



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:56 AM UTC

PDB ID : 8BR8 / pdb_00008br8
EMDB ID : EMD-16211
Title : Giardia ribosome in POST-T state (A1)
Authors : Majumdar, S.; Emmerich, A.G.; Sanyal, S.
Deposited on : 2022-11-22
Resolution : 3.35 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
MolProbity : 4-5-2 with Phenix2.0
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

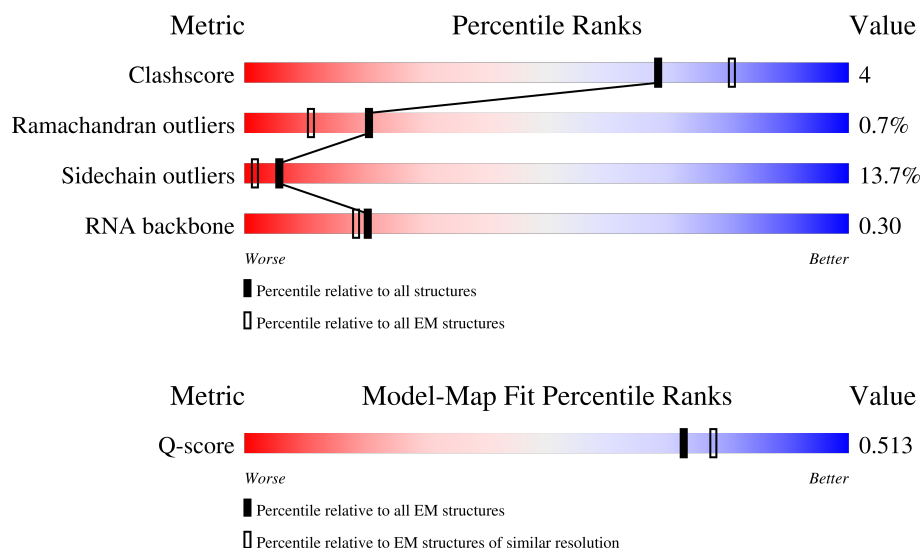
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.35 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	14390 (2.85 - 3.85)

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	LA	251	
2	LB	379	
3	LC	316	

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Mol	Chain	Length	Quality of chain
4	LD	142	
5	LE	121	
6	LF	297	
7	LG	51	
8	LH	235	
9	LI	225	
10	LJ	185	
11	LK	210	
12	LL	173	
13	LM	234	
14	LN	131	
15	LO	204	
16	LP	197	
17	LQ	164	
18	LR	179	
19	LS	196	
20	LT	173	
21	LU	159	
22	LV	124	
23	LW	142	
24	LX	189	
25	LY	141	
26	LZ	135	
27	La	135	
28	Lb	149	

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Mol	Chain	Length	Quality of chain
29	Lc	62	
30	Ld	109	
31	Le	106	
32	Lf	136	
33	Lg	123	
34	Lh	120	
35	Li	124	
36	Lj	90	
37	Lk	89	
38	Ll	77	
39	Ln	217	
40	Lo	25	
41	Lp	106	
42	Lq	94	
43	Ls	127	
44	Lt	2697	
45	Lu	75	
46	SA	245	
47	SB	242	
48	SC	217	
49	SD	248	
50	SE	268	
51	SF	190	
52	SG	248	
53	SH	190	

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Mol	Chain	Length	Quality of chain
54	SI	174	
55	SJ	130	
56	SK	189	
57	SL	134	
58	SM	154	
59	SO	143	
60	SP	154	
61	SQ	145	
62	SR	145	
63	ST	158	
64	SU	137	
65	SV	154	
66	SW	139	
67	SX	126	
68	SY	89	
69	Sb	132	
70	Sc	88	
71	Sd	109	
72	Se	81	
73	Sg	64	
74	Sh	51	
75	Sj	69	
76	St	1454	

2 Entry composition

There are 76 unique types of molecules in this entry. The entry contains 174771 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 protein called Ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	LA	248	Total	C	N	O	S	0	0
			1864	1151	381	320	12		

- Molecule 2 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	LB	377	Total	C	N	O	S	0	0
			2978	1880	564	513	21		

- Molecule 3 is a protein called Ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LC	309	Total	C	N	O	S	0	0
			2412	1516	469	419	8		

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LD	142	Total	C	N	O	P	0	0
			3038	1350	563	983	142		

- Molecule 5 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LE	117	Total	C	N	O	P	0	0
			2502	1116	457	812	117		

- Molecule 6 is a protein called Ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LF	293	Total	C	N	O	S	0	0
			2355	1490	439	418	8		

- Molecule 7 is a protein called Ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	LG	50	Total	C	N	O	0	0
			439	281	94	64		

- Molecule 8 is a protein called Ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LH	213	Total	C	N	O	S	0	0
			1726	1097	314	310	5		

- Molecule 9 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LI	188	Total	C	N	O	S	0	0
			1502	956	276	265	5		

- Molecule 10 is a protein called Ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LJ	184	Total	C	N	O	S	0	0
			1452	917	264	261	10		

- Molecule 11 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LK	156	Total	C	N	O	S	0	0
			1270	798	245	223	4		

- Molecule 12 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LL	167	Total	C	N	O	S	0	0
			1340	845	249	241	5		

- Molecule 13 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LM	201	Total	C	N	O	S	0	0
			1605	999	325	274	7		

- Molecule 14 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LN	130	Total	C	N	O	S	0	0
			1024	649	186	183	6		

- Molecule 15 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LO	203	Total	C	N	O	S	0	0
			1708	1080	357	265	6		

- Molecule 16 is a protein called Ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LP	193	Total	C	N	O	S	0	0
			1570	988	305	265	12		

- Molecule 17 is a protein called Ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LQ	154	Total	C	N	O	S	0	0
			1239	784	240	211	4		

- Molecule 18 is a protein called Ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LR	178	Total	C	N	O	S	0	0
			1402	871	279	243	9		

- Molecule 19 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LS	192	Total	C	N	O	S	0	0
			1592	983	334	270	5		

- Molecule 20 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LT	170	Total	C	N	O	S	0	0
			1423	899	272	243	9		

- Molecule 21 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LU	157	Total	C	N	O	S	0	0
			1264	789	260	208	7		

- Molecule 22 is a protein called Ribosomal L22e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LV	100	Total	C	N	O	S	0	0
			820	523	140	155	2		

- Molecule 23 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LW	132	Total	C	N	O	S	0	0
			1015	641	193	176	5		

- Molecule 24 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LX	63	Total	C	N	O	S	0	0
			538	340	109	82	7		

- Molecule 25 is a protein called Ribosomal protein L23A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LY	115	Total	C	N	O	S	0	0
			931	598	168	162	3		

- Molecule 26 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LZ	133	Total	C	N	O	S	0	0
			1076	665	219	184	8		

- Molecule 27 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	La	119	Total	C	N	O	S	0	0
			957	608	181	163	5		

- Molecule 28 is a protein called Ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Lb	148	Total	C	N	O	S	0	0
			1201	759	240	199	3		

- Molecule 29 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Lc	52	Total	C	N	O	S	0	0
			434	260	99	73	2		

- Molecule 30 is a protein called Ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ld	107	Total	C	N	O	S	0	0
			804	506	141	153	4		

- Molecule 31 is a protein called Ribosomal protein L31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Le	100	Total	C	N	O		0	0
			818	518	158	142			

- Molecule 32 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lf	127	Total	C	N	O	S	0	0
			1050	667	211	166	6		

- Molecule 33 is a protein called Ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lg	98	Total	C	N	O	S	0	0
			778	498	147	130	3		

- Molecule 34 is a protein called Ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lh	95	Total	C	N	O	S	0	0
			765	473	159	129	4		

- Molecule 35 is a protein called Ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Li	122	Total	C	N	O	S	0	0
			983	623	192	163	5		

- Molecule 36 is a protein called Ribosomal protein L36-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lj	89	Total	C	N	O	S	0	0
			731	462	146	119	4		

- Molecule 37 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lk	85	Total	C	N	O	S	0	0
			689	420	148	114	7		

- Molecule 38 is a protein called Ribosomal L38e.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ll	72	Total	C	N	O	S	0	0
			558	353	99	102	4		

- Molecule 39 is a protein called Ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ln	200	Total	C	N	O	S	0	0
			1592	1025	278	284	5		

- Molecule 40 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lo	25	Total	C	N	O	S	0	0
			227	140	57	27	3		

- Molecule 41 is a protein called Ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lp	93	Total	C	N	O	S	0	0
			767	478	159	125	5		

- Molecule 42 is a protein called Ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lq	90	Total	C	N	O	S	0	0
			700	432	143	119	6		

- Molecule 43 is a protein called Ubiquitin/Ribosomal protein L40e.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ls	47	Total	C	N	O	S	0	0
			388	234	83	64	7		

- Molecule 44 is a RNA chain called Large Subunit rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lt	2593	Total	C	N	O	P	0	0
			55643	24727	10311	18012	2593		

- Molecule 45 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lu	57	Total	C	N	O	P	0	0
			1221	546	228	391	56		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SA	196	Total	C	N	O	S	0	0
			1569	1013	274	274	8		

- Molecule 47 is a protein called Ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SB	199	Total	C	N	O	S	0	0
			1529	976	277	272	4		

- Molecule 48 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SC	208	Total	C	N	O	S	0	0
			1648	1038	304	290	16		

- Molecule 49 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SD	231	Total	C	N	O	S	0	0
			1868	1180	349	326	13		

- Molecule 50 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SE	260	Total	C	N	O	S	0	0
			2085	1333	384	356	12		

- Molecule 51 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SF	184	Total	C	N	O	S	0	0
			1429	889	272	259	9		

- Molecule 52 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SG	205	Total	C	N	O	S	0	0
			1617	1017	307	283	10		

- Molecule 53 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SH	184	Total	C	N	O	S	0	0
			1481	948	258	268	7		

- Molecule 54 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SI	173	Total	C	N	O	S	0	0
			1357	850	260	244	3		

- Molecule 55 is a protein called Ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SJ	129	Total	C	N	O	S	0	0
			1031	659	192	177	3		

- Molecule 56 is a protein called Ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SK	176	Total	C	N	O	S	0	0
			1423	889	281	247	6		

- Molecule 57 is a protein called Ribosomal protein S10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SL	98	Total	C	N	O	S	0	0
			802	519	134	146	3		

- Molecule 58 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SM	151	Total	C	N	O	S	0	0
			1251	794	246	205	6		

- Molecule 59 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SO	139	Total	C	N	O	S	0	0
			1080	683	213	181	3		

- Molecule 60 is a protein called Ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SP	150	Total	C	N	O	S	0	0
			1192	758	228	201	5		

- Molecule 61 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SQ	126	Total	C	N	O	S	0	0
			925	569	190	163	3		

- Molecule 62 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SR	101	Total	C	N	O	S	0	0
			831	530	161	132	8		

- Molecule 63 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	ST	151	Total	C	N	O	S	0	0
			1180	736	229	212	3		

- Molecule 64 is a protein called Ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SU	110	Total	C	N	O	S	0	0
			886	550	171	160	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SU	104	THR	ALA	conflict	UNP A8BRG5

- Molecule 65 is a protein called Ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SV	140	Total	C	N	O	S	0	0
			1113	685	226	196	6		

- Molecule 66 is a protein called Ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SW	137	Total	C	N	O	S	0	0
			1071	680	202	186	3		

- Molecule 67 is a protein called Ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SX	100	Total	C	N	O	S	0	0
			794	507	145	137	5		

- Molecule 68 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SY	86	Total	C	N	O	S	0	0
			651	403	120	122	6		

- Molecule 69 is a protein called Ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Sb	119	Total	C	N	O	S	0	0
			945	600	178	161	6		

- Molecule 70 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Sc	75	Total	C	N	O	S	0	0
			597	377	107	107	6		

- Molecule 71 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Sd	98	Total	C	N	O	S	0	0
			796	491	164	134	7		

- Molecule 72 is a protein called Ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Se	80	Total	C	N	O	S	0	0
			629	397	110	116	6		

- Molecule 73 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Sg	63	Total	C	N	O	S	0	0
			505	311	100	92	2		

- Molecule 74 is a protein called Ribosomal protein S29A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sh	50	Total	C	N	O	S	0	0
			417	264	80	67	6		

- Molecule 75 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sj	62	Total	C	N	O	S	0	0
			502	315	104	82	1		

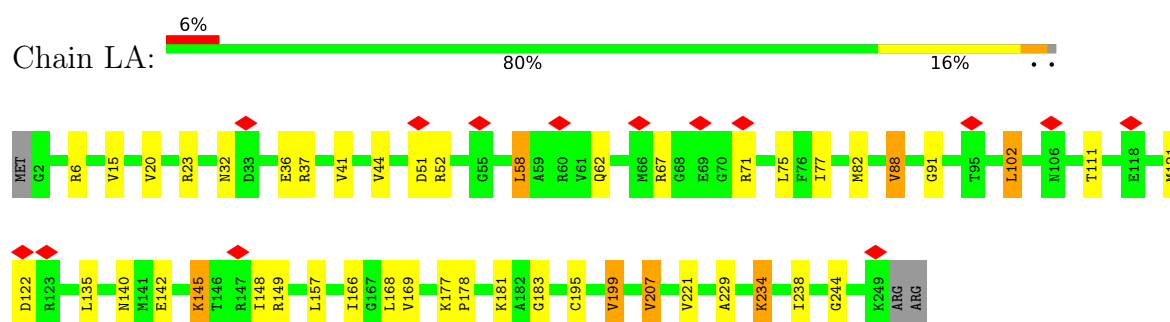
- Molecule 76 is a RNA chain called Small Subunit rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
76	St	1454	31176	13861	5772	10090	1453	0	0

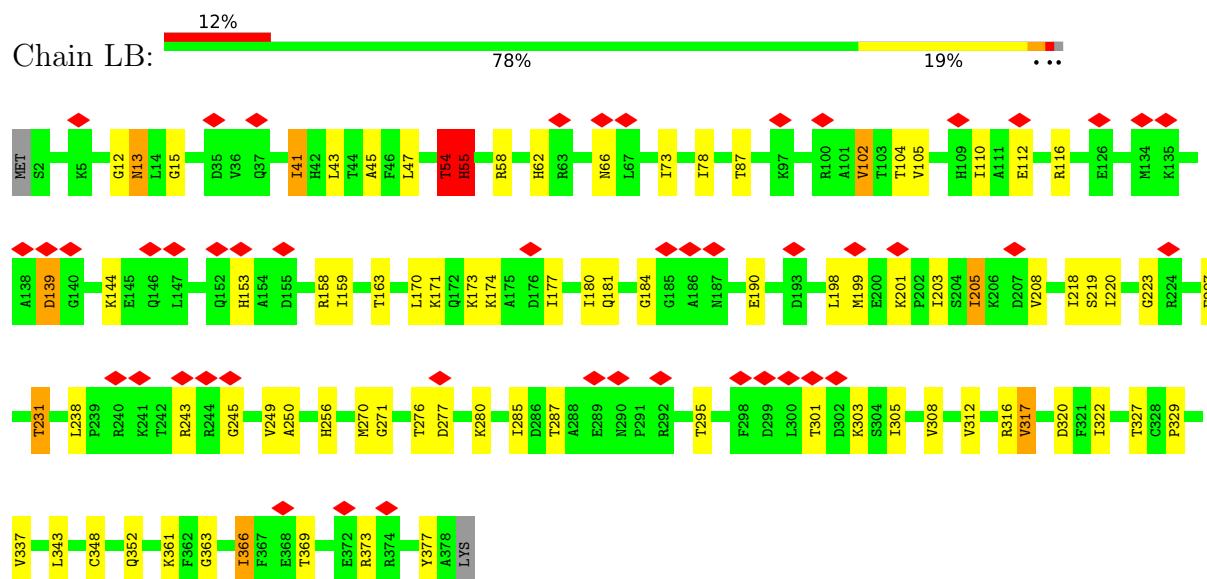
3 Residue-property plots [i](#)

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

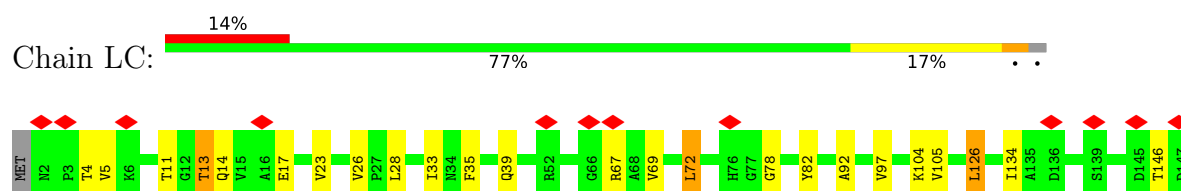
• Molecule 1: Ribosomal protein L2

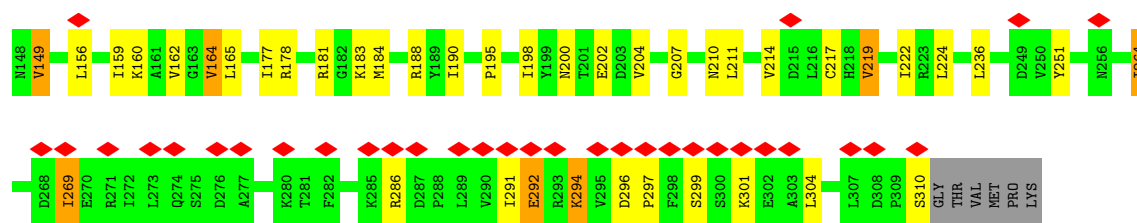


• Molecule 2: Ribosomal protein L3



• Molecule 3: Ribosomal protein L4

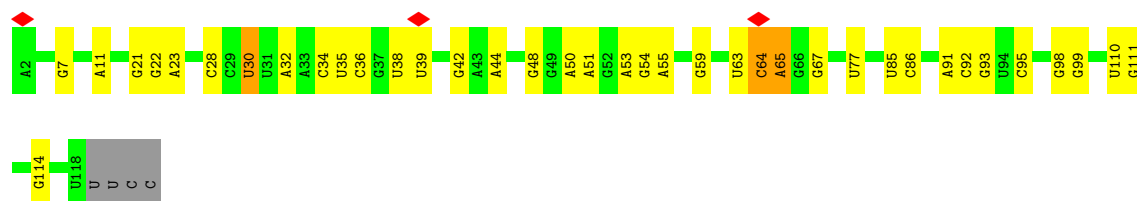




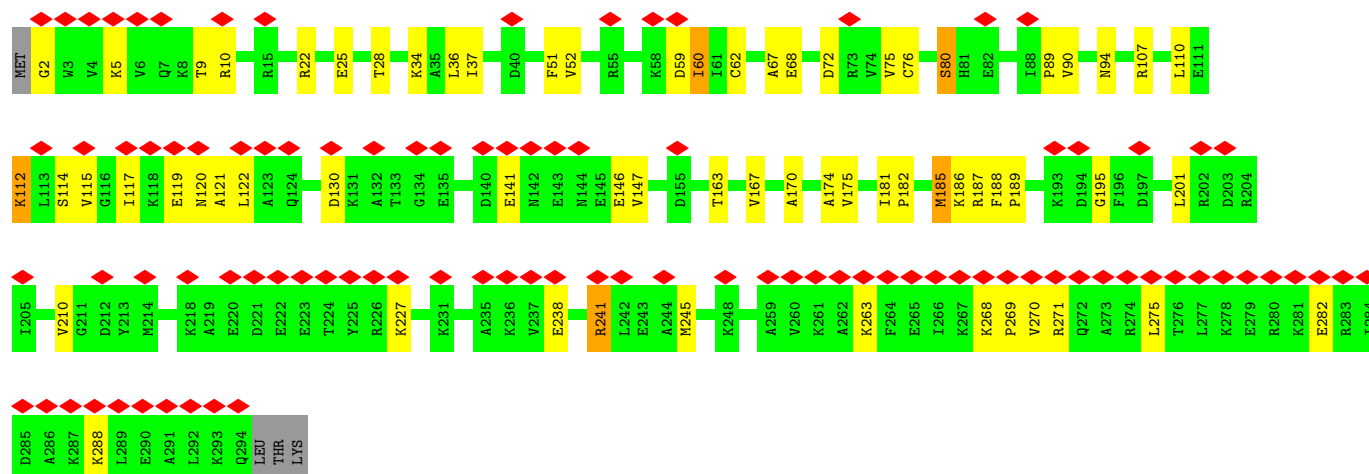
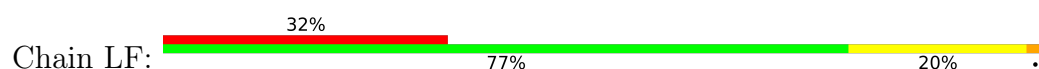
• Molecule 4: 5.8S rRNA



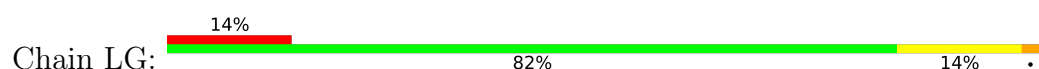
• Molecule 5: 5S rRNA

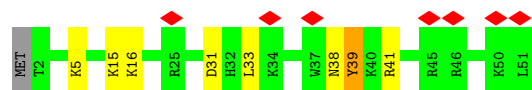


• Molecule 6: Ribosomal protein L5

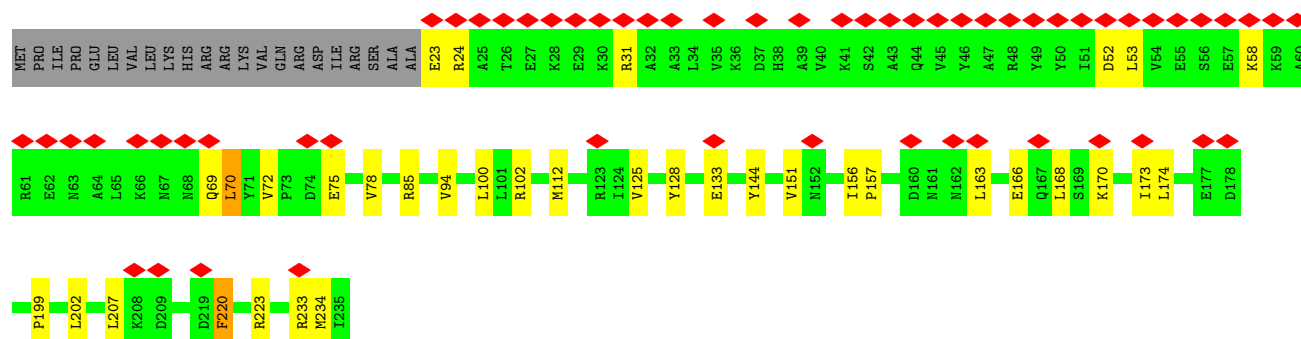
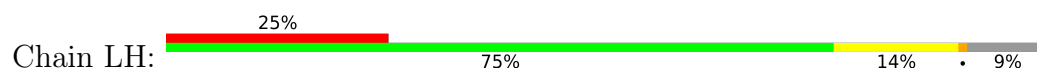


• Molecule 7: Ribosomal protein L39

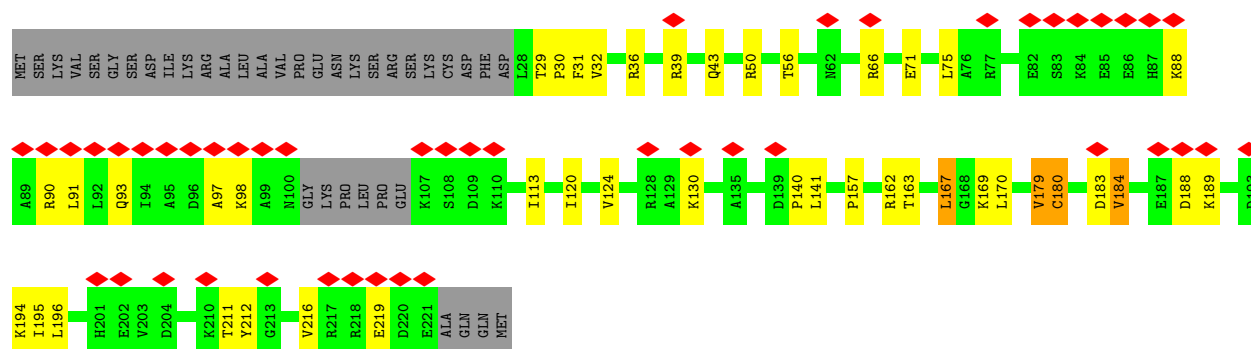




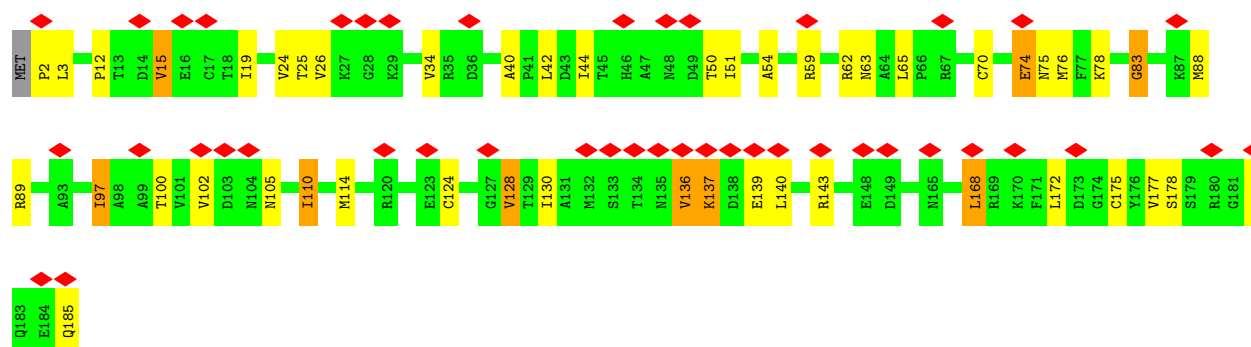
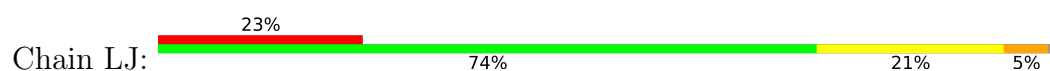
- Molecule 8: Ribosomal protein L7



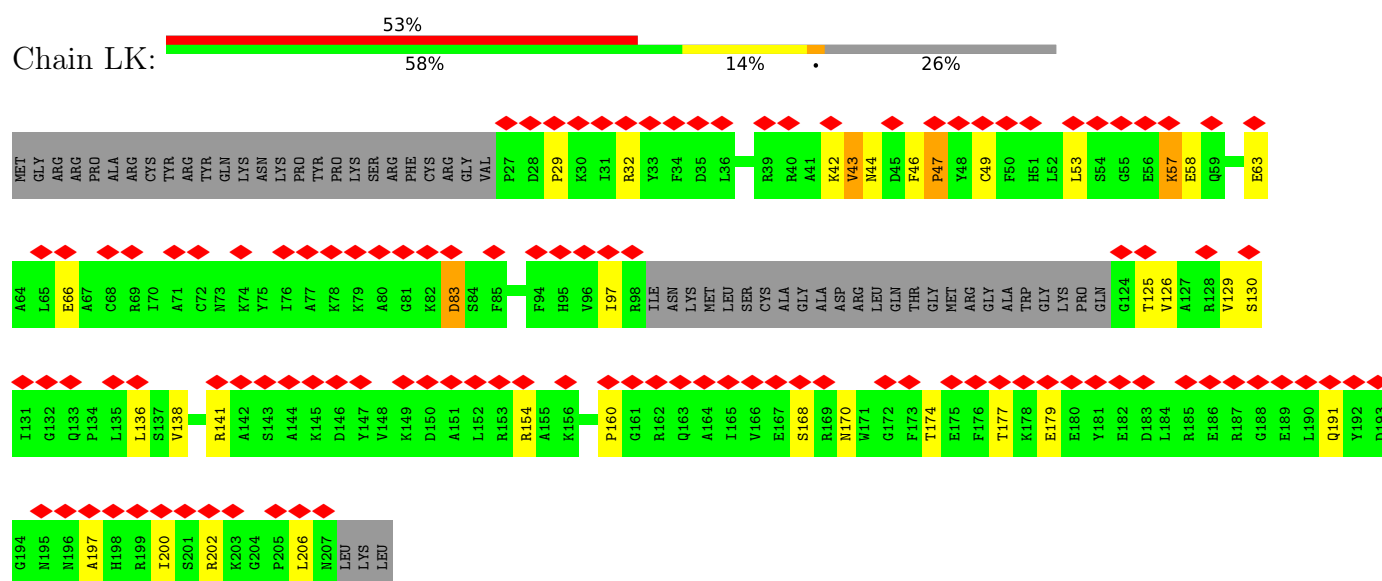
- Molecule 9: 60S ribosomal protein L7a



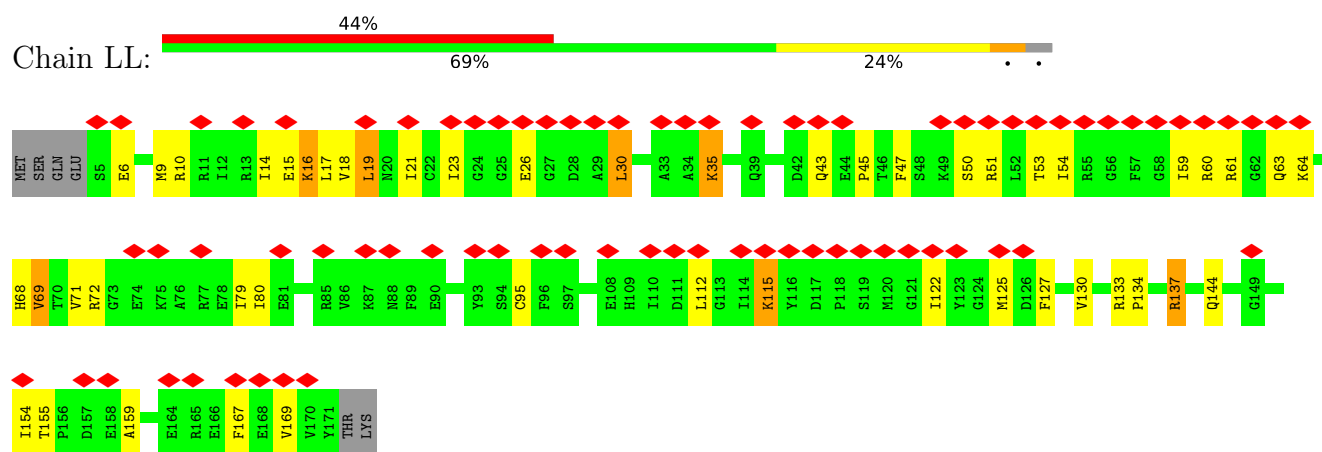
- Molecule 10: Ribosomal protein L6



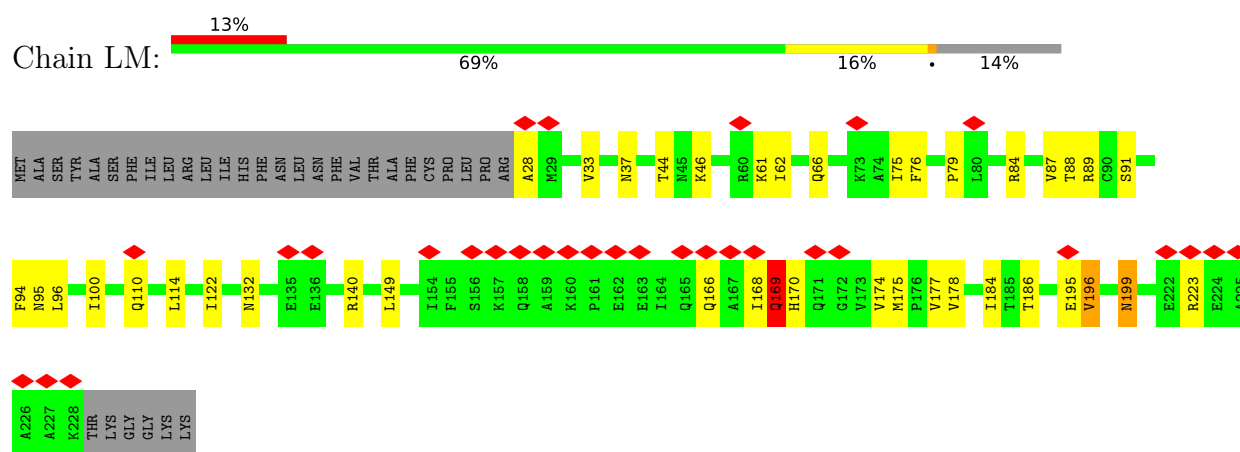
- Molecule 11: Ribosomal protein L10



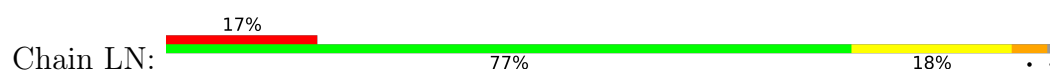
• Molecule 12: Ribosomal protein L11

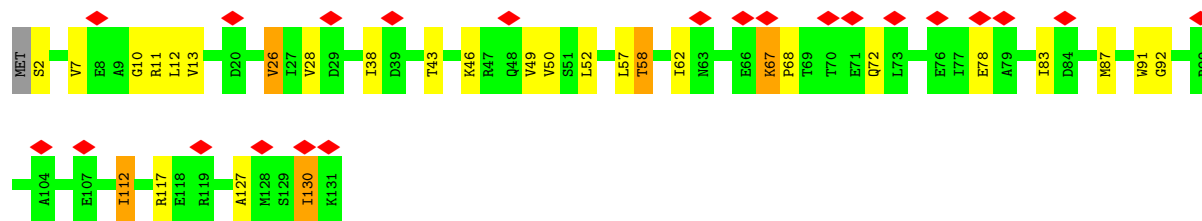


• Molecule 13: 60S ribosomal protein L13

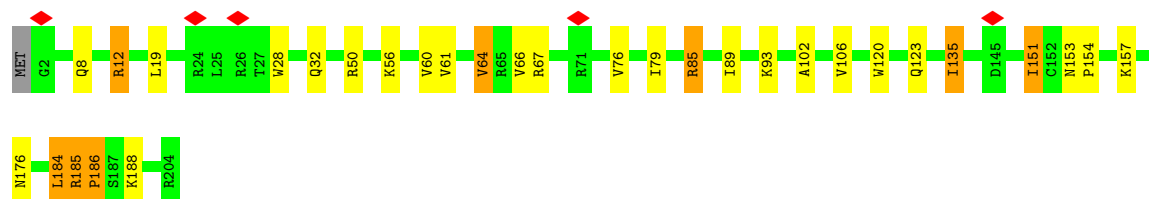
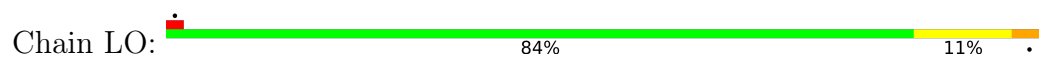


• Molecule 14: Ribosomal protein L14

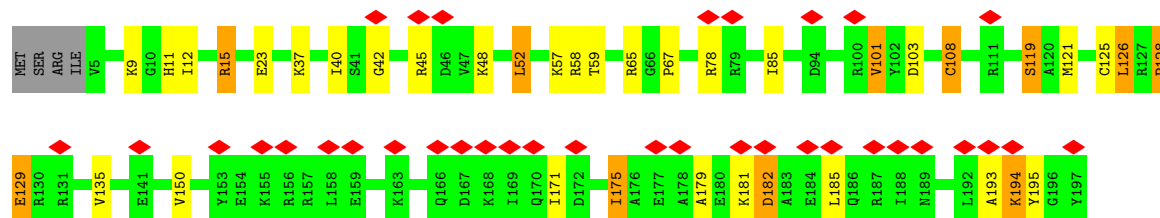
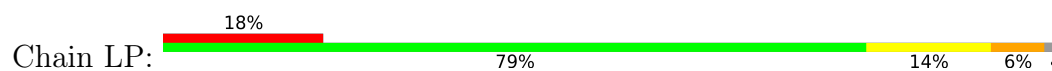




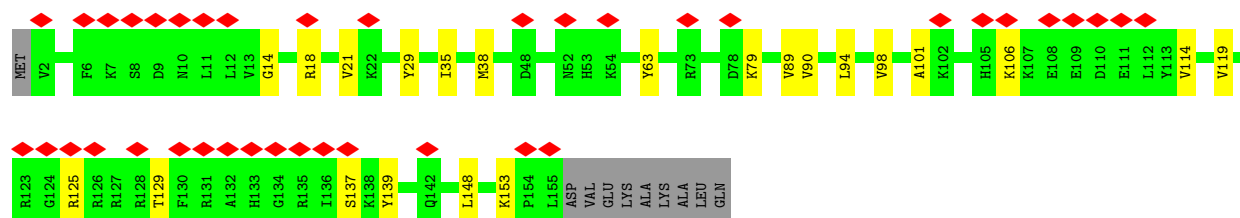
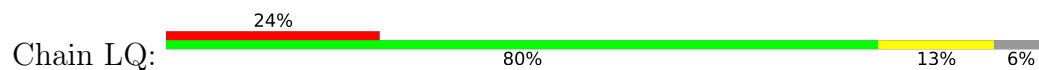
• Molecule 15: Ribosomal protein L15



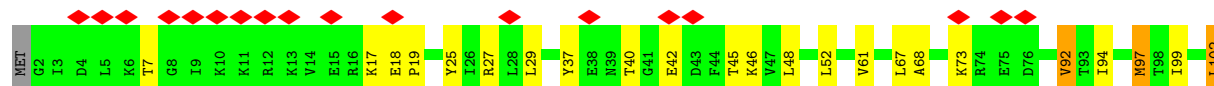
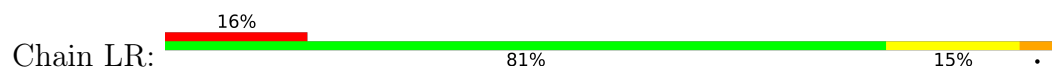
• Molecule 16: Ribosomal protein L13a

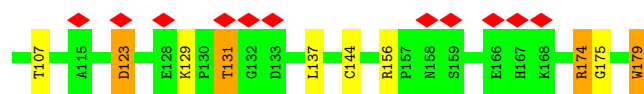


• Molecule 17: Ribosomal protein L17

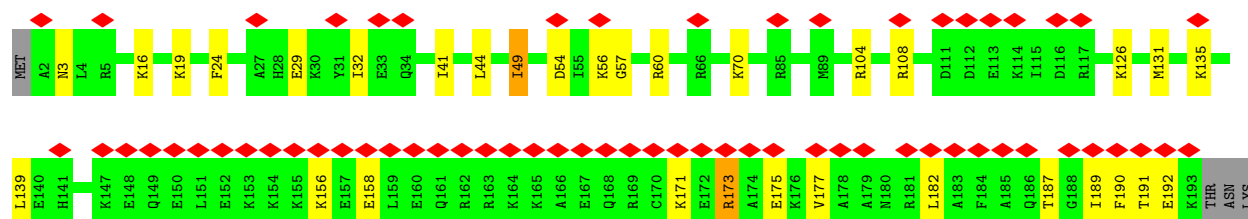
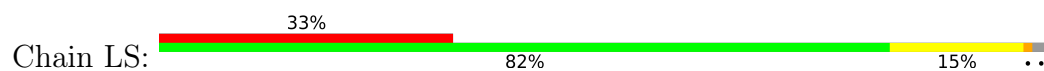


• Molecule 18: Ribosomal protein L18

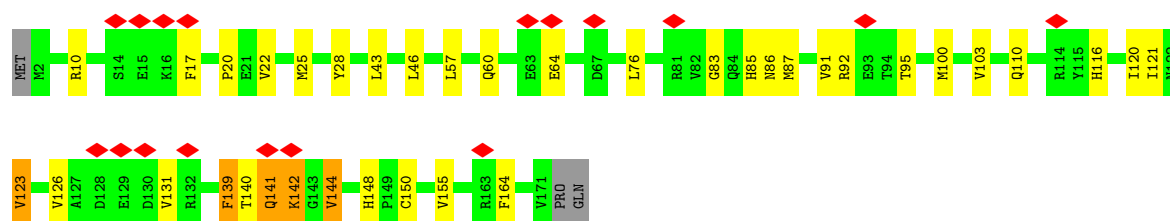
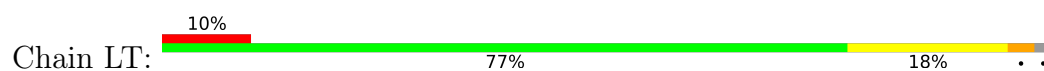




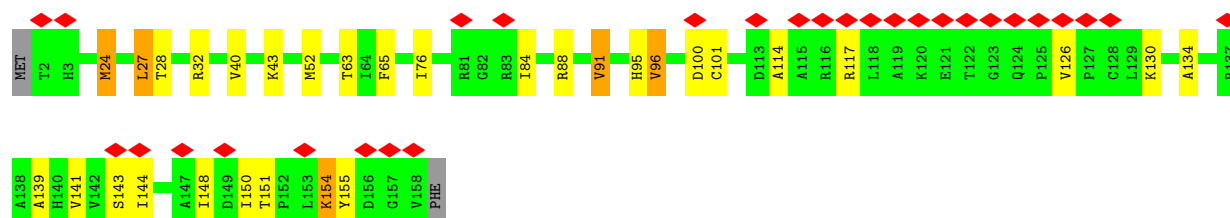
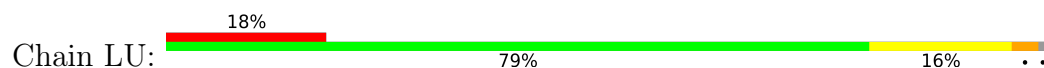
• Molecule 19: Ribosomal protein L19



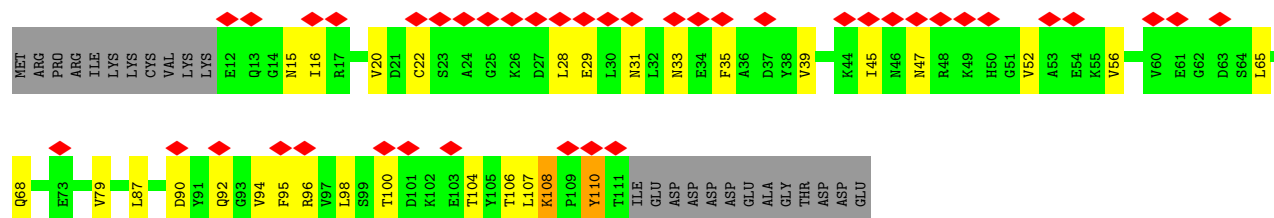
• Molecule 20: 60S ribosomal protein L18a



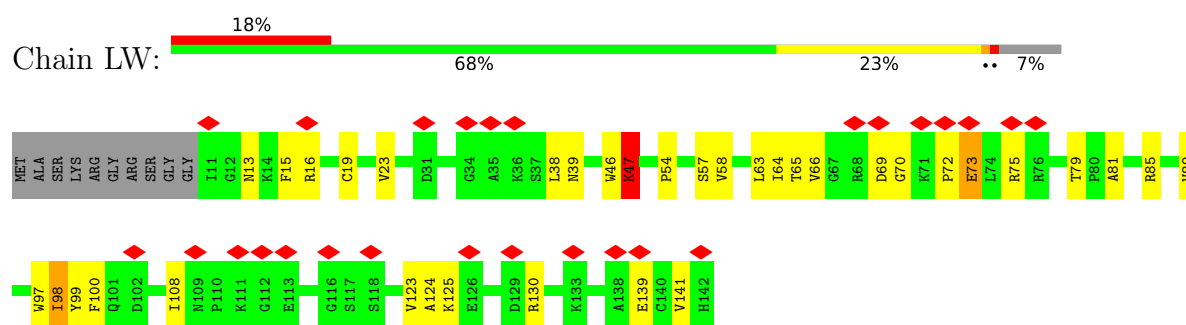
• Molecule 21: Ribosomal protein L21



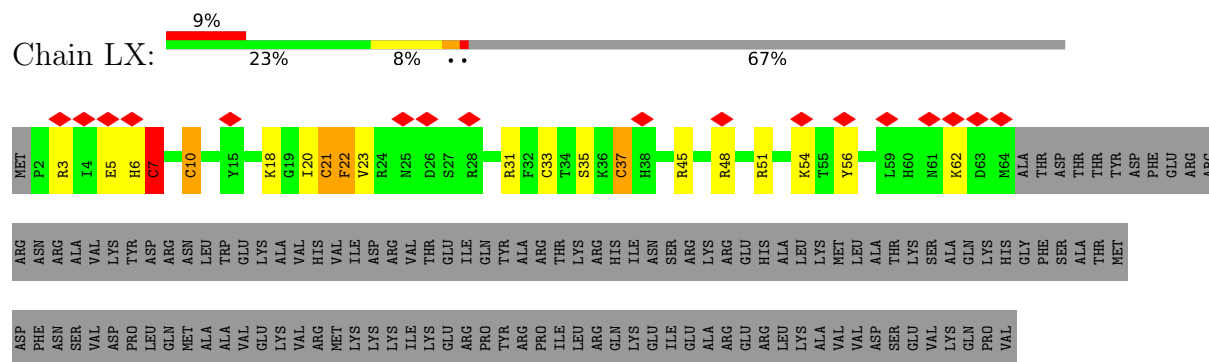
• Molecule 22: Ribosomal L22e



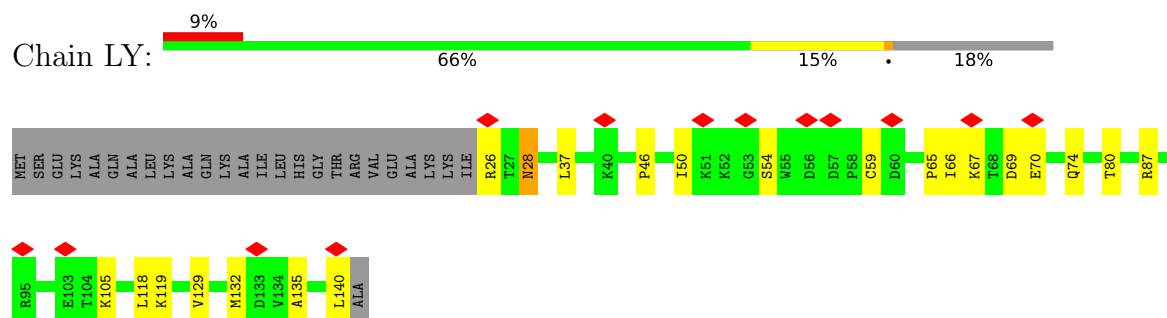
• Molecule 23: Ribosomal protein L23



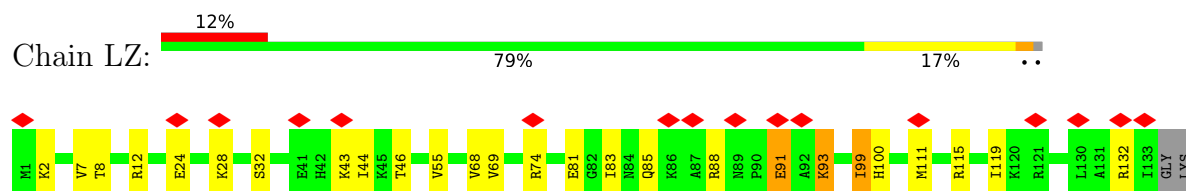
• Molecule 24: Ribosomal protein L24



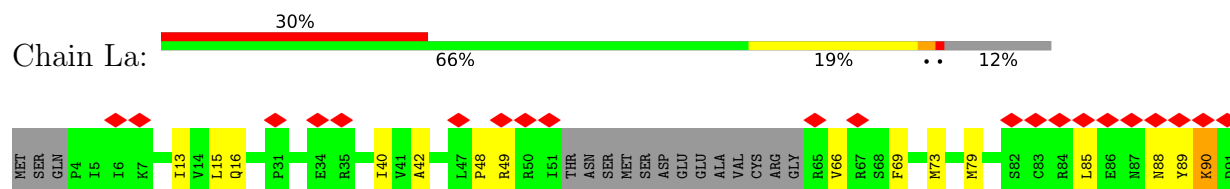
• Molecule 25: Ribosomal protein L23A

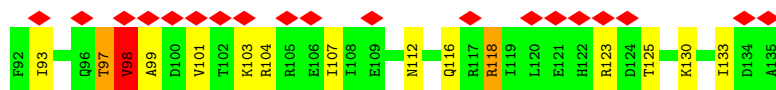


• Molecule 26: Ribosomal protein L26

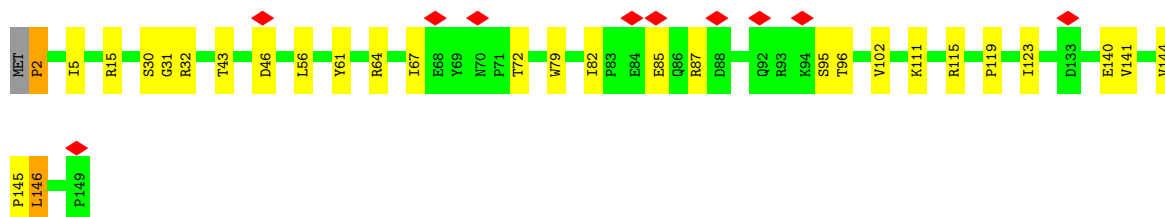
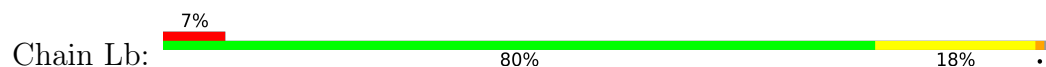


• Molecule 27: 60S ribosomal protein L27

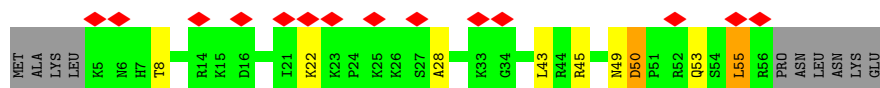




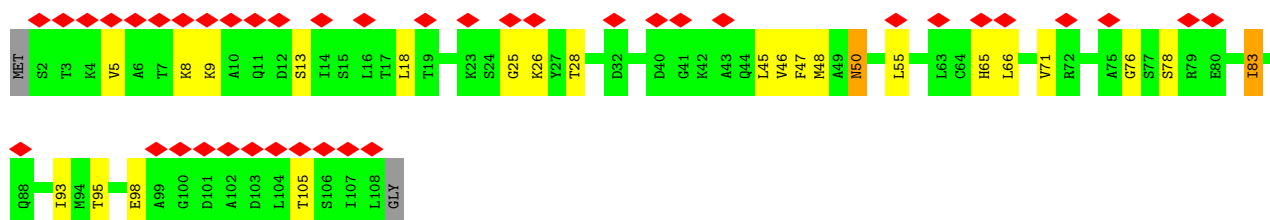
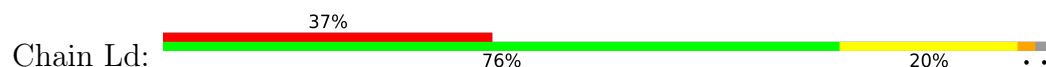
- Molecule 28: Ribosomal protein L27a



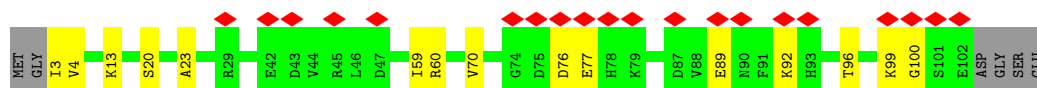
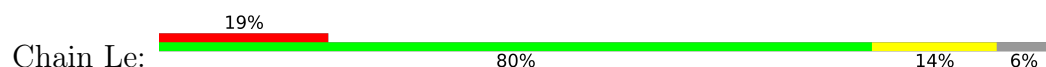
- Molecule 29: 60S ribosomal protein L29



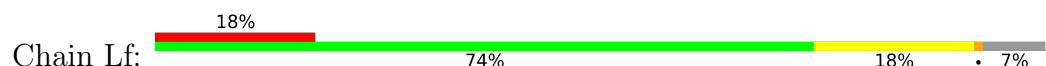
- Molecule 30: Ribosomal protein L30

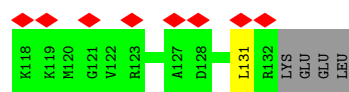


- Molecule 31: Ribosomal protein L31B

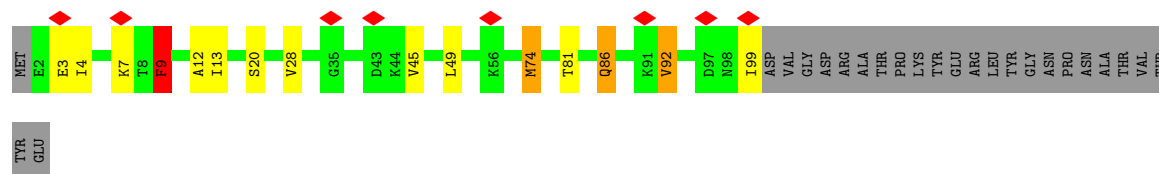


- Molecule 32: Ribosomal protein L32

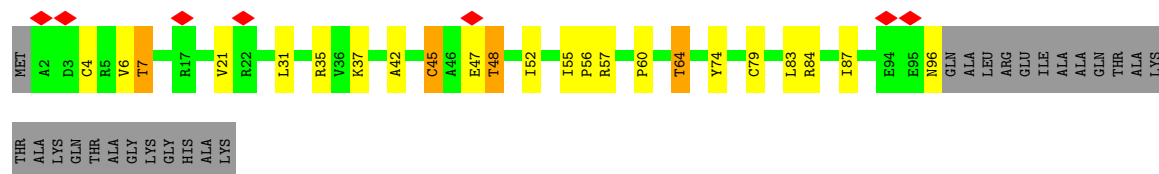




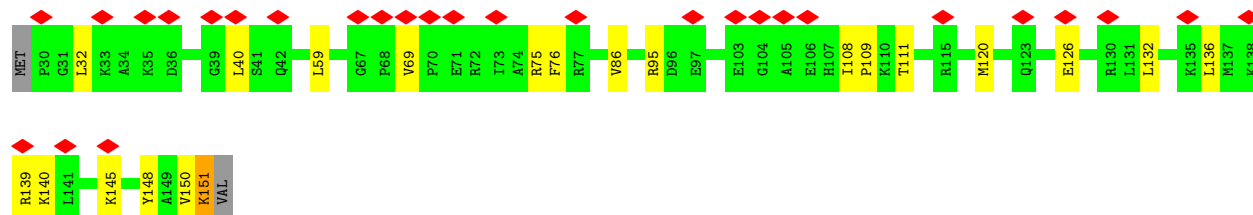
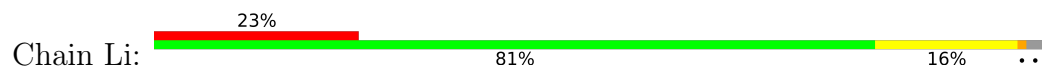
- Molecule 33: Ribosomal protein L35a



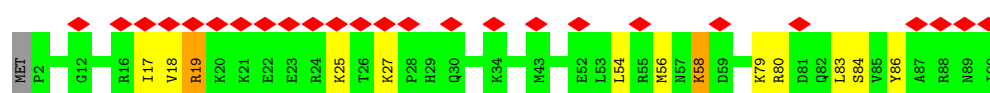
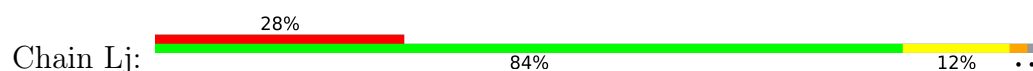
- Molecule 34: Ribosomal protein L34



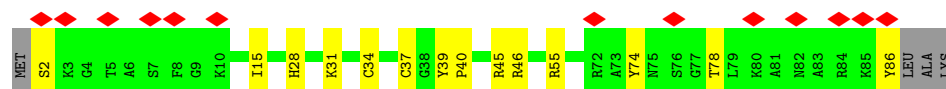
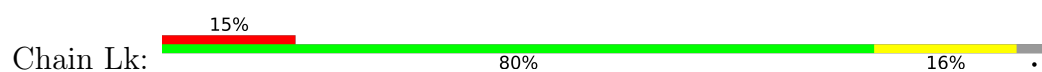
- Molecule 35: Ribosomal protein L29



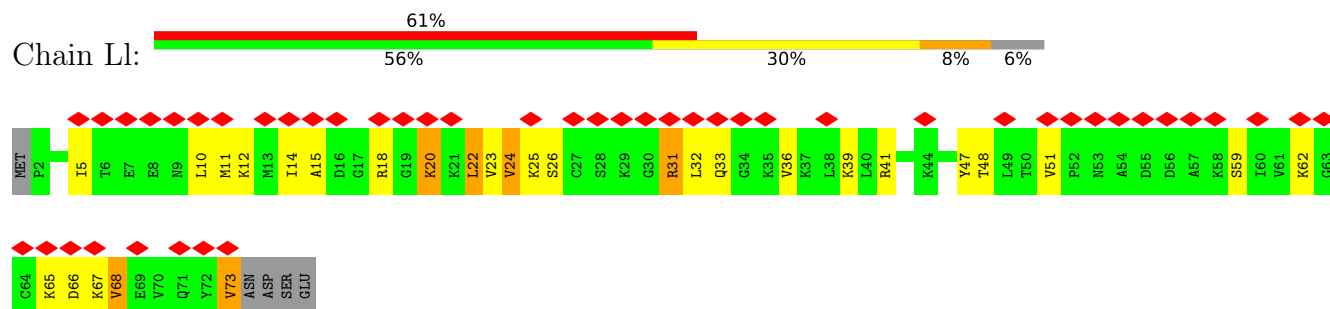
- Molecule 36: Ribosomal protein L36-1



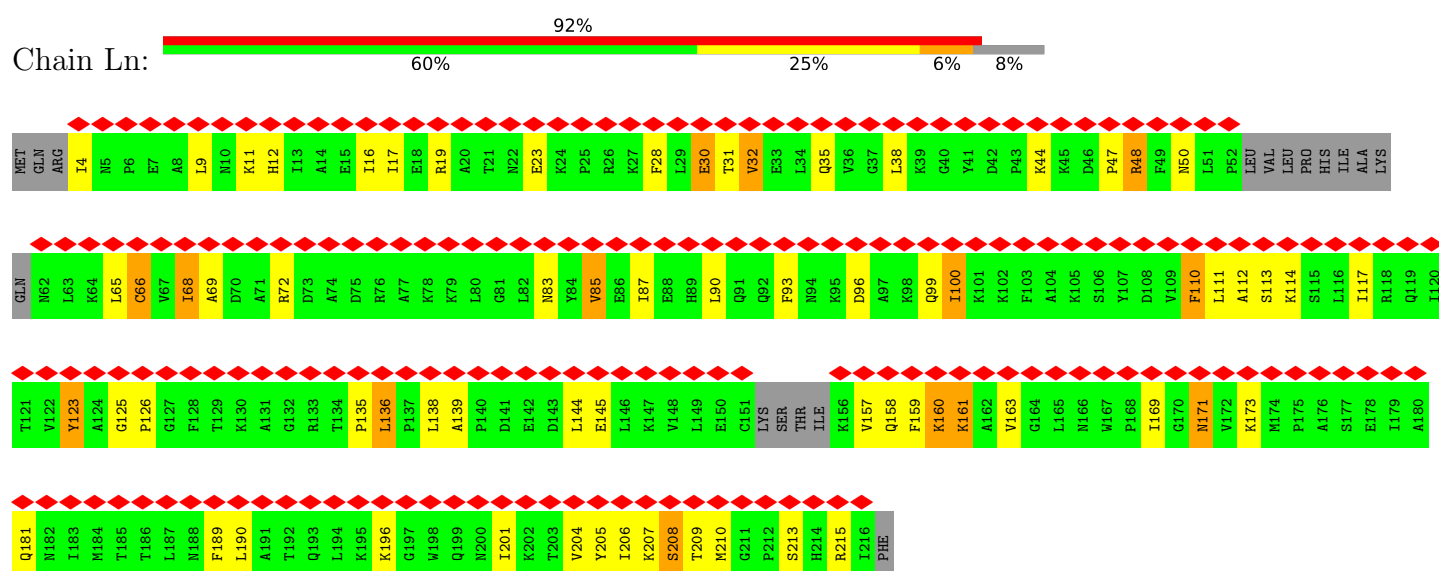
- Molecule 37: Ribosomal protein L37



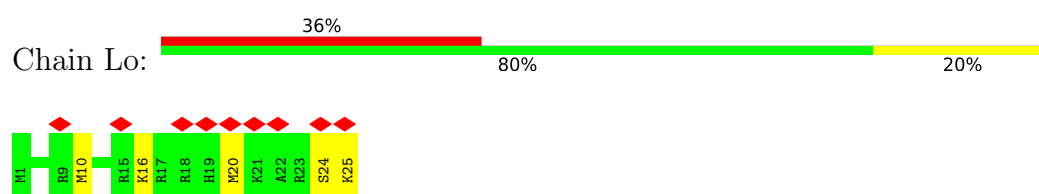
- Molecule 38: Ribosomal L38e



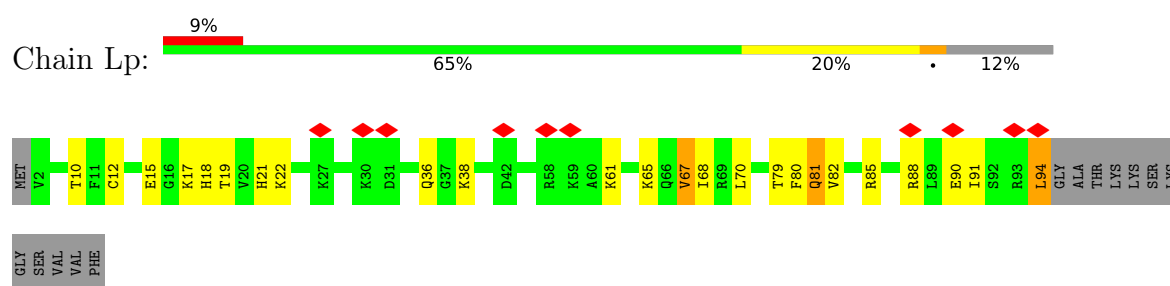
- Molecule 39: Ribosomal protein L10a



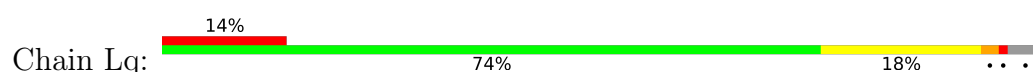
- Molecule 40: 60S ribosomal protein L41

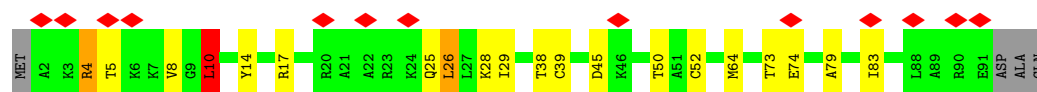


- Molecule 41: Ribosomal protein L44

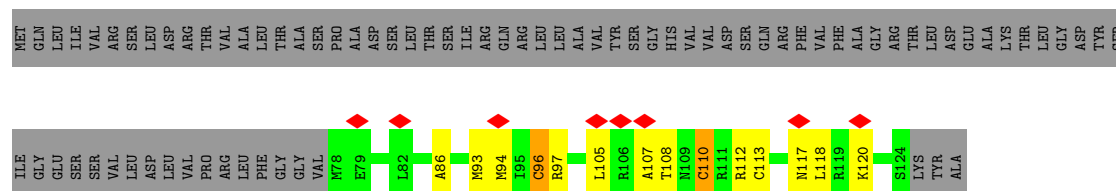


- Molecule 42: Ribosomal protein L37a

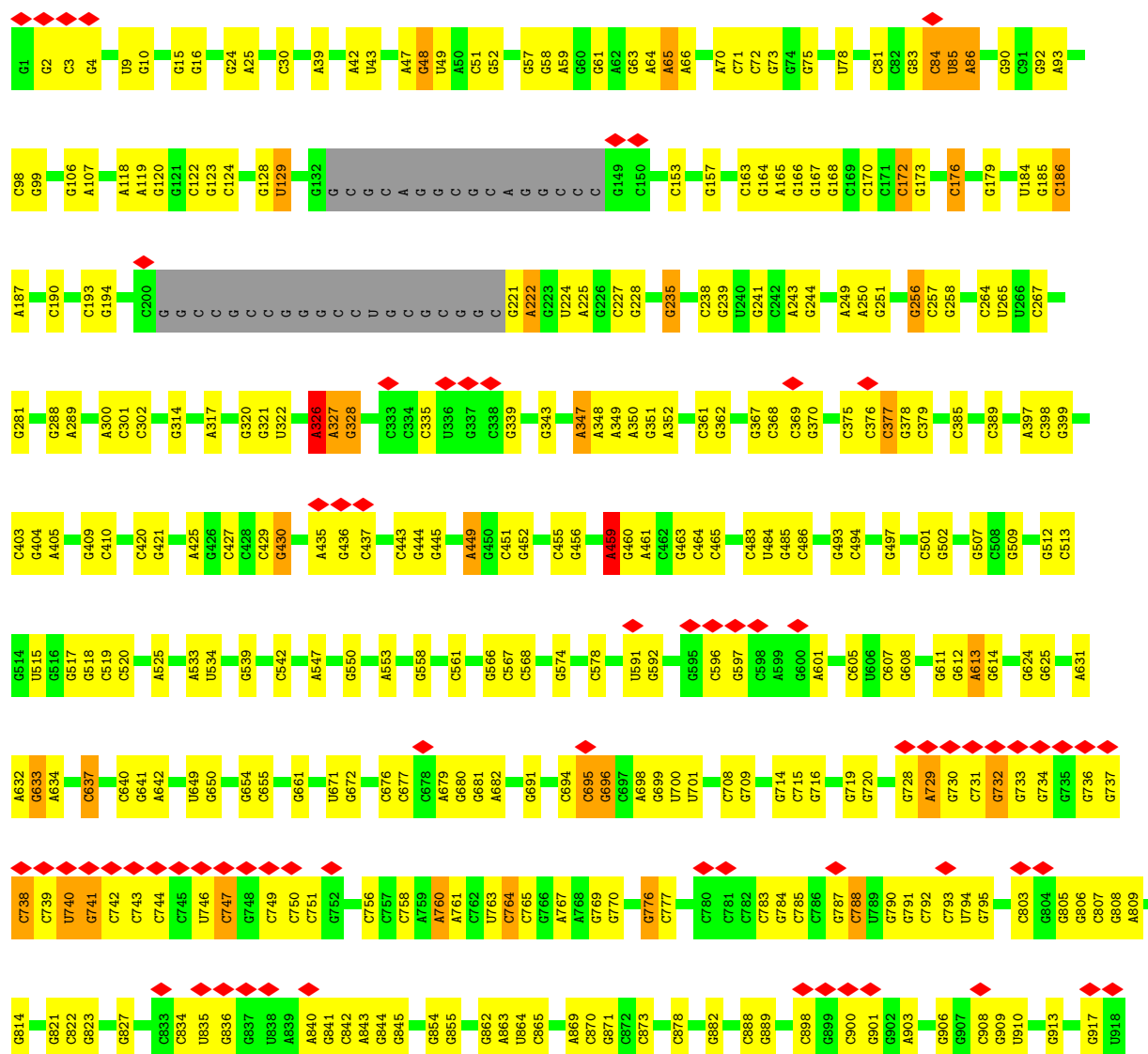


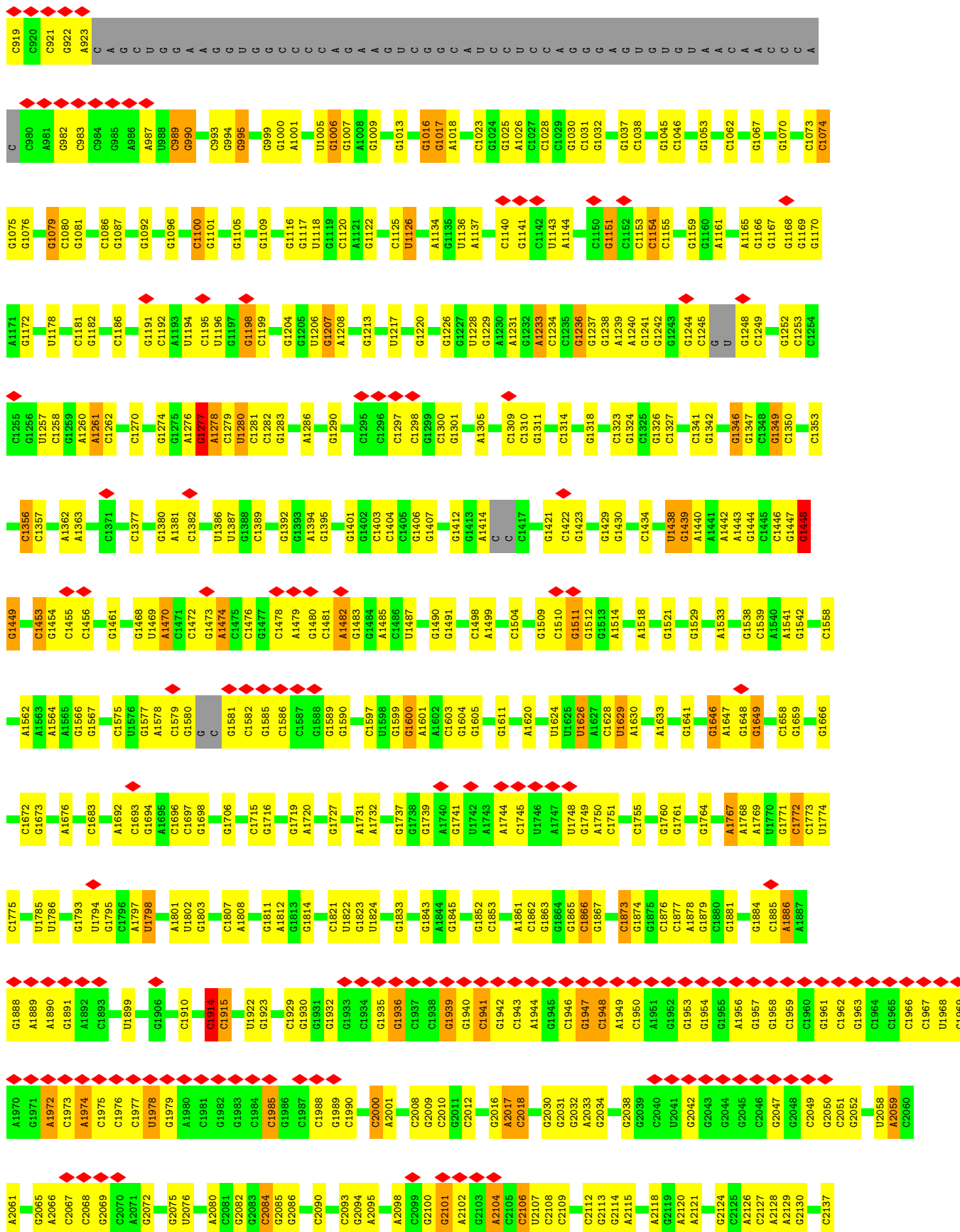


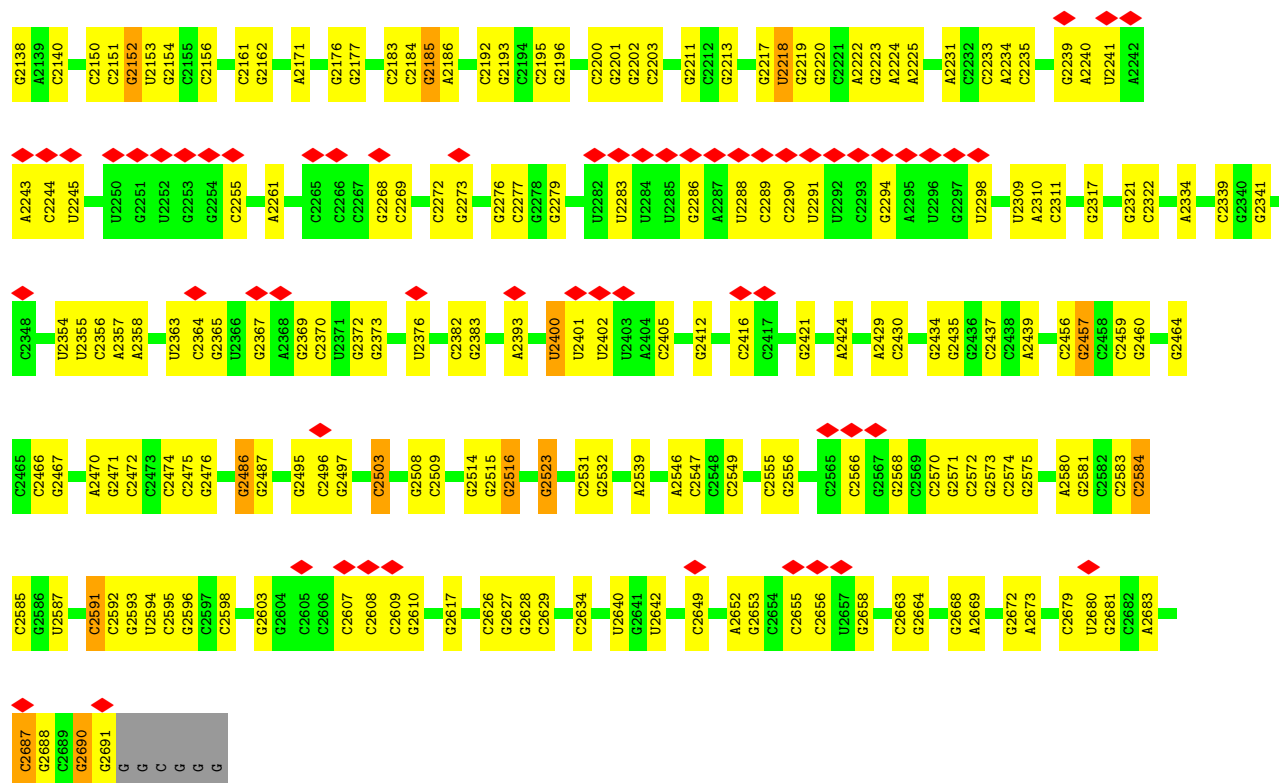
• Molecule 43: Ubiquitin/Ribosomal protein L40e



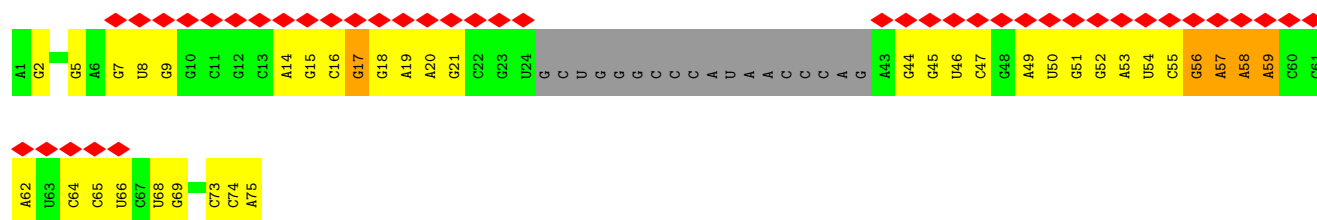
• Molecule 44: Large Subunit rRNA



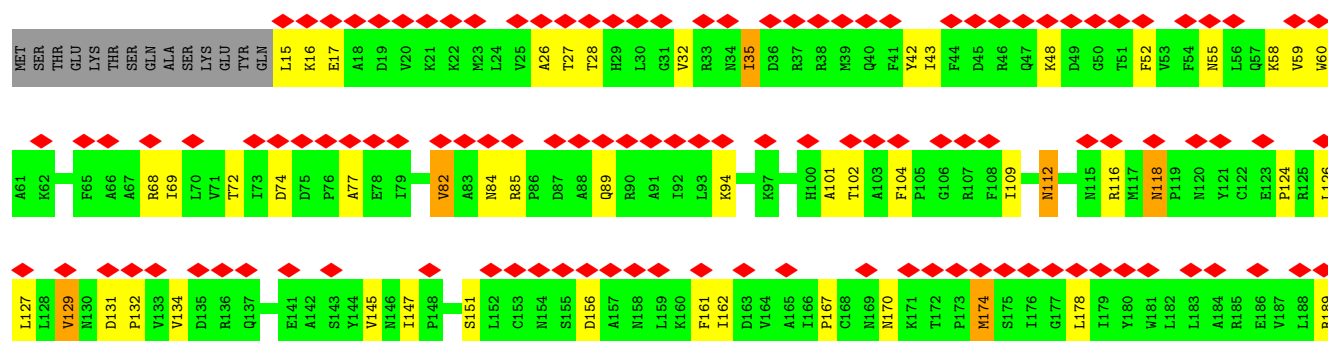


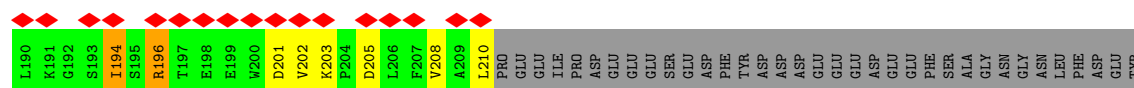


• Molecule 45: E-site tRNA

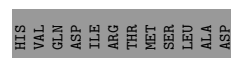
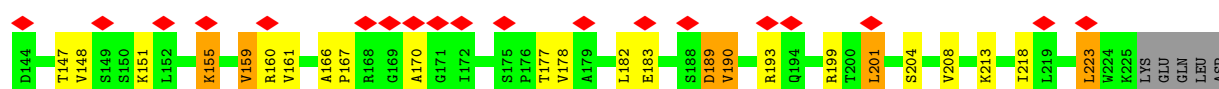
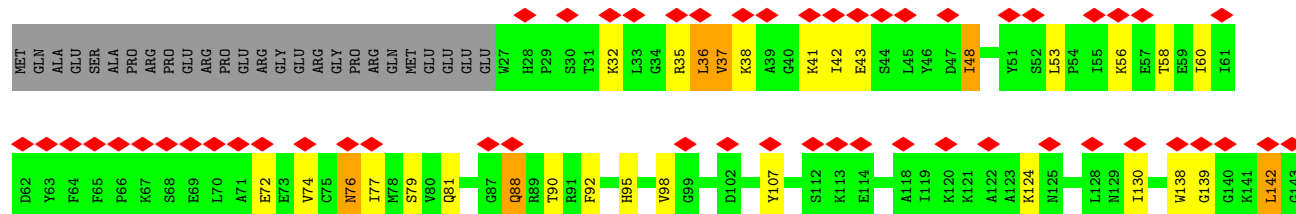


• Molecule 46: 40S ribosomal protein SA

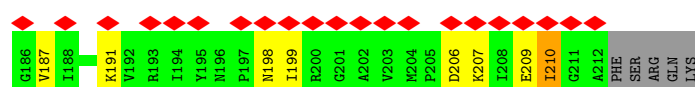
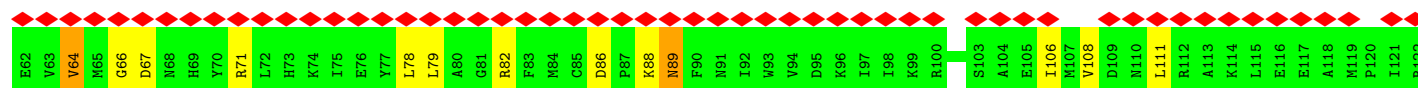
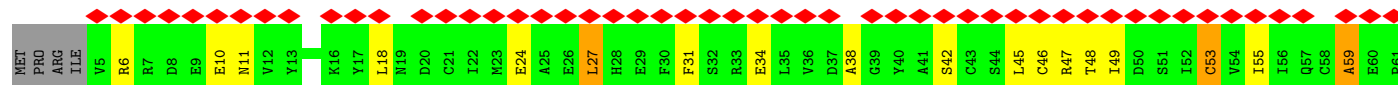
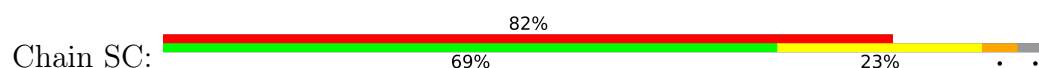




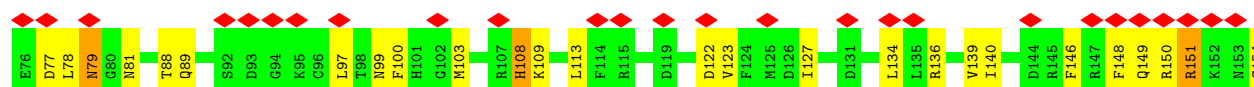
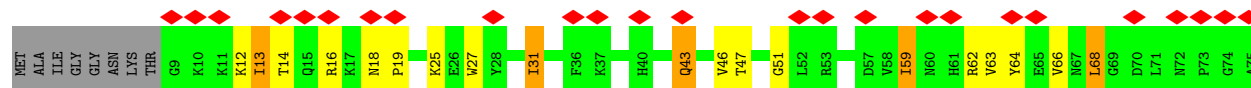
• Molecule 47: Ribosomal protein S2

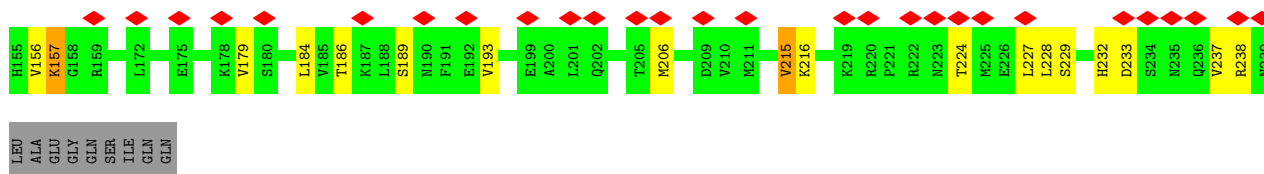


• Molecule 48: Ribosomal protein S3

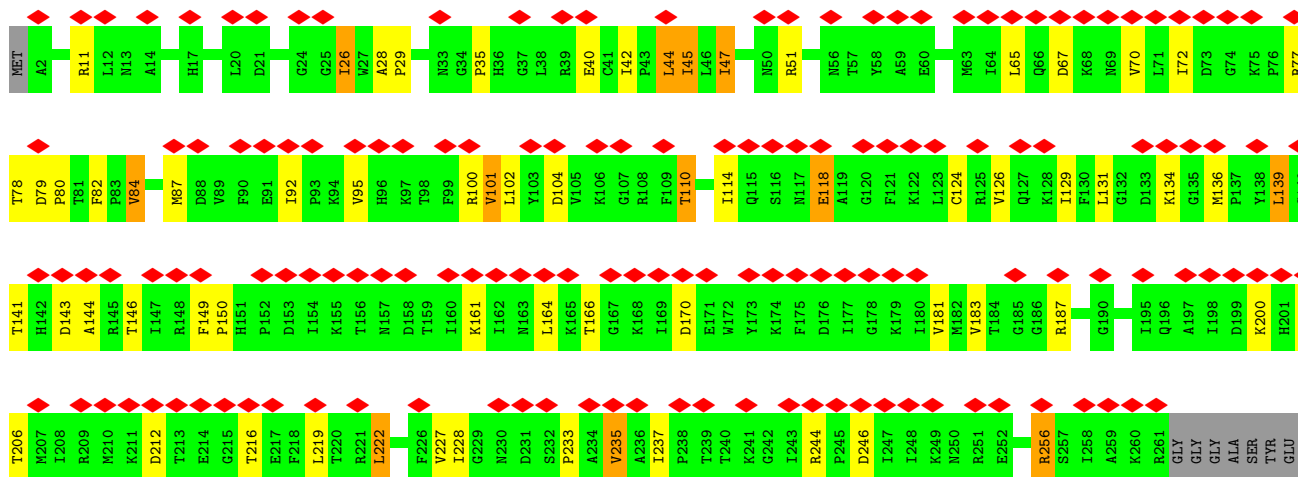
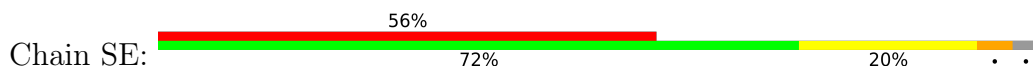


• Molecule 49: 40S ribosomal protein S3a

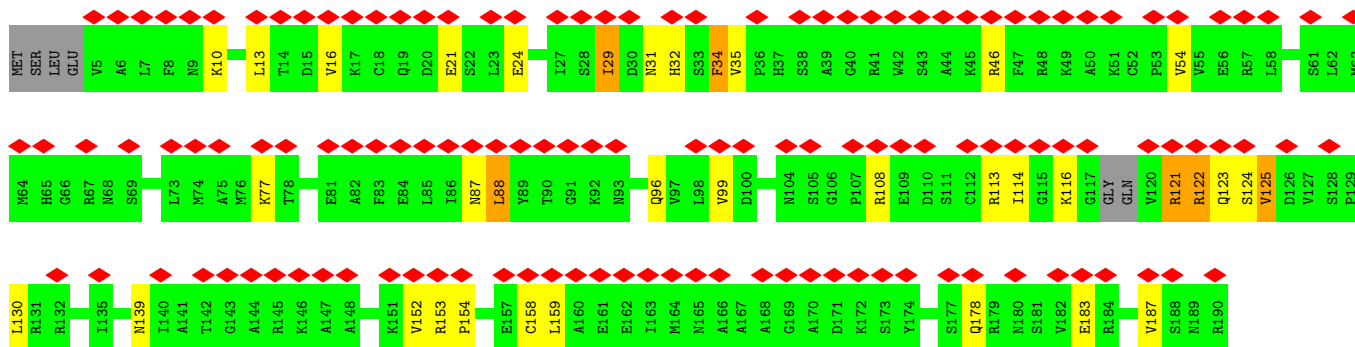
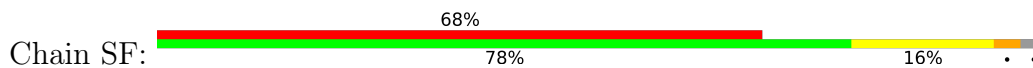




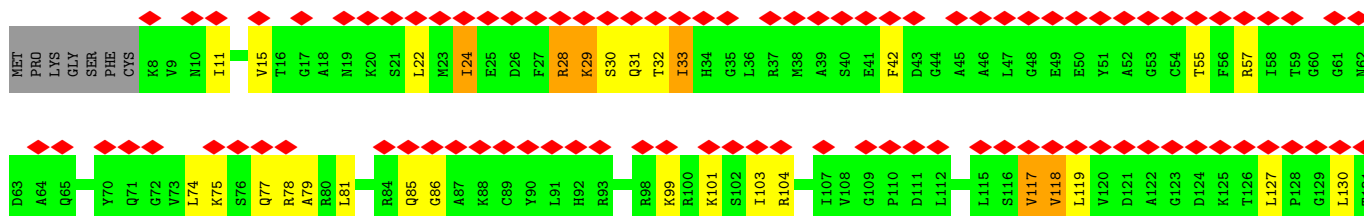
• Molecule 50: 40S ribosomal protein S4

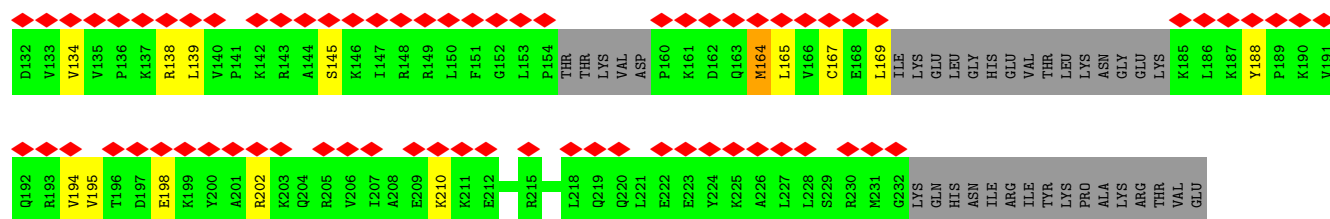


• Molecule 51: Ribosomal protein S5

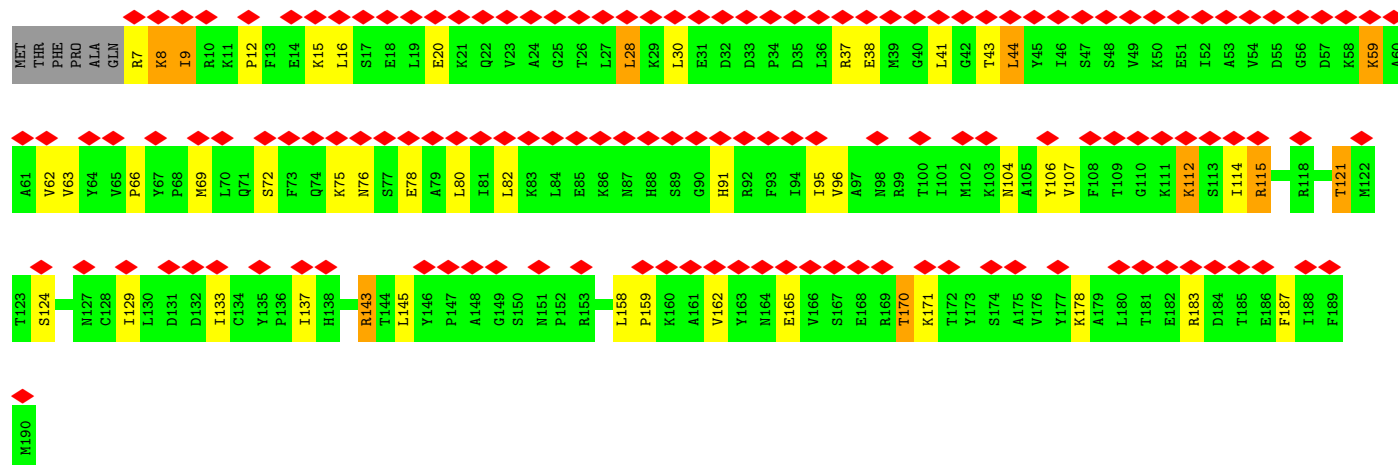
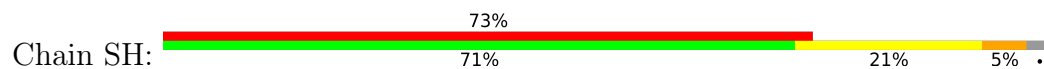


• Molecule 52: 40S ribosomal protein S6

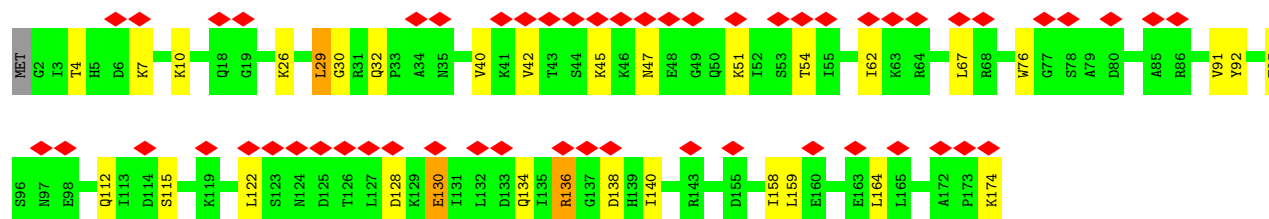
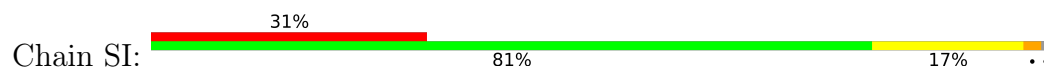




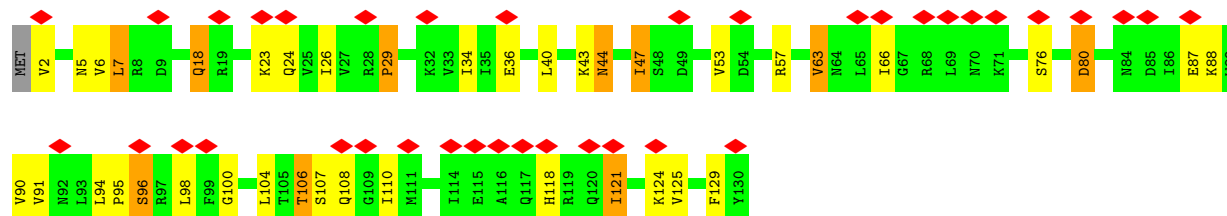
• Molecule 53: 40S ribosomal protein S7



• Molecule 54: 40S ribosomal protein S8

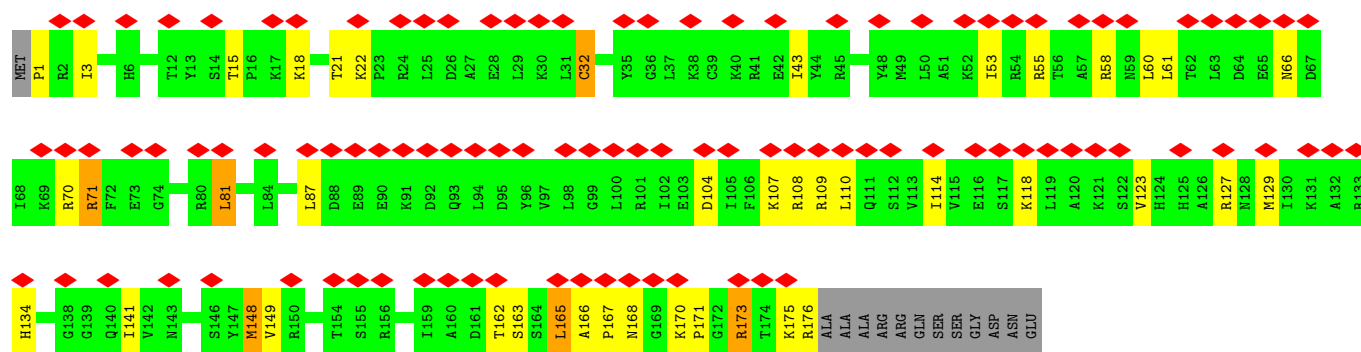


• Molecule 55: Ribosomal protein S15A



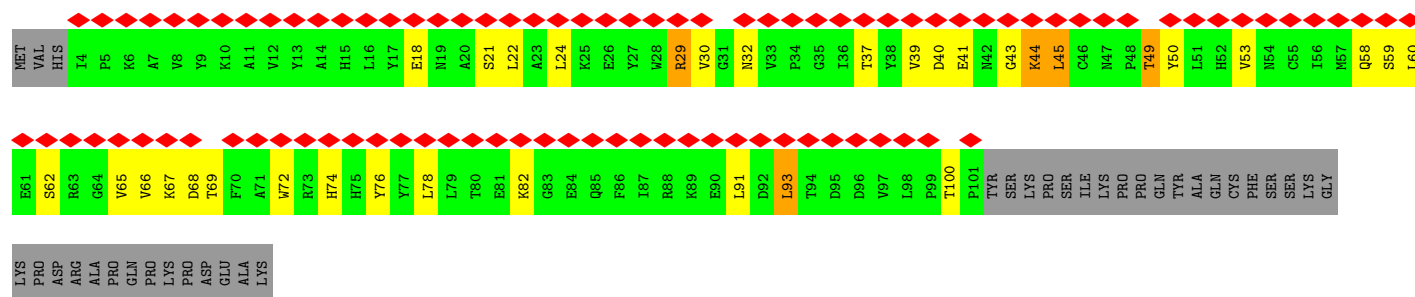
• Molecule 56: Ribosomal protein S9

Chain SK: 



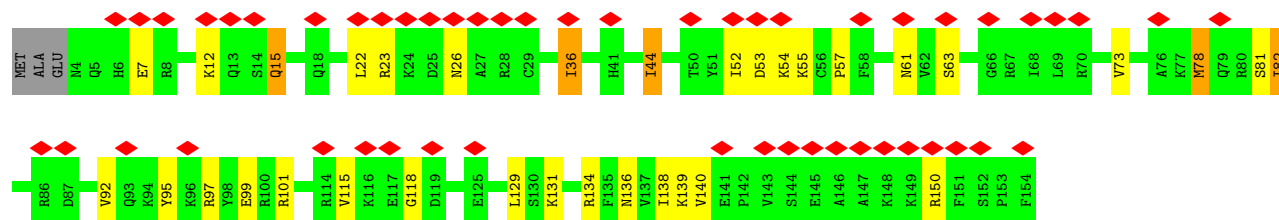
• Molecule 57: Ribosomal protein S10B

Chain SL: 



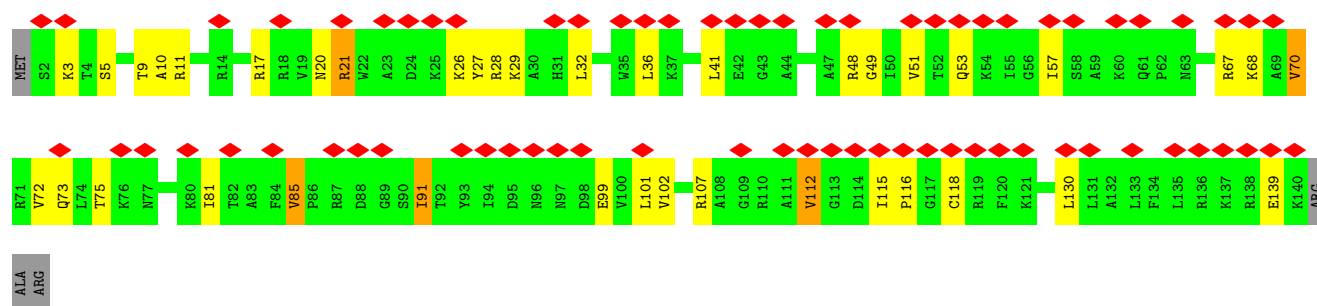
• Molecule 58: Ribosomal protein S11

Chain SM: 



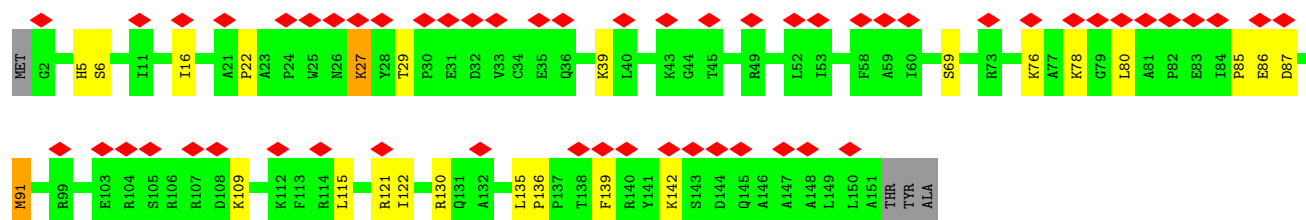
• Molecule 59: Ribosomal protein S23

Chain SO: 



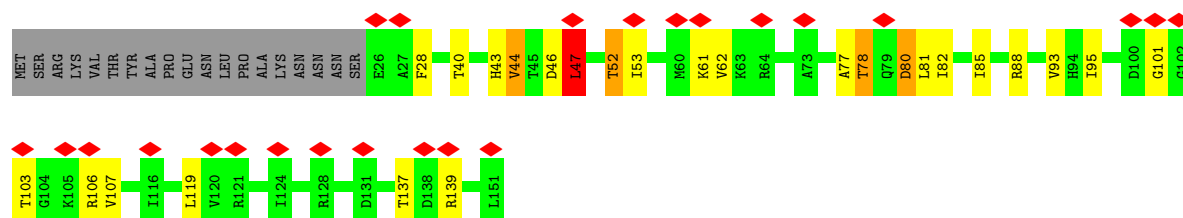
- Molecule 60: Ribosomal protein S13

Chain SP: 



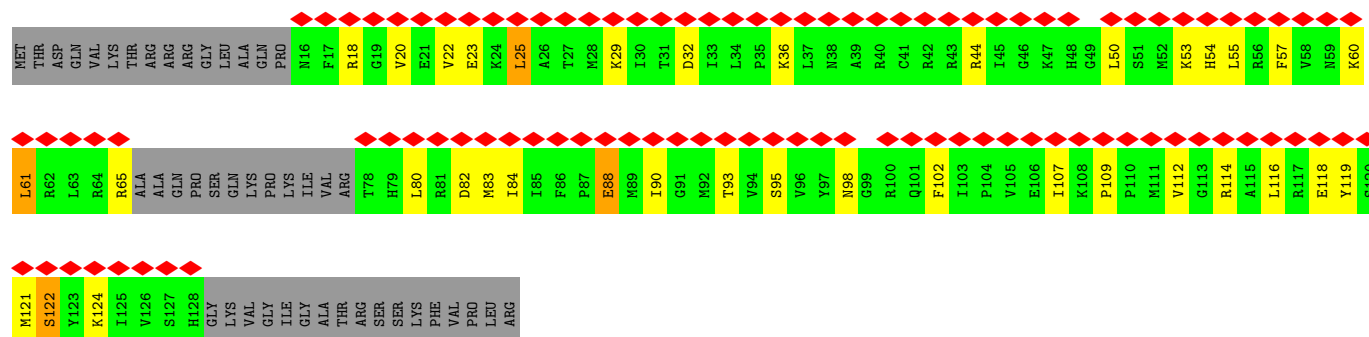
- Molecule 61: Ribosomal protein S14

Chain SQ: 



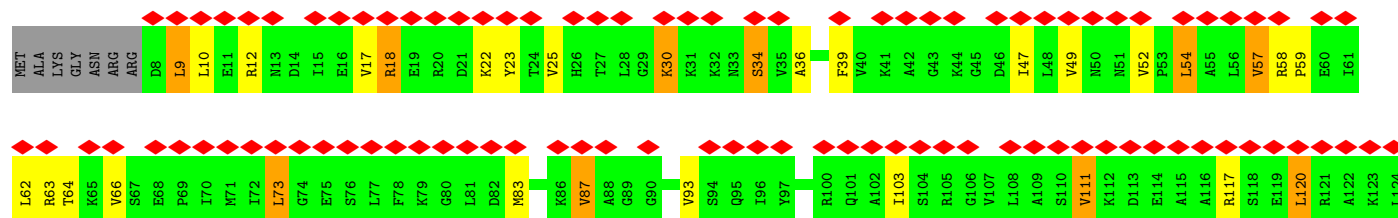
- Molecule 62: Ribosomal protein S15

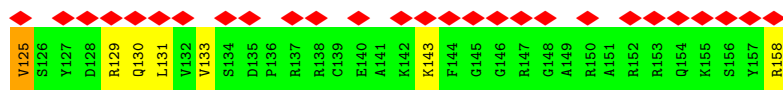
Chain SR: 



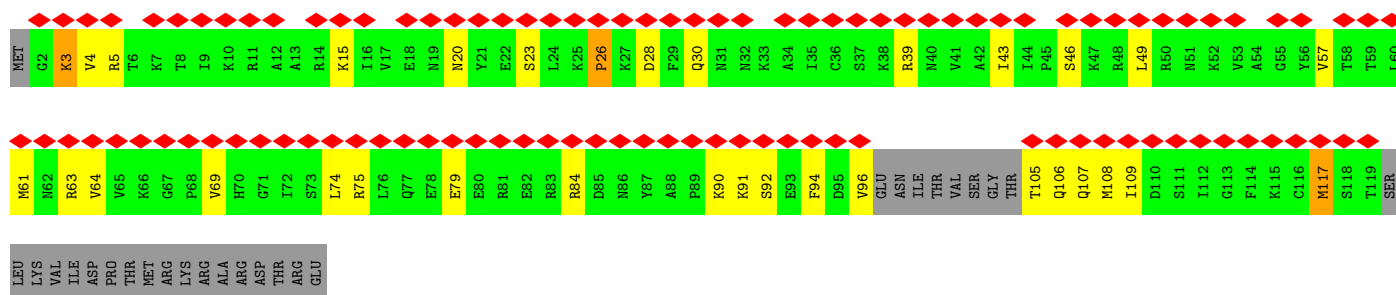
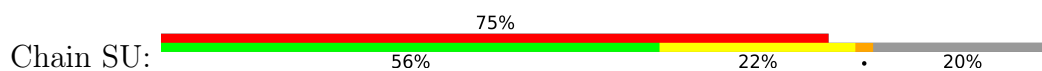
- Molecule 63: Ribosomal protein S16

Chain ST: 

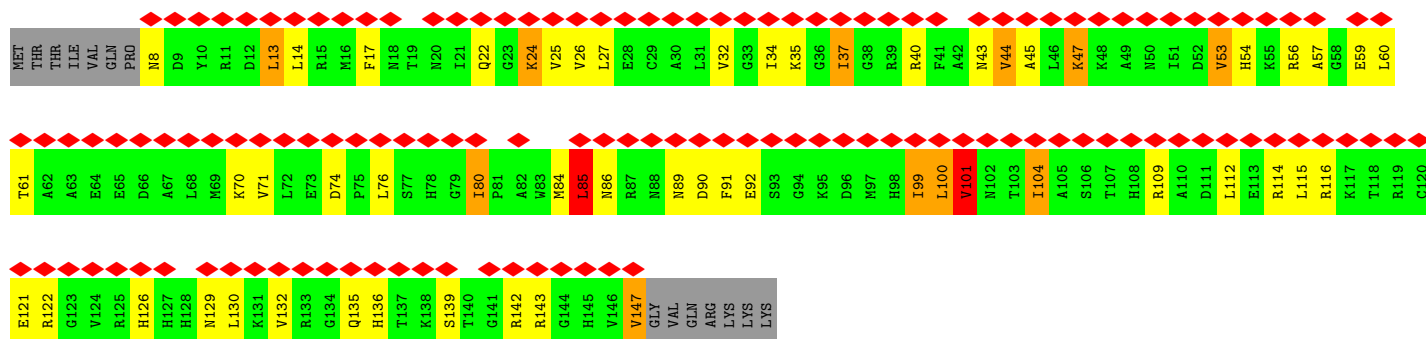
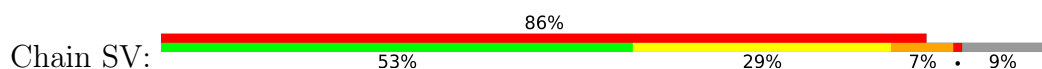




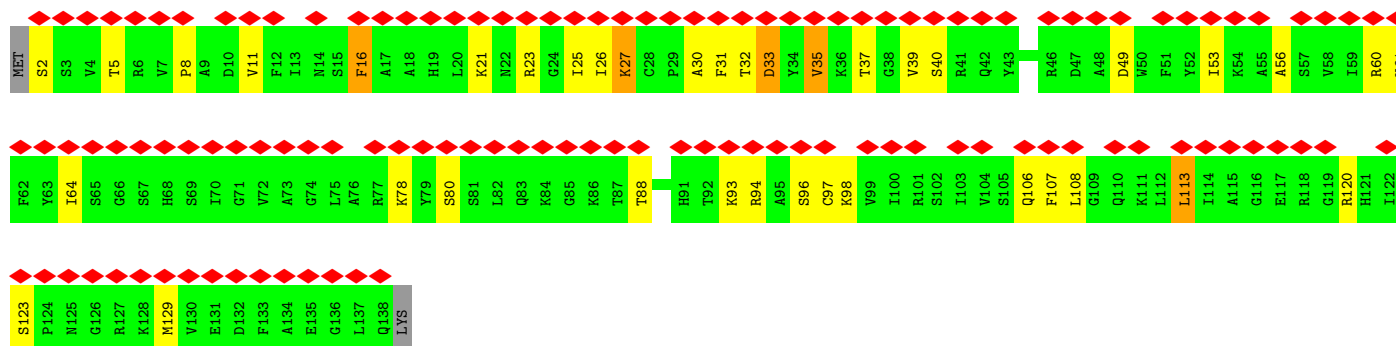
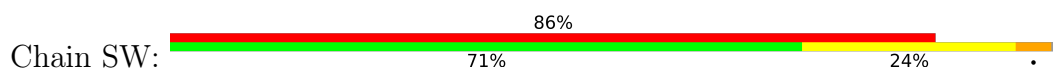
• Molecule 64: Ribosomal protein S17



• Molecule 65: Ribosomal protein S18

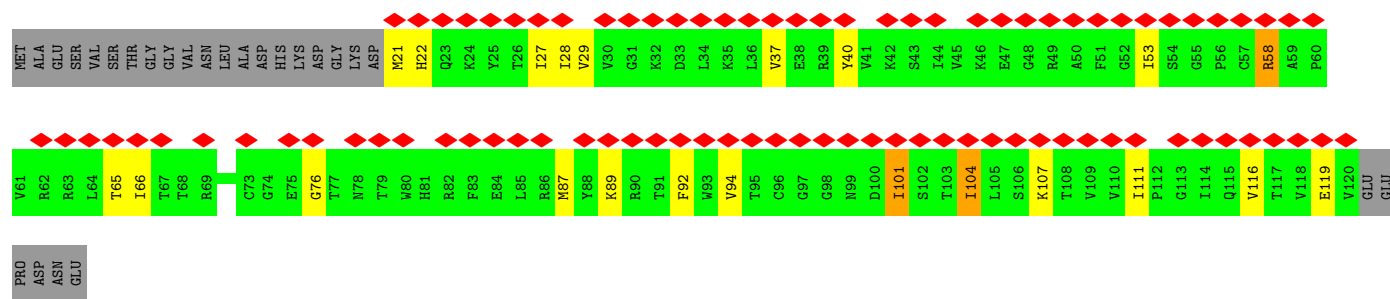


• Molecule 66: Ribosomal protein S19

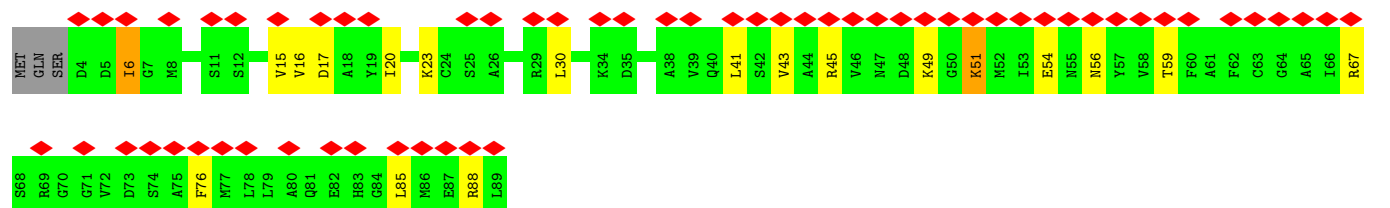
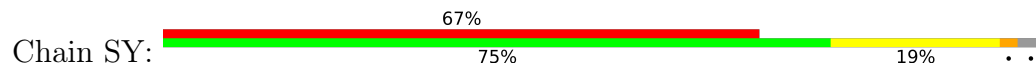


• Molecule 67: Ribosomal protein S20

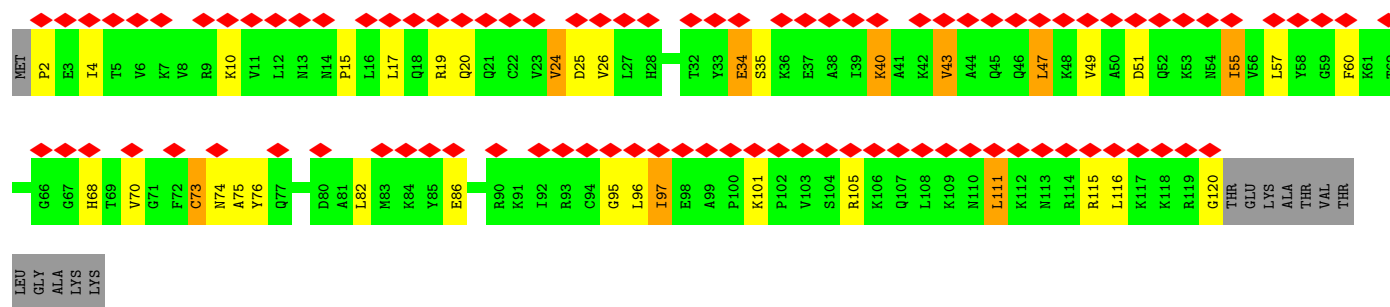




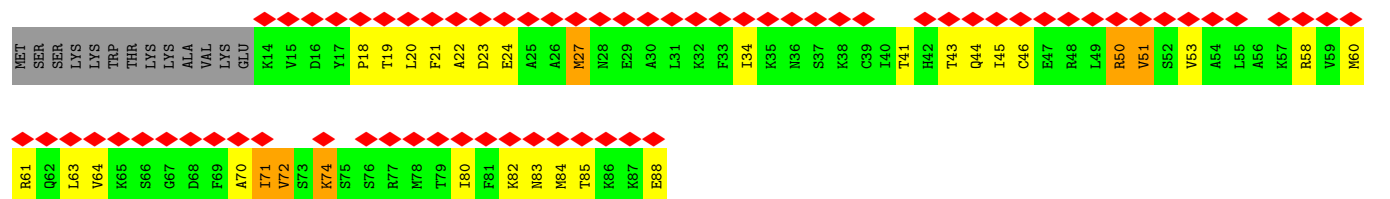
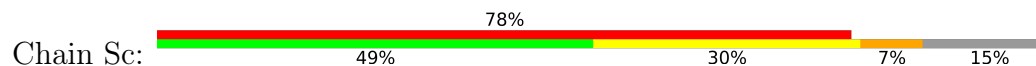
• Molecule 68: 40S ribosomal protein S21



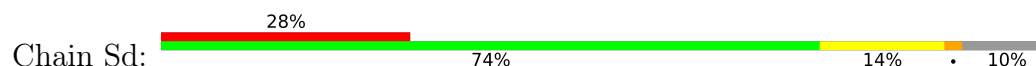
• Molecule 69: Ribosomal protein S24

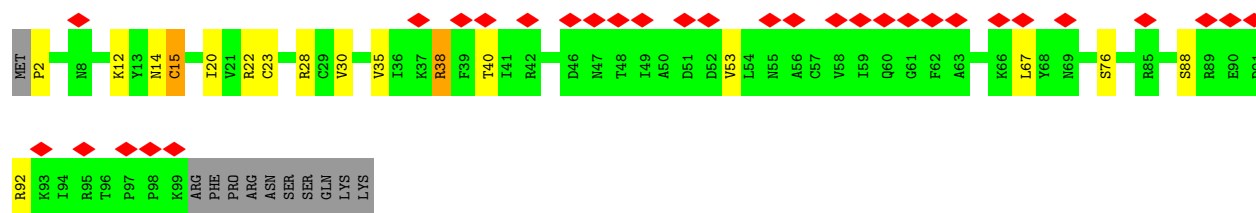


• Molecule 70: 40S ribosomal protein S25

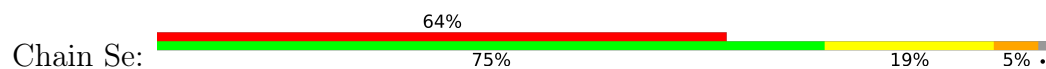


• Molecule 71: 40S ribosomal protein S26

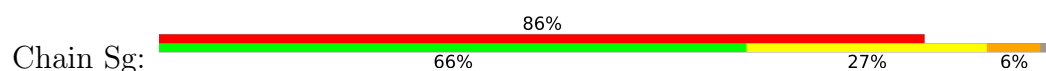




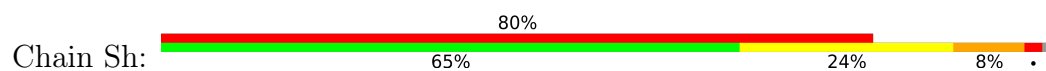
• Molecule 72: Ribosomal protein S27



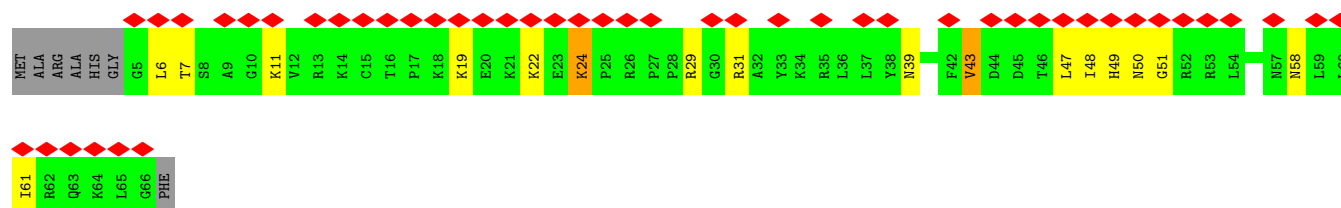
• Molecule 73: Ribosomal protein S28



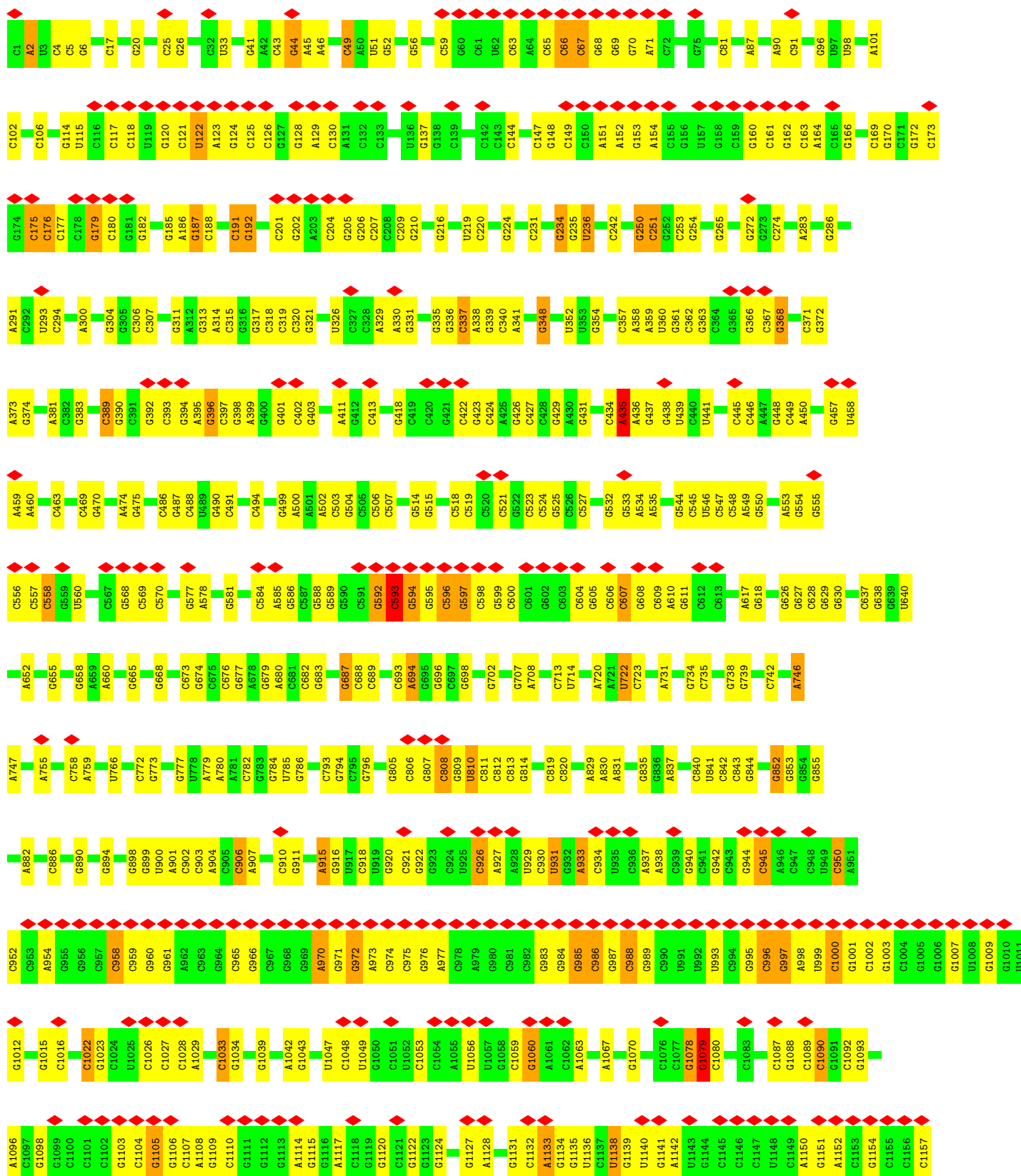
• Molecule 74: Ribosomal protein S29A

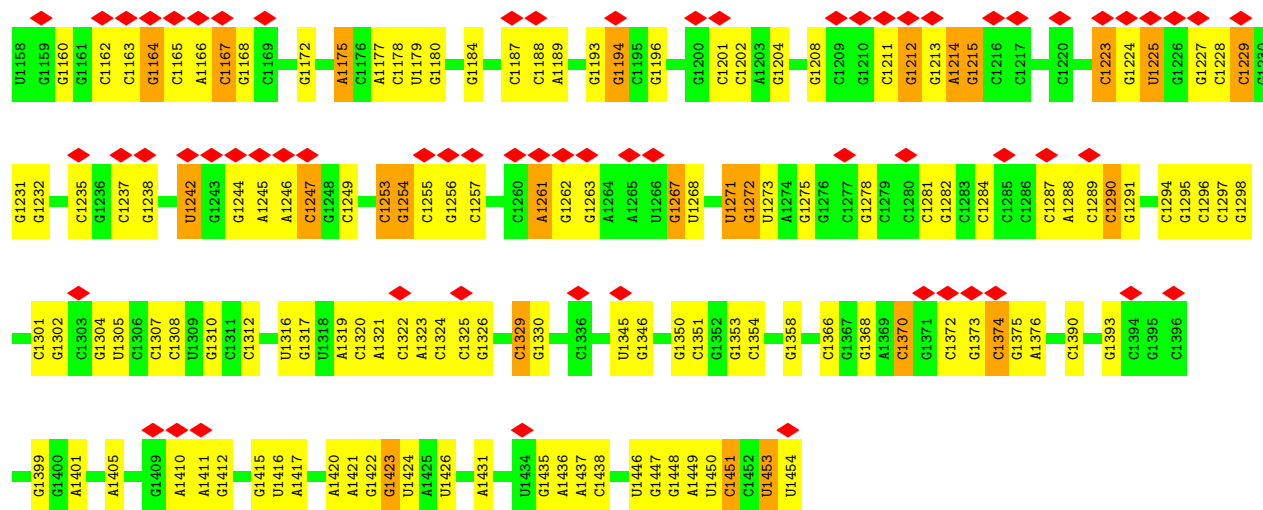


• Molecule 75: 40S ribosomal protein S30



• Molecule 76: Small Subunit rRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29181	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.0	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	19.404	Depositor
Minimum map value	-10.312	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.7	Depositor
Map size (Å)	410.0, 410.0, 410.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	LA	0.94	0/1897	1.33	2/2549 (0.1%)
2	LB	0.92	0/3049	1.31	13/4118 (0.3%)
3	LC	0.93	0/2463	1.29	3/3342 (0.1%)
4	LD	0.60	0/3393	0.76	0/5292
5	LE	0.57	0/2798	0.74	0/4361
6	LF	0.89	0/2398	1.31	4/3216 (0.1%)
7	LG	0.85	0/450	1.27	1/601 (0.2%)
8	LH	0.88	0/1756	1.30	3/2367 (0.1%)
9	LI	0.91	0/1528	1.29	4/2063 (0.2%)
10	LJ	0.92	0/1479	1.33	6/1997 (0.3%)
11	LK	0.91	0/1296	1.27	1/1736 (0.1%)
12	LL	0.90	0/1365	1.26	3/1833 (0.2%)
13	LM	0.89	0/1628	1.33	4/2180 (0.2%)
14	LN	0.91	1/1037 (0.1%)	1.35	3/1390 (0.2%)
15	LO	0.88	0/1751	1.27	3/2346 (0.1%)
16	LP	0.89	0/1602	1.37	10/2149 (0.5%)
17	LQ	0.89	0/1265	1.28	1/1692 (0.1%)
18	LR	0.92	0/1425	1.28	3/1907 (0.2%)
19	LS	0.85	0/1609	1.29	5/2129 (0.2%)
20	LT	0.88	0/1457	1.24	0/1957
21	LU	0.91	0/1290	1.27	1/1735 (0.1%)
22	LV	0.85	0/836	1.35	3/1126 (0.3%)
23	LW	0.90	0/1035	1.31	3/1396 (0.2%)
24	LX	0.88	0/553	1.41	5/736 (0.7%)
25	LY	0.91	0/951	1.26	0/1286
26	LZ	0.90	0/1091	1.29	3/1454 (0.2%)
27	La	0.93	0/974	1.35	1/1313 (0.1%)
28	Lb	0.93	1/1231 (0.1%)	1.26	4/1647 (0.2%)
29	Lc	0.90	0/441	1.35	2/583 (0.3%)
30	Ld	0.93	0/812	1.42	3/1097 (0.3%)
31	Le	0.90	0/832	1.28	1/1118 (0.1%)
32	Lf	0.88	0/1074	1.27	4/1432 (0.3%)
33	Lg	0.93	0/793	1.35	4/1062 (0.4%)
34	Lh	0.92	0/780	1.32	4/1048 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	Li	0.88	0/996	1.30	2/1328 (0.2%)
36	Lj	0.86	0/741	1.36	3/982 (0.3%)
37	Lk	0.89	0/705	1.27	1/934 (0.1%)
38	Ll	0.90	0/562	1.37	2/749 (0.3%)
39	Ln	0.95	0/1621	1.32	3/2183 (0.1%)
40	Lo	0.79	0/229	1.24	0/291
41	Lp	0.89	0/778	1.24	0/1029
42	Lq	0.88	0/709	1.35	1/945 (0.1%)
43	Ls	0.89	0/392	1.40	0/522
44	Lt	0.59	0/62214	0.76	29/97098 (0.0%)
45	Lu	0.59	0/1366	0.75	0/2127
46	SA	0.92	0/1603	1.30	5/2178 (0.2%)
47	SB	0.93	0/1561	1.34	4/2107 (0.2%)
48	SC	0.92	0/1674	1.34	8/2248 (0.4%)
49	SD	0.90	0/1903	1.31	3/2562 (0.1%)
50	SE	0.96	0/2131	1.30	6/2874 (0.2%)
51	SF	0.94	0/1451	1.30	3/1950 (0.2%)
52	SG	0.93	0/1637	1.27	0/2185
53	SH	0.93	0/1508	1.27	2/2032 (0.1%)
54	SI	0.92	0/1378	1.28	3/1848 (0.2%)
55	SJ	0.95	0/1048	1.36	5/1412 (0.4%)
56	SK	0.92	0/1443	1.29	3/1930 (0.2%)
57	SL	0.90	0/824	1.29	0/1122
58	SM	0.93	0/1280	1.25	3/1712 (0.2%)
59	SO	0.91	0/1095	1.34	2/1467 (0.1%)
60	SP	0.89	0/1215	1.31	3/1632 (0.2%)
61	SQ	0.94	0/937	1.44	4/1258 (0.3%)
62	SR	0.93	0/845	1.35	3/1127 (0.3%)
63	ST	0.94	0/1192	1.31	2/1594 (0.1%)
64	SU	0.90	0/895	1.40	3/1193 (0.3%)
65	SV	0.91	0/1129	1.40	6/1514 (0.4%)
66	SW	0.96	0/1095	1.35	5/1473 (0.3%)
67	SX	0.90	0/809	1.33	0/1092
68	SY	0.96	0/659	1.31	1/883 (0.1%)
69	Sb	0.90	0/960	1.32	3/1284 (0.2%)
70	Sc	0.95	0/603	1.35	3/802 (0.4%)
71	Sd	0.91	0/809	1.29	0/1088
72	Se	0.95	0/643	1.33	3/871 (0.3%)
73	Sg	0.97	0/508	1.34	5/677 (0.7%)
74	Sh	0.85	0/425	1.44	3/563 (0.5%)
75	Sj	0.90	0/510	1.34	2/679 (0.3%)
76	St	0.60	0/34858	0.77	22/54401 (0.0%)
All	All	0.75	2/187280 (0.0%)	1.02	263/274204 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Lb	145	PRO	C-O	-5.19	1.19	1.24
14	LN	67	LYS	N-CA	5.17	1.50	1.46

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	SD	79	ASN	CB-CA-C	10.97	120.69	109.83
61	SQ	80	ASP	N-CA-C	-10.38	100.48	113.55
62	SR	109	PRO	N-CA-C	10.16	123.09	110.70
76	St	1416	U	C2'-C3'-O3'	10.10	124.65	109.50
76	St	1079	G	C2'-C3'-O3'	10.01	128.72	113.70
14	LN	67	LYS	CB-CA-C	9.79	119.51	111.00
44	Lt	776	G	C2'-C3'-O3'	9.65	123.98	109.50
19	LS	41	ILE	N-CA-C	-9.60	103.56	111.81
23	LW	47	LYS	N-CA-C	-9.16	98.71	110.53
44	Lt	1277	G	C2'-C3'-O3'	8.92	122.88	109.50
44	Lt	2591	C	C2'-C3'-O3'	8.50	122.26	109.50
44	Lt	1448	G	C2'-C3'-O3'	8.42	126.33	113.70
64	SU	26	PRO	N-CA-C	8.40	124.66	113.40
13	LM	110	GLN	N-CA-C	-8.36	103.22	113.41
2	LB	139	ASP	N-CA-C	-8.33	103.31	113.97
23	LW	47	LYS	CA-C-N	-8.29	114.85	121.82
23	LW	47	LYS	C-N-CA	-8.29	114.85	121.82
56	SK	32	CYS	N-CA-C	-8.19	103.81	113.88
66	SW	31	PHE	N-CA-C	-8.02	103.71	113.97
44	Lt	1349	G	C2'-C3'-O3'	8.01	125.72	113.70
29	Lc	50	ASP	CB-CA-C	8.00	125.94	110.17
11	LK	154	ARG	N-CA-C	-7.96	103.78	113.97
44	Lt	1356	C	C2'-C3'-O3'	7.87	125.51	113.70
36	Lj	19	ARG	N-CA-C	-7.82	102.38	112.23
30	Ld	105	THR	CB-CA-C	-7.79	98.65	110.88
6	LF	146	GLU	N-CA-C	-7.72	103.99	113.41
44	Lt	1914	C	C2'-C3'-O3'	7.69	125.23	113.70
29	Lc	28	ALA	N-CA-C	-7.68	103.52	113.12
76	St	122	U	C2'-C3'-O3'	7.57	125.05	113.70
16	LP	193	ALA	N-CA-C	-7.53	103.98	113.02
44	Lt	2017	A	C2'-C3'-O3'	7.45	120.68	109.50
49	SD	148	PHE	CA-C-O	-7.44	115.01	119.55
44	Lt	1972	A	C2'-C3'-O3'	7.39	120.59	109.50
15	LO	12	ARG	N-CA-C	-7.31	104.17	113.23
44	Lt	2687	C	C2'-C3'-O3'	7.29	120.43	109.50
12	LL	95	CYS	N-CA-C	-7.22	104.46	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	Lt	2574	C	C2'-C3'-O3'	7.22	124.53	113.70
74	Sh	120	CYS	CB-CA-C	-7.18	94.79	109.65
60	SP	115	LEU	N-CA-C	-7.16	104.17	113.12
47	SB	38	LYS	N-CA-C	-7.16	104.36	113.23
2	LB	184	GLY	CA-C-N	-7.15	115.87	122.80
2	LB	184	GLY	C-N-CA	-7.15	115.87	122.80
76	St	599	G	C2'-C3'-O3'	7.14	124.41	113.70
75	Sj	50	ASN	N-CA-C	-7.10	103.93	112.59
76	St	1187	C	C4'-C3'-O3'	7.10	123.65	113.00
66	SW	49	ASP	N-CA-C	-7.06	102.98	112.94
70	Sc	64	VAL	N-CA-C	-7.06	104.10	111.58
39	Ln	171	ASN	N-CA-C	-7.00	104.73	113.20
76	St	435	A	C2'-C3'-O3'	6.96	124.13	113.70
44	Lt	1252	G	C2'-C3'-O3'	6.94	124.11	113.70
33	Lg	20	SER	N-CA-C	-6.92	99.22	109.81
16	LP	128	PRO	CA-C-O	-6.91	113.15	121.03
55	SJ	100	GLY	CA-C-O	-6.91	117.06	122.52
76	St	588	G	C2'-C3'-O3'	6.89	124.03	113.70
76	St	593	C	C4'-C3'-O3'	6.84	119.67	109.40
75	Sj	51	GLY	N-CA-C	-6.81	105.66	115.27
32	Lf	113	ILE	N-CA-C	-6.81	104.36	111.58
66	SW	21	LYS	N-CA-C	-6.76	105.17	113.41
55	SJ	76	SER	CA-C-O	-6.75	113.38	119.86
16	LP	179	ALA	N-CA-C	-6.75	105.01	113.18
53	SH	38	GLU	N-CA-C	-6.75	104.52	112.89
35	Li	75	ARG	N-CA-C	-6.74	105.18	113.41
44	Lt	2627	G	C4'-C3'-O3'	6.73	123.09	113.00
24	LX	10	CYS	CB-CA-C	-6.66	99.73	110.79
76	St	1261	A	C2'-C3'-O3'	6.60	119.41	109.50
46	SA	205	ASP	N-CA-C	-6.59	105.06	113.23
54	SI	40	VAL	N-CA-C	-6.58	106.32	112.83
44	Lt	1511	G	C2'-C3'-O3'	6.56	123.54	113.70
63	ST	131	LEU	N-CA-C	-6.55	104.22	111.36
35	Li	86	VAL	N-CA-C	-6.50	104.69	111.58
44	Lt	2584	C	C2'-C3'-O3'	6.44	119.16	109.50
76	St	175	C	C2'-C3'-O3'	6.44	119.16	109.50
55	SJ	57	ARG	CB-CA-C	-6.43	107.15	116.54
10	LJ	62	ARG	N-CA-C	-6.42	105.43	113.20
48	SC	167	GLY	CA-C-O	-6.38	117.86	122.45
73	Sg	57	GLU	N-CA-C	-6.37	105.15	113.17
47	SB	213	LYS	N-CA-C	-6.33	105.48	113.72
48	SC	89	ASN	N-CA-C	-6.31	104.41	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	LJ	83	GLY	CA-C-O	-6.30	117.88	122.23
47	SB	36	LEU	N-CA-C	-6.30	105.59	113.28
50	SE	45	ILE	N-CA-C	-6.29	104.14	111.00
76	St	44	G	C2'-C3'-O3'	6.28	118.92	109.50
46	SA	196	ARG	N-CA-C	-6.25	105.61	113.18
10	LJ	74	GLU	N-CA-C	-6.24	104.73	112.90
33	Lg	86	GLN	N-CA-C	-6.21	105.46	113.16
76	St	1288	A	C2'-C3'-O3'	-6.20	100.21	109.50
16	LP	128	PRO	N-CA-C	-6.19	101.46	110.80
76	St	187	G	C2'-C3'-O3'	6.17	118.75	109.50
38	Ll	32	LEU	N-CA-C	-6.17	104.64	111.36
2	LB	256	HIS	CA-C-O	-6.14	113.42	119.69
2	LB	12	GLY	CA-C-O	-6.12	118.24	122.22
61	SQ	46	ASP	CA-C-O	-6.12	115.33	122.37
62	SR	118	GLU	N-CA-C	-6.11	105.99	113.50
44	Lt	459	A	C2'-C3'-O3'	6.10	122.85	113.70
61	SQ	137	THR	N-CA-C	-6.08	104.66	111.28
37	Lk	74	TYR	N-CA-C	-6.07	104.58	112.23
9	LI	140	PRO	N-CA-C	-6.07	99.98	112.47
47	SB	199	ARG	N-CA-C	-6.05	105.39	112.89
16	LP	42	GLY	CA-C-O	-6.04	118.06	122.23
8	LH	220	PHE	CA-CB-CG	6.03	119.83	113.80
50	SE	149	PHE	CA-C-O	-6.03	115.83	120.48
1	LA	244	GLY	CA-C-O	-6.03	118.07	122.23
16	LP	175	ILE	N-CA-C	-6.02	105.20	111.58
33	Lg	9	PHE	CA-CB-CG	6.01	119.81	113.80
22	LV	52	VAL	N-CA-C	-6.01	104.65	110.72
61	SQ	46	ASP	CB-CA-C	-6.01	102.66	112.03
7	LG	39	TYR	CB-CA-C	5.97	122.30	110.42
44	Lt	2355	U	C2'-C3'-O3'	5.95	118.43	109.50
6	LF	195	GLY	CA-C-O	-5.92	118.05	122.37
48	SC	27	LEU	N-CA-C	-5.91	104.19	111.40
30	Ld	25	GLY	CA-C-O	-5.91	118.06	122.37
44	Lt	1074	C	C4'-C3'-O3'	5.89	118.24	109.40
28	Lb	31	GLY	CA-C-O	-5.89	118.16	122.23
10	LJ	105	ASN	N-CA-C	-5.88	106.05	113.23
15	LO	186	PRO	N-CA-C	-5.88	105.06	113.47
38	Ll	66	ASP	N-CA-C	-5.88	106.07	113.18
2	LB	256	HIS	CB-CA-C	5.86	117.33	109.42
36	Lj	56	MET	N-CA-C	-5.85	102.66	110.55
58	SM	57	PRO	CB-CA-C	-5.84	102.62	111.44
53	SH	43	THR	N-CA-C	-5.84	105.74	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Lb	96	THR	N-CA-C	-5.81	106.81	114.31
6	LF	186	LYS	N-CA-C	-5.81	104.54	111.69
13	LM	84	ARG	CB-CA-C	5.81	117.61	108.84
60	SP	22	PRO	N-CA-C	-5.80	102.48	111.13
69	Sb	95	GLY	N-CA-C	-5.79	107.33	115.32
44	Lt	1236	G	C2'-C3'-O3'	5.78	122.36	113.70
44	Lt	1472	C	C2'-C3'-O3'	5.77	122.35	113.70
2	LB	361	LYS	N-CA-C	-5.76	106.25	113.28
69	Sb	15	PRO	N-CA-C	-5.76	106.17	114.18
24	LX	22	PHE	CA-CB-CG	5.76	119.56	113.80
34	Lh	74	TYR	N-CA-C	-5.75	105.57	112.58
48	SC	199	ILE	N-CA-C	-5.75	106.71	112.17
49	SD	148	PHE	O-C-N	5.74	125.87	120.71
56	SK	1	PRO	CA-N-CD	-5.73	103.97	112.00
76	St	808	C	C2'-C3'-O3'	5.73	118.09	109.50
76	St	1138	U	C2'-C3'-O3'	5.71	118.06	109.50
39	Ln	173	LYS	N-CA-C	-5.70	105.91	112.92
44	Lt	1079	G	C4'-C3'-O3'	5.68	117.92	109.40
16	LP	194	LYS	CB-CA-C	5.66	118.22	110.06
26	LZ	81	GLU	CA-C-N	-5.66	116.70	123.44
26	LZ	81	GLU	C-N-CA	-5.66	116.70	123.44
44	Lt	694	C	C2'-C3'-O3'	5.66	122.19	113.70
32	Lf	95	LYS	N-CA-C	-5.65	105.72	113.30
48	SC	31	PHE	N-CA-C	-5.64	104.75	111.69
3	LC	251	TYR	CB-CA-C	5.64	121.50	110.67
50	SE	26	ILE	N-CA-C	-5.63	105.03	110.72
44	Lt	1074	C	C2'-C3'-O3'	5.63	117.94	109.50
27	La	112	ASN	CB-CA-C	5.62	120.41	110.85
76	St	1193	G	C2'-C3'-O3'	5.62	122.13	113.70
19	LS	49	ILE	N-CA-C	-5.61	105.04	110.42
19	LS	70	LYS	N-CA-C	-5.61	105.17	112.23
69	Sb	34	GLU	CA-C-O	-5.60	115.64	122.64
72	Se	70	ASN	N-CA-C	-5.59	106.04	112.92
9	LI	141	LEU	N-CA-C	-5.59	106.30	113.01
42	Lq	10	LEU	N-CA-C	-5.59	106.42	113.18
64	SU	90	LYS	CB-CA-C	-5.57	110.17	116.63
8	LH	223	ARG	N-CA-C	-5.57	106.48	113.72
44	Lt	2584	C	C4'-C3'-O3'	5.57	117.75	109.40
10	LJ	63	ASN	N-CA-C	-5.56	106.33	113.23
12	LL	6	GLU	N-CA-C	-5.56	106.70	112.93
76	St	1138	U	C4'-C3'-O3'	5.55	117.72	109.40
76	St	950	C	C2'-C3'-O3'	-5.55	101.18	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	LB	366	ILE	N-CA-C	-5.53	107.40	113.43
50	SE	42	ILE	CA-C-O	-5.53	116.08	119.51
56	SK	165	LEU	N-CA-C	-5.51	106.32	113.16
59	SO	5	SER	CA-C-N	-5.51	118.38	122.18
59	SO	5	SER	C-N-CA	-5.51	118.38	122.18
6	LF	170	ALA	N-CA-C	-5.50	105.30	112.23
9	LI	124	VAL	N-CA-C	-5.50	105.00	111.00
32	Lf	76	PHE	CB-CA-C	-5.50	99.49	109.38
24	LX	7	CYS	CB-CA-C	-5.48	99.82	109.62
50	SE	149	PHE	CB-CA-C	5.48	115.76	111.00
9	LI	167	LEU	N-CA-C	-5.47	105.73	112.90
17	LQ	139	TYR	N-CA-C	-5.47	103.88	110.88
33	Lg	3	GLU	N-CA-C	-5.46	106.66	113.38
34	Lh	48	THR	N-CA-CB	5.45	119.70	110.49
18	LR	144	CYS	N-CA-C	-5.45	106.55	114.12
31	Le	76	ASP	CA-C-O	-5.45	115.52	121.84
28	Lb	2	PRO	CA-N-CD	-5.44	104.39	112.00
58	SM	129	LEU	N-CA-C	-5.43	106.82	113.50
64	SU	26	PRO	CB-CA-C	-5.42	104.43	112.55
48	SC	66	GLY	CA-C-O	-5.40	118.25	122.52
76	St	191	C	C2'-C3'-O3'	5.40	121.80	113.70
63	ST	9	LEU	CA-C-O	-5.39	116.17	122.37
74	Sh	120	CYS	CA-CB-SG	5.39	126.79	114.40
44	Lt	1277	G	C4'-C3'-O3'	5.39	117.48	109.40
44	Lt	459	A	C3'-C2'-O2'	5.38	118.77	110.70
62	SR	119	TYR	CB-CA-C	5.38	120.28	110.11
44	Lt	2640	U	C2'-C3'-O3'	-5.38	105.64	113.70
60	SP	122	ILE	N-CA-C	-5.37	105.14	111.00
21	LU	100	ASP	N-CA-C	-5.37	105.33	111.07
66	SW	78	LYS	N-CA-C	-5.34	106.60	113.23
76	St	90	A	C4'-C3'-O3'	5.34	117.42	109.40
19	LS	19	LYS	N-CA-C	-5.34	106.72	113.18
1	LA	195	CYS	N-CA-C	-5.33	105.83	114.09
32	Lf	76	PHE	CA-CB-CG	5.33	119.13	113.80
2	LB	171	LYS	CB-CA-C	-5.32	104.14	112.12
44	Lt	71	C	C4'-C3'-O3'	5.32	120.97	113.00
10	LJ	136	VAL	CA-C-O	-5.31	115.15	121.05
50	SE	67	ASP	N-CA-C	-5.31	106.65	113.02
65	SV	135	GLN	CA-C-N	-5.31	115.67	123.00
65	SV	135	GLN	C-N-CA	-5.31	115.67	123.00
24	LX	48	ARG	N-CA-C	-5.30	106.32	112.89
28	Lb	61	TYR	CB-CA-C	5.30	119.59	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	SF	77	LYS	N-CA-C	-5.29	105.41	111.07
70	Sc	83	ASN	CB-CA-C	5.29	118.36	109.89
3	LC	82	TYR	CB-CA-C	-5.29	104.22	111.73
72	Se	105	SER	CA-C-N	-5.29	117.52	123.02
72	Se	105	SER	C-N-CA	-5.29	117.52	123.02
30	Ld	78	SER	N-CA-C	-5.28	105.98	112.90
51	SF	34	PHE	CA-C-O	-5.28	115.67	120.95
51	SF	130	LEU	N-CA-C	-5.28	104.44	112.04
18	LR	102	LEU	N-CA-C	-5.28	106.34	112.89
14	LN	117	ARG	N-CA-C	-5.27	105.59	112.23
76	St	592	G	C2'-C3'-O3'	-5.27	101.60	109.50
58	SM	52	ILE	CA-C-O	-5.25	115.69	120.73
73	Sg	37	ILE	CA-C-O	-5.25	117.53	121.68
13	LM	37	ASN	N-CA-C	-5.24	106.47	112.92
2	LB	208	VAL	N-CA-C	-5.23	107.06	111.56
34	Lh	64	THR	N-CA-CB	5.23	119.33	110.49
24	LX	37	CYS	N-CA-C	-5.23	105.58	111.28
2	LB	377	TYR	CB-CA-C	5.23	119.74	110.85
15	LO	89	ILE	N-CA-CB	-5.23	107.35	111.64
65	SV	142	ARG	N-CA-C	-5.22	105.48	111.07
34	Lh	47	GLU	CA-C-O	-5.22	114.69	120.38
54	SI	67	LEU	N-CA-C	-5.22	105.74	112.68
66	SW	32	THR	N-CA-C	-5.22	106.92	113.28
68	SY	17	ASP	CA-CB-CG	5.21	117.81	112.60
44	Lt	326	A	C4'-C3'-O3'	5.21	117.21	109.40
48	SC	59	ALA	CA-C-N	-5.17	115.63	122.56
48	SC	59	ALA	C-N-CA	-5.17	115.63	122.56
73	Sg	19	ARG	N-CA-C	-5.17	105.85	113.61
65	SV	59	GLU	N-CA-C	-5.17	106.08	114.09
65	SV	45	ALA	N-CA-C	5.16	117.31	111.11
26	LZ	132	ARG	CB-CA-C	5.16	118.77	111.86
73	Sg	10	ILE	N-CA-C	-5.15	107.38	111.81
55	SJ	44	ASN	N-CA-C	-5.15	105.89	113.61
76	St	1253	C	C4'-C3'-O3'	5.14	120.71	113.00
55	SJ	88	LYS	N-CA-C	-5.11	105.79	111.36
73	Sg	16	THR	CA-C-O	-5.11	115.57	121.49
46	SA	27	THR	N-CA-C	-5.10	107.01	113.23
12	LL	159	ALA	N-CA-C	-5.09	105.38	112.45
46	SA	27	THR	CB-CA-C	5.09	119.75	111.26
46	SA	84	ASN	N-CA-C	-5.08	107.46	113.97
19	LS	190	PHE	N-CA-C	-5.08	105.78	112.94
22	LV	28	LEU	N-CA-C	-5.08	106.67	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	LC	78	GLY	N-CA-C	-5.08	108.23	115.64
54	SI	30	GLY	CA-C-O	-5.07	117.16	121.57
18	LR	175	GLY	CA-C-O	-5.07	117.62	122.13
65	SV	142	ARG	CB-CA-C	-5.06	102.93	110.88
2	LB	54	THR	CB-CA-C	-5.06	100.34	110.42
36	Lj	79	LYS	N-CA-C	-5.06	105.47	111.69
16	LP	119	SER	N-CA-C	-5.05	105.68	111.14
39	Ln	125	GLY	CA-C-O	-5.05	116.51	119.69
13	LM	169	GLN	CB-CA-C	-5.04	101.03	109.65
16	LP	182	ASP	N-CA-C	-5.03	106.40	112.54
14	LN	91	TRP	N-CA-C	-5.03	105.80	111.28
22	LV	94	VAL	CA-C-O	-5.03	116.41	121.59
8	LH	100	LEU	N-CA-C	-5.02	105.90	112.23
16	LP	65	ARG	N-CA-C	-5.02	106.85	113.17
70	Sc	51	VAL	CA-C-O	-5.01	115.55	119.46
2	LB	249	VAL	N-CA-C	-5.00	103.05	109.30
74	Sh	103	ARG	CA-C-O	-5.00	115.69	121.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	LA	1864	0	1922	17	0
2	LB	2978	0	3011	25	0
3	LC	2412	0	2493	35	0
4	LD	3038	0	1556	4	0
5	LE	2502	0	1268	7	0
6	LF	2355	0	2416	22	0
7	LG	439	0	479	4	0
8	LH	1726	0	1761	13	0
9	LI	1502	0	1584	16	0
10	LJ	1452	0	1495	20	0
11	LK	1270	0	1276	10	0
12	LL	1340	0	1356	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	LM	1605	0	1704	11	0
14	LN	1024	0	1091	11	0
15	LO	1708	0	1785	17	0
16	LP	1570	0	1605	18	0
17	LQ	1239	0	1276	9	0
18	LR	1402	0	1478	15	0
19	LS	1592	0	1697	9	0
20	LT	1423	0	1426	19	0
21	LU	1264	0	1303	11	0
22	LV	820	0	805	6	0
23	LW	1015	0	1057	24	0
24	LX	538	0	547	11	0
25	LY	931	0	979	8	0
26	LZ	1076	0	1140	10	0
27	La	957	0	999	15	0
28	Lb	1201	0	1233	13	0
29	Lc	434	0	453	4	0
30	Ld	804	0	847	4	0
31	Le	818	0	857	4	0
32	Lf	1050	0	1108	14	0
33	Lg	778	0	816	5	0
34	Lh	765	0	793	10	0
35	Li	983	0	1081	8	0
36	Lj	731	0	794	3	0
37	Lk	689	0	683	4	0
38	Ll	558	0	612	13	0
39	Ln	1592	0	1667	20	0
40	Lo	227	0	272	2	0
41	Lp	767	0	822	10	0
42	Lq	700	0	741	10	0
43	Ls	388	0	401	7	0
44	Lt	55643	0	28280	211	0
45	Lu	1221	0	621	7	0
46	SA	1569	0	1610	29	0
47	SB	1529	0	1580	25	0
48	SC	1648	0	1689	16	0
49	SD	1868	0	1927	26	0
50	SE	2085	0	2174	22	0
51	SF	1429	0	1457	15	0
52	SG	1617	0	1716	14	0
53	SH	1481	0	1544	19	0
54	SI	1357	0	1421	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	SJ	1031	0	1082	12	0
56	SK	1423	0	1515	20	0
57	SL	802	0	790	12	0
58	SM	1251	0	1287	12	0
59	SO	1080	0	1165	23	0
60	SP	1192	0	1265	10	0
61	SQ	925	0	933	13	0
62	SR	831	0	891	13	0
63	ST	1180	0	1250	15	0
64	SU	886	0	933	13	0
65	SV	1113	0	1136	28	0
66	SW	1071	0	1093	15	0
67	SX	794	0	836	9	0
68	SY	651	0	655	6	0
69	Sb	945	0	1004	15	0
70	Sc	597	0	636	12	0
71	Sd	796	0	825	6	0
72	Se	629	0	623	8	0
73	Sg	505	0	540	5	0
74	Sh	417	0	416	9	0
75	Sj	502	0	547	6	0
76	St	31176	0	15856	134	0
All	All	174771	0	131986	1137	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 (1137) 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)
3:LC:11:THR:HG23	3:LC:13:THR:HG22	1.41	1.00
9:LI:50:ARG:HG2	44:Lt:2000:C:H5'	1.61	0.82
6:LF:2:GLY:HA3	44:Lt:729:A:H1'	1.61	0.81
3:LC:11:THR:CG2	3:LC:13:THR:HG22	2.09	0.81
19:LS:57:GLY:HA2	44:Lt:1504:C:H4'	1.61	0.81
49:SD:103:MET:HB3	49:SD:215:VAL:HG13	1.66	0.77
68:SY:6:ILE:HD13	68:SY:20:ILE:HG21	1.68	0.76
44:Lt:2459:C:H2'	44:Lt:2460:G:C8	2.20	0.75
30:Ld:50:ASN:HB3	30:Ld:76:GLY:HA2	1.69	0.75
32:Lf:81:ILE:HD11	32:Lf:91:PHE:CE2	2.23	0.74
66:SW:113:LEU:HD21	66:SW:120:ARG:HD3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Lf:81:ILE:HD11	32:Lf:91:PHE:HE2	1.51	0.74
32:Lf:91:PHE:HZ	32:Lf:99:ALA:HA	1.53	0.73
62:SR:124:LYS:HD3	76:St:926:C:H4'	1.71	0.72
65:SV:26:VAL:HA	65:SV:56:ARG:HA	1.72	0.72
6:LF:114:SER:HB2	6:LF:121:ALA:HB1	1.73	0.71
76:St:191:C:H2'	76:St:192:G:H8	1.54	0.71
11:LK:170:ASN:HA	11:LK:177:THR:HA	1.70	0.71
17:LQ:35:ILE:HA	17:LQ:38:MET:HE2	1.71	0.70
49:SD:229:SER:HA	49:SD:233:ASP:HB2	1.74	0.70
53:SH:137:ILE:HG21	53:SH:162:VAL:HG21	1.73	0.70
67:SX:101:ILE:HA	67:SX:104:ILE:HB	1.74	0.70
47:SB:48:ILE:HG22	47:SB:53:LEU:HB2	1.74	0.70
50:SE:11:ARG:HA	50:SE:28:ALA:HB2	1.74	0.69
3:LC:11:THR:HG23	3:LC:13:THR:CG2	2.22	0.69
15:LO:154:PRO:HB2	44:Lt:57:G:H5''	1.73	0.69
23:LW:13:ASN:HD21	44:Lt:2435:G:H1'	1.57	0.69
45:Lu:9:G:H1'	45:Lu:44:G:H2'	1.72	0.69
47:SB:77:ILE:HD11	47:SB:92:PHE:HB3	1.74	0.69
39:Ln:90:LEU:HD23	39:Ln:123:TYR:HB3	1.74	0.69
39:Ln:32:VAL:HB	39:Ln:169:ILE:HB	1.76	0.68
4:LD:126:C:H5''	15:LO:60:VAL:HG21	1.74	0.68
19:LS:173:ARG:HA	76:St:607:C:H42	1.59	0.68
10:LJ:26:VAL:HG11	10:LJ:76:MET:HB3	1.76	0.68
37:Lk:28:HIS:HB3	37:Lk:31:LYS:HG2	1.74	0.67
21:LU:114:ALA:HA	21:LU:117:ARG:HE	1.59	0.67
44:Lt:1311:G:H1	44:Lt:1453:C:H5	1.43	0.67
57:SL:60:LEU:HB3	57:SL:65:VAL:HB	1.78	0.66
18:LR:179:TRP:HB3	44:Lt:2154:G:H4'	1.75	0.66
76:St:1420:A:H2	76:St:1423:G:H1	1.43	0.66
9:LI:93:GLN:HA	9:LI:97:ALA:HB3	1.78	0.66
20:LT:22:VAL:HG11	21:LU:144:ILE:HG22	1.76	0.66
24:LX:45:ARG:HB3	44:Lt:1600:G:H2'	1.76	0.66
53:SH:12:PRO:HB2	53:SH:16:LEU:HD12	1.76	0.66
27:La:97:THR:C	27:La:99:ALA:H	2.03	0.66
50:SE:44:LEU:HD12	50:SE:82:PHE:HB3	1.77	0.66
10:LJ:124:CYS:HB3	10:LJ:128:VAL:HG22	1.78	0.65
32:Lf:91:PHE:CZ	32:Lf:99:ALA:HA	2.31	0.65
56:SK:127:ARG:HD2	75:Sj:31:ARG:HD3	1.79	0.65
63:ST:83:MET:HE1	63:ST:103:ILE:HA	1.78	0.65
66:SW:30:ALA:HA	66:SW:33:ASP:HB3	1.79	0.65
47:SB:178:VAL:HG13	47:SB:208:VAL:HG21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Ln:110:PHE:HB3	39:Ln:135:PRO:HA	1.78	0.65
76:St:66:C:H3'	76:St:67:C:H4'	1.77	0.65
2:LB:223:GLY:HA2	2:LB:271:GLY:HA3	1.80	0.64
44:Lt:1767:A:H2	44:Lt:1774:U:H3	1.44	0.64
6:LF:185:MET:HA	6:LF:188:PHE:HD2	1.62	0.64
44:Lt:1985:C:H4'	44:Lt:1985:C:OP1	1.96	0.64
62:SR:57:PHE:HA	62:SR:60:LYS:HE2	1.78	0.64
39:Ln:48:ARG:HA	39:Ln:159:PHE:HB2	1.78	0.64
4:LD:133:G:H1	44:Lt:9:U:H3	1.44	0.64
76:St:915:A:H2'	76:St:916:G:C8	2.33	0.64
76:St:734:G:H4'	76:St:1431:A:H4'	1.80	0.64
31:Le:4:VAL:H	31:Le:100:GLY:HA3	1.63	0.63
56:SK:162:THR:HA	56:SK:167:PRO:HG2	1.80	0.63
27:La:15:LEU:HB3	34:Lh:84:ARG:HG3	1.80	0.63
65:SV:37:ILE:HG13	65:SV:101:VAL:HA	1.81	0.63
10:LJ:172:LEU:HB3	43:Ls:86:ALA:HB1	1.80	0.63
61:SQ:44:VAL:HG11	61:SQ:85:ILE:HG21	1.78	0.63
15:LO:93:LYS:HD2	44:Lt:244:G:H1'	1.81	0.63
65:SV:13:LEU:HB3	65:SV:22:GLN:HA	1.81	0.62
38:Ll:20:LYS:HD3	38:Ll:68:VAL:HG22	1.80	0.62
23:LW:38:LEU:HD22	23:LW:64:ILE:HD13	1.79	0.62
46:SA:43:ILE:HD12	46:SA:52:PHE:HB3	1.80	0.62
51:SF:114:ILE:HD11	51:SF:125:VAL:HG12	1.81	0.62
39:Ln:112:ALA:HB2	39:Ln:135:PRO:HB2	1.82	0.62
76:St:1022:C:H2'	76:St:1023:G:H8	1.65	0.62
12:LL:45:PRO:HB3	12:LL:69:VAL:HG22	1.82	0.61
13:LM:28:ALA:HB3	44:Lt:821:G:H5'	1.81	0.61
23:LW:58:VAL:HG11	23:LW:124:ALA:HB3	1.80	0.61
28:Lb:2:PRO:HD2	44:Lt:509:G:H5''	1.82	0.61
5:LE:30:U:H3	5:LE:48:G:H1	1.48	0.61
76:St:1284:C:H1'	76:St:1287:C:H41	1.66	0.61
44:Lt:157:G:H1	44:Lt:172:C:H5	1.46	0.61
10:LJ:78:LYS:HB3	10:LJ:182:LEU:HD11	1.81	0.61
14:LN:10:GLY:HA2	14:LN:26:VAL:HG13	1.81	0.61
39:Ln:114:LYS:HB2	39:Ln:139:ALA:HB2	1.83	0.61
66:SW:26:ILE:HD13	66:SW:106:GLN:HB2	1.83	0.61
39:Ln:66:CYS:HA	39:Ln:83:ASN:HB3	1.82	0.61
32:Lf:69:ARG:HG2	44:Lt:1092:G:H5''	1.82	0.61
32:Lf:91:PHE:CZ	32:Lf:99:ALA:CA	2.84	0.61
76:St:5:C:H2'	76:St:6:G:H8	1.66	0.60
76:St:358:A:H2'	76:St:359:A:H8	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SX:58:ARG:HB2	76:St:1090:C:H4'	1.83	0.60
29:Lc:45:ARG:HH22	44:Lt:788:C:H5'	1.65	0.60
39:Ln:31:THR:H	39:Ln:209:THR:HG23	1.65	0.60
44:Lt:1958:G:H1'	44:Lt:1974:A:H2	1.66	0.60
55:SJ:7:LEU:HG	55:SJ:34:ILE:HG12	1.84	0.60
59:SO:26:LYS:NZ	76:St:486:C:H41	1.99	0.60
12:LL:167:PHE:HB2	12:LL:169:VAL:HG23	1.82	0.60
43:Ls:96:CYS:HB2	43:Ls:118:LEU:HD12	1.82	0.60
48:SC:78:LEU:HD21	57:SL:76:TYR:HB3	1.83	0.60
44:Lt:403:C:H2'	44:Lt:404:G:C8	2.37	0.60
76:St:1246:A:H1'	76:St:1247:C:H6	1.66	0.60
18:LR:67:LEU:HD13	18:LR:99:ILE:HD13	1.83	0.60
44:Lt:1947:G:H5''	44:Lt:1948:C:H4'	1.84	0.59
59:SO:85:VAL:HG23	59:SO:130:LEU:HD11	1.84	0.59
76:St:931:U:H3	76:St:942:G:H1	1.49	0.59
76:St:1132:C:H3'	76:St:1133:A:H4'	1.82	0.59
35:Li:126:GLU:HG2	37:Lk:86:TYR:HB3	1.83	0.59
26:LZ:2:LYS:HD2	26:LZ:7:VAL:HB	1.82	0.59
18:LR:68:ALA:HA	18:LR:97:MET:HE1	1.84	0.59
46:SA:131:ASP:HB3	46:SA:134:VAL:HG22	1.83	0.59
53:SH:121:THR:HG22	53:SH:124:SER:H	1.68	0.59
66:SW:2:SER:N	66:SW:5:THR:HG1	2.01	0.59
47:SB:32:LYS:HD2	47:SB:35:ARG:HE	1.66	0.59
58:SM:101:ARG:HG2	59:SO:11:ARG:HH22	1.68	0.59
50:SE:65:LEU:HD13	50:SE:80:PRO:HA	1.84	0.59
18:LR:174:ARG:HD3	28:Lb:56:LEU:HD11	1.84	0.59
34:Lh:56:PRO:HA	44:Lt:1404:C:H5''	1.85	0.59
44:Lt:695:C:H2'	44:Lt:696:G:H4'	1.84	0.59
44:Lt:403:C:H2'	44:Lt:404:G:H8	1.68	0.58
55:SJ:6:VAL:HG22	55:SJ:34:ILE:HD11	1.85	0.58
63:ST:111:VAL:HB	63:ST:117:ARG:HB2	1.84	0.58
18:LR:19:PRO:HG2	18:LR:27:ARG:HD2	1.85	0.58
9:LI:75:LEU:HD11	9:LI:188:ASP:HB3	1.85	0.58
46:SA:59:VAL:HG22	46:SA:167:PRO:HB2	1.86	0.58
3:LC:294:LYS:HB2	8:LH:157:PRO:HB3	1.86	0.58
25:LY:46:PRO:HD2	35:Li:109:PRO:HG3	1.86	0.58
44:Lt:1629:U:H1'	44:Lt:2400:U:H5''	1.86	0.58
56:SK:18:LYS:HE2	76:St:434:C:H5'	1.86	0.58
59:SO:107:ARG:HB2	59:SO:112:VAL:HG12	1.86	0.58
56:SK:171:PRO:HB2	76:St:396:G:H5'	1.86	0.58
5:LE:95:C:H4'	20:LT:116:HIS:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LK:43:VAL:HG11	11:LK:197:ALA:HB2	1.86	0.58
76:St:975:C:H2'	76:St:976:G:H8	1.68	0.58
3:LC:297:PRO:HG2	8:LH:144:TYR:HB3	1.86	0.57
16:LP:58:ARG:HA	16:LP:67:PRO:HD2	1.85	0.57
16:LP:40:ILE:HD11	16:LP:135:VAL:HG23	1.86	0.57
44:Lt:61:G:H22	44:Lt:78:U:H4'	1.69	0.57
46:SA:112:ASN:HD22	46:SA:118:ASN:HD22	1.49	0.57
1:LA:23:ARG:HG2	1:LA:52:ARG:HB3	1.86	0.57
76:St:1175:A:H4'	76:St:1231:G:H4'	1.86	0.57
34:Lh:35:ARG:HE	34:Lh:37:LYS:HG2	1.69	0.57
11:LK:160:PRO:HG3	44:Lt:2277:C:H5''	1.86	0.57
32:Lf:31:VAL:HB	44:Lt:403:C:H5''	1.86	0.57
54:SI:10:LYS:HG3	76:St:251:C:H5''	1.87	0.57
76:St:1107:C:H2'	76:St:1108:A:C8	2.40	0.57
76:St:1135:G:H2'	76:St:1136:U:C6	2.40	0.57
76:St:830:A:H2'	76:St:831:A:C8	2.40	0.57
6:LF:238:GLU:HB3	6:LF:241:ARG:HB2	1.87	0.56
76:St:707:G:H2'	76:St:708:A:C8	2.40	0.56
2:LB:13:ASN:HD22	2:LB:15:GLY:H	1.53	0.56
44:Lt:328:G:H1'	44:Lt:351:G:H21	1.70	0.56
46:SA:124:PRO:HD2	46:SA:147:ILE:HD13	1.87	0.56
76:St:191:C:H2'	76:St:192:G:C8	2.37	0.56
3:LC:11:THR:CG2	3:LC:13:THR:CG2	2.80	0.56
14:LN:112:ILE:HG12	16:LP:195:TYR:HB3	1.86	0.56
2:LB:227:GLU:HB2	2:LB:270:MET:HB2	1.86	0.56
17:LQ:63:TYR:HB2	17:LQ:79:LYS:HD2	1.88	0.56
44:Lt:1582:C:H2'	44:Lt:1585:G:C8	2.41	0.56
12:LL:54:ILE:HB	12:LL:59:ILE:HD12	1.86	0.56
46:SA:132:PRO:HB3	46:SA:162:ILE:HD11	1.88	0.56
46:SA:161:PHE:HA	68:SY:67:ARG:HG2	1.87	0.56
63:ST:125:VAL:HG22	63:ST:129:ARG:HG2	1.88	0.56
65:SV:130:LEU:HD23	65:SV:147:VAL:HG11	1.86	0.56
2:LB:343:LEU:HD21	44:Lt:2516:G:H5'	1.88	0.56
44:Lt:98:C:H2'	44:Lt:99:G:C8	2.41	0.56
48:SC:86:ASP:HB2	48:SC:89:ASN:HB2	1.87	0.56
61:SQ:78:THR:C	61:SQ:80:ASP:H	2.13	0.56
76:St:179:G:H22	76:St:596:C:H3'	1.71	0.56
3:LC:162:VAL:HG23	3:LC:164:VAL:HG23	1.88	0.56
76:St:996:C:H2'	76:St:997:G:C8	2.41	0.56
38:LI:65:LYS:HB3	38:LI:67:LYS:HG2	1.88	0.56
57:SL:40:ASP:HB3	57:SL:43:GLY:HA3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SV:27:LEU:HD11	65:SV:60:LEU:HD13	1.86	0.56
50:SE:35:PRO:HA	50:SE:144:ALA:HB3	1.87	0.55
55:SJ:44:ASN:HD22	55:SJ:129:PHE:HZ	1.54	0.55
76:St:1033:C:H2'	76:St:1034:G:C8	2.40	0.55
47:SB:161:VAL:HG21	47:SB:208:VAL:HA	1.88	0.55
66:SW:16:PHE:HB3	66:SW:56:ALA:HB1	1.87	0.55
1:LA:36:GLU:HG3	1:LA:91:GLY:HA2	1.88	0.55
44:Lt:2058:U:H3'	44:Lt:2059:A:H5''	1.88	0.55
48:SC:78:LEU:HD13	57:SL:21:SER:HB2	1.88	0.55
59:SO:26:LYS:HA	59:SO:29:LYS:HG2	1.89	0.55
65:SV:89:ASN:HB2	76:St:1238:G:H5'	1.89	0.55
55:SJ:80:ASP:HA	55:SJ:124:LYS:HA	1.88	0.55
65:SV:27:LEU:HD12	65:SV:57:ALA:HA	1.88	0.55
24:LX:7:CYS:SG	24:LX:33:CYS:N	2.70	0.55
59:SO:57:ILE:HD11	59:SO:116:PRO:HD2	1.89	0.55
65:SV:126:HIS:HE1	76:St:1235:C:H5''	1.71	0.55
28:Lb:64:ARG:HB2	28:Lb:67:ILE:HB	1.88	0.55
33:Lg:12:ALA:HB3	33:Lg:92:VAL:HG22	1.88	0.55
20:LT:121:ILE:HD13	21:LU:154:LYS:HG2	1.88	0.55
34:Lh:4:CYS:HB3	34:Lh:31:LEU:HD22	1.87	0.55
76:St:1167:C:H2'	76:St:1168:G:H8	1.72	0.55
8:LH:69:GLN:HA	21:LU:143:SER:HA	1.88	0.55
44:Lt:83:G:H5'	44:Lt:445:G:H4'	1.87	0.55
49:SD:149:GLN:HA	76:St:810:U:H3'	1.88	0.55
13:LM:28:ALA:HA	44:Lt:512:G:H21	1.71	0.55
65:SV:99:ILE:HG22	65:SV:104:ILE:HG12	1.89	0.55
66:SW:35:VAL:HG21	76:St:1201:C:H4'	1.87	0.55
76:St:1329:C:H2'	76:St:1330:G:C8	2.42	0.55
1:LA:177:LYS:HG3	42:Lq:26:LEU:HD21	1.89	0.54
49:SD:89:GLN:HB2	49:SD:228:LEU:HD11	1.87	0.54
62:SR:29:LYS:HB3	62:SR:32:ASP:HB2	1.88	0.54
76:St:1022:C:H2'	76:St:1023:G:C8	2.42	0.54
3:LC:72:LEU:HD21	44:Lt:1126:U:H5'	1.88	0.54
44:Lt:760:A:H1'	44:Lt:2058:U:H5'	1.90	0.54
44:Lt:910:U:H5	44:Lt:995:G:H1	1.56	0.54
6:LF:269:PRO:HB2	6:LF:271:ARG:HD3	1.89	0.54
44:Lt:1939:G:H2'	44:Lt:1940:G:C8	2.43	0.54
38:Ll:15:ALA:HA	38:Ll:20:LYS:HG2	1.90	0.54
5:LE:55:A:H4'	12:LL:10:ARG:HD2	1.90	0.54
27:La:16:GLN:HE21	44:Lt:1305:A:H5'	1.73	0.54
47:SB:37:VAL:HG21	47:SB:60:ILE:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:St:1271:U:H4'	76:St:1272:G:H4'	1.88	0.54
23:LW:89:VAL:HG22	23:LW:97:TRP:HE3	1.72	0.54
76:St:945:C:H5	76:St:1162:C:H2'	1.72	0.54
2:LB:245:GLY:HA3	44:Lt:1521:G:H5''	1.89	0.54
9:LI:36:ARG:HG3	9:LI:39:ARG:HH21	1.73	0.54
34:Lh:60:PRO:HB2	44:Lt:1446:C:H4'	1.89	0.54
32:Lf:79:HIS:HB2	32:Lf:91:PHE:CZ	2.42	0.54
16:LP:12:ILE:HD11	16:LP:126:LEU:HD23	1.90	0.53
23:LW:15:PHE:HE1	44:Lt:2457:G:H5'	1.73	0.53
2:LB:287:THR:HA	2:LB:320:ASP:HA	1.90	0.53
14:LN:7:VAL:HG22	14:LN:57:LEU:HD11	1.89	0.53
76:St:5:C:H2'	76:St:6:G:C8	2.43	0.53
17:LQ:21:VAL:HG11	17:LQ:89:VAL:HG11	1.90	0.53
44:Lt:790:G:N2	44:Lt:792:C:H3'	2.24	0.53
39:Ln:69:ALA:HA	39:Ln:113:SER:HB2	1.91	0.53
10:LJ:12:PRO:HG2	10:LJ:15:VAL:HB	1.91	0.53
44:Lt:2690:G:H3'	44:Lt:2691:G:H8	1.73	0.53
50:SE:206:THR:HB	50:SE:222:LEU:HD22	1.91	0.53
76:St:320:C:H2'	76:St:321:G:C8	2.43	0.53
32:Lf:81:ILE:CD1	32:Lf:91:PHE:HE2	2.20	0.53
49:SD:31:ILE:HB	49:SD:232:HIS:NE2	2.23	0.53
11:LK:49:CYS:HB3	11:LK:168:SER:HB3	1.89	0.53
15:LO:135:ILE:HG13	15:LO:151:ILE:HD13	1.91	0.53
34:Lh:83:LEU:O	34:Lh:87:ILE:HG12	2.08	0.52
46:SA:82:VAL:HB	46:SA:104:PHE:HB2	1.90	0.52
3:LC:291:ILE:HD12	8:LH:156:ILE:HD12	1.90	0.52
64:SU:63:ARG:HH22	76:St:1105:G:H1	1.56	0.52
39:Ln:35:GLN:HG3	44:Lt:1978:U:H1'	1.92	0.52
39:Ln:205:TYR:HB3	39:Ln:213:SER:HB2	1.90	0.52
46:SA:55:ASN:HB3	46:SA:58:LYS:HE3	1.91	0.52
76:St:975:C:H2'	76:St:976:G:C8	2.44	0.52
48:SC:209:GLU:HB2	64:SU:43:ILE:HB	1.90	0.52
50:SE:161:LYS:HE3	50:SE:170:ASP:HB2	1.92	0.52
3:LC:14:GLN:NE2	3:LC:17:GLU:HG2	2.24	0.52
6:LF:182:PRO:HB2	44:Lt:2171:A:H4'	1.91	0.52
17:LQ:137:SER:HB2	44:Lt:1845:G:H5'	1.91	0.52
55:SJ:47:ILE:HD11	55:SJ:63:VAL:HG13	1.92	0.52
75:Sj:39:ASN:HA	75:Sj:43:VAL:HG12	1.91	0.52
20:LT:100:MET:HE1	20:LT:120:ILE:HG13	1.92	0.52
23:LW:72:PRO:HG3	23:LW:75:ARG:HH21	1.74	0.52
44:Lt:224:U:H2'	44:Lt:225:A:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:Ls:112:ARG:HE	44:Lt:2523:G:H5''	1.74	0.52
48:SC:18:LEU:HB2	67:SX:87:MET:HE1	1.89	0.52
6:LF:51:PHE:CZ	6:LF:174:ALA:HB2	2.45	0.52
58:SM:131:LYS:HB2	76:St:250:G:H3'	1.91	0.52
59:SO:68:LYS:HD2	75:Sj:6:LEU:HD12	1.90	0.52
23:LW:47:LYS:HZ1	44:Lt:2459:C:H4'	1.74	0.52
44:Lt:398:C:H2'	44:Lt:399:G:C8	2.45	0.52
44:Lt:452:G:H21	44:Lt:455:C:H5	1.57	0.52
47:SB:155:LYS:HB3	47:SB:160:ARG:HD3	1.92	0.52
56:SK:53:ILE:HD13	56:SK:81:LEU:HD21	1.92	0.52
69:Sb:10:LYS:HB2	76:St:555:G:H1	1.74	0.52
39:Ln:93:PHE:HB3	39:Ln:100:ILE:HG12	1.92	0.52
49:SD:13:ILE:HG12	49:SD:18:ASN:HB2	1.92	0.52
76:St:306:C:H2'	76:St:307:C:C6	2.44	0.52
43:Ls:110:CYS:SG	43:Ls:113:CYS:N	2.80	0.51
16:LP:78:ARG:HB2	16:LP:101:VAL:HG21	1.92	0.51
44:Lt:1346:G:H2'	44:Lt:1347:G:C8	2.45	0.51
63:ST:59:PRO:HB2	63:ST:62:LEU:HB2	1.91	0.51
76:St:1194:G:H4'	76:St:1212:G:H21	1.75	0.51
6:LF:34:LYS:HA	21:LU:27:LEU:HD11	1.91	0.51
64:SU:106:GLN:HA	64:SU:109:ILE:HD12	1.92	0.51
76:St:546:U:H2'	76:St:547:C:H6	1.74	0.51
35:Li:59:LEU:HD13	35:Li:76:PHE:HA	1.91	0.51
48:SC:210:ILE:HD12	64:SU:15:LYS:HG2	1.92	0.51
73:Sg:17:SER:C	73:Sg:19:ARG:H	2.19	0.51
3:LC:67:ARG:HB2	3:LC:69:VAL:HG22	1.91	0.51
3:LC:198:ILE:HD13	3:LC:217:CYS:HB3	1.92	0.51
11:LK:47:PRO:HD2	11:LK:141:ARG:HA	1.92	0.51
55:SJ:26:ILE:HG13	72:Se:48:LEU:HD13	1.93	0.51
65:SV:8:ASN:N	70:Sc:21:PHE:HB3	2.25	0.51
67:SX:27:ILE:HB	67:SX:92:PHE:HB2	1.92	0.51
44:Lt:326:A:H1'	44:Lt:327:A:H5''	1.93	0.51
47:SB:95:HIS:HB3	47:SB:107:TYR:HE2	1.75	0.51
20:LT:83:GLY:O	20:LT:85:HIS:NE2	2.44	0.51
76:St:988:C:H2'	76:St:989:G:C8	2.45	0.51
2:LB:227:GLU:HG3	2:LB:231:THR:HB	1.93	0.51
50:SE:124:CYS:HB3	50:SE:141:THR:HB	1.92	0.51
50:SE:131:LEU:HG	76:St:182:G:H1'	1.93	0.51
51:SF:88:LEU:HD11	70:Sc:72:VAL:HG21	1.92	0.51
9:LI:167:LEU:HD22	9:LI:179:VAL:HB	1.92	0.51
49:SD:59:ILE:HG22	49:SD:62:ARG:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:ST:130:GLN:HA	63:ST:133:VAL:HB	1.93	0.51
2:LB:174:LYS:HD2	44:Lt:2626:C:H5'	1.93	0.50
41:Lp:67:VAL:HG12	41:Lp:80:PHE:HB3	1.93	0.50
72:Se:75:GLU:HG3	72:Se:123:GLN:HB2	1.92	0.50
76:St:1033:C:H2'	76:St:1034:G:H8	1.76	0.50
48:SC:143:ILE:HG23	48:SC:191:LYS:HB2	1.92	0.50
70:Sc:22:ALA:HB3	70:Sc:27:MET:HG2	1.93	0.50
5:LE:28:C:H5''	12:LL:137:ARG:HG2	1.91	0.50
9:LI:39:ARG:O	9:LI:43:GLN:HG2	2.11	0.50
44:Lt:1341:C:H2'	44:Lt:1342:G:C8	2.46	0.50
47:SB:159:VAL:HG21	47:SB:204:SER:HA	1.93	0.50
51:SF:114:ILE:HD12	51:SF:123:GLN:HB2	1.94	0.50
71:Sd:38:ARG:HD2	76:St:1453:U:H2'	1.93	0.50
76:St:1002:C:H2'	76:St:1003:G:C8	2.46	0.50
16:LP:15:ARG:HH22	44:Lt:1017:G:H4'	1.75	0.50
24:LX:51:ARG:HA	24:LX:56:TYR:HD2	1.75	0.50
44:Lt:2192:C:H2'	44:Lt:2193:G:C8	2.46	0.50
8:LH:202:LEU:HB3	8:LH:234:MET:HB3	1.93	0.50
18:LR:179:TRP:CH2	28:Lb:46:ASP:HA	2.46	0.50
26:LZ:83:ILE:HG21	26:LZ:99:ILE:HD11	1.94	0.50
27:La:98:VAL:HG12	27:La:107:ILE:HD11	1.94	0.50
34:Lh:52:ILE:HD11	34:Lh:55:ILE:HD12	1.94	0.50
44:Lt:1877:C:H2'	44:Lt:1878:A:C8	2.46	0.50
53:SH:66:PRO:HB2	53:SH:69:MET:HG3	1.93	0.50
74:Sh:120:CYS:HB2	74:Sh:123:CYS:H	1.77	0.50
23:LW:99:TYR:CZ	24:LX:22:PHE:HB2	2.46	0.50
46:SA:189:ARG:HG3	46:SA:194:ILE:HD12	1.94	0.50
51:SF:113:ARG:HA	51:SF:122:ARG:HA	1.94	0.50
62:SR:98:ASN:HB2	62:SR:122:SER:HA	1.94	0.50
5:LE:64:C:H5'	5:LE:65:A:H5''	1.94	0.50
32:Lf:91:PHE:CZ	32:Lf:99:ALA:HB2	2.47	0.50
47:SB:81:GLN:HB3	47:SB:88:GLN:HB3	1.93	0.50
47:SB:193:ARG:HD3	76:St:2:A:H1'	1.94	0.50
1:LA:229:ALA:HB3	1:LA:234:LYS:HG3	1.94	0.49
2:LB:102:VAL:HG11	2:LB:153:HIS:HB2	1.93	0.49
12:LL:53:THR:HG23	12:LL:60:ARG:HA	1.93	0.49
12:LL:133:ARG:HG3	12:LL:154:ILE:HD11	1.94	0.49
15:LO:120:TRP:HE1	15:LO:123:GLN:HB2	1.77	0.49
27:La:97:THR:C	27:La:99:ALA:N	2.69	0.49
44:Lt:2084:C:H2'	44:Lt:2085:G:C8	2.47	0.49
2:LB:45:ALA:H	2:LB:180:ILE:HG23	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LB:78:ILE:HG12	2:LB:305:ILE:HD11	1.94	0.49
22:LV:96:ARG:HD2	22:LV:110:TYR:HA	1.94	0.49
25:LY:74:GLN:HG3	25:LY:80:THR:HB	1.94	0.49
76:St:320:C:H2'	76:St:321:G:H8	1.77	0.49
76:St:628:C:H2'	76:St:629:G:C8	2.47	0.49
76:St:693:C:H2'	76:St:694:A:C8	2.46	0.49
5:LE:36:C:H5'	6:LF:163:THR:HB	1.94	0.49
44:Lt:1442:A:H2'	44:Lt:1443:A:C8	2.47	0.49
50:SE:100:ARG:HB2	50:SE:114:ILE:HD13	1.94	0.49
1:LA:111:THR:HG23	42:Lq:83:ILE:HD12	1.93	0.49
11:LK:29:PRO:HG3	11:LK:125:THR:HG21	1.94	0.49
50:SE:29:PRO:HB3	50:SE:45:ILE:HD12	1.94	0.49
14:LN:127:ALA:HA	16:LP:175:ILE:HD12	1.94	0.49
61:SQ:103:THR:HG22	61:SQ:139:ARG:HB2	1.95	0.49
71:Sd:22:ARG:HA	71:Sd:28:ARG:O	2.12	0.49
76:St:1078:G:H2'	76:St:1079:G:C8	2.47	0.49
3:LC:296:ASP:HB3	3:LC:299:SER:HB3	1.94	0.49
16:LP:108:CYS:HA	44:Lt:2603:G:H4'	1.95	0.49
52:SG:24:ILE:HG21	52:SG:29:LYS:HG2	1.95	0.49
53:SH:112:LYS:HE3	53:SH:114:ILE:HD13	1.94	0.49
76:St:96:G:H4'	76:St:533:G:H21	1.77	0.49
17:LQ:14:GLY:HA3	17:LQ:101:ALA:HB2	1.95	0.49
53:SH:106:TYR:HA	53:SH:115:ARG:HA	1.93	0.49
44:Lt:1198:G:H21	44:Lt:1474:A:H8	1.60	0.49
63:ST:23:TYR:CG	63:ST:39:PHE:HB3	2.46	0.49
70:Sc:58:ARG:HA	70:Sc:61:ARG:HE	1.78	0.49
76:St:1281:C:H2'	76:St:1282:G:C8	2.48	0.49
12:LL:17:LEU:HD22	12:LL:80:ILE:HG13	1.95	0.49
23:LW:98:ILE:HG13	23:LW:99:TYR:N	2.28	0.49
76:St:1249:C:H4'	76:St:1287:C:H4'	1.95	0.49
6:LF:60:ILE:H	6:LF:80:SER:HB3	1.78	0.49
44:Lt:2156:C:H5'	44:Lt:2185:G:H5''	1.95	0.49
49:SD:19:PRO:HB2	61:SQ:88:ARG:HH21	1.78	0.49
52:SG:78:ARG:HA	52:SG:104:ARG:HA	1.95	0.49
76:St:1267:G:H2'	76:St:1268:U:C6	2.48	0.49
3:LC:210:ASN:HD22	44:Lt:176:C:H6	1.59	0.48
38:Ll:14:ILE:HG23	38:Ll:18:ARG:HB3	1.95	0.48
70:Sc:70:ALA:HB2	70:Sc:84:MET:HG2	1.95	0.48
51:SF:116:LYS:HG2	51:SF:121:ARG:HB3	1.95	0.48
53:SH:37:ARG:HD3	53:SH:76:ASN:HD21	1.78	0.48
58:SM:73:VAL:HB	58:SM:118:GLY:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LI:43:GLN:HG3	15:LO:28:TRP:HH2	1.76	0.48
29:Lc:49:ASN:HB3	44:Lt:785:C:H4'	1.94	0.48
44:Lt:1542:G:H21	44:Lt:1821:C:H1'	1.79	0.48
66:SW:80:SER:HB2	66:SW:94:ARG:HA	1.94	0.48
69:Sb:57:LEU:HD23	69:Sb:73:CYS:HB3	1.95	0.48
2:LB:43:LEU:HD12	2:LB:203:ILE:HG21	1.96	0.48
15:LO:28:TRP:O	15:LO:32:GLN:HG2	2.12	0.48
20:LT:17:PHE:HD2	20:LT:20:PRO:HG3	1.79	0.48
44:Lt:2042:G:C8	44:Lt:2288:U:H5''	2.48	0.48
65:SV:143:ARG:CZ	65:SV:143:ARG:HA	2.43	0.48
20:LT:83:GLY:O	20:LT:85:HIS:CD2	2.67	0.48
28:Lb:115:ARG:HG3	44:Lt:459:A:H8	1.77	0.48
58:SM:95:TYR:C	58:SM:97:ARG:H	2.22	0.48
59:SO:20:ASN:HD22	76:St:852:G:H1	1.60	0.48
62:SR:25:LEU:HD11	62:SR:112:VAL:HG11	1.95	0.48
65:SV:84:MET:O	65:SV:85:LEU:HB2	2.13	0.48
9:LI:43:GLN:HG3	15:LO:28:TRP:CH2	2.48	0.48
17:LQ:29:TYR:HA	17:LQ:119:VAL:HG21	1.95	0.48
17:LQ:90:VAL:HG13	17:LQ:148:LEU:HD11	1.96	0.48
51:SF:154:PRO:HD3	70:Sc:43:THR:HG21	1.95	0.48
76:St:51:U:H2'	76:St:52:G:C8	2.47	0.48
3:LC:200:ASN:HB2	3:LC:219:VAL:HG21	1.95	0.48
12:LL:23:ILE:HB	12:LL:30:LEU:HD22	1.94	0.48
12:LL:47:PHE:HB3	12:LL:64:LYS:HG3	1.96	0.48
46:SA:77:ALA:HA	46:SA:101:ALA:HA	1.95	0.48
53:SH:9:ILE:HA	53:SH:12:PRO:HD2	1.96	0.48
61:SQ:101:GLY:HA2	61:SQ:106:ARG:HD3	1.95	0.48
34:Lh:42:ALA:HB2	34:Lh:57:ARG:HG2	1.94	0.48
48:SC:166:THR:HG22	76:St:1070:G:H5''	1.95	0.48
62:SR:18:ARG:HG3	62:SR:36:LYS:HE3	1.95	0.48
76:St:1167:C:H2'	76:St:1168:G:C8	2.49	0.48
44:Lt:1429:G:H2'	44:Lt:1430:G:C8	2.49	0.48
44:Lt:1443:A:H3'	44:Lt:1444:G:H8	1.77	0.48
44:Lt:2161:C:H2'	44:Lt:2162:G:C8	2.48	0.48
53:SH:72:SER:HA	53:SH:75:LYS:HG2	1.96	0.48
36:Lj:80:ARG:HE	36:Lj:80:ARG:HB3	1.43	0.48
38:LI:31:ARG:HD3	38:LI:31:ARG:HA	1.80	0.48
48:SC:38:ALA:HB1	48:SC:64:VAL:HG22	1.95	0.48
63:ST:36:ALA:HB2	63:ST:87:VAL:HG13	1.96	0.48
1:LA:145:LYS:HB3	1:LA:157:LEU:HD12	1.96	0.47
55:SJ:106:THR:HG21	55:SJ:121:ILE:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SV:17:PHE:HB3	65:SV:101:VAL:HG21	1.95	0.47
72:Se:74:LEU:HD23	72:Se:122:ARG:HB2	1.96	0.47
44:Lt:47:A:H4'	44:Lt:48:G:H5'	1.95	0.47
64:SU:26:PRO:HA	64:SU:61:MET:HB3	1.96	0.47
23:LW:58:VAL:HG11	23:LW:124:ALA:CB	2.43	0.47
29:Lc:53:GLN:HG2	29:Lc:55:LEU:HG	1.95	0.47
44:Lt:740:U:H3'	44:Lt:741:G:H8	1.78	0.47
44:Lt:783:C:H2'	44:Lt:784:G:H8	1.79	0.47
49:SD:136:ARG:HB3	49:SD:216:LYS:HG2	1.97	0.47
60:SP:78:LYS:HB3	60:SP:80:LEU:HD22	1.96	0.47
69:Sb:40:LYS:HB2	69:Sb:40:LYS:HE2	1.70	0.47
72:Se:106:ILE:HG23	72:Se:113:ALA:HB3	1.96	0.47
76:St:722:U:H2'	76:St:723:C:O4'	2.13	0.47
2:LB:238:LEU:HD21	2:LB:250:ALA:HB2	1.96	0.47
3:LC:184:MET:HE2	3:LC:184:MET:HB3	1.75	0.47
38:Ll:5:ILE:HB	38:Ll:47:TYR:HB3	1.96	0.47
44:Lt:1582:C:H2'	44:Lt:1585:G:H8	1.78	0.47
46:SA:196:ARG:HD3	68:SY:51:LYS:HD3	1.95	0.47
52:SG:30:SER:HA	52:SG:33:ILE:HG23	1.96	0.47
53:SH:8:LYS:HD3	53:SH:28:LEU:HD22	1.95	0.47
56:SK:81:LEU:HB3	56:SK:87:LEU:HB2	1.96	0.47
59:SO:70:VAL:HG22	59:SO:72:VAL:HG22	1.97	0.47
36:Lj:58:LYS:HA	36:Lj:58:LYS:HD3	1.70	0.47
44:Lt:533:A:H5''	44:Lt:637:C:H41	1.80	0.47
44:Lt:700:U:H2'	44:Lt:701:U:C6	2.49	0.47
44:Lt:729:A:H61	44:Lt:750:C:H1'	1.79	0.47
56:SK:66:ASN:HA	56:SK:71:ARG:HE	1.79	0.47
9:LI:120:ILE:HG13	9:LI:180:CYS:HB3	1.96	0.47
17:LQ:94:LEU:HD11	17:LQ:114:VAL:HG22	1.97	0.47
19:LS:126:LYS:HA	44:Lt:558:G:H4'	1.95	0.47
44:Lt:1181:C:H2'	44:Lt:1182:G:C8	2.50	0.47
63:ST:120:LEU:HD12	63:ST:120:LEU:HA	1.78	0.47
64:SU:3:LYS:HE2	76:St:1120:G:H1'	1.96	0.47
76:St:746:A:H2	76:St:766:U:H3	1.60	0.47
76:St:1000:C:H2'	76:St:1001:G:C8	2.50	0.47
16:LP:9:LYS:HA	16:LP:37:LYS:HB2	1.96	0.47
23:LW:23:VAL:HG13	23:LW:54:PRO:HB2	1.96	0.47
44:Lt:98:C:H2'	44:Lt:99:G:H8	1.78	0.47
48:SC:46:CYS:HB2	48:SC:53:CYS:HB3	1.53	0.47
50:SE:79:ASP:HB3	50:SE:82:PHE:HB2	1.96	0.47
56:SK:104:ASP:HA	56:SK:107:LYS:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Sb:97:ILE:HD12	69:Sb:97:ILE:HA	1.81	0.47
3:LC:177:ILE:HG23	3:LC:188:ARG:HG3	1.96	0.47
19:LS:44:LEU:HD22	19:LS:49:ILE:HD12	1.97	0.47
32:Lf:92:MET:H	32:Lf:92:MET:HG3	1.46	0.47
44:Lt:61:G:N2	44:Lt:78:U:H4'	2.30	0.47
44:Lt:1957:G:H21	44:Lt:1974:A:H1'	1.79	0.47
48:SC:24:GLU:HA	48:SC:27:LEU:HD12	1.95	0.47
60:SP:85:PRO:HD3	60:SP:135:LEU:HD21	1.97	0.47
69:Sb:116:LEU:HA	69:Sb:120:GLY:HA2	1.96	0.47
1:LA:102:LEU:HD21	1:LA:166:ILE:HD11	1.97	0.47
9:LI:66:ARG:HD2	9:LI:66:ARG:HA	1.43	0.47
44:Lt:607:C:H2'	44:Lt:608:G:H8	1.79	0.47
44:Lt:1884:G:H3'	44:Lt:1886:A:H5''	1.97	0.47
65:SV:126:HIS:CE1	76:St:1235:C:H5''	2.50	0.47
76:St:673:C:H2'	76:St:674:G:C8	2.49	0.47
76:St:1290:C:H2'	76:St:1291:G:C8	2.50	0.47
3:LC:35:PHE:O	3:LC:39:GLN:HG2	2.15	0.46
3:LC:202:GLU:HB3	3:LC:204:VAL:HG13	1.97	0.46
23:LW:19:CYS:HA	23:LW:57:SER:HB3	1.97	0.46
23:LW:47:LYS:CD	23:LW:47:LYS:H	2.28	0.46
44:Lt:1935:G:H2'	44:Lt:1936:G:C8	2.50	0.46
44:Lt:2486:G:H2'	44:Lt:2487:G:H8	1.80	0.46
45:Lu:17:G:H1	45:Lu:54:U:H1'	1.79	0.46
52:SG:99:LYS:HE3	52:SG:101:LYS:HE3	1.95	0.46
55:SJ:18:GLN:HE21	55:SJ:18:GLN:HB3	1.44	0.46
61:SQ:43:HIS:NE2	61:SQ:52:THR:HB	2.30	0.46
74:Sh:120:CYS:HB2	74:Sh:123:CYS:HB2	1.42	0.46
9:LI:32:VAL:HG21	25:LY:26:ARG:HD3	1.97	0.46
11:LK:57:LYS:HG2	11:LK:130:SER:HA	1.97	0.46
44:Lt:2161:C:H2'	44:Lt:2162:G:H8	1.80	0.46
44:Lt:2663:C:H2'	44:Lt:2664:G:C8	2.50	0.46
15:LO:184:LEU:HB3	15:LO:188:LYS:HG2	1.97	0.46
19:LS:29:GLU:HA	19:LS:32:ILE:HD12	1.96	0.46
24:LX:10:CYS:N	24:LX:37:CYS:SG	2.86	0.46
56:SK:60:LEU:HD22	56:SK:70:ARG:HA	1.96	0.46
73:Sg:12:VAL:HA	73:Sg:25:VAL:HG12	1.97	0.46
76:St:1164:G:N3	76:St:1164:G:H2'	2.30	0.46
3:LC:92:ALA:HB1	44:Lt:520:C:H5''	1.98	0.46
44:Lt:224:U:H2'	44:Lt:225:A:H8	1.81	0.46
44:Lt:328:G:H1'	44:Lt:351:G:N2	2.29	0.46
44:Lt:1194:U:H2'	44:Lt:1196:U:C5	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LF:189:PRO:HD2	6:LF:201:LEU:HD13	1.98	0.46
44:Lt:84:C:H1'	44:Lt:85:U:C6	2.50	0.46
44:Lt:85:U:HO2'	44:Lt:86:A:H8	1.61	0.46
53:SH:158:LEU:HD11	53:SH:187:PHE:HD2	1.80	0.46
58:SM:99:GLU:HG2	59:SO:10:ALA:HB3	1.98	0.46
3:LC:104:LYS:HE3	44:Lt:507:G:H5''	1.98	0.46
23:LW:13:ASN:ND2	44:Lt:2435:G:H1'	2.29	0.46
44:Lt:749:C:H2'	44:Lt:750:C:O4'	2.16	0.46
46:SA:129:VAL:HG23	46:SA:151:SER:HB2	1.98	0.46
73:Sg:26:LYS:HD3	73:Sg:36:GLN:HB3	1.98	0.46
74:Sh:88:ARG:HH11	76:St:958:C:H1'	1.80	0.46
75:Sj:58:ASN:HB3	75:Sj:61:ILE:HG12	1.96	0.46
76:St:209:C:H2'	76:St:210:G:C8	2.50	0.46
76:St:548:C:H2'	76:St:549:A:C8	2.51	0.46
13:LM:184:ILE:HG13	28:Lb:82:ILE:HA	1.97	0.46
13:LM:199:ASN:HD22	13:LM:199:ASN:HA	1.57	0.46
16:LP:11:HIS:HA	16:LP:121:MET:HA	1.98	0.46
18:LR:48:LEU:HD12	18:LR:48:LEU:HA	1.77	0.46
32:Lf:30:PHE:HB2	32:Lf:33:VAL:HG23	1.98	0.46
44:Lt:15:G:H2'	44:Lt:16:G:C8	2.51	0.46
50:SE:181:VAL:HG12	50:SE:227:VAL:HA	1.96	0.46
74:Sh:100:ARG:HD3	74:Sh:100:ARG:HA	1.76	0.46
76:St:253:C:H2'	76:St:254:G:C8	2.51	0.46
3:LC:264:ILE:HD13	3:LC:269:ILE:HG12	1.98	0.46
10:LJ:168:LEU:HD13	10:LJ:168:LEU:HA	1.85	0.46
39:Ln:157:VAL:HG21	39:Ln:189:PHE:HD2	1.81	0.46
45:Lu:53:A:H2	45:Lu:57:A:H8	1.63	0.46
1:LA:82:MET:HE2	1:LA:88:VAL:HG11	1.97	0.46
3:LC:183:LYS:HA	3:LC:188:ARG:HA	1.98	0.46
7:LG:38:ASN:HD22	7:LG:41:ARG:HG3	1.81	0.46
12:LL:21:ILE:HD11	12:LL:125:MET:HE2	1.98	0.46
15:LO:56:LYS:HG2	44:Lt:129:U:H4'	1.97	0.46
39:Ln:96:ASP:HB3	39:Ln:99:GLN:HB2	1.98	0.46
46:SA:85:ARG:HG3	46:SA:134:VAL:HG21	1.97	0.46
52:SG:75:LYS:HE2	52:SG:79:ALA:HB2	1.98	0.46
55:SJ:6:VAL:HG23	55:SJ:29:PRO:HG2	1.97	0.46
75:Sj:22:LYS:HB3	75:Sj:24:LYS:HZ3	1.81	0.46
4:LD:139:U:H2'	4:LD:140:G:C8	2.51	0.46
33:Lg:86:GLN:HE22	44:Lt:377:C:H5'	1.81	0.46
44:Lt:1141:G:C4	44:Lt:1482:A:H1'	2.51	0.46
53:SH:59:LYS:O	53:SH:91:HIS:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SV:100:LEU:HD12	65:SV:101:VAL:HG23	1.97	0.46
2:LB:158:ARG:HG2	2:LB:181:GLN:HA	1.97	0.45
2:LB:243:ARG:HG2	44:Lt:2370:C:H5'	1.98	0.45
25:LY:105:LYS:HA	25:LY:105:LYS:HD3	1.68	0.45
42:Lq:79:ALA:O	42:Lq:83:ILE:HG12	2.17	0.45
44:Lt:567:C:H2'	44:Lt:568:C:C6	2.51	0.45
66:SW:40:SER:HB3	66:SW:93:LYS:HB2	1.97	0.45
75:Sj:29:ARG:HB2	76:St:389:C:H2'	1.97	0.45
1:LA:177:LYS:HB2	42:Lq:29:ILE:HG21	1.98	0.45
52:SG:42:PHE:HE1	52:SG:117:VAL:HG21	1.81	0.45
56:SK:110:LEU:O	56:SK:114:ILE:HG12	2.16	0.45
58:SM:73:VAL:HG13	58:SM:82:ILE:HG13	1.99	0.45
62:SR:54:HIS:HA	62:SR:80:LEU:HD13	1.97	0.45
66:SW:8:PRO:HB2	66:SW:11:VAL:HG23	1.98	0.45
28:Lb:2:PRO:HB2	28:Lb:5:ILE:HG12	1.98	0.45
44:Lt:1866:C:H2'	44:Lt:1867:G:H8	1.80	0.45
57:SL:29:ARG:H	57:SL:29:ARG:HG2	1.61	0.45
76:St:687:G:H1	76:St:698:G:H1	1.65	0.45
1:LA:62:GLN:HG2	1:LA:71:ARG:HE	1.80	0.45
8:LH:85:ARG:HB3	8:LH:128:TYR:CD2	2.52	0.45
20:LT:87:MET:HG3	44:Lt:913:G:H4'	1.99	0.45
44:Lt:2016:G:H4'	44:Lt:2018:C:C2	2.51	0.45
49:SD:81:ASN:HD22	49:SD:109:LYS:HD3	1.81	0.45
56:SK:170:LYS:HD2	56:SK:175:LYS:HA	1.97	0.45
76:St:637:C:H2'	76:St:638:G:C8	2.51	0.45
8:LH:102:ARG:HB3	8:LH:199:PRO:HG3	1.99	0.45
20:LT:28:TYR:CE1	20:LT:123:VAL:HG11	2.51	0.45
23:LW:47:LYS:CE	44:Lt:2459:C:H4'	2.47	0.45
27:La:90:LYS:HB3	27:La:90:LYS:HE3	1.70	0.45
41:Lp:67:VAL:HG13	41:Lp:82:VAL:HG22	1.97	0.45
44:Lt:404:G:H2'	44:Lt:405:A:C8	2.51	0.45
47:SB:37:VAL:HG23	47:SB:42:ILE:HG13	1.97	0.45
47:SB:76:ASN:HB2	47:SB:201:LEU:HD22	1.97	0.45
48:SC:111:LEU:HB2	48:SC:128:ILE:HG13	1.99	0.45
2:LB:41:ILE:H	2:LB:41:ILE:HG12	1.52	0.45
20:LT:92:ARG:HH11	20:LT:139:PHE:HB2	1.82	0.45
26:LZ:111:MET:HE1	26:LZ:119:ILE:HD12	1.97	0.45
44:Lt:420:C:H2'	44:Lt:421:G:H8	1.81	0.45
52:SG:85:GLN:HA	52:SG:86:GLY:HA2	1.79	0.45
53:SH:137:ILE:HD12	53:SH:162:VAL:HG11	1.99	0.45
54:SI:115:SER:HB3	54:SI:138:ASP:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:St:367:C:H4'	76:St:368:G:C8	2.51	0.45
2:LB:277:ASP:HB2	2:LB:329:PRO:HD3	1.97	0.45
22:LV:31:ASN:C	22:LV:33:ASN:H	2.23	0.45
26:LZ:28:LYS:HE3	44:Lt:193:C:H5''	1.98	0.45
27:La:73:MET:HB3	27:La:73:MET:HE2	1.80	0.45
39:Ln:30:GLU:HG2	39:Ln:208:SER:HB2	1.98	0.45
46:SA:69:ILE:HG21	68:SY:41:LEU:HD12	1.98	0.45
51:SF:183:GLU:O	51:SF:187:VAL:HG23	2.17	0.45
60:SP:136:PRO:HG2	60:SP:139:PHE:HB2	1.98	0.45
69:Sb:24:VAL:HG11	69:Sb:57:LEU:HD22	1.98	0.45
2:LB:205:ILE:H	2:LB:205:ILE:HG13	1.39	0.45
3:LC:156:LEU:HG	3:LC:211:LEU:HD21	1.98	0.45
25:LY:65:PRO:HB2	25:LY:140:LEU:HD21	1.98	0.45
42:Lq:4:ARG:H	42:Lq:4:ARG:HG2	1.30	0.45
44:Lt:1421:G:H2'	44:Lt:1422:C:C6	2.51	0.45
44:Lt:1448:G:H2'	44:Lt:1449:G:C8	2.52	0.45
44:Lt:2570:C:H2'	44:Lt:2571:G:H8	1.82	0.45
46:SA:17:GLU:CD	46:SA:17:GLU:H	2.25	0.45
46:SA:174:MET:HG3	46:SA:208:VAL:HG11	1.99	0.45
49:SD:146:PHE:HA	49:SD:206:MET:HG3	1.98	0.45
50:SE:77:ARG:HA	50:SE:77:ARG:HD3	1.62	0.45
71:Sd:2:PRO:HB3	76:St:886:C:H5''	1.98	0.45
76:St:1246:A:H1'	76:St:1247:C:H2'	1.99	0.45
9:LI:130:LYS:O	9:LI:157:PRO:HD2	2.16	0.45
14:LN:68:PRO:O	14:LN:72:GLN:HB3	2.17	0.45
44:Lt:92:G:H2'	44:Lt:93:A:C8	2.52	0.45
76:St:1370:C:H42	76:St:1374:C:H42	1.65	0.45
3:LC:178:ARG:HB3	3:LC:190:ILE:HG13	1.99	0.45
13:LM:79:PRO:HB3	13:LM:170:HIS:HB3	1.99	0.45
35:Li:95:ARG:HH22	35:Li:111:THR:HB	1.81	0.45
38:Ll:48:THR:HB	44:Lt:1412:G:H4'	1.98	0.45
44:Lt:164:G:H2'	44:Lt:165:A:C8	2.51	0.45
47:SB:72:GLU:HB2	47:SB:98:VAL:HG12	1.99	0.45
56:SK:22:LYS:HD2	56:SK:22:LYS:HA	1.79	0.45
59:SO:51:VAL:HG13	59:SO:70:VAL:HG23	1.97	0.45
61:SQ:61:LYS:HG3	61:SQ:77:ALA:HA	1.98	0.45
67:SX:66:ILE:HD11	74:Sh:117:LEU:HD13	1.98	0.45
76:St:965:C:H2'	76:St:966:G:C8	2.52	0.45
24:LX:21:CYS:HB3	24:LX:31:ARG:HD2	1.99	0.44
26:LZ:74:ARG:H	26:LZ:74:ARG:HG2	1.52	0.44
27:La:15:LEU:HD21	27:La:79:MET:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SL:44:LYS:H	57:SL:44:LYS:HD3	1.82	0.44
61:SQ:78:THR:HG22	61:SQ:82:ILE:HG13	1.99	0.44
6:LF:147:VAL:HA	44:Lt:792:C:H5'	1.99	0.44
7:LG:38:ASN:HB3	7:LG:41:ARG:HG3	1.98	0.44
10:LJ:19:ILE:HD11	10:LJ:51:ILE:HD13	1.98	0.44
33:Lg:4:ILE:HA	33:Lg:7:LYS:HE2	1.99	0.44
44:Lt:51:C:H2'	44:Lt:52:G:H8	1.81	0.44
66:SW:129:MET:HE2	66:SW:129:MET:HB3	1.85	0.44
8:LH:151:VAL:HG21	8:LH:163:LEU:HD11	1.99	0.44
20:LT:10:ARG:HG2	20:LT:57:LEU:HD21	1.99	0.44
23:LW:66:VAL:CG1	23:LW:70:GLY:HA3	2.47	0.44
27:La:97:THR:HG23	27:La:103:LYS:HE2	1.98	0.44
28:Lb:72:THR:HG22	28:Lb:111:LYS:HB3	1.98	0.44
39:Ln:111:LEU:HA	39:Ln:136:LEU:H	1.80	0.44
44:Lt:1362:A:H2'	44:Lt:1363:A:C8	2.52	0.44
46:SA:116:ARG:HE	47:SB:56:LYS:HB3	1.82	0.44
50:SE:139:LEU:HD23	50:SE:150:PRO:HB3	2.00	0.44
59:SO:115:ILE:HG12	59:SO:118:CYS:HB2	1.98	0.44
62:SR:121:MET:HG3	65:SV:121:GLU:HG2	2.00	0.44
76:St:921:C:H5''	76:St:933:A:H61	1.81	0.44
37:Lk:15:ILE:HD13	37:Lk:15:ILE:HA	1.79	0.44
51:SF:153:ARG:HD3	51:SF:158:CYS:HB3	1.98	0.44
52:SG:164:MET:HE2	52:SG:164:MET:HB2	1.93	0.44
57:SL:45:LEU:HD13	57:SL:45:LEU:HA	1.88	0.44
62:SR:61:LEU:HD13	62:SR:61:LEU:HA	1.82	0.44
62:SR:65:ARG:HA	62:SR:65:ARG:HD3	1.86	0.44
62:SR:95:SER:HB3	62:SR:102:PHE:HB3	1.99	0.44
66:SW:107:PHE:HB3	66:SW:113:LEU:HB3	1.99	0.44
76:St:1201:C:H2'	76:St:1202:C:C6	2.52	0.44
8:LH:70:LEU:HD12	21:LU:144:ILE:HG21	1.99	0.44
13:LM:196:VAL:HG11	28:Lb:146:LEU:HA	2.00	0.44
16:LP:52:LEU:HD13	16:LP:52:LEU:HA	1.70	0.44
19:LS:24:PHE:HB3	19:LS:32:ILE:HD13	2.00	0.44
26:LZ:91:GLU:H	26:LZ:91:GLU:HG3	1.45	0.44
44:Lt:361:C:H2'	44:Lt:362:G:C8	2.52	0.44
44:Lt:2150:C:H2'	44:Lt:2152:G:C8	2.52	0.44
57:SL:72:TRP:HA	74:Sh:104:ILE:HA	1.99	0.44
59:SO:17:ARG:HD3	59:SO:17:ARG:HA	1.73	0.44
59:SO:85:VAL:HG11	59:SO:91:ILE:HG23	1.98	0.44
73:Sg:6:ASN:HB2	73:Sg:50:ILE:HG22	2.00	0.44
76:St:358:A:H2'	76:St:359:A:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LR:25:TYR:CZ	18:LR:29:LEU:HD11	2.53	0.44
31:Le:23:ALA:HB3	31:Le:59:ILE:O	2.17	0.44
44:Lt:1277:G:H4'	44:Lt:1470:A:H4'	2.00	0.44
71:Sd:14:ASN:HB2	76:St:819:C:H4'	1.99	0.44
76:St:900:U:H2'	76:St:901:A:C8	2.53	0.44
1:LA:207:VAL:HG11	44:Lt:633:G:C5	2.53	0.44
10:LJ:19:ILE:HG12	10:LJ:24:VAL:HG13	1.99	0.44
12:LL:60:ARG:O	12:LL:63:GLN:HB2	2.18	0.44
21:LU:91:VAL:HG22	21:LU:96:VAL:HG22	2.00	0.44
27:La:118:ARG:HD3	27:La:123:ARG:NH2	2.33	0.44
31:Le:20:SER:O	31:Le:60:ARG:HA	2.17	0.44
39:Ln:160:LYS:HB3	39:Ln:161:LYS:H	1.65	0.44
44:Lt:222:A:H61	44:Lt:249:A:H5''	1.82	0.44
44:Lt:903:A:N6	44:Lt:1000:G:H2'	2.32	0.44
44:Lt:1278:A:H4'	44:Lt:1280:U:C5	2.53	0.44
48:SC:168:HIS:N	48:SC:169:PRO:HD2	2.32	0.44
52:SG:138:ARG:HD2	76:St:148:G:H21	1.83	0.44
53:SH:159:PRO:O	53:SH:162:VAL:HG22	2.17	0.44
76:St:910:C:H4'	76:St:1275:G:H4'	1.99	0.44
76:St:1242:U:H3	76:St:1246:A:H2	1.66	0.44
76:St:1294:C:H2'	76:St:1295:G:C8	2.53	0.44
12:LL:79:ILE:HG22	12:LL:127:PHE:HE2	1.83	0.44
13:LM:79:PRO:HD2	35:Li:148:TYR:CE2	2.52	0.44
24:LX:54:LYS:HE3	24:LX:54:LYS:HB3	1.74	0.44
42:Lq:38:THR:HA	42:Lq:45:ASP:HA	1.99	0.44
53:SH:143:ARG:HD3	55:SJ:53:VAL:HG13	1.99	0.44
54:SI:134:GLN:HE22	54:SI:164:LEU:HD11	1.83	0.44
70:Sc:50:ARG:HE	70:Sc:50:ARG:HB2	1.42	0.44
16:LP:128:PRO:HD3	44:Lt:1016:G:C6	2.53	0.44
23:LW:46:TRP:CE2	23:LW:54:PRO:HA	2.52	0.44
27:La:98:VAL:HA	27:La:104:ARG:HG3	2.00	0.44
28:Lb:79:TRP:HE3	28:Lb:87:ARG:HG3	1.83	0.44
40:Lo:16:LYS:HG3	40:Lo:20:MET:HE2	2.00	0.44
41:Lp:15:GLU:HB3	41:Lp:17:LYS:HG2	1.99	0.44
41:Lp:22:LYS:O	41:Lp:70:LEU:HA	2.18	0.44
47:SB:170:ALA:O	47:SB:189:ASP:HB3	2.17	0.44
49:SD:12:LYS:HD3	49:SD:12:LYS:HA	1.80	0.44
50:SE:47:ILE:HD12	50:SE:47:ILE:HA	1.91	0.44
54:SI:26:LYS:O	54:SI:29:LEU:HB3	2.17	0.44
60:SP:91:MET:HB2	60:SP:91:MET:HE2	1.73	0.44
63:ST:54:LEU:HD12	63:ST:66:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Sb:49:VAL:C	69:Sb:51:ASP:H	2.26	0.44
72:Se:76:ILE:HG13	72:Se:85:VAL:HG13	1.98	0.44
72:Se:109:GLY:HA2	76:St:626:G:H1'	1.99	0.44
3:LC:33:ILE:HG23	3:LC:224:LEU:HD11	2.00	0.43
3:LC:286:ARG:HE	3:LC:286:ARG:HB3	1.62	0.43
13:LM:184:ILE:HD12	28:Lb:102:VAL:HG22	1.99	0.43
20:LT:25:MET:HE2	20:LT:25:MET:HB3	1.82	0.43
22:LV:15:ASN:HB3	22:LV:68:GLN:HE22	1.83	0.43
33:Lg:74:MET:HB3	33:Lg:74:MET:HE3	1.63	0.43
44:Lt:119:A:N1	44:Lt:129:U:H5	2.16	0.43
44:Lt:1228:U:H2'	44:Lt:1229:G:C8	2.53	0.43
44:Lt:1270:C:H5'	44:Lt:1362:A:H1'	2.00	0.43
57:SL:24:LEU:HD11	57:SL:53:VAL:HG12	1.99	0.43
69:Sb:43:VAL:HG22	69:Sb:55:ILE:HD12	2.00	0.43
2:LB:55:HIS:HE1	24:LX:18:LYS:HD2	1.83	0.43
9:LI:183:ASP:O	9:LI:184:VAL:HB	2.17	0.43
12:LL:19:LEU:HD13	12:LL:19:LEU:HA	1.81	0.43
21:LU:24:MET:H	21:LU:24:MET:HG3	1.56	0.43
26:LZ:93:LYS:H	26:LZ:93:LYS:HG3	1.71	0.43
47:SB:151:LYS:H	55:SJ:95:PRO:HB3	1.83	0.43
50:SE:233:PRO:HG2	50:SE:237:ILE:HD13	1.99	0.43
58:SM:36:ILE:H	58:SM:36:ILE:HG13	1.52	0.43
60:SP:142:LYS:HA	60:SP:142:LYS:HD3	1.76	0.43
64:SU:49:LEU:HD12	64:SU:49:LEU:HA	1.90	0.43
67:SX:29:VAL:O	67:SX:89:LYS:HA	2.18	0.43
70:Sc:18:PRO:HB2	70:Sc:51:VAL:HA	1.99	0.43
76:St:373:A:H3'	76:St:374:G:H8	1.82	0.43
76:St:597:G:O5'	76:St:597:G:H8	2.00	0.43
41:Lp:21:HIS:HB3	41:Lp:70:LEU:HB3	1.99	0.43
46:SA:178:LEU:HB2	64:SU:94:PHE:CZ	2.53	0.43
60:SP:78:LYS:HD3	60:SP:78:LYS:HA	1.72	0.43
14:LN:57:LEU:HG	20:LT:148:HIS:HD2	1.83	0.43
22:LV:106:THR:HG22	22:LV:107:LEU:H	1.83	0.43
44:Lt:738:C:H1'	44:Lt:740:U:H5''	2.01	0.43
44:Lt:2655:C:H2'	44:Lt:2656:C:C6	2.52	0.43
67:SX:76:GLY:HA3	76:St:1023:G:H4'	2.00	0.43
76:St:1301:C:H2'	76:St:1302:G:C8	2.53	0.43
6:LF:114:SER:HA	6:LF:117:ILE:CG2	2.48	0.43
10:LJ:88:MET:HE2	10:LJ:175:CYS:HB3	2.00	0.43
20:LT:17:PHE:CD2	20:LT:20:PRO:HG3	2.53	0.43
43:Ls:93:MET:HB3	43:Ls:93:MET:HE2	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Lt:361:C:H2'	44:Lt:362:G:H8	1.83	0.43
64:SU:75:ARG:HA	64:SU:75:ARG:HD3	1.65	0.43
1:LA:6:ARG:HH12	1:LA:199:VAL:H	1.66	0.43
3:LC:149:VAL:HG22	3:LC:207:GLY:HA3	2.01	0.43
10:LJ:15:VAL:HG13	10:LJ:26:VAL:HG23	2.00	0.43
10:LJ:83:GLY:HA3	10:LJ:185:GLN:HA	2.00	0.43
11:LK:46:PHE:HZ	11:LK:83:ASP:O	2.02	0.43
12:LL:115:LYS:HB2	12:LL:115:LYS:HE2	1.84	0.43
15:LO:85:ARG:HE	15:LO:85:ARG:HB2	1.47	0.43
19:LS:60:ARG:HE	19:LS:60:ARG:HB3	1.51	0.43
42:Lq:14:TYR:O	42:Lq:17:ARG:HG2	2.18	0.43
46:SA:15:LEU:HD13	46:SA:60:TRP:CG	2.53	0.43
53:SH:44:LEU:HD12	53:SH:69:MET:HE2	2.00	0.43
65:SV:47:LYS:H	65:SV:47:LYS:HG2	1.44	0.43
76:St:176:C:H2'	76:St:177:C:C6	2.53	0.43
6:LF:25:GLU:O	12:LL:144:GLN:HA	2.19	0.43
7:LG:31:ASP:HB2	7:LG:33:LEU:HG	2.00	0.43
23:LW:73:GLU:H	23:LW:73:GLU:HG3	1.55	0.43
44:Lt:2101:G:H1	44:Lt:2104:A:H62	1.67	0.43
46:SA:35:ILE:HD11	46:SA:43:ILE:HG13	2.00	0.43
63:ST:57:VAL:HG21	63:ST:66:VAL:HG21	2.00	0.43
72:Se:105:SER:HB2	72:Se:112:CYS:SG	2.59	0.43
14:LN:7:VAL:HG11	14:LN:52:LEU:HD11	2.00	0.43
20:LT:142:LYS:HE2	20:LT:142:LYS:HB3	1.89	0.43
23:LW:125:LYS:HA	23:LW:141:VAL:CG1	2.48	0.43
34:Lh:7:THR:HA	44:Lt:1170:G:H21	1.82	0.43
44:Lt:235:G:H1	44:Lt:256:G:N2	2.17	0.43
44:Lt:822:C:H2'	44:Lt:823:G:C8	2.54	0.43
44:Lt:1300:C:H2'	44:Lt:1301:G:C8	2.53	0.43
44:Lt:1958:G:H1'	44:Lt:1974:A:C2	2.52	0.43
57:SL:91:LEU:HB2	57:SL:93:LEU:HD22	2.00	0.43
59:SO:32:LEU:HD12	59:SO:32:LEU:HA	1.91	0.43
65:SV:44:VAL:HG23	65:SV:53:VAL:HG11	2.00	0.43
1:LA:58:LEU:HD23	1:LA:75:LEU:HD21	2.01	0.43
6:LF:37:ILE:HD12	6:LF:67:ALA:HB2	1.99	0.43
8:LH:72:VAL:HB	21:LU:139:ALA:O	2.19	0.43
10:LJ:97:ILE:HG22	10:LJ:110:ILE:HG22	2.00	0.43
10:LJ:114:MET:HE2	10:LJ:114:MET:HB2	1.94	0.43
13:LM:76:PHE:O	13:LM:169:GLN:HG2	2.19	0.43
39:Ln:11:LYS:HB3	39:Ln:11:LYS:HE3	1.78	0.43
42:Lq:28:LYS:HB3	42:Lq:28:LYS:HE3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Lt:227:C:H2'	44:Lt:228:G:C8	2.54	0.43
44:Lt:420:C:H2'	44:Lt:421:G:C8	2.53	0.43
44:Lt:732:G:H2'	44:Lt:733:G:O4'	2.19	0.43
44:Lt:2059:A:H62	44:Lt:2067:C:H41	1.67	0.43
45:Lu:17:G:H4'	45:Lu:59:A:C2	2.54	0.43
46:SA:26:ALA:HB2	46:SA:178:LEU:HD22	2.00	0.43
48:SC:147:LYS:HB3	48:SC:150:ALA:O	2.19	0.43
48:SC:172:ILE:H	48:SC:172:ILE:HG12	1.63	0.43
53:SH:170:THR:HG23	53:SH:187:PHE:HB2	2.01	0.43
59:SO:21:ARG:HD3	59:SO:27:TYR:CE2	2.54	0.43
69:Sb:20:GLN:HB2	69:Sb:75:ALA:HB3	2.00	0.43
76:St:906:C:H3'	76:St:907:A:H8	1.82	0.43
76:St:1214:A:H2'	76:St:1215:G:C8	2.54	0.43
76:St:1307:C:H2'	76:St:1308:C:C6	2.54	0.43
12:LL:15:GLU:HG3	12:LL:72:ARG:HH21	1.83	0.43
19:LS:3:ASN:HA	44:Lt:1155:C:H4'	2.01	0.43
25:LY:135:ALA:HB1	25:LY:140:LEU:HB2	2.00	0.43
30:Ld:26:LYS:HB3	30:Ld:26:LYS:HE3	1.77	0.43
48:SC:59:ALA:HB2	48:SC:106:ILE:HD13	2.00	0.43
59:SO:49:GLY:HA2	59:SO:75:THR:HG23	2.00	0.43
61:SQ:78:THR:HG21	61:SQ:119:LEU:HG	2.00	0.43
62:SR:90:ILE:HA	62:SR:107:ILE:HG22	2.01	0.43
66:SW:113:LEU:HA	66:SW:123:SER:H	1.84	0.43
67:SX:58:ARG:H	67:SX:58:ARG:HG2	1.62	0.43
76:St:772:C:H2'	76:St:773:G:C8	2.53	0.43
3:LC:269:ILE:HD13	3:LC:269:ILE:HA	1.87	0.42
10:LJ:40:ALA:HB1	10:LJ:65:LEU:HD13	2.01	0.42
15:LO:64:VAL:HG13	15:LO:102:ALA:HB1	2.01	0.42
16:LP:23:GLU:HG3	20:LT:164:PHE:HZ	1.83	0.42
35:Li:139:ARG:HE	35:Li:139:ARG:HB2	1.44	0.42
44:Lt:264:C:H2'	44:Lt:265:U:C6	2.54	0.42
44:Lt:671:U:H2'	44:Lt:672:G:H8	1.83	0.42
46:SA:26:ALA:HA	64:SU:94:PHE:HE1	1.84	0.42
49:SD:109:LYS:O	49:SD:113:LEU:HG	2.19	0.42
51:SF:21:GLU:HA	51:SF:24:GLU:HG2	2.01	0.42
51:SF:125:VAL:HG11	73:Sg:22:ILE:HD11	2.01	0.42
55:SJ:90:VAL:HG13	55:SJ:94:LEU:HD12	1.99	0.42
59:SO:48:ARG:HB3	76:St:348:G:H5'	2.01	0.42
69:Sb:74:ASN:HB3	69:Sb:76:TYR:CE1	2.54	0.42
74:Sh:127:ASN:O	74:Sh:131:ILE:HG12	2.18	0.42
76:St:676:C:H2'	76:St:677:G:C8	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:St:986:C:H2'	76:St:988:C:O2	2.19	0.42
1:LA:51:ASP:HB2	1:LA:58:LEU:HD22	2.01	0.42
6:LF:110:LEU:HD23	6:LF:110:LEU:HA	1.82	0.42
16:LP:45:ARG:H	16:LP:45:ARG:HG2	1.54	0.42
18:LR:92:VAL:HG21	28:Lb:119:PRO:HB3	2.00	0.42
24:LX:3:ARG:NE	24:LX:3:ARG:HA	2.34	0.42
32:Lf:14:ILE:HG23	32:Lf:68:THR:HB	2.00	0.42
37:Lk:39:TYR:CG	37:Lk:40:PRO:HA	2.55	0.42
44:Lt:449:A:H61	44:Lt:459:A:H5''	1.84	0.42
44:Lt:1086:C:H2'	44:Lt:1087:G:C8	2.54	0.42
44:Lt:1961:G:N3	44:Lt:1961:G:H2'	2.34	0.42
63:ST:18:ARG:HD2	63:ST:18:ARG:HA	1.67	0.42
64:SU:117:MET:HE2	64:SU:117:MET:HB3	1.84	0.42
76:St:318:C:H2'	76:St:319:C:C6	2.54	0.42
2:LB:54:THR:HG23	2:LB:78:ILE:HD11	2.01	0.42
2:LB:66:ASN:HB2	23:LW:15:PHE:CE2	2.54	0.42
44:Lt:2120:A:H2'	44:Lt:2121:A:C8	2.54	0.42
56:SK:22:LYS:HD3	76:St:435:A:H4'	2.01	0.42
58:SM:78:MET:HB2	58:SM:81:SER:HB3	2.00	0.42
63:ST:47:ILE:HB	63:ST:54:LEU:HD22	2.00	0.42
66:SW:23:ARG:HB2	66:SW:25:ILE:HG13	2.01	0.42
70:Sc:41:THR:HB	70:Sc:44:GLN:HG3	2.01	0.42
3:LC:126:LEU:HD22	3:LC:126:LEU:HA	1.82	0.42
14:LN:112:ILE:HD13	14:LN:112:ILE:HA	1.89	0.42
41:Lp:94:LEU:HD13	41:Lp:94:LEU:HA	1.77	0.42
44:Lt:714:G:H1'	44:Lt:764:C:H42	1.85	0.42
44:Lt:989:C:H2'	44:Lt:990:G:C8	2.54	0.42
45:Lu:55:C:H2'	45:Lu:56:G:C8	2.54	0.42
46:SA:94:LYS:HA	46:SA:94:LYS:HD3	1.91	0.42
49:SD:99:ASN:HB3	49:SD:100:PHE:H	1.61	0.42
49:SD:157:LYS:HE3	49:SD:157:LYS:HB2	1.90	0.42
58:SM:78:MET:H	58:SM:78:MET:HG3	1.66	0.42
63:ST:83:MET:HE2	63:ST:83:MET:HB3	1.89	0.42
71:Sd:12:LYS:HG2	71:Sd:15:CYS:HB3	2.01	0.42
76:St:1316:U:H2'	76:St:1317:G:C8	2.54	0.42
3:LC:160:LYS:HA	3:LC:165:LEU:HB2	2.01	0.42
23:LW:47:LYS:H	23:LW:47:LYS:HD3	1.85	0.42
39:Ln:68:ILE:HB	39:Ln:85:VAL:HG23	2.01	0.42
44:Lt:1326:G:H2'	44:Lt:1327:C:C6	2.54	0.42
46:SA:42:TYR:HA	46:SA:58:LYS:HD2	2.01	0.42
50:SE:114:ILE:HB	50:SE:118:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SK:108:ARG:HB2	56:SK:148:MET:HE3	2.01	0.42
56:SK:109:ARG:HH12	56:SK:127:ARG:HH21	1.68	0.42
57:SL:32:ASN:HB3	57:SL:49:THR:HA	2.02	0.42
3:LC:104:LYS:HE3	3:LC:104:LYS:HB2	1.73	0.42
10:LJ:130:ILE:HD11	10:LJ:140:LEU:HB3	2.02	0.42
18:LR:97:MET:HB3	18:LR:97:MET:HE2	1.62	0.42
22:LV:98:LEU:HD12	22:LV:108:LYS:HG3	2.02	0.42
23:LW:64:ILE:HG12	23:LW:81:ALA:HB2	2.02	0.42
27:La:88:ASN:O	27:La:90:LYS:N	2.52	0.42
44:Lt:835:U:H2'	44:Lt:836:G:C8	2.55	0.42
44:Lt:2555:C:H2'	44:Lt:2556:G:O4'	2.18	0.42
46:SA:203:LYS:HE2	46:SA:203:LYS:HB3	1.86	0.42
54:SI:32:GLN:HE21	54:SI:32:GLN:HB3	1.73	0.42
56:SK:108:ARG:HD3	56:SK:108:ARG:HA	1.62	0.42
11:LK:191:GLN:HG2	11:LK:200:ILE:HA	2.00	0.42
17:LQ:129:THR:HB	17:LQ:137:SER:OG	2.20	0.42
18:LR:37:TYR:CE1	18:LR:46:LYS:HB2	2.55	0.42
18:LR:102:LEU:HD23	18:LR:102:LEU:HA	1.84	0.42
47:SB:138:TRP:HB2	47:SB:147:THR:HG21	2.02	0.42
50:SE:256:ARG:HD3	76:St:558:C:H5''	2.02	0.42
58:SM:63:SER:HB2	76:St:186:A:H2	1.84	0.42
65:SV:56:ARG:HE	65:SV:56:ARG:HB2	1.77	0.42
69:Sb:47:LEU:HA	69:Sb:47:LEU:HD13	1.81	0.42
76:St:970:A:OP2	76:St:972:G:H4'	2.18	0.42
8:LH:24:ARG:HA	8:LH:24:ARG:HD3	1.53	0.42
23:LW:85:ARG:HG2	23:LW:100:PHE:CD1	2.54	0.42
24:LX:51:ARG:HD3	44:Lt:2642:U:H2'	2.01	0.42
44:Lt:760:A:H2'	44:Lt:761:A:C8	2.55	0.42
44:Lt:790:G:H22	44:Lt:792:C:H3'	1.83	0.42
44:Lt:903:A:H61	44:Lt:1000:G:H2'	1.85	0.42
44:Lt:1100:C:H2'	44:Lt:1101:G:C8	2.55	0.42
44:Lt:1873:C:H3'	44:Lt:1874:G:H8	1.84	0.42
44:Lt:1941:C:H6	44:Lt:1941:C:H2'	1.71	0.42
49:SD:13:ILE:HA	49:SD:16:ARG:O	2.19	0.42
50:SE:87:MET:HE1	50:SE:235:VAL:HG11	2.01	0.42
56:SK:166:ALA:N	56:SK:167:PRO:HD3	2.34	0.42
60:SP:135:LEU:HD23	60:SP:135:LEU:HA	1.82	0.42
64:SU:20:ASN:HB3	64:SU:23:SER:HB2	2.02	0.42
65:SV:92:GLU:HG2	65:SV:114:ARG:HH12	1.84	0.42
66:SW:27:LYS:HE3	66:SW:27:LYS:HB3	1.87	0.42
4:LD:46:C:H5''	7:LG:15:LYS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LT:141:GLN:HE21	20:LT:141:GLN:HB2	1.48	0.42
21:LU:65:PHE:CE2	21:LU:88:ARG:HB3	2.55	0.42
36:Lj:83:LEU:HA	36:Lj:86:TYR:HD1	1.85	0.42
43:Ls:97:ARG:HD3	44:Lt:2269:C:H2'	2.01	0.42
44:Lt:65:A:N6	44:Lt:75:G:H1'	2.35	0.42
44:Lt:1207:G:C2	44:Lt:1281:C:H4'	2.54	0.42
47:SB:166:ALA:HB3	47:SB:189:ASP:HB2	2.02	0.42
51:SF:16:VAL:HG13	51:SF:96:GLN:HA	2.01	0.42
54:SI:130:GLU:H	54:SI:130:GLU:HG3	1.50	0.42
62:SR:88:GLU:H	62:SR:88:GLU:HG3	1.50	0.42
76:St:506:C:H2'	76:St:507:C:C6	2.55	0.42
76:St:1059:C:H2'	76:St:1060:G:C8	2.55	0.42
2:LB:250:ALA:HB1	44:Lt:2369:G:N3	2.35	0.42
11:LK:42:LYS:HA	11:LK:42:LYS:HD3	1.76	0.42
43:Ls:107:ALA:O	43:Ls:118:LEU:HD22	2.20	0.42
44:Lt:2382:C:H2'	44:Lt:2383:G:C8	2.55	0.42
51:SF:116:LYS:HA	51:SF:116:LYS:HD2	1.89	0.42
59:SO:51:VAL:HG22	59:SO:70:VAL:HG21	2.02	0.42
60:SP:5:HIS:HD2	60:SP:121:ARG:HE	1.68	0.42
6:LF:112:LYS:O	6:LF:115:VAL:HG22	2.20	0.41
9:LI:50:ARG:HD3	9:LI:216:VAL:O	2.19	0.41
10:LJ:25:THR:HG23	10:LJ:34:VAL:HG22	2.02	0.41
10:LJ:136:VAL:O	10:LJ:137:LYS:HB3	2.20	0.41
12:LL:16:LYS:HB3	12:LL:16:LYS:HE2	1.90	0.41
15:LO:67:ARG:HD3	44:Lt:1228:U:H5''	2.01	0.41
15:LO:186:PRO:HB3	44:Lt:61:G:H21	1.85	0.41
16:LP:59:THR:HA	44:Lt:1006:G:C6	2.55	0.41
38:Ll:22:LEU:HD22	38:Ll:24:VAL:HG22	2.01	0.41
38:Ll:67:LYS:HG2	38:Ll:67:LYS:H	1.62	0.41
44:Lt:81:C:H1'	44:Lt:430:G:H21	1.85	0.41
44:Lt:347:A:H2'	44:Lt:348:A:C8	2.55	0.41
44:Lt:2570:C:H2'	44:Lt:2571:G:C8	2.55	0.41
49:SD:122:ASP:HB3	49:SD:140:ILE:HG13	2.02	0.41
56:SK:134:HIS:ND1	56:SK:163:SER:HB2	2.35	0.41
69:Sb:19:ARG:HA	69:Sb:76:TYR:HA	2.01	0.41
69:Sb:57:LEU:HB3	69:Sb:60:PHE:CE1	2.55	0.41
70:Sc:70:ALA:HB2	70:Sc:84:MET:HE2	2.02	0.41
74:Sh:122:ARG:H	74:Sh:122:ARG:HG2	1.21	0.41
76:St:147:C:H2'	76:St:148:G:C8	2.54	0.41
12:LL:45:PRO:HA	12:LL:69:VAL:HG13	2.02	0.41
18:LR:156:ARG:HA	18:LR:156:ARG:HD2	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Lb:67:ILE:HD11	44:Lt:70:A:H3'	2.02	0.41
38:Ll:26:SER:HA	38:Ll:73:VAL:HG13	2.03	0.41
42:Lq:10:LEU:H	42:Lq:10:LEU:HG	1.52	0.41
44:Lt:1914:C:H2'	44:Lt:1915:C:C6	2.55	0.41
44:Lt:1935:G:H21	44:Lt:1985:C:H41	1.68	0.41
52:SG:57:ARG:HB3	52:SG:118:VAL:HG12	2.02	0.41
53:SH:16:LEU:HD23	53:SH:16:LEU:HA	1.89	0.41
53:SH:171:LYS:HE2	53:SH:171:LYS:HB3	1.87	0.41
60:SP:130:ARG:HD2	60:SP:139:PHE:O	2.21	0.41
68:SY:49:LYS:HE3	68:SY:49:LYS:HB3	1.86	0.41
76:St:679:G:H2'	76:St:680:A:C8	2.55	0.41
76:St:1223:C:H4'	76:St:1229:C:H42	1.84	0.41
76:St:1374:C:H2'	76:St:1375:G:O4'	2.19	0.41
6:LF:112:LYS:HA	6:LF:115:VAL:HG13	2.01	0.41
6:LF:114:SER:HA	6:LF:117:ILE:HG22	2.01	0.41
12:LL:9:MET:O	12:LL:134:PRO:HD2	2.19	0.41
35:Li:151:LYS:HE3	35:Li:151:LYS:HB3	1.95	0.41
51:SF:29:ILE:H	51:SF:29:ILE:HG13	1.66	0.41
59:SO:81:ILE:HD11	59:SO:102:VAL:HG21	2.02	0.41
2:LB:363:GLY:HA2	44:Lt:2503:C:H5''	2.03	0.41
12:LL:59:ILE:H	12:LL:59:ILE:HG13	1.62	0.41
18:LR:42:GLU:HG2	18:LR:131:THR:O	2.21	0.41
25:LY:28:ASN:HD22	25:LY:28:ASN:HA	1.54	0.41
26:LZ:100:HIS:CG	44:Lt:184:U:H4'	2.56	0.41
30:Ld:8:LYS:HA	30:Ld:8:LYS:HD3	1.90	0.41
52:SG:28:ARG:C	52:SG:30:SER:H	2.28	0.41
59:SO:57:ILE:HG23	59:SO:67:ARG:HB2	2.03	0.41
65:SV:26:VAL:HG13	65:SV:54:HIS:HA	2.02	0.41
65:SV:86:ASN:HB3	65:SV:99:ILE:H	1.85	0.41
76:St:49:C:H2'	76:St:337:C:H41	1.85	0.41
76:St:812:C:H2'	76:St:813:C:C6	2.55	0.41
8:LH:168:LEU:HB3	8:LH:173:ILE:HB	2.01	0.41
9:LI:29:THR:N	9:LI:30:PRO:HD2	2.36	0.41
13:LM:89:ARG:HB2	13:LM:94:PHE:HB3	2.02	0.41
44:Lt:989:C:H2'	44:Lt:990:G:H8	1.86	0.41
44:Lt:1274:G:N2	44:Lt:1276:A:H3'	2.36	0.41
46:SA:68:ARG:O	46:SA:72:THR:HG23	2.20	0.41
47:SB:182:LEU:HD13	47:SB:190:VAL:HG11	2.02	0.41
49:SD:64:TYR:HE1	49:SD:88:THR:HG23	1.86	0.41
50:SE:51:ARG:HH12	50:SE:110:THR:HA	1.84	0.41
51:SF:29:ILE:HA	51:SF:32:HIS:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SK:173:ARG:HH11	56:SK:173:ARG:HB3	1.85	0.41
65:SV:143:ARG:HA	65:SV:143:ARG:NH1	2.36	0.41
76:St:546:U:H2'	76:St:547:C:C6	2.53	0.41
1:LA:178:PRO:HD3	42:Lq:25:GLN:HG2	2.02	0.41
8:LH:94:VAL:HG13	8:LH:125:VAL:HG12	2.02	0.41
10:LJ:3:LEU:HD12	10:LJ:3:LEU:HA	1.90	0.41
14:LN:130:ILE:HD13	14:LN:130:ILE:HA	1.81	0.41
38:Ll:5:ILE:HD12	38:Ll:5:ILE:HA	1.94	0.41
44:Lt:163:C:H1'	44:Lt:186:C:H41	1.86	0.41
44:Lt:243:A:H2'	44:Lt:244:G:C8	2.55	0.41
44:Lt:1233:A:H2'	44:Lt:1234:C:C6	2.55	0.41
44:Lt:1626:U:H2'	44:Lt:1630:A:N1	2.36	0.41
44:Lt:2067:C:H2'	44:Lt:2069:G:H8	1.85	0.41
45:Lu:15:G:H2'	45:Lu:58:A:H61	1.85	0.41
47:SB:142:LEU:HD13	47:SB:142:LEU:HA	1.82	0.41
47:SB:167:PRO:HG3	56:SK:58:ARG:HD2	2.01	0.41
50:SE:84:VAL:HG23	50:SE:101:VAL:HG21	2.02	0.41
63:ST:30:LYS:HA	63:ST:34:SER:O	2.21	0.41
70:Sc:71:ILE:HG21	70:Sc:74:LYS:HB2	2.01	0.41
76:St:234:G:H1'	76:St:236:U:C2	2.56	0.41
14:LN:12:LEU:HB3	14:LN:58:THR:OG1	2.21	0.41
15:LO:50:ARG:HD3	44:Lt:221:G:H1'	2.03	0.41
16:LP:171:ILE:O	16:LP:175:ILE:HG12	2.21	0.41
19:LS:104:ARG:HG2	19:LS:108:ARG:HE	1.84	0.41
27:La:48:PRO:HA	27:La:66:VAL:HG22	2.03	0.41
35:Li:136:LEU:HD23	35:Li:136:LEU:HA	1.95	0.41
44:Lt:1136:U:H2'	44:Lt:1137:A:H8	1.86	0.41
44:Lt:1151:G:H1'	44:Lt:1154:C:N4	2.35	0.41
44:Lt:1438:U:H4'	44:Lt:1439:G:C4	2.56	0.41
51:SF:152:VAL:HA	76:St:1225:U:C4	2.56	0.41
52:SG:139:LEU:HD23	76:St:63:C:C4	2.56	0.41
59:SO:26:LYS:HZ2	76:St:486:C:H41	1.69	0.41
65:SV:22:GLN:HB3	65:SV:24:LYS:HG3	2.03	0.41
65:SV:56:ARG:HB3	70:Sc:20:LEU:HD13	2.03	0.41
69:Sb:111:LEU:HD13	69:Sb:111:LEU:HA	1.85	0.41
2:LB:316:ARG:O	2:LB:317:VAL:C	2.63	0.41
3:LC:195:PRO:HG2	3:LC:214:VAL:HG22	2.02	0.41
24:LX:7:CYS:HB3	24:LX:10:CYS:H	1.86	0.41
29:Lc:43:LEU:HD12	29:Lc:43:LEU:HA	1.93	0.41
32:Lf:91:PHE:CE2	32:Lf:99:ALA:HB2	2.56	0.41
49:SD:150:ARG:HH21	49:SD:151:ARG:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SI:76:TRP:HB2	54:SI:158:ILE:HD12	2.01	0.41
76:St:362:C:H2'	76:St:363:G:C8	2.55	0.41
76:St:970:A:H1'	76:St:972:G:H21	1.86	0.41
1:LA:32:ASN:HB3	1:LA:121:MET:HE3	2.03	0.41
10:LJ:75:ASN:HA	10:LJ:78:LYS:HE2	2.03	0.41
12:LL:35:LYS:HA	12:LL:35:LYS:HD3	1.75	0.41
12:LL:68:HIS:CD2	44:Lt:2106:C:H5''	2.56	0.41
15:LO:176:ASN:HD22	44:Lt:241:G:H5''	1.86	0.41
16:LP:48:LYS:HE2	16:LP:48:LYS:HB3	1.79	0.41
16:LP:52:LEU:HD11	44:Lt:2549:C:H5'	2.03	0.41
26:LZ:93:LYS:HE3	26:LZ:93:LYS:HB2	1.91	0.41
30:Ld:83:ILE:HD13	30:Ld:83:ILE:HA	1.87	0.41
33:Lg:49:LEU:HD22	33:Lg:99:ILE:HA	2.03	0.41
38:Ll:59:SER:HA	38:Ll:62:LYS:HD2	2.03	0.41
44:Lt:51:C:H2'	44:Lt:52:G:C8	2.56	0.41
44:Lt:746:U:H2'	44:Lt:747:C:C6	2.56	0.41
44:Lt:1261:A:N1	44:Lt:1468:G:H1'	2.36	0.41
44:Lt:1646:G:H5''	44:Lt:1649:G:H1'	2.03	0.41
44:Lt:2672:G:H2'	44:Lt:2673:A:C8	2.56	0.41
49:SD:151:ARG:HE	49:SD:151:ARG:H	1.68	0.41
49:SD:228:LEU:HD23	49:SD:228:LEU:HA	1.96	0.41
52:SG:28:ARG:C	52:SG:30:SER:N	2.78	0.41
54:SI:45:LYS:HG3	54:SI:47:ASN:H	1.85	0.41
57:SL:21:SER:HB3	57:SL:78:LEU:HD23	2.03	0.41
61:SQ:78:THR:C	61:SQ:80:ASP:N	2.78	0.41
65:SV:40:ARG:HH11	65:SV:80:ILE:HG12	1.85	0.41
66:SW:16:PHE:HD2	66:SW:16:PHE:HA	1.76	0.41
76:St:367:C:H4'	76:St:368:G:H8	1.85	0.41
2:LB:112:GLU:O	2:LB:116:ARG:HG3	2.20	0.41
20:LT:86:ASN:HD21	21:LU:155:TYR:H	1.69	0.41
26:LZ:111:MET:O	26:LZ:115:ARG:HB2	2.21	0.41
41:Lp:65:LYS:HG3	41:Lp:85:ARG:HG2	2.03	0.41
49:SD:27:TRP:HB3	49:SD:43:GLN:HG2	2.03	0.41
49:SD:68:LEU:HD11	49:SD:189:SER:HA	2.03	0.41
54:SI:136:ARG:HE	54:SI:136:ARG:HB2	1.65	0.41
64:SU:108:MET:HE3	64:SU:108:MET:HB3	1.85	0.41
76:St:983:G:N2	76:St:985:G:H3'	2.35	0.41
31:Le:13:LYS:HE2	31:Le:13:LYS:HB3	1.78	0.40
34:Lh:45:CYS:SG	34:Lh:79:CYS:N	2.93	0.40
44:Lt:1282:C:H2'	44:Lt:1283:G:C8	2.56	0.40
46:SA:15:LEU:HD12	46:SA:16:LYS:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SB:124:LYS:HB3	47:SB:124:LYS:HE2	1.83	0.40
49:SD:64:TYR:HD2	61:SQ:47:LEU:HB3	1.86	0.40
49:SD:108:HIS:CD2	49:SD:108:HIS:H	2.37	0.40
50:SE:92:ILE:HB	50:SE:95:VAL:HG12	2.03	0.40
52:SG:138:ARG:H	52:SG:138:ARG:HG2	1.56	0.40
54:SI:122:LEU:HD23	54:SI:122:LEU:HA	1.93	0.40
67:SX:104:ILE:HA	67:SX:107:LYS:HD2	2.03	0.40
69:Sb:25:ASP:HB3	69:Sb:68:HIS:HE1	1.87	0.40
6:LF:22:ARG:HB2	6:LF:28:THR:HG22	2.03	0.40
39:Ln:48:ARG:H	39:Ln:48:ARG:HG2	1.46	0.40
41:Lp:81:GLN:HE21	41:Lp:81:GLN:HB3	1.54	0.40
44:Lt:1768:A:H61	44:Lt:1798:U:H1'	1.85	0.40
45:Lu:68:U:H2'	45:Lu:69:G:C8	2.56	0.40
47:SB:41:LYS:HE2	47:SB:41:LYS:HB2	1.81	0.40
61:SQ:82:ILE:HD11	61:SQ:119:LEU:HA	2.03	0.40
65:SV:99:ILE:HD13	65:SV:99:ILE:HA	1.85	0.40
74:Sh:125:LYS:HB2	74:Sh:125:LYS:HE3	1.90	0.40
76:St:593:C:H4'	76:St:594:G:OP1	2.21	0.40
1:LA:183:GLY:HA2	44:Lt:613:A:H5''	2.03	0.40
3:LC:264:ILE:HG12	18:LR:123:ASP:HB3	2.02	0.40
6:LF:187:ARG:HA	6:LF:187:ARG:HD3	1.91	0.40
10:LJ:143:ARG:HB3	10:LJ:185:GLN:C	2.46	0.40
23:LW:139:GLU:H	23:LW:139:GLU:HG3	1.71	0.40
38:Ll:5:ILE:HG21	38:Ll:11:MET:HE2	2.02	0.40
41:Lp:61:LYS:HG2	44:Lt:2218:U:OP2	2.21	0.40
44:Lt:85:U:O2'	44:Lt:86:A:H8	2.04	0.40
44:Lt:1403:C:H2'	44:Lt:1404:C:C6	2.56	0.40
58:SM:15:GLN:HE21	58:SM:15:GLN:HB2	1.67	0.40
60:SP:27:LYS:HB3	60:SP:27:LYS:HE2	1.54	0.40
76:St:469:C:H2'	76:St:470:G:H8	1.85	0.40
76:St:1253:C:H2'	76:St:1254:G:O4'	2.21	0.40
3:LC:134:ILE:HG22	3:LC:236:LEU:HD22	2.03	0.40
9:LI:196:LEU:HD23	9:LI:196:LEU:HA	1.92	0.40
13:LM:169:GLN:HE21	13:LM:169:GLN:HB3	1.62	0.40
15:LO:8:GLN:O	15:LO:12:ARG:HG2	2.21	0.40
20:LT:139:PHE:HA	20:LT:144:VAL:HG11	2.03	0.40
27:La:42:ALA:HA	27:La:69:PHE:O	2.22	0.40
27:La:93:ILE:HG12	27:La:107:ILE:HD12	2.04	0.40
40:Lo:24:SER:O	40:Lo:25:LYS:C	2.64	0.40
41:Lp:68:ILE:HD12	41:Lp:91:ILE:HD11	2.04	0.40
44:Lt:1772:C:H2'	44:Lt:1773:C:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Lt:2085:G:H2'	44:Lt:2086:G:C8	2.56	0.40
47:SB:223:LEU:HD13	68:SY:30:LEU:HD11	2.04	0.40
49:SD:16:ARG:HD2	49:SD:16:ARG:HA	1.90	0.40
58:SM:44:ILE:HD13	58:SM:44:ILE:HA	1.88	0.40
63:ST:73:LEU:HD12	63:ST:73:LEU:HA	1.76	0.40
65:SV:70:LYS:HA	65:SV:70:LYS:HD3	1.84	0.40
5:LE:67:G:H5'	6:LF:10:ARG:HG3	2.02	0.40
12:LL:51:ARG:HA	12:LL:51:ARG:HD3	1.91	0.40
14:LN:87:MET:HA	14:LN:92:GLY:HA3	2.03	0.40
22:LV:35:PHE:O	22:LV:39:VAL:HG22	2.22	0.40
25:LY:87:ARG:HA	25:LY:119:LYS:HD2	2.03	0.40
44:Lt:451:C:H2'	44:Lt:452:G:C8	2.57	0.40
44:Lt:519:C:H2'	44:Lt:520:C:C6	2.56	0.40
44:Lt:842:C:H2'	44:Lt:843:A:C8	2.57	0.40
46:SA:124:PRO:HD2	46:SA:147:ILE:CD1	2.52	0.40
59:SO:68:LYS:CB	59:SO:91:ILE:HG12	2.52	0.40
61:SQ:44:VAL:HG12	61:SQ:81:LEU:HD21	2.04	0.40
71:Sd:92:ARG:HB3	76:St:1451:C:O2	2.21	0.40
72:Se:120:ARG:O	72:Se:121:TYR:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	
1	LA	246/251 (98%)	235 (96%)	11 (4%)	0	100	100
2	LB	375/379 (99%)	355 (95%)	16 (4%)	4 (1%)	11	36
3	LC	307/316 (97%)	298 (97%)	8 (3%)	1 (0%)	36	63
6	LF	291/297 (98%)	280 (96%)	10 (3%)	1 (0%)	36	63
7	LG	48/51 (94%)	44 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	LH	211/235 (90%)	205 (97%)	5 (2%)	1 (0%)	24	52
9	LI	184/225 (82%)	171 (93%)	11 (6%)	2 (1%)	11	36
10	LJ	182/185 (98%)	163 (90%)	15 (8%)	4 (2%)	5	23
11	LK	152/210 (72%)	146 (96%)	5 (3%)	1 (1%)	18	46
12	LL	165/173 (95%)	157 (95%)	8 (5%)	0	100	100
13	LM	199/234 (85%)	187 (94%)	10 (5%)	2 (1%)	12	38
14	LN	128/131 (98%)	123 (96%)	5 (4%)	0	100	100
15	LO	201/204 (98%)	192 (96%)	8 (4%)	1 (0%)	24	52
16	LP	191/197 (97%)	185 (97%)	4 (2%)	2 (1%)	12	38
17	LQ	152/164 (93%)	146 (96%)	5 (3%)	1 (1%)	18	46
18	LR	176/179 (98%)	168 (96%)	7 (4%)	1 (1%)	21	49
19	LS	190/196 (97%)	186 (98%)	4 (2%)	0	100	100
20	LT	168/173 (97%)	164 (98%)	4 (2%)	0	100	100
21	LU	155/159 (98%)	145 (94%)	8 (5%)	2 (1%)	9	32
22	LV	98/124 (79%)	86 (88%)	9 (9%)	3 (3%)	3	17
23	LW	130/142 (92%)	126 (97%)	4 (3%)	0	100	100
24	LX	61/189 (32%)	57 (93%)	4 (7%)	0	100	100
25	LY	113/141 (80%)	108 (96%)	4 (4%)	1 (1%)	14	41
26	LZ	131/135 (97%)	127 (97%)	4 (3%)	0	100	100
27	La	115/135 (85%)	104 (90%)	9 (8%)	2 (2%)	7	27
28	Lb	146/149 (98%)	136 (93%)	8 (6%)	2 (1%)	9	30
29	Lc	50/62 (81%)	46 (92%)	3 (6%)	1 (2%)	6	24
30	Ld	105/109 (96%)	102 (97%)	3 (3%)	0	100	100
31	Le	98/106 (92%)	94 (96%)	4 (4%)	0	100	100
32	Lf	125/136 (92%)	121 (97%)	4 (3%)	0	100	100
33	Lg	96/123 (78%)	94 (98%)	1 (1%)	1 (1%)	12	38
34	Lh	93/120 (78%)	89 (96%)	1 (1%)	3 (3%)	3	17
35	Li	120/124 (97%)	112 (93%)	8 (7%)	0	100	100
36	Lj	87/90 (97%)	81 (93%)	5 (6%)	1 (1%)	11	36
37	Lk	83/89 (93%)	78 (94%)	5 (6%)	0	100	100
38	Ll	70/77 (91%)	68 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	Ln	194/217 (89%)	180 (93%)	12 (6%)	2 (1%)	12	38
40	Lo	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
41	Lp	91/106 (86%)	88 (97%)	3 (3%)	0	100	100
42	Lq	88/94 (94%)	87 (99%)	1 (1%)	0	100	100
43	Ls	45/127 (35%)	44 (98%)	1 (2%)	0	100	100
46	SA	194/245 (79%)	188 (97%)	5 (3%)	1 (0%)	24	52
47	SB	197/242 (81%)	186 (94%)	10 (5%)	1 (0%)	24	52
48	SC	206/217 (95%)	193 (94%)	12 (6%)	1 (0%)	24	52
49	SD	229/248 (92%)	217 (95%)	10 (4%)	2 (1%)	14	41
50	SE	258/268 (96%)	241 (93%)	15 (6%)	2 (1%)	16	44
51	SF	180/190 (95%)	174 (97%)	5 (3%)	1 (1%)	21	49
52	SG	199/248 (80%)	189 (95%)	10 (5%)	0	100	100
53	SH	182/190 (96%)	169 (93%)	12 (7%)	1 (0%)	24	52
54	SI	171/174 (98%)	165 (96%)	4 (2%)	2 (1%)	10	33
55	SJ	127/130 (98%)	121 (95%)	4 (3%)	2 (2%)	7	28
56	SK	174/189 (92%)	167 (96%)	6 (3%)	1 (1%)	21	49
57	SL	96/134 (72%)	94 (98%)	2 (2%)	0	100	100
58	SM	149/154 (97%)	135 (91%)	12 (8%)	2 (1%)	9	32
59	SO	137/143 (96%)	132 (96%)	3 (2%)	2 (2%)	8	29
60	SP	148/154 (96%)	142 (96%)	6 (4%)	0	100	100
61	SQ	124/145 (86%)	116 (94%)	7 (6%)	1 (1%)	16	44
62	SR	97/145 (67%)	94 (97%)	3 (3%)	0	100	100
63	ST	149/158 (94%)	143 (96%)	6 (4%)	0	100	100
64	SU	106/137 (77%)	100 (94%)	4 (4%)	2 (2%)	6	25
65	SV	138/154 (90%)	120 (87%)	14 (10%)	4 (3%)	3	18
66	SW	135/139 (97%)	126 (93%)	8 (6%)	1 (1%)	18	46
67	SX	98/126 (78%)	95 (97%)	3 (3%)	0	100	100
68	SY	84/89 (94%)	78 (93%)	5 (6%)	1 (1%)	10	33
69	Sb	117/132 (89%)	110 (94%)	6 (5%)	1 (1%)	14	41
70	Sc	73/88 (83%)	65 (89%)	7 (10%)	1 (1%)	9	30
71	Sd	96/109 (88%)	92 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	Se	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
73	Sg	61/64 (95%)	56 (92%)	5 (8%)	0	100	100
74	Sh	48/51 (94%)	44 (92%)	3 (6%)	1 (2%)	5	23
75	Sj	60/69 (87%)	56 (93%)	4 (7%)	0	100	100
All	All	9994/11192 (89%)	9480 (95%)	445 (4%)	69 (1%)	20	46

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	LV	45	ILE
27	La	89	TYR
27	La	98	VAL
29	Lc	50	ASP
48	SC	210	ILE
58	SM	53	ASP
74	Sh	104	ILE
2	LB	303	LYS
2	LB	317	VAL
3	LC	292	GLU
8	LH	207	LEU
9	LI	184	VAL
16	LP	129	GLU
34	Lh	7	THR
34	Lh	48	THR
2	LB	55	HIS
2	LB	173	LYS
9	LI	163	THR
10	LJ	54	ALA
10	LJ	137	LYS
11	LK	47	PRO
16	LP	181	LYS
22	LV	47	ASN
22	LV	95	PHE
28	Lb	15	ARG
28	Lb	95	SER
33	Lg	9	PHE
47	SB	139	GLY
54	SI	92	TYR
54	SI	128	ASP
65	SV	90	ASP
13	LM	91	SER

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Mol	Chain	Res	Type
15	LO	185	ARG
17	LQ	153	LYS
21	LU	101	CYS
21	LU	134	ALA
34	Lh	64	THR
36	Lj	27	LYS
39	Ln	47	PRO
50	SE	244	ARG
56	SK	148	MET
59	SO	3	LYS
61	SQ	47	LEU
64	SU	46	SER
64	SU	92	SER
65	SV	101	VAL
66	SW	27	LYS
69	Sb	35	SER
10	LJ	59	ARG
13	LM	168	ILE
18	LR	174	ARG
25	LY	54	SER
46	SA	109	ILE
49	SD	51	GLY
51	SF	35	VAL
53	SH	115	ARG
55	SJ	96	SER
58	SM	150	ARG
59	SO	99	GLU
65	SV	44	VAL
65	SV	85	LEU
70	Sc	24	GLU
10	LJ	177	VAL
50	SE	143	ASP
55	SJ	29	PRO
68	SY	16	VAL
6	LF	89	PRO
39	Ln	126	PRO
49	SD	59	ILE

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	
1	LA	189/192 (98%)	164 (87%)	25 (13%)	4	15
2	LB	311/313 (99%)	268 (86%)	43 (14%)	3	14
3	LC	257/263 (98%)	233 (91%)	24 (9%)	8	30
6	LF	238/242 (98%)	203 (85%)	35 (15%)	3	12
7	LG	47/48 (98%)	44 (94%)	3 (6%)	16	42
8	LH	184/204 (90%)	169 (92%)	15 (8%)	10	35
9	LI	166/198 (84%)	147 (89%)	19 (11%)	5	20
10	LJ	163/164 (99%)	147 (90%)	16 (10%)	7	27
11	LK	133/177 (75%)	115 (86%)	18 (14%)	4	15
12	LL	143/149 (96%)	125 (87%)	18 (13%)	4	17
13	LM	169/197 (86%)	141 (83%)	28 (17%)	2	9
14	LN	110/111 (99%)	93 (84%)	17 (16%)	2	10
15	LO	174/175 (99%)	160 (92%)	14 (8%)	11	36
16	LP	161/165 (98%)	146 (91%)	15 (9%)	8	30
17	LQ	131/139 (94%)	127 (97%)	4 (3%)	35	59
18	LR	154/155 (99%)	137 (89%)	17 (11%)	6	22
19	LS	163/167 (98%)	146 (90%)	17 (10%)	7	24
20	LT	151/154 (98%)	132 (87%)	19 (13%)	4	17
21	LU	131/133 (98%)	111 (85%)	20 (15%)	3	10
22	LV	88/110 (80%)	74 (84%)	14 (16%)	2	10
23	LW	108/114 (95%)	96 (89%)	12 (11%)	6	21
24	LX	61/174 (35%)	53 (87%)	8 (13%)	4	15
25	LY	104/123 (85%)	93 (89%)	11 (11%)	6	23
26	LZ	114/115 (99%)	99 (87%)	15 (13%)	4	15
27	La	105/119 (88%)	92 (88%)	13 (12%)	4	18
28	Lb	126/127 (99%)	117 (93%)	9 (7%)	13	39
29	Lc	48/57 (84%)	45 (94%)	3 (6%)	16	43
30	Ld	91/92 (99%)	73 (80%)	18 (20%)	1	5
31	Le	88/92 (96%)	81 (92%)	7 (8%)	11	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Lf	113/120 (94%)	99 (88%)	14 (12%)	4	18
33	Lg	82/103 (80%)	75 (92%)	7 (8%)	10	33
34	Lh	84/100 (84%)	80 (95%)	4 (5%)	23	49
35	Li	105/107 (98%)	95 (90%)	10 (10%)	8	29
36	Lj	77/78 (99%)	70 (91%)	7 (9%)	9	30
37	Lk	71/74 (96%)	64 (90%)	7 (10%)	7	27
38	Ll	63/68 (93%)	48 (76%)	15 (24%)	1	2
39	Ln	173/189 (92%)	130 (75%)	43 (25%)	0	2
40	Lo	22/22 (100%)	21 (96%)	1 (4%)	24	51
41	Lp	83/93 (89%)	71 (86%)	12 (14%)	3	13
42	Lq	70/73 (96%)	59 (84%)	11 (16%)	2	10
43	Ls	43/110 (39%)	36 (84%)	7 (16%)	2	10
46	SA	171/217 (79%)	150 (88%)	21 (12%)	4	18
47	SB	163/201 (81%)	141 (86%)	22 (14%)	4	15
48	SC	173/182 (95%)	139 (80%)	34 (20%)	1	5
49	SD	208/220 (94%)	176 (85%)	32 (15%)	2	10
50	SE	228/232 (98%)	195 (86%)	33 (14%)	3	13
51	SF	152/157 (97%)	134 (88%)	18 (12%)	5	19
52	SG	174/213 (82%)	143 (82%)	31 (18%)	2	7
53	SH	165/170 (97%)	136 (82%)	29 (18%)	2	8
54	SI	147/148 (99%)	132 (90%)	15 (10%)	7	25
55	SJ	114/115 (99%)	89 (78%)	25 (22%)	1	3
56	SK	155/164 (94%)	137 (88%)	18 (12%)	5	20
57	SL	87/119 (73%)	65 (75%)	22 (25%)	0	1
58	SM	134/136 (98%)	114 (85%)	20 (15%)	3	12
59	SO	111/114 (97%)	98 (88%)	13 (12%)	5	19
60	SP	125/130 (96%)	114 (91%)	11 (9%)	9	31
61	SQ	87/113 (77%)	76 (87%)	11 (13%)	4	17
62	SR	92/128 (72%)	75 (82%)	17 (18%)	1	7
63	ST	125/130 (96%)	101 (81%)	24 (19%)	1	5
64	SU	99/124 (80%)	82 (83%)	17 (17%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	SV	118/131 (90%)	86 (73%)	32 (27%)	0	1
66	SW	113/115 (98%)	98 (87%)	15 (13%)	4	15
67	SX	89/110 (81%)	75 (84%)	14 (16%)	2	10
68	SY	69/72 (96%)	57 (83%)	12 (17%)	2	8
69	Sb	103/113 (91%)	83 (81%)	20 (19%)	1	5
70	Sc	67/79 (85%)	50 (75%)	17 (25%)	0	1
71	Sd	92/103 (89%)	81 (88%)	11 (12%)	5	19
72	Se	72/73 (99%)	65 (90%)	7 (10%)	8	28
73	Sg	56/57 (98%)	45 (80%)	11 (20%)	1	5
74	Sh	44/45 (98%)	34 (77%)	10 (23%)	1	3
75	Sj	54/58 (93%)	46 (85%)	8 (15%)	3	12
All	All	8681/9575 (91%)	7496 (86%)	1185 (14%)	6	14

All (1185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	LA	15	VAL
1	LA	20	VAL
1	LA	37	ARG
1	LA	41	VAL
1	LA	44	VAL
1	LA	58	LEU
1	LA	67	ARG
1	LA	77	ILE
1	LA	88	VAL
1	LA	102	LEU
1	LA	122	ASP
1	LA	135	LEU
1	LA	140	ASN
1	LA	142	GLU
1	LA	145	LYS
1	LA	148	ILE
1	LA	149	ARG
1	LA	168	LEU
1	LA	169	VAL
1	LA	181	LYS
1	LA	199	VAL
1	LA	207	VAL

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Mol	Chain	Res	Type
1	LA	221	VAL
1	LA	234	LYS
1	LA	238	ILE
2	LB	13	ASN
2	LB	41	ILE
2	LB	47	LEU
2	LB	54	THR
2	LB	55	HIS
2	LB	58	ARG
2	LB	62	HIS
2	LB	73	ILE
2	LB	87	THR
2	LB	102	VAL
2	LB	104	THR
2	LB	105	VAL
2	LB	110	ILE
2	LB	139	ASP
2	LB	144	LYS
2	LB	159	ILE
2	LB	163	THR
2	LB	170	LEU
2	LB	177	ILE
2	LB	190	GLU
2	LB	198	LEU
2	LB	199	MET
2	LB	201	LYS
2	LB	205	ILE
2	LB	218	ILE
2	LB	219	SER
2	LB	220	ILE
2	LB	231	THR
2	LB	276	THR
2	LB	280	LYS
2	LB	285	ILE
2	LB	295	THR
2	LB	301	THR
2	LB	308	VAL
2	LB	312	VAL
2	LB	322	ILE
2	LB	327	THR
2	LB	337	VAL
2	LB	348	CYS

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Mol	Chain	Res	Type
2	LB	352	GLN
2	LB	366	ILE
2	LB	369	THR
2	LB	373	ARG
3	LC	4	THR
3	LC	5	VAL
3	LC	13	THR
3	LC	23	VAL
3	LC	26	VAL
3	LC	28	LEU
3	LC	72	LEU
3	LC	97	VAL
3	LC	105	VAL
3	LC	126	LEU
3	LC	146	THR
3	LC	149	VAL
3	LC	159	ILE
3	LC	164	VAL
3	LC	181	ARG
3	LC	219	VAL
3	LC	222	ILE
3	LC	264	ILE
3	LC	269	ILE
3	LC	292	GLU
3	LC	294	LYS
3	LC	301	LYS
3	LC	304	LEU
3	LC	310	SER
6	LF	5	LYS
6	LF	9	THR
6	LF	36	LEU
6	LF	52	VAL
6	LF	59	ASP
6	LF	60	ILE
6	LF	62	CYS
6	LF	68	GLU
6	LF	72	ASP
6	LF	75	VAL
6	LF	76	CYS
6	LF	80	SER
6	LF	90	VAL
6	LF	94	ASN

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Mol	Chain	Res	Type
6	LF	107	ARG
6	LF	112	LYS
6	LF	119	GLU
6	LF	120	ASN
6	LF	122	LEU
6	LF	130	ASP
6	LF	141	GLU
6	LF	167	VAL
6	LF	175	VAL
6	LF	181	ILE
6	LF	185	MET
6	LF	210	VAL
6	LF	227	LYS
6	LF	241	ARG
6	LF	245	MET
6	LF	263	LYS
6	LF	268	LYS
6	LF	270	VAL
6	LF	275	LEU
6	LF	282	GLU
6	LF	288	LYS
7	LG	5	LYS
7	LG	16	LYS
7	LG	39	TYR
8	LH	23	GLU
8	LH	31	ARG
8	LH	52	ASP
8	LH	53	LEU
8	LH	58	LYS
8	LH	70	LEU
8	LH	75	GLU
8	LH	78	VAL
8	LH	112	MET
8	LH	133	GLU
8	LH	166	GLU
8	LH	170	LYS
8	LH	174	LEU
8	LH	220	PHE
8	LH	233	ARG
9	LI	31	PHE
9	LI	56	THR
9	LI	71	GLU

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Mol	Chain	Res	Type
9	LI	88	LYS
9	LI	90	ARG
9	LI	91	LEU
9	LI	98	LYS
9	LI	113	ILE
9	LI	162	ARG
9	LI	169	LYS
9	LI	170	LEU
9	LI	179	VAL
9	LI	180	CYS
9	LI	189	LYS
9	LI	194	LYS
9	LI	195	ILE
9	LI	211	THR
9	LI	212	TYR
9	LI	219	GLU
10	LJ	2	PRO
10	LJ	15	VAL
10	LJ	42	LEU
10	LJ	44	ILE
10	LJ	50	THR
10	LJ	70	CYS
10	LJ	74	GLU
10	LJ	89	ARG
10	LJ	97	ILE
10	LJ	100	THR
10	LJ	102	VAL
10	LJ	110	ILE
10	LJ	128	VAL
10	LJ	139	GLU
10	LJ	168	LEU
10	LJ	178	SER
11	LK	32	ARG
11	LK	43	VAL
11	LK	44	ASN
11	LK	53	LEU
11	LK	57	LYS
11	LK	58	GLU
11	LK	63	GLU
11	LK	66	GLU
11	LK	83	ASP
11	LK	97	ILE

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Mol	Chain	Res	Type
11	LK	126	VAL
11	LK	129	VAL
11	LK	136	LEU
11	LK	138	VAL
11	LK	174	THR
11	LK	179	GLU
11	LK	202	ARG
11	LK	206	LEU
12	LL	14	ILE
12	LL	16	LYS
12	LL	18	VAL
12	LL	19	LEU
12	LL	26	GLU
12	LL	30	LEU
12	LL	35	LYS
12	LL	43	GLN
12	LL	50	SER
12	LL	61	ARG
12	LL	69	VAL
12	LL	71	VAL
12	LL	112	LEU
12	LL	115	LYS
12	LL	122	ILE
12	LL	130	VAL
12	LL	137	ARG
12	LL	155	THR
13	LM	33	VAL
13	LM	44	THR
13	LM	46	LYS
13	LM	61	LYS
13	LM	62	ILE
13	LM	66	GLN
13	LM	75	ILE
13	LM	87	VAL
13	LM	88	THR
13	LM	95	ASN
13	LM	96	LEU
13	LM	100	ILE
13	LM	114	LEU
13	LM	122	ILE
13	LM	132	ASN
13	LM	140	ARG

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Mol	Chain	Res	Type
13	LM	149	LEU
13	LM	166	GLN
13	LM	169	GLN
13	LM	174	VAL
13	LM	175	MET
13	LM	177	VAL
13	LM	178	VAL
13	LM	186	THR
13	LM	195	GLU
13	LM	196	VAL
13	LM	199	ASN
13	LM	223	ARG
14	LN	2	SER
14	LN	11	ARG
14	LN	13	VAL
14	LN	26	VAL
14	LN	28	VAL
14	LN	38	ILE
14	LN	43	THR
14	LN	46	LYS
14	LN	49	VAL
14	LN	50	VAL
14	LN	58	THR
14	LN	62	ILE
14	LN	67	LYS
14	LN	78	GLU
14	LN	83	ILE
14	LN	112	ILE
14	LN	130	ILE
15	LO	19	LEU
15	LO	61	VAL
15	LO	64	VAL
15	LO	66	VAL
15	LO	76	VAL
15	LO	79	ILE
15	LO	85	ARG
15	LO	106	VAL
15	LO	135	ILE
15	LO	151	ILE
15	LO	153	ASN
15	LO	157	LYS
15	LO	184	LEU

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Mol	Chain	Res	Type
15	LO	185	ARG
16	LP	15	ARG
16	LP	52	LEU
16	LP	57	LYS
16	LP	85	ILE
16	LP	101	VAL
16	LP	103	ASP
16	LP	108	CYS
16	LP	119	SER
16	LP	125	CYS
16	LP	126	LEU
16	LP	129	GLU
16	LP	150	VAL
16	LP	182	ASP
16	LP	185	LEU
16	LP	194	LYS
17	LQ	18	ARG
17	LQ	98	VAL
17	LQ	106	LYS
17	LQ	125	ARG
18	LR	7	THR
18	LR	17	LYS
18	LR	18	GLU
18	LR	40	THR
18	LR	45	THR
18	LR	52	LEU
18	LR	61	VAL
18	LR	73	LYS
18	LR	92	VAL
18	LR	94	ILE
18	LR	97	MET
18	LR	107	THR
18	LR	123	ASP
18	LR	129	LYS
18	LR	131	THR
18	LR	137	LEU
18	LR	179	TRP
19	LS	16	LYS
19	LS	54	ASP
19	LS	56	LYS
19	LS	131	MET
19	LS	135	LYS

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Mol	Chain	Res	Type
19	LS	139	LEU
19	LS	156	LYS
19	LS	158	GLU
19	LS	171	LYS
19	LS	173	ARG
19	LS	175	GLU
19	LS	177	VAL
19	LS	182	LEU
19	LS	187	THR
19	LS	189	ILE
19	LS	191	THR
19	LS	192	GLU
20	LT	43	LEU
20	LT	46	LEU
20	LT	60	GLN
20	LT	64	GLU
20	LT	76	LEU
20	LT	91	VAL
20	LT	95	THR
20	LT	103	VAL
20	LT	110	GLN
20	LT	123	VAL
20	LT	126	VAL
20	LT	131	VAL
20	LT	139	PHE
20	LT	140	THR
20	LT	141	GLN
20	LT	142	LYS
20	LT	144	VAL
20	LT	150	CYS
20	LT	155	VAL
21	LU	24	MET
21	LU	27	LEU
21	LU	28	THR
21	LU	32	ARG
21	LU	40	VAL
21	LU	43	LYS
21	LU	52	MET
21	LU	63	THR
21	LU	76	ILE
21	LU	84	ILE
21	LU	91	VAL

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Mol	Chain	Res	Type
21	LU	95	HIS
21	LU	96	VAL
21	LU	126	VAL
21	LU	130	LYS
21	LU	141	VAL
21	LU	148	ILE
21	LU	150	ILE
21	LU	151	THR
21	LU	154	LYS
22	LV	16	ILE
22	LV	20	VAL
22	LV	22	CYS
22	LV	29	GLU
22	LV	56	VAL
22	LV	65	LEU
22	LV	79	VAL
22	LV	87	LEU
22	LV	90	ASP
22	LV	92	GLN
22	LV	100	THR
22	LV	104	THR
22	LV	108	LYS
22	LV	110	TYR
23	LW	16	ARG
23	LW	39	ASN
23	LW	47	LYS
23	LW	63	LEU
23	LW	65	THR
23	LW	69	ASP
23	LW	73	GLU
23	LW	79	THR
23	LW	98	ILE
23	LW	108	ILE
23	LW	123	VAL
23	LW	130	ARG
24	LX	5	GLU
24	LX	6	HIS
24	LX	7	CYS
24	LX	20	ILE
24	LX	21	CYS
24	LX	23	VAL
24	LX	35	SER

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Mol	Chain	Res	Type
24	LX	62	LYS
25	LY	28	ASN
25	LY	37	LEU
25	LY	50	ILE
25	LY	59	CYS
25	LY	66	ILE
25	LY	67	LYS
25	LY	69	ASP
25	LY	70	GLU
25	LY	118	LEU
25	LY	129	VAL
25	LY	132	MET
26	LZ	8	THR
26	LZ	12	ARG
26	LZ	24	GLU
26	LZ	32	SER
26	LZ	43	LYS
26	LZ	44	ILE
26	LZ	46	THR
26	LZ	55	VAL
26	LZ	68	VAL
26	LZ	69	VAL
26	LZ	85	GLN
26	LZ	88	ARG
26	LZ	91	GLU
26	LZ	93	LYS
26	LZ	99	ILE
27	La	13	ILE
27	La	40	ILE
27	La	49	ARG
27	La	85	LEU
27	La	90	LYS
27	La	97	THR
27	La	98	VAL
27	La	101	VAL
27	La	116	GLN
27	La	118	ARG
27	La	125	THR
27	La	130	LYS
27	La	133	ILE
28	Lb	30	SER
28	Lb	32	ARG

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Mol	Chain	Res	Type
28	Lb	43	THR
28	Lb	85	GLU
28	Lb	123	ILE
28	Lb	140	GLU
28	Lb	141	VAL
28	Lb	144	VAL
28	Lb	146	LEU
29	Lc	8	THR
29	Lc	22	LYS
29	Lc	55	LEU
30	Ld	5	VAL
30	Ld	9	LYS
30	Ld	13	SER
30	Ld	18	LEU
30	Ld	28	THR
30	Ld	45	LEU
30	Ld	46	VAL
30	Ld	47	PHE
30	Ld	48	MET
30	Ld	50	ASN
30	Ld	55	LEU
30	Ld	65	HIS
30	Ld	66	LEU
30	Ld	71	VAL
30	Ld	83	ILE
30	Ld	93	ILE
30	Ld	95	THR
30	Ld	98	GLU
31	Le	3	ILE
31	Le	70	VAL
31	Le	77	GLU
31	Le	89	GLU
31	Le	92	LYS
31	Le	96	THR
31	Le	99	LYS
32	Lf	9	LEU
32	Lf	23	ILE
32	Lf	28	GLU
32	Lf	38	ARG
32	Lf	44	ASP
32	Lf	55	ARG
32	Lf	60	ILE

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Mol	Chain	Res	Type
32	Lf	72	LEU
32	Lf	79	HIS
32	Lf	92	MET
32	Lf	94	ASN
32	Lf	101	ILE
32	Lf	114	LEU
32	Lf	131	LEU
33	Lg	9	PHE
33	Lg	13	ILE
33	Lg	28	VAL
33	Lg	45	VAL
33	Lg	74	MET
33	Lg	81	THR
33	Lg	92	VAL
34	Lh	6	VAL
34	Lh	21	VAL
34	Lh	45	CYS
34	Lh	96	ASN
35	Li	32	LEU
35	Li	40	LEU
35	Li	69	VAL
35	Li	108	ILE
35	Li	120	MET
35	Li	132	LEU
35	Li	140	LYS
35	Li	145	LYS
35	Li	150	VAL
35	Li	151	LYS
36	Lj	17	ILE
36	Lj	18	VAL
36	Lj	19	ARG
36	Lj	25	LYS
36	Lj	54	LEU
36	Lj	58	LYS
36	Lj	84	SER
37	Lk	2	SER
37	Lk	34	CYS
37	Lk	37	CYS
37	Lk	45	ARG
37	Lk	46	ARG
37	Lk	55	ARG
37	Lk	78	THR

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Mol	Chain	Res	Type
38	Ll	10	LEU
38	Ll	12	LYS
38	Ll	20	LYS
38	Ll	22	LEU
38	Ll	23	VAL
38	Ll	24	VAL
38	Ll	25	LYS
38	Ll	31	ARG
38	Ll	33	GLN
38	Ll	36	VAL
38	Ll	39	LYS
38	Ll	41	ARG
38	Ll	51	VAL
38	Ll	68	VAL
38	Ll	73	VAL
39	Ln	4	ILE
39	Ln	9	LEU
39	Ln	12	HIS
39	Ln	16	ILE
39	Ln	17	ILE
39	Ln	19	ARG
39	Ln	23	GLU
39	Ln	28	PHE
39	Ln	30	GLU
39	Ln	32	VAL
39	Ln	38	LEU
39	Ln	44	LYS
39	Ln	48	ARG
39	Ln	50	ASN
39	Ln	65	LEU
39	Ln	66	CYS
39	Ln	68	ILE
39	Ln	72	ARG
39	Ln	85	VAL
39	Ln	87	ILE
39	Ln	100	ILE
39	Ln	110	PHE
39	Ln	117	ILE
39	Ln	123	TYR
39	Ln	136	LEU
39	Ln	138	LEU
39	Ln	144	LEU

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Mol	Chain	Res	Type
39	Ln	145	GLU
39	Ln	158	GLN
39	Ln	160	LYS
39	Ln	161	LYS
39	Ln	163	VAL
39	Ln	171	ASN
39	Ln	181	GLN
39	Ln	190	LEU
39	Ln	196	LYS
39	Ln	201	ILE
39	Ln	204	VAL
39	Ln	206	ILE
39	Ln	207	LYS
39	Ln	208	SER
39	Ln	210	MET
39	Ln	215	ARG
40	Lo	10	MET
41	Lp	10	THR
41	Lp	12	CYS
41	Lp	18	HIS
41	Lp	19	THR
41	Lp	36	GLN
41	Lp	38	LYS
41	Lp	67	VAL
41	Lp	79	THR
41	Lp	81	GLN
41	Lp	88	ARG
41	Lp	90	GLU
41	Lp	94	LEU
42	Lq	4	ARG
42	Lq	5	THR
42	Lq	8	VAL
42	Lq	10	LEU
42	Lq	26	LEU
42	Lq	39	CYS
42	Lq	50	THR
42	Lq	52	CYS
42	Lq	64	MET
42	Lq	73	THR
42	Lq	74	GLU
43	Ls	94	MET
43	Ls	96	CYS

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Mol	Chain	Res	Type
43	Ls	105	LEU
43	Ls	108	THR
43	Ls	110	CYS
43	Ls	117	ASN
43	Ls	120	LYS
46	SA	28	THR
46	SA	32	VAL
46	SA	35	ILE
46	SA	48	LYS
46	SA	74	ASP
46	SA	82	VAL
46	SA	89	GLN
46	SA	102	THR
46	SA	112	ASN
46	SA	118	ASN
46	SA	126	LEU
46	SA	127	LEU
46	SA	129	VAL
46	SA	145	VAL
46	SA	156	ASP
46	SA	170	ASN
46	SA	174	MET
46	SA	194	ILE
46	SA	201	ASP
46	SA	202	VAL
46	SA	210	LEU
47	SB	36	LEU
47	SB	37	VAL
47	SB	43	GLU
47	SB	48	ILE
47	SB	58	THR
47	SB	74	VAL
47	SB	76	ASN
47	SB	79	SER
47	SB	88	GLN
47	SB	90	THR
47	SB	130	ILE
47	SB	142	LEU
47	SB	148	VAL
47	SB	155	LYS
47	SB	159	VAL
47	SB	177	THR

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Mol	Chain	Res	Type
47	SB	183	GLU
47	SB	189	ASP
47	SB	190	VAL
47	SB	201	LEU
47	SB	218	ILE
47	SB	223	LEU
48	SC	6	ARG
48	SC	10	GLU
48	SC	11	ASN
48	SC	34	GLU
48	SC	42	SER
48	SC	45	LEU
48	SC	47	ARG
48	SC	48	THR
48	SC	49	ILE
48	SC	53	CYS
48	SC	55	ILE
48	SC	64	VAL
48	SC	67	ASP
48	SC	71	ARG
48	SC	79	LEU
48	SC	82	ARG
48	SC	88	LYS
48	SC	108	VAL
48	SC	142	VAL
48	SC	143	ILE
48	SC	144	VAL
48	SC	148	LEU
48	SC	149	ARG
48	SC	154	ARG
48	SC	163	LEU
48	SC	172	ILE
48	SC	174	LEU
48	SC	179	ARG
48	SC	181	ILE
48	SC	184	ARG
48	SC	187	VAL
48	SC	198	ASN
48	SC	206	ASP
48	SC	207	LYS
49	SD	13	ILE
49	SD	14	THR

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Mol	Chain	Res	Type
49	SD	25	LYS
49	SD	31	ILE
49	SD	43	GLN
49	SD	46	VAL
49	SD	47	THR
49	SD	63	VAL
49	SD	66	VAL
49	SD	68	LEU
49	SD	77	ASP
49	SD	78	LEU
49	SD	79	ASN
49	SD	97	LEU
49	SD	108	HIS
49	SD	123	VAL
49	SD	127	ILE
49	SD	134	LEU
49	SD	139	VAL
49	SD	151	ARG
49	SD	154	CYS
49	SD	156	VAL
49	SD	157	LYS
49	SD	179	VAL
49	SD	184	LEU
49	SD	186	THR
49	SD	193	VAL
49	SD	215	VAL
49	SD	224	THR
49	SD	227	LEU
49	SD	237	VAL
49	SD	238	ARG
50	SE	26	ILE
50	SE	40	GLU
50	SE	44	LEU
50	SE	47	ILE
50	SE	70	VAL
50	SE	72	ILE
50	SE	78	THR
50	SE	84	VAL
50	SE	101	VAL
50	SE	102	LEU
50	SE	104	ASP
50	SE	110	THR

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Mol	Chain	Res	Type
50	SE	118	GLU
50	SE	126	VAL
50	SE	129	ILE
50	SE	134	LYS
50	SE	136	MET
50	SE	139	LEU
50	SE	146	THR
50	SE	164	LEU
50	SE	166	THR
50	SE	183	VAL
50	SE	187	ARG
50	SE	200	LYS
50	SE	202	MET
50	SE	212	ASP
50	SE	216	THR
50	SE	219	LEU
50	SE	222	LEU
50	SE	228	ILE
50	SE	235	VAL
50	SE	246	ASP
50	SE	256	ARG
51	SF	10	LYS
51	SF	13	LEU
51	SF	29	ILE
51	SF	31	ASN
51	SF	34	PHE
51	SF	46	ARG
51	SF	54	VAL
51	SF	87	ASN
51	SF	88	LEU
51	SF	99	VAL
51	SF	108	ARG
51	SF	121	ARG
51	SF	122	ARG
51	SF	124	SER
51	SF	125	VAL
51	SF	139	ASN
51	SF	159	LEU
51	SF	178	GLN
52	SG	11	ILE
52	SG	15	VAL
52	SG	22	LEU

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Mol	Chain	Res	Type
52	SG	24	ILE
52	SG	28	ARG
52	SG	29	LYS
52	SG	31	GLN
52	SG	32	THR
52	SG	33	ILE
52	SG	55	THR
52	SG	74	LEU
52	SG	77	GLN
52	SG	81	LEU
52	SG	103	ILE
52	SG	117	VAL
52	SG	118	VAL
52	SG	119	LEU
52	SG	127	LEU
52	SG	130	LEU
52	SG	134	VAL
52	SG	145	SER
52	SG	164	MET
52	SG	165	LEU
52	SG	167	CYS
52	SG	169	LEU
52	SG	188	TYR
52	SG	194	VAL
52	SG	195	VAL
52	SG	198	GLU
52	SG	202	ARG
52	SG	210	LYS
53	SH	7	ARG
53	SH	8	LYS
53	SH	9	ILE
53	SH	15	LYS
53	SH	20	GLU
53	SH	28	LEU
53	SH	30	LEU
53	SH	41	LEU
53	SH	44	LEU
53	SH	59	LYS
53	SH	62	VAL
53	SH	63	VAL
53	SH	78	GLU
53	SH	80	LEU

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Mol	Chain	Res	Type
53	SH	82	LEU
53	SH	95	ILE
53	SH	96	VAL
53	SH	104	ASN
53	SH	107	VAL
53	SH	112	LYS
53	SH	121	THR
53	SH	129	ILE
53	SH	133	ILE
53	SH	143	ARG
53	SH	145	LEU
53	SH	165	GLU
53	SH	170	THR
53	SH	178	LYS
53	SH	183	ARG
54	SI	4	THR
54	SI	7	LYS
54	SI	29	LEU
54	SI	42	VAL
54	SI	51	LYS
54	SI	54	THR
54	SI	62	ILE
54	SI	91	VAL
54	SI	95	THR
54	SI	112	GLN
54	SI	130	GLU
54	SI	136	ARG
54	SI	140	ILE
54	SI	159	LEU
54	SI	174	LYS
55	SJ	2	VAL
55	SJ	5	ASN
55	SJ	7	LEU
55	SJ	18	GLN
55	SJ	23	LYS
55	SJ	24	GLN
55	SJ	36	GLU
55	SJ	40	LEU
55	SJ	43	LYS
55	SJ	47	ILE
55	SJ	63	VAL
55	SJ	66	ILE

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Mol	Chain	Res	Type
55	SJ	80	ASP
55	SJ	87	GLU
55	SJ	91	VAL
55	SJ	96	SER
55	SJ	98	LEU
55	SJ	104	LEU
55	SJ	106	THR
55	SJ	107	SER
55	SJ	108	GLN
55	SJ	110	ILE
55	SJ	118	HIS
55	SJ	121	ILE
55	SJ	125	VAL
56	SK	3	ILE
56	SK	15	THR
56	SK	21	THR
56	SK	32	CYS
56	SK	43	ILE
56	SK	55	ARG
56	SK	61	LEU
56	SK	71	ARG
56	SK	81	LEU
56	SK	118	LYS
56	SK	123	VAL
56	SK	129	MET
56	SK	141	ILE
56	SK	149	VAL
56	SK	165	LEU
56	SK	168	ASN
56	SK	173	ARG
56	SK	176	ARG
57	SL	18	GLU
57	SL	22	LEU
57	SL	29	ARG
57	SL	30	VAL
57	SL	37	THR
57	SL	39	VAL
57	SL	41	GLU
57	SL	44	LYS
57	SL	45	LEU
57	SL	49	THR
57	SL	50	TYR

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Mol	Chain	Res	Type
57	SL	58	GLN
57	SL	59	SER
57	SL	62	SER
57	SL	66	VAL
57	SL	67	LYS
57	SL	68	ASP
57	SL	69	THR
57	SL	74	HIS
57	SL	82	LYS
57	SL	93	LEU
57	SL	100	THR
58	SM	7	GLU
58	SM	12	LYS
58	SM	15	GLN
58	SM	22	LEU
58	SM	23	ARG
58	SM	26	ASN
58	SM	36	ILE
58	SM	44	ILE
58	SM	54	LYS
58	SM	55	LYS
58	SM	61	ASN
58	SM	78	MET
58	SM	82	ILE
58	SM	92	VAL
58	SM	115	VAL
58	SM	134	ARG
58	SM	136	ASN
58	SM	138	ILE
58	SM	139	LYS
58	SM	140	VAL
59	SO	9	THR
59	SO	21	ARG
59	SO	28	ARG
59	SO	36	LEU
59	SO	41	LEU
59	SO	53	GLN
59	SO	70	VAL
59	SO	73	GLN
59	SO	85	VAL
59	SO	91	ILE
59	SO	101	LEU

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Mol	Chain	Res	Type
59	SO	112	VAL
59	SO	139	GLU
60	SP	6	SER
60	SP	16	ILE
60	SP	27	LYS
60	SP	29	THR
60	SP	39	LYS
60	SP	69	SER
60	SP	76	LYS
60	SP	86	GLU
60	SP	87	ASP
60	SP	91	MET
60	SP	109	LYS
61	SQ	28	PHE
61	SQ	40	THR
61	SQ	44	VAL
61	SQ	47	LEU
61	SQ	52	THR
61	SQ	53	ILE
61	SQ	62	VAL
61	SQ	78	THR
61	SQ	93	VAL
61	SQ	95	ILE
61	SQ	107	VAL
62	SR	20	VAL
62	SR	22	VAL
62	SR	23	GLU
62	SR	25	LEU
62	SR	44	ARG
62	SR	50	LEU
62	SR	53	LYS
62	SR	55	LEU
62	SR	61	LEU
62	SR	82	ASP
62	SR	83	MET
62	SR	84	ILE
62	SR	88	GLU
62	SR	93	THR
62	SR	114	ARG
62	SR	116	LEU
62	SR	122	SER
63	ST	9	LEU

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Mol	Chain	Res	Type
63	ST	10	LEU
63	ST	12	ARG
63	ST	17	VAL
63	ST	18	ARG
63	ST	22	LYS
63	ST	25	VAL
63	ST	30	LYS
63	ST	34	SER
63	ST	49	VAL
63	ST	52	VAL
63	ST	54	LEU
63	ST	57	VAL
63	ST	58	ARG
63	ST	63	ARG
63	ST	64	THR
63	ST	73	LEU
63	ST	87	VAL
63	ST	93	VAL
63	ST	111	VAL
63	ST	120	LEU
63	ST	125	VAL
63	ST	143	LYS
63	ST	158	ARG
64	SU	3	LYS
64	SU	4	VAL
64	SU	5	ARG
64	SU	28	ASP
64	SU	30	GLN
64	SU	39	ARG
64	SU	57	VAL
64	SU	64	VAL
64	SU	69	VAL
64	SU	74	LEU
64	SU	79	GLU
64	SU	84	ARG
64	SU	91	LYS
64	SU	96	VAL
64	SU	105	THR
64	SU	107	GLN
64	SU	117	MET
65	SV	13	LEU
65	SV	14	LEU

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Mol	Chain	Res	Type
65	SV	24	LYS
65	SV	25	VAL
65	SV	32	VAL
65	SV	34	ILE
65	SV	35	LYS
65	SV	37	ILE
65	SV	43	ASN
65	SV	47	LYS
65	SV	53	VAL
65	SV	61	THR
65	SV	71	VAL
65	SV	74	ASP
65	SV	76	LEU
65	SV	80	ILE
65	SV	85	LEU
65	SV	91	PHE
65	SV	99	ILE
65	SV	100	LEU
65	SV	101	VAL
65	SV	104	ILE
65	SV	109	ARG
65	SV	112	LEU
65	SV	115	LEU
65	SV	116	ARG
65	SV	122	ARG
65	SV	129	ASN
65	SV	132	VAL
65	SV	136	HIS
65	SV	139	SER
65	SV	147	VAL
66	SW	16	PHE
66	SW	33	ASP
66	SW	35	VAL
66	SW	37	THR
66	SW	39	VAL
66	SW	53	ILE
66	SW	60	ARG
66	SW	61	HIS
66	SW	64	ILE
66	SW	88	THR
66	SW	96	SER
66	SW	97	CYS

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Mol	Chain	Res	Type
66	SW	98	LYS
66	SW	108	LEU
66	SW	113	LEU
67	SX	21	MET
67	SX	22	HIS
67	SX	28	ILE
67	SX	37	VAL
67	SX	40	TYR
67	SX	53	ILE
67	SX	58	ARG
67	SX	65	THR
67	SX	94	VAL
67	SX	101	ILE
67	SX	104	ILE
67	SX	111	ILE
67	SX	116	VAL
67	SX	119	GLU
68	SY	6	ILE
68	SY	15	VAL
68	SY	23	LYS
68	SY	43	VAL
68	SY	45	ARG
68	SY	51	LYS
68	SY	54	GLU
68	SY	56	ASN
68	SY	59	THR
68	SY	76	PHE
68	SY	85	LEU
68	SY	88	ARG
69	Sb	2	PRO
69	Sb	4	ILE
69	Sb	17	LEU
69	Sb	24	VAL
69	Sb	26	VAL
69	Sb	34	GLU
69	Sb	40	LYS
69	Sb	43	VAL
69	Sb	47	LEU
69	Sb	55	ILE
69	Sb	70	VAL
69	Sb	73	CYS
69	Sb	82	LEU

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Mol	Chain	Res	Type
69	Sb	86	GLU
69	Sb	96	LEU
69	Sb	97	ILE
69	Sb	101	LYS
69	Sb	105	ARG
69	Sb	111	LEU
69	Sb	115	ARG
70	Sc	19	THR
70	Sc	23	ASP
70	Sc	27	MET
70	Sc	34	ILE
70	Sc	45	ILE
70	Sc	46	CYS
70	Sc	50	ARG
70	Sc	53	VAL
70	Sc	60	MET
70	Sc	63	LEU
70	Sc	71	ILE
70	Sc	72	VAL
70	Sc	74	LYS
70	Sc	80	ILE
70	Sc	82	LYS
70	Sc	85	THR
70	Sc	88	GLU
71	Sd	15	CYS
71	Sd	20	ILE
71	Sd	23	CYS
71	Sd	30	VAL
71	Sd	35	VAL
71	Sd	38	ARG
71	Sd	40	THR
71	Sd	53	VAL
71	Sd	67	LEU
71	Sd	76	SER
71	Sd	88	SER
72	Se	45	ASN
72	Se	85	VAL
72	Se	86	VAL
72	Se	95	VAL
72	Se	106	ILE
72	Se	118	VAL
72	Se	123	GLN

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Mol	Chain	Res	Type
73	Sg	16	THR
73	Sg	22	ILE
73	Sg	26	LYS
73	Sg	27	VAL
73	Sg	33	GLU
73	Sg	38	ILE
73	Sg	41	VAL
73	Sg	51	LEU
73	Sg	52	VAL
73	Sg	58	ARG
73	Sg	61	ARG
74	Sh	87	MET
74	Sh	96	ILE
74	Sh	104	ILE
74	Sh	105	CYS
74	Sh	111	VAL
74	Sh	112	TYR
74	Sh	117	LEU
74	Sh	119	ILE
74	Sh	122	ARG
74	Sh	125	LYS
75	Sj	7	THR
75	Sj	11	LYS
75	Sj	19	LYS
75	Sj	24	LYS
75	Sj	43	VAL
75	Sj	47	LEU
75	Sj	48	ILE
75	Sj	49	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (224) such sidechains are listed below:

Mol	Chain	Res	Type
1	LA	50	HIS
1	LA	73	ASN
1	LA	97	HIS
1	LA	140	ASN
1	LA	218	HIS
2	LB	13	ASN
2	LB	181	GLN
2	LB	261	GLN
2	LB	281	GLN

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Mol	Chain	Res	Type
2	LB	345	HIS
2	LB	347	ASN
2	LB	352	GLN
2	LB	375	GLN
3	LC	57	GLN
3	LC	93	HIS
3	LC	109	GLN
3	LC	210	ASN
3	LC	232	HIS
3	LC	266	GLN
6	LF	81	HIS
6	LF	138	HIS
6	LF	144	ASN
6	LF	250	HIS
6	LF	256	ASN
7	LG	22	ASN
7	LG	38	ASN
8	LH	63	ASN
8	LH	105	GLN
8	LH	201	GLN
9	LI	48	GLN
9	LI	62	ASN
9	LI	172	HIS
9	LI	201	HIS
10	LJ	104	ASN
10	LJ	115	HIS
11	LK	59	GLN
11	LK	163	GLN
12	LL	139	ASN
12	LL	144	GLN
12	LL	147	HIS
13	LM	49	ASN
13	LM	81	GLN
13	LM	92	GLN
13	LM	95	ASN
13	LM	169	GLN
13	LM	199	ASN
14	LN	4	HIS
14	LN	63	ASN
14	LN	96	GLN
15	LO	32	GLN
15	LO	41	HIS

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Mol	Chain	Res	Type
15	LO	153	ASN
16	LP	28	HIS
16	LP	56	HIS
16	LP	60	ASN
16	LP	69	HIS
16	LP	145	GLN
16	LP	146	HIS
16	LP	166	GLN
16	LP	189	ASN
17	LQ	105	HIS
17	LQ	142	GLN
17	LQ	145	HIS
18	LR	31	ASN
18	LR	158	ASN
18	LR	167	HIS
19	LS	3	ASN
19	LS	28	HIS
19	LS	67	HIS
19	LS	146	GLN
19	LS	161	GLN
19	LS	180	ASN
20	LT	3	GLN
20	LT	60	GLN
20	LT	61	HIS
20	LT	86	ASN
20	LT	141	GLN
20	LT	154	HIS
21	LU	26	ASN
21	LU	38	GLN
21	LU	105	HIS
22	LV	33	ASN
22	LV	68	GLN
23	LW	13	ASN
23	LW	142	HIS
24	LX	6	HIS
24	LX	38	HIS
24	LX	40	ASN
24	LX	60	HIS
25	LY	110	ASN
27	La	16	GLN
27	La	19	HIS
27	La	74	ASN

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Mol	Chain	Res	Type
27	La	88	ASN
27	La	96	GLN
28	Lb	14	HIS
28	Lb	16	GLN
28	Lb	39	GLN
28	Lb	49	HIS
28	Lb	62	HIS
28	Lb	66	ASN
28	Lb	70	ASN
29	Lc	11	ASN
29	Lc	42	ASN
30	Ld	33	GLN
30	Ld	37	ASN
31	Le	85	ASN
32	Lf	11	HIS
32	Lf	50	GLN
32	Lf	79	HIS
32	Lf	94	ASN
35	Li	91	ASN
35	Li	107	HIS
36	Lj	7	ASN
36	Lj	30	GLN
36	Lj	38	GLN
36	Lj	49	HIS
36	Lj	61	HIS
37	Lk	32	HIS
38	Ll	71	GLN
39	Ln	35	GLN
39	Ln	62	ASN
39	Ln	166	ASN
39	Ln	171	ASN
39	Ln	193	GLN
39	Ln	214	HIS
41	Lp	18	HIS
41	Lp	45	GLN
41	Lp	81	GLN
43	Ls	90	ASN
43	Ls	98	HIS
46	SA	34	ASN
46	SA	55	ASN
46	SA	112	ASN
46	SA	130	ASN

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Mol	Chain	Res	Type
46	SA	146	ASN
47	SB	76	ASN
47	SB	88	GLN
47	SB	146	HIS
48	SC	198	ASN
49	SD	81	ASN
49	SD	190	ASN
49	SD	202	GLN
49	SD	223	ASN
50	SE	127	GLN
51	SF	32	HIS
51	SF	68	ASN
51	SF	87	ASN
51	SF	123	GLN
51	SF	139	ASN
52	SG	10	ASN
52	SG	19	ASN
52	SG	77	GLN
52	SG	85	GLN
52	SG	204	GLN
52	SG	220	GLN
53	SH	87	ASN
53	SH	98	ASN
53	SH	138	HIS
53	SH	155	GLN
54	SI	5	HIS
54	SI	112	GLN
54	SI	134	GLN
54	SI	139	HIS
54	SI	150	GLN
55	SJ	18	GLN
55	SJ	24	GLN
55	SJ	44	ASN
55	SJ	56	HIS
55	SJ	117	GLN
56	SK	125	HIS
56	SK	143	ASN
57	SL	52	HIS
57	SL	54	ASN
58	SM	15	GLN
58	SM	41	HIS
58	SM	48	ASN

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Mol	Chain	Res	Type
58	SM	61	ASN
59	SO	20	ASN
59	SO	31	HIS
59	SO	73	GLN
60	SP	5	HIS
60	SP	36	GLN
60	SP	62	GLN
61	SQ	32	HIS
61	SQ	76	GLN
62	SR	48	HIS
63	ST	51	ASN
63	ST	84	ASN
63	ST	130	GLN
64	SU	30	GLN
64	SU	31	ASN
64	SU	51	ASN
65	SV	8	ASN
65	SV	22	GLN
65	SV	43	ASN
65	SV	78	HIS
65	SV	98	HIS
65	SV	126	HIS
65	SV	129	ASN
65	SV	135	GLN
65	SV	145	HIS
66	SW	83	GLN
66	SW	138	GLN
67	SX	78	ASN
67	SX	115	GLN
68	SY	55	ASN
68	SY	81	GLN
69	Sb	14	ASN
69	Sb	54	ASN
69	Sb	68	HIS
69	Sb	77	GLN
70	Sc	28	ASN
70	Sc	36	ASN
70	Sc	42	HIS
70	Sc	62	GLN
71	Sd	17	HIS
71	Sd	19	ASN
71	Sd	82	HIS

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Mol	Chain	Res	Type
72	Se	45	ASN
72	Se	57	GLN
73	Sg	24	GLN
73	Sg	36	GLN
75	Sj	57	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	LD	141/142 (99%)	43 (30%)	11 (7%)
44	Lt	2588/2697 (95%)	779 (30%)	0
45	Lu	55/75 (73%)	29 (52%)	0
5	LE	116/121 (95%)	32 (27%)	5 (4%)
76	St	1453/1454 (99%)	501 (34%)	0
All	All	4353/4489 (96%)	1384 (31%)	16 (0%)

All (1384) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	LD	9	C
4	LD	12	C
4	LD	17	G
4	LD	20	G
4	LD	21	C
4	LD	22	C
4	LD	23	U
4	LD	24	C
4	LD	27	C
4	LD	29	C
4	LD	31	G
4	LD	39	C
4	LD	40	G
4	LD	47	G
4	LD	50	G
4	LD	52	G
4	LD	54	A
4	LD	59	G
4	LD	60	A
4	LD	64	G
4	LD	71	G
4	LD	72	G

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Mol	Chain	Res	Type
4	LD	73	A
4	LD	74	C
4	LD	76	C
4	LD	77	G
4	LD	80	C
4	LD	81	G
4	LD	85	C
4	LD	86	G
4	LD	87	A
4	LD	88	G
4	LD	94	C
4	LD	104	A
4	LD	105	A
4	LD	106	C
4	LD	108	C
4	LD	112	G
4	LD	117	C
4	LD	118	C
4	LD	119	G
4	LD	126	C
4	LD	133	G
5	LE	7	G
5	LE	11	A
5	LE	21	G
5	LE	22	G
5	LE	23	A
5	LE	30	U
5	LE	32	A
5	LE	34	C
5	LE	35	U
5	LE	38	U
5	LE	39	U
5	LE	42	G
5	LE	44	A
5	LE	50	A
5	LE	51	A
5	LE	53	A
5	LE	54	G
5	LE	59	G
5	LE	63	U
5	LE	64	C
5	LE	65	A

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Mol	Chain	Res	Type
5	LE	77	U
5	LE	85	U
5	LE	86	C
5	LE	91	A
5	LE	92	C
5	LE	93	G
5	LE	98	G
5	LE	99	G
5	LE	110	U
5	LE	111	G
5	LE	114	G
44	Lt	2	G
44	Lt	3	C
44	Lt	4	G
44	Lt	10	G
44	Lt	24	G
44	Lt	25	A
44	Lt	30	C
44	Lt	39	A
44	Lt	42	A
44	Lt	43	U
44	Lt	48	G
44	Lt	49	U
44	Lt	58	G
44	Lt	59	A
44	Lt	63	G
44	Lt	64	A
44	Lt	65	A
44	Lt	66	A
44	Lt	72	C
44	Lt	73	G
44	Lt	84	C
44	Lt	85	U
44	Lt	86	A
44	Lt	90	G
44	Lt	106	G
44	Lt	107	A
44	Lt	118	A
44	Lt	120	G
44	Lt	122	C
44	Lt	123	G
44	Lt	124	C

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Mol	Chain	Res	Type
44	Lt	128	G
44	Lt	129	U
44	Lt	153	C
44	Lt	166	G
44	Lt	167	G
44	Lt	168	G
44	Lt	170	C
44	Lt	172	C
44	Lt	173	G
44	Lt	176	C
44	Lt	179	G
44	Lt	185	G
44	Lt	186	C
44	Lt	187	A
44	Lt	190	C
44	Lt	194	G
44	Lt	222	A
44	Lt	235	G
44	Lt	238	C
44	Lt	239	G
44	Lt	250	A
44	Lt	251	G
44	Lt	256	G
44	Lt	257	C
44	Lt	258	G
44	Lt	267	C
44	Lt	281	G
44	Lt	288	G
44	Lt	289	A
44	Lt	300	A
44	Lt	301	C
44	Lt	302	C
44	Lt	314	G
44	Lt	317	A
44	Lt	320	G
44	Lt	321	G
44	Lt	322	U
44	Lt	326	A
44	Lt	327	A
44	Lt	328	G
44	Lt	335	C
44	Lt	339	G

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Mol	Chain	Res	Type
44	Lt	343	G
44	Lt	347	A
44	Lt	349	A
44	Lt	350	A
44	Lt	352	A
44	Lt	367	G
44	Lt	368	C
44	Lt	369	C
44	Lt	370	G
44	Lt	375	C
44	Lt	376	C
44	Lt	377	C
44	Lt	378	G
44	Lt	379	C
44	Lt	385	C
44	Lt	389	C
44	Lt	397	A
44	Lt	409	G
44	Lt	410	C
44	Lt	425	A
44	Lt	427	C
44	Lt	429	C
44	Lt	430	G
44	Lt	435	A
44	Lt	436	G
44	Lt	437	C
44	Lt	443	C
44	Lt	444	G
44	Lt	449	A
44	Lt	456	G
44	Lt	459	A
44	Lt	460	G
44	Lt	461	A
44	Lt	463	G
44	Lt	464	C
44	Lt	465	C
44	Lt	483	C
44	Lt	484	U
44	Lt	485	G
44	Lt	486	C
44	Lt	493	G
44	Lt	494	C

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Mol	Chain	Res	Type
44	Lt	497	G
44	Lt	501	C
44	Lt	502	G
44	Lt	513	C
44	Lt	515	U
44	Lt	517	G
44	Lt	518	G
44	Lt	525	A
44	Lt	534	U
44	Lt	539	G
44	Lt	542	C
44	Lt	547	A
44	Lt	550	G
44	Lt	553	A
44	Lt	561	C
44	Lt	566	G
44	Lt	574	G
44	Lt	578	C
44	Lt	591	U
44	Lt	592	G
44	Lt	596	C
44	Lt	597	G
44	Lt	601	A
44	Lt	605	C
44	Lt	611	G
44	Lt	612	G
44	Lt	613	A
44	Lt	614	G
44	Lt	624	G
44	Lt	625	G
44	Lt	631	A
44	Lt	632	A
44	Lt	633	G
44	Lt	634	A
44	Lt	637	C
44	Lt	640	C
44	Lt	641	G
44	Lt	642	A
44	Lt	649	U
44	Lt	650	G
44	Lt	654	G
44	Lt	655	C

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Mol	Chain	Res	Type
44	Lt	661	G
44	Lt	676	C
44	Lt	677	C
44	Lt	679	A
44	Lt	680	G
44	Lt	681	G
44	Lt	682	A
44	Lt	691	G
44	Lt	695	C
44	Lt	696	G
44	Lt	698	A
44	Lt	699	G
44	Lt	708	C
44	Lt	709	G
44	Lt	715	C
44	Lt	716	G
44	Lt	719	G
44	Lt	720	G
44	Lt	728	G
44	Lt	729	A
44	Lt	730	G
44	Lt	731	C
44	Lt	732	G
44	Lt	734	G
44	Lt	736	G
44	Lt	737	G
44	Lt	738	C
44	Lt	739	C
44	Lt	740	U
44	Lt	741	G
44	Lt	742	C
44	Lt	743	C
44	Lt	744	C
44	Lt	747	C
44	Lt	751	C
44	Lt	756	C
44	Lt	758	C
44	Lt	760	A
44	Lt	763	U
44	Lt	764	C
44	Lt	765	C
44	Lt	767	A

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Mol	Chain	Res	Type
44	Lt	769	G
44	Lt	770	G
44	Lt	776	G
44	Lt	777	C
44	Lt	787	G
44	Lt	788	C
44	Lt	791	G
44	Lt	793	C
44	Lt	794	U
44	Lt	795	G
44	Lt	803	C
44	Lt	805	G
44	Lt	806	G
44	Lt	807	C
44	Lt	808	G
44	Lt	809	A
44	Lt	814	G
44	Lt	827	G
44	Lt	834	C
44	Lt	840	A
44	Lt	841	G
44	Lt	844	G
44	Lt	845	G
44	Lt	854	G
44	Lt	855	G
44	Lt	862	G
44	Lt	863	A
44	Lt	864	U
44	Lt	865	C
44	Lt	869	A
44	Lt	870	C
44	Lt	871	G
44	Lt	873	C
44	Lt	878	C
44	Lt	882	G
44	Lt	888	C
44	Lt	889	G
44	Lt	898	C
44	Lt	900	C
44	Lt	901	G
44	Lt	906	G
44	Lt	908	C

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Mol	Chain	Res	Type
44	Lt	909	G
44	Lt	917	G
44	Lt	919	C
44	Lt	921	C
44	Lt	922	G
44	Lt	923	A
44	Lt	982	G
44	Lt	983	C
44	Lt	987	A
44	Lt	989	C
44	Lt	990	G
44	Lt	993	C
44	Lt	994	G
44	Lt	995	G
44	Lt	999	G
44	Lt	1001	A
44	Lt	1005	U
44	Lt	1006	G
44	Lt	1007	G
44	Lt	1009	G
44	Lt	1013	G
44	Lt	1016	G
44	Lt	1017	G
44	Lt	1018	A
44	Lt	1023	C
44	Lt	1025	G
44	Lt	1026	A
44	Lt	1028	C
44	Lt	1030	G
44	Lt	1031	C
44	Lt	1032	G
44	Lt	1037	G
44	Lt	1038	C
44	Lt	1045	G
44	Lt	1046	C
44	Lt	1053	G
44	Lt	1062	C
44	Lt	1067	G
44	Lt	1070	G
44	Lt	1073	C
44	Lt	1074	C
44	Lt	1075	G

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Mol	Chain	Res	Type
44	Lt	1076	G
44	Lt	1079	G
44	Lt	1080	C
44	Lt	1081	G
44	Lt	1096	G
44	Lt	1100	C
44	Lt	1105	G
44	Lt	1109	G
44	Lt	1116	G
44	Lt	1117	G
44	Lt	1118	U
44	Lt	1120	C
44	Lt	1122	G
44	Lt	1125	C
44	Lt	1126	U
44	Lt	1134	A
44	Lt	1140	C
44	Lt	1143	U
44	Lt	1144	A
44	Lt	1151	G
44	Lt	1153	C
44	Lt	1154	C
44	Lt	1159	G
44	Lt	1161	A
44	Lt	1165	A
44	Lt	1166	G
44	Lt	1167	G
44	Lt	1168	G
44	Lt	1169	G
44	Lt	1172	G
44	Lt	1178	U
44	Lt	1186	C
44	Lt	1191	G
44	Lt	1192	C
44	Lt	1195	C
44	Lt	1198	G
44	Lt	1199	C
44	Lt	1204	G
44	Lt	1206	U
44	Lt	1207	G
44	Lt	1208	A
44	Lt	1213	G

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Mol	Chain	Res	Type
44	Lt	1217	U
44	Lt	1220	G
44	Lt	1226	G
44	Lt	1231	A
44	Lt	1233	A
44	Lt	1236	G
44	Lt	1237	G
44	Lt	1238	G
44	Lt	1239	A
44	Lt	1240	A
44	Lt	1241	G
44	Lt	1242	G
44	Lt	1244	G
44	Lt	1245	C
44	Lt	1248	G
44	Lt	1249	C
44	Lt	1253	C
44	Lt	1257	U
44	Lt	1258	C
44	Lt	1260	A
44	Lt	1261	A
44	Lt	1262	C
44	Lt	1277	G
44	Lt	1278	A
44	Lt	1279	C
44	Lt	1280	U
44	Lt	1286	A
44	Lt	1290	G
44	Lt	1297	C
44	Lt	1298	C
44	Lt	1309	C
44	Lt	1310	C
44	Lt	1314	C
44	Lt	1318	G
44	Lt	1323	C
44	Lt	1324	G
44	Lt	1346	G
44	Lt	1349	G
44	Lt	1350	C
44	Lt	1353	C
44	Lt	1356	C
44	Lt	1357	C

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Mol	Chain	Res	Type
44	Lt	1377	C
44	Lt	1380	G
44	Lt	1381	A
44	Lt	1382	C
44	Lt	1386	U
44	Lt	1387	U
44	Lt	1389	C
44	Lt	1392	G
44	Lt	1394	A
44	Lt	1395	G
44	Lt	1401	G
44	Lt	1406	G
44	Lt	1407	G
44	Lt	1414	A
44	Lt	1423	G
44	Lt	1434	C
44	Lt	1438	U
44	Lt	1439	G
44	Lt	1440	A
44	Lt	1447	G
44	Lt	1448	G
44	Lt	1449	G
44	Lt	1453	C
44	Lt	1454	G
44	Lt	1455	C
44	Lt	1456	C
44	Lt	1461	G
44	Lt	1469	U
44	Lt	1470	A
44	Lt	1473	G
44	Lt	1474	A
44	Lt	1476	C
44	Lt	1478	C
44	Lt	1479	A
44	Lt	1480	G
44	Lt	1481	C
44	Lt	1482	A
44	Lt	1483	G
44	Lt	1485	A
44	Lt	1487	U
44	Lt	1490	G
44	Lt	1491	G

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Mol	Chain	Res	Type
44	Lt	1498	C
44	Lt	1499	A
44	Lt	1509	G
44	Lt	1510	C
44	Lt	1511	G
44	Lt	1512	G
44	Lt	1514	A
44	Lt	1518	A
44	Lt	1529	G
44	Lt	1533	A
44	Lt	1538	G
44	Lt	1539	C
44	Lt	1541	A
44	Lt	1558	C
44	Lt	1562	A
44	Lt	1564	A
44	Lt	1566	G
44	Lt	1567	G
44	Lt	1575	C
44	Lt	1577	G
44	Lt	1578	A
44	Lt	1579	C
44	Lt	1580	G
44	Lt	1581	G
44	Lt	1586	C
44	Lt	1589	G
44	Lt	1590	G
44	Lt	1597	C
44	Lt	1599	G
44	Lt	1600	G
44	Lt	1601	A
44	Lt	1603	C
44	Lt	1604	G
44	Lt	1605	G
44	Lt	1611	G
44	Lt	1620	A
44	Lt	1624	U
44	Lt	1626	U
44	Lt	1628	C
44	Lt	1629	U
44	Lt	1633	A
44	Lt	1641	G

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Mol	Chain	Res	Type
44	Lt	1646	G
44	Lt	1647	A
44	Lt	1648	G
44	Lt	1649	G
44	Lt	1658	C
44	Lt	1659	G
44	Lt	1666	G
44	Lt	1672	C
44	Lt	1673	G
44	Lt	1676	A
44	Lt	1683	C
44	Lt	1692	A
44	Lt	1693	C
44	Lt	1694	G
44	Lt	1696	C
44	Lt	1697	C
44	Lt	1698	G
44	Lt	1706	G
44	Lt	1715	C
44	Lt	1716	G
44	Lt	1719	G
44	Lt	1720	A
44	Lt	1727	G
44	Lt	1731	A
44	Lt	1732	A
44	Lt	1737	G
44	Lt	1739	G
44	Lt	1741	G
44	Lt	1744	A
44	Lt	1745	C
44	Lt	1748	U
44	Lt	1749	G
44	Lt	1750	A
44	Lt	1751	C
44	Lt	1755	C
44	Lt	1760	G
44	Lt	1761	G
44	Lt	1764	G
44	Lt	1767	A
44	Lt	1769	A
44	Lt	1771	G
44	Lt	1772	C

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Mol	Chain	Res	Type
44	Lt	1775	C
44	Lt	1785	U
44	Lt	1786	U
44	Lt	1793	G
44	Lt	1794	U
44	Lt	1795	G
44	Lt	1797	A
44	Lt	1798	U
44	Lt	1801	A
44	Lt	1802	U
44	Lt	1803	G
44	Lt	1807	C
44	Lt	1808	A
44	Lt	1811	G
44	Lt	1812	A
44	Lt	1814	G
44	Lt	1822	U
44	Lt	1823	G
44	Lt	1824	U
44	Lt	1833	G
44	Lt	1843	G
44	Lt	1852	G
44	Lt	1853	C
44	Lt	1861	A
44	Lt	1862	C
44	Lt	1863	G
44	Lt	1865	G
44	Lt	1866	C
44	Lt	1873	C
44	Lt	1876	C
44	Lt	1879	G
44	Lt	1881	G
44	Lt	1885	C
44	Lt	1886	A
44	Lt	1888	G
44	Lt	1889	A
44	Lt	1890	A
44	Lt	1891	G
44	Lt	1899	U
44	Lt	1910	C
44	Lt	1914	C
44	Lt	1915	C

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Mol	Chain	Res	Type
44	Lt	1922	U
44	Lt	1923	G
44	Lt	1929	C
44	Lt	1930	G
44	Lt	1932	G
44	Lt	1936	G
44	Lt	1939	G
44	Lt	1941	C
44	Lt	1942	G
44	Lt	1943	C
44	Lt	1944	A
44	Lt	1946	C
44	Lt	1947	G
44	Lt	1948	C
44	Lt	1949	A
44	Lt	1950	C
44	Lt	1953	G
44	Lt	1954	G
44	Lt	1956	A
44	Lt	1959	C
44	Lt	1962	C
44	Lt	1963	G
44	Lt	1966	C
44	Lt	1967	C
44	Lt	1968	U
44	Lt	1969	G
44	Lt	1972	A
44	Lt	1973	C
44	Lt	1974	A
44	Lt	1975	C
44	Lt	1976	C
44	Lt	1977	C
44	Lt	1978	U
44	Lt	1979	G
44	Lt	1985	C
44	Lt	1988	C
44	Lt	1989	G
44	Lt	1990	C
44	Lt	2000	C
44	Lt	2001	A
44	Lt	2008	C
44	Lt	2009	G

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Mol	Chain	Res	Type
44	Lt	2010	C
44	Lt	2012	C
44	Lt	2017	A
44	Lt	2018	C
44	Lt	2030	G
44	Lt	2031	G
44	Lt	2032	G
44	Lt	2033	A
44	Lt	2034	G
44	Lt	2038	G
44	Lt	2047	G
44	Lt	2049	C
44	Lt	2050	G
44	Lt	2051	C
44	Lt	2052	G
44	Lt	2059	A
44	Lt	2061	A
44	Lt	2065	G
44	Lt	2066	A
44	Lt	2068	C
44	Lt	2072	G
44	Lt	2075	G
44	Lt	2076	U
44	Lt	2080	A
44	Lt	2082	G
44	Lt	2084	C
44	Lt	2090	C
44	Lt	2093	C
44	Lt	2094	G
44	Lt	2095	A
44	Lt	2098	A
44	Lt	2100	G
44	Lt	2101	G
44	Lt	2102	A
44	Lt	2104	A
44	Lt	2106	C
44	Lt	2107	U
44	Lt	2108	C
44	Lt	2109	C
44	Lt	2112	C
44	Lt	2113	G
44	Lt	2114	G

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Mol	Chain	Res	Type
44	Lt	2115	A
44	Lt	2118	A
44	Lt	2124	G
44	Lt	2126	A
44	Lt	2127	C
44	Lt	2128	A
44	Lt	2129	A
44	Lt	2130	G
44	Lt	2137	C
44	Lt	2138	G
44	Lt	2140	C
44	Lt	2151	C
44	Lt	2152	G
44	Lt	2153	U
44	Lt	2176	G
44	Lt	2177	G
44	Lt	2183	C
44	Lt	2184	C
44	Lt	2185	G
44	Lt	2186	A
44	Lt	2195	C
44	Lt	2196	G
44	Lt	2200	C
44	Lt	2201	G
44	Lt	2202	G
44	Lt	2203	C
44	Lt	2211	G
44	Lt	2213	G
44	Lt	2217	G
44	Lt	2218	U
44	Lt	2219	G
44	Lt	2220	G
44	Lt	2222	A
44	Lt	2223	G
44	Lt	2224	A
44	Lt	2225	A
44	Lt	2231	A
44	Lt	2233	C
44	Lt	2234	A
44	Lt	2235	C
44	Lt	2239	G
44	Lt	2240	A

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Mol	Chain	Res	Type
44	Lt	2241	U
44	Lt	2243	A
44	Lt	2244	C
44	Lt	2245	U
44	Lt	2255	C
44	Lt	2261	A
44	Lt	2268	G
44	Lt	2272	C
44	Lt	2273	G
44	Lt	2276	G
44	Lt	2279	G
44	Lt	2283	U
44	Lt	2286	G
44	Lt	2289	C
44	Lt	2290	C
44	Lt	2291	U
44	Lt	2294	G
44	Lt	2298	U
44	Lt	2309	U
44	Lt	2310	A
44	Lt	2311	C
44	Lt	2317	G
44	Lt	2321	G
44	Lt	2322	C
44	Lt	2334	A
44	Lt	2339	C
44	Lt	2341	G
44	Lt	2354	U
44	Lt	2356	C
44	Lt	2357	A
44	Lt	2358	A
44	Lt	2363	U
44	Lt	2364	C
44	Lt	2365	G
44	Lt	2367	G
44	Lt	2372	G
44	Lt	2373	G
44	Lt	2376	U
44	Lt	2393	A
44	Lt	2400	U
44	Lt	2401	U
44	Lt	2402	U

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Mol	Chain	Res	Type
44	Lt	2405	C
44	Lt	2412	G
44	Lt	2416	C
44	Lt	2421	G
44	Lt	2424	A
44	Lt	2429	A
44	Lt	2430	C
44	Lt	2434	G
44	Lt	2437	C
44	Lt	2439	A
44	Lt	2456	C
44	Lt	2457	G
44	Lt	2464	G
44	Lt	2466	C
44	Lt	2467	G
44	Lt	2470	A
44	Lt	2471	G
44	Lt	2472	C
44	Lt	2474	C
44	Lt	2475	C
44	Lt	2476	G
44	Lt	2486	G
44	Lt	2495	G
44	Lt	2496	C
44	Lt	2497	G
44	Lt	2503	C
44	Lt	2508	G
44	Lt	2509	C
44	Lt	2514	G
44	Lt	2515	G
44	Lt	2516	G
44	Lt	2523	G
44	Lt	2531	C
44	Lt	2532	G
44	Lt	2539	A
44	Lt	2546	A
44	Lt	2547	C
44	Lt	2566	C
44	Lt	2568	G
44	Lt	2572	C
44	Lt	2573	G
44	Lt	2575	G

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Mol	Chain	Res	Type
44	Lt	2580	A
44	Lt	2581	G
44	Lt	2583	C
44	Lt	2584	C
44	Lt	2585	C
44	Lt	2587	U
44	Lt	2591	C
44	Lt	2592	C
44	Lt	2593	G
44	Lt	2594	U
44	Lt	2595	C
44	Lt	2596	G
44	Lt	2598	C
44	Lt	2607	C
44	Lt	2608	C
44	Lt	2609	C
44	Lt	2610	G
44	Lt	2617	G
44	Lt	2628	G
44	Lt	2629	C
44	Lt	2634	C
44	Lt	2649	C
44	Lt	2652	A
44	Lt	2653	G
44	Lt	2658	G
44	Lt	2668	G
44	Lt	2669	A
44	Lt	2679	C
44	Lt	2680	U
44	Lt	2681	G
44	Lt	2683	A
44	Lt	2687	C
44	Lt	2688	G
44	Lt	2690	G
45	Lu	2	G
45	Lu	5	G
45	Lu	7	G
45	Lu	8	U
45	Lu	14	A
45	Lu	16	C
45	Lu	17	G
45	Lu	18	G

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Mol	Chain	Res	Type
45	Lu	19	A
45	Lu	20	A
45	Lu	21	G
45	Lu	45	G
45	Lu	46	U
45	Lu	47	C
45	Lu	49	A
45	Lu	50	U
45	Lu	51	G
45	Lu	52	G
45	Lu	56	G
45	Lu	57	A
45	Lu	58	A
45	Lu	59	A
45	Lu	62	A
45	Lu	64	C
45	Lu	65	C
45	Lu	66	U
45	Lu	73	C
45	Lu	74	C
45	Lu	75	A
76	St	2	A
76	St	4	C
76	St	17	C
76	St	20	G
76	St	25	C
76	St	26	G
76	St	33	U
76	St	41	G
76	St	43	C
76	St	44	G
76	St	45	A
76	St	46	A
76	St	49	C
76	St	56	G
76	St	59	C
76	St	65	C
76	St	66	C
76	St	67	C
76	St	68	G
76	St	69	G
76	St	70	G

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Mol	Chain	Res	Type
76	St	71	A
76	St	81	C
76	St	87	A
76	St	91	C
76	St	98	U
76	St	101	A
76	St	102	C
76	St	106	C
76	St	114	G
76	St	115	U
76	St	117	C
76	St	118	C
76	St	120	G
76	St	121	C
76	St	122	U
76	St	123	A
76	St	124	G
76	St	125	C
76	St	126	C
76	St	128	G
76	St	129	A
76	St	130	C
76	St	137	G
76	St	144	C
76	St	149	C
76	St	151	A
76	St	152	A
76	St	153	G
76	St	154	A
76	St	160	G
76	St	161	C
76	St	162	G
76	St	163	C
76	St	164	A
76	St	166	G
76	St	169	C
76	St	170	G
76	St	172	G
76	St	173	C
76	St	175	C
76	St	176	C
76	St	179	G

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Mol	Chain	Res	Type
76	St	180	C
76	St	185	G
76	St	187	G
76	St	188	C
76	St	192	G
76	St	201	C
76	St	202	G
76	St	204	C
76	St	205	G
76	St	206	G
76	St	207	C
76	St	216	G
76	St	219	U
76	St	220	C
76	St	224	G
76	St	231	C
76	St	234	G
76	St	235	G
76	St	236	U
76	St	242	C
76	St	250	G
76	St	251	C
76	St	265	G
76	St	272	G
76	St	274	C
76	St	283	A
76	St	286	G
76	St	291	A
76	St	293	U
76	St	294	C
76	St	300	A
76	St	304	G
76	St	311	G
76	St	313	G
76	St	314	A
76	St	315	C
76	St	317	G
76	St	326	U
76	St	329	A
76	St	330	A
76	St	331	G
76	St	335	G

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Mol	Chain	Res	Type
76	St	336	G
76	St	337	C
76	St	338	A
76	St	339	G
76	St	340	C
76	St	341	A
76	St	348	G
76	St	352	U
76	St	354	G
76	St	357	C
76	St	360	U
76	St	361	G
76	St	366	G
76	St	368	G
76	St	371	C
76	St	372	G
76	St	381	A
76	St	383	G
76	St	389	C
76	St	390	G
76	St	392	G
76	St	393	C
76	St	394	G
76	St	395	A
76	St	396	G
76	St	397	C
76	St	398	G
76	St	399	A
76	St	401	G
76	St	402	C
76	St	403	G
76	St	411	A
76	St	413	C
76	St	418	G
76	St	422	C
76	St	423	G
76	St	424	C
76	St	426	G
76	St	427	C
76	St	429	G
76	St	431	G
76	St	435	A

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Mol	Chain	Res	Type
76	St	436	A
76	St	437	G
76	St	438	G
76	St	439	U
76	St	441	U
76	St	445	C
76	St	446	C
76	St	448	G
76	St	449	C
76	St	450	A
76	St	457	G
76	St	458	U
76	St	459	A
76	St	460	A
76	St	463	C
76	St	474	A
76	St	475	G
76	St	487	G
76	St	488	C
76	St	490	G
76	St	491	C
76	St	494	C
76	St	499	G
76	St	500	A
76	St	502	A
76	St	503	C
76	St	504	G
76	St	514	G
76	St	515	G
76	St	518	C
76	St	519	C
76	St	521	C
76	St	523	C
76	St	524	C
76	St	525	G
76	St	527	C
76	St	532	G
76	St	534	A
76	St	535	A
76	St	544	G
76	St	545	C
76	St	550	G

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Mol	Chain	Res	Type
76	St	553	A
76	St	554	G
76	St	556	C
76	St	557	C
76	St	558	C
76	St	560	U
76	St	568	G
76	St	569	C
76	St	570	C
76	St	577	G
76	St	578	A
76	St	581	G
76	St	584	C
76	St	585	A
76	St	586	G
76	St	589	G
76	St	592	G
76	St	593	C
76	St	594	G
76	St	595	G
76	St	596	C
76	St	597	G
76	St	598	C
76	St	600	C
76	St	604	C
76	St	605	G
76	St	606	C
76	St	607	C
76	St	608	G
76	St	609	C
76	St	610	A
76	St	611	G
76	St	617	A
76	St	618	G
76	St	627	G
76	St	630	G
76	St	640	U
76	St	652	A
76	St	655	G
76	St	658	G
76	St	660	A
76	St	665	G

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Mol	Chain	Res	Type
76	St	668	G
76	St	682	C
76	St	683	G
76	St	687	G
76	St	688	C
76	St	689	C
76	St	694	A
76	St	696	G
76	St	702	G
76	St	713	C
76	St	714	U
76	St	720	A
76	St	722	U
76	St	731	A
76	St	735	C
76	St	738	G
76	St	739	G
76	St	742	C
76	St	746	A
76	St	747	A
76	St	755	A
76	St	758	C
76	St	759	A
76	St	777	G
76	St	779	A
76	St	780	A
76	St	782	C
76	St	784	G
76	St	785	U
76	St	786	G
76	St	793	C
76	St	794	G
76	St	796	G
76	St	805	G
76	St	806	C
76	St	807	G
76	St	808	C
76	St	809	G
76	St	810	U
76	St	811	C
76	St	814	G
76	St	820	C

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Mol	Chain	Res	Type
76	St	829	A
76	St	835	G
76	St	837	A
76	St	840	C
76	St	841	U
76	St	842	C
76	St	843	C
76	St	844	G
76	St	852	G
76	St	853	G
76	St	855	G
76	St	882	A
76	St	890	G
76	St	894	G
76	St	898	G
76	St	899	G
76	St	902	C
76	St	903	C
76	St	904	A
76	St	906	C
76	St	911	G
76	St	915	A
76	St	918	C
76	St	920	G
76	St	922	G
76	St	926	C
76	St	927	A
76	St	929	U
76	St	930	C
76	St	931	U
76	St	933	A
76	St	934	C
76	St	937	A
76	St	938	A
76	St	940	G
76	St	944	G
76	St	945	C
76	St	950	C
76	St	952	C
76	St	954	A
76	St	958	C
76	St	959	C

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Mol	Chain	Res	Type
76	St	960	G
76	St	961	G
76	St	970	A
76	St	971	G
76	St	972	G
76	St	973	A
76	St	974	C
76	St	977	A
76	St	984	G
76	St	985	G
76	St	986	C
76	St	987	G
76	St	988	C
76	St	993	U
76	St	995	G
76	St	996	C
76	St	997	G
76	St	998	A
76	St	999	U
76	St	1000	C
76	St	1007	G
76	St	1009	G
76	St	1012	G
76	St	1015	G
76	St	1016	C
76	St	1022	C
76	St	1026	C
76	St	1027	C
76	St	1028	C
76	St	1029	A
76	St	1033	C
76	St	1039	G
76	St	1042	A
76	St	1043	G
76	St	1047	U
76	St	1048	C
76	St	1049	U
76	St	1053	C
76	St	1056	U
76	St	1060	G
76	St	1063	A
76	St	1067	A

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Mol	Chain	Res	Type
76	St	1078	G
76	St	1079	G
76	St	1080	C
76	St	1087	C
76	St	1088	G
76	St	1089	C
76	St	1090	C
76	St	1092	C
76	St	1093	G
76	St	1096	A
76	St	1098	G
76	St	1103	G
76	St	1104	C
76	St	1105	G
76	St	1106	G
76	St	1109	G
76	St	1110	C
76	St	1114	A
76	St	1115	G
76	St	1117	A
76	St	1122	G
76	St	1124	G
76	St	1127	G
76	St	1128	A
76	St	1131	G
76	St	1133	A
76	St	1134	G
76	St	1138	U
76	St	1139	G
76	St	1140	U
76	St	1141	G
76	St	1142	A
76	St	1150	A
76	St	1151	G
76	St	1152	A
76	St	1154	G
76	St	1157	C
76	St	1160	G
76	St	1163	C
76	St	1164	G
76	St	1165	C
76	St	1166	A

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Mol	Chain	Res	Type
76	St	1167	C
76	St	1172	G
76	St	1175	A
76	St	1177	A
76	St	1178	C
76	St	1179	U
76	St	1180	G
76	St	1184	G
76	St	1188	C
76	St	1189	A
76	St	1194	G
76	St	1196	G
76	St	1204	G
76	St	1208	G
76	St	1211	C
76	St	1212	G
76	St	1213	G
76	St	1214	A
76	St	1215	G
76	St	1223	C
76	St	1224	G
76	St	1225	U
76	St	1227	G
76	St	1228	C
76	St	1229	C
76	St	1232	G
76	St	1237	C
76	St	1242	U
76	St	1244	G
76	St	1245	A
76	St	1247	C
76	St	1254	G
76	St	1255	C
76	St	1256	G
76	St	1257	C
76	St	1261	A
76	St	1262	G
76	St	1263	G
76	St	1267	G
76	St	1271	U
76	St	1272	G
76	St	1273	U

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Mol	Chain	Res	Type
76	St	1278	G
76	St	1289	C
76	St	1290	C
76	St	1296	C
76	St	1297	C
76	St	1298	G
76	St	1304	G
76	St	1305	U
76	St	1310	G
76	St	1312	C
76	St	1319	A
76	St	1320	C
76	St	1321	A
76	St	1322	C
76	St	1323	A
76	St	1324	C
76	St	1325	C
76	St	1326	G
76	St	1329	C
76	St	1345	U
76	St	1346	G
76	St	1350	G
76	St	1351	C
76	St	1353	G
76	St	1354	C
76	St	1358	G
76	St	1366	C
76	St	1368	G
76	St	1370	C
76	St	1372	C
76	St	1373	G
76	St	1374	C
76	St	1376	A
76	St	1390	C
76	St	1393	G
76	St	1399	G
76	St	1401	A
76	St	1405	A
76	St	1410	A
76	St	1411	A
76	St	1412	G
76	St	1415	G

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Mol	Chain	Res	Type
76	St	1417	A
76	St	1421	A
76	St	1422	G
76	St	1423	G
76	St	1424	U
76	St	1426	U
76	St	1435	G
76	St	1436	A
76	St	1437	A
76	St	1438	C
76	St	1446	U
76	St	1447	G
76	St	1448	G
76	St	1449	A
76	St	1450	U
76	St	1451	C
76	St	1453	U
76	St	1454	U

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	LD	23	U
4	LD	39	C
4	LD	49	G
4	LD	59	G
4	LD	72	G
4	LD	73	A
4	LD	76	C
4	LD	87	A
4	LD	88	G
4	LD	111	C
4	LD	132	C
5	LE	38	U
5	LE	50	A
5	LE	63	U
5	LE	85	U
5	LE	110	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

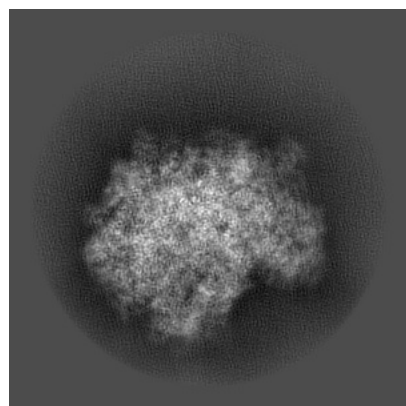
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16211. These allow visual inspection of the internal detail of the map and identification of artifacts.

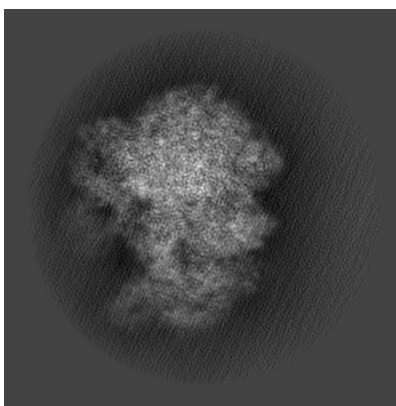
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

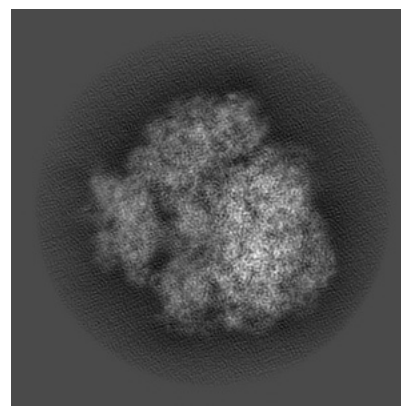
6.1.1 Primary map



X

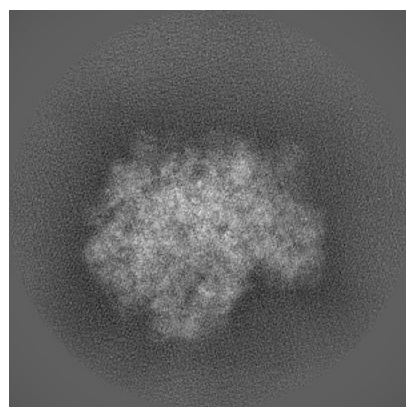


Y

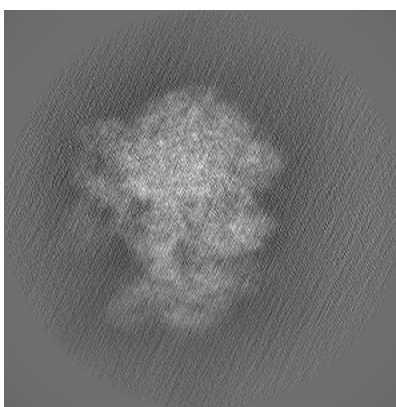


Z

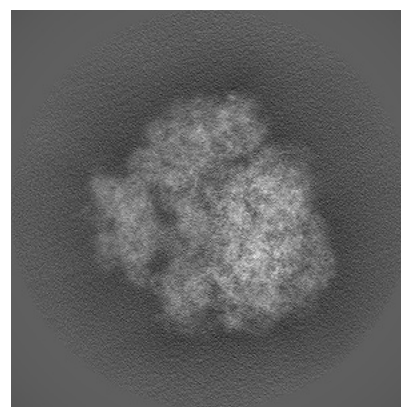
6.1.2 Raw map



X



Y

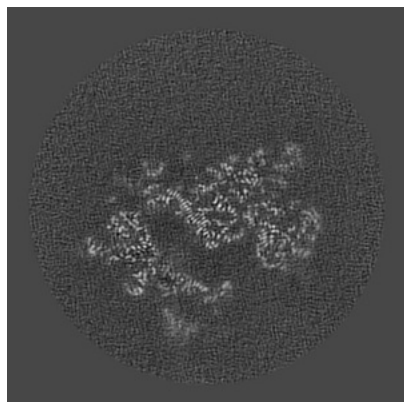


Z

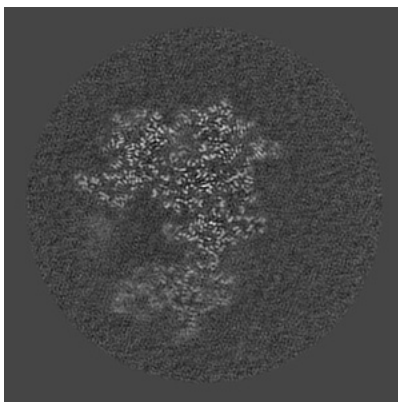
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

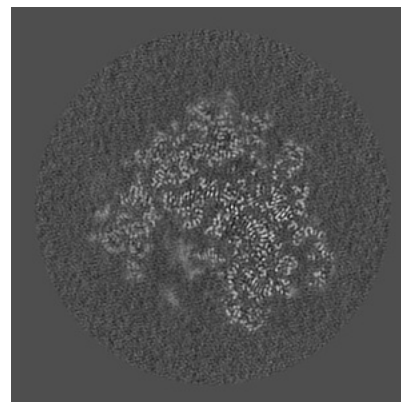
6.2.1 Primary map



X Index: 250

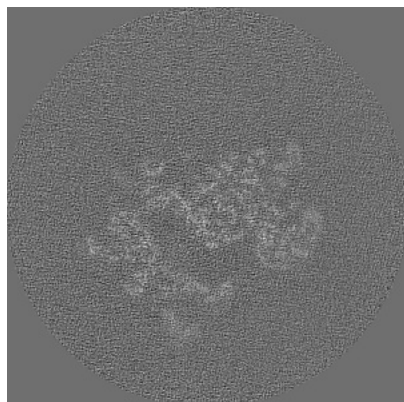


Y Index: 250

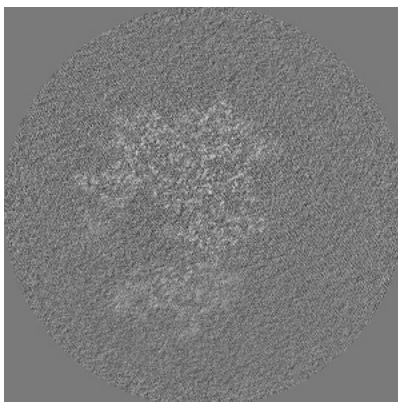


Z Index: 250

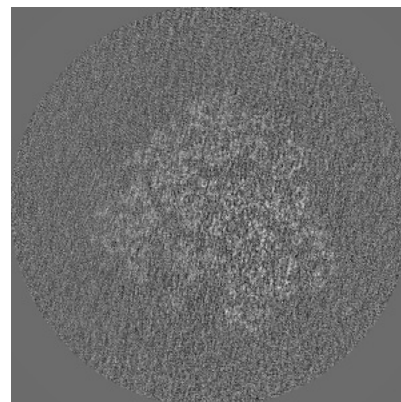
6.2.2 Raw map



X Index: 250



Y Index: 250

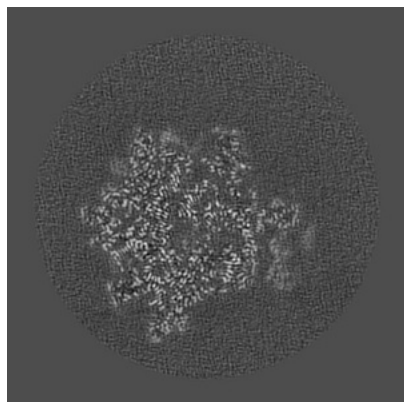


Z Index: 250

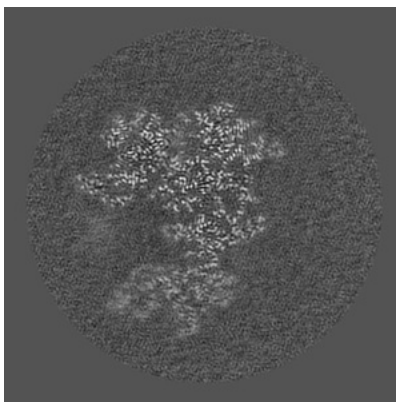
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

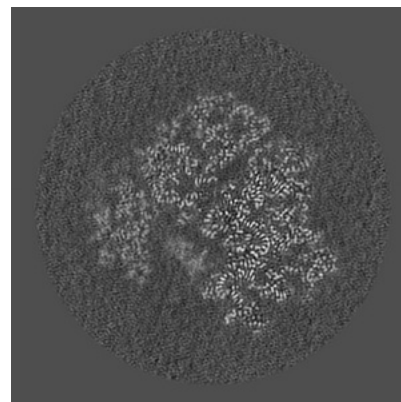
6.3.1 Primary map



X Index: 307

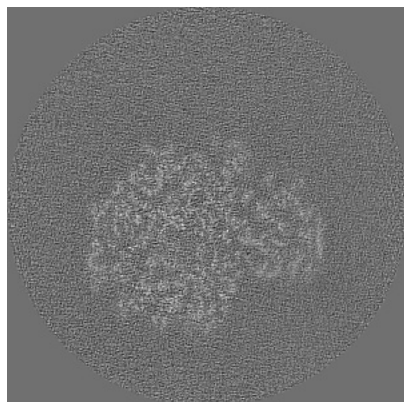


Y Index: 252

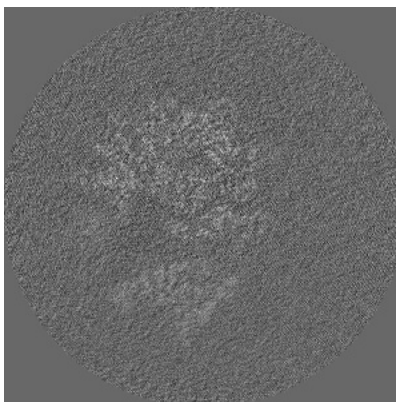


Z Index: 241

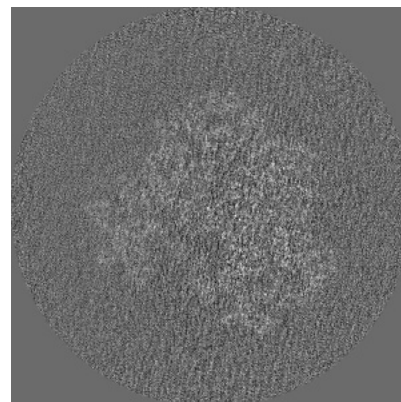
6.3.2 Raw map



X Index: 278



Y Index: 242

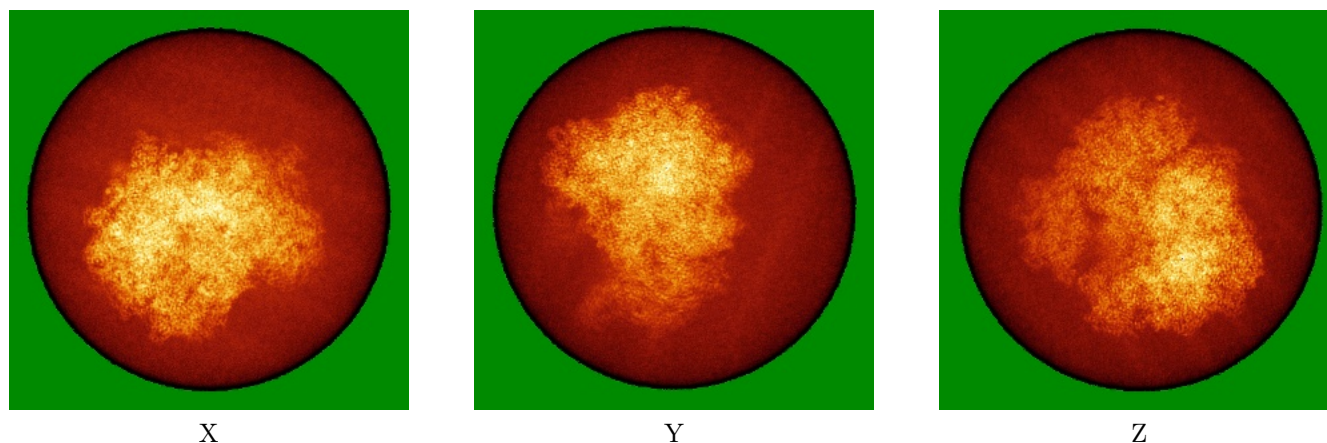


Z Index: 236

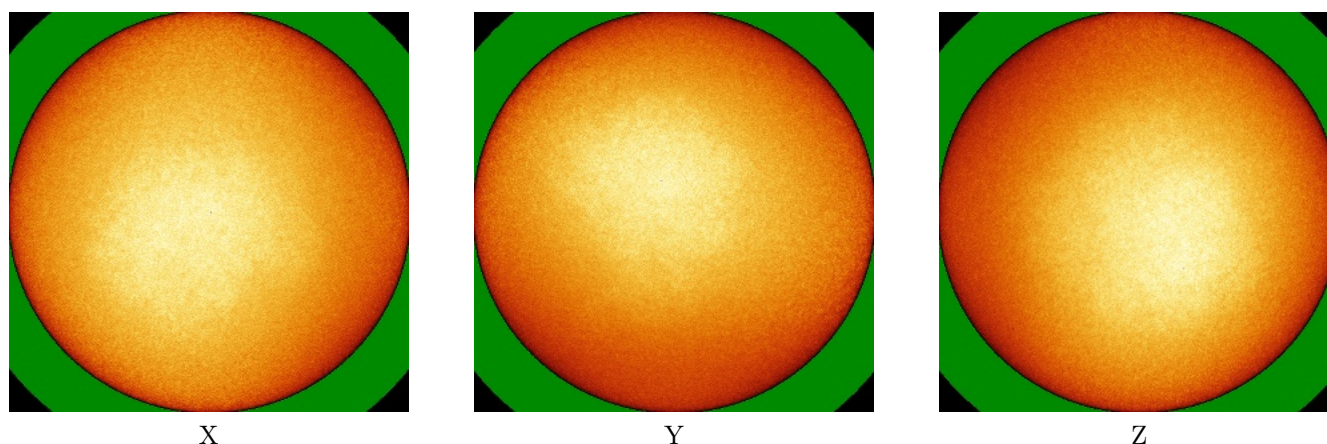
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

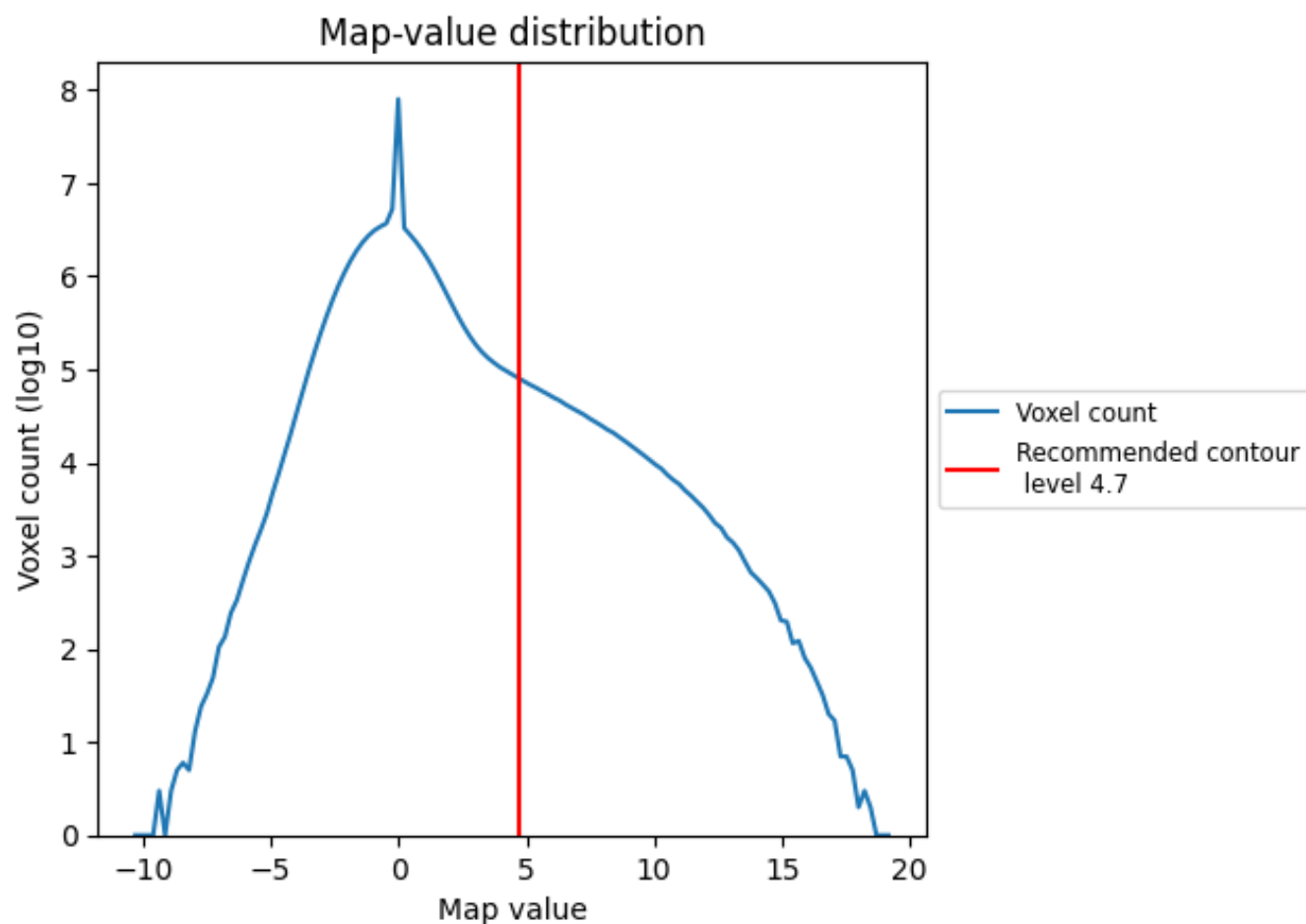
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

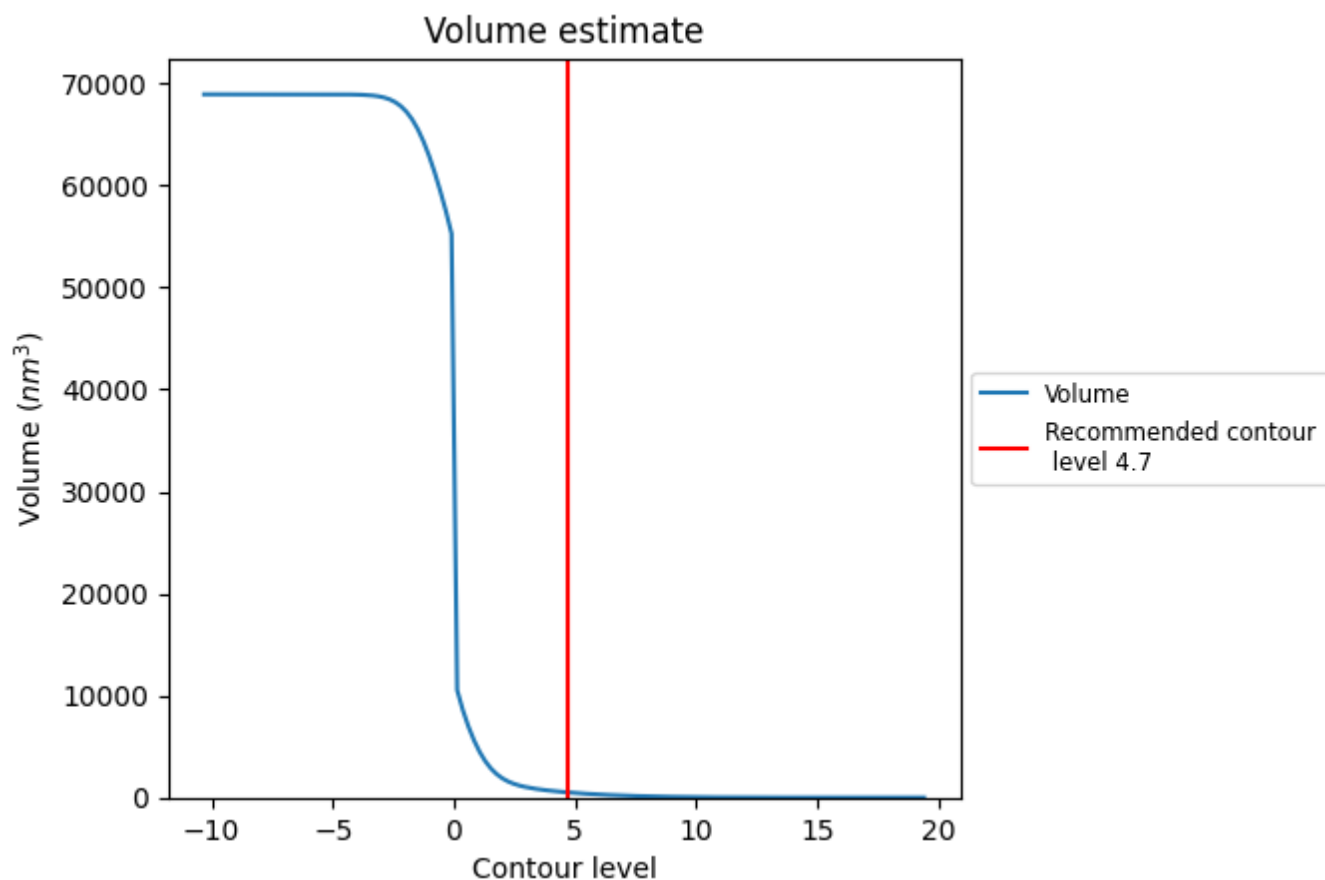
This section contains the results of statistical analysis of the map.

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.

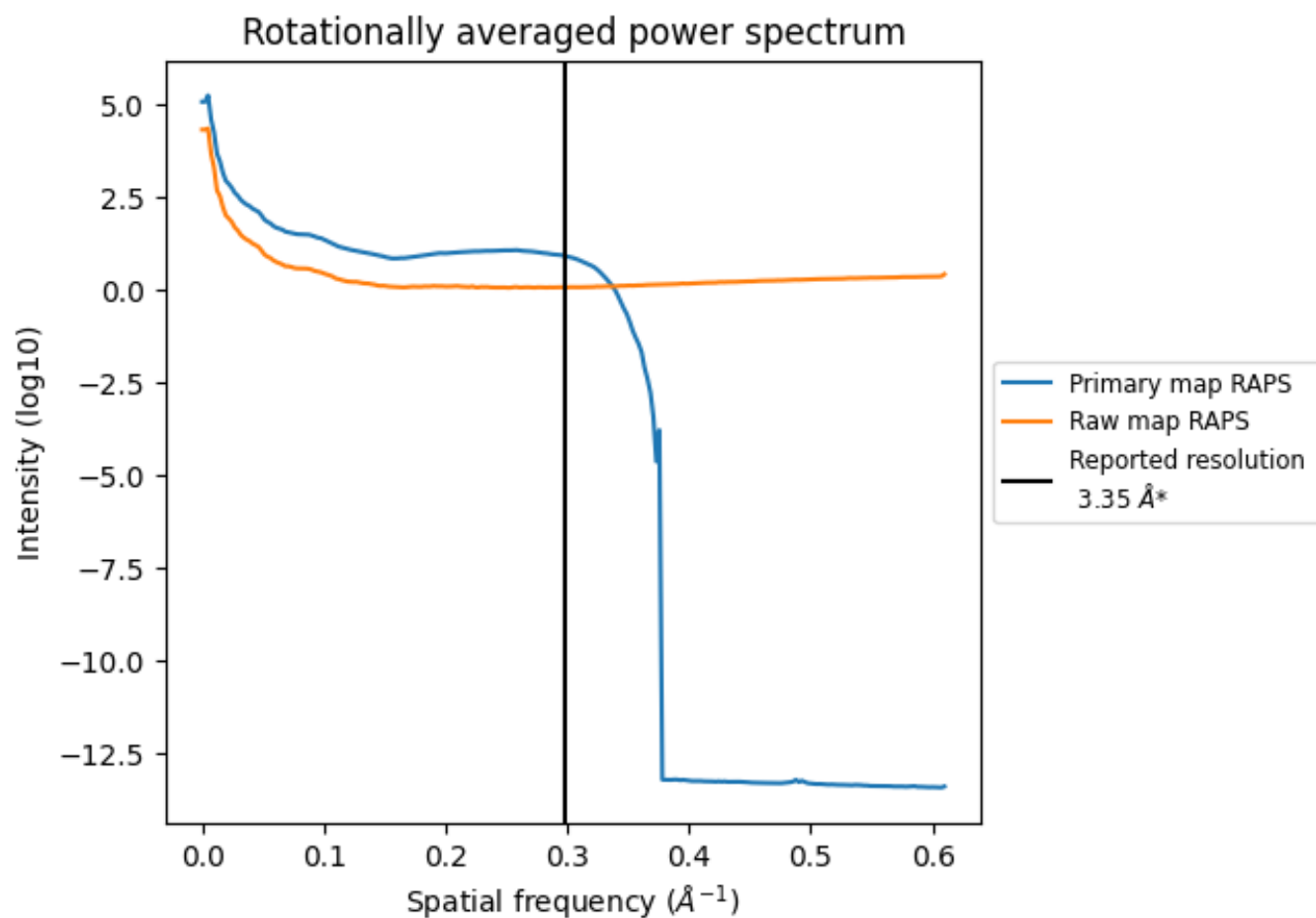
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 506 nm³; this corresponds to an approximate mass of 457 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 ⓘ

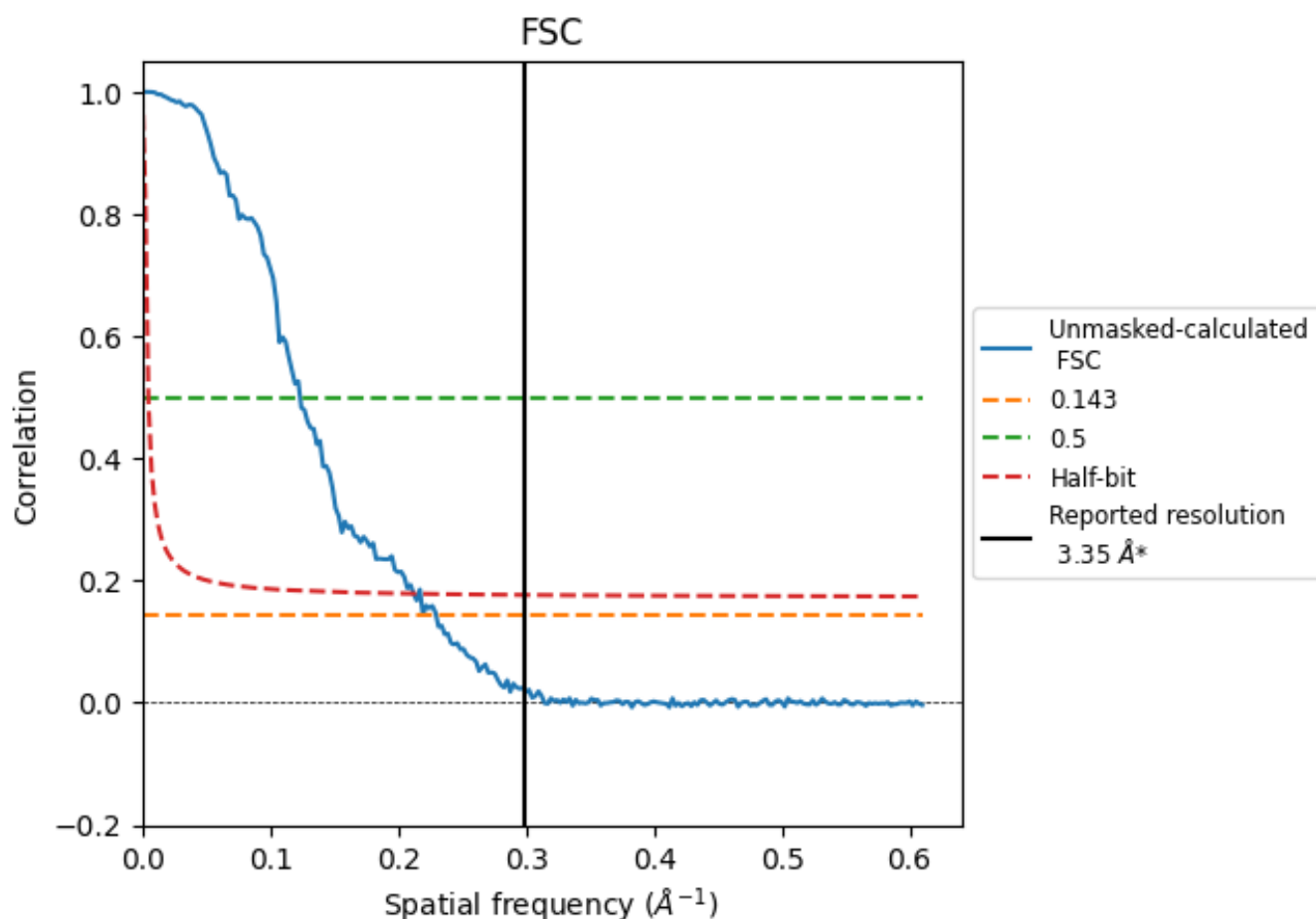


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.299 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.35	8.10	4.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.35 differs from the reported value 3.35 by more than 10 %

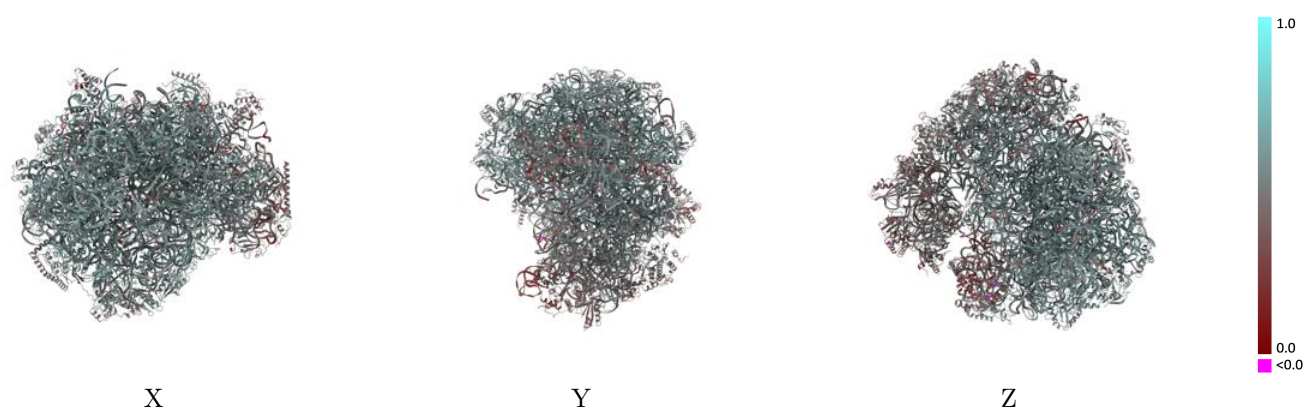
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16211 and PDB model 8BR8. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)

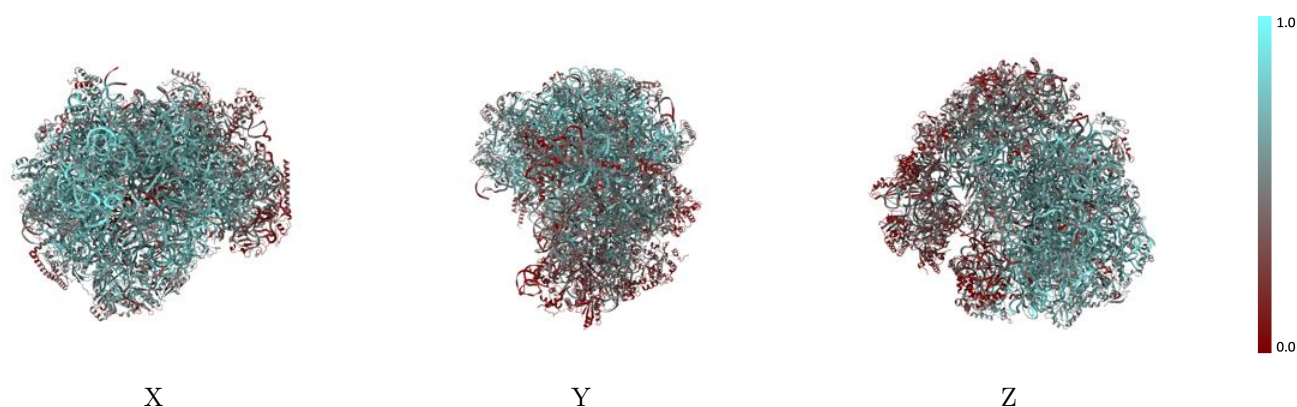
This section was not generated.

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



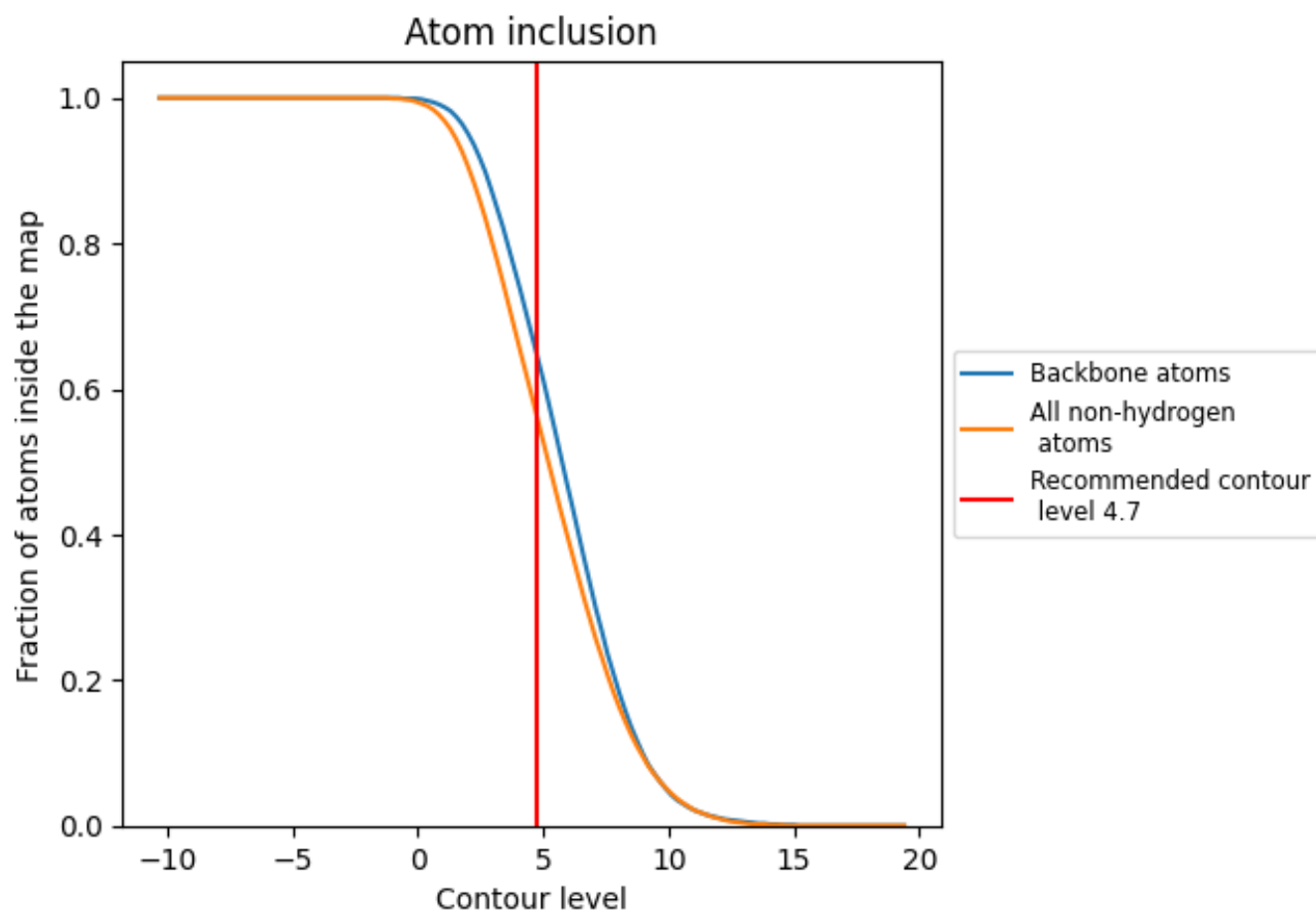
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 57% 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 (4.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5680	 0.5130
LA	 0.6440	 0.5730
LB	 0.6170	 0.5550
LC	 0.6070	 0.5510
LD	 0.7530	 0.5500
LE	 0.7290	 0.5400
LF	 0.4750	 0.5040
LG	 0.6220	 0.5640
LH	 0.5340	 0.5310
LI	 0.5110	 0.5150
LJ	 0.5210	 0.5210
LK	 0.2940	 0.4730
LL	 0.4260	 0.4900
LM	 0.5910	 0.5350
LN	 0.5370	 0.5160
LO	 0.7030	 0.5790
LP	 0.5770	 0.5390
LQ	 0.5540	 0.5460
LR	 0.5740	 0.5550
LS	 0.5120	 0.5120
LT	 0.6140	 0.5480
LU	 0.5910	 0.5450
LV	 0.4560	 0.4850
LW	 0.5750	 0.5570
LX	 0.5730	 0.5170
LY	 0.6110	 0.5530
LZ	 0.6040	 0.5420
La	 0.4770	 0.5070
Lb	 0.6710	 0.5650
Lc	 0.5460	 0.5360
Ld	 0.4620	 0.5030
Le	 0.5480	 0.5440
Lf	 0.5760	 0.5570
Lg	 0.6190	 0.5600
Lh	 0.6330	 0.5670



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Chain	Atom inclusion	Q-score
Li	 0.5480	 0.5280
Lj	 0.4900	 0.5010
Lk	 0.6640	 0.5630
Ll	 0.3460	 0.4470
Ln	 0.0250	 0.2830
Lo	 0.4950	 0.5270
Lp	 0.6170	 0.5680
Lq	 0.6190	 0.5700
Ls	 0.5780	 0.5400
Lt	 0.7180	 0.5460
Lu	 0.2640	 0.3560
SA	 0.3410	 0.4660
SB	 0.4700	 0.5030
SC	 0.2150	 0.4170
SD	 0.4700	 0.4990
SE	 0.3920	 0.4930
SF	 0.3000	 0.4560
SG	 0.2270	 0.4250
SH	 0.2510	 0.4350
SI	 0.4850	 0.5160
SJ	 0.4910	 0.5170
SK	 0.3730	 0.4700
SL	 0.1050	 0.3710
SM	 0.4550	 0.5200
SO	 0.4060	 0.5190
SP	 0.4800	 0.5320
SQ	 0.5380	 0.5370
SR	 0.0900	 0.4050
ST	 0.2290	 0.4220
SU	 0.1410	 0.3910
SV	 0.1610	 0.3920
SW	 0.2390	 0.4060
SX	 0.1740	 0.4130
SY	 0.3120	 0.4620
Sb	 0.2490	 0.4220
Sc	 0.1760	 0.3890
Sd	 0.5120	 0.5230
Se	 0.3370	 0.4540
Sg	 0.2250	 0.4360
Sh	 0.2390	 0.4220
Sj	 0.2440	 0.4490
St	 0.5670	 0.4860