	3792	0	2859	33	0
18	LJ	3911	0	3906	46	0
19	LK	1068	0	1120	14	0
20	LL	3982	0	3983	58	0
21	LM	9380	0	6279	49	0
22	LN	5263	0	5270	53	0
23	LO	6639	0	6524	64	0
24	LP	3220	0	3272	30	0
25	LQ	6707	0	6738	80	0
26	LR	6207	0	6247	62	0
27	LS	3793	0	3770	37	0
28	LT	6876	0	6853	60	0
29	LU	3756	0	3708	47	0
30	LV	3286	0	3208	44	0
31	LW	4237	0	4239	38	0
32	LX	6720	0	6840	86	0
32	LY	6179	0	5745	58	0
33	LZ	1524	0	1567	18	0
34	NA	2075	0	1915	22	0
35	NB	1873	0	1638	15	0
36	NC	777	0	684	12	0
37	ND	609	0	671	11	0
38	NE	1649	0	1669	27	0
39	NF	1135	0	1197	8	0
40	NG	875	0	905	11	0
41	NH	8693	0	8806	100	0
42	NI	1953	0	1933	27	0
43	NK	2107	0	2184	18	0
44	NM	1838	0	1933	22	0
45	NN	1930	0	1738	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	NQ	595	0	609	5	0
47	NV	64	0	72	0	0
48	OA	888	0	484	6	0
49	SA	3035	0	3059	31	0
50	SB	3357	0	3471	47	0
51	SC	1871	0	1916	18	0
51	SD	1817	0	1857	24	0
52	SE	916	0	964	4	0
52	SF	916	0	964	10	0
53	SG	3672	0	3690	24	0
54	SH	2781	0	2878	35	0
55	SI	6577	0	6743	64	0
56	SJ	1678	0	1756	30	0
56	SK	1793	0	1874	31	0
57	SL	1384	0	1465	14	0
58	SM	2296	0	2325	14	0
59	SN	2053	0	2168	11	0
60	SP	18367	0	17934	211	0
61	SQ	1280	0	1331	22	0
62	SR	792	0	847	10	0
63	SS	2267	0	2300	47	0
64	ST	4448	0	4337	53	0
65	SU	4370	0	4365	55	0
66	SV	869	0	554	7	0
67	SW	1565	0	1647	20	0
68	SY	1953	0	2050	29	0
69	SZ	1314	0	649	1	0
70	L0	3	0	0	0	0
70	L1	26	0	0	0	0
70	L2	2	0	0	0	0
70	NH	1	0	0	0	0
70	SI	1	0	0	0	0
70	SM	1	0	0	0	0
71	NH	31	0	12	1	0
72	NQ	1	0	0	0	0
72	SL	1	0	0	0	0
73	SI	32	0	12	1	0
All	All	245176	0	221207	2066	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 4.

All (2066) 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)
31:LW:433:LEU:HD21	33:LZ:16:VAL:HG21	1.38	1.04
8:L7:67:LEU:HD22	8:L7:94:ALA:HB2	1.39	1.01
2:L1:384:G:O2'	9:L8:22:ARG:NH2	2.01	0.93
36:NC:68:MET:HE1	45:NN:190:ILE:HD13	1.52	0.91
60:SP:2065:VAL:HG21	63:SS:262:LEU:HD13	1.50	0.91
56:SJ:176:ARG:NH2	56:SJ:223:GLU:OE2	2.05	0.89
2:L1:1657:U:OP2	25:LQ:450:ARG:NH1	2.08	0.87
26:LR:10:ILE:HD12	26:LR:370:LEU:HD22	1.55	0.87
2:L1:1509:C:O2'	59:SN:194:ASP:OD2	1.92	0.86
22:LN:448:THR:HG1	22:LN:475:THR:HG1	1.20	0.86
31:LW:552:ARG:NH1	41:NH:791:LYS:O	2.08	0.86
1:L0:296:C:O2'	28:LT:68:LEU:O	1.94	0.84
42:NI:55:LEU:O	42:NI:123:THR:OG1	1.95	0.84
22:LN:140:ASN:OD1	51:SD:292:LYS:NZ	2.11	0.83
19:LK:412:THR:OG1	19:LK:415:GLU:OE1	1.97	0.82
32:LX:368:GLN:NE2	32:LY:380:GLN:OE1	2.12	0.81
10:L9:157:ASP:OD2	10:L9:158:PHE:N	2.14	0.81
55:SI:1086:MET:SD	68:SY:80:SER:OG	2.37	0.81
2:L1:1193:A:HO2'	56:SJ:152:SER:HG	1.24	0.81
2:L1:1534:G:O6	18:LJ:79:ARG:NH2	2.14	0.80
16:LH:139:GLU:OE2	16:LH:172:ARG:NH2	2.15	0.80
2:L1:440:U:OP2	55:SI:222:ASN:ND2	2.13	0.80
37:ND:111:GLU:OE2	65:SU:25:ASN:ND2	2.14	0.80
32:LX:366:THR:OG1	32:LY:380:GLN:NE2	2.14	0.80
2:L1:1482:C:O2'	11:LC:72:GLY:O	2.00	0.80
49:SA:261:GLN:NE2	49:SA:262:ASP:O	2.14	0.79
32:LY:824:GLU:OE2	32:LY:923:TYR:OH	1.99	0.79
2:L1:405:C:OP1	7:L6:93:LYS:NZ	2.15	0.79
7:L6:92:ARG:NH2	30:LV:52:ASP:OD2	2.15	0.79
11:LC:98:ASP:OD2	28:LT:488:ASN:ND2	2.15	0.79
20:LL:153:ILE:HG22	20:LL:163:LEU:HD22	1.64	0.79
56:SK:104:ILE:N	56:SK:246:GLU:OE2	2.16	0.79
60:SP:717:GLN:NE2	60:SP:718:PRO:O	2.16	0.78
2:L1:541:A:OP1	35:NB:556:LYS:NZ	2.16	0.78
4:L3:45:LEU:HD21	4:L3:49:LYS:HE2	1.65	0.78
32:LY:666:THR:HG21	36:NC:117:LEU:HD23	1.65	0.78
32:LY:862:LEU:HD13	32:LY:917:MET:HE1	1.65	0.78
22:LN:448:THR:OG1	22:LN:475:THR:OG1	2.01	0.78
20:LL:520:MET:O	20:LL:524:SER:OG	2.01	0.78
28:LT:885:MET:SD	28:LT:912:TRP:NE1	2.57	0.78
32:LY:287:ARG:NH1	32:LY:471:ASP:O	2.17	0.77
51:SD:309:TYR:OH	68:SY:127:PHE:O	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SH:60:THR:O	64:ST:108:LYS:NZ	2.16	0.77
64:ST:482:GLN:NE2	65:SU:504:ASP:OD1	2.17	0.77
21:LM:356:ALA:O	21:LM:360:ARG:NH1	2.17	0.77
27:LS:165:ARG:NH2	28:LT:219:ASP:OD2	2.16	0.77
57:SL:93:LYS:NZ	57:SL:95:ASN:OD1	2.17	0.77
28:LT:807:VAL:O	67:SW:244:ARG:NH1	2.17	0.77
35:NB:380:ARG:NH2	65:SU:114:SER:O	2.17	0.77
7:L6:10:ASN:ND2	7:L6:124:LEU:O	2.17	0.77
60:SP:1735:SER:OG	60:SP:1737:ASN:OD1	2.01	0.77
1:L0:86:C:N4	16:LH:318:GLU:OE1	2.18	0.77
2:L1:904:G:N2	43:NK:216:ALA:O	2.18	0.77
2:L1:1463:C:O3'	64:ST:64:ARG:NH1	2.18	0.77
2:L1:351:C:O3'	12:LD:103:ARG:NH1	2.18	0.77
2:L1:569:C:O2	62:SR:63:GLN:NE2	2.18	0.77
14:LF:76:TYR:OH	14:LF:86:GLU:OE2	2.01	0.77
26:LR:194:ARG:NH1	26:LR:244:GLU:OE1	2.18	0.77
32:LX:527:HIS:HB3	55:SI:416:LEU:HD11	1.66	0.77
37:ND:114:GLU:OE2	65:SU:25:ASN:ND2	2.17	0.77
41:NH:749:SER:N	41:NH:787:GLU:OE1	2.17	0.77
20:LL:433:THR:OG1	20:LL:467:ASP:OD2	2.03	0.76
29:LU:371:ASN:ND2	57:SL:107:GLU:OE2	2.18	0.76
2:L1:1040:G:O2'	29:LU:433:GLU:OE1	2.02	0.76
17:LI:680:ASP:OD1	19:LK:483:LYS:NZ	2.18	0.75
28:LT:803:ASN:O	28:LT:810:ARG:NH1	2.19	0.75
26:LR:427:TYR:OH	26:LR:469:PRO:O	2.04	0.75
28:LT:827:SER:OG	28:LT:829:ASP:OD1	2.04	0.75
60:SP:668:GLY:O	60:SP:671:THR:OG1	2.04	0.75
2:L1:861:U:O2'	13:LE:56:HIS:O	2.03	0.75
54:SH:111:LYS:NZ	55:SI:921:GLU:OE2	2.18	0.75
4:L3:16:ARG:NH2	4:L3:19:ASN:OD1	2.20	0.75
6:L5:97:LEU:O	6:L5:180:ARG:NH2	2.19	0.75
23:LO:358:SER:OG	23:LO:359:ARG:NH1	2.19	0.75
41:NH:707:PHE:O	41:NH:918:ARG:NH1	2.19	0.75
2:L1:1231:U:HO2'	2:L1:1258:U:HO2'	1.21	0.74
2:L1:1618:C:OP2	23:LO:505:ARG:NH2	2.19	0.74
42:NI:210:ASP:O	46:NQ:80:ARG:NH1	2.20	0.74
2:L1:75:U:O4	60:SP:6:GLN:N	2.20	0.74
29:LU:250:ARG:O	63:SS:447:ASN:ND2	2.20	0.74
4:L3:115:ARG:NH1	34:NA:342:THR:OG1	2.19	0.74
68:SY:167:THR:N	68:SY:170:GLN:OE1	2.21	0.74
1:L0:272:A:O2'	68:SY:228:GLY:O	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L0:337:G:OP1	38:NE:209:ARG:NH2	2.20	0.74
21:LM:22:ARG:NH2	29:LU:20:GLN:O	2.19	0.74
18:LJ:273:ILE:HD13	18:LJ:307:VAL:HG13	1.70	0.74
38:NE:282:ASP:OD2	38:NE:285:ARG:NH1	2.20	0.74
60:SP:1345:LEU:HD21	60:SP:1393:MET:HE2	1.69	0.73
12:LD:12:ALA:O	12:LD:14:GLN:NE2	2.21	0.73
25:LQ:840:MET:HE2	25:LQ:886:GLU:HB2	1.68	0.73
22:LN:216:GLN:NE2	22:LN:219:ASP:OD2	2.21	0.73
60:SP:1948:SER:O	60:SP:1985:ARG:NH2	2.22	0.73
9:L8:59:ARG:NH1	30:LV:334:GLU:OE2	2.21	0.73
32:LY:400:LEU:O	32:LY:404:TYR:OH	2.06	0.73
41:NH:963:LYS:O	41:NH:966:SER:OG	2.05	0.73
32:LX:547:LYS:O	32:LX:637:ARG:NH2	2.21	0.73
28:LT:307:GLN:NE2	50:SB:422:THR:O	2.21	0.73
49:SA:199:TYR:OH	49:SA:223:ILE:O	2.06	0.73
2:L1:318:U:O4	43:NK:295:ARG:NH2	2.21	0.73
17:LI:651:GLU:O	17:LI:655:LEU:HD23	1.89	0.73
24:LP:206:ILE:HG21	63:SS:363:LEU:HD11	1.71	0.73
30:LV:148:LYS:NZ	45:NN:477:ALA:O	2.21	0.73
60:SP:1651:ARG:NH1	60:SP:1744:GLU:OE1	2.22	0.73
14:LF:36:SER:OG	14:LF:38:ASP:OD1	2.06	0.73
60:SP:325:GLU:OE2	60:SP:328:ARG:NH1	2.21	0.73
11:LC:50:GLU:OE1	11:LC:82:ARG:NH2	2.23	0.72
26:LR:362:LEU:HD12	26:LR:405:THR:HG21	1.69	0.72
60:SP:582:LEU:HD11	60:SP:608:MET:HE3	1.71	0.72
29:LU:92:ILE:HD12	29:LU:136:MET:HE3	1.71	0.72
20:LL:115:ASN:OD1	20:LL:131:LEU:N	2.23	0.72
2:L1:331:A:OP1	9:L8:56:ARG:NH1	2.23	0.72
2:L1:1042:G:OP1	29:LU:439:ARG:NH2	2.23	0.72
32:LX:790:SER:OG	32:LY:892:ARG:NH1	2.22	0.72
2:L1:414:C:O2'	32:LX:70:ARG:NH1	2.22	0.71
25:LQ:20:ASN:OD1	25:LQ:339:LYS:NZ	2.22	0.71
27:LS:137:ILE:O	27:LS:143:THR:OG1	2.08	0.71
27:LS:278:ASP:OD2	27:LS:281:THR:OG1	2.07	0.71
7:L6:68:LEU:HD11	30:LV:47:VAL:HG21	1.71	0.71
22:LN:391:VAL:HG23	22:LN:404:MET:HE1	1.70	0.71
23:LO:841:ASP:OD1	25:LQ:903:GLN:NE2	2.23	0.71
56:SJ:51:GLU:OE2	56:SJ:118:ARG:NH1	2.23	0.71
60:SP:1762:SER:OG	60:SP:1765:GLU:OE1	2.08	0.71
32:LX:165:THR:O	55:SI:410:LYS:NZ	2.23	0.71
49:SA:257:ILE:HD12	50:SB:138:LYS:HD3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SB:7:GLU:OE2	51:SD:231:ARG:NE	2.24	0.71
42:NI:151:HIS:ND1	42:NI:154:GLU:OE1	2.24	0.71
7:L6:20:ASP:OD1	7:L6:23:ARG:NH1	2.24	0.71
21:LM:166:ASN:ND2	50:SB:408:THR:O	2.23	0.71
26:LR:111:ASP:OD2	26:LR:113:THR:OG1	2.08	0.71
50:SB:319:ILE:HD12	50:SB:326:LEU:HD22	1.73	0.71
16:LH:464:LYS:NZ	16:LH:466:GLU:OE1	2.23	0.71
22:LN:532:ASN:OD1	22:LN:546:GLY:N	2.23	0.71
27:LS:321:MET:HE1	27:LS:375:VAL:HG11	1.71	0.71
22:LN:631:GLU:OE2	22:LN:652:THR:OG1	2.05	0.71
60:SP:1966:PHE:O	60:SP:1970:THR:OG1	2.08	0.71
32:LX:400:LEU:O	32:LX:404:TYR:OH	2.07	0.71
50:SB:14:LEU:HD13	50:SB:79:ILE:HD12	1.72	0.70
2:L1:918:U:O2'	40:NG:35:GLY:O	2.09	0.70
8:L7:7:LYS:NZ	8:L7:39:ARG:O	2.24	0.70
60:SP:993:THR:HG22	60:SP:997:MET:HE2	1.74	0.70
7:L6:119:GLN:NE2	7:L6:120:GLU:O	2.23	0.70
30:LV:120:ASP:OD1	30:LV:122:SER:OG	2.07	0.70
16:LH:559:LYS:NZ	16:LH:708:ASP:OD2	2.23	0.70
36:NC:96:ARG:HD2	45:NN:337:MET:HE1	1.74	0.70
64:ST:499:VAL:O	64:ST:502:SER:OG	2.09	0.70
2:L1:1084:A:N6	38:NE:309:SER:O	2.25	0.70
2:L1:1609:U:O2'	6:L5:105:GLY:O	2.08	0.70
1:L0:320:A:OP1	23:LO:249:ARG:NH1	2.25	0.70
24:LP:38:ASP:OD1	24:LP:42:ARG:NH2	2.25	0.69
64:ST:703:GLN:NE2	65:SU:484:PHE:O	2.26	0.69
11:LC:114:ARG:NH2	23:LO:513:GLU:O	2.25	0.69
41:NH:833:TYR:OH	42:NI:97:GLU:OE2	2.05	0.69
64:ST:95:ARG:NH1	64:ST:758:ASP:OD1	2.25	0.69
64:ST:719:GLU:OE1	64:ST:720:ASN:ND2	2.24	0.69
68:SY:158:MET:HE1	68:SY:161:ARG:NH2	2.07	0.69
26:LR:662:GLN:NE2	26:LR:666:GLU:OE2	2.26	0.69
41:NH:584:GLU:OE2	41:NH:616:LYS:NZ	2.23	0.69
17:LI:650:LEU:HB3	17:LI:655:LEU:HD21	1.73	0.69
16:LH:675:ARG:NH2	17:LI:492:GLU:OE2	2.25	0.69
30:LV:103:ASP:OD1	30:LV:104:PHE:N	2.26	0.69
54:SH:338:PHE:CG	55:SI:772:MET:HE1	2.27	0.69
16:LH:714:ASP:OD1	16:LH:715:GLU:N	2.26	0.69
52:SE:94:SER:OG	68:SY:248:ARG:NH1	2.26	0.69
25:LQ:220:THR:HG23	25:LQ:259:ILE:HD11	1.74	0.69
56:SJ:125:ASN:ND2	56:SJ:157:GLU:OE1	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LX:43:LEU:HD21	55:SI:371:VAL:HG21	1.75	0.69
65:SU:154:ALA:O	65:SU:157:SER:OG	2.10	0.69
42:NI:132:ALA:O	42:NI:136:ASN:ND2	2.26	0.68
53:SG:185:LEU:HD13	53:SG:527:VAL:HG11	1.75	0.68
25:LQ:7:ARG:NH2	25:LQ:70:GLY:O	2.27	0.68
53:SG:522:THR:OG1	53:SG:542:SER:OG	2.05	0.68
60:SP:643:LYS:NZ	60:SP:683:ASP:OD2	2.26	0.68
2:L1:407:A:OP1	7:L6:94:ARG:NH1	2.26	0.68
17:LI:570:LEU:HD21	17:LI:637:LEU:HD21	1.74	0.68
38:NE:198:GLN:NE2	43:NK:208:GLU:OE1	2.26	0.68
21:LM:784:SER:O	50:SB:84:LYS:NZ	2.23	0.68
30:LV:58:ALA:HB3	30:LV:76:THR:HG21	1.75	0.68
35:NB:376:VAL:HG12	65:SU:53:ARG:HH11	1.56	0.68
2:L1:95:G:HO2'	2:L1:460:A:HO2'	1.40	0.68
68:SY:73:ASP:OD1	68:SY:74:ALA:N	2.26	0.68
20:LL:185:PRO:O	20:LL:215:TYR:OH	2.11	0.68
32:LX:164:MET:HE3	32:LX:190:LEU:HD21	1.76	0.68
32:LX:520:ARG:NH1	32:LX:556:MET:O	2.27	0.68
60:SP:2140:ILE:HD12	63:SS:256:VAL:HG22	1.74	0.68
1:L0:125:G:OP1	65:SU:145:ASN:ND2	2.27	0.68
7:L6:67:VAL:HG21	7:L6:73:ILE:HD11	1.76	0.68
25:LQ:941:THR:HG23	34:NA:466:GLU:OE2	1.93	0.67
60:SP:474:ASN:OD1	60:SP:716:TYR:OH	2.10	0.67
19:LK:404:ASP:HA	19:LK:407:MET:HE2	1.76	0.67
21:LM:86:GLN:NE2	21:LM:90:GLU:OE1	2.26	0.67
60:SP:491:LEU:HD12	60:SP:491:LEU:O	1.94	0.67
23:LO:130:ASP:OD1	28:LT:25:SER:OG	2.08	0.67
26:LR:570:THR:OG1	26:LR:572:GLU:OE2	2.06	0.67
41:NH:1037:LEU:HD22	41:NH:1050:ILE:HG22	1.76	0.67
49:SA:257:ILE:HD12	50:SB:138:LYS:CD	2.24	0.67
60:SP:1099:LEU:HD21	60:SP:1139:ASN:ND2	2.09	0.67
63:SS:331:GLN:OE1	63:SS:335:GLN:NE2	2.28	0.67
8:L7:134:GLU:OE1	39:NF:21:ASN:ND2	2.27	0.67
20:LL:18:CYS:SG	20:LL:65:TRP:NE1	2.67	0.67
66:SV:138:GLU:OE1	68:SY:195:LEU:HD11	1.94	0.67
16:LH:136:LEU:HD23	16:LH:139:GLU:HB2	1.76	0.67
53:SG:200:ASP:HB2	53:SG:211:LEU:HD11	1.75	0.67
55:SI:831:ARG:NH1	55:SI:835:HIS:O	2.28	0.67
20:LL:454:GLU:OE2	20:LL:487:ARG:NH1	2.27	0.67
16:LH:244:ILE:HD13	16:LH:283:VAL:HG21	1.77	0.67
25:LQ:928:GLU:OE2	25:LQ:932:ASN:ND2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SB:118:ARG:NH2	51:SD:261:LEU:O	2.28	0.67
67:SW:174:LEU:HD11	67:SW:182:ILE:HD11	1.76	0.67
18:LJ:29:GLN:OE1	18:LJ:332:LYS:NZ	2.25	0.67
29:LU:361:LYS:NZ	63:SS:887:PRO:O	2.28	0.67
41:NH:620:ASN:ND2	41:NH:623:GLU:OE2	2.27	0.67
3:L2:82:G:OP1	50:SB:366:LYS:NZ	2.26	0.67
1:L0:333:G:O6	33:LZ:25:GLN:NE2	2.28	0.66
27:LS:449:ASP:OD1	27:LS:494:TYR:OH	2.09	0.66
29:LU:267:ILE:HD12	29:LU:279:THR:HG22	1.77	0.66
8:L7:121:VAL:O	8:L7:125:ILE:HD12	1.94	0.66
26:LR:406:ALA:HB2	26:LR:440:VAL:HG23	1.76	0.66
38:NE:164:LEU:HD11	38:NE:213:MET:HE3	1.78	0.66
40:NG:37:GLU:OE1	44:NM:64:ARG:NH2	2.27	0.66
64:ST:475:ARG:NH2	65:SU:511:SER:O	2.29	0.66
22:LN:541:ALA:HB2	22:LN:555:LEU:HD11	1.77	0.66
30:LV:218:LEU:HD11	30:LV:255:TYR:CE2	2.30	0.66
44:NM:127:VAL:HG11	44:NM:176:VAL:HG21	1.76	0.66
65:SU:297:ASP:OD1	65:SU:298:PHE:N	2.29	0.66
2:L1:168:A:OP1	7:L6:140:ASN:ND2	2.29	0.66
2:L1:325:G:OP1	12:LD:134:THR:OG1	2.13	0.66
21:LM:778:SER:O	21:LM:782:VAL:N	2.28	0.66
35:NB:606:VAL:N	51:SC:302:GLU:OE2	2.29	0.66
38:NE:118:ARG:NH1	54:SH:228:ASP:OD2	2.28	0.66
60:SP:1988:PRO:O	63:SS:439:ARG:NH1	2.28	0.66
2:L1:486:G:OP1	61:SQ:190:LYS:NZ	2.20	0.66
25:LQ:867:GLU:OE2	25:LQ:871:GLN:NE2	2.28	0.66
48:OA:1408:ASP:OD2	48:OA:1413:ILE:N	2.29	0.66
2:L1:416:A:N6	32:LX:68:SER:OG	2.27	0.66
16:LH:682:ASN:CG	16:LH:689:ILE:HD11	2.21	0.66
64:ST:800:GLU:OE1	64:ST:803:ARG:NH2	2.29	0.66
2:L1:467:G:O2'	2:L1:469:C:OP2	2.14	0.66
57:SL:156:ASN:O	57:SL:156:ASN:ND2	2.27	0.66
67:SW:96:SER:O	67:SW:97:ARG:NH1	2.29	0.66
32:LX:827:ARG:NH2	32:LX:928:LEU:O	2.29	0.66
2:L1:1655:A:N1	2:L1:1745:G:O6	2.29	0.65
3:L2:256:G:OP1	49:SA:382:LYS:NZ	2.29	0.65
22:LN:88:GLU:OE1	22:LN:527:TYR:OH	2.09	0.65
41:NH:656:ARG:NH2	44:NM:241:GLY:O	2.29	0.65
2:L1:321:C:N4	30:LV:135:THR:OG1	2.29	0.65
2:L1:1045:C:OP1	44:NM:153:HIS:NE2	2.21	0.65
16:LH:16:SER:OG	16:LH:465:ASN:OD1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LJ:140:LEU:O	18:LJ:152:TRP:N	2.29	0.65
20:LL:436:THR:N	65:SU:297:ASP:OD2	2.29	0.65
27:LS:511:LEU:HD13	27:LS:544:VAL:HG21	1.78	0.65
5:L4:98:ASN:ND2	5:L4:116:ASP:OD1	2.30	0.65
44:NM:59:ASP:OD1	44:NM:60:ALA:N	2.29	0.65
22:LN:681:ILE:HG22	22:LN:683:ASP:H	1.61	0.65
41:NH:622:SER:OG	41:NH:623:GLU:OE1	2.09	0.65
55:SI:91:ARG:O	55:SI:95:LYS:N	2.27	0.65
20:LL:209:ASP:N	20:LL:231:ASP:OD2	2.29	0.65
37:ND:166:LEU:O	68:SY:140:ARG:NH2	2.30	0.65
56:SK:156:GLU:OE1	56:SK:156:GLU:N	2.30	0.65
66:SV:135:VAL:HG13	68:SY:195:LEU:HD13	1.77	0.65
3:L2:30:A:N6	29:LU:341:GLU:OE2	2.30	0.65
16:LH:671:ILE:HD11	16:LH:750:LEU:HD11	1.79	0.65
32:LY:540:LEU:HD23	32:LY:585:VAL:HG23	1.77	0.65
60:SP:1419:SER:O	60:SP:1422:SER:OG	2.14	0.65
28:LT:604:SER:OG	28:LT:606:ASP:OD1	2.12	0.64
38:NE:149:LEU:HD13	43:NK:197:ILE:HD12	1.79	0.64
59:SN:96:LEU:HD21	59:SN:180:LEU:HD12	1.79	0.64
60:SP:1667:ALA:HA	60:SP:1670:LEU:HD13	1.80	0.64
60:SP:1942:LEU:HD22	63:SS:455:ILE:HD11	1.77	0.64
41:NH:349:LEU:HD22	41:NH:394:THR:HG22	1.77	0.64
68:SY:215:GLN:NE2	68:SY:219:ASP:OD2	2.31	0.64
49:SA:263:ILE:HD12	49:SA:267:ASP:OD2	1.98	0.64
64:ST:563:GLU:N	64:ST:563:GLU:OE1	2.30	0.64
41:NH:177:ASN:OD1	41:NH:178:TYR:N	2.29	0.64
65:SU:509:ALA:O	65:SU:512:SER:OG	2.06	0.64
3:L2:37:G:O4'	31:LW:431:ARG:NH2	2.30	0.64
3:L2:112:U:OP1	52:SF:46:ARG:NH2	2.31	0.64
33:LZ:34:ARG:NH2	57:SL:16:THR:O	2.30	0.64
2:L1:1767:G:O2'	67:SW:203:GLY:O	2.13	0.64
16:LH:197:ILE:HD11	16:LH:213:LYS:HG3	1.80	0.64
25:LQ:287:ARG:NH1	25:LQ:323:SER:O	2.30	0.64
60:SP:749:LYS:O	60:SP:756:SER:OG	2.15	0.64
18:LJ:132:PHE:CD1	18:LJ:140:LEU:HD13	2.31	0.64
2:L1:592:A:O3'	10:L9:39:LYS:NZ	2.31	0.64
9:L8:70:GLU:OE1	12:LD:24:LYS:NZ	2.28	0.64
54:SH:301:MET:HE3	54:SH:354:ILE:HD13	1.80	0.64
21:LM:193:THR:OG1	21:LM:241:ILE:HD11	1.98	0.63
25:LQ:580:ASP:OD2	25:LQ:623:PHE:N	2.31	0.63
32:LY:502:PHE:O	32:LY:506:GLY:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SM:243:GLU:OE1	58:SM:243:GLU:N	2.31	0.63
60:SP:1428:THR:OG1	60:SP:1431:PHE:O	2.16	0.63
67:SW:129:ARG:NH1	67:SW:131:ASN:OD1	2.31	0.63
1:L0:234:A:C5	18:LJ:360:MET:HE1	2.33	0.63
26:LR:188:GLU:OE1	26:LR:188:GLU:N	2.31	0.63
26:LR:561:SER:OG	26:LR:563:ASP:OD1	2.16	0.63
29:LU:186:ASP:OD1	29:LU:187:SER:N	2.31	0.63
55:SI:826:LYS:HE2	55:SI:926:ILE:HD13	1.79	0.63
60:SP:1992:GLU:OE2	60:SP:1994:SER:OG	2.16	0.63
20:LL:580:TYR:OH	20:LL:585:ASP:OD2	2.16	0.63
63:SS:432:ASP:OD1	63:SS:433:ILE:HD12	1.99	0.63
2:L1:416:A:N1	32:LX:59:TYR:OH	2.32	0.63
2:L1:864:U:O2	46:NQ:22:LYS:NZ	2.32	0.63
24:LP:33:MET:SD	31:LW:66:LEU:HD23	2.39	0.63
24:LP:41:HIS:NE2	29:LU:21:GLU:O	2.29	0.63
25:LQ:400:SER:OG	25:LQ:402:ASP:OD1	2.09	0.63
55:SI:923:ASP:OD1	55:SI:924:VAL:N	2.32	0.63
60:SP:264:THR:O	60:SP:313:ARG:NH1	2.32	0.63
60:SP:283:SER:O	60:SP:329:LYS:NZ	2.31	0.63
60:SP:1946:LYS:HD2	63:SS:455:ILE:HG23	1.80	0.63
16:LH:656:ASP:OD1	16:LH:657:SER:N	2.32	0.63
23:LO:288:ASP:O	23:LO:292:PHE:N	2.31	0.63
25:LQ:619:MET:HE1	25:LQ:661:TRP:CZ3	2.34	0.63
37:ND:178:VAL:HG12	68:SY:135:ILE:HB	1.80	0.63
41:NH:887:ALA:HA	41:NH:1051:LEU:HD21	1.81	0.63
51:SD:204:GLY:HA3	51:SD:221:ILE:HD12	1.80	0.63
2:L1:192:U:H3	2:L1:193:U:HO2'	1.45	0.62
4:L3:70:VAL:HG12	4:L3:74:GLN:OE1	1.98	0.62
19:LK:394:HIS:ND1	19:LK:405:ASP:OD2	2.32	0.62
54:SH:12:GLN:NE2	54:SH:34:GLU:OE2	2.32	0.62
63:SS:244:LEU:HD21	63:SS:263:LEU:HD13	1.81	0.62
4:L3:26:ILE:HG23	4:L3:31:ALA:HB2	1.79	0.62
16:LH:381:SER:OG	20:LL:349:ASP:OD1	2.18	0.62
28:LT:95:GLU:OE2	28:LT:97:LYS:NZ	2.32	0.62
44:NM:30:PHE:N	44:NM:46:THR:O	2.32	0.62
56:SK:69:ASN:OD1	56:SK:70:CYS:N	2.32	0.62
32:LY:541:TYR:OH	32:LY:552:ASP:OD1	2.15	0.62
16:LH:582:LEU:HD11	16:LH:613:LEU:HD11	1.81	0.62
20:LL:111:ASP:OD2	20:LL:112:LEU:N	2.32	0.62
32:LY:779:LYS:NZ	32:LY:822:ASN:OD1	2.33	0.62
32:LY:917:MET:HA	32:LY:917:MET:HE3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SB:208:ILE:HD12	50:SB:223:LEU:HD13	1.80	0.62
53:SG:184:ARG:NH2	53:SG:200:ASP:OD2	2.32	0.62
56:SJ:41:MET:HE3	56:SJ:110:LEU:HD12	1.81	0.62
60:SP:267:SER:O	60:SP:313:ARG:NH2	2.32	0.62
16:LH:720:ILE:HG12	16:LH:745:ILE:HD13	1.82	0.62
30:LV:218:LEU:HD11	30:LV:255:TYR:HE2	1.65	0.62
49:SA:185:ASP:OD1	49:SA:285:ARG:NE	2.31	0.62
54:SH:54:ARG:NH2	64:ST:114:ASP:OD2	2.33	0.62
64:ST:563:GLU:OE2	65:SU:503:TYR:OH	2.17	0.62
23:LO:669:ASP:O	23:LO:672:THR:OG1	2.13	0.62
23:LO:669:ASP:OD1	23:LO:670:LEU:N	2.32	0.62
60:SP:365:PHE:O	60:SP:369:SER:OG	2.16	0.62
64:ST:461:SER:O	64:ST:465:LYS:NZ	2.25	0.62
68:SY:235:ASP:OD1	68:SY:236:SER:N	2.33	0.62
2:L1:49:C:OP2	2:L1:425:A:N6	2.25	0.62
31:LW:125:LEU:HD21	31:LW:398:ILE:HD13	1.81	0.62
50:SB:219:SER:OG	50:SB:220:GLU:OE1	2.18	0.62
52:SF:10:PRO:HG3	52:SF:125:LEU:HD23	1.82	0.62
54:SH:283:ILE:O	55:SI:634:ARG:NH1	2.33	0.62
56:SK:35:ASP:O	56:SK:40:ARG:NH2	2.32	0.62
16:LH:147:SER:OG	16:LH:148:GLU:OE1	2.09	0.62
16:LH:245:LEU:HD22	16:LH:249:THR:HG21	1.81	0.62
21:LM:218:ILE:HD12	21:LM:263:VAL:HG21	1.82	0.62
16:LH:40:ASP:OD2	16:LH:42:ARG:NH2	2.33	0.61
18:LJ:53:HIS:NE2	18:LJ:311:THR:O	2.33	0.61
65:SU:318:LEU:HD21	65:SU:354:TYR:CD1	2.33	0.61
2:L1:447:U:O2'	5:L4:27:TYR:O	2.18	0.61
8:L7:186:PRO:O	8:L7:187:SER:OG	2.13	0.61
22:LN:469:LEU:O	22:LN:473:THR:OG1	2.12	0.61
25:LQ:589:ILE:HG21	25:LQ:621:VAL:HG11	1.82	0.61
50:SB:45:ALA:HB1	50:SB:79:ILE:HD11	1.81	0.61
60:SP:1617:VAL:HG11	60:SP:1661:ILE:HG13	1.82	0.61
60:SP:2068:LEU:HD23	60:SP:2105:ALA:HB1	1.81	0.61
64:ST:395:ASP:OD1	64:ST:396:LEU:N	2.32	0.61
2:L1:67:A:O2'	2:L1:69:G:OP1	2.18	0.61
16:LH:753:LYS:NZ	17:LI:430:LEU:O	2.21	0.61
60:SP:201:ARG:NH2	60:SP:241:THR:O	2.34	0.61
2:L1:932:U:OP2	44:NM:155:TYR:OH	2.12	0.61
4:L3:26:ILE:HD11	4:L3:30:TYR:CD2	2.36	0.61
50:SB:122:GLU:O	51:SD:236:MET:HE2	2.01	0.61
16:LH:418:ASN:OD1	16:LH:419:HIS:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LL:113:MET:HE3	20:LL:160:VAL:HG13	1.82	0.61
54:SH:67:ILE:HD12	64:ST:114:ASP:OD1	2.01	0.61
18:LJ:404:ALA:HB2	18:LJ:417:VAL:HG11	1.83	0.61
21:LM:309:GLN:N	21:LM:309:GLN:OE1	2.34	0.61
55:SI:98:LEU:HD11	55:SI:354:ILE:HD11	1.83	0.61
2:L1:188:A:N6	2:L1:197:A:O2'	2.33	0.61
32:LX:502:PHE:HE2	32:LX:507:THR:HG22	1.65	0.61
35:NB:372:PHE:O	35:NB:376:VAL:HG13	2.00	0.61
65:SU:116:GLY:O	65:SU:119:SER:OG	2.08	0.61
14:LF:38:ASP:OD1	14:LF:39:GLU:N	2.33	0.61
25:LQ:840:MET:HE2	25:LQ:886:GLU:CB	2.31	0.61
43:NK:141:ARG:NH1	43:NK:191:MET:O	2.34	0.61
65:SU:325:GLU:OE2	65:SU:329:ARG:NH2	2.33	0.61
55:SI:952:PHE:CD2	55:SI:958:VAL:HG22	2.35	0.61
55:SI:1106:GLU:OE1	61:SQ:115:ARG:NH2	2.34	0.61
54:SH:104:LEU:HD12	54:SH:141:MET:SD	2.41	0.60
59:SN:35:ASP:OD1	59:SN:37:HIS:NE2	2.34	0.60
16:LH:856:GLU:OE1	21:LM:378:TYR:N	2.34	0.60
18:LJ:248:ARG:NH2	18:LJ:289:ASN:O	2.34	0.60
19:LK:459:LEU:HD23	19:LK:467:LEU:HD11	1.83	0.60
21:LM:1594:PHE:O	21:LM:1598:LEU:N	2.34	0.60
50:SB:91:GLU:OE2	51:SD:231:ARG:NH1	2.34	0.60
51:SD:198:GLU:O	51:SD:222:GLU:N	2.34	0.60
63:SS:357:ASP:OD1	63:SS:358:SER:N	2.34	0.60
2:L1:763:G:OP2	10:L9:79:ARG:NH2	2.33	0.60
28:LT:592:ASP:OD1	28:LT:593:PHE:N	2.34	0.60
31:LW:17:ASN:ND2	31:LW:64:ASP:OD2	2.33	0.60
1:L0:156:U:O2'	1:L0:157:U:O5'	2.20	0.60
23:LO:146:PHE:N	23:LO:167:ASP:OD2	2.34	0.60
56:SJ:94:GLN:OE1	56:SK:94:GLN:NE2	2.34	0.60
60:SP:2103:PHE:CE1	60:SP:2141:VAL:HG13	2.36	0.60
20:LL:72:ASP:OD1	20:LL:73:THR:N	2.34	0.60
23:LO:484:GLU:OE2	23:LO:815:TYR:OH	2.19	0.60
34:NA:312:GLU:OE2	34:NA:316:ASN:ND2	2.34	0.60
41:NH:899:LEU:HD11	41:NH:909:TYR:CE2	2.36	0.60
60:SP:2376:VAL:O	60:SP:2380:GLY:N	2.33	0.60
28:LT:879:GLU:HG3	28:LT:880:LEU:HD12	1.82	0.60
56:SK:137:PHE:CE1	56:SK:141:MET:HE3	2.36	0.60
58:SM:12:TYR:OH	58:SM:75:ASP:OD2	2.16	0.60
60:SP:1140:GLN:O	60:SP:1188:LYS:NZ	2.21	0.60
20:LL:227:VAL:HG11	28:LT:563:ASP:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LX:356:ARG:NH2	32:LY:379:GLY:O	2.35	0.60
60:SP:1308:LEU:HD22	60:SP:1347:LEU:HD22	1.82	0.60
6:L5:55:ASP:OD2	6:L5:57:SER:OG	2.19	0.60
22:LN:384:VAL:HG22	22:LN:391:VAL:HG22	1.82	0.60
29:LU:304:HIS:NE2	29:LU:322:THR:OG1	2.34	0.60
1:L0:262:U:OP2	59:SN:164:ARG:NH2	2.34	0.60
27:LS:544:VAL:HG22	27:LS:551:VAL:HG22	1.82	0.60
45:NN:180:LEU:O	45:NN:183:THR:OG1	2.16	0.60
55:SI:82:LYS:N	73:SI:2001:GTP:O1B	2.35	0.60
65:SU:450:GLU:OE2	65:SU:451:SER:N	2.35	0.60
2:L1:931:C:O2'	44:NM:118:GLN:O	2.20	0.59
6:L5:94:THR:HG22	6:L5:114:ILE:HG13	1.84	0.59
16:LH:200:ASN:OD1	16:LH:201:ILE:N	2.34	0.59
34:NA:493:GLN:O	34:NA:497:ASN:ND2	2.34	0.59
2:L1:57:G:OP2	14:LF:116:LYS:NZ	2.29	0.59
60:SP:871:ASP:OD1	60:SP:889:LYS:NZ	2.35	0.59
60:SP:1951:THR:N	60:SP:1989:ASP:OD2	2.35	0.59
4:L3:30:TYR:O	4:L3:33:THR:OG1	2.20	0.59
8:L7:17:GLU:HG3	8:L7:46:ILE:HG22	1.82	0.59
16:LH:778:ASP:OD1	16:LH:779:ILE:N	2.35	0.59
53:SG:372:TRP:HE3	53:SG:373:MET:HE2	1.66	0.59
60:SP:35:GLU:OE1	60:SP:35:GLU:N	2.36	0.59
60:SP:976:TYR:O	60:SP:980:ASN:ND2	2.34	0.59
60:SP:1085:VAL:HG23	60:SP:1086:VAL:HG23	1.84	0.59
36:NC:63:LEU:HD11	45:NN:290:ARG:HG2	1.84	0.59
41:NH:1233:ASN:ND2	41:NH:1235:GLU:OE2	2.35	0.59
51:SC:103:GLU:OE1	61:SQ:134:ARG:NH1	2.35	0.59
51:SD:106:LEU:HD22	51:SD:156:MET:HE3	1.84	0.59
1:L0:326:C:O2'	1:L0:327:A:OP1	2.20	0.59
2:L1:319:U:O4	43:NK:295:ARG:NE	2.36	0.59
16:LH:537:ASN:ND2	16:LH:538:GLU:OE2	2.36	0.59
29:LU:231:GLU:OE2	29:LU:250:ARG:NH1	2.35	0.59
56:SJ:123:GLU:HB2	56:SJ:163:ILE:HD12	1.85	0.59
2:L1:486:G:HO2'	61:SQ:135:HIS:HE2	1.50	0.59
40:NG:25:ASP:OD1	40:NG:26:THR:N	2.36	0.59
56:SJ:192:TYR:O	56:SJ:196:LEU:HD23	2.03	0.59
60:SP:615:VAL:HG13	60:SP:619:LEU:HD23	1.83	0.59
2:L1:427:C:O2'	2:L1:459:G:N3	2.33	0.59
22:LN:144:ILE:HD12	22:LN:158:VAL:HG12	1.85	0.59
27:LS:376:LEU:CD1	27:LS:409:ILE:HD11	2.32	0.59
32:LX:892:ARG:NH2	32:LY:790:SER:OG	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SQ:173:ILE:HD12	61:SQ:173:ILE:H	1.67	0.59
3:L2:90:C:O2'	3:L2:91:C:OP1	2.20	0.59
4:L3:45:LEU:HD21	4:L3:49:LYS:CE	2.32	0.59
60:SP:374:LEU:O	60:SP:378:HIS:N	2.34	0.59
8:L7:10:SER:OG	8:L7:44:LYS:O	2.21	0.59
27:LS:350:SER:O	27:LS:380:ASN:ND2	2.35	0.59
2:L1:7:G:OP2	38:NE:294:ARG:NH2	2.33	0.59
32:LX:64:LEU:HD21	32:LX:153:LYS:HE3	1.85	0.59
50:SB:14:LEU:HD12	50:SB:75:LEU:HD23	1.85	0.59
23:LO:497:ILE:CD1	23:LO:532:VAL:HG11	2.33	0.58
55:SI:628:VAL:O	55:SI:628:VAL:HG12	2.03	0.58
1:L0:87:C:O2	16:LH:332:GLN:NE2	2.36	0.58
2:L1:474:A:O2'	2:L1:475:A:O5'	2.20	0.58
17:LI:706:TYR:CZ	17:LI:708:MET:HE3	2.38	0.58
31:LW:46:LEU:HD21	63:SS:856:GLN:HG2	1.86	0.58
34:NA:473:THR:OG1	34:NA:487:ALA:O	2.09	0.58
49:SA:281:LEU:HD11	50:SB:265:PHE:CZ	2.39	0.58
56:SJ:180:LEU:HD12	56:SJ:206:VAL:HG22	1.84	0.58
16:LH:177:THR:OG1	16:LH:186:GLU:OE2	2.13	0.58
25:LQ:538:ARG:NH1	25:LQ:539:VAL:O	2.37	0.58
32:LX:801:ALA:O	32:LX:805:ILE:HD12	2.03	0.58
21:LM:79:ILE:O	21:LM:124:ARG:NH1	2.37	0.58
22:LN:205:CYS:SG	22:LN:211:ARG:NH1	2.76	0.58
26:LR:454:LEU:N	26:LR:466:TRP:O	2.36	0.58
37:ND:124:ASP:OD2	65:SU:21:ARG:NH1	2.37	0.58
41:NH:1189:LEU:HD11	48:OA:1470:GLY:O	2.04	0.58
20:LL:369:PHE:O	20:LL:524:SER:OG	2.21	0.58
32:LY:888:ILE:HG23	32:LY:898:ILE:HD11	1.85	0.58
41:NH:199:ASN:OD1	41:NH:200:GLY:N	2.36	0.58
56:SJ:48:ALA:HB1	56:SJ:50:LEU:HD13	1.86	0.58
67:SW:25:ILE:HD11	67:SW:30:ASN:HB2	1.86	0.58
18:LJ:250:ASN:OD1	18:LJ:282:LYS:NZ	2.35	0.58
41:NH:1158:LYS:O	41:NH:1187:LYS:NZ	2.36	0.58
60:SP:1138:SER:HA	60:SP:1181:ILE:HD13	1.85	0.58
60:SP:1987:LEU:HD23	63:SS:442:LEU:HD21	1.86	0.58
13:LE:64:GLN:OE1	29:LU:263:ARG:NH2	2.37	0.58
13:LE:79:PHE:CE2	38:NE:321:VAL:HG21	2.39	0.58
32:LX:851:ASP:OD2	32:LX:852:TYR:N	2.37	0.58
45:NN:240:ASN:OD1	45:NN:275:LEU:HD11	2.02	0.58
29:LU:116:LEU:HD12	29:LU:137:LEU:O	2.04	0.58
50:SB:30:GLN:O	50:SB:37:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SK:77:LEU:HD11	56:SK:82:ARG:HB2	1.86	0.58
2:L1:501:U:O2'	2:L1:502:U:OP2	2.19	0.57
14:LF:51:GLU:OE2	60:SP:36:LYS:N	2.31	0.57
64:ST:729:ASP:OD1	64:ST:734:ARG:NH1	2.37	0.57
17:LI:707:THR:O	17:LI:708:MET:HE2	2.04	0.57
2:L1:31:C:OP1	62:SR:140:LYS:NZ	2.28	0.57
2:L1:248:U:O2'	2:L1:249:U:OP1	2.18	0.57
13:LE:75:ILE:HD13	38:NE:319:LEU:HD23	1.86	0.57
22:LN:107:VAL:O	22:LN:524:LYS:NZ	2.38	0.57
60:SP:1711:ASP:OD2	60:SP:1762:SER:OG	2.14	0.57
60:SP:2077:GLN:HA	60:SP:2080:MET:HE2	1.85	0.57
60:SP:1385:ASN:O	60:SP:1388:SER:OG	2.14	0.57
22:LN:139:CYS:SG	22:LN:144:ILE:HD11	2.44	0.57
24:LP:126:TYR:O	24:LP:130:HIS:ND1	2.30	0.57
41:NH:520:ASN:OD1	41:NH:521:LEU:N	2.37	0.57
1:L0:168:G:H22	1:L0:227:U:H3	1.53	0.57
28:LT:627:ASN:ND2	28:LT:647:THR:OG1	2.37	0.57
32:LX:588:ILE:HG22	32:LX:635:ILE:HD13	1.87	0.57
32:LY:843:ASP:OD2	32:LY:921:SER:OG	2.15	0.57
53:SG:164:GLN:NE2	53:SG:528:GLU:O	2.37	0.57
54:SH:185:ARG:NH2	54:SH:349:ASP:OD1	2.38	0.57
65:SU:31:ILE:HD13	65:SU:59:LEU:HD13	1.86	0.57
68:SY:154:THR:HG22	68:SY:166:LEU:O	2.04	0.57
26:LR:30:LYS:O	26:LR:45:LEU:N	2.36	0.57
27:LS:401:GLU:OE1	27:LS:401:GLU:N	2.38	0.57
52:SF:22:ASP:OD1	53:SG:342:ARG:NH2	2.36	0.57
60:SP:312:ASP:OD1	60:SP:313:ARG:N	2.37	0.57
60:SP:993:THR:HG22	60:SP:997:MET:CE	2.34	0.57
17:LI:708:MET:HE1	22:LN:34:HIS:HA	1.87	0.57
24:LP:391:TYR:CE2	24:LP:395:ILE:HD11	2.39	0.57
28:LT:331:GLY:O	28:LT:332:SER:OG	2.22	0.57
30:LV:82:HIS:CD2	30:LV:91:LEU:HD11	2.40	0.57
32:LX:838:ASP:OD1	32:LX:841:ARG:NH2	2.34	0.57
60:SP:2071:PRO:O	60:SP:2076:ARG:NH2	2.37	0.57
5:L4:93:ASP:OD1	5:L4:94:ALA:N	2.37	0.57
26:LR:255:LYS:HE3	26:LR:257:ILE:HD11	1.87	0.57
2:L1:1231:U:O2'	2:L1:1258:U:O2'	2.04	0.57
6:L5:161:ASP:OD1	6:L5:162:VAL:N	2.36	0.57
29:LU:303:ASP:OD2	29:LU:339:SER:N	2.38	0.57
39:NF:116:ILE:HD11	43:NK:252:PRO:HB3	1.87	0.57
41:NH:1209:ASP:OD1	42:NI:10:LYS:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SI:56:VAL:HG22	62:SR:52:ILE:CD1	2.35	0.57
60:SP:1662:SER:HB2	60:SP:1701:MET:HE2	1.86	0.57
54:SH:208:MET:HE3	54:SH:241:TRP:HZ3	1.68	0.56
59:SN:53:ILE:HG23	59:SN:153:MET:HE2	1.86	0.56
5:L4:103:TYR:O	5:L4:182:TYR:OH	2.22	0.56
30:LV:319:ASP:OD1	30:LV:320:ILE:N	2.38	0.56
31:LW:482:ASP:OD2	31:LW:512:ARG:NH1	2.38	0.56
43:NK:119:ASP:OD1	43:NK:120:ASP:N	2.37	0.56
43:NK:218:GLU:N	43:NK:218:GLU:OE2	2.38	0.56
55:SI:56:VAL:HG22	62:SR:52:ILE:HD12	1.85	0.56
16:LH:197:ILE:HD11	16:LH:213:LYS:CG	2.34	0.56
30:LV:74:THR:HG21	30:LV:101:ASN:HB3	1.87	0.56
33:LZ:115:MET:HE3	33:LZ:127:ALA:HB1	1.88	0.56
60:SP:1777:LEU:HD21	60:SP:1789:LEU:CD2	2.35	0.56
4:L3:103:ASN:ND2	64:ST:740:MET:SD	2.75	0.56
21:LM:45:TYR:CE2	29:LU:16:VAL:HG11	2.40	0.56
41:NH:765:LEU:O	41:NH:914:ARG:NH1	2.38	0.56
43:NK:106:ARG:O	43:NK:107:SER:OG	2.20	0.56
50:SB:319:ILE:HD12	50:SB:326:LEU:CD2	2.35	0.56
68:SY:92:SER:OG	68:SY:94:ASP:OD1	2.21	0.56
9:L8:106:ALA:HB2	9:L8:165:LEU:HG	1.88	0.56
64:ST:383:THR:OG1	64:ST:385:ASP:OD1	2.11	0.56
68:SY:94:ASP:OD1	68:SY:95:GLN:N	2.38	0.56
2:L1:1681:A:N6	2:L1:1720:G:C6	2.74	0.56
41:NH:551:GLU:N	41:NH:551:GLU:OE1	2.38	0.56
56:SK:68:LEU:HD21	56:SK:77:LEU:HD13	1.87	0.56
60:SP:489:SER:OG	60:SP:493:ASN:OD1	2.18	0.56
5:L4:208:VAL:HG13	5:L4:210:ILE:HD11	1.86	0.56
9:L8:8:ARG:NH2	9:L8:28:GLU:OE2	2.39	0.56
35:NB:529:ALA:O	35:NB:532:VAL:HG12	2.06	0.56
41:NH:315:ILE:HB	41:NH:553:VAL:HG23	1.87	0.56
44:NM:244:VAL:HG13	44:NM:244:VAL:O	2.06	0.56
49:SA:155:GLY:HA2	51:SC:233:LEU:HD23	1.87	0.56
60:SP:1450:PHE:CD1	60:SP:1465:ALA:HB1	2.40	0.56
2:L1:532:U:OP1	10:L9:132:ARG:NH2	2.39	0.56
53:SG:372:TRP:CE3	53:SG:373:MET:HE2	2.41	0.56
65:SU:10:ASP:OD2	65:SU:14:ARG:NH2	2.38	0.56
31:LW:96:ASP:OD2	31:LW:98:SER:OG	2.17	0.56
25:LQ:588:ILE:HB	25:LQ:602:LEU:HD11	1.88	0.56
25:LQ:762:GLU:OE2	25:LQ:791:ASN:N	2.38	0.56
26:LR:733:ASP:OD1	26:LR:734:GLU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:SS:351:LEU:O	63:SS:351:LEU:HD23	2.06	0.56
1:L0:150:G:O4'	18:LJ:380:ARG:NH2	2.39	0.55
2:L1:330:G:OP2	9:L8:172:ARG:NH1	2.39	0.55
8:L7:94:ALA:HB3	8:L7:96:ARG:HH12	1.72	0.55
22:LN:279:HIS:HD1	22:LN:301:ASP:CG	2.13	0.55
22:LN:473:THR:HG21	22:LN:496:PHE:HZ	1.72	0.55
28:LT:854:SER:HB2	28:LT:895:VAL:HG21	1.88	0.55
30:LV:359:ILE:HG22	30:LV:359:ILE:O	2.05	0.55
31:LW:545:VAL:HG21	42:NI:181:LYS:HG2	1.88	0.55
32:LX:243:ASP:OD1	32:LX:244:VAL:HG23	2.06	0.55
32:LX:309:PHE:HB2	32:LX:384:VAL:HG12	1.87	0.55
49:SA:226:LYS:NZ	49:SA:260:GLY:O	2.40	0.55
64:ST:481:MET:HE1	64:ST:501:PHE:CZ	2.40	0.55
11:LC:97:VAL:HG12	11:LC:98:ASP:H	1.70	0.55
18:LJ:510:LEU:HD23	19:LK:505:MET:HE1	1.88	0.55
23:LO:708:ASP:OD1	23:LO:709:THR:N	2.39	0.55
26:LR:560:TRP:NE1	26:LR:567:VAL:HG22	2.21	0.55
30:LV:58:ALA:HB3	30:LV:76:THR:CG2	2.35	0.55
32:LX:540:LEU:HD23	32:LX:585:VAL:HG12	1.88	0.55
32:LX:617:LEU:CD2	32:LX:761:VAL:HG21	2.35	0.55
41:NH:110:LEU:HD13	41:NH:512:LEU:HD11	1.87	0.55
41:NH:369:TRP:HE1	41:NH:495:THR:HG21	1.70	0.55
11:LC:40:GLU:OE1	11:LC:42:GLU:N	2.40	0.55
20:LL:21:THR:HG21	20:LL:310:THR:HG21	1.88	0.55
28:LT:646:VAL:HG13	28:LT:647:THR:HG23	1.88	0.55
55:SI:1057:ILE:HD11	68:SY:15:GLU:OE2	2.06	0.55
2:L1:486:G:O2'	61:SQ:135:HIS:NE2	2.35	0.55
21:LM:157:LEU:HD11	21:LM:168:VAL:HG21	1.88	0.55
32:LX:507:THR:HG21	32:LX:647:MET:HE1	1.87	0.55
49:SA:328:GLN:OE1	49:SA:332:THR:HG21	2.07	0.55
60:SP:825:GLU:OE1	60:SP:828:ARG:NH2	2.40	0.55
60:SP:1196:SER:O	60:SP:1242:LYS:NZ	2.38	0.55
3:L2:313:A:OP1	61:SQ:166:ARG:NH1	2.40	0.55
18:LJ:388:PHE:CE1	18:LJ:413:LEU:HD11	2.42	0.55
25:LQ:206:GLU:OE1	25:LQ:206:GLU:N	2.39	0.55
31:LW:510:ASP:OD1	31:LW:511:GLU:N	2.38	0.55
43:NK:288:GLN:O	43:NK:291:ARG:N	2.38	0.55
44:NM:127:VAL:CG1	44:NM:176:VAL:HG21	2.35	0.55
13:LE:44:HIS:NE2	13:LE:112:ASP:OD2	2.37	0.55
21:LM:35:TYR:OH	61:SQ:82:LEU:HD12	2.06	0.55
40:NG:37:GLU:OE2	44:NM:47:LEU:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:NH:164:ASP:OD2	41:NH:598:LYS:NZ	2.31	0.55
42:NI:217:GLY:N	46:NQ:75:GLU:OE1	2.38	0.55
60:SP:1436:ASP:OD2	60:SP:1480:SER:OG	2.10	0.55
23:LO:497:ILE:HD13	23:LO:532:VAL:HG11	1.89	0.55
34:NA:383:ARG:NH2	58:SM:212:ALA:O	2.39	0.55
2:L1:390:G:H22	2:L1:407:A:H2	1.55	0.55
22:LN:144:ILE:HD12	22:LN:158:VAL:CG1	2.36	0.55
32:LX:21:LYS:HB2	32:LX:477:ALA:HB2	1.88	0.55
32:LY:841:ARG:HD2	32:LY:854:VAL:HG12	1.88	0.55
60:SP:905:LEU:HD12	60:SP:956:PHE:HE1	1.71	0.55
24:LP:268:ASP:OD1	24:LP:269:ILE:N	2.40	0.55
25:LQ:483:SER:OG	25:LQ:543:ASP:OD2	2.22	0.55
32:LY:508:PRO:O	32:LY:649:TYR:OH	2.22	0.55
33:LZ:62:SER:O	33:LZ:71:ARG:NH1	2.40	0.55
60:SP:1919:ILE:HD12	60:SP:1958:MET:HE3	1.88	0.55
2:L1:163:G:OP2	2:L1:163:G:N2	2.29	0.55
2:L1:1638:G:OP2	2:L1:1638:G:N2	2.36	0.55
17:LI:650:LEU:HD13	19:LK:506:LEU:HD13	1.89	0.55
18:LJ:494:GLU:OE1	20:LL:533:ARG:NH1	2.39	0.55
32:LX:164:MET:CE	32:LX:190:LEU:HD21	2.37	0.55
32:LX:798:ALA:N	32:LX:901:GLU:OE2	2.39	0.55
54:SH:22:VAL:HG11	54:SH:105:TYR:HD1	1.71	0.55
8:L7:168:SER:O	8:L7:172:VAL:HG23	2.07	0.54
17:LI:650:LEU:CD1	19:LK:506:LEU:HD13	2.36	0.54
32:LX:27:VAL:HG13	32:LX:152:LEU:HD13	1.88	0.54
2:L1:1583:A:O2'	6:L5:76:ARG:NH2	2.40	0.54
14:LF:121:THR:HG21	14:LF:123:LYS:HE3	1.88	0.54
18:LJ:420:GLU:OE2	18:LJ:424:ARG:NH1	2.40	0.54
27:LS:272:LEU:HD11	27:LS:314:THR:HG21	1.88	0.54
41:NH:777:ASP:O	41:NH:780:GLN:NE2	2.41	0.54
60:SP:1261:ILE:HD12	60:SP:1291:LEU:HD22	1.89	0.54
64:ST:601:PRO:O	64:ST:675:TYR:OH	2.25	0.54
2:L1:192:U:N3	2:L1:193:U:O2'	2.40	0.54
3:L2:24:U:O2'	3:L2:25:U:OP2	2.25	0.54
3:L2:324:U:N3	50:SB:323:GLU:OE2	2.40	0.54
22:LN:684:GLU:OE1	22:LN:684:GLU:N	2.36	0.54
23:LO:667:GLY:HA3	34:NA:454:VAL:HG21	1.88	0.54
38:NE:149:LEU:HD12	38:NE:150:GLN:N	2.23	0.54
41:NH:542:SER:O	41:NH:546:THR:HG23	2.07	0.54
44:NM:172:LEU:O	44:NM:176:VAL:HG22	2.07	0.54
68:SY:213:GLN:O	68:SY:217:ARG:NE	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LH:604:PHE:HA	17:LI:592:ARG:HH12	1.72	0.54
16:LH:879:ILE:HD12	21:LM:215:CYS:SG	2.47	0.54
17:LI:359:LYS:N	17:LI:386:THR:O	2.38	0.54
20:LL:443:GLN:NE2	65:SU:333:GLU:O	2.41	0.54
28:LT:778:ALA:HA	67:SW:238:THR:HG21	1.89	0.54
33:LZ:65:PRO:HD3	38:NE:203:ILE:HG22	1.87	0.54
56:SK:49:SER:C	56:SK:50:LEU:HD12	2.32	0.54
64:ST:565:VAL:HG11	64:ST:660:ILE:HD11	1.90	0.54
23:LO:839:THR:N	28:LT:882:GLU:OE1	2.40	0.54
37:ND:110:ALA:O	65:SU:90:TRP:NE1	2.41	0.54
42:NI:54:PHE:C	42:NI:55:LEU:HD12	2.32	0.54
2:L1:249:U:N3	12:LD:63:LEU:HD21	2.23	0.54
2:L1:1632:C:N4	25:LQ:940:GLY:O	2.40	0.54
16:LH:720:ILE:HD12	16:LH:774:PHE:CD2	2.41	0.54
23:LO:288:ASP:OD2	23:LO:295:ILE:HD11	2.08	0.54
24:LP:12:ILE:HG21	31:LW:62:ALA:HB1	1.90	0.54
24:LP:173:ARG:NH1	63:SS:335:GLN:OE1	2.38	0.54
32:LY:24:SER:HA	32:LY:482:ILE:HD11	1.90	0.54
49:SA:281:LEU:HD11	50:SB:265:PHE:HZ	1.72	0.54
57:SL:19:THR:O	57:SL:28:ASN:ND2	2.37	0.54
58:SM:241:THR:OG1	58:SM:244:GLY:O	2.22	0.54
60:SP:334:ASN:O	60:SP:337:THR:OG1	2.19	0.54
63:SS:248:MET:HE2	63:SS:257:ILE:HG23	1.88	0.54
63:SS:360:PHE:CD2	63:SS:387:MET:HE1	2.43	0.54
8:L7:159:VAL:HG23	8:L7:185:ILE:HG21	1.89	0.54
21:LM:276:LEU:HD23	21:LM:279:MET:CE	2.37	0.54
37:ND:168:LYS:O	68:SY:140:ARG:NH2	2.41	0.54
56:SJ:176:ARG:HD2	56:SJ:196:LEU:HD11	1.89	0.54
2:L1:416:A:O4'	32:LX:104:ARG:NH1	2.41	0.54
21:LM:718:ARG:O	21:LM:722:ASN:N	2.37	0.54
30:LV:313:PRO:HG2	30:LV:317:ILE:HD11	1.89	0.54
56:SJ:206:VAL:HG21	56:SJ:238:CYS:SG	2.48	0.54
62:SR:90:ASP:OD2	62:SR:91:GLY:N	2.41	0.54
2:L1:763:G:N2	2:L1:774:A:N7	2.56	0.54
8:L7:163:ASP:O	63:SS:277:ARG:NH1	2.40	0.54
16:LH:495:ILE:HD11	16:LH:509:THR:HB	1.89	0.54
21:LM:91:ILE:HD12	31:LW:97:VAL:HG21	1.88	0.54
29:LU:66:HIS:N	29:LU:370:GLY:O	2.40	0.54
31:LW:107:SER:OG	31:LW:109:LYS:NZ	2.41	0.54
4:L3:18:LEU:HD22	4:L3:73:MET:CE	2.38	0.54
18:LJ:510:LEU:HD23	19:LK:505:MET:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LQ:941:THR:HG23	34:NA:466:GLU:CD	2.33	0.54
60:SP:1917:ILE:O	60:SP:1920:THR:OG1	2.21	0.54
2:L1:332:U:OP1	9:L8:31:ARG:NH1	2.39	0.53
2:L1:438:A:H1'	2:L1:465:G:H22	1.73	0.53
15:LG:29:ARG:NH2	25:LQ:824:MET:O	2.41	0.53
17:LI:614:ILE:CD1	17:LI:634:LEU:HD21	2.38	0.53
32:LX:200:VAL:HG21	32:LX:210:LEU:HD11	1.89	0.53
55:SI:819:GLU:OE1	55:SI:819:GLU:N	2.41	0.53
7:L6:65:GLN:OE1	7:L6:66:GLY:N	2.38	0.53
16:LH:627:ASP:OD1	16:LH:628:ASP:N	2.41	0.53
25:LQ:171:CYS:HB2	25:LQ:177:LEU:HD13	1.90	0.53
31:LW:19:ASN:OD1	31:LW:20:LYS:N	2.40	0.53
54:SH:208:MET:HE3	54:SH:241:TRP:CZ3	2.43	0.53
60:SP:1876:LEU:HD22	60:SP:1917:ILE:HD12	1.89	0.53
60:SP:1927:SER:OG	60:SP:1929:GLU:OE1	2.21	0.53
26:LR:631:MET:HE3	26:LR:644:TRP:O	2.09	0.53
31:LW:283:ASP:OD1	31:LW:284:ARG:N	2.41	0.53
65:SU:415:MET:HE3	65:SU:458:ALA:O	2.09	0.53
2:L1:8:U:O2	38:NE:239:ARG:NE	2.38	0.53
9:L8:11:ARG:NH1	9:L8:15:GLY:O	2.40	0.53
30:LV:287:ASN:OD1	30:LV:302:ARG:NE	2.41	0.53
45:NN:333:MET:O	45:NN:337:MET:N	2.39	0.53
60:SP:2103:PHE:HE1	60:SP:2141:VAL:HG13	1.72	0.53
2:L1:1595:U:OP1	55:SI:945:THR:OG1	2.25	0.53
16:LH:97:THR:HG21	16:LH:132:PHE:CE2	2.44	0.53
24:LP:62:ASN:OD1	27:LS:22:LEU:HD22	2.08	0.53
29:LU:68:ASP:OD2	29:LU:69:GLY:N	2.37	0.53
35:NB:376:VAL:HG11	65:SU:54:PHE:HD2	1.74	0.53
41:NH:741:ILE:HG21	41:NH:753:ILE:CD1	2.38	0.53
44:NM:126:THR:OG1	44:NM:136:ARG:NH1	2.42	0.53
49:SA:182:ASP:OD1	49:SA:183:GLN:N	2.42	0.53
63:SS:793:GLU:N	63:SS:793:GLU:OE1	2.41	0.53
67:SW:124:LEU:HB3	67:SW:126:LEU:HD23	1.89	0.53
21:LM:390:LEU:O	21:LM:394:LEU:N	2.41	0.53
28:LT:335:VAL:HG23	28:LT:336:VAL:HG23	1.90	0.53
29:LU:291:MET:HE1	63:SS:295:VAL:HG11	1.90	0.53
32:LX:748:ARG:NE	32:LX:750:THR:O	2.42	0.53
32:LY:309:PHE:HB2	32:LY:384:VAL:HG22	1.89	0.53
32:LY:540:LEU:HD11	32:LY:640:THR:C	2.34	0.53
44:NM:87:ARG:NH1	44:NM:100:PHE:O	2.41	0.53
53:SG:409:ASP:OD1	53:SG:410:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SI:616:ASP:OD1	55:SI:617:THR:N	2.39	0.53
2:L1:1680:G:H21	2:L1:1681:A:H61	1.57	0.53
23:LO:269:HIS:NE2	23:LO:312:GLN:O	2.39	0.53
50:SB:48:SER:HB2	50:SB:75:LEU:HD12	1.90	0.53
60:SP:2095:LEU:O	60:SP:2099:SER:N	2.42	0.53
66:SV:143:GLN:OE1	68:SY:128:LYS:HE2	2.09	0.53
2:L1:1633:A:O2'	23:LO:415:ASP:OD2	2.27	0.53
12:LD:55:ASP:OD2	12:LD:58:CYS:N	2.41	0.53
32:LX:529:VAL:HB	55:SI:416:LEU:HD12	1.91	0.53
32:LY:17:GLY:O	32:LY:21:LYS:N	2.42	0.53
38:NE:149:LEU:HD13	43:NK:197:ILE:CD1	2.38	0.53
56:SJ:180:LEU:CD1	56:SJ:206:VAL:HG22	2.38	0.53
8:L7:152:VAL:HG23	8:L7:181:ILE:HD11	1.91	0.53
17:LI:706:TYR:CE2	17:LI:708:MET:HE3	2.43	0.53
18:LJ:312:ALA:HB3	18:LJ:316:ARG:HH11	1.74	0.53
24:LP:192:PHE:CZ	63:SS:351:LEU:HD21	2.43	0.53
30:LV:319:ASP:O	30:LV:332:ALA:N	2.41	0.53
32:LX:765:VAL:HG23	32:LX:774:LEU:HD22	1.89	0.53
60:SP:1449:ASP:O	60:SP:1453:ASN:ND2	2.38	0.53
63:SS:319:THR:O	63:SS:319:THR:HG23	2.09	0.53
18:LJ:118:LEU:HD11	18:LJ:157:ALA:CB	2.40	0.52
23:LO:485:ASN:O	23:LO:486:SER:OG	2.24	0.52
30:LV:74:THR:HG21	30:LV:101:ASN:CB	2.40	0.52
32:LX:617:LEU:HD23	32:LX:761:VAL:HG21	1.90	0.52
60:SP:1134:MET:HE3	60:SP:1181:ILE:HD12	1.92	0.52
2:L1:1584:G:N2	2:L1:1611:A:OP2	2.24	0.52
23:LO:567:ASP:OD1	23:LO:576:ARG:NH2	2.43	0.52
24:LP:391:TYR:CZ	24:LP:395:ILE:HD11	2.43	0.52
31:LW:378:VAL:HG11	31:LW:381:LEU:HD11	1.90	0.52
18:LJ:238:ASP:O	18:LJ:242:ASN:N	2.41	0.52
27:LS:504:THR:HG23	27:LS:504:THR:O	2.09	0.52
28:LT:174:ALA:O	28:LT:175:THR:OG1	2.21	0.52
30:LV:264:ILE:HD12	30:LV:302:ARG:O	2.10	0.52
31:LW:507:ASN:OD1	31:LW:508:VAL:HG23	2.10	0.52
32:LX:233:GLU:O	32:LX:237:LEU:HD23	2.10	0.52
36:NC:93:MET:HE2	36:NC:93:MET:HA	1.91	0.52
41:NH:480:MET:HE2	41:NH:485:TYR:HA	1.91	0.52
60:SP:137:ASP:O	60:SP:140:ILE:HG22	2.10	0.52
63:SS:376:ARG:NH1	63:SS:379:GLU:OE1	2.43	0.52
16:LH:413:SER:OG	16:LH:414:ILE:N	2.43	0.52
18:LJ:132:PHE:CE1	18:LJ:140:LEU:HD13	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LL:472:LEU:HD23	20:LL:473:LYS:O	2.10	0.52
23:LO:356:ASP:O	23:LO:689:THR:OG1	2.18	0.52
32:LX:6:ILE:CG1	55:SI:373:ILE:HD13	2.39	0.52
41:NH:515:ILE:HG23	41:NH:948:TYR:CD1	2.44	0.52
54:SH:100:VAL:HG13	54:SH:168:LEU:HD12	1.91	0.52
55:SI:925:ASN:OD1	55:SI:926:ILE:N	2.42	0.52
56:SK:163:ILE:HD12	56:SK:170:HIS:CD2	2.44	0.52
60:SP:1151:ILE:HG23	60:SP:1201:LEU:HD22	1.92	0.52
60:SP:2101:SER:OG	63:SS:262:LEU:HD21	2.09	0.52
5:L4:21:ASP:OD2	5:L4:24:SER:N	2.42	0.52
56:SK:77:LEU:HD23	56:SK:84:ILE:HG22	1.91	0.52
28:LT:726:GLY:O	28:LT:728:ARG:NH1	2.42	0.52
60:SP:1027:ILE:HG23	60:SP:1085:VAL:HG21	1.91	0.52
65:SU:65:LYS:HA	65:SU:65:LYS:HE3	1.90	0.52
18:LJ:85:TYR:O	18:LJ:86:SER:OG	2.18	0.52
30:LV:56:SER:OG	30:LV:77:TYR:O	2.28	0.52
60:SP:1610:MET:HA	60:SP:1610:MET:HE3	1.91	0.52
32:LY:341:ASP:OD1	32:LY:342:ILE:N	2.43	0.52
32:LY:370:ILE:CD1	32:LY:378:LEU:HD21	2.40	0.52
2:L1:6:G:O6	29:LU:419:VAL:HG22	2.09	0.52
16:LH:724:ILE:HG21	16:LH:762:TYR:CD2	2.44	0.52
23:LO:4:ASP:O	23:LO:706:THR:HG22	2.09	0.52
52:SE:46:ARG:HE	68:SY:108:ARG:HD2	1.75	0.52
60:SP:121:PHE:HD2	60:SP:162:LEU:HD11	1.74	0.52
61:SQ:120:ASP:OD2	61:SQ:173:ILE:HD13	2.10	0.52
26:LR:457:ALA:HB1	26:LR:494:ILE:HG21	1.91	0.52
26:LR:561:SER:O	26:LR:565:PHE:N	2.43	0.52
29:LU:215:LEU:O	29:LU:216:SER:OG	2.27	0.52
29:LU:267:ILE:CD1	29:LU:279:THR:HG22	2.40	0.52
34:NA:504:ASP:OD2	34:NA:505:GLY:N	2.42	0.52
35:NB:376:VAL:HG11	65:SU:54:PHE:CD2	2.44	0.52
55:SI:1086:MET:HE1	68:SY:81:SER:O	2.10	0.52
60:SP:389:ILE:O	60:SP:393:PHE:N	2.43	0.52
2:L1:207:U:O2	9:L8:178:ARG:NH2	2.43	0.51
2:L1:1492:A:OP1	61:SQ:210:LYS:NZ	2.31	0.51
8:L7:166:LEU:HD11	8:L7:185:ILE:CD1	2.38	0.51
16:LH:671:ILE:CD1	16:LH:750:LEU:HD11	2.39	0.51
28:LT:894:ASP:OD1	28:LT:895:VAL:N	2.42	0.51
32:LX:510:PRO:O	32:LX:652:ARG:NE	2.43	0.51
32:LX:757:GLU:OE1	32:LX:757:GLU:N	2.43	0.51
32:LY:144:GLY:N	32:LY:475:ARG:O	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:NE:303:GLU:O	57:SL:112:LYS:NZ	2.42	0.51
41:NH:763:THR:HG21	41:NH:935:GLU:OE2	2.09	0.51
56:SK:31:LEU:HD23	56:SK:40:ARG:HD3	1.91	0.51
9:L8:43:ILE:HG22	9:L8:57:ALA:HA	1.92	0.51
20:LL:509:HIS:O	20:LL:513:LEU:HD23	2.09	0.51
31:LW:125:LEU:HD21	31:LW:398:ILE:CD1	2.40	0.51
50:SB:133:ASP:OD1	50:SB:134:ASN:N	2.43	0.51
51:SC:239:CYS:SG	51:SC:240:VAL:N	2.83	0.51
54:SH:137:LEU:HD12	54:SH:296:LEU:HD22	1.93	0.51
54:SH:338:PHE:CB	55:SI:772:MET:HE1	2.40	0.51
60:SP:322:VAL:O	60:SP:368:ASN:ND2	2.43	0.51
3:L2:86:A:O2'	50:SB:336:THR:O	2.26	0.51
41:NH:209:MET:HE3	41:NH:214:PHE:CZ	2.45	0.51
41:NH:1083:GLN:OE1	41:NH:1083:GLN:N	2.43	0.51
2:L1:628:G:N2	2:L1:629:U:O4	2.43	0.51
7:L6:57:ASP:OD1	7:L6:60:GLY:N	2.44	0.51
22:LN:312:ASN:OD1	22:LN:313:LYS:N	2.44	0.51
26:LR:222:LEU:CD2	26:LR:234:LEU:HD12	2.41	0.51
27:LS:376:LEU:HD13	27:LS:409:ILE:HD11	1.91	0.51
60:SP:1037:LEU:O	60:SP:1048:ARG:NH1	2.43	0.51
16:LH:372:LEU:HD21	16:LH:374:LEU:HD21	1.92	0.51
16:LH:769:ASN:OD1	16:LH:770:TYR:N	2.43	0.51
23:LO:14:VAL:O	23:LO:31:SER:OG	2.16	0.51
28:LT:743:ARG:NH2	34:NA:480:GLN:O	2.44	0.51
32:LX:578:ARG:NH1	55:SI:429:ALA:O	2.44	0.51
59:SN:56:ILE:HD12	66:SV:192:ALA:HA	1.92	0.51
2:L1:1229:G:N2	2:L1:1255:G:O2'	2.43	0.51
32:LX:6:ILE:HG13	55:SI:373:ILE:HD13	1.92	0.51
32:LX:190:LEU:HD23	55:SI:407:ILE:HD11	1.91	0.51
41:NH:840:LEU:HD21	41:NH:842:ILE:HD11	1.93	0.51
53:SG:185:LEU:HD13	53:SG:527:VAL:CG1	2.41	0.51
56:SK:140:LEU:HB2	56:SK:141:MET:HE2	1.92	0.51
60:SP:497:ILE:HD11	60:SP:525:ILE:HG22	1.93	0.51
60:SP:1372:MET:HE3	60:SP:1423:TYR:CD1	2.46	0.51
63:SS:313:PHE:O	63:SS:315:LEU:N	2.44	0.51
5:L4:129:VAL:HG22	5:L4:139:VAL:HG12	1.93	0.51
16:LH:302:SER:OG	16:LH:344:CYS:N	2.43	0.51
25:LQ:149:ASP:O	25:LQ:153:GLU:N	2.42	0.51
49:SA:229:LEU:HD11	49:SA:255:ALA:HB3	1.93	0.51
49:SA:254:ASN:O	49:SA:254:ASN:ND2	2.43	0.51
56:SK:222:ASP:OD1	56:SK:223:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SN:194:ASP:OD1	59:SN:194:ASP:N	2.42	0.51
60:SP:484:ILE:O	60:SP:487:LYS:NZ	2.44	0.51
60:SP:1539:ASN:OD1	60:SP:1540:GLN:N	2.43	0.51
6:L5:120:ILE:HD12	18:LJ:117:LEU:CD2	2.41	0.51
7:L6:57:ASP:OD1	7:L6:61:PHE:N	2.44	0.51
16:LH:343:ASP:OD2	16:LH:344:CYS:N	2.44	0.51
17:LI:674:GLU:O	17:LI:678:LEU:HD23	2.10	0.51
20:LL:22:VAL:HG12	20:LL:27:GLN:HG2	1.93	0.51
20:LL:302:ASN:ND2	20:LL:316:ASN:OD1	2.44	0.51
22:LN:424:ASP:OD2	22:LN:444:ARG:NH1	2.43	0.51
23:LO:363:ALA:HB2	23:LO:393:VAL:CG2	2.41	0.51
23:LO:467:ASP:OD1	23:LO:468:ALA:N	2.43	0.51
32:LY:278:THR:OG1	32:LY:463:ARG:NH2	2.43	0.51
1:L0:407:A:O2'	55:SI:1086:MET:O	2.29	0.51
2:L1:70:C:OP2	7:L6:164:LYS:NZ	2.42	0.51
27:LS:364:GLN:NE2	27:LS:369:ASN:OD1	2.44	0.51
42:NI:266:LYS:HA	42:NI:266:LYS:HE3	1.92	0.51
60:SP:1640:CYS:HB3	60:SP:1680:THR:HG21	1.92	0.51
2:L1:298:C:OP2	5:L4:37:LYS:NZ	2.40	0.51
4:L3:45:LEU:HD23	4:L3:45:LEU:C	2.35	0.51
16:LH:682:ASN:O	16:LH:686:GLY:N	2.40	0.51
23:LO:707:ASN:OD1	23:LO:708:ASP:N	2.43	0.51
32:LX:775:VAL:HG11	32:LX:820:HIS:NE2	2.26	0.51
36:NC:96:ARG:CD	45:NN:337:MET:HE1	2.40	0.51
55:SI:99:ASN:OD1	55:SI:100:ASP:N	2.44	0.51
56:SK:113:TYR:CD2	56:SK:167:ILE:HD11	2.46	0.51
27:LS:307:GLN:O	27:LS:310:GLN:NE2	2.44	0.50
34:NA:348:ASP:OD1	64:ST:766:ARG:NH2	2.43	0.50
60:SP:922:MET:HE1	60:SP:956:PHE:CD1	2.45	0.50
60:SP:1425:VAL:HG21	60:SP:1437:MET:HG2	1.92	0.50
2:L1:1608:U:OP1	11:LC:15:SER:OG	2.29	0.50
21:LM:130:LYS:O	28:LT:330:GLN:NE2	2.43	0.50
28:LT:807:VAL:HG13	67:SW:248:VAL:HG11	1.93	0.50
41:NH:203:ILE:HD11	41:NH:290:PHE:CE2	2.46	0.50
41:NH:253:GLN:NE2	41:NH:273:SER:OG	2.44	0.50
44:NM:99:ASN:OD1	44:NM:100:PHE:N	2.42	0.50
21:LM:717:GLU:O	21:LM:721:VAL:N	2.35	0.50
27:LS:224:ASN:OD1	27:LS:225:SER:N	2.44	0.50
32:LY:548:ASN:OD1	32:LY:549:SER:N	2.45	0.50
48:OA:1520:MET:O	48:OA:1523:LEU:N	2.44	0.50
2:L1:1085:G:N7	38:NE:302:ARG:NH2	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LD:118:GLN:N	12:LD:118:GLN:OE1	2.45	0.50
25:LQ:529:GLU:OE1	25:LQ:529:GLU:N	2.45	0.50
50:SB:3:TYR:OH	50:SB:82:ASP:OD2	2.27	0.50
55:SI:124:ASP:OD1	55:SI:126:ASN:N	2.45	0.50
67:SW:131:ASN:O	67:SW:135:LYS:N	2.45	0.50
16:LH:374:LEU:HD23	16:LH:381:SER:HA	1.94	0.50
26:LR:8:LYS:NZ	26:LR:10:ILE:HD11	2.26	0.50
27:LS:156:ASN:OD1	27:LS:159:HIS:ND1	2.37	0.50
43:NK:52:TYR:CE1	43:NK:56:ILE:HD13	2.46	0.50
50:SB:14:LEU:HD12	50:SB:75:LEU:CD2	2.42	0.50
4:L3:109:LEU:HD22	64:ST:747:GLU:HG3	1.94	0.50
24:LP:203:MET:O	24:LP:207:ASN:N	2.43	0.50
26:LR:469:PRO:HG3	26:LR:480:ILE:HD11	1.93	0.50
30:LV:273:ASP:OD1	30:LV:273:ASP:N	2.45	0.50
32:LX:259:GLN:NE2	32:LX:288:GLY:O	2.45	0.50
49:SA:222:PHE:O	49:SA:224:LYS:NZ	2.44	0.50
49:SA:223:ILE:O	49:SA:223:ILE:HG23	2.11	0.50
60:SP:1876:LEU:HD22	60:SP:1917:ILE:CD1	2.41	0.50
65:SU:99:LYS:HE3	65:SU:147:THR:HG23	1.94	0.50
4:L3:45:LEU:HD13	4:L3:85:PHE:HE2	1.77	0.50
26:LR:12:LEU:HD11	26:LR:378:PRO:HG2	1.93	0.50
44:NM:57:ALA:O	44:NM:61:LEU:HD23	2.12	0.50
60:SP:497:ILE:HD11	60:SP:525:ILE:CG2	2.42	0.50
2:L1:563:U:O3'	58:SM:278:ARG:NH1	2.44	0.50
20:LL:310:THR:O	20:LL:310:THR:HG22	2.12	0.50
27:LS:519:SER:HB2	27:LS:535:ARG:HD2	1.94	0.50
31:LW:116:ILE:HG22	31:LW:127:ILE:HG22	1.93	0.50
4:L3:18:LEU:HD22	4:L3:73:MET:HE3	1.94	0.50
9:L8:60:ILE:HG21	9:L8:179:CYS:SG	2.52	0.50
16:LH:378:ASP:OD1	16:LH:380:THR:HG22	2.12	0.50
25:LQ:502:PHE:HE2	25:LQ:522:LEU:HD21	1.77	0.50
41:NH:975:LEU:HD11	41:NH:977:LEU:HD21	1.93	0.50
51:SD:156:MET:HE2	51:SD:156:MET:HA	1.93	0.50
55:SI:65:ASP:OD2	55:SI:66:ASP:N	2.45	0.50
60:SP:1308:LEU:HD21	60:SP:1351:PHE:CE1	2.47	0.50
24:LP:320:ILE:HD12	24:LP:335:ILE:HG23	1.94	0.49
25:LQ:414:LEU:CD1	25:LQ:447:LEU:HD21	2.42	0.49
26:LR:579:GLN:NE2	26:LR:620:LEU:O	2.45	0.49
31:LW:14:GLU:OE1	31:LW:14:GLU:N	2.45	0.49
56:SJ:55:ILE:HD12	56:SJ:76:LEU:HD21	1.94	0.49
56:SJ:97:LEU:HD22	56:SJ:130:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SP:358:VAL:HB	60:SP:389:ILE:HD11	1.94	0.49
60:SP:603:LEU:O	60:SP:607:LEU:HD23	2.12	0.49
60:SP:1249:LEU:O	60:SP:1253:ASN:ND2	2.40	0.49
32:LY:789:LEU:HD23	32:LY:793:PHE:HB2	1.94	0.49
48:OA:1408:ASP:OD2	48:OA:1412:SER:N	2.46	0.49
50:SB:152:LEU:HD21	51:SD:221:ILE:HD13	1.94	0.49
60:SP:1312:SER:N	60:SP:1318:GLU:O	2.41	0.49
60:SP:1527:LEU:HD21	60:SP:1590:LEU:HD21	1.93	0.49
63:SS:827:GLN:OE1	63:SS:827:GLN:N	2.45	0.49
2:L1:1169:G:N1	2:L1:1575:G:OP2	2.36	0.49
16:LH:282:ILE:HD13	16:LH:293:LEU:HD13	1.93	0.49
21:LM:1742:GLU:O	21:LM:1746:ARG:N	2.38	0.49
32:LY:749:GLN:NE2	32:LY:792:ASP:OD2	2.45	0.49
54:SH:125:HIS:NE2	54:SH:263:ASP:OD1	2.41	0.49
56:SJ:125:ASN:O	56:SJ:128:VAL:HG12	2.12	0.49
56:SJ:176:ARG:CD	56:SJ:196:LEU:HD11	2.43	0.49
60:SP:2070:TYR:O	60:SP:2076:ARG:NH2	2.45	0.49
65:SU:156:TRP:CD1	65:SU:218:LYS:HD2	2.48	0.49
16:LH:495:ILE:O	16:LH:495:ILE:HG23	2.12	0.49
18:LJ:108:TYR:CE1	18:LJ:116:ILE:HG23	2.47	0.49
24:LP:80:THR:HG23	24:LP:80:THR:O	2.12	0.49
24:LP:411:ARG:HD2	24:LP:437:ILE:HG23	1.94	0.49
30:LV:138:PRO:CG	45:NN:464:LEU:HD13	2.42	0.49
32:LY:276:ASN:ND2	32:LY:464:GLN:OE1	2.44	0.49
41:NH:856:THR:HG22	41:NH:858:ARG:H	1.76	0.49
41:NH:1206:PRO:HA	41:NH:1212:VAL:HG12	1.95	0.49
60:SP:1946:LYS:CD	63:SS:455:ILE:HG23	2.42	0.49
5:L4:111:VAL:HG23	5:L4:111:VAL:O	2.13	0.49
28:LT:179:LYS:HB3	28:LT:190:LEU:HD11	1.95	0.49
28:LT:593:PHE:CZ	28:LT:600:ILE:HD11	2.48	0.49
32:LX:855:ILE:HG22	32:LX:855:ILE:O	2.13	0.49
39:NF:87:ASP:OD1	39:NF:88:LEU:N	2.45	0.49
43:NK:112:GLN:O	43:NK:174:MET:HE1	2.13	0.49
49:SA:213:ASN:OD1	49:SA:214:TYR:N	2.46	0.49
58:SM:83:ILE:HG22	58:SM:84:MET:HE2	1.94	0.49
60:SP:757:ILE:O	60:SP:761:THR:HG23	2.12	0.49
60:SP:1523:TYR:OH	60:SP:1551:LEU:O	2.25	0.49
60:SP:2153:ASP:OD1	60:SP:2154:ASN:N	2.45	0.49
64:ST:385:ASP:OD1	64:ST:386:ALA:N	2.45	0.49
64:ST:555:ARG:NH2	65:SU:522:GLU:OE2	2.44	0.49
5:L4:216:ASN:OD1	5:L4:217:THR:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L6:32:ILE:HD13	7:L6:52:ILE:HG22	1.95	0.49
8:L7:70:PHE:O	8:L7:74:GLN:N	2.46	0.49
16:LH:817:SER:O	16:LH:821:ILE:HD12	2.12	0.49
21:LM:268:LEU:HD11	27:LS:219:LYS:CE	2.42	0.49
23:LO:423:ARG:NH1	23:LO:460:VAL:O	2.46	0.49
25:LQ:161:SER:OG	25:LQ:187:LYS:NZ	2.30	0.49
27:LS:183:ASP:OD1	28:LT:281:ARG:NH1	2.43	0.49
32:LX:174:THR:O	32:LX:681:ARG:NH2	2.46	0.49
39:NF:79:GLY:O	42:NI:259:ARG:NH1	2.46	0.49
60:SP:1600:THR:O	60:SP:1609:ARG:NH2	2.46	0.49
7:L6:23:ARG:O	7:L6:26:VAL:HG12	2.12	0.49
18:LJ:504:ILE:HD11	20:LL:499:ASN:OD1	2.12	0.49
20:LL:227:VAL:HG11	28:LT:563:ASP:CG	2.38	0.49
23:LO:103:LYS:HB3	23:LO:152:LEU:HD11	1.95	0.49
25:LQ:759:GLY:HA3	25:LQ:805:ILE:HD11	1.95	0.49
60:SP:1511:ILE:HG21	60:SP:1547:LEU:HD11	1.93	0.49
60:SP:1928:ASP:OD1	60:SP:1929:GLU:N	2.46	0.49
64:ST:516:LEU:HD23	65:SU:515:LEU:HD12	1.94	0.49
2:L1:1699:G:N2	2:L1:1702:A:OP2	2.45	0.49
26:LR:406:ALA:HB2	26:LR:440:VAL:CG2	2.41	0.49
33:LZ:153:ASN:OD1	33:LZ:154:MET:N	2.46	0.49
41:NH:232:LEU:HD13	41:NH:296:ILE:HD11	1.95	0.49
49:SA:217:ALA:O	49:SA:221:LEU:HD23	2.13	0.49
51:SD:234:ILE:HG22	51:SD:235:GLY:O	2.12	0.49
60:SP:906:THR:O	60:SP:912:SER:OG	2.30	0.49
60:SP:2121:MET:HE2	60:SP:2121:MET:HA	1.94	0.49
67:SW:25:ILE:HD13	67:SW:160:LYS:HG2	1.95	0.49
2:L1:18:C:O4'	57:SL:162:GLN:NE2	2.45	0.49
2:L1:862:A:H3'	39:NF:16:ILE:HD13	1.94	0.49
22:LN:586:THR:OG1	22:LN:588:ASP:OD1	2.15	0.49
32:LX:496:LEU:HD23	32:LX:539:ALA:HB1	1.95	0.49
40:NG:36:LYS:HG2	44:NM:64:ARG:NH1	2.28	0.49
41:NH:396:LEU:O	41:NH:400:LEU:HD23	2.13	0.49
41:NH:1037:LEU:CD2	41:NH:1050:ILE:HG22	2.40	0.49
65:SU:98:PHE:CE1	65:SU:102:LEU:HD11	2.47	0.49
65:SU:417:HIS:NE2	65:SU:422:ILE:HD11	2.28	0.49
3:L2:332:G:H21	16:LH:869:MET:CE	2.25	0.49
16:LH:236:ASN:C	16:LH:237:LEU:HD22	2.38	0.49
31:LW:302:ASP:O	31:LW:306:PHE:N	2.46	0.49
32:LX:857:ASP:OD1	32:LX:858:MET:N	2.46	0.49
56:SJ:73:HIS:O	56:SJ:77:LEU:HD23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SJ:179:THR:HG23	56:SJ:221:VAL:HG21	1.95	0.49
65:SU:185:TYR:CG	65:SU:222:LEU:HD11	2.48	0.49
33:LZ:115:MET:HE2	33:LZ:131:ILE:HD11	1.95	0.48
38:NE:164:LEU:HD11	38:NE:213:MET:CE	2.43	0.48
41:NH:469:ASP:O	41:NH:473:LYS:N	2.45	0.48
4:L3:23:ASP:O	4:L3:26:ILE:HG22	2.12	0.48
23:LO:33:VAL:HG23	23:LO:33:VAL:O	2.13	0.48
29:LU:305:VAL:HG21	29:LU:426:ALA:HB1	1.94	0.48
32:LX:94:PHE:CZ	32:LX:98:ILE:HD11	2.48	0.48
41:NH:503:VAL:HG23	41:NH:504:GLN:CD	2.38	0.48
54:SH:337:VAL:HG22	54:SH:354:ILE:CG1	2.43	0.48
60:SP:1139:ASN:OD1	60:SP:1140:GLN:N	2.45	0.48
60:SP:1181:ILE:O	60:SP:1184:SER:OG	2.28	0.48
60:SP:1193:ASN:O	60:SP:1196:SER:OG	2.20	0.48
65:SU:417:HIS:CE1	65:SU:422:ILE:HD11	2.48	0.48
13:LE:79:PHE:HE2	38:NE:321:VAL:HG21	1.78	0.48
28:LT:334:ASP:OD1	28:LT:335:VAL:N	2.44	0.48
30:LV:312:GLU:O	30:LV:366:LYS:NZ	2.26	0.48
41:NH:176:PHE:CD2	41:NH:230:VAL:HG21	2.48	0.48
51:SD:111:MET:HE1	51:SD:190:PRO:N	2.28	0.48
53:SG:327:ASP:OD1	53:SG:328:ILE:N	2.46	0.48
54:SH:23:LEU:HD11	54:SH:329:ILE:HD13	1.95	0.48
32:LX:894:ASN:O	32:LX:897:THR:OG1	2.30	0.48
50:SB:240:GLU:HG3	50:SB:241:VAL:HG13	1.94	0.48
55:SI:1119:ILE:HD13	61:SQ:194:ILE:HD12	1.95	0.48
2:L1:-7:A:O2'	2:L1:-6:A:O5'	2.29	0.48
2:L1:418:G:O2'	7:L6:72:ARG:NH2	2.45	0.48
5:L4:95:THR:O	5:L4:95:THR:HG22	2.12	0.48
16:LH:495:ILE:HD12	16:LH:510:TYR:O	2.14	0.48
16:LH:627:ASP:O	16:LH:659:ILE:HD12	2.14	0.48
20:LL:255:ILE:HD11	20:LL:301:LEU:HD13	1.96	0.48
25:LQ:51:ILE:HD12	25:LQ:61:SER:OG	2.14	0.48
25:LQ:177:LEU:CB	25:LQ:191:LEU:HD21	2.43	0.48
26:LR:143:HIS:HE2	26:LR:173:LYS:HB2	1.77	0.48
26:LR:342:ASP:OD1	26:LR:343:MET:N	2.47	0.48
26:LR:552:SER:OG	26:LR:553:GLY:N	2.46	0.48
27:LS:512:ASP:O	68:SY:248:ARG:NH2	2.46	0.48
28:LT:258:THR:OG1	28:LT:306:GLY:N	2.45	0.48
32:LX:293:LEU:HD21	32:LX:409:ALA:HB2	1.95	0.48
55:SI:134:ILE:CD1	55:SI:245:LEU:HD13	2.43	0.48
60:SP:458:ILE:HG22	60:SP:491:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SQ:180:ASP:OD1	61:SQ:181:GLU:N	2.46	0.48
65:SU:400:PRO:HB2	65:SU:495:MET:HE1	1.94	0.48
8:L7:166:LEU:HD21	8:L7:185:ILE:HD11	1.94	0.48
16:LH:27:SER:OG	16:LH:171:TYR:OH	2.30	0.48
20:LL:113:MET:HE3	20:LL:160:VAL:CG1	2.44	0.48
25:LQ:680:SER:OG	25:LQ:682:ARG:NH1	2.47	0.48
25:LQ:799:LYS:NZ	25:LQ:807:ASP:OD1	2.46	0.48
41:NH:404:GLY:N	41:NH:455:SER:OG	2.46	0.48
65:SU:466:LEU:HA	65:SU:469:LEU:HD12	1.96	0.48
17:LI:432:ASP:OD1	17:LI:433:ASP:N	2.45	0.48
23:LO:261:ALA:HB2	23:LO:281:SER:OG	2.13	0.48
25:LQ:199:THR:OG1	26:LR:667:GLN:OE1	2.30	0.48
30:LV:39:ASN:OD1	30:LV:40:ASP:N	2.46	0.48
56:SJ:169:ASP:OD1	56:SJ:170:HIS:N	2.46	0.48
61:SQ:167:LYS:O	61:SQ:170:LYS:NZ	2.47	0.48
1:L0:382:U:O5'	38:NE:280:LYS:NZ	2.41	0.48
9:L8:58:LEU:HD12	30:LV:57:GLU:HG3	1.96	0.48
24:LP:324:ASP:OD1	24:LP:373:TYR:OH	2.27	0.48
25:LQ:115:LEU:HD22	25:LQ:153:GLU:HG2	1.94	0.48
35:NB:378:GLN:NE2	35:NB:379:SER:O	2.46	0.48
41:NH:1063:ARG:HH12	41:NH:1067:LEU:HD21	1.79	0.48
56:SK:229:ASN:OD1	56:SK:230:TYR:N	2.47	0.48
57:SL:97:LEU:HB3	57:SL:128:LEU:HD13	1.96	0.48
60:SP:441:ASP:OD1	60:SP:442:LYS:N	2.46	0.48
60:SP:2084:ASN:O	60:SP:2088:THR:HG22	2.13	0.48
64:ST:573:LEU:HD23	64:ST:593:LEU:HD21	1.96	0.48
65:SU:46:ASP:OD1	65:SU:47:GLU:N	2.46	0.48
7:L6:161:GLU:OE2	7:L6:168:THR:OG1	2.20	0.48
17:LI:498:SER:HB2	17:LI:531:LEU:HD12	1.95	0.48
32:LX:738:LYS:NZ	32:LX:806:GLU:OE2	2.36	0.48
41:NH:501:ASN:OD1	41:NH:503:VAL:HG22	2.14	0.48
52:SF:23:VAL:HG21	52:SF:117:VAL:HG21	1.95	0.48
55:SI:750:TRP:NE1	55:SI:754:GLN:OE1	2.46	0.48
60:SP:1324:ILE:HG21	60:SP:1363:LEU:HD21	1.95	0.48
64:ST:677:ASP:OD1	64:ST:678:PHE:N	2.47	0.48
8:L7:23:ALA:O	8:L7:27:LEU:HD23	2.13	0.48
20:LL:225:VAL:HG23	20:LL:225:VAL:O	2.14	0.48
21:LM:285:ASN:OD1	27:LS:205:ILE:HD12	2.13	0.48
22:LN:514:LEU:HD23	22:LN:515:GLU:O	2.14	0.48
26:LR:81:GLN:NE2	40:NG:69:ALA:HB1	2.28	0.48
28:LT:192:ASN:O	28:LT:196:GLY:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LU:316:THR:OG1	29:LU:318:ASP:OD1	2.32	0.48
34:NA:466:GLU:OE2	34:NA:466:GLU:N	2.47	0.48
60:SP:1613:ALA:HB1	60:SP:1639:ILE:HD11	1.95	0.48
61:SQ:199:THR:HG22	61:SQ:199:THR:O	2.13	0.48
2:L1:40:A:H62	2:L1:467:G:H21	1.62	0.47
13:LE:92:ASN:O	57:SL:79:LYS:NZ	2.46	0.47
13:LE:108:ALA:HB3	13:LE:111:MET:HE1	1.95	0.47
32:LY:516:PHE:CD2	32:LY:568:LEU:HD12	2.48	0.47
32:LY:785:PHE:CZ	32:LY:789:LEU:HD21	2.49	0.47
41:NH:390:THR:O	41:NH:394:THR:OG1	2.22	0.47
60:SP:1087:VAL:O	60:SP:1091:ILE:HG23	2.13	0.47
2:L1:1226:A:O2'	2:L1:1256:A:N1	2.40	0.47
9:L8:87:ASN:OD1	9:L8:88:ASN:N	2.47	0.47
26:LR:316:VAL:O	26:LR:320:LEU:N	2.40	0.47
27:LS:151:ASN:OD1	27:LS:152:GLU:N	2.47	0.47
29:LU:13:TYR:OH	31:LW:69:GLU:OE1	2.32	0.47
32:LY:864:LEU:HD22	32:LY:890:LEU:HD21	1.96	0.47
36:NC:114:GLU:O	36:NC:118:ALA:N	2.47	0.47
36:NC:131:MET:HE3	36:NC:131:MET:HA	1.96	0.47
49:SA:206:LEU:HD21	49:SA:219:LEU:HD22	1.95	0.47
2:L1:333:A:OP2	9:L8:48:THR:OG1	2.31	0.47
5:L4:141:THR:OG1	5:L4:143:ASP:OD1	2.31	0.47
16:LH:574:LEU:HD11	16:LH:622:ILE:HD13	1.96	0.47
25:LQ:135:ARG:NH2	25:LQ:174:GLU:OE1	2.47	0.47
29:LU:92:ILE:CD1	29:LU:136:MET:HE3	2.43	0.47
32:LX:297:ILE:HD11	32:LX:385:VAL:HG21	1.96	0.47
41:NH:397:MET:O	41:NH:401:LEU:HD23	2.14	0.47
50:SB:63:ILE:HB	51:SD:232:MET:HE1	1.96	0.47
56:SK:143:GLN:NE2	64:ST:718:GLU:O	2.47	0.47
60:SP:1134:MET:CE	60:SP:1181:ILE:HD12	2.44	0.47
60:SP:1273:LYS:NZ	60:SP:1401:ASN:OD1	2.47	0.47
64:ST:394:LEU:HD12	64:ST:398:ASP:OD2	2.14	0.47
21:LM:218:ILE:HD12	21:LM:263:VAL:CG2	2.45	0.47
23:LO:400:GLN:HG3	23:LO:401:VAL:HG23	1.96	0.47
25:LQ:446:ILE:HD12	25:LQ:479:LEU:HD21	1.95	0.47
31:LW:183:GLU:OE1	33:LZ:41:ARG:NH1	2.47	0.47
32:LX:94:PHE:CE2	32:LX:98:ILE:HD11	2.49	0.47
59:SN:217:GLN:NE2	59:SN:221:ASN:OD1	2.46	0.47
64:ST:576:ILE:O	64:ST:576:ILE:HG22	2.14	0.47
1:L0:467:A:N1	1:L0:468:A:N6	2.62	0.47
2:L1:31:C:O3'	62:SR:139:LYS:NZ	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LF:86:GLU:O	60:SP:13:ARG:NH2	2.42	0.47
16:LH:404:SER:OG	16:LH:405:ALA:N	2.47	0.47
16:LH:654:THR:C	16:LH:655:LEU:HD22	2.39	0.47
23:LO:507:GLN:N	23:LO:507:GLN:OE1	2.47	0.47
25:LQ:472:HIS:ND1	25:LQ:494:ASP:OD2	2.40	0.47
26:LR:235:LYS:NZ	26:LR:273:GLU:OE2	2.46	0.47
27:LS:45:ILE:H	27:LS:45:ILE:HD12	1.80	0.47
28:LT:354:SER:O	28:LT:631:ASN:ND2	2.45	0.47
29:LU:11:ASP:OD1	29:LU:12:ASP:N	2.47	0.47
41:NH:742:PHE:CD1	41:NH:750:VAL:HG21	2.49	0.47
51:SC:245:ALA:O	51:SC:246:GLN:NE2	2.47	0.47
55:SI:748:ASP:OD1	55:SI:749:THR:N	2.47	0.47
60:SP:481:TRP:HA	60:SP:484:ILE:HD12	1.95	0.47
60:SP:495:GLU:OE2	60:SP:495:GLU:N	2.43	0.47
60:SP:1027:ILE:CG2	60:SP:1085:VAL:HG21	2.45	0.47
3:L2:59:G:H5'	23:LO:570:THR:HG23	1.97	0.47
8:L7:17:GLU:CG	8:L7:46:ILE:HG22	2.45	0.47
13:LE:93:LEU:HD13	38:NE:311:VAL:HG21	1.95	0.47
21:LM:238:LEU:HD22	21:LM:264:PHE:HZ	1.80	0.47
21:LM:262:VAL:HG13	21:LM:301:LYS:HG2	1.96	0.47
21:LM:363:LEU:HD13	21:LM:366:ILE:HD12	1.96	0.47
23:LO:62:ASP:OD1	23:LO:63:LEU:N	2.47	0.47
26:LR:333:ILE:HG23	26:LR:379:LEU:HB3	1.97	0.47
32:LY:494:VAL:HG22	32:LY:539:ALA:HB2	1.96	0.47
32:LY:859:ILE:HD11	32:LY:885:LEU:HD12	1.97	0.47
56:SK:90:ASP:OD1	56:SK:91:ILE:N	2.48	0.47
60:SP:323:PHE:HB2	60:SP:364:LEU:HD13	1.95	0.47
5:L4:72:VAL:HG11	5:L4:82:TYR:CE2	2.50	0.47
16:LH:438:THR:HG22	16:LH:764:SER:OG	2.15	0.47
16:LH:555:VAL:HG13	16:LH:555:VAL:O	2.14	0.47
18:LJ:432:TYR:O	18:LJ:470:TYR:OH	2.32	0.47
22:LN:345:ASP:OD2	22:LN:360:SER:OG	2.25	0.47
23:LO:73:ILE:HG21	23:LO:99:CYS:HB2	1.97	0.47
23:LO:419:TYR:OH	34:NA:477:GLU:OE2	2.27	0.47
23:LO:649:GLU:N	23:LO:649:GLU:OE1	2.48	0.47
26:LR:362:LEU:CD1	26:LR:405:THR:HG21	2.44	0.47
28:LT:626:ASP:OD1	28:LT:627:ASN:N	2.46	0.47
32:LY:516:PHE:HD2	32:LY:568:LEU:HD12	1.79	0.47
36:NC:100:ILE:CG2	45:NN:336:LEU:HD13	2.44	0.47
39:NF:16:ILE:H	39:NF:16:ILE:HD12	1.80	0.47
49:SA:174:ILE:HD12	49:SA:296:MET:SD	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SP:1549:VAL:HG13	60:SP:1614:GLU:OE1	2.14	0.47
60:SP:1680:THR:HG23	60:SP:1681:LEU:HG	1.97	0.47
61:SQ:155:ASP:OD1	61:SQ:156:LYS:N	2.48	0.47
65:SU:381:LYS:HB2	65:SU:415:MET:HE1	1.97	0.47
8:L7:48:GLU:OE2	8:L7:88:ARG:NE	2.47	0.47
8:L7:163:ASP:OD1	63:SS:277:ARG:NH1	2.46	0.47
18:LJ:42:VAL:HG23	18:LJ:42:VAL:O	2.15	0.47
20:LL:25:ASP:OD2	20:LL:25:ASP:N	2.48	0.47
28:LT:369:ALA:HB1	28:LT:414:ILE:HD13	1.97	0.47
51:SD:175:ALA:HB1	51:SD:181:VAL:HG21	1.97	0.47
53:SG:278:ASP:OD1	53:SG:279:ARG:N	2.47	0.47
56:SJ:99:LEU:HD21	56:SJ:238:CYS:HB3	1.97	0.47
60:SP:587:ASP:OD1	60:SP:664:LYS:NZ	2.33	0.47
60:SP:1220:LEU:O	60:SP:1223:SER:OG	2.24	0.47
60:SP:1436:ASP:OD1	60:SP:1437:MET:N	2.47	0.47
60:SP:2065:VAL:HG21	63:SS:262:LEU:CD1	2.32	0.47
64:ST:659:GLU:OE1	64:ST:659:GLU:N	2.47	0.47
8:L7:173:TYR:CE1	8:L7:177:THR:HG21	2.50	0.47
23:LO:192:ASP:OD1	23:LO:193:TYR:N	2.42	0.47
24:LP:182:TRP:CG	24:LP:277:CYS:HG	2.32	0.47
28:LT:621:ASP:OD1	28:LT:622:GLY:N	2.47	0.47
33:LZ:156:ASP:OD1	58:SM:7:ARG:NH1	2.47	0.47
50:SB:115:ASP:OD1	51:SD:322:ARG:NH2	2.48	0.47
53:SG:168:ASN:O	53:SG:172:PHE:N	2.43	0.47
60:SP:233:LEU:O	60:SP:237:THR:HG22	2.15	0.47
60:SP:1887:LEU:HD12	60:SP:1924:LEU:HD22	1.97	0.47
2:L1:878:G:O2'	39:NF:108:ASP:OD1	2.27	0.47
27:LS:16:ASP:OD1	27:LS:17:GLU:N	2.44	0.47
28:LT:933:ALA:O	28:LT:937:THR:HG22	2.15	0.47
32:LX:428:GLN:NE2	32:LX:643:GLU:OE2	2.48	0.47
60:SP:70:ILE:O	60:SP:70:ILE:HG22	2.15	0.47
64:ST:453:ASN:OD1	64:ST:454:ALA:N	2.48	0.47
22:LN:61:THR:HG21	22:LN:681:ILE:HD13	1.97	0.46
24:LP:192:PHE:HZ	63:SS:351:LEU:HD21	1.80	0.46
26:LR:295:PRO:O	26:LR:296:ILE:HD13	2.15	0.46
29:LU:305:VAL:HG21	29:LU:426:ALA:CB	2.45	0.46
46:NQ:40:CYS:SG	46:NQ:42:ASN:ND2	2.85	0.46
54:SH:130:ILE:HD12	54:SH:166:VAL:HG11	1.96	0.46
60:SP:1394:LEU:HD12	60:SP:1398:LEU:HG	1.98	0.46
60:SP:1453:ASN:HB2	60:SP:1465:ALA:HB2	1.96	0.46
60:SP:1967:ILE:HD13	60:SP:2006:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:298:C:O3'	5:L4:30:ARG:NH2	2.49	0.46
2:L1:1681:A:H2'	2:L1:1682:U:O4'	2.16	0.46
8:L7:126:LEU:HD21	8:L7:152:VAL:HG21	1.96	0.46
10:L9:56:ALA:O	10:L9:60:LEU:HD23	2.15	0.46
16:LH:437:THR:HG22	16:LH:710:LEU:HD21	1.97	0.46
16:LH:822:PHE:CD2	20:LL:91:LEU:HD21	2.51	0.46
24:LP:350:SER:N	24:LP:354:ASP:OD2	2.48	0.46
25:LQ:177:LEU:HB3	25:LQ:191:LEU:HD21	1.96	0.46
26:LR:386:GLY:HA3	26:LR:426:ILE:HD11	1.97	0.46
29:LU:263:ARG:NH1	29:LU:265:ASN:OD1	2.48	0.46
32:LY:888:ILE:HG23	32:LY:898:ILE:CD1	2.46	0.46
41:NH:313:ASN:ND2	41:NH:327:PRO:O	2.47	0.46
41:NH:693:LYS:O	41:NH:695:GLN:NE2	2.48	0.46
55:SI:631:ILE:O	55:SI:631:ILE:HG22	2.15	0.46
56:SK:31:LEU:HD23	56:SK:40:ARG:CG	2.46	0.46
57:SL:156:ASN:HD22	57:SL:156:ASN:C	2.17	0.46
2:L1:-5:G:OP2	31:LW:41:LYS:NZ	2.34	0.46
7:L6:105:ASP:OD1	7:L6:105:ASP:O	2.34	0.46
26:LR:62:GLN:OE1	26:LR:82:ALA:HB2	2.15	0.46
32:LX:896:ASP:OD1	32:LX:896:ASP:N	2.47	0.46
38:NE:107:VAL:HG23	38:NE:107:VAL:O	2.15	0.46
60:SP:1158:ILE:O	60:SP:1208:MET:HE3	2.15	0.46
69:SZ:415:VAL:O	69:SZ:418:HIS:N	2.49	0.46
3:L2:62:C:O2'	28:LT:447:ASN:O	2.32	0.46
16:LH:16:SER:HG	16:LH:465:ASN:CG	2.22	0.46
16:LH:289:GLN:OE1	22:LN:310:ASN:ND2	2.48	0.46
17:LI:571:PHE:O	17:LI:574:ARG:NH2	2.48	0.46
18:LJ:504:ILE:HA	18:LJ:507:MET:HE3	1.97	0.46
29:LU:242:ASN:OD1	29:LU:263:ARG:N	2.48	0.46
51:SC:220:ILE:HD12	51:SC:233:LEU:HD22	1.98	0.46
65:SU:531:ASP:OD1	65:SU:532:ASN:N	2.49	0.46
22:LN:80:ASN:ND2	22:LN:88:GLU:OE2	2.47	0.46
25:LQ:185:MET:HE1	26:LR:663:VAL:HG21	1.98	0.46
27:LS:417:GLY:HA2	27:LS:473:ILE:HG21	1.98	0.46
32:LY:597:GLU:OE1	32:LY:597:GLU:N	2.49	0.46
60:SP:1001:VAL:HG12	60:SP:1005:ASN:OD1	2.16	0.46
1:L0:394:U:OP1	33:LZ:108:ARG:NH2	2.48	0.46
2:L1:1681:A:N6	2:L1:1720:G:N1	2.64	0.46
16:LH:366:ASN:OD1	16:LH:367:SER:N	2.49	0.46
21:LM:359:ASP:OD2	21:LM:362:LYS:N	2.46	0.46
28:LT:724:SER:HB3	28:LT:880:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LV:189:ASN:O	30:LV:193:GLY:N	2.49	0.46
41:NH:188:SER:N	71:NH:1300:ATP:O2B	2.41	0.46
41:NH:217:LYS:HD3	41:NH:220:LEU:HD23	1.97	0.46
53:SG:331:LEU:HD12	53:SG:407:MET:HE3	1.98	0.46
56:SK:146:HIS:O	64:ST:67:ARG:NH2	2.49	0.46
56:SK:189:VAL:HG13	56:SK:244:GLY:HA3	1.96	0.46
59:SN:96:LEU:HD21	59:SN:180:LEU:CD1	2.44	0.46
64:ST:391:VAL:O	64:ST:391:VAL:HG12	2.16	0.46
2:L1:959:U:OP2	46:NQ:20:LYS:NZ	2.48	0.46
3:L2:23:U:O4	3:L2:28:A:N6	2.49	0.46
3:L2:31:G:N7	29:LU:345:THR:HG21	2.30	0.46
13:LE:130:TYR:CZ	38:NE:308:ILE:HG21	2.51	0.46
16:LH:89:VAL:HG22	16:LH:110:PHE:O	2.16	0.46
17:LI:632:THR:HB	19:LK:492:ILE:HD12	1.98	0.46
25:LQ:884:LYS:HD2	26:LR:807:ASP:OD2	2.16	0.46
56:SJ:53:HIS:CB	56:SJ:68:LEU:HD21	2.45	0.46
2:L1:936:G:OP1	2:L1:1074:G:N2	2.39	0.46
25:LQ:21:ALA:HB3	25:LQ:44:SER:OG	2.16	0.46
27:LS:43:ASP:OD1	27:LS:43:ASP:N	2.48	0.46
28:LT:613:ASP:O	28:LT:617:GLY:N	2.48	0.46
49:SA:159:SER:OG	51:SC:219:PRO:O	2.31	0.46
53:SG:61:ASP:OD1	53:SG:64:ARG:NH2	2.48	0.46
56:SJ:179:THR:HG22	56:SJ:205:PHE:HB2	1.98	0.46
60:SP:1981:TYR:CD2	63:SS:455:ILE:HB	2.51	0.46
16:LH:244:ILE:CD1	16:LH:283:VAL:HG21	2.45	0.46
23:LO:351:LEU:HD23	23:LO:696:ALA:HB2	1.97	0.46
23:LO:678:GLU:O	23:LO:698:THR:HG21	2.16	0.46
29:LU:227:PHE:CE1	29:LU:249:LEU:HD11	2.51	0.46
41:NH:585:MET:HE2	41:NH:613:VAL:HG23	1.97	0.46
41:NH:1233:ASN:OD1	41:NH:1234:PHE:N	2.49	0.46
50:SB:45:ALA:CB	50:SB:79:ILE:HD11	2.45	0.46
53:SG:209:LYS:O	53:SG:211:LEU:HD12	2.15	0.46
64:ST:488:ASN:HB2	64:ST:492:ALA:HB2	1.98	0.46
65:SU:98:PHE:CE1	65:SU:126:LEU:HD11	2.51	0.46
16:LH:717:THR:HG23	16:LH:718:GLY:N	2.31	0.46
25:LQ:360:ASN:O	25:LQ:391:ARG:NH2	2.49	0.46
25:LQ:836:ILE:HD12	25:LQ:853:ILE:HG23	1.97	0.46
26:LR:519:ASN:O	26:LR:523:GLY:N	2.46	0.46
42:NI:64:ILE:HD12	42:NI:86:GLU:HA	1.98	0.46
60:SP:84:ASP:OD1	60:SP:85:LYS:N	2.49	0.46
9:L8:32:GLN:OE1	9:L8:32:GLN:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LE:105:THR:HG23	13:LE:105:THR:O	2.16	0.45
25:LQ:200:HIS:CD2	25:LQ:242:LEU:HD23	2.51	0.45
28:LT:716:ILE:H	28:LT:716:ILE:HD12	1.81	0.45
34:NA:311:ILE:HD11	55:SI:1032:LEU:HA	1.98	0.45
54:SH:23:LEU:CD1	54:SH:329:ILE:HD13	2.46	0.45
54:SH:136:GLY:O	54:SH:293:GLN:NE2	2.37	0.45
60:SP:625:ILE:HD13	60:SP:642:ILE:HD13	1.98	0.45
8:L7:73:VAL:HG22	8:L7:73:VAL:O	2.16	0.45
11:LC:97:VAL:HG12	11:LC:98:ASP:N	2.31	0.45
16:LH:321:MET:HE2	16:LH:334:LEU:HB3	1.98	0.45
31:LW:489:ASP:OD1	31:LW:489:ASP:N	2.48	0.45
41:NH:203:ILE:HD11	41:NH:290:PHE:CD2	2.51	0.45
42:NI:67:MET:HE2	42:NI:126:LEU:HD22	1.98	0.45
60:SP:517:ASP:OD1	60:SP:765:ARG:NH1	2.48	0.45
60:SP:841:ILE:O	60:SP:844:VAL:HG22	2.16	0.45
7:L6:27:PHE:CE1	7:L6:36:VAL:HG21	2.51	0.45
17:LI:632:THR:HB	19:LK:492:ILE:CD1	2.47	0.45
17:LI:703:LEU:HD23	17:LI:704:PRO:O	2.17	0.45
20:LL:116:GLN:OE1	20:LL:128:GLN:NE2	2.49	0.45
35:NB:599:LYS:NZ	61:SQ:138:LYS:O	2.48	0.45
41:NH:524:ASP:OD2	41:NH:619:VAL:N	2.50	0.45
65:SU:181:THR:HG23	65:SU:222:LEU:HD12	1.99	0.45
6:L5:23:VAL:O	6:L5:23:VAL:HG23	2.17	0.45
9:L8:6:ASP:OD2	9:L8:6:ASP:N	2.49	0.45
17:LI:497:ILE:HG22	17:LI:497:ILE:O	2.16	0.45
21:LM:91:ILE:CD1	31:LW:97:VAL:HG21	2.46	0.45
23:LO:89:VAL:HG11	23:LO:92:HIS:NE2	2.32	0.45
23:LO:637:GLU:O	57:SL:8:ARG:NH1	2.49	0.45
25:LQ:292:ILE:HG23	25:LQ:324:PHE:HB3	1.98	0.45
28:LT:177:LEU:HD23	50:SB:432:ASP:O	2.16	0.45
32:LY:686:GLU:O	32:LY:690:THR:HG23	2.16	0.45
41:NH:1202:CYS:SG	41:NH:1203:ASN:N	2.89	0.45
42:NI:135:ASN:OD1	42:NI:136:ASN:N	2.49	0.45
52:SF:19:GLN:HG2	52:SF:117:VAL:HG22	1.98	0.45
60:SP:2143:LYS:HB3	63:SS:251:ILE:HD11	1.98	0.45
2:L1:58:U:O2'	2:L1:451:A:N3	2.45	0.45
24:LP:324:ASP:OD2	24:LP:372:ARG:NH2	2.49	0.45
25:LQ:536:CYS:N	25:LQ:549:SER:OG	2.49	0.45
25:LQ:619:MET:HE3	25:LQ:635:LYS:CG	2.46	0.45
28:LT:231:ILE:HG23	28:LT:240:ARG:HG3	1.99	0.45
29:LU:258:ILE:HG22	29:LU:464:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SF:61:ILE:H	52:SF:61:ILE:HD12	1.82	0.45
60:SP:456:GLU:OE2	60:SP:456:GLU:N	2.45	0.45
60:SP:1929:GLU:OE1	60:SP:1929:GLU:N	2.46	0.45
1:L0:471:C:O3'	31:LW:143:GLN:NE2	2.43	0.45
2:L1:1682:U:O2	2:L1:1720:G:N2	2.49	0.45
11:LC:101:SER:O	11:LC:105:LEU:HD13	2.17	0.45
12:LD:55:ASP:OD1	12:LD:82:ARG:NH1	2.50	0.45
18:LJ:460:ALA:HA	20:LL:543:LEU:HD12	1.97	0.45
32:LX:275:LEU:O	32:LX:404:TYR:N	2.50	0.45
32:LX:517:VAL:HG22	32:LX:565:PHE:CE1	2.52	0.45
35:NB:395:ASP:OD1	35:NB:395:ASP:N	2.49	0.45
45:NN:197:GLN:NE2	45:NN:411:GLU:OE2	2.49	0.45
51:SD:103:GLU:HB2	51:SD:105:LEU:HD11	1.98	0.45
55:SI:54:LEU:HB3	62:SR:77:ILE:HG21	1.99	0.45
60:SP:1261:ILE:HD12	60:SP:1291:LEU:CD2	2.46	0.45
61:SQ:59:LEU:HD11	63:SS:382:LEU:HD11	1.99	0.45
63:SS:248:MET:O	63:SS:251:ILE:HG22	2.17	0.45
5:L4:72:VAL:HG11	5:L4:82:TYR:HE2	1.82	0.45
18:LJ:109:ASP:OD1	18:LJ:117:LEU:HD11	2.17	0.45
21:LM:134:MET:HE2	21:LM:134:MET:HA	1.98	0.45
21:LM:362:LYS:O	21:LM:365:ILE:N	2.50	0.45
24:LP:278:MET:HE3	24:LP:312:LEU:HD22	1.99	0.45
32:LX:426:LEU:O	32:LX:430:LEU:HD23	2.16	0.45
32:LY:378:LEU:HD22	32:LY:384:VAL:CG2	2.47	0.45
42:NI:13:PHE:CE1	42:NI:40:LYS:HE3	2.51	0.45
60:SP:1778:MET:HA	60:SP:1778:MET:HE3	1.99	0.45
2:L1:67:A:HO2'	2:L1:69:G:P	2.39	0.45
25:LQ:632:SER:OG	25:LQ:642:TRP:NE1	2.47	0.45
28:LT:819:LYS:NZ	28:LT:823:GLU:OE2	2.50	0.45
32:LY:775:VAL:HG21	32:LY:815:SER:HB2	1.98	0.45
41:NH:270:ILE:CD1	41:NH:294:LEU:HD23	2.47	0.45
49:SA:257:ILE:HD12	50:SB:138:LYS:HD2	1.97	0.45
58:SM:123:VAL:HG12	58:SM:125:PRO:HD2	1.98	0.45
2:L1:334:G:O6	9:L8:5:ARG:NH2	2.50	0.45
29:LU:6:ILE:HD12	31:LW:409:ALA:HA	1.99	0.45
30:LV:416:LEU:HD23	30:LV:416:LEU:O	2.17	0.45
41:NH:158:VAL:HG11	41:NH:237:HIS:HB2	1.98	0.45
41:NH:189:PHE:CG	41:NH:203:ILE:HD12	2.52	0.45
52:SF:51:PHE:CE1	52:SF:53:ILE:HD11	2.51	0.45
67:SW:269:ARG:NH2	67:SW:272:GLU:OE1	2.46	0.45
2:L1:748:U:O2'	13:LE:122:SER:OG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:1767:G:OP2	67:SW:211:LYS:NZ	2.45	0.45
16:LH:612:SER:C	16:LH:613:LEU:HD22	2.42	0.45
26:LR:575:THR:OG1	26:LR:596:ASP:OD2	2.34	0.45
27:LS:264:LEU:HD11	27:LS:272:LEU:HD22	1.99	0.45
27:LS:325:ASP:OD1	27:LS:326:LEU:N	2.50	0.45
41:NH:427:LYS:O	41:NH:431:THR:HG22	2.17	0.45
64:ST:506:ILE:HD11	65:SU:529:VAL:HG23	1.98	0.45
65:SU:118:ASP:O	65:SU:122:VAL:HG22	2.17	0.45
3:L2:39:C:OP2	31:LW:424:GLN:NE2	2.50	0.44
16:LH:144:VAL:HG12	16:LH:153:ILE:HG22	1.99	0.44
22:LN:681:ILE:HG22	22:LN:683:ASP:N	2.30	0.44
23:LO:379:CYS:O	34:NA:480:GLN:NE2	2.50	0.44
23:LO:491:ALA:HB1	23:LO:518:VAL:HG11	2.00	0.44
23:LO:564:PHE:N	23:LO:567:ASP:OD2	2.45	0.44
25:LQ:479:LEU:HD21	25:LQ:488:LEU:HD11	1.99	0.44
32:LX:4:LYS:N	55:SI:373:ILE:O	2.47	0.44
32:LX:412:ILE:HG23	32:LX:420:ARG:HG3	1.99	0.44
39:NF:45:LEU:O	42:NI:258:TYR:OH	2.35	0.44
41:NH:655:LEU:HD13	41:NH:665:HIS:CD2	2.52	0.44
50:SB:116:ILE:HG22	50:SB:120:ILE:HD12	1.99	0.44
1:L0:395:C:O4'	33:LZ:108:ARG:NH1	2.50	0.44
7:L6:161:GLU:OE2	7:L6:169:TYR:N	2.51	0.44
17:LI:592:ARG:HD2	17:LI:592:ARG:N	2.32	0.44
24:LP:183:TYR:CZ	24:LP:322:LEU:HD12	2.52	0.44
24:LP:320:ILE:HD11	24:LP:338:VAL:HG11	1.99	0.44
25:LQ:212:VAL:HG22	25:LQ:217:LEU:HD12	1.98	0.44
50:SB:225:GLU:OE1	50:SB:225:GLU:N	2.43	0.44
51:SD:117:VAL:HG23	51:SD:118:TYR:HD2	1.82	0.44
55:SI:127:ALA:O	55:SI:131:ILE:HD12	2.17	0.44
3:L2:115:G:O2'	3:L2:257:A:N3	2.39	0.44
4:L3:45:LEU:HD13	4:L3:85:PHE:CE2	2.52	0.44
7:L6:142:ARG:O	7:L6:146:GLY:N	2.50	0.44
12:LD:22:ASN:ND2	12:LD:25:VAL:HG23	2.33	0.44
20:LL:62:CYS:SG	20:LL:110:ILE:HG22	2.57	0.44
22:LN:401:ILE:O	22:LN:416:LEU:HD12	2.18	0.44
28:LT:608:THR:OG1	28:LT:610:ARG:NH1	2.50	0.44
29:LU:298:LEU:O	29:LU:457:ARG:NH2	2.50	0.44
30:LV:218:LEU:HD21	30:LV:255:TYR:CD2	2.52	0.44
30:LV:221:GLU:N	30:LV:221:GLU:OE2	2.50	0.44
31:LW:185:HIS:ND1	33:LZ:24:ASP:OD2	2.48	0.44
32:LX:571:ILE:H	32:LX:571:ILE:HD12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:NH:1149:LEU:HD22	41:NH:1226:PHE:CE2	2.53	0.44
51:SC:282:ALA:HB2	51:SC:312:ASP:OD1	2.17	0.44
51:SD:171:LEU:N	51:SD:237:VAL:HG21	2.32	0.44
60:SP:2107:VAL:O	60:SP:2111:PHE:N	2.42	0.44
1:L0:309:A:H61	50:SB:431:ALA:HB3	1.81	0.44
8:L7:133:THR:HG21	8:L7:162:ILE:HG21	1.99	0.44
20:LL:364:THR:HG22	20:LL:365:SER:N	2.33	0.44
20:LL:441:LEU:HD13	20:LL:456:VAL:HG11	1.99	0.44
22:LN:186:GLN:OE1	22:LN:188:ALA:N	2.41	0.44
22:LN:466:ASP:O	22:LN:466:ASP:OD2	2.36	0.44
24:LP:167:ILE:HD11	63:SS:327:PHE:CD1	2.53	0.44
26:LR:8:LYS:HZ2	26:LR:10:ILE:HD11	1.81	0.44
26:LR:626:MET:HE3	26:LR:627:ASN:OD1	2.17	0.44
32:LY:306:SER:N	32:LY:382:GLU:OE1	2.48	0.44
60:SP:334:ASN:C	60:SP:334:ASN:HD22	2.25	0.44
64:ST:542:PHE:CE1	64:ST:546:LEU:HD11	2.52	0.44
21:LM:469:LEU:O	21:LM:473:SER:N	2.51	0.44
21:LM:786:TYR:O	50:SB:84:LYS:NZ	2.50	0.44
22:LN:595:ASN:ND2	22:LN:612:THR:HG22	2.33	0.44
25:LQ:201:ILE:HD12	26:LR:660:LYS:HA	1.99	0.44
26:LR:36:VAL:O	26:LR:36:VAL:HG13	2.17	0.44
27:LS:122:GLU:OE1	27:LS:122:GLU:N	2.50	0.44
27:LS:554:ASN:OD1	27:LS:555:TRP:N	2.51	0.44
32:LX:527:HIS:CB	55:SI:416:LEU:HD11	2.41	0.44
32:LY:238:LYS:NZ	32:LY:252:SER:O	2.40	0.44
43:NK:186:VAL:HG22	43:NK:199:HIS:HB3	2.00	0.44
53:SG:569:ASP:OD1	53:SG:570:GLN:N	2.51	0.44
54:SH:57:GLU:O	64:ST:108:LYS:NZ	2.41	0.44
55:SI:153:MET:HA	55:SI:153:MET:HE3	1.98	0.44
56:SK:159:LEU:HD12	56:SK:159:LEU:N	2.32	0.44
60:SP:1320:ASP:O	60:SP:1324:ILE:HG22	2.17	0.44
67:SW:167:ASP:OD1	67:SW:168:LEU:N	2.51	0.44
2:L1:1194:A:N6	56:SJ:129:ARG:O	2.49	0.44
16:LH:292:LEU:C	16:LH:293:LEU:HD12	2.42	0.44
18:LJ:108:TYR:HE1	18:LJ:116:ILE:HG23	1.81	0.44
18:LJ:266:SER:OG	18:LJ:267:PRO:HD2	2.17	0.44
21:LM:153:SER:O	21:LM:169:ARG:NH2	2.51	0.44
25:LQ:92:ASP:CB	25:LQ:109:MET:HE1	2.47	0.44
49:SA:129:ARG:NH1	51:SC:261:LEU:O	2.46	0.44
2:L1:486:G:HO2'	61:SQ:135:HIS:CE1	2.36	0.44
9:L8:152:ILE:HG22	9:L8:153:GLU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LE:79:PHE:CE1	13:LE:125:ILE:HG21	2.53	0.44
20:LL:277:LYS:NZ	20:LL:319:TRP:O	2.39	0.44
23:LO:154:TRP:CH2	23:LO:161:ILE:HD11	2.53	0.44
37:ND:173:ARG:NH2	68:SY:144:ASN:O	2.50	0.44
41:NH:901:ASN:O	41:NH:981:LYS:NZ	2.51	0.44
42:NI:108:MET:HE2	42:NI:187:HIS:CD2	2.53	0.44
55:SI:303:LYS:C	55:SI:304:LEU:HD12	2.42	0.44
60:SP:1428:THR:HG23	60:SP:1428:THR:O	2.18	0.44
64:ST:481:MET:HE1	64:ST:501:PHE:CE2	2.53	0.44
68:SY:185:MET:SD	68:SY:185:MET:N	2.91	0.44
4:L3:29:VAL:HG21	4:L3:54:LEU:HD23	1.99	0.44
23:LO:621:MET:HG2	23:LO:627:LEU:HD11	2.00	0.44
41:NH:623:GLU:OE1	41:NH:623:GLU:N	2.51	0.44
56:SK:49:SER:O	56:SK:50:LEU:HD12	2.18	0.44
61:SQ:180:ASP:OD1	61:SQ:182:ALA:N	2.51	0.44
64:ST:469:GLU:OE1	64:ST:469:GLU:N	2.49	0.44
64:ST:781:MET:N	64:ST:781:MET:HE2	2.33	0.44
1:L0:370:U:O2	1:L0:372:A:N6	2.51	0.44
8:L7:64:VAL:HG12	8:L7:94:ALA:HB1	2.00	0.44
23:LO:434:ASN:CG	23:LO:450:LEU:HD23	2.43	0.44
37:ND:112:LEU:HD21	65:SU:90:TRP:CG	2.53	0.44
41:NH:781:ASP:OD1	41:NH:782:VAL:N	2.51	0.44
42:NI:55:LEU:HB3	42:NI:58:LEU:HD21	2.00	0.44
60:SP:1224:LEU:HD21	60:SP:1247:LEU:HD12	2.00	0.44
63:SS:373:MET:HE3	63:SS:373:MET:HA	1.99	0.44
64:ST:391:VAL:HG11	64:ST:399:HIS:ND1	2.33	0.44
64:ST:434:ILE:O	64:ST:437:SER:OG	2.32	0.44
65:SU:515:LEU:O	65:SU:515:LEU:HD23	2.18	0.44
8:L7:136:VAL:N	8:L7:153:LEU:O	2.51	0.43
12:LD:42:PHE:CE2	12:LD:140:VAL:HG11	2.53	0.43
17:LI:614:ILE:HG13	17:LI:638:LEU:HD12	2.00	0.43
25:LQ:559:PHE:O	25:LQ:563:MET:N	2.48	0.43
30:LV:400:TYR:CZ	30:LV:401:MET:HE1	2.53	0.43
31:LW:196:LEU:CD2	31:LW:207:THR:HG22	2.48	0.43
32:LX:283:ALA:HB3	32:LX:289:LYS:HD3	2.00	0.43
45:NN:190:ILE:HG21	45:NN:421:LEU:HD22	1.99	0.43
56:SJ:93:HIS:O	56:SJ:97:LEU:HD23	2.18	0.43
60:SP:230:GLU:OE1	60:SP:234:ILE:HD11	2.17	0.43
60:SP:314:ILE:HG21	60:SP:343:ILE:HD11	1.99	0.43
60:SP:1643:LEU:HD22	60:SP:1654:VAL:HG11	2.00	0.43
19:LK:459:LEU:CD2	19:LK:467:LEU:HD11	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LL:197:ILE:HD13	20:LL:244:ILE:HD11	2.00	0.43
22:LN:95:LYS:O	22:LN:97:ARG:NH1	2.47	0.43
22:LN:97:ARG:NE	37:ND:191:PRO:O	2.42	0.43
26:LR:115:THR:C	26:LR:116:LEU:HD22	2.43	0.43
32:LY:617:LEU:HD23	32:LY:617:LEU:C	2.43	0.43
35:NB:437:ASP:OD2	56:SJ:91:ILE:HD12	2.18	0.43
40:NG:27:PHE:CD1	40:NG:43:THR:HG22	2.54	0.43
41:NH:756:VAL:O	41:NH:756:VAL:HG12	2.18	0.43
44:NM:191:GLU:OE2	44:NM:194:ASN:ND2	2.51	0.43
51:SC:155:ILE:HD11	51:SC:162:LEU:HD21	2.00	0.43
56:SK:218:ASP:HA	56:SK:221:VAL:HG12	2.00	0.43
4:L3:56:LYS:HD3	18:LJ:39:HIS:CE1	2.54	0.43
5:L4:199:GLU:CD	5:L4:209:HIS:HE2	2.25	0.43
8:L7:75:THR:HG23	8:L7:76:LYS:N	2.33	0.43
18:LJ:125:HIS:NE2	56:SK:19:LEU:O	2.49	0.43
20:LL:68:LEU:CD2	20:LL:74:VAL:HG23	2.48	0.43
23:LO:339:LEU:HD11	23:LO:378:PHE:CE1	2.52	0.43
25:LQ:619:MET:HE3	25:LQ:635:LYS:HG3	1.99	0.43
25:LQ:922:ASP:OD1	25:LQ:922:ASP:N	2.51	0.43
29:LU:305:VAL:O	29:LU:305:VAL:HG22	2.18	0.43
31:LW:152:GLU:OE1	31:LW:170:GLN:NE2	2.46	0.43
31:LW:206:VAL:HG11	31:LW:247:MET:HE2	2.00	0.43
32:LX:425:LYS:NZ	32:LX:544:SER:O	2.46	0.43
32:LY:430:LEU:HD22	32:LY:465:LEU:HD22	2.00	0.43
34:NA:373:ILE:HG21	58:SM:245:VAL:HG21	2.00	0.43
41:NH:976:ILE:HD11	41:NH:1017:TYR:CE1	2.52	0.43
43:NK:300:ALA:O	43:NK:304:ILE:HD12	2.18	0.43
56:SJ:218:ASP:OD1	56:SJ:219:GLU:N	2.51	0.43
58:SM:138:ASP:OD2	58:SM:209:LEU:HD23	2.18	0.43
1:L0:452:A:H1'	55:SI:1083:ILE:HG22	1.99	0.43
5:L4:121:TYR:OH	5:L4:235:TYR:O	2.18	0.43
8:L7:26:GLU:OE1	8:L7:84:LYS:NZ	2.41	0.43
16:LH:612:SER:OG	16:LH:662:VAL:HG23	2.19	0.43
20:LL:222:THR:HG23	20:LL:222:THR:O	2.17	0.43
21:LM:1028:LEU:O	21:LM:1031:THR:N	2.51	0.43
23:LO:760:ILE:HA	23:LO:763:ILE:HD12	2.00	0.43
52:SF:61:ILE:HD12	53:SG:451:ILE:O	2.18	0.43
53:SG:157:LEU:HD11	53:SG:189:THR:HB	2.01	0.43
56:SJ:186:VAL:HG11	56:SK:252:LEU:HD21	1.99	0.43
60:SP:375:THR:HG22	60:SP:411:PHE:HE1	1.83	0.43
2:L1:1572:G:O6	56:SK:151:ARG:NH2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L5:34:GLN:O	6:L5:37:GLN:HB3	2.19	0.43
14:LF:31:ASN:OD1	14:LF:31:ASN:O	2.36	0.43
18:LJ:509:GLN:OE1	19:LK:502:ARG:NH2	2.52	0.43
22:LN:388:GLN:NE2	22:LN:436:ASP:O	2.43	0.43
23:LO:254:HIS:CD2	23:LO:292:PHE:CE2	3.06	0.43
32:LY:896:ASP:OD1	32:LY:897:THR:N	2.51	0.43
38:NE:207:ARG:NH2	58:SM:60:GLN:OE1	2.51	0.43
41:NH:1081:ASN:O	41:NH:1084:THR:OG1	2.27	0.43
42:NI:108:MET:HE2	42:NI:187:HIS:NE2	2.32	0.43
51:SC:269:ILE:CD1	51:SC:293:LEU:HD11	2.47	0.43
52:SE:10:PRO:HB2	52:SE:124:LEU:HD21	2.01	0.43
56:SK:43:VAL:HG11	56:SK:99:LEU:HD11	1.99	0.43
60:SP:1151:ILE:HD13	60:SP:1198:PHE:HE1	1.83	0.43
60:SP:1352:LEU:HD13	60:SP:1355:ILE:HD11	1.99	0.43
60:SP:1655:ARG:O	60:SP:1659:GLY:N	2.50	0.43
2:L1:475:A:OP2	10:L9:126:ARG:NH2	2.52	0.43
5:L4:100:ARG:NH2	5:L4:118:GLU:O	2.51	0.43
8:L7:94:ALA:HB3	8:L7:96:ARG:NH1	2.33	0.43
16:LH:152:ARG:HB3	16:LH:173:LEU:HD11	1.99	0.43
16:LH:736:THR:HG22	16:LH:737:ILE:N	2.33	0.43
23:LO:362:THR:HG22	23:LO:701:LEU:HD21	2.00	0.43
25:LQ:71:ALA:O	25:LQ:74:ALA:HB3	2.18	0.43
29:LU:133:GLN:NE2	29:LU:168:ASN:O	2.51	0.43
35:NB:595:LYS:O	61:SQ:134:ARG:NH2	2.50	0.43
43:NK:226:MET:HE2	43:NK:226:MET:HA	2.00	0.43
61:SQ:120:ASP:CG	61:SQ:173:ILE:HD13	2.43	0.43
66:SV:201:ASP:OD2	66:SV:202:SER:N	2.51	0.43
2:L1:1679:G:N2	2:L1:1723:U:O4	2.52	0.43
3:L2:325:C:N4	50:SB:318:GLN:OE1	2.44	0.43
16:LH:381:SER:HG	20:LL:349:ASP:CG	2.22	0.43
16:LH:414:ILE:H	16:LH:414:ILE:HD12	1.84	0.43
23:LO:852:THR:HG22	23:LO:853:ASP:N	2.34	0.43
25:LQ:179:SER:OG	25:LQ:189:TRP:NE1	2.44	0.43
25:LQ:486:LYS:HD2	25:LQ:486:LYS:N	2.34	0.43
25:LQ:840:MET:HA	25:LQ:840:MET:HE3	2.00	0.43
26:LR:494:ILE:HD11	26:LR:508:THR:HB	2.01	0.43
28:LT:342:TYR:HH	28:LT:345:SER:HG	1.40	0.43
32:LY:859:ILE:HD11	32:LY:885:LEU:CD1	2.49	0.43
32:LY:861:MET:O	32:LY:865:LEU:HD23	2.18	0.43
41:NH:971:LYS:H	48:OA:1414:LEU:HD11	1.83	0.43
50:SB:385:ASP:N	50:SB:385:ASP:OD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SP:1526:LEU:HD11	60:SP:1530:TYR:OH	2.18	0.43
60:SP:1778:MET:SD	60:SP:1864:LEU:HD22	2.59	0.43
66:SV:131:LEU:HD23	66:SV:132:GLU:N	2.34	0.43
20:LL:575:GLU:O	20:LL:578:VAL:HG22	2.19	0.43
22:LN:285:CYS:HB2	22:LN:336:ILE:HG22	2.00	0.43
25:LQ:444:LEU:HD23	25:LQ:458:ASP:HA	2.00	0.43
25:LQ:880:ILE:CG2	26:LR:810:LEU:HD21	2.48	0.43
27:LS:148:THR:O	31:LW:80:LEU:HD11	2.17	0.43
32:LX:861:MET:HE2	32:LX:861:MET:HA	1.99	0.43
44:NM:14:LYS:HE2	44:NM:14:LYS:HA	2.01	0.43
55:SI:198:VAL:HG12	55:SI:199:TYR:CD1	2.54	0.43
65:SU:49:GLU:O	65:SU:53:ARG:N	2.44	0.43
11:LC:103:ASN:ND2	23:LO:554:ASP:OD2	2.44	0.43
13:LE:83:ILE:HG23	13:LE:84:GLY:N	2.34	0.43
16:LH:849:ASP:OD1	16:LH:851:GLU:N	2.52	0.43
18:LJ:208:SER:C	18:LJ:209:LEU:HD12	2.44	0.43
21:LM:258:HIS:CE1	21:LM:282:ILE:HG23	2.54	0.43
21:LM:559:ASN:N	21:LM:597:HIS:O	2.48	0.43
26:LR:25:VAL:HG12	26:LR:294:LEU:HD13	2.00	0.43
27:LS:41:ASN:ND2	27:LS:43:ASP:OD1	2.40	0.43
28:LT:437:GLU:OE2	28:LT:441:ARG:NH2	2.52	0.43
28:LT:850:ARG:HH21	67:SW:266:VAL:HG12	1.84	0.43
55:SI:164:MET:HE2	62:SR:143:PRO:HB3	2.00	0.43
60:SP:1421:LEU:O	60:SP:1425:VAL:HG23	2.19	0.43
63:SS:382:LEU:HG	63:SS:386:LEU:HD23	2.01	0.43
63:SS:435:ARG:NE	63:SS:435:ARG:HA	2.33	0.43
64:ST:573:LEU:HD22	64:ST:591:ILE:HD12	2.01	0.43
2:L1:1059:U:O2'	42:NI:229:LYS:NZ	2.52	0.43
2:L1:1636:C:O2'	25:LQ:814:MET:HE3	2.19	0.43
10:L9:85:VAL:HG23	10:L9:103:ASP:HB3	2.01	0.43
20:LL:516:ILE:HD12	20:LL:517:PRO:HD2	2.01	0.43
25:LQ:453:GLU:HG3	25:LQ:469:GLU:HA	2.01	0.43
25:LQ:502:PHE:CE2	25:LQ:522:LEU:HD21	2.54	0.43
25:LQ:529:GLU:OE2	38:NE:96:VAL:HG12	2.19	0.43
32:LX:775:VAL:HG11	32:LX:820:HIS:CE1	2.54	0.43
34:NA:384:ARG:NH2	58:SM:78:ALA:O	2.49	0.43
41:NH:578:ILE:HG21	41:NH:617:LEU:HD12	2.00	0.43
41:NH:1185:LEU:HD11	48:OA:1407:PHE:CE2	2.54	0.43
42:NI:9:MET:O	42:NI:12:GLY:N	2.45	0.43
56:SJ:227:LEU:HD11	56:SJ:240:LYS:HB3	2.00	0.43
60:SP:642:ILE:HD12	60:SP:669:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SP:1463:GLN:HB2	60:SP:1503:ILE:HD13	2.00	0.43
67:SW:205:ILE:HD11	67:SW:251:ILE:CG1	2.49	0.43
16:LH:431:SER:O	16:LH:434:GLN:NE2	2.50	0.42
41:NH:814:LEU:HD21	41:NH:821:TYR:HB2	2.01	0.42
54:SH:183:ILE:HG21	54:SH:310:ARG:HE	1.83	0.42
2:L1:1595:U:P	55:SI:945:THR:HG1	2.40	0.42
16:LH:77:ILE:HD13	16:LH:117:ILE:HD11	2.00	0.42
21:LM:132:THR:OG1	21:LM:155:ILE:HD11	2.19	0.42
21:LM:157:LEU:HD11	21:LM:168:VAL:CG2	2.48	0.42
25:LQ:126:LEU:HD23	25:LQ:169:PHE:CD2	2.54	0.42
27:LS:414:ILE:HD11	27:LS:420:ARG:HE	1.84	0.42
28:LT:217:VAL:HG23	28:LT:220:ILE:HB	1.99	0.42
29:LU:248:ASP:O	29:LU:252:ASN:N	2.52	0.42
30:LV:195:LEU:HD23	30:LV:195:LEU:O	2.19	0.42
32:LX:384:VAL:HG22	32:LX:404:TYR:HE2	1.84	0.42
38:NE:200:ASP:OD1	38:NE:201:GLN:N	2.51	0.42
41:NH:591:ASP:OD1	41:NH:591:ASP:N	2.52	0.42
41:NH:1169:ILE:HD12	41:NH:1180:ASN:ND2	2.34	0.42
50:SB:2:ALA:HB3	50:SB:17:ALA:HB3	2.01	0.42
51:SC:253:ILE:HD13	51:SC:269:ILE:HG21	2.00	0.42
51:SD:182:SER:HB3	51:SD:210:MET:HE2	1.99	0.42
52:SE:13:ASP:O	52:SE:17:THR:HG23	2.19	0.42
60:SP:1555:LEU:HD21	60:SP:1586:ILE:HD11	2.01	0.42
60:SP:1919:ILE:O	60:SP:1922:ILE:HG22	2.19	0.42
6:L5:90:ILE:O	6:L5:94:THR:HG23	2.18	0.42
10:L9:57:ARG:HG3	57:SL:87:MET:HE3	2.01	0.42
16:LH:357:ILE:C	16:LH:358:LEU:HD12	2.44	0.42
30:LV:253:TYR:HE1	30:LV:265:ILE:HG23	1.84	0.42
30:LV:267:ASP:OD1	30:LV:269:GLY:N	2.52	0.42
30:LV:360:THR:HA	30:LV:363:LEU:HD23	2.00	0.42
41:NH:796:ILE:HG23	41:NH:797:THR:N	2.34	0.42
49:SA:74:VAL:HG11	49:SA:112:GLU:OE2	2.19	0.42
55:SI:366:MET:SD	55:SI:366:MET:N	2.92	0.42
60:SP:10:SER:O	60:SP:15:ARG:NH2	2.50	0.42
60:SP:264:THR:HG22	60:SP:266:SER:H	1.83	0.42
60:SP:1864:LEU:HD11	60:SP:1868:LEU:HD11	2.00	0.42
67:SW:25:ILE:HG22	67:SW:182:ILE:HD13	1.99	0.42
1:L0:236:C:N4	68:SY:230:LYS:O	2.53	0.42
16:LH:265:ASP:OD1	16:LH:266:ASN:N	2.51	0.42
16:LH:664:LEU:HD12	16:LH:664:LEU:O	2.19	0.42
17:LI:457:CYS:SG	17:LI:458:ASN:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:422:LEU:HD13	22:LN:444:ARG:HH21	1.83	0.42
22:LN:575:ILE:HD12	22:LN:582:VAL:HG22	2.00	0.42
25:LQ:464:LEU:HD21	25:LQ:467:THR:OG1	2.19	0.42
29:LU:263:ARG:NH1	29:LU:282:GLU:OE1	2.53	0.42
50:SB:39:LEU:HD23	50:SB:127:LEU:HD12	2.01	0.42
52:SF:10:PRO:HB2	52:SF:124:LEU:HD21	2.00	0.42
53:SG:443:LEU:HD23	53:SG:473:PHE:CZ	2.54	0.42
54:SH:180:MET:HE1	54:SH:254:TRP:CH2	2.54	0.42
59:SN:36:ILE:HD11	59:SN:204:ILE:HG13	2.01	0.42
8:L7:81:LEU:HD12	8:L7:90:VAL:HG21	2.02	0.42
16:LH:497:ASP:OD2	16:LH:498:LEU:N	2.52	0.42
29:LU:292:ARG:O	63:SS:288:TYR:OH	2.27	0.42
30:LV:162:LEU:O	30:LV:162:LEU:HD23	2.19	0.42
41:NH:715:SER:O	41:NH:719:THR:HG23	2.19	0.42
42:NI:67:MET:CE	42:NI:126:LEU:HD22	2.50	0.42
51:SC:269:ILE:HD11	51:SC:293:LEU:HD11	2.01	0.42
51:SD:93:HIS:NE2	51:SD:162:LEU:HD13	2.34	0.42
53:SG:241:THR:HG21	53:SG:285:SER:HA	2.00	0.42
60:SP:2110:SER:OG	60:SP:2122:ALA:HB3	2.20	0.42
2:L1:249:U:H3	12:LD:63:LEU:HD21	1.84	0.42
2:L1:563:U:H4'	58:SM:278:ARG:HG3	2.02	0.42
2:L1:1176:G:OP1	55:SI:978:ARG:NH2	2.51	0.42
7:L6:18:ILE:HD12	7:L6:23:ARG:HD2	2.01	0.42
16:LH:341:ILE:HG21	16:LH:344:CYS:SG	2.60	0.42
21:LM:57:GLU:O	21:LM:60:SER:OG	2.27	0.42
24:LP:332:ASP:N	24:LP:332:ASP:OD1	2.52	0.42
25:LQ:351:LEU:O	25:LQ:367:ILE:N	2.42	0.42
42:NI:13:PHE:HE1	42:NI:40:LYS:HE3	1.84	0.42
60:SP:590:MET:HE2	60:SP:770:TYR:OH	2.20	0.42
64:ST:648:SER:O	64:ST:652:LYS:NZ	2.41	0.42
65:SU:347:PRO:O	65:SU:351:HIS:ND1	2.49	0.42
1:L0:483:U:O2'	49:SA:46:LYS:NZ	2.35	0.42
2:L1:249:U:C2	12:LD:63:LEU:HD21	2.55	0.42
5:L4:112:HIS:NE2	5:L4:238:LEU:O	2.52	0.42
16:LH:457:VAL:HG12	16:LH:473:LEU:HD13	2.01	0.42
16:LH:604:PHE:CE2	16:LH:626:PHE:CE2	3.07	0.42
16:LH:821:ILE:HD12	16:LH:821:ILE:H	1.84	0.42
26:LR:563:ASP:OD2	26:LR:564:THR:HG23	2.20	0.42
29:LU:26:ARG:NH1	31:LW:412:ASP:OD2	2.52	0.42
32:LY:262:ALA:HB2	32:LY:470:LEU:HD21	2.02	0.42
34:NA:359:SER:O	34:NA:362:THR:OG1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SN:250:THR:HG22	59:SN:251:SER:N	2.35	0.42
60:SP:608:MET:O	60:SP:612:GLY:N	2.50	0.42
60:SP:1277:GLU:OE1	60:SP:1280:LEU:HD13	2.19	0.42
60:SP:1662:SER:CB	60:SP:1701:MET:HE2	2.49	0.42
64:ST:388:LEU:O	64:ST:392:LYS:N	2.52	0.42
1:L0:153:U:O4	1:L0:154:A:N6	2.53	0.42
9:L8:113:PHE:CE2	9:L8:152:ILE:HD11	2.54	0.42
11:LC:118:ILE:HD11	23:LO:515:TYR:CE1	2.54	0.42
13:LE:86:ILE:HD12	13:LE:104:LEU:HD11	2.00	0.42
16:LH:148:GLU:HG2	16:LH:148:GLU:O	2.20	0.42
22:LN:541:ALA:HB3	22:LN:553:LEU:HB2	2.01	0.42
23:LO:661:LEU:HD22	33:LZ:50:ILE:HD11	2.02	0.42
25:LQ:846:LEU:HD21	25:LQ:890:ALA:HB2	2.00	0.42
25:LQ:854:CYS:HB3	26:LR:799:LEU:HD12	2.01	0.42
27:LS:242:ASN:OD1	27:LS:586:VAL:HG23	2.20	0.42
29:LU:227:PHE:HE1	29:LU:249:LEU:HD11	1.84	0.42
32:LX:253:LEU:O	32:LX:255:LYS:NZ	2.49	0.42
41:NH:376:SER:OG	41:NH:377:SER:N	2.53	0.42
55:SI:56:VAL:HG23	62:SR:101:GLU:CG	2.50	0.42
57:SL:67:ILE:HD11	57:SL:86:MET:HE1	2.01	0.42
60:SP:219:LEU:HD21	60:SP:270:ARG:HB3	2.01	0.42
2:L1:79:C:OP1	7:L6:159:ARG:NH2	2.47	0.42
2:L1:448:C:OP1	5:L4:49:ARG:NH2	2.50	0.42
2:L1:1132:A:H4'	54:SH:231:ARG:HH21	1.85	0.42
7:L6:31:ARG:N	7:L6:34:GLN:OE1	2.53	0.42
10:L9:29:LYS:NZ	10:L9:33:GLU:OE2	2.45	0.42
16:LH:443:ASN:O	16:LH:447:LYS:N	2.49	0.42
17:LI:510:ILE:HD11	17:LI:522:THR:OG1	2.19	0.42
21:LM:1008:PHE:O	21:LM:1012:SER:N	2.47	0.42
23:LO:689:THR:HG23	23:LO:823:SER:HA	2.01	0.42
28:LT:601:VAL:HG22	28:LT:611:THR:HG22	2.02	0.42
40:NG:82:LYS:NZ	44:NM:67:GLU:OE1	2.53	0.42
49:SA:129:ARG:NH2	51:SC:261:LEU:O	2.52	0.42
51:SD:249:GLN:HA	51:SD:252:ILE:HD12	2.01	0.42
55:SI:952:PHE:HD2	55:SI:958:VAL:HG22	1.79	0.42
60:SP:1247:LEU:O	60:SP:1251:VAL:HG12	2.20	0.42
60:SP:1534:LEU:HD13	60:SP:1597:ILE:HD13	2.02	0.42
60:SP:1908:GLU:OE1	60:SP:1908:GLU:N	2.50	0.42
64:ST:387:LEU:O	64:ST:387:LEU:HD23	2.19	0.42
67:SW:113:TRP:CH2	67:SW:130:MET:HB2	2.55	0.42
2:L1:36:C:N4	2:L1:473:A:H61	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:630:A:N6	2:L1:969:C:O2'	2.53	0.42
4:L3:45:LEU:HD23	4:L3:45:LEU:O	2.20	0.42
16:LH:38:SER:OG	16:LH:40:ASP:OD1	2.22	0.42
16:LH:658:GLU:OE1	16:LH:658:GLU:N	2.48	0.42
18:LJ:16:LEU:HD12	20:LL:489:ALA:HB1	2.02	0.42
20:LL:160:VAL:HG23	20:LL:160:VAL:O	2.20	0.42
20:LL:518:ASN:OD1	20:LL:518:ASN:N	2.52	0.42
21:LM:216:CYS:O	21:LM:220:VAL:HG23	2.19	0.42
28:LT:307:GLN:HG2	50:SB:421:MET:HE3	2.00	0.42
30:LV:211:SER:C	30:LV:212:ARG:HD2	2.45	0.42
32:LX:625:GLU:OE1	32:LX:625:GLU:N	2.52	0.42
33:LZ:121:ALA:HB3	33:LZ:127:ALA:HB2	2.02	0.42
41:NH:1155:LEU:HD23	42:NI:93:PHE:HB3	2.02	0.42
44:NM:48:VAL:HG22	44:NM:64:ARG:HH21	1.85	0.42
60:SP:1147:ILE:O	60:SP:1151:ILE:HD12	2.20	0.42
63:SS:357:ASP:OD2	63:SS:359:LYS:HD2	2.20	0.42
1:L0:298:A:OP2	28:LT:103:ARG:NH2	2.49	0.41
12:LD:30:ARG:NH2	12:LD:50:GLU:O	2.51	0.41
13:LE:75:ILE:HD11	38:NE:321:VAL:HG13	2.02	0.41
18:LJ:357:PHE:O	18:LJ:360:MET:HB3	2.19	0.41
18:LJ:467:LEU:HD22	20:LL:550:THR:HG21	2.02	0.41
21:LM:1056:ALA:O	21:LM:1061:LYS:N	2.49	0.41
22:LN:110:GLU:OE1	22:LN:110:GLU:N	2.52	0.41
22:LN:554:ASP:O	22:LN:558:ARG:N	2.48	0.41
24:LP:148:ILE:HD13	24:LP:184:GLU:HG3	2.01	0.41
24:LP:199:ARG:HB2	63:SS:386:LEU:HD12	2.02	0.41
26:LR:40:ILE:HD12	26:LR:67:LEU:HD13	2.02	0.41
32:LX:493:ASP:OD1	32:LX:493:ASP:O	2.38	0.41
32:LY:494:VAL:HG21	32:LY:535:GLU:O	2.20	0.41
35:NB:221:ALA:HB3	35:NB:222:PRO:HD3	2.01	0.41
49:SA:152:LEU:HD11	51:SC:215:PRO:O	2.19	0.41
56:SK:145:LEU:O	64:ST:67:ARG:NH1	2.53	0.41
60:SP:1556:ARG:NH2	60:SP:1664:ILE:HD12	2.35	0.41
60:SP:1777:LEU:HD21	60:SP:1789:LEU:HD22	2.02	0.41
64:ST:560:TYR:OH	65:SU:388:LEU:O	2.35	0.41
65:SU:380:ILE:HD11	65:SU:405:LEU:HD12	2.02	0.41
8:L7:49:ILE:HD11	8:L7:172:VAL:HG22	2.01	0.41
9:L8:56:ARG:NH1	9:L8:174:GLY:O	2.52	0.41
17:LI:603:SER:OG	17:LI:606:ASP:OD2	2.36	0.41
20:LL:113:MET:HE1	20:LL:159:SER:HA	2.02	0.41
20:LL:481:LEU:HD21	20:LL:505:CYS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LN:382:VAL:HG11	22:LN:755:ILE:HD13	2.01	0.41
26:LR:160:ILE:HG23	26:LR:160:ILE:O	2.19	0.41
49:SA:191:PHE:HB2	49:SA:278:VAL:HG22	2.02	0.41
50:SB:409:THR:HG23	50:SB:409:THR:O	2.20	0.41
51:SC:175:ALA:HB1	51:SC:181:VAL:HG21	2.03	0.41
54:SH:315:LYS:O	54:SH:318:ILE:HG22	2.20	0.41
60:SP:1020:ASN:OD1	60:SP:1021:SER:N	2.53	0.41
60:SP:1279:ASN:ND2	60:SP:1280:LEU:HD12	2.35	0.41
2:L1:1533:C:H2'	2:L1:1534:G:O4'	2.20	0.41
16:LH:581:GLY:C	16:LH:582:LEU:HD22	2.44	0.41
20:LL:440:ILE:H	20:LL:440:ILE:HD12	1.86	0.41
26:LR:251:ASP:OD1	26:LR:252:GLY:N	2.50	0.41
26:LR:730:ILE:O	26:LR:730:ILE:HG22	2.19	0.41
28:LT:428:GLU:OE1	28:LT:428:GLU:N	2.51	0.41
32:LX:421:SER:HB3	32:LX:543:SER:HA	2.02	0.41
32:LX:601:ASN:O	32:LX:604:SER:OG	2.23	0.41
32:LY:344:GLN:OE1	32:LY:344:GLN:N	2.53	0.41
33:LZ:44:TYR:CD2	33:LZ:103:VAL:HG11	2.55	0.41
41:NH:313:ASN:OD1	41:NH:314:CYS:N	2.52	0.41
41:NH:855:LEU:HD23	41:NH:856:THR:N	2.34	0.41
60:SP:635:ALA:HB1	60:SP:676:PRO:HG2	2.02	0.41
60:SP:1416:GLU:O	60:SP:1419:SER:OG	2.27	0.41
65:SU:190:ASP:OD1	65:SU:190:ASP:N	2.53	0.41
4:L3:23:ASP:OD1	4:L3:24:GLY:N	2.53	0.41
20:LL:95:VAL:HG13	20:LL:95:VAL:O	2.19	0.41
20:LL:296:ILE:HG23	20:LL:296:ILE:O	2.20	0.41
20:LL:510:GLY:O	20:LL:514:VAL:HG23	2.20	0.41
25:LQ:45:ALA:N	25:LQ:48:ASP:O	2.42	0.41
29:LU:6:ILE:HD11	29:LU:8:ARG:CZ	2.51	0.41
32:LX:106:VAL:HG12	32:LX:107:TYR:O	2.20	0.41
32:LY:894:ASN:OD1	32:LY:895:ILE:N	2.53	0.41
40:NG:47:LYS:NZ	40:NG:66:ASP:OD1	2.41	0.41
54:SH:66:GLU:OE2	54:SH:67:ILE:N	2.52	0.41
54:SH:337:VAL:HG22	54:SH:354:ILE:HG12	2.02	0.41
56:SK:246:GLU:HA	56:SK:251:ILE:HD12	2.02	0.41
60:SP:302:PHE:CE2	60:SP:314:ILE:HG23	2.55	0.41
60:SP:470:ILE:CG2	60:SP:479:ILE:HD11	2.50	0.41
60:SP:1720:ILE:O	60:SP:1724:ASN:ND2	2.54	0.41
2:L1:475:A:OP1	10:L9:130:THR:HG21	2.21	0.41
2:L1:1680:G:HO2'	2:L1:1681:A:H2	1.68	0.41
4:L3:18:LEU:HD13	4:L3:73:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L7:92:PHE:C	8:L7:93:LEU:HD22	2.45	0.41
17:LI:592:ARG:O	17:LI:596:LYS:N	2.36	0.41
18:LJ:226:ILE:HD13	18:LJ:239:LEU:HD21	2.02	0.41
21:LM:360:ARG:HD2	21:LM:394:LEU:HD22	2.02	0.41
24:LP:96:TYR:HB3	24:LP:113:TYR:CD1	2.55	0.41
26:LR:249:LEU:HD21	26:LR:316:VAL:HG11	2.02	0.41
26:LR:431:ILE:HG22	26:LR:431:ILE:O	2.20	0.41
28:LT:738:ASP:OD1	28:LT:739:VAL:N	2.54	0.41
32:LX:805:ILE:HD12	32:LX:805:ILE:H	1.85	0.41
41:NH:220:LEU:HD13	41:NH:314:CYS:O	2.20	0.41
41:NH:1038:GLN:OE1	41:NH:1038:GLN:N	2.54	0.41
43:NK:300:ALA:O	43:NK:303:PHE:N	2.47	0.41
51:SD:161:GLU:C	51:SD:162:LEU:HD12	2.46	0.41
54:SH:111:LYS:NZ	54:SH:363:SER:O	2.52	0.41
54:SH:284:SER:CB	55:SI:631:ILE:HD11	2.51	0.41
55:SI:826:LYS:CE	55:SI:926:ILE:HD13	2.46	0.41
60:SP:514:PHE:CD2	60:SP:518:MET:HE1	2.55	0.41
60:SP:641:ARG:O	60:SP:645:VAL:HG22	2.20	0.41
63:SS:387:MET:HA	63:SS:387:MET:HE3	2.02	0.41
68:SY:118:LEU:HD11	68:SY:205:LEU:HD13	2.03	0.41
2:L1:406:U:H2'	2:L1:407:A:C8	2.55	0.41
4:L3:18:LEU:HD13	4:L3:73:MET:CE	2.50	0.41
15:LG:65:ARG:O	15:LG:67:ARG:NH1	2.54	0.41
18:LJ:257:CYS:SG	18:LJ:258:LEU:N	2.93	0.41
18:LJ:429:VAL:HG13	22:LN:775:VAL:HG23	2.01	0.41
20:LL:197:ILE:HG22	20:LL:198:THR:HG23	2.03	0.41
33:LZ:159:THR:HG22	33:LZ:160:TRP:N	2.35	0.41
34:NA:498:VAL:HG13	34:NA:498:VAL:O	2.20	0.41
38:NE:239:ARG:NH1	38:NE:286:ARG:O	2.54	0.41
41:NH:638:MET:HE1	41:NH:643:ALA:HB2	2.02	0.41
60:SP:648:GLU:O	60:SP:652:THR:HG22	2.20	0.41
65:SU:15:LEU:HD21	65:SU:23:GLN:O	2.21	0.41
65:SU:196:GLN:OE1	65:SU:260:ASN:ND2	2.49	0.41
1:L0:156:U:O2'	1:L0:157:U:O4'	2.26	0.41
2:L1:259:U:H3'	2:L1:260:U:H5''	2.03	0.41
8:L7:142:TYR:HE1	13:LE:35:ILE:HG23	1.85	0.41
14:LF:103:ALA:O	14:LF:108:ARG:NH1	2.48	0.41
18:LJ:94:LYS:O	18:LJ:110:SER:OG	2.30	0.41
18:LJ:140:LEU:O	18:LJ:151:LEU:HD12	2.19	0.41
18:LJ:391:ASN:ND2	18:LJ:403:ASN:OD1	2.54	0.41
20:LL:74:VAL:HG13	20:LL:90:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LX:6:ILE:HD12	32:LX:205:LEU:CD1	2.51	0.41
32:LX:786:LEU:O	32:LX:890:LEU:HD23	2.20	0.41
40:NG:18:ARG:N	40:NG:29:HIS:O	2.43	0.41
41:NH:583:ILE:CD1	41:NH:615:VAL:HG13	2.51	0.41
41:NH:721:VAL:HG23	41:NH:722:LEU:HD12	2.01	0.41
41:NH:1071:ALA:O	41:NH:1075:LEU:HD23	2.20	0.41
50:SB:116:ILE:HG22	50:SB:120:ILE:CD1	2.51	0.41
50:SB:131:MET:HE1	50:SB:139:MET:HE3	2.03	0.41
51:SD:302:GLU:OE1	51:SD:302:GLU:HA	2.21	0.41
54:SH:305:LYS:O	54:SH:307:ASP:N	2.54	0.41
55:SI:929:VAL:HG21	55:SI:1006:TRP:HB3	2.02	0.41
60:SP:389:ILE:O	60:SP:389:ILE:HG22	2.21	0.41
60:SP:562:VAL:HG21	60:SP:607:LEU:HD22	2.01	0.41
60:SP:2103:PHE:CD1	60:SP:2141:VAL:HG22	2.56	0.41
65:SU:378:SER:OG	65:SU:453:PRO:O	2.39	0.41
2:L1:73:U:O2'	2:L1:74:U:O4'	2.36	0.41
2:L1:1680:G:H21	2:L1:1681:A:N6	2.17	0.41
4:L3:68:ARG:O	4:L3:72:ILE:HG12	2.21	0.41
12:LD:70:ILE:C	12:LD:71:LEU:HD22	2.46	0.41
22:LN:541:ALA:CB	22:LN:555:LEU:HD11	2.48	0.41
23:LO:289:LEU:HD11	23:LO:292:PHE:CE1	2.56	0.41
25:LQ:814:MET:SD	25:LQ:815:SER:N	2.93	0.41
30:LV:194:LEU:HD11	45:NN:494:PHE:CE1	2.56	0.41
32:LX:283:ALA:HB2	32:LX:470:LEU:HB2	2.02	0.41
32:LX:705:LEU:HD11	55:SI:416:LEU:HD22	2.02	0.41
36:NC:58:VAL:O	45:NN:182:GLN:NE2	2.45	0.41
41:NH:515:ILE:O	41:NH:515:ILE:HG22	2.21	0.41
54:SH:337:VAL:HG22	54:SH:354:ILE:HG13	2.02	0.41
55:SI:113:ARG:NH2	55:SI:230:MET:O	2.52	0.41
60:SP:1193:ASN:ND2	60:SP:1196:SER:OG	2.49	0.41
60:SP:1545:VAL:O	60:SP:1549:VAL:HG23	2.20	0.41
60:SP:1976:ASP:OD1	60:SP:1977:THR:N	2.53	0.41
60:SP:1991:ASN:OD1	60:SP:1992:GLU:N	2.53	0.41
1:L0:237:A:OP2	18:LJ:356:ASN:N	2.49	0.41
1:L0:280:A:H5'	28:LT:406:THR:HG21	2.02	0.41
1:L0:321:G:H5''	23:LO:250:ILE:HD12	2.03	0.41
2:L1:-7:A:N6	29:LU:290:ASP:OD2	2.50	0.41
2:L1:187:G:O2'	60:SP:1100:GLN:NE2	2.54	0.41
2:L1:447:U:H2'	2:L1:448:C:O4'	2.21	0.41
2:L1:1712:A:H2'	2:L1:1713:G:H8	1.86	0.41
5:L4:130:GLN:NE2	5:L4:138:TYR:OH	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L4:199:GLU:OE2	5:L4:209:HIS:NE2	2.43	0.41
6:L5:143:ARG:HD2	15:LG:55:VAL:HG11	2.03	0.41
9:L8:8:ARG:NH1	9:L8:22:ARG:O	2.53	0.41
9:L8:171:SER:OG	9:L8:172:ARG:N	2.52	0.41
11:LC:60:PHE:CZ	11:LC:89:LEU:HD22	2.56	0.41
13:LE:77:PRO:O	13:LE:79:PHE:N	2.54	0.41
16:LH:688:VAL:HG13	17:LI:425:VAL:HG21	2.03	0.41
21:LM:193:THR:HG23	21:LM:241:ILE:HG12	2.03	0.41
22:LN:402:TRP:CE2	22:LN:416:LEU:HD13	2.56	0.41
23:LO:497:ILE:HD11	23:LO:532:VAL:HG11	2.03	0.41
25:LQ:223:ASP:OD2	25:LQ:224:SER:N	2.54	0.41
25:LQ:539:VAL:HG22	25:LQ:546:LEU:HD13	2.03	0.41
25:LQ:758:LEU:HD23	25:LQ:793:VAL:HG11	2.03	0.41
32:LX:548:ASN:OD1	32:LX:637:ARG:NH2	2.54	0.41
32:LY:694:LYS:O	32:LY:694:LYS:HD3	2.19	0.41
42:NI:78:TYR:O	42:NI:80:THR:HG23	2.21	0.41
44:NM:32:ILE:HG23	44:NM:43:VAL:HG23	2.02	0.41
49:SA:302:ASN:ND2	49:SA:390:ASP:OD1	2.50	0.41
53:SG:159:CYS:SG	53:SG:160:ILE:N	2.94	0.41
53:SG:481:ILE:H	53:SG:481:ILE:HD12	1.86	0.41
55:SI:153:MET:HE1	55:SI:197:GLU:HG3	2.03	0.41
55:SI:247:ASP:N	55:SI:272:TYR:O	2.50	0.41
60:SP:311:ILE:HD11	60:SP:343:ILE:HG23	2.02	0.41
60:SP:670:LEU:HD22	60:SP:681:VAL:HG11	2.01	0.41
60:SP:1290:GLU:N	60:SP:1293:ARG:HH21	2.19	0.41
60:SP:1987:LEU:CD2	63:SS:442:LEU:HD21	2.51	0.41
60:SP:2064:MET:HE3	60:SP:2083:ILE:HD13	2.02	0.41
63:SS:387:MET:HE3	63:SS:391:GLU:OE2	2.21	0.41
65:SU:53:ARG:NE	65:SU:118:ASP:OD2	2.41	0.41
66:SV:131:LEU:HD21	66:SV:135:VAL:CG1	2.51	0.41
67:SW:117:TYR:N	67:SW:118:PRO:CD	2.83	0.41
2:L1:248:U:O2'	2:L1:249:U:P	2.79	0.41
5:L4:86:PHE:CE1	5:L4:87:MET:HE3	2.56	0.41
9:L8:21:PHE:C	9:L8:22:ARG:HG2	2.46	0.41
16:LH:234:SER:OG	16:LH:235:VAL:HG23	2.21	0.41
16:LH:692:PHE:HB3	17:LI:430:LEU:HD12	2.03	0.41
26:LR:457:ALA:HB1	26:LR:494:ILE:HD13	2.03	0.41
26:LR:626:MET:HE3	26:LR:627:ASN:CG	2.45	0.41
30:LV:131:LEU:HD21	30:LV:134:THR:CG2	2.51	0.41
30:LV:232:THR:O	30:LV:233:THR:HG23	2.20	0.41
31:LW:462:ASN:OD1	31:LW:464:LYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LY:666:THR:CG2	36:NC:117:LEU:HD23	2.43	0.41
33:LZ:170:LEU:HD22	68:SY:62:GLU:O	2.22	0.41
34:NA:365:LEU:HD22	58:SM:227:ARG:NH2	2.36	0.41
41:NH:891:ALA:HA	41:NH:894:ARG:NH1	2.36	0.41
49:SA:373:GLY:O	49:SA:376:SER:OG	2.24	0.41
64:ST:512:ASP:OD1	64:ST:513:GLN:N	2.53	0.41
15:LG:12:VAL:HG22	15:LG:30:VAL:HG12	2.03	0.40
21:LM:218:ILE:HD11	21:LM:260:ILE:HA	2.02	0.40
22:LN:40:ASP:OD1	22:LN:40:ASP:N	2.54	0.40
22:LN:274:GLN:OE1	22:LN:320:TRP:N	2.44	0.40
23:LO:348:THR:O	23:LO:682:THR:HG21	2.21	0.40
24:LP:64:ASN:HB2	24:LP:88:ILE:HG21	2.03	0.40
28:LT:64:ASN:OD1	50:SB:421:MET:HG3	2.21	0.40
32:LX:104:ARG:NH1	32:LX:105:TYR:O	2.55	0.40
32:LX:384:VAL:HG13	32:LX:404:TYR:CE2	2.56	0.40
37:ND:112:LEU:HD11	65:SU:90:TRP:CE3	2.56	0.40
41:NH:169:PRO:HA	41:NH:172:THR:HG22	2.02	0.40
41:NH:218:ASP:O	41:NH:224:CYS:N	2.53	0.40
54:SH:333:PHE:CD2	54:SH:357:ILE:HD13	2.56	0.40
56:SK:31:LEU:HD23	56:SK:40:ARG:HG2	2.03	0.40
60:SP:1345:LEU:HD21	60:SP:1393:MET:CE	2.45	0.40
60:SP:1903:LEU:O	60:SP:1940:LYS:NZ	2.54	0.40
61:SQ:112:ASN:OD1	61:SQ:113:MET:N	2.54	0.40
64:ST:650:VAL:HG23	64:ST:651:TRP:N	2.36	0.40
12:LD:46:LYS:O	12:LD:49:ILE:N	2.55	0.40
17:LI:614:ILE:HD12	17:LI:634:LEU:HD21	2.03	0.40
17:LI:673:THR:HG23	19:LK:490:GLU:HG3	2.03	0.40
20:LL:36:ARG:O	20:LL:44:THR:OG1	2.13	0.40
21:LM:287:ASP:OD1	21:LM:288:ALA:N	2.54	0.40
22:LN:682:THR:OG1	22:LN:684:GLU:OE1	2.33	0.40
23:LO:215:VAL:HG11	23:LO:292:PHE:CE1	2.56	0.40
26:LR:44:ASP:OD2	26:LR:46:THR:N	2.43	0.40
26:LR:698:LEU:HD13	26:LR:759:THR:HG21	2.03	0.40
27:LS:178:VAL:HG23	28:LT:220:ILE:CD1	2.51	0.40
28:LT:342:TYR:OH	28:LT:345:SER:OG	2.16	0.40
29:LU:306:SER:OG	29:LU:307:ALA:N	2.54	0.40
32:LY:764:ASN:OD1	32:LY:765:VAL:N	2.53	0.40
40:NG:48:VAL:HG21	40:NG:53:ASP:HB2	2.03	0.40
42:NI:50:SER:O	42:NI:127:LYS:NZ	2.39	0.40
53:SG:158:THR:HG21	53:SG:240:LEU:HA	2.03	0.40
56:SJ:68:LEU:HD22	56:SJ:77:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SP:470:ILE:O	60:SP:470:ILE:HG13	2.20	0.40
60:SP:1151:ILE:HD12	60:SP:1151:ILE:H	1.85	0.40
60:SP:2065:VAL:CG2	63:SS:262:LEU:HD13	2.36	0.40
62:SR:70:LYS:O	62:SR:87:VAL:N	2.53	0.40
64:ST:685:LEU:HD23	64:ST:685:LEU:C	2.46	0.40
68:SY:75:LYS:HD2	68:SY:77:LEU:HD13	2.03	0.40
9:L8:38:ILE:HD11	9:L8:96:LEU:HD11	2.03	0.40
10:L9:68:LYS:NZ	10:L9:72:GLU:OE1	2.29	0.40
16:LH:749:ASP:OD1	16:LH:749:ASP:C	2.64	0.40
18:LJ:488:LYS:HD3	20:LL:551:ILE:HD13	2.02	0.40
22:LN:363:SER:O	22:LN:367:GLY:N	2.47	0.40
25:LQ:764:GLU:OE2	25:LQ:834:LYS:NZ	2.42	0.40
30:LV:311:MET:HE1	30:LV:329:PHE:CG	2.55	0.40
32:LX:17:GLY:O	32:LX:21:LYS:N	2.54	0.40
41:NH:172:THR:O	41:NH:172:THR:HG23	2.22	0.40
52:SF:13:ASP:O	52:SF:17:THR:HG23	2.21	0.40
55:SI:298:VAL:HG13	55:SI:791:ILE:HG23	2.03	0.40
60:SP:2152:VAL:HA	60:SP:2158:LEU:HD21	2.02	0.40
7:L6:18:ILE:HG23	7:L6:23:ARG:HH11	1.87	0.40
12:LD:94:ILE:O	12:LD:94:ILE:HG23	2.20	0.40
22:LN:389:ARG:NH2	22:LN:405:GLY:O	2.54	0.40
23:LO:340:LYS:HB3	34:NA:479:ALA:HB3	2.03	0.40
25:LQ:445:VAL:O	25:LQ:456:LEU:HD12	2.21	0.40
25:LQ:577:LEU:HD21	34:NA:591:ILE:HG22	2.03	0.40
26:LR:616:HIS:CG	26:LR:620:LEU:HD21	2.56	0.40
29:LU:342:ILE:HG21	29:LU:419:VAL:HG12	2.02	0.40
30:LV:27:ASP:O	30:LV:30:ALA:N	2.50	0.40
30:LV:115:VAL:HG13	30:LV:125:PHE:CE1	2.56	0.40
31:LW:197:ASP:HB2	31:LW:247:MET:HE1	2.03	0.40
35:NB:605:SER:HB2	51:SC:302:GLU:CD	2.47	0.40
41:NH:301:LYS:HG2	41:NH:301:LYS:O	2.22	0.40
42:NI:37:MET:SD	42:NI:55:LEU:HD23	2.61	0.40
51:SC:110:ASN:OD1	51:SC:112:ALA:N	2.55	0.40
60:SP:1308:LEU:HD23	60:SP:1350:THR:HB	2.02	0.40
63:SS:432:ASP:OD1	63:SS:433:ILE:N	2.55	0.40
1:L0:461:A:C2	57:SL:13:VAL:HG21	2.57	0.40
2:L1:139:C:OP2	7:L6:187:LYS:NZ	2.49	0.40
4:L3:76:PRO:HA	4:L3:81:ILE:HD12	2.03	0.40
16:LH:152:ARG:NH1	16:LH:175:ALA:HB2	2.37	0.40
16:LH:656:ASP:OD2	16:LH:676:THR:OG1	2.40	0.40
16:LH:678:LEU:HD12	16:LH:678:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LL:143:ASN:OD1	20:LL:144:ASN:N	2.54	0.40
22:LN:108:ASN:O	22:LN:108:ASN:OD1	2.39	0.40
26:LR:266:ILE:HD11	26:LR:283:LYS:CA	2.52	0.40
30:LV:361:GLU:OE2	32:LY:918:ARG:NH1	2.55	0.40
32:LX:23:ARG:CB	32:LX:482:ILE:HD12	2.51	0.40
32:LY:329:PHE:HB3	32:LY:334:TYR:HB2	2.03	0.40
36:NC:58:VAL:HG21	45:NN:179:ILE:HG12	2.03	0.40
41:NH:583:ILE:HD12	41:NH:615:VAL:HG22	2.04	0.40
41:NH:799:LEU:HD11	41:NH:856:THR:HG21	2.04	0.40
41:NH:1080:LEU:CD1	41:NH:1085:ILE:HD11	2.52	0.40
50:SB:57:LEU:O	50:SB:61:ASN:ND2	2.44	0.40
55:SI:115:LEU:HD11	55:SI:227:ILE:CG2	2.52	0.40
60:SP:1182:LEU:C	60:SP:1182:LEU:HD23	2.47	0.40
60:SP:1967:ILE:CD1	60:SP:2006:LEU:HD23	2.52	0.40
67:SW:196:ASP:O	67:SW:200:ARG:N	2.52	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	91/146 (62%)	89 (98%)	2 (2%)	0	100	100
5	L4	242/261 (93%)	240 (99%)	2 (1%)	0	100	100
6	L5	202/225 (90%)	200 (99%)	2 (1%)	0	100	100
7	L6	202/236 (86%)	201 (100%)	1 (0%)	0	100	100
8	L7	165/190 (87%)	161 (98%)	4 (2%)	0	100	100
9	L8	166/200 (83%)	165 (99%)	1 (1%)	0	100	100
10	L9	169/197 (86%)	169 (100%)	0	0	100	100
11	LC	123/143 (86%)	122 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	LD	135/156 (86%)	132 (98%)	3 (2%)	0	100	100
13	LE	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
14	LF	128/135 (95%)	126 (98%)	2 (2%)	0	100	100
15	LG	60/67 (90%)	60 (100%)	0	0	100	100
16	LH	790/896 (88%)	774 (98%)	16 (2%)	0	100	100
17	LI	582/713 (82%)	574 (99%)	8 (1%)	0	100	100
18	LJ	489/513 (95%)	473 (97%)	16 (3%)	0	100	100
19	LK	130/575 (23%)	130 (100%)	0	0	100	100
20	LL	496/643 (77%)	486 (98%)	10 (2%)	0	100	100
21	LM	1597/1769 (90%)	1567 (98%)	30 (2%)	0	100	100
22	LN	649/776 (84%)	639 (98%)	10 (2%)	0	100	100
23	LO	829/923 (90%)	819 (99%)	10 (1%)	0	100	100
24	LP	376/440 (86%)	372 (99%)	4 (1%)	0	100	100
25	LQ	831/943 (88%)	813 (98%)	18 (2%)	0	100	100
26	LR	785/817 (96%)	767 (98%)	18 (2%)	0	100	100
27	LS	469/594 (79%)	457 (97%)	12 (3%)	0	100	100
28	LT	865/939 (92%)	844 (98%)	21 (2%)	0	100	100
29	LU	456/489 (93%)	448 (98%)	8 (2%)	0	100	100
30	LV	401/707 (57%)	388 (97%)	13 (3%)	0	100	100
31	LW	531/554 (96%)	522 (98%)	9 (2%)	0	100	100
32	LX	826/1056 (78%)	812 (98%)	14 (2%)	0	100	100
32	LY	834/1056 (79%)	822 (99%)	12 (1%)	0	100	100
33	LZ	179/183 (98%)	178 (99%)	1 (1%)	0	100	100
34	NA	274/593 (46%)	270 (98%)	4 (2%)	0	100	100
35	NB	255/610 (42%)	253 (99%)	2 (1%)	0	100	100
36	NC	111/357 (31%)	109 (98%)	2 (2%)	0	100	100
37	ND	70/214 (33%)	70 (100%)	0	0	100	100
38	NE	207/346 (60%)	206 (100%)	1 (0%)	0	100	100
39	NF	139/151 (92%)	138 (99%)	1 (1%)	0	100	100
40	NG	117/137 (85%)	114 (97%)	3 (3%)	0	100	100
41	NH	1063/1237 (86%)	1044 (98%)	19 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	NI	232/297 (78%)	224 (97%)	8 (3%)	0	100	100
43	NK	253/316 (80%)	251 (99%)	2 (1%)	0	100	100
44	NM	224/255 (88%)	222 (99%)	2 (1%)	0	100	100
45	NN	257/534 (48%)	257 (100%)	0	0	100	100
46	NQ	77/82 (94%)	76 (99%)	1 (1%)	0	100	100
47	NV	6/733 (1%)	6 (100%)	0	0	100	100
48	OA	167/1729 (10%)	166 (99%)	1 (1%)	0	100	100
49	SA	379/504 (75%)	376 (99%)	3 (1%)	0	100	100
50	SB	434/511 (85%)	427 (98%)	7 (2%)	0	100	100
51	SC	237/327 (72%)	233 (98%)	4 (2%)	0	100	100
51	SD	228/327 (70%)	223 (98%)	5 (2%)	0	100	100
52	SE	119/126 (94%)	115 (97%)	4 (3%)	0	100	100
52	SF	119/126 (94%)	118 (99%)	1 (1%)	0	100	100
53	SG	453/573 (79%)	444 (98%)	9 (2%)	0	100	100
54	SH	358/367 (98%)	349 (98%)	9 (2%)	0	100	100
55	SI	799/1183 (68%)	785 (98%)	14 (2%)	0	100	100
56	SJ	207/252 (82%)	206 (100%)	1 (0%)	0	100	100
56	SK	225/252 (89%)	219 (97%)	6 (3%)	0	100	100
57	SL	169/189 (89%)	164 (97%)	5 (3%)	0	100	100
58	SM	278/290 (96%)	276 (99%)	2 (1%)	0	100	100
59	SN	251/274 (92%)	249 (99%)	2 (1%)	0	100	100
60	SP	2334/2493 (94%)	2303 (99%)	31 (1%)	0	100	100
61	SQ	147/217 (68%)	139 (95%)	8 (5%)	0	100	100
62	SR	102/145 (70%)	101 (99%)	1 (1%)	0	100	100
63	SS	262/899 (29%)	255 (97%)	7 (3%)	0	100	100
64	ST	566/810 (70%)	560 (99%)	6 (1%)	0	100	100
65	SU	528/552 (96%)	523 (99%)	5 (1%)	0	100	100
66	SV	141/206 (68%)	140 (99%)	1 (1%)	0	100	100
67	SW	193/274 (70%)	188 (97%)	5 (3%)	0	100	100
68	SY	227/250 (91%)	226 (100%)	1 (0%)	0	100	100
69	SZ	255/483 (53%)	252 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	26388/35893 (74%)	25947 (98%)	441 (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	88/129 (68%)	88 (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	175/201 (87%)	175 (100%)	0	100	100
8	L7	149/170 (88%)	149 (100%)	0	100	100
9	L8	137/161 (85%)	137 (100%)	0	100	100
10	L9	147/166 (89%)	147 (100%)	0	100	100
11	LC	105/119 (88%)	105 (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	745/826 (90%)	745 (100%)	0	100	100
17	LI	244/657 (37%)	244 (100%)	0	100	100
18	LJ	437/454 (96%)	437 (100%)	0	100	100
19	LK	124/533 (23%)	124 (100%)	0	100	100
20	LL	452/574 (79%)	452 (100%)	0	100	100
21	LM	421/1633 (26%)	421 (100%)	0	100	100
22	LN	603/713 (85%)	603 (100%)	0	100	100
23	LO	729/811 (90%)	729 (100%)	0	100	100
24	LP	360/414 (87%)	360 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	LQ	746/832 (90%)	746 (100%)	0	100	100
26	LR	698/719 (97%)	698 (100%)	0	100	100
27	LS	423/528 (80%)	423 (100%)	0	100	100
28	LT	763/819 (93%)	763 (100%)	0	100	100
29	LU	415/443 (94%)	415 (100%)	0	100	100
30	LV	366/636 (58%)	366 (100%)	0	100	100
31	LW	465/480 (97%)	465 (100%)	0	100	100
32	LX	751/934 (80%)	751 (100%)	0	100	100
32	LY	592/934 (63%)	592 (100%)	0	100	100
33	LZ	170/172 (99%)	170 (100%)	0	100	100
34	NA	194/535 (36%)	194 (100%)	0	100	100
35	NB	149/538 (28%)	149 (100%)	0	100	100
36	NC	59/315 (19%)	59 (100%)	0	100	100
37	ND	70/196 (36%)	70 (100%)	0	100	100
38	NE	166/304 (55%)	166 (100%)	0	100	100
39	NF	121/128 (94%)	121 (100%)	0	100	100
40	NG	90/105 (86%)	90 (100%)	0	100	100
41	NH	982/1125 (87%)	982 (100%)	0	100	100
42	NI	220/274 (80%)	220 (100%)	0	100	100
43	NK	233/289 (81%)	233 (100%)	0	100	100
44	NM	205/224 (92%)	205 (100%)	0	100	100
45	NN	175/482 (36%)	175 (100%)	0	100	100
46	NQ	68/71 (96%)	68 (100%)	0	100	100
47	NV	7/671 (1%)	7 (100%)	0	100	100
48	OA	14/1544 (1%)	14 (100%)	0	100	100
49	SA	328/435 (75%)	328 (100%)	0	100	100
50	SB	360/433 (83%)	360 (100%)	0	100	100
51	SC	200/240 (83%)	200 (100%)	0	100	100
51	SD	197/240 (82%)	197 (100%)	0	100	100
52	SE	100/104 (96%)	100 (100%)	0	100	100
52	SF	100/104 (96%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	SG	399/503 (79%)	399 (100%)	0	100	100
54	SH	307/312 (98%)	307 (100%)	0	100	100
55	SI	718/1039 (69%)	718 (100%)	0	100	100
56	SJ	192/222 (86%)	192 (100%)	0	100	100
56	SK	205/222 (92%)	205 (100%)	0	100	100
57	SL	155/169 (92%)	155 (100%)	0	100	100
58	SM	251/258 (97%)	251 (100%)	0	100	100
59	SN	236/256 (92%)	236 (100%)	0	100	100
60	SP	1956/2307 (85%)	1956 (100%)	0	100	100
61	SQ	140/200 (70%)	140 (100%)	0	100	100
62	SR	86/120 (72%)	86 (100%)	0	100	100
63	SS	251/808 (31%)	251 (100%)	0	100	100
64	ST	441/732 (60%)	441 (100%)	0	100	100
65	SU	490/506 (97%)	490 (100%)	0	100	100
66	SV	42/192 (22%)	42 (100%)	0	100	100
67	SW	172/238 (72%)	172 (100%)	0	100	100
68	SY	218/234 (93%)	218 (100%)	0	100	100
69	SZ	14/424 (3%)	14 (100%)	0	100	100
All	All	21401/31991 (67%)	21401 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (174) such sidechains are listed below:

Mol	Chain	Res	Type
4	L3	55	HIS
5	L4	50	ASN
5	L4	67	GLN
5	L4	130	GLN
5	L4	142	HIS
6	L5	131	GLN
9	L8	119	GLN
10	L9	112	GLN
10	L9	176	ASN
11	LC	74	HIS

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Mol	Chain	Res	Type
12	LD	14	GLN
12	LD	81	HIS
12	LD	138	ASN
13	LE	24	GLN
13	LE	42	GLN
14	LF	29	HIS
16	LH	115	HIS
16	LH	131	HIS
16	LH	150	ASN
16	LH	189	HIS
16	LH	194	HIS
16	LH	352	ASN
16	LH	410	ASN
16	LH	568	ASN
16	LH	631	GLN
16	LH	738	ASN
17	LI	529	HIS
17	LI	677	ASN
18	LJ	44	HIS
18	LJ	210	ASN
18	LJ	391	ASN
19	LK	398	ASN
19	LK	450	ASN
20	LL	280	GLN
20	LL	297	ASN
21	LM	10	GLN
21	LM	86	GLN
21	LM	227	ASN
22	LN	108	ASN
22	LN	381	ASN
22	LN	574	HIS
22	LN	731	HIS
23	LO	88	ASN
23	LO	91	HIS
23	LO	254	HIS
23	LO	349	ASN
23	LO	746	ASN
25	LQ	172	GLN
25	LQ	200	HIS
25	LQ	275	GLN
25	LQ	383	HIS
25	LQ	451	ASN

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Mol	Chain	Res	Type
25	LQ	628	HIS
25	LQ	677	HIS
25	LQ	865	HIS
26	LR	299	ASN
26	LR	433	HIS
26	LR	488	HIS
26	LR	579	GLN
26	LR	735	GLN
27	LS	309	GLN
27	LS	310	GLN
27	LS	372	HIS
27	LS	388	HIS
27	LS	520	ASN
28	LT	263	HIS
28	LT	291	HIS
28	LT	330	GLN
28	LT	338	GLN
28	LT	627	ASN
28	LT	736	HIS
28	LT	779	HIS
29	LU	350	HIS
29	LU	384	ASN
31	LW	124	HIS
31	LW	278	ASN
31	LW	410	ASN
31	LW	506	GLN
31	LW	517	GLN
31	LW	535	GLN
32	LX	231	GLN
32	LX	344	GLN
32	LX	363	HIS
32	LX	368	GLN
32	LX	601	ASN
32	LY	380	GLN
32	LY	545	HIS
32	LY	623	GLN
32	LY	718	HIS
32	LY	740	ASN
32	LY	752	ASN
33	LZ	27	HIS
33	LZ	59	ASN
33	LZ	74	HIS

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Mol	Chain	Res	Type
33	LZ	116	HIS
34	NA	443	ASN
34	NA	455	HIS
34	NA	497	ASN
35	NB	378	GLN
35	NB	382	HIS
35	NB	513	HIS
36	NC	120	GLN
38	NE	156	GLN
41	NH	582	GLN
41	NH	634	HIS
41	NH	1228	ASN
42	NI	148	HIS
43	NK	143	GLN
44	NM	16	GLN
44	NM	209	ASN
49	SA	95	ASN
49	SA	176	GLN
49	SA	183	GLN
49	SA	261	GLN
49	SA	297	HIS
50	SB	334	HIS
50	SB	344	HIS
51	SC	93	HIS
51	SD	93	HIS
52	SF	113	GLN
53	SG	177	ASN
53	SG	465	GLN
53	SG	547	HIS
53	SG	570	GLN
54	SH	42	ASN
54	SH	176	GLN
54	SH	181	HIS
54	SH	317	GLN
55	SI	112	HIS
55	SI	200	GLN
55	SI	761	GLN
55	SI	776	GLN
55	SI	803	ASN
55	SI	893	ASN
55	SI	986	HIS
55	SI	1065	ASN

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Mol	Chain	Res	Type
55	SI	1114	GLN
56	SJ	111	GLN
56	SK	26	GLN
56	SK	111	GLN
58	SM	18	GLN
58	SM	182	GLN
59	SN	207	HIS
59	SN	248	ASN
60	SP	745	HIS
60	SP	802	ASN
60	SP	1057	GLN
60	SP	1193	ASN
60	SP	1356	ASN
60	SP	1458	GLN
60	SP	1483	HIS
60	SP	1516	GLN
60	SP	1786	GLN
60	SP	1957	GLN
60	SP	2159	ASN
61	SQ	126	HIS
63	SS	282	HIS
63	SS	447	ASN
63	SS	876	GLN
64	ST	107	ASN
64	ST	399	HIS
64	ST	432	HIS
64	ST	438	ASN
64	ST	617	HIS
64	ST	697	HIS
64	ST	713	HIS
65	SU	25	ASN
65	SU	42	GLN
65	SU	133	HIS
65	SU	228	HIS
65	SU	304	ASN
65	SU	457	HIS
65	SU	474	HIS
68	SY	6	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L0	442/700 (63%)	82 (18%)	1 (0%)
2	L1	1180/1808 (65%)	197 (16%)	1 (0%)
3	L2	170/333 (51%)	27 (15%)	0
All	All	1792/2841 (63%)	306 (17%)	2 (0%)

All (306) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L0	7	A
1	L0	61	U
1	L0	62	C
1	L0	63	G
1	L0	64	U
1	L0	83	U
1	L0	85	G
1	L0	86	C
1	L0	91	U
1	L0	95	A
1	L0	103	G
1	L0	104	A
1	L0	109	C
1	L0	110	G
1	L0	114	G
1	L0	122	U
1	L0	123	C
1	L0	125	G
1	L0	127	U
1	L0	128	C
1	L0	129	U
1	L0	130	G
1	L0	141	A
1	L0	142	U
1	L0	144	C
1	L0	148	G
1	L0	151	U
1	L0	156	U
1	L0	171	G
1	L0	176	U
1	L0	177	U
1	L0	190	U
1	L0	200	A
1	L0	219	U
1	L0	227	U

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Mol	Chain	Res	Type
1	L0	235	A
1	L0	240	C
1	L0	256	U
1	L0	259	G
1	L0	260	A
1	L0	267	U
1	L0	279	A
1	L0	280	A
1	L0	281	G
1	L0	295	A
1	L0	297	U
1	L0	304	U
1	L0	305	A
1	L0	306	G
1	L0	310	U
1	L0	311	C
1	L0	316	U
1	L0	325	U
1	L0	326	C
1	L0	354	G
1	L0	360	C
1	L0	365	G
1	L0	369	G
1	L0	370	U
1	L0	371	G
1	L0	372	A
1	L0	373	U
1	L0	381	G
1	L0	382	U
1	L0	383	G
1	L0	386	A
1	L0	391	C
1	L0	395	C
1	L0	407	A
1	L0	427	A
1	L0	430	C
1	L0	431	A
1	L0	432	C
1	L0	461	A
1	L0	462	G
1	L0	464	G
1	L0	468	A

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Mol	Chain	Res	Type
1	L0	474	A
1	L0	481	U
1	L0	482	A
1	L0	487	A
1	L0	488	U
2	L1	-6	A
2	L1	-1	G
2	L1	5	U
2	L1	18	C
2	L1	23	G
2	L1	25	C
2	L1	34	G
2	L1	35	U
2	L1	39	A
2	L1	57	G
2	L1	60	U
2	L1	67	A
2	L1	71	A
2	L1	73	U
2	L1	74	U
2	L1	76	A
2	L1	77	U
2	L1	88	U
2	L1	100	A
2	L1	103	A
2	L1	104	A
2	L1	114	C
2	L1	116	U
2	L1	127	G
2	L1	128	U
2	L1	140	A
2	L1	145	A
2	L1	153	G
2	L1	160	C
2	L1	164	A
2	L1	168	A
2	L1	187	G
2	L1	188	A
2	L1	190	C
2	L1	192	U
2	L1	193	U
2	L1	195	G

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Mol	Chain	Res	Type
2	L1	196	G
2	L1	201	G
2	L1	202	A
2	L1	204	G
2	L1	249	U
2	L1	260	U
2	L1	261	U
2	L1	265	A
2	L1	267	U
2	L1	275	C
2	L1	276	C
2	L1	277	U
2	L1	278	U
2	L1	279	G
2	L1	280	U
2	L1	299	A
2	L1	316	A
2	L1	320	U
2	L1	321	C
2	L1	322	G
2	L1	333	A
2	L1	334	G
2	L1	337	G
2	L1	387	A
2	L1	388	G
2	L1	393	C
2	L1	400	A
2	L1	402	C
2	L1	423	G
2	L1	424	C
2	L1	425	A
2	L1	426	G
2	L1	428	A
2	L1	435	C
2	L1	437	A
2	L1	438	A
2	L1	439	U
2	L1	444	C
2	L1	447	U
2	L1	453	U
2	L1	454	U
2	L1	456	A

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Mol	Chain	Res	Type
2	L1	457	G
2	L1	467	G
2	L1	468	A
2	L1	475	A
2	L1	477	A
2	L1	495	C
2	L1	496	G
2	L1	501	U
2	L1	505	A
2	L1	506	A
2	L1	516	G
2	L1	539	G
2	L1	542	A
2	L1	545	A
2	L1	551	G
2	L1	552	G
2	L1	564	G
2	L1	565	C
2	L1	575	C
2	L1	579	A
2	L1	583	C
2	L1	594	A
2	L1	635	A
2	L1	752	A
2	L1	765	G
2	L1	766	U
2	L1	774	A
2	L1	803	A
2	L1	863	A
2	L1	893	U
2	L1	898	A
2	L1	906	A
2	L1	933	A
2	L1	935	U
2	L1	951	A
2	L1	960	U
2	L1	965	U
2	L1	970	A
2	L1	1027	A
2	L1	1030	A
2	L1	1033	C
2	L1	1036	A

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Mol	Chain	Res	Type
2	L1	1040	G
2	L1	1062	A
2	L1	1064	G
2	L1	1076	A
2	L1	1079	U
2	L1	1084	A
2	L1	1085	G
2	L1	1114	G
2	L1	1122	G
2	L1	1128	C
2	L1	1132	A
2	L1	1158	C
2	L1	1159	C
2	L1	1167	G
2	L1	1175	U
2	L1	1191	U
2	L1	1192	C
2	L1	1193	A
2	L1	1207	C
2	L1	1208	A
2	L1	1218	G
2	L1	1219	A
2	L1	1227	A
2	L1	1228	G
2	L1	1230	A
2	L1	1232	U
2	L1	1258	U
2	L1	1267	G
2	L1	1268	G
2	L1	1269	U
2	L1	1270	G
2	L1	1435	G
2	L1	1436	A
2	L1	1437	U
2	L1	1438	G
2	L1	1440	C
2	L1	1461	C
2	L1	1472	C
2	L1	1473	U
2	L1	1474	G
2	L1	1485	C
2	L1	1492	A

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Mol	Chain	Res	Type
2	L1	1493	A
2	L1	1506	G
2	L1	1577	A
2	L1	1590	G
2	L1	1595	U
2	L1	1596	C
2	L1	1601	G
2	L1	1602	C
2	L1	1611	A
2	L1	1618	C
2	L1	1619	C
2	L1	1633	A
2	L1	1651	A
2	L1	1654	G
2	L1	1657	U
2	L1	1658	G
2	L1	1661	U
2	L1	1664	C
2	L1	1680	G
2	L1	1683	C
2	L1	1697	G
2	L1	1701	A
2	L1	1703	C
2	L1	1705	C
2	L1	1715	G
2	L1	1716	C
2	L1	1721	A
2	L1	1745	G
2	L1	1747	G
2	L1	1756	A
2	L1	1778	G
2	L1	1780	G
2	L1	1781	A
2	L1	1782	A
3	L2	4	G
3	L2	14	A
3	L2	22	A
3	L2	24	U
3	L2	25	U
3	L2	27	U
3	L2	28	A
3	L2	29	U

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Mol	Chain	Res	Type
3	L2	30	A
3	L2	34	A
3	L2	35	U
3	L2	38	U
3	L2	48	A
3	L2	56	A
3	L2	61	G
3	L2	62	C
3	L2	77	U
3	L2	90	C
3	L2	91	C
3	L2	109	G
3	L2	118	A
3	L2	252	C
3	L2	308	U
3	L2	313	A
3	L2	324	U
3	L2	325	C
3	L2	329	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L0	381	G
2	L1	248	U

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

2 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	$\# Z > 2$
27	SEP	LS	128	27	8,9,10	1.60	1 (12%)	7,12,14	1.28	1 (14%)
23	SEP	LO	651	23	8,9,10	1.58	1 (12%)	7,12,14	1.35	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SEP	LS	128	27	-	0/6/8/10	-
23	SEP	LO	651	23	-	1/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	LS	128	SEP	P-O1P	3.49	1.61	1.50
23	LO	651	SEP	P-O1P	3.45	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	LO	651	SEP	OG-CB-CA	2.90	110.97	108.14
27	LS	128	SEP	OG-CB-CA	2.71	110.78	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	LO	651	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 36 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
73	GTP	SI	2001	70	33,34,34	1.82	4 (12%)	50,54,54	1.47	7 (14%)
71	ATP	NH	1300	70	32,33,33	0.31	0	48,52,52	0.69	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
73	GTP	SI	2001	70	-	6/22/38/38	0/3/3/3
71	ATP	NH	1300	70	-	3/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	SI	2001	GTP	C5-N7	6.62	1.52	1.39
73	SI	2001	GTP	C8-N9	-4.29	1.27	1.37
73	SI	2001	GTP	C4-N9	-3.86	1.28	1.38
73	SI	2001	GTP	C4-N3	2.27	1.39	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	SI	2001	GTP	C8-N9-C4	7.19	119.51	106.03
73	SI	2001	GTP	N9-C4-N3	2.71	131.38	125.95
73	SI	2001	GTP	C6-C5-N7	2.52	134.88	130.29
73	SI	2001	GTP	C1'-N9-C8	-2.26	120.32	126.73
73	SI	2001	GTP	C1'-N9-C4	-2.14	120.17	126.49
73	SI	2001	GTP	C5-C4-N9	-2.10	101.90	105.66
73	SI	2001	GTP	C8-N7-C5	-2.10	100.53	104.26

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
71	NH	1300	ATP	PB-O3B-PG-O2G
71	NH	1300	ATP	PB-O3B-PG-O3G

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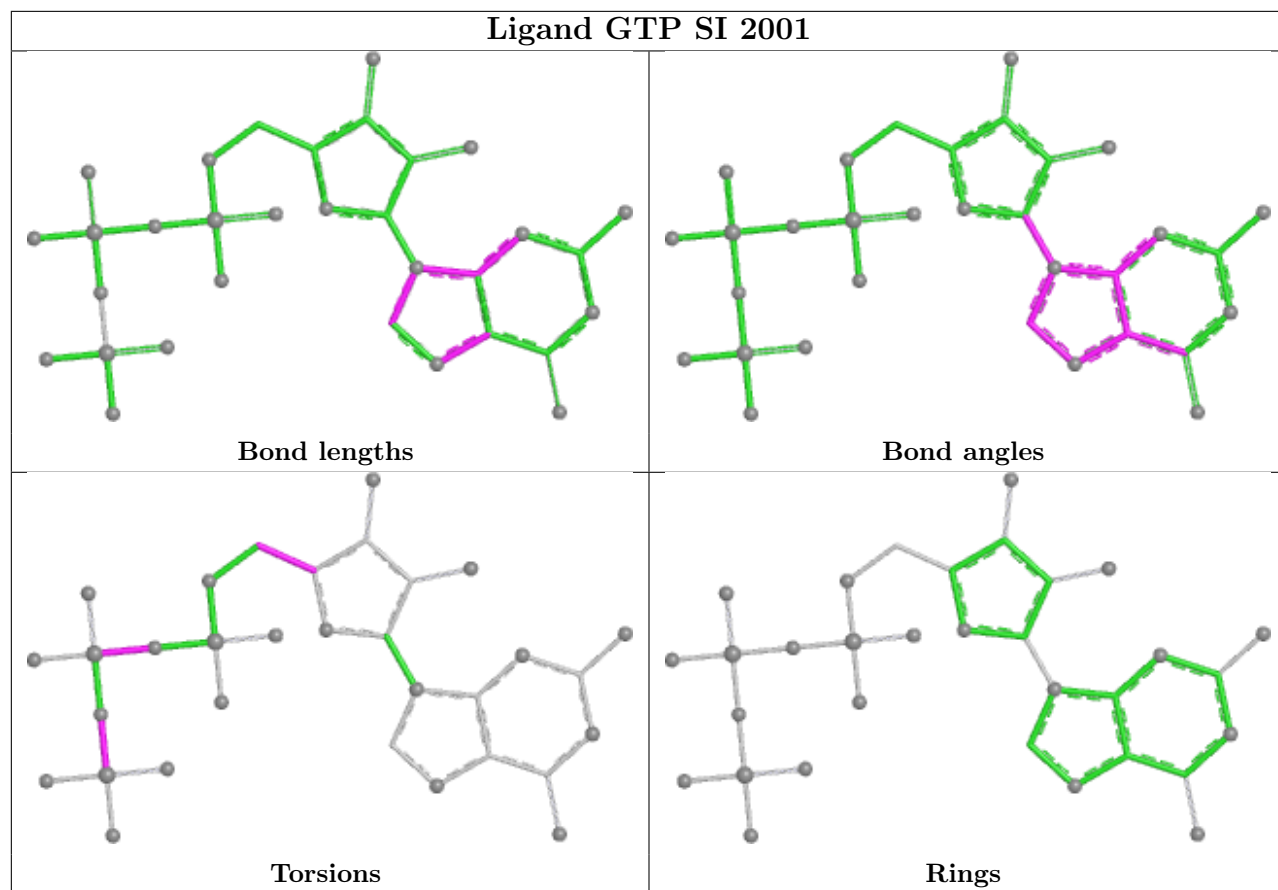
Mol	Chain	Res	Type	Atoms
73	SI	2001	GTP	PB-O3B-PG-O3G
73	SI	2001	GTP	O4'-C4'-C5'-O5'
73	SI	2001	GTP	C3'-C4'-C5'-O5'
73	SI	2001	GTP	PA-O3A-PB-O1B
73	SI	2001	GTP	PB-O3B-PG-O1G
73	SI	2001	GTP	PA-O3A-PB-O2B
71	NH	1300	ATP	PA-O3A-PB-O2B

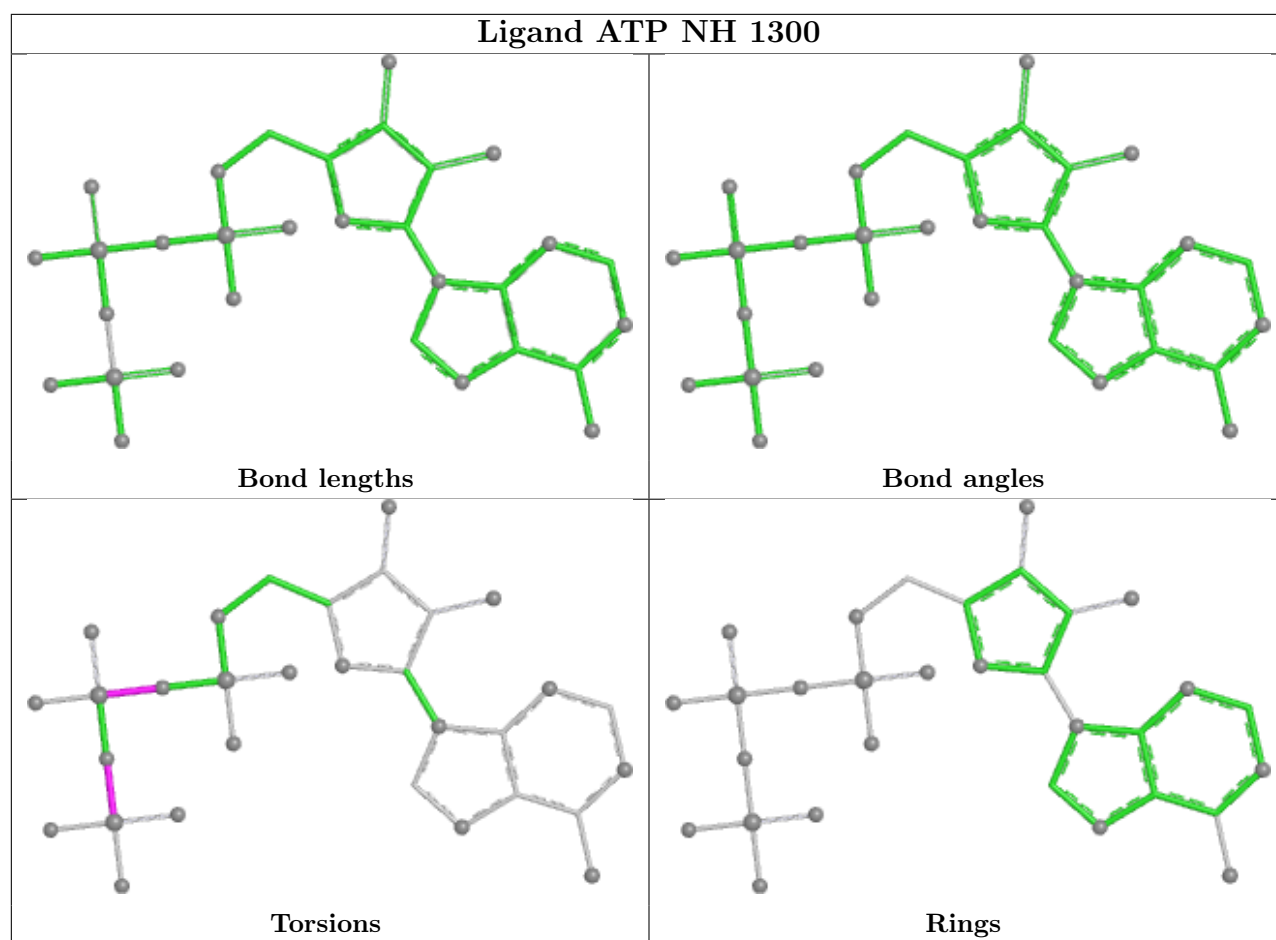
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
73	SI	2001	GTP	1	0
71	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.

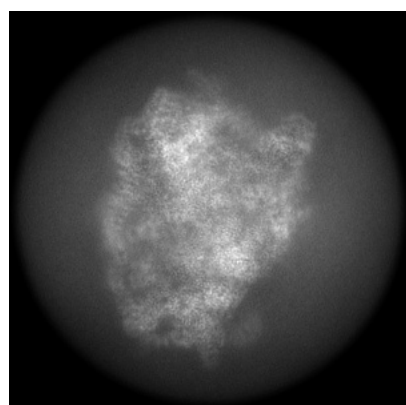
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49078. These allow visual inspection of the internal detail of the map and identification of artifacts.

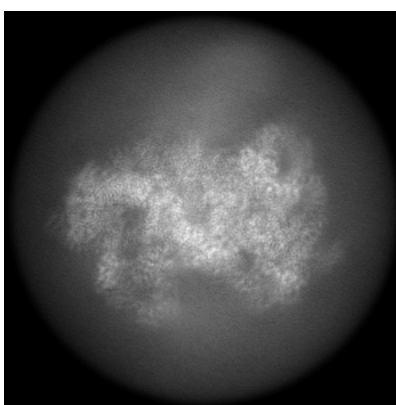
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

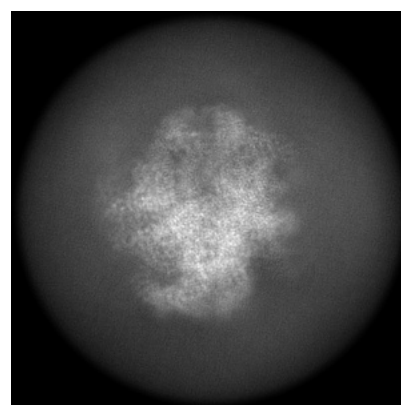
6.1.1 Primary map



X



Y

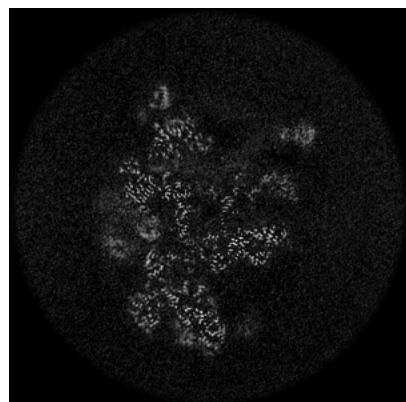


Z

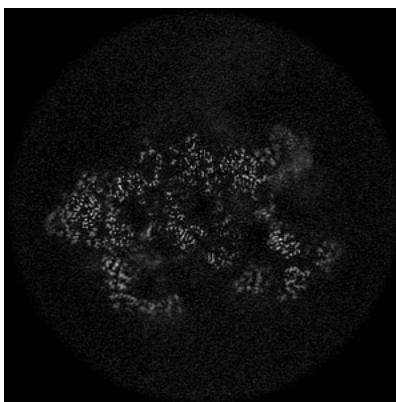
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

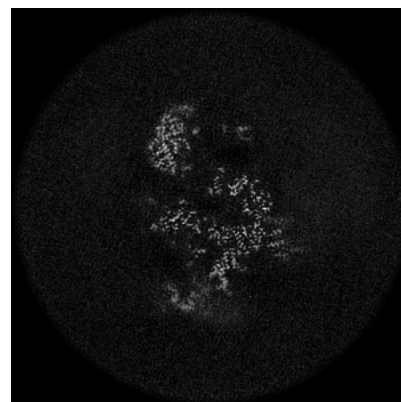
6.2.1 Primary map



X Index: 252



Y Index: 252

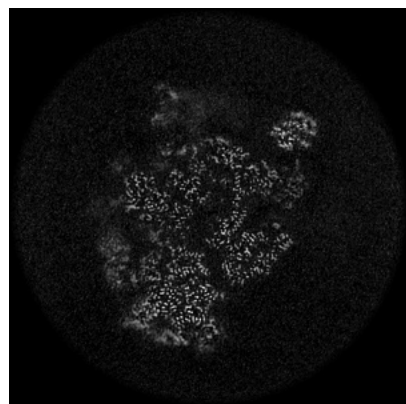


Z Index: 252

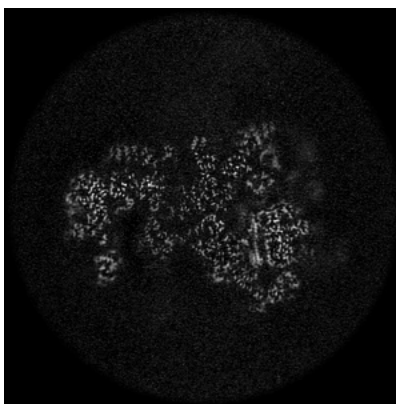
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

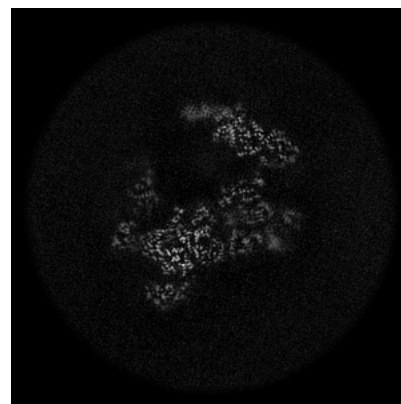
6.3.1 Primary map



X Index: 268



Y Index: 223

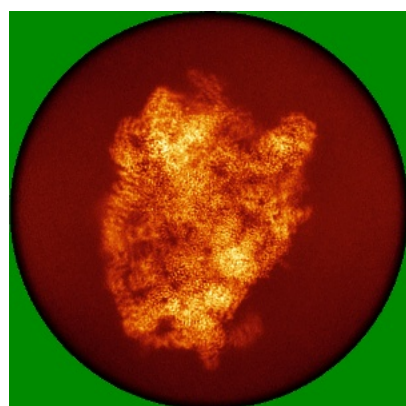


Z Index: 333

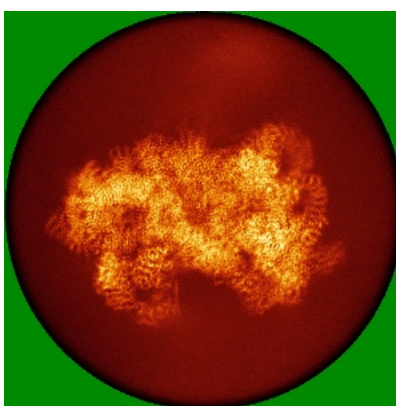
The images above show the largest variance slices of the map in three orthogonal directions.

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

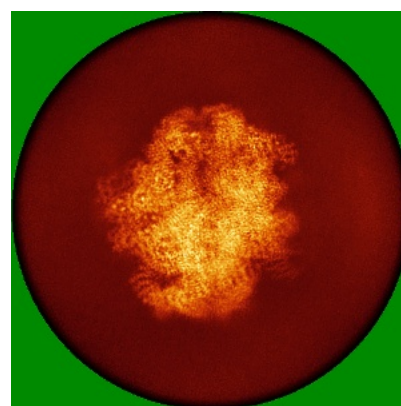
6.4.1 Primary map



X



Y

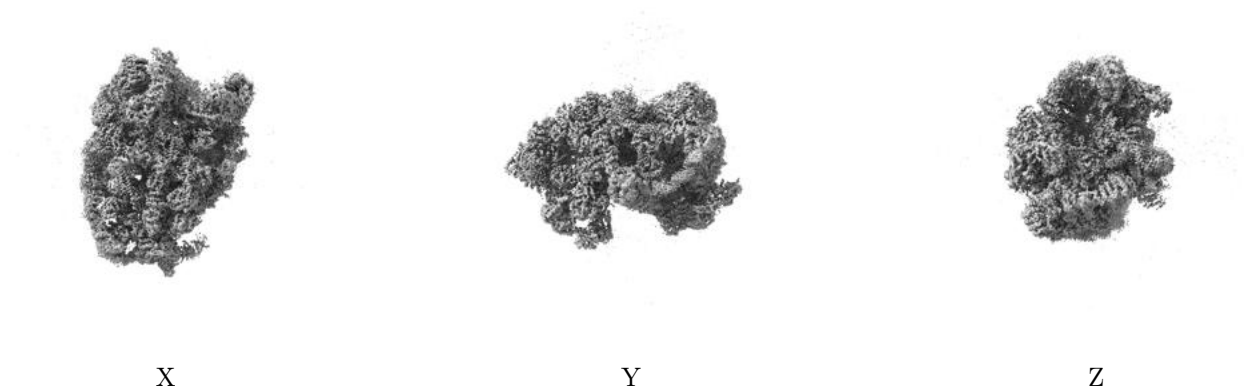


Z

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

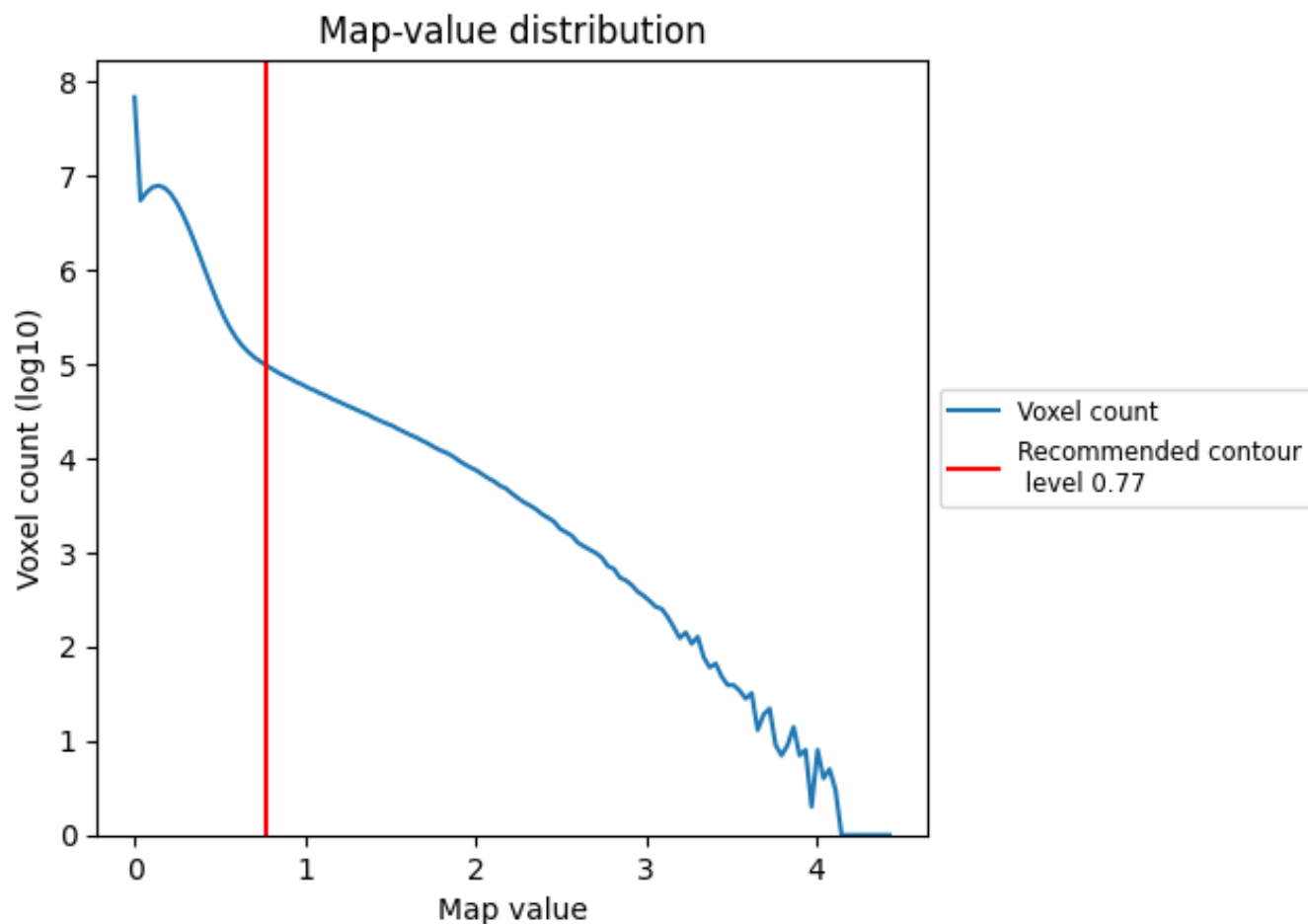
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

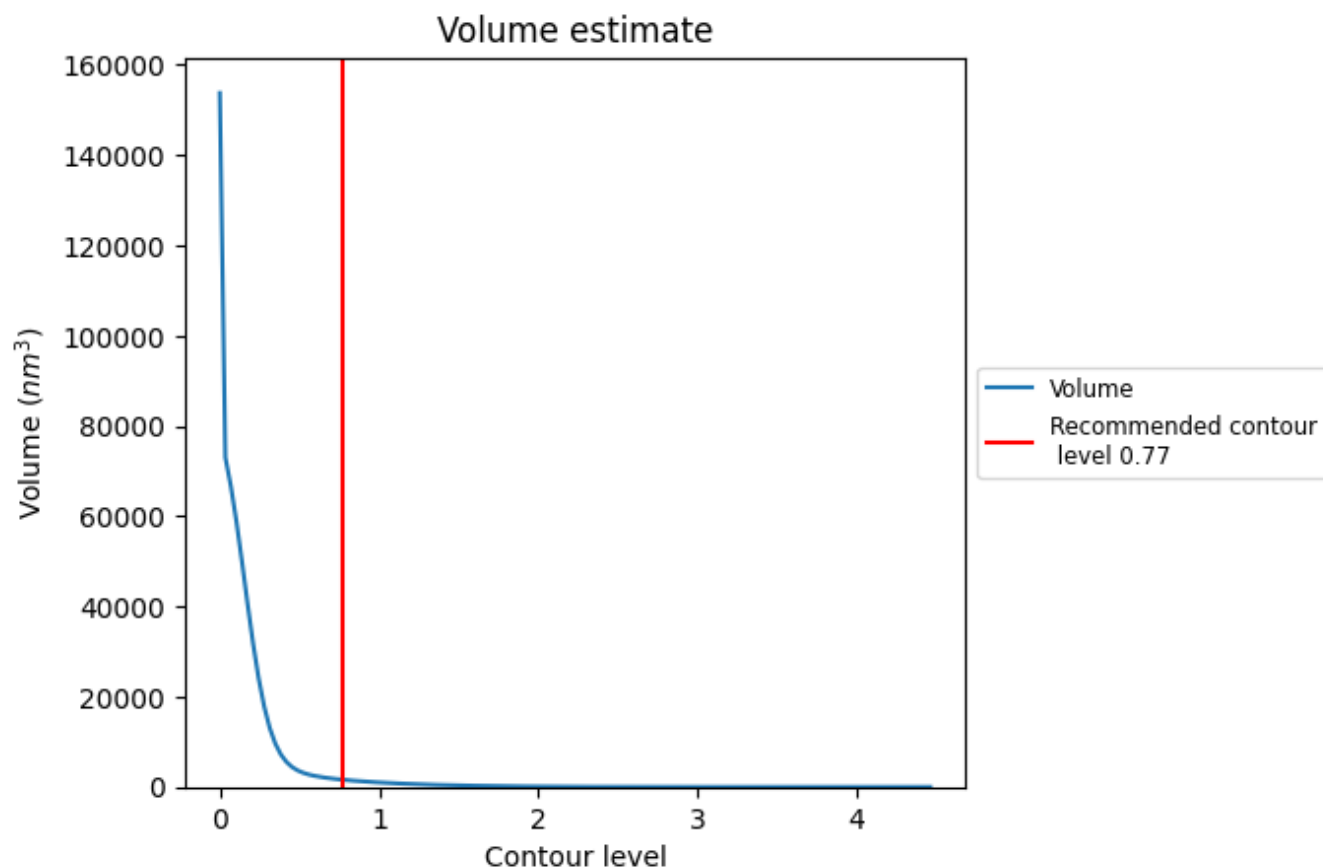
This section contains the results of statistical analysis of the map.

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.

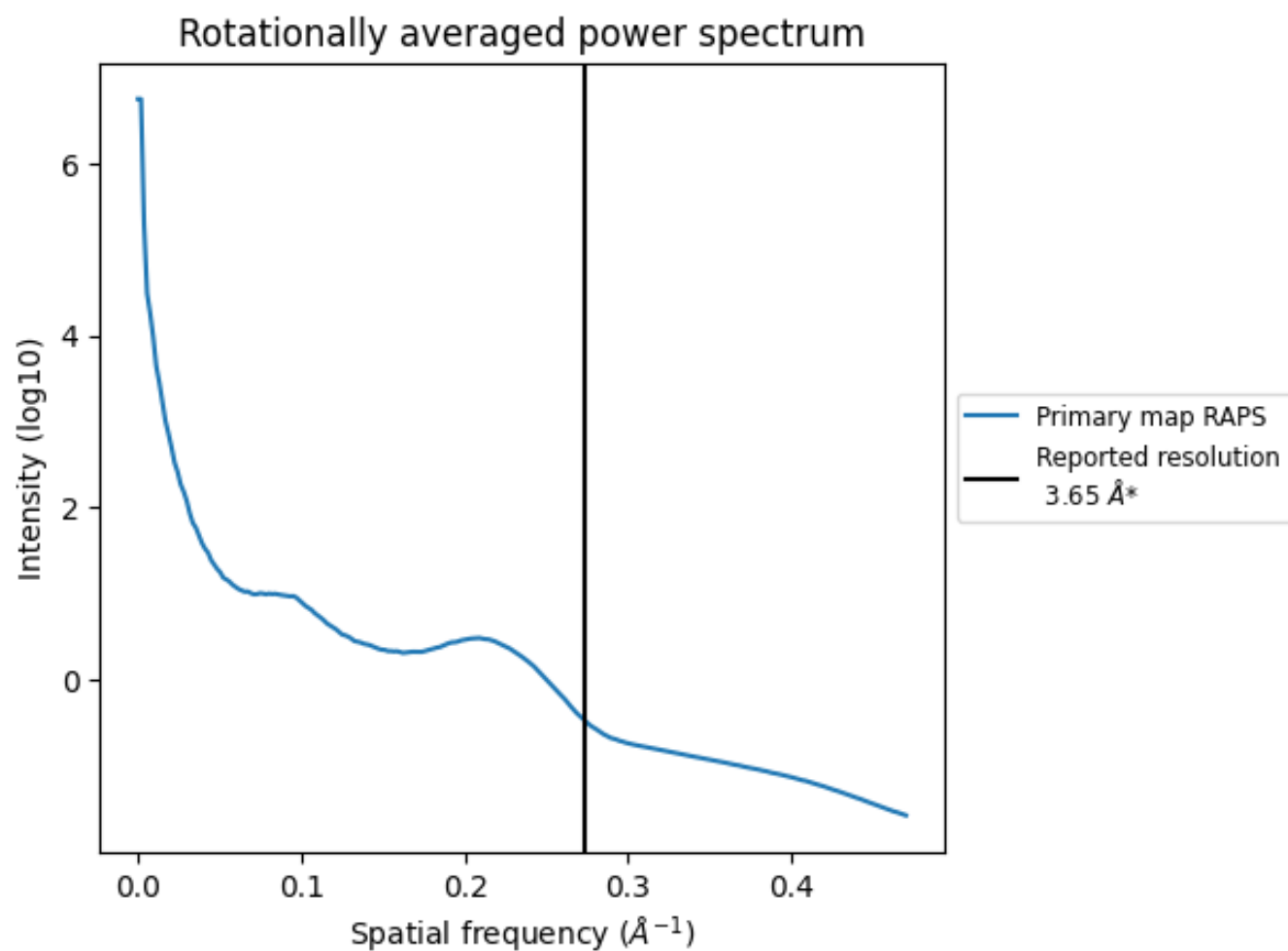
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1608 nm^3 ; this corresponds to an approximate mass of 1453 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 0.274 Å⁻¹

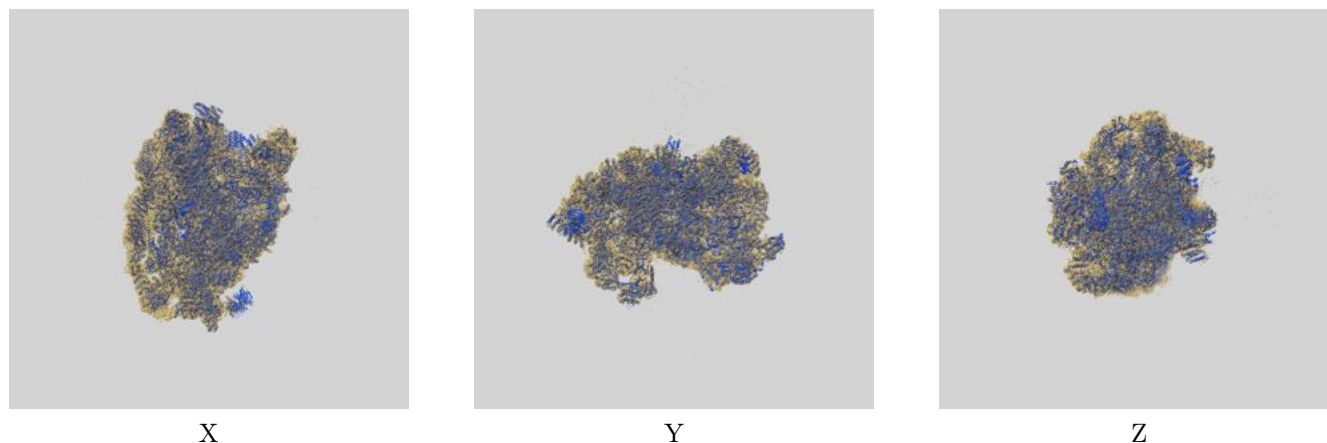
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

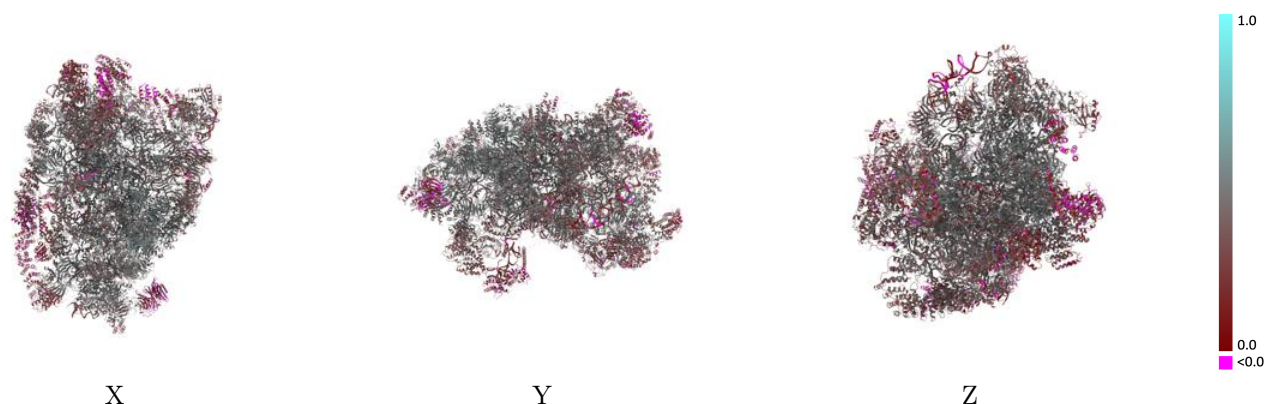
This section contains information regarding the fit between EMDB map EMD-49078 and PDB model 9N6Y. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



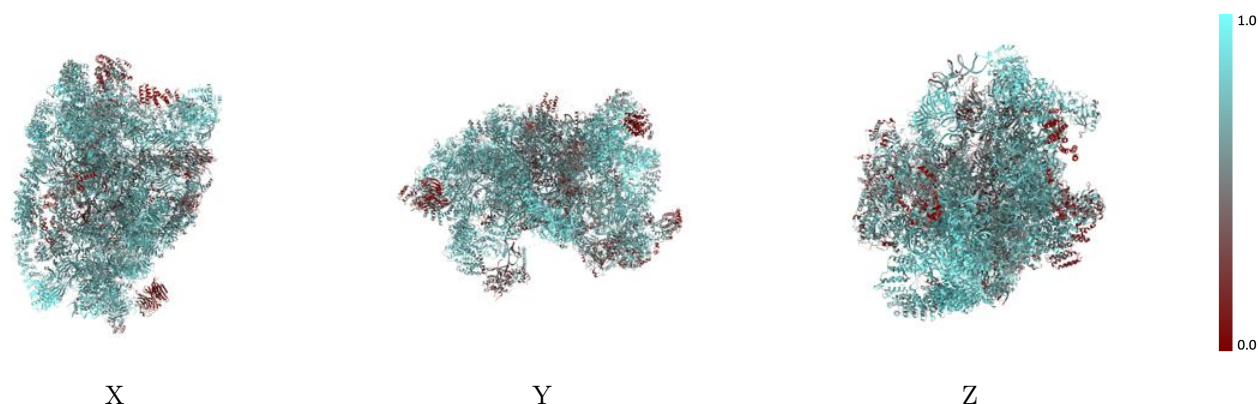
The images above show the 3D surface view of the map at the recommended contour level 0.77 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



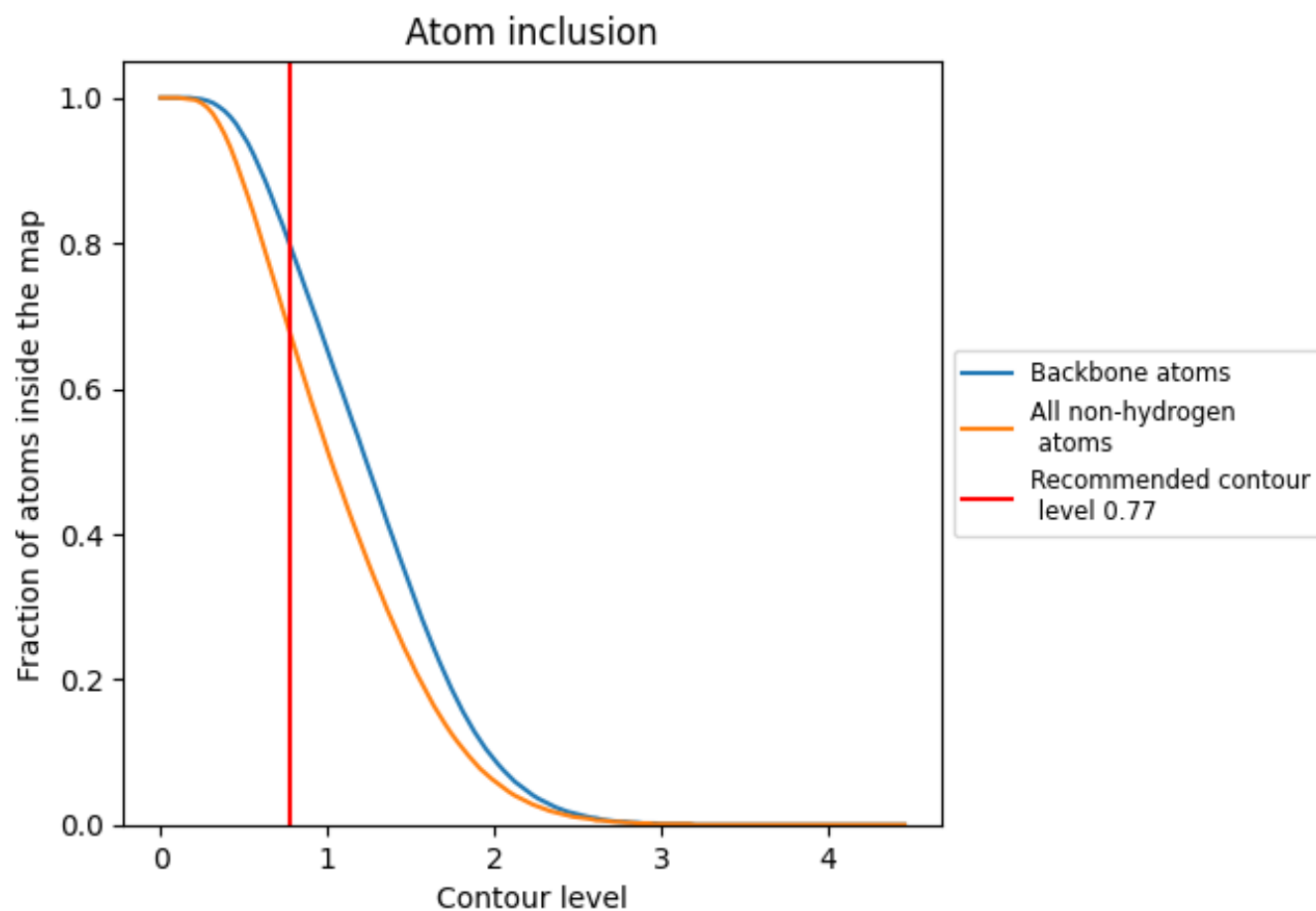
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.77).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 68% 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 (0.77) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6810	 0.4010
L0	 0.6940	 0.3980
L1	 0.8000	 0.3920
L2	 0.7530	 0.4080
L3	 0.0910	 0.2740
L4	 0.7840	 0.4640
L5	 0.6940	 0.4680
L6	 0.8190	 0.4260
L7	 0.6260	 0.3410
L8	 0.8280	 0.4520
L9	 0.6910	 0.4680
LC	 0.6830	 0.4820
LD	 0.7200	 0.4140
LE	 0.7600	 0.4650
LF	 0.8420	 0.4770
LG	 0.6700	 0.4950
LH	 0.7580	 0.4560
LI	 0.3630	 0.2570
LJ	 0.7600	 0.4590
LK	 0.5930	 0.3480
LL	 0.7320	 0.4500
LM	 0.7660	 0.3260
LN	 0.7760	 0.4410
LO	 0.7290	 0.4960
LP	 0.5210	 0.3740
LQ	 0.7750	 0.3980
LR	 0.4890	 0.3680
LS	 0.7410	 0.4780
LT	 0.7040	 0.4830
LU	 0.7650	 0.4930
LV	 0.7650	 0.4400
LW	 0.6730	 0.4870
LX	 0.5620	 0.3450
LY	 0.5860	 0.3440
LZ	 0.7160	 0.5090



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Chain	Atom inclusion	Q-score
NA	 0.5650	 0.3930
NB	 0.5600	 0.3300
NC	 0.3920	 0.2840
ND	 0.6200	 0.3780
NE	 0.5310	 0.4260
NF	 0.7320	 0.4500
NG	 0.5610	 0.4580
NH	 0.8150	 0.4070
NI	 0.6390	 0.3410
NK	 0.5730	 0.4290
NM	 0.6390	 0.4630
NN	 0.4300	 0.2800
NQ	 0.7720	 0.4610
NV	 0.4220	 0.4460
OA	 0.0790	 0.1320
SA	 0.5890	 0.4170
SB	 0.5980	 0.3780
SC	 0.6580	 0.4860
SD	 0.6180	 0.4130
SE	 0.7550	 0.4720
SF	 0.6680	 0.4760
SG	 0.6990	 0.4540
SH	 0.6040	 0.4320
SI	 0.6500	 0.4430
SJ	 0.7400	 0.3440
SK	 0.8000	 0.3900
SL	 0.6600	 0.4920
SM	 0.6340	 0.4770
SN	 0.5540	 0.4290
SP	 0.6980	 0.3340
SQ	 0.4680	 0.4280
SR	 0.6440	 0.4840
SS	 0.4140	 0.3320
ST	 0.6100	 0.3270
SU	 0.7340	 0.3430
SV	 0.6590	 0.3260
SW	 0.4020	 0.3890
SY	 0.6270	 0.4440
SZ	 0.4440	 0.2110