



Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 01:54 pm BST

PDB ID : 7NQH / pdb_00007nqh
EMDB ID : EMD-12527
Title : 55S mammalian mitochondrial ribosome with mtRF1a and P-site tRNAMet
Authors : Kummer, E.; Schubert, K.; Ban, N.
Deposited on : 2021-03-01
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

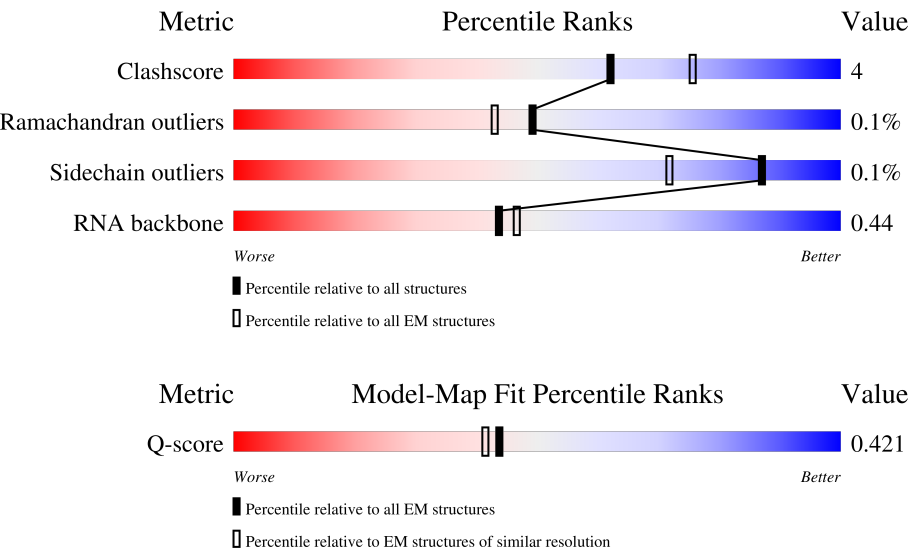
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	CL	198	
1	DL	198	
1	EL	198	

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Mol	Chain	Length	Quality of chain
1	FL	198	
1	GL	198	
1	HL	198	
2	B0	148	
3	B1	256	
4	B2	252	
5	BB	73	
6	BD	306	
7	BE	399	
8	BF	294	
9	BI	268	
10	BJ	262	
11	BK	192	
12	BL	362	
13	BN	178	
14	BO	145	
15	BP	296	
16	BQ	251	
17	BR	169	
18	BS	180	
19	BT	292	
20	BU	149	
21	BV	209	
22	BW	210	
23	BX	150	

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Mol	Chain	Length	Quality of chain
24	BY	216	
25	Ba	423	
26	Bb	380	
27	B3	161	
28	Bc	334	
29	Bd	206	
30	Be	135	
31	Bf	142	
32	Bg	159	
33	Bh	332	
34	Bi	306	
35	Bj	279	
36	Bk	269	
37	Bl	166	
38	Bm	198	
39	Bn	128	
40	Bo	124	
41	Bp	112	
42	Bq	138	
43	Bt	102	
44	Bu	205	
45	Bv	222	
46	Bw	433	
47	Bx	196	
48	AA	962	

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Mol	Chain	Length	Quality of chain
49	B4	126	
50	B5	188	
51	B6	65	
52	B7	95	
53	AB	289	
54	AC	167	
55	AE	430	
56	AF	276	
57	AG	240	
58	AI	397	
59	AJ	200	
60	AK	196	
61	AL	139	
62	AN	128	
63	AO	239	
64	AP	135	
65	AQ	130	
66	AR	143	
67	AU	87	
68	AV	71	
69	AX	9	
70	AZ	18	
71	Aa	382	
72	Ab	190	
73	Ac	173	

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Mol	Chain	Length	Quality of chain
74	Ad	205	
75	B8	188	
76	Ae	455	
77	Af	188	
78	Ag	410	
79	Ah	387	
80	Ai	106	
81	Aj	218	
82	Ak	325	
83	Am	118	
84	An	199	
85	Ao	699	
86	Ap	258	
87	B9	100	
88	BA	1571	

2 Entry composition [i](#)

There are 94 unique types of molecules in this entry. The entry contains 174617 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 Mitochondrial ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	CL	45	Total	C	N	O	0	0
			317	203	52	62		
1	DL	27	Total	C	N	O	0	0
			213	137	33	43		
1	EL	28	Total	C	N	O	0	0
			222	143	35	44		
1	FL	27	Total	C	N	O	0	0
			213	137	33	43		
1	GL	27	Total	C	N	O	0	0
			213	137	33	43		
1	HL	26	Total	C	N	O	0	0
			205	131	32	42		

- Molecule 2 is a protein called Mitochondrial ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B0	110	Total	C	N	O	S	0	0
			857	553	156	145	3		

- Molecule 3 is a protein called Mitochondrial ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B1	244	Total	C	N	O	S	0	0
			2036	1315	363	353	5		

- Molecule 4 is a protein called Mitochondrial ribosomal protein L47.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B2	179	Total	C	N	O	S	0	0
			1548	992	290	260	6		

- Molecule 5 is a RNA chain called tRNA(Phe) in LSU.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BB	67	Total	C	N	O	P	0	0
			1427	640	261	459	67		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	72	C	-	insertion	GB 76262549
BB	73	A	-	insertion	GB 76262549

- Molecule 6 is a protein called uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BD	210	Total	C	N	O	S	0	0
			1625	1016	323	278	8		

- Molecule 7 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BE	279	Total	C	N	O	S	0	0
			2192	1406	389	388	9		

- Molecule 8 is a protein called Mitochondrial ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BF	223	Total	C	N	O	S	0	0
			1792	1155	330	301	6		

- Molecule 9 is a protein called Mitochondrial ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	BI	98	Total	C	N	O	0	0
			805	509	155	141		

- Molecule 10 is a protein called Mitochondrial ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BJ	212	Total	C	N	O	S	0	0
			1705	1100	306	290	9		

- Molecule 11 is a protein called Mitochondrial ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BK	176	Total	C	N	O	S	0	0
			1303	830	236	235	2		

- Molecule 12 is a protein called Peptide chain release factor 1-like, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BL	250	Total	C	N	O	S	0	0
			2003	1253	362	380	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BL	-6	SER	-	expression tag	UNP Q9UGC7
BL	-4	GLY	PRO	conflict	UNP Q9UGC7
BL	-3	SER	ALA	conflict	UNP Q9UGC7
BL	-2	GLY	ARG	conflict	UNP Q9UGC7
BL	-1	SER	ARG	conflict	UNP Q9UGC7
BL	0	GLY	PRO	conflict	UNP Q9UGC7

- Molecule 13 is a protein called uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BN	177	Total	C	N	O	S	0	0
			1444	926	258	253	7		

- Molecule 14 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BO	115	Total	C	N	O	S	0	0
			896	562	176	154	4		

- Molecule 15 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BP	288	Total	C	N	O	S	0	0
			2312	1473	430	403	6		

- Molecule 16 is a protein called uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BQ	222	Total	C	N	O	S	0	0
			1803	1156	331	306	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	237	HIS	TYR	conflict	UNP F1RI89

- Molecule 17 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BR	153	Total	C	N	O	S	0	0
			1240	777	236	222	5		

- Molecule 18 is a protein called Mitochondrial ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BS	143	Total	C	N	O	S	0	0
			1168	733	227	204	4		

- Molecule 19 is a protein called Mitochondrial ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BT	240	Total	C	N	O	S	0	0
			1954	1253	338	354	9		

- Molecule 20 is a protein called Mitochondrial ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BU	140	Total	C	N	O	S	0	0
			1159	732	239	185	3		

- Molecule 21 is a protein called Mitochondrial ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BV	155	Total	C	N	O	S	0	0
			1231	789	219	219	4		

- Molecule 22 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BW	166	Total	C	N	O	S	0	0
			1374	876	258	234	6		

- Molecule 23 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BX	149	Total	C	N	O	S	0	0
			1181	752	227	200	2		

- Molecule 24 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BY	206	Total	C	N	O	S	0	0
			1678	1056	308	309	5		

- Molecule 25 is a protein called Mitochondrial ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ba	393	Total	C	N	O	S	0	0
			3173	2040	556	565	12		

- Molecule 26 is a protein called Mitochondrial ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Bb	354	Total	C	N	O	S	0	0
			2952	1876	542	525	9		

- Molecule 27 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B3	118	Total	C	N	O	S	0	0
			968	622	178	165	3		

- Molecule 28 is a protein called Mitochondrial ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Bc	295	Total	C	N	O	S	0	0
			2408	1541	410	441	16		

- Molecule 29 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Bd	138	Total	C	N	O	S	0	0
			1158	729	211	217	1		

- Molecule 30 is a protein called Mitochondrial ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Be	122	Total	C	N	O	S	0	0
			972	628	168	173	3		

- Molecule 31 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bf	108	Total	C	N	O	S	0	0
			827	519	154	150	4		

- Molecule 32 is a protein called Mitochondrial ribosomal protein L43.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bg	148	Total	C	N	O	S	0	0
			1167	727	225	212	3		

- Molecule 33 is a protein called mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bh	289	Total	C	N	O	S	0	0
			2319	1486	399	426	8		

- Molecule 34 is a protein called Mitochondrial ribosomal protein L45.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bi	260	Total	C	N	O	S	0	0
			2138	1370	379	379	10		

- Molecule 35 is a protein called Mitochondrial ribosomal protein L46.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bj	217	Total	C	N	O	S	0	0
			1775	1137	311	321	6		

- Molecule 36 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Bk	155	Total	C	N	O	S	0	0
			1246	796	214	231	5		

- Molecule 37 is a protein called Mrpl34.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bl	133	Total	C	N	O	S	0	0
			1097	709	192	194	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bl	59	ARG	LYS	conflict	UNP A0A0R4J8D6

- Molecule 38 is a protein called Mitochondrial ribosomal protein L50.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bm	109	Total	C	N	O	S	0	0
			893	568	160	162	3		

- Molecule 39 is a protein called Mitochondrial ribosomal protein L51.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bn	97	Total	C	N	O	S	0	0
			837	539	166	128	4		

- Molecule 40 is a protein called mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bo	97	Total	C	N	O	S	0	0
			772	481	148	141	2		

- Molecule 41 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bp	97	Total	C	N	O	S	0	0
			742	459	143	134	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bp	12	ALA	SER	conflict	UNP A0A341D604
Bp	107	SER	GLY	conflict	UNP A0A341D604

- Molecule 42 is a protein called mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bq	68	Total	C	N	O	S	0	0
			542	344	102	95	1		

- Molecule 43 is a protein called Mitochondrial ribosomal protein L57.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bt	94	Total	C	N	O	S	0	0
			780	485	168	126	1		

- Molecule 44 is a protein called mL62 (ICT1).

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bu	151	Total	C	N	O	S	0	0
			1198	738	233	222	5		

- Molecule 45 is a protein called mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Bv	135	Total	C	N	O	S	0	0
			1131	692	223	211	5		

- Molecule 46 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Bw	387	Total	C	N	O	S	0	0
			3126	2011	548	555	12		

- Molecule 47 is a protein called Mitochondrial ribosomal protein S18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Bx	162	Total	C	N	O	S	0	0
			1325	845	249	224	7		

- Molecule 48 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AA	960	Total	C	N	O	P	0	0
			20411	9162	3708	6581	960		

- Molecule 49 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B4	63	Total	C	N	O	S	0	0
			479	299	95	82	3		

- Molecule 50 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B5	110	Total	C	N	O	S	0	0
			902	553	181	162	6		

- Molecule 51 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B6	52	Total	C	N	O	S	0	0
			425	274	78	71	2		

- Molecule 52 is a protein called Mitochondrial ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B7	46	Total	C	N	O	S	0	0
			387	239	89	58	1		

- Molecule 53 is a protein called Mitochondrial ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AB	220	Total	C	N	O	S	0	0
			1762	1126	326	304	6		

- Molecule 54 is a protein called Mitochondrial ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AC	132	Total	C	N	O	S	0	0
			1075	695	195	181	4		

- Molecule 55 is a protein called Mitochondrial ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AE	343	Total	C	N	O	S	0	0
			2732	1707	527	487	11		

- Molecule 56 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AF	122	Total	C	N	O	S	0	0
			981	620	178	177	6		

- Molecule 57 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AG	206	Total	C	N	O	S	0	0
			1693	1075	310	297	11		

- Molecule 58 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AI	328	Total	C	N	O	S	0	0
			2650	1678	478	481	13		

- Molecule 59 is a protein called Mitochondrial ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AJ	140	Total	C	N	O	S	0	0
			1155	746	197	208	4		

- Molecule 60 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AK	137	Total	C	N	O	S	0	0
			1007	631	193	180	3		

- Molecule 61 is a protein called Mitochondrial ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AL	109	Total	C	N	O	S	0	0
			840	524	172	138	6		

- Molecule 62 is a protein called Mitochondrial ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AN	101	Total	C	N	O	S	0	0
			858	534	174	144	6		

- Molecule 63 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AO	175	Total	C	N	O	S	0	0
			1448	919	272	248	9		

- Molecule 64 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AP	117	Total	C	N	O	S	0	0
			932	588	184	155	5		

- Molecule 65 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AQ	112	Total	C	N	O	S	0	0
			875	568	153	151	3		

- Molecule 66 is a protein called Mitochondrial ribosomal protein S18C.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AR	97	Total	C	N	O	S	0	0
			784	507	132	138	7		

- Molecule 67 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AU	86	Total	C	N	O	S	0	0
			734	453	148	125	8		

- Molecule 68 is a RNA chain called tRNAMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AV	71	Total	C	N	O	P	0	0
			1498	673	264	491	70		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AV	69	C	-	insertion	GB 1208989970
AV	70	C	-	insertion	GB 1208989970
AV	71	A	-	insertion	GB 1208989970

- Molecule 69 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AX	9	Total	C	N	O	P	0	0
			188	86	35	59	8		

- Molecule 70 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
70	AZ	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 71 is a protein called Mitochondrial ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Aa	292	Total	C	N	O	S	0	0
			2378	1518	409	442	9		

- Molecule 72 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Ab	135	Total	C	N	O	S	0	0
			1101	709	199	192	1		

- Molecule 73 is a protein called Mitochondrial ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Ac	169	Total	C	N	O	S	0	0
			1367	876	236	245	10		

- Molecule 74 is a protein called Mitochondrial ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Ad	177	Total	C	N	O	S	0	0
			1467	904	288	273	2		

- Molecule 75 is a protein called Mitochondrial ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	B8	95	Total	C	N	O	S	0	0
			833	539	163	129	2		

- Molecule 76 is a protein called Mitochondrial ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Ae	388	Total	C	N	O	S	0	0
			3109	1971	535	589	14		

- Molecule 77 is a protein called Mitoribosomal protein ms28, mrps28.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Af	99	Total	C	N	O	S	0	0
			778	494	134	146	4		

- Molecule 78 is a protein called Death associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ag	353	Total	C	N	O	S	0	0
			2875	1837	515	513	10		

- Molecule 79 is a protein called Mitochondrial ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Ah	120	Total	C	N	O	S	0	0
			1015	659	168	185	3		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	180	UNK	-	insertion	UNP F1RME2
Ah	181	GLN	-	insertion	UNP F1RME2
Ah	182	LYS	-	insertion	UNP F1RME2
Ah	184	GLY	-	insertion	UNP F1RME2
Ah	185	GLU	LYS	conflict	UNP F1RME2
Ah	187	PRO	LYS	conflict	UNP F1RME2
Ah	189	ILE	LEU	conflict	UNP F1RME2
Ah	190	SER	ILE	conflict	UNP F1RME2
Ah	237	SER	-	insertion	UNP F1RME2
Ah	238	PHE	-	insertion	UNP F1RME2

- Molecule 80 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Ai	99	Total	C	N	O	S	0	0
			824	522	156	143	3		

- Molecule 81 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Aj	213	Total	C	N	O	S	0	0
			1788	1131	338	311	8		

- Molecule 82 is a protein called Mitochondrial ribosomal protein S35.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Ak	275	Total	C	N	O	S	0	0
			2222	1414	380	419	9		

- Molecule 83 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Am	116	Total	C	N	O	S	0	0
			930	577	185	160	8		

- Molecule 84 is a protein called Aurora kinase A interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	An	72	Total	C	N	O	S	0	0
			639	407	139	92	1		

- Molecule 85 is a protein called Pentatricopeptide repeat domain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Ao	572	Total	C	N	O	S	0	0
			4526	2898	770	834	24		

- Molecule 86 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Ap	190	Total	C	N	O	S	0	0
			1564	991	292	273	8		

- Molecule 87 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	B9	38	Total	C	N	O	S	0	0
			335	214	70	47	4		

- Molecule 88 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	BA	1544	Total	C	N	O	P	0	0
			32844	14750	5972	10578	1544		

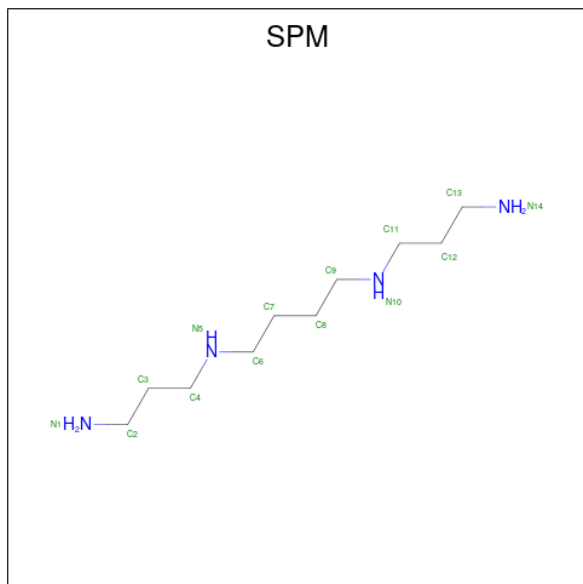
- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	B0	1	Total	Mg	0
			1	1	
89	BB	1	Total	Mg	0
			1	1	
89	BD	3	Total	Mg	0
			3	3	
89	BE	1	Total	Mg	0
			1	1	
89	BP	3	Total	Mg	0
			3	3	
89	BR	1	Total	Mg	0
			1	1	
89	B3	2	Total	Mg	0
			2	2	
89	Be	1	Total	Mg	0
			1	1	
89	Bl	1	Total	Mg	0
			1	1	
89	Bt	2	Total	Mg	0
			2	2	
89	AA	104	Total	Mg	0
			104	104	
89	AB	1	Total	Mg	0
			1	1	
89	AL	2	Total	Mg	0
			2	2	
89	Ag	1	Total	Mg	0
			1	1	
89	Am	1	Total	Mg	0
			1	1	
89	An	1	Total	Mg	0
			1	1	
89	BA	197	Total	Mg	0
			197	197	

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

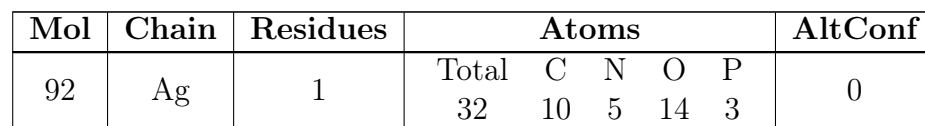
Mol	Chain	Residues	Atoms		AltConf
90	Bx	1	Total	Zn	0
			1	1	
90	B5	1	Total	Zn	0
			1	1	
90	AR	1	Total	Zn	0
			1	1	
90	Ac	1	Total	Zn	0
			1	1	
90	Ap	1	Total	Zn	0
			1	1	
90	B9	1	Total	Zn	0
			1	1	

- Molecule 91 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
91	AA	1	Total	C	N	0
			14	10	4	
91	BA	1	Total	C	N	0
			14	10	4	
91	BA	1	Total	C	N	0
			14	10	4	

- Molecule 92 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



-
- The chemical structure of 5-GMP (5'-guanylate) is shown. It consists of a guanine base (a purine ring system with an amino group at C2 and a carbonyl group at C6) linked to a ribose sugar at the C5' position. The ribose sugar is further linked to a phosphate group at the C3' position. The atoms are labeled with their respective symbols: N1, N2, N3, N7, N9 for nitrogen; C2, C3, C4, C5, C6, C8, C9 for carbon; O1, O2, O3, O4, O5, O6 for oxygen; and P for phosphorus. The phosphate group is shown with its terminal hydroxyl groups (OP1, OP2, OP3) and a double-bonded oxygen (O5').

Mol	Chain	Residues	Atoms					AltConf
93	BA	1	Total 24	C 10	N 5	O 8	P 1	0
93	BA	1	Total 24	C 10	N 5	O 8	P 1	0

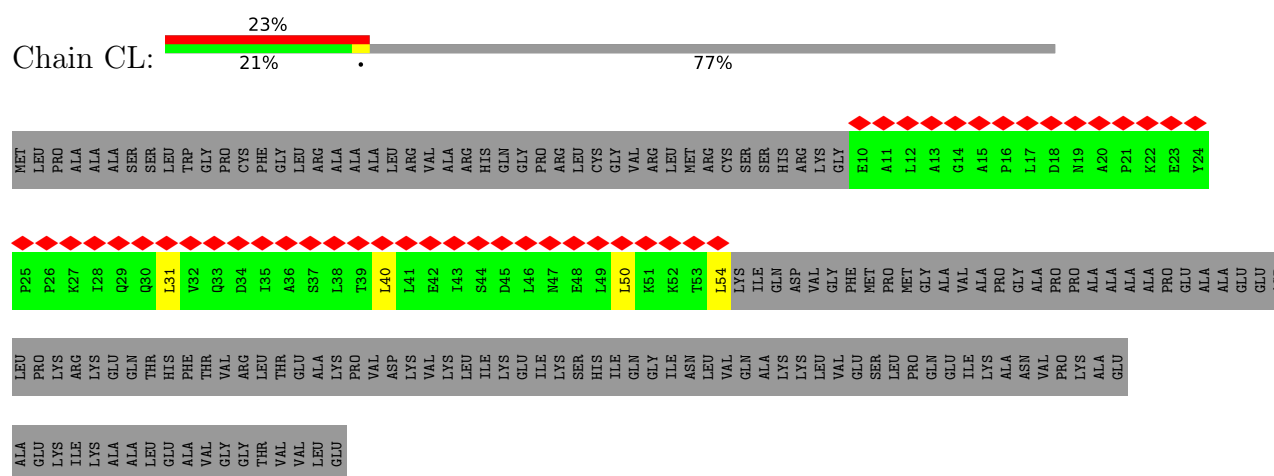
- 

Mol	Chain	Residues	Atoms		AltConf
94	Ag	3	Total 3	O 3	0

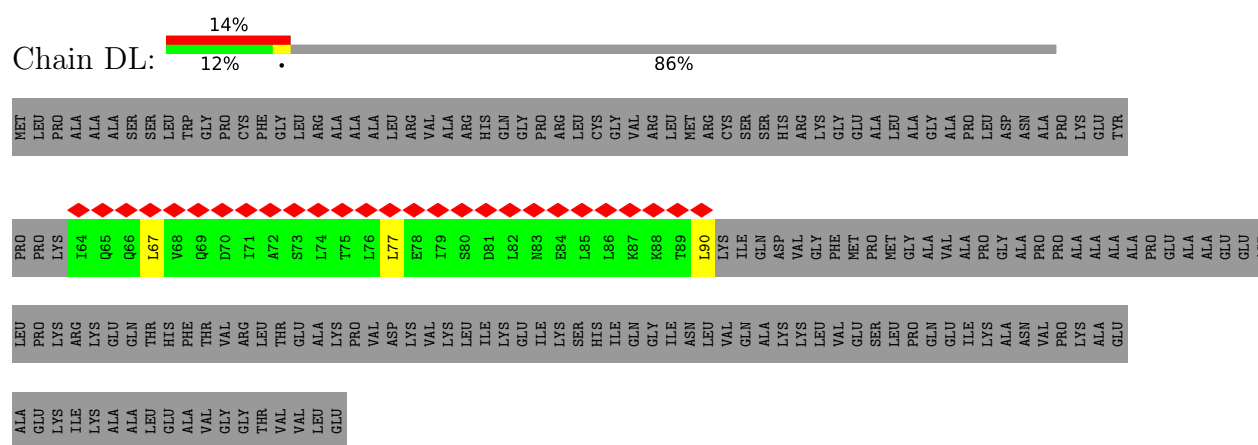
3 Residue-property plots [i](#)

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.

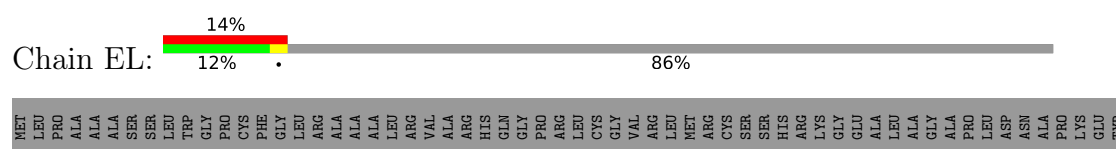
- Molecule 1: Mitochondrial ribosomal protein L12

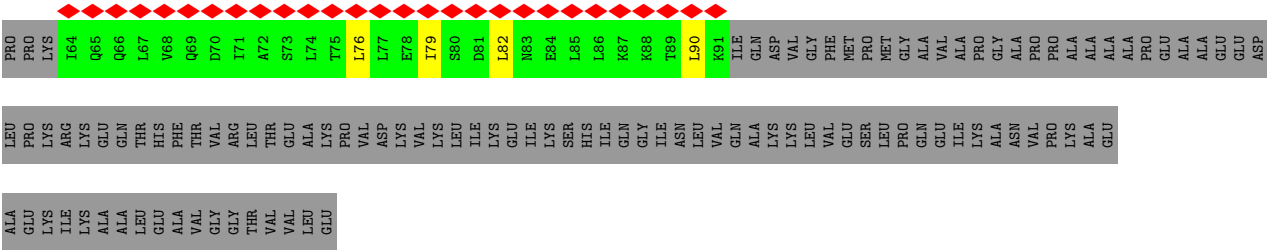


- Molecule 1: Mitochondrial ribosomal protein L12

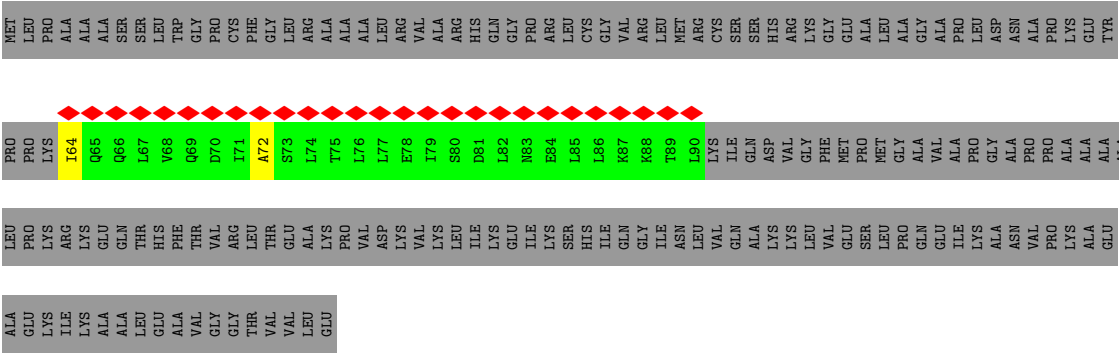


- Molecule 1: Mitochondrial ribosomal protein L12

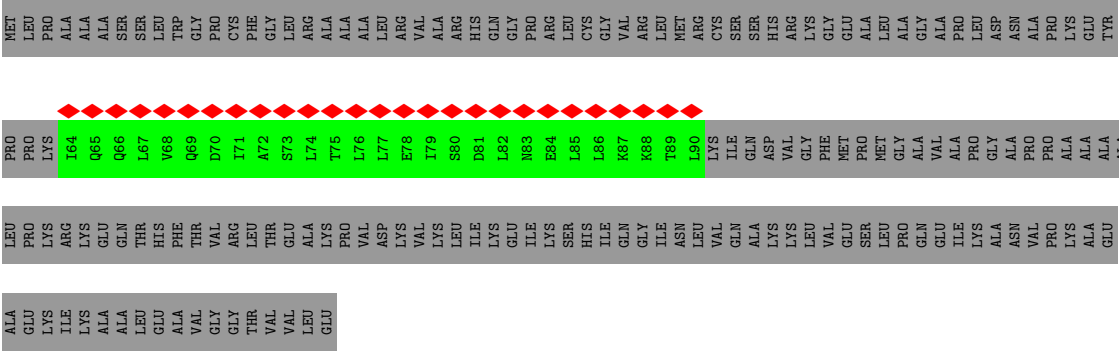




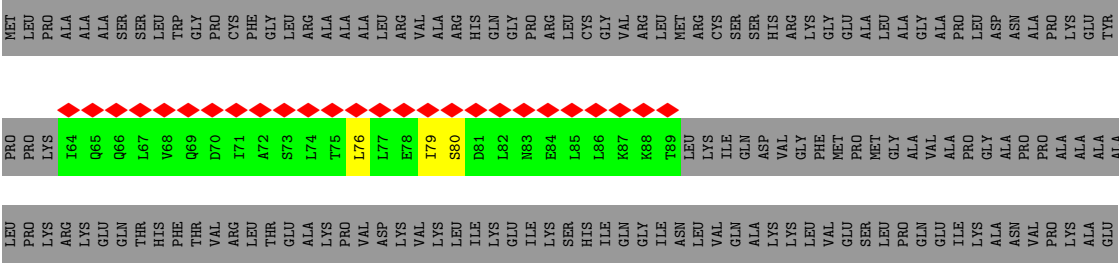
• Molecule 1: Mitochondrial ribosomal protein L12



• Molecule 1: Mitochondrial ribosomal protein L12



• Molecule 1: Mitochondrial ribosomal protein L12



ALA
GLU
LYS
ILE
LYS
VAL
ALA
ALA
GLU
LEU
ARG
THR
ALA
VAL
GLY
GLY
THR
VAL
VAL
LEU
GLU

• Molecule 2: Mitochondrial ribosomal protein L27

Chain B0:  70% 26%

MET
ALA
LEU
ALA
VAL
LEU
ALA
LEU
ARG
THR
ALA
VAL
GLY
GLY
THR
VAL
VAL
LEU
GLU
SER
PRO
PRO
GLN
ALA
ALA
ALA
LEU
ALA
VAL
ARG
TYR
ALA
SER
LYS
LYS
THR
THR
GLY
GLY
SER
S39
P77
L83
N86
K87
C88
L92
Q122
V125
L148

• Molecule 3: Mitochondrial ribosomal protein L28

Chain B1:  19% 85% 10% 5%

MET
P2
V6
L10
W11
K12
R15
L16
W17
H177
E18
G19
L24
P25
R30
E33
E34
A35
R36
V41
K55
R59
E63
D64
E83
N94
D95
K96
K99
E113
D120
K121
R122
F123
D133
G140
I145
E161
K156
L161
K162
R163
L166
L167
R168
Q172
D173
P174
Q175
L176
H177
P178
D179
D180
P181
A182
D189
F194
A199
E200
A201
E202
G205
D209
E210
A211
V212
E213
L218
K221
D222
P223
I224
F227
E232
E233
L234
Q237
L238
Q239
Q240
Q241
A242
L243
S244
E245
PRO
ALA
VAL
VAL
GLN
THR
ARG
ALA
SER
ARG
LYS

• Molecule 4: Mitochondrial ribosomal protein L47

Chain B2:  7% 64% 7% 29%

MET
ALA
ALA
ALA
GLY
LEU
ALA
VAL
PHE
CYS
ARG
ARG
VAL
SER
SER
ALA
ALA
LEU
LYS
LYS
ALA
CYS
ARG
LEU
LEU
ILE
PRO
GLN
ALA
PRO
SER
THR
SER
CYS
ARG
PHE
SER
PRO
SER
LEU
LEU
PRO
LYS
ASN
THR
PRO
ASN
VAL
THR
SER
PHE
HIS
HIS
PHE
THR
THR
PHE
SER
ARG
TLE
PHE
HIS
THR
F235
L236
Q237
E238
K239
PHE
SER
ARG
G65
E68
D71
G77
E78
E79
L92
R93
N94
K95
D99
F127
D142
D145
K146
V147
E150
D153
L158
K164
A165
F175
K184
Q185
K195
R212
P213
R214
T215
E216
L228
E229
R230
F235
L236
Q237
E238
K239
F240
P241
H242
L243
SER
GLU
THR
GLN
LYS
SER
SER
HIS
VAL

• Molecule 5: tRNA(Phe) in LSU

Chain BB:  38% 63% 26% 8%

G1
U2
U3
A4
A5
U6
G7
U8
A9
U13
A14
A15
A
U
U
U
A
U20
C21
A22
A23
A32
C33
U34
G35
U40
G41
C42
C43
U44
A45
G46
A47
U48
G49
A50
G51
C52
C53
U54
C55
A
C
A58
G59
C60
U61
C62
C63
A64
U65
A66
A67
A68
C69
A70
C71
C72
A73

• Molecule 6: uL2m

Frequency	Percentage
Daily	60%
Weekly	8%
Monthly	31%



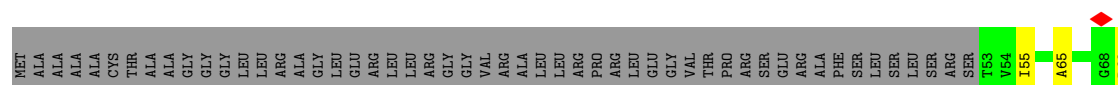
Frequency	Percentage
Daily	60%
Weekly	10%
Monthly	30%

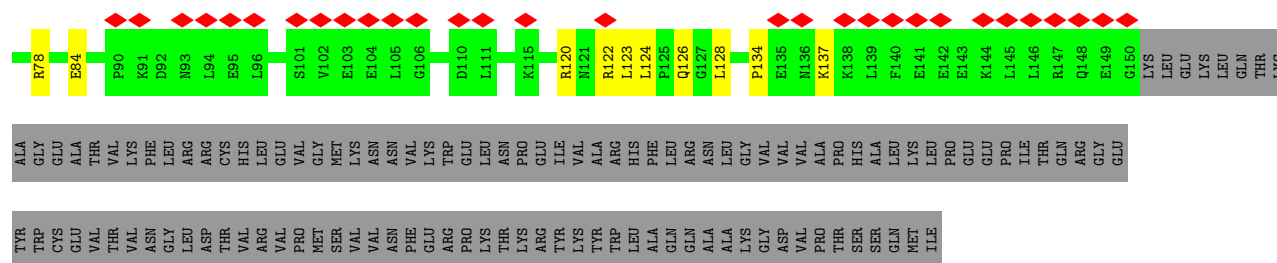


Response	Percentage
Yes	67%
No	9%
Don't know	24%

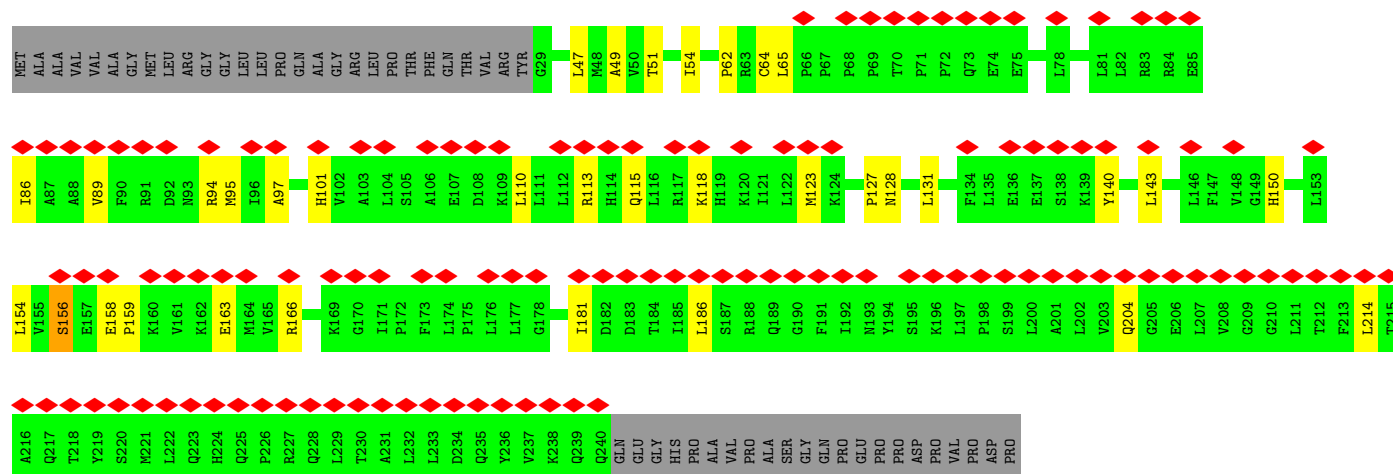


Category	Percentage
Very bad	12%
Bad	32%
Good	5%
Very good	63%

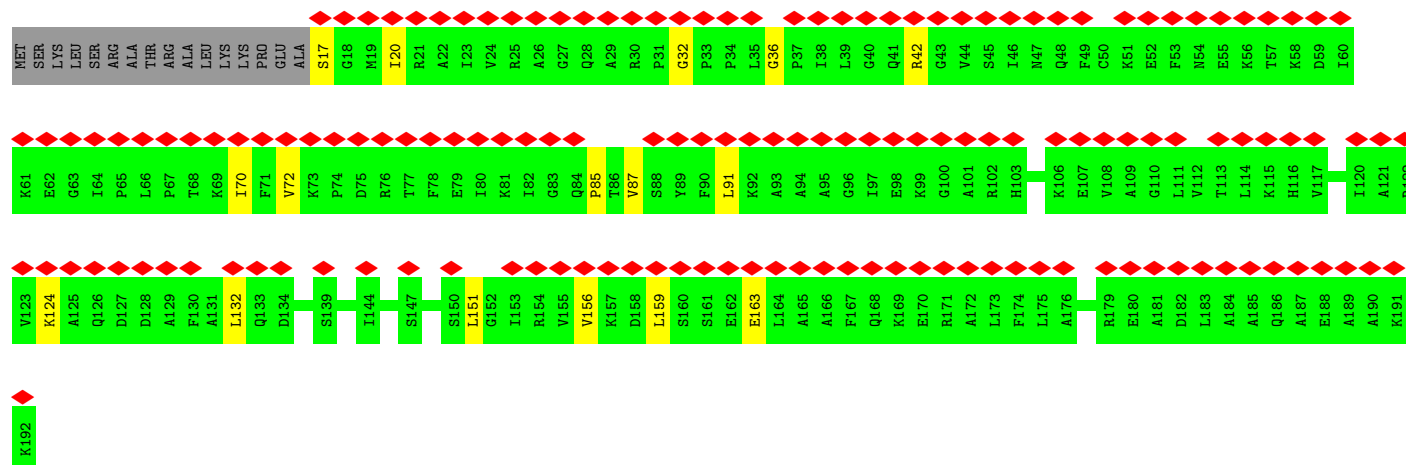
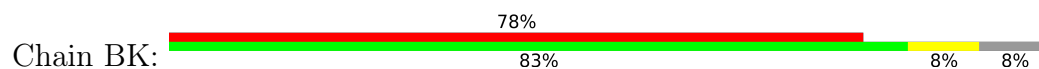




• Molecule 10: Mitochondrial ribosomal protein L10

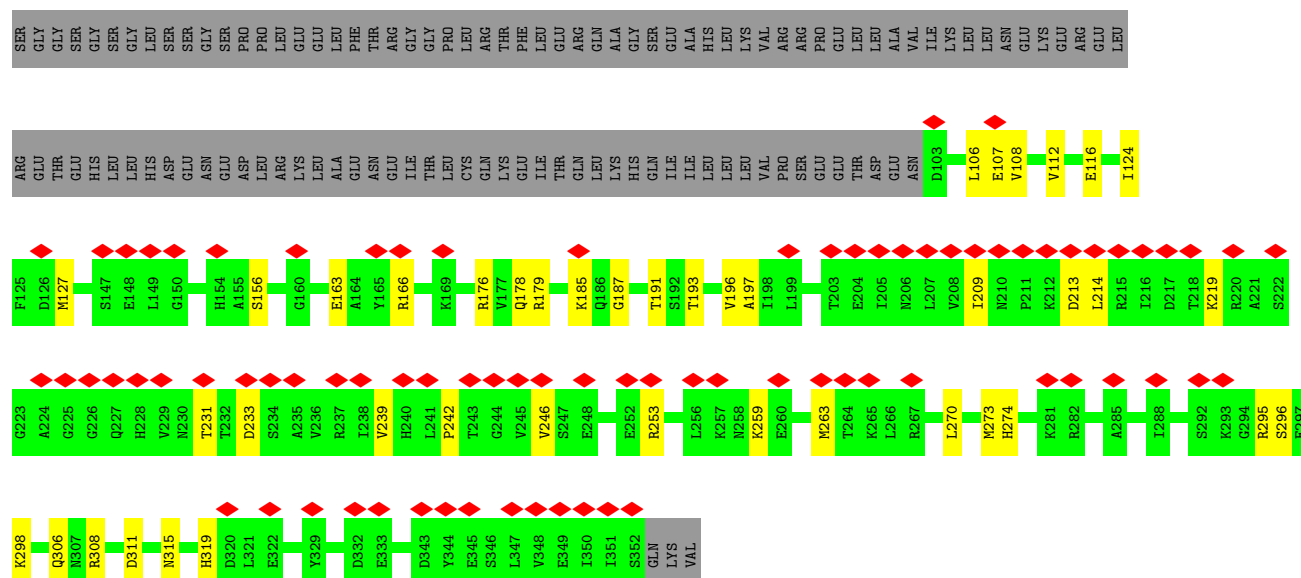


• Molecule 11: Mitochondrial ribosomal protein L11

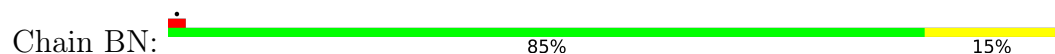


• Molecule 12: Peptide chain release factor 1-like, mitochondrial

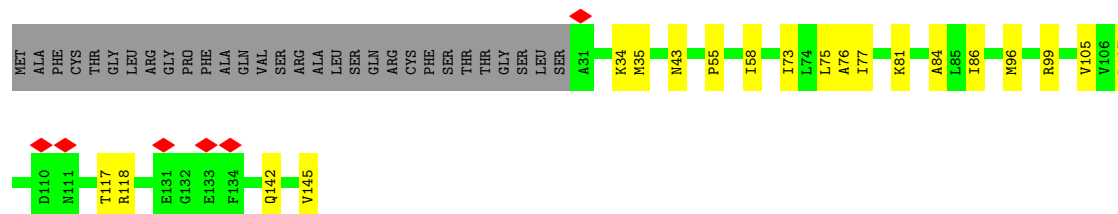




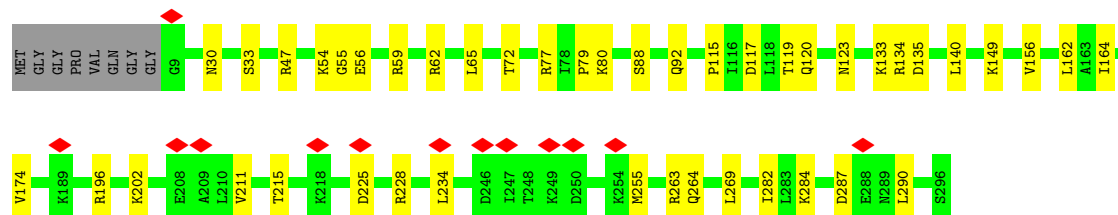
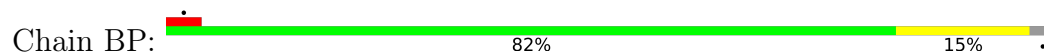
• Molecule 13: uL13m



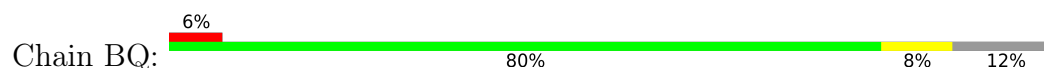
• Molecule 14: uL14m

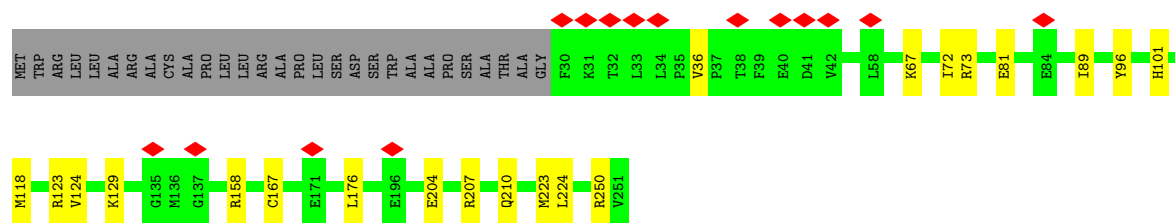


• Molecule 15: uL15m

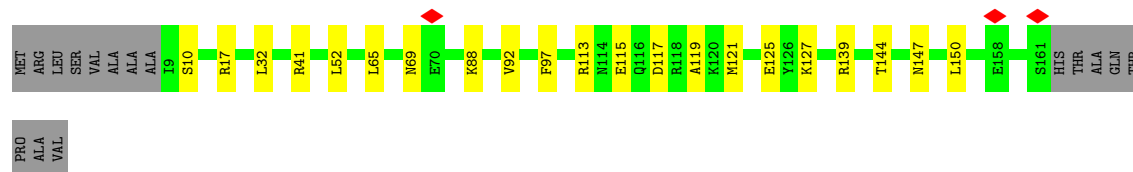
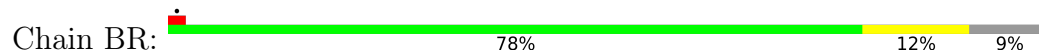


• Molecule 16: uL16m

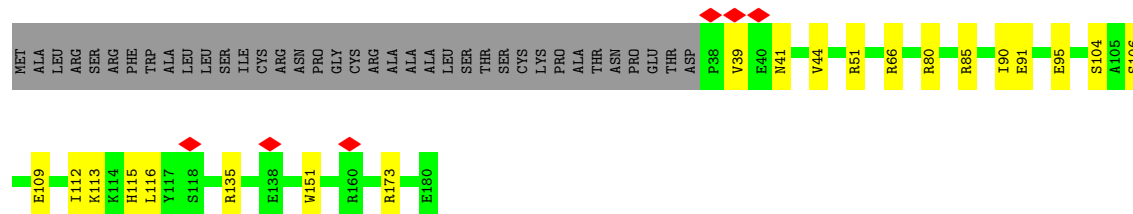




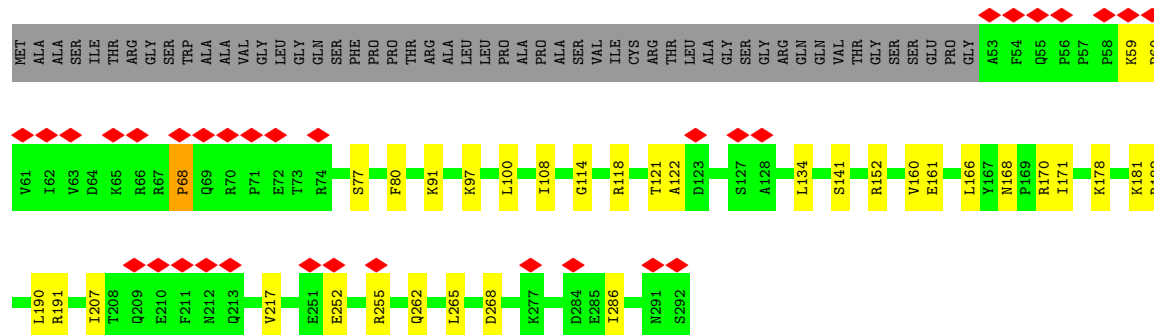
- Molecule 17: bL17m



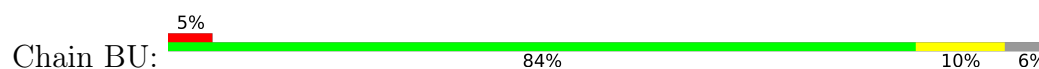
- Molecule 18: Mitochondrial ribosomal protein L18



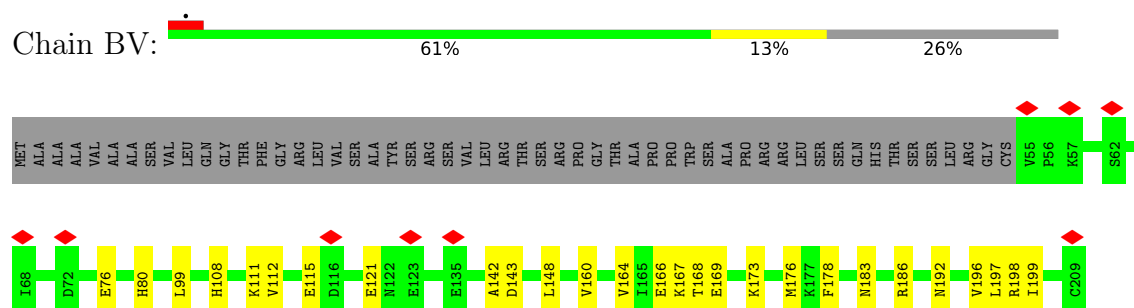
- Molecule 19: Mitochondrial ribosomal protein L19



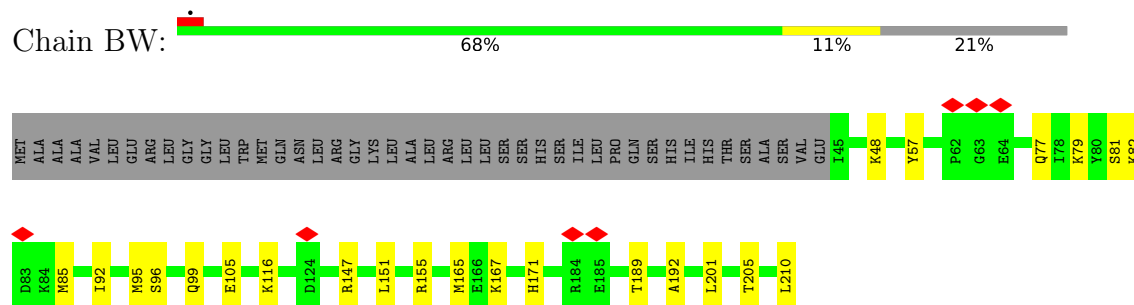
- Molecule 20: Mitochondrial ribosomal protein L20



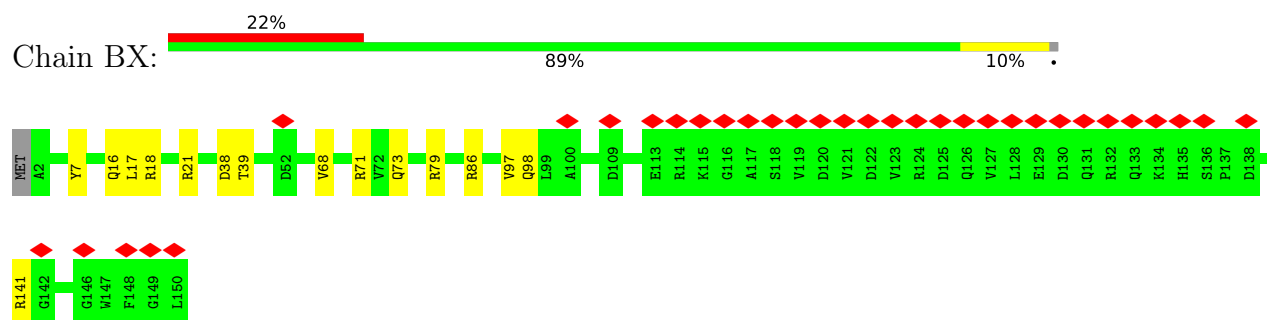
- Molecule 21: Mitochondrial ribosomal protein L21



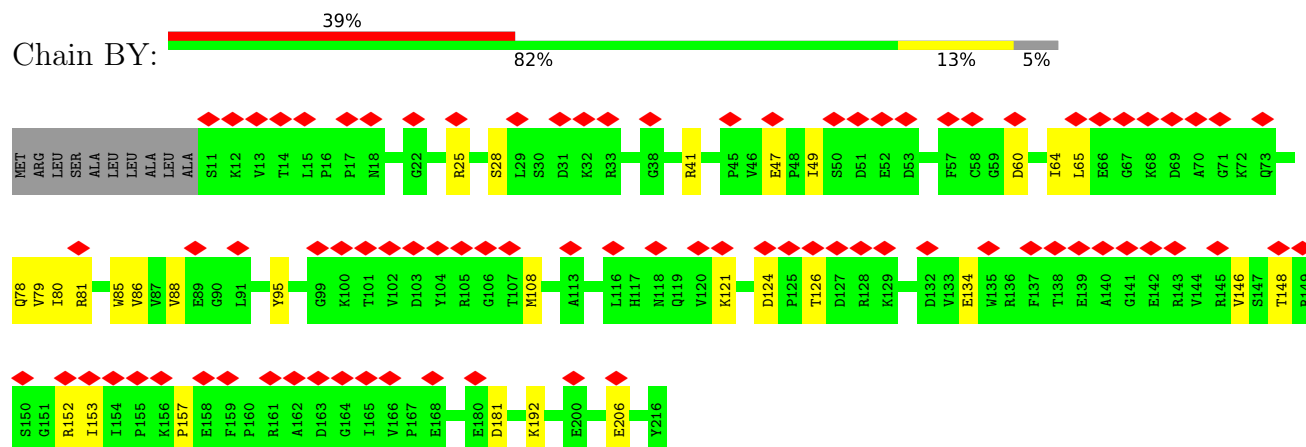
- Molecule 22: uL22m



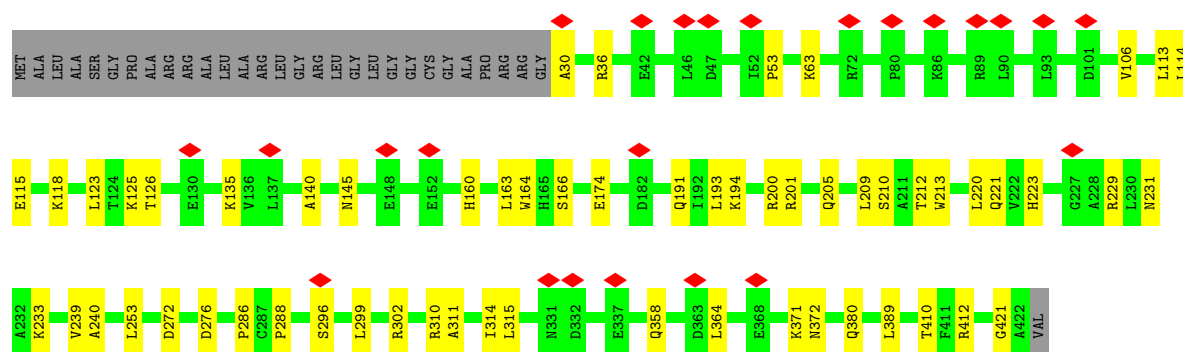
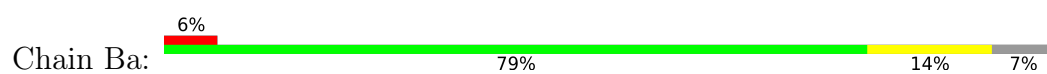
- Molecule 23: uL23m



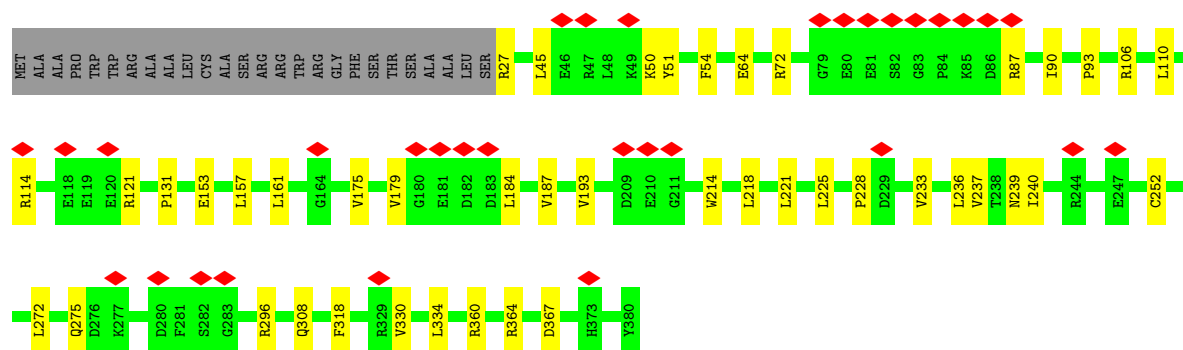
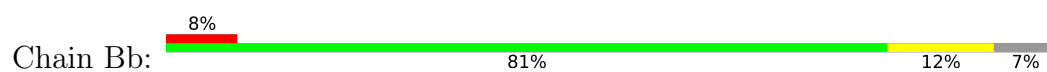
- Molecule 24: uL24m



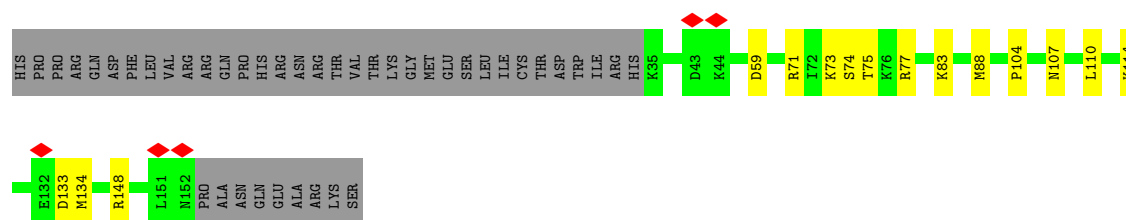
- Molecule 25: Mitochondrial ribosomal protein L37



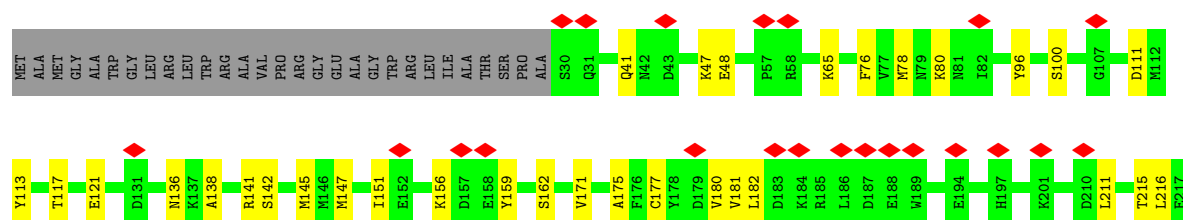
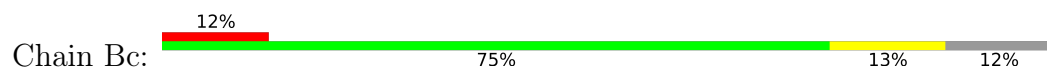
• Molecule 26: Mitochondrial ribosomal protein L38

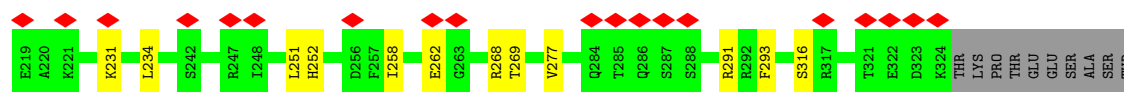


• Molecule 27: uL30m

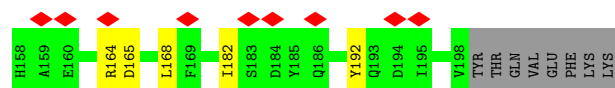
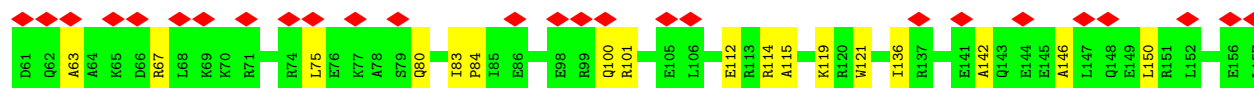
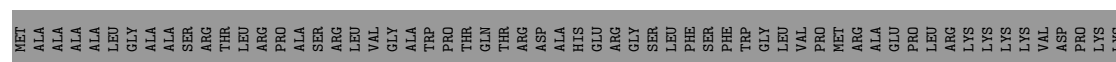


• Molecule 28: Mitochondrial ribosomal protein L39

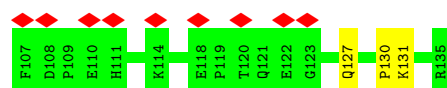
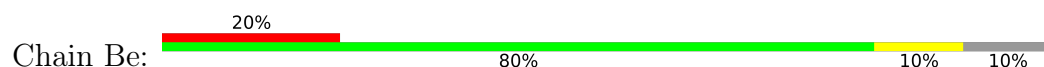




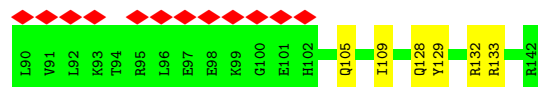
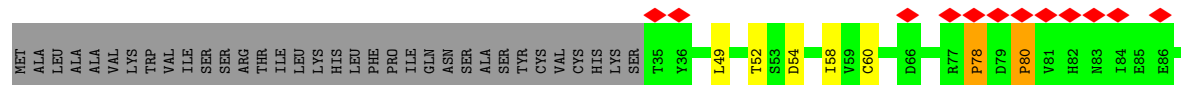
• Molecule 29: mL40



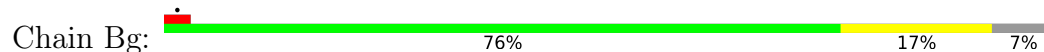
• Molecule 30: Mitochondrial ribosomal protein L41



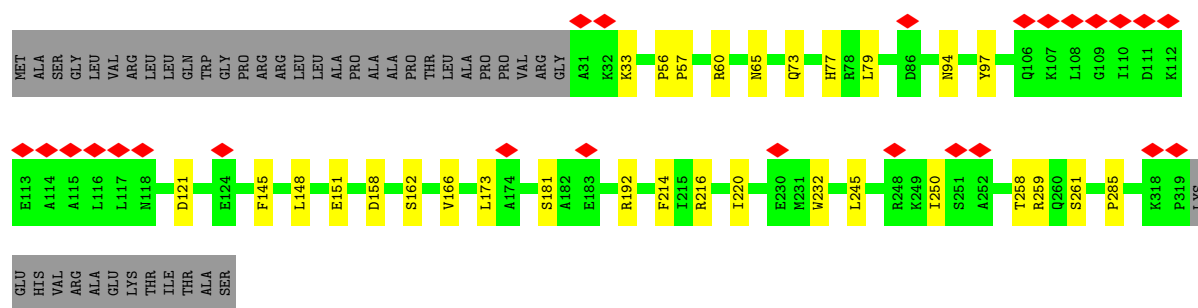
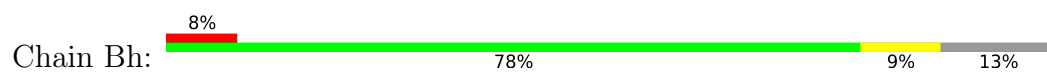
• Molecule 31: mL42



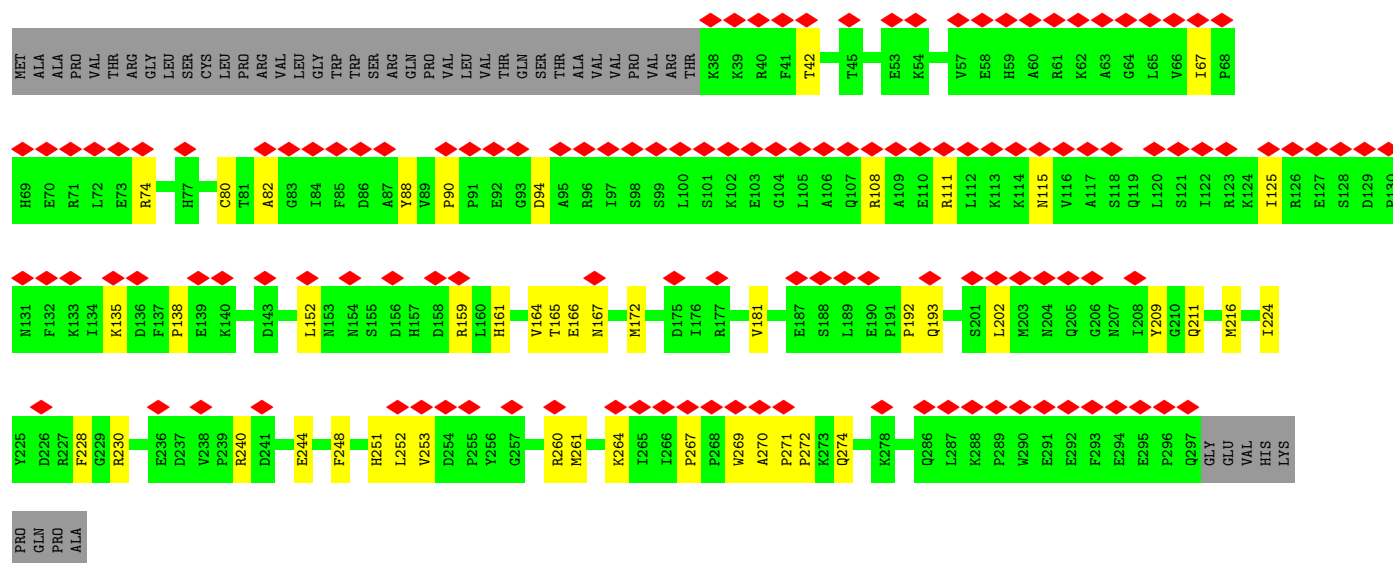
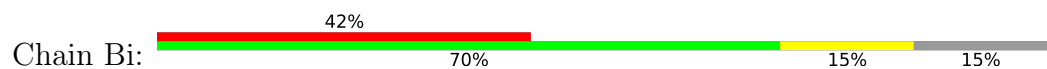
• Molecule 32: Mitochondrial ribosomal protein L43



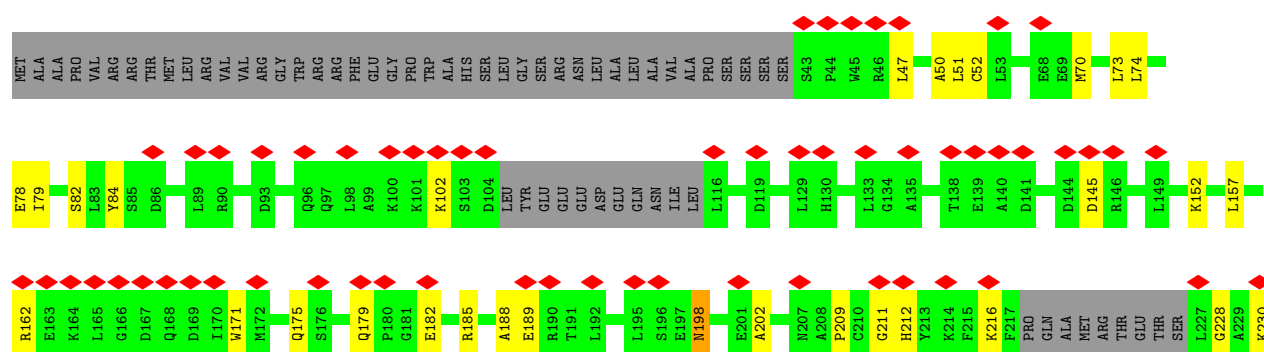
• Molecule 33: mL44

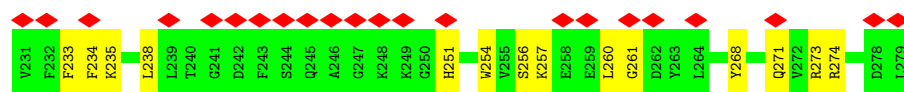


• Molecule 34: Mitochondrial ribosomal protein L45

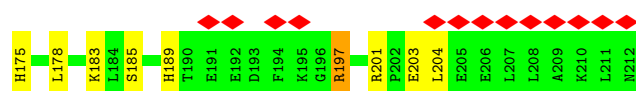
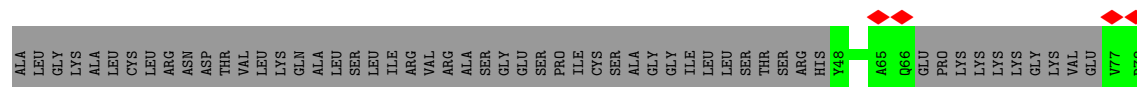
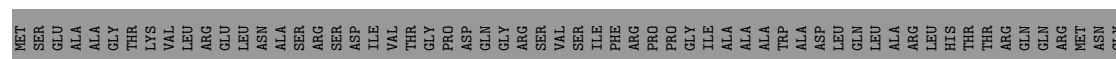


• Molecule 35: Mitochondrial ribosomal protein L46

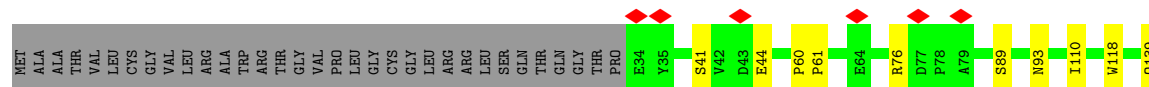




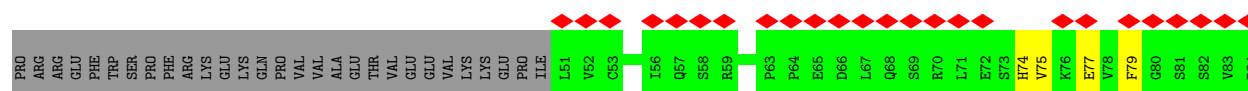
- Molecule 36: 39S ribosomal protein L48, mitochondrial



- Molecule 37: Mrpl34

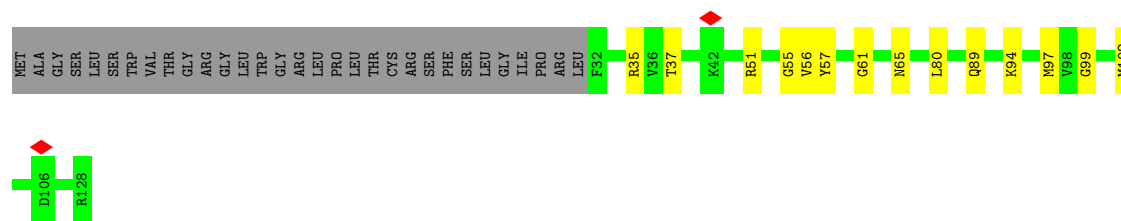


- Molecule 38: Mitochondrial ribosomal protein L50

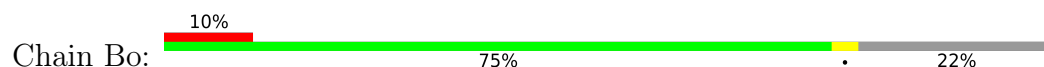


- Molecule 39: Mitochondrial ribosomal protein L51

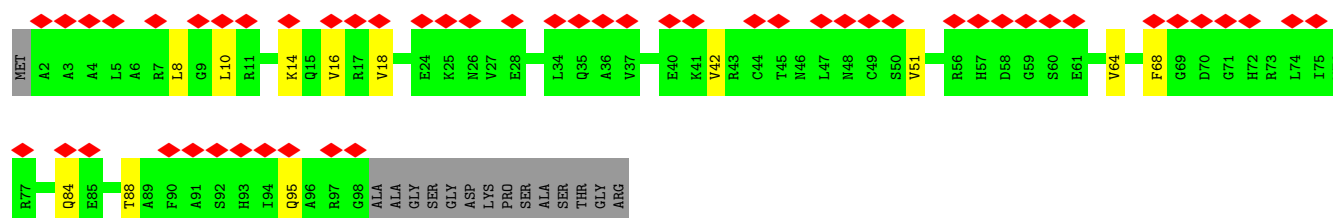
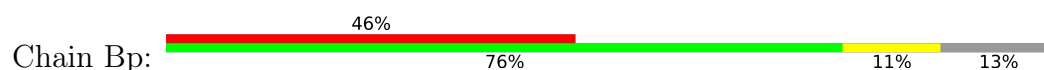




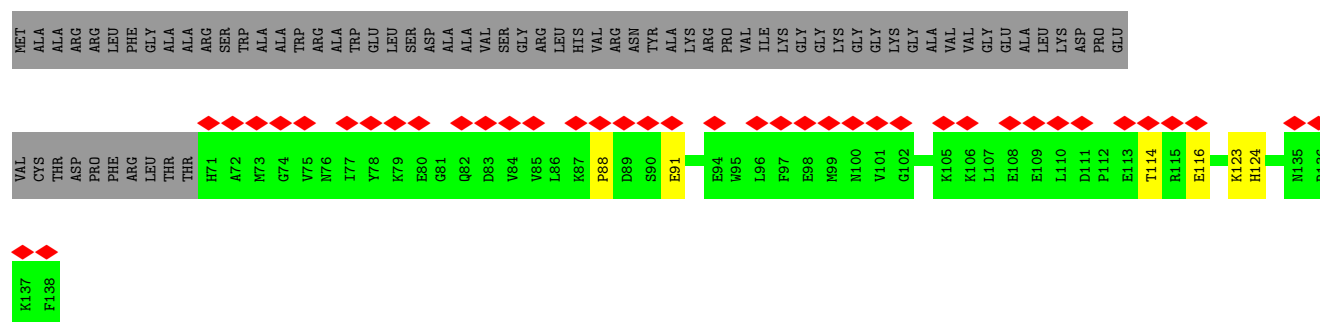
- Molecule 40: mL52



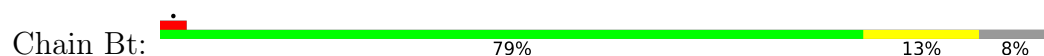
- Molecule 41: mL53



- Molecule 42: mL54

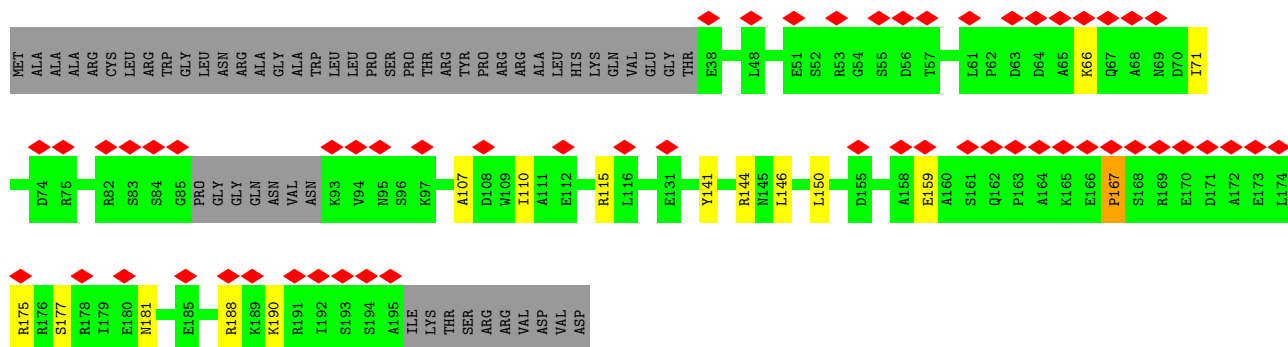


- Molecule 43: Mitochondrial ribosomal protein L57

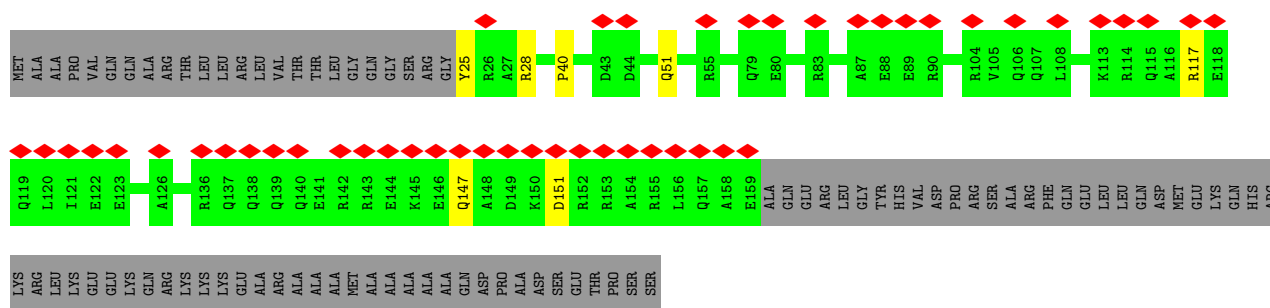


- Molecule 44: mL62 (ICT1)

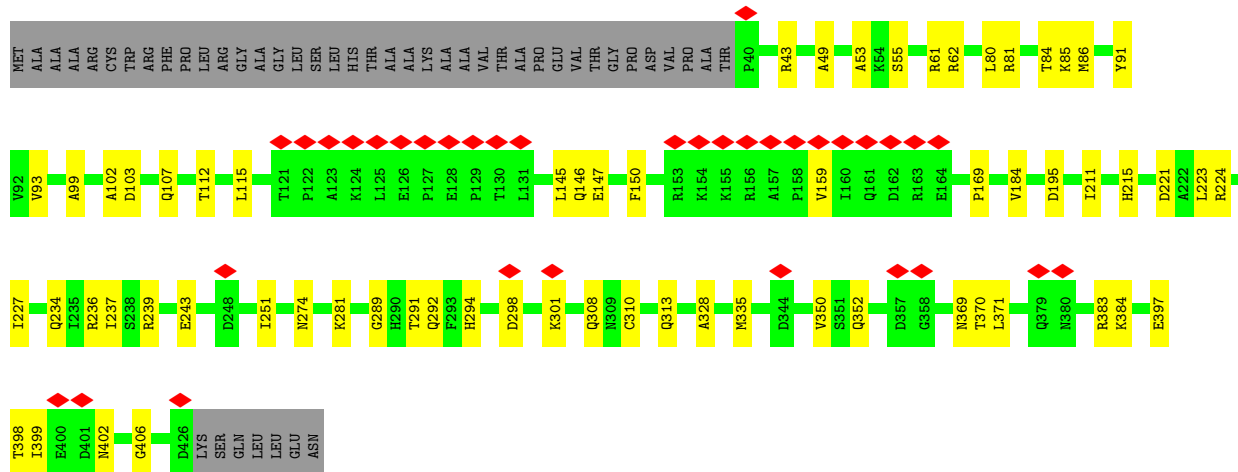
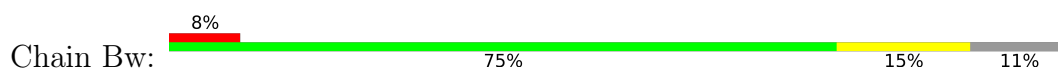




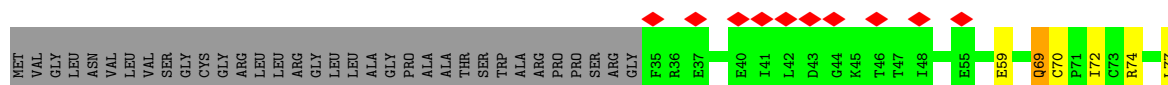
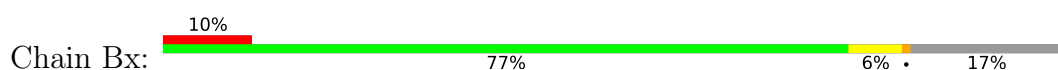
• Molecule 45: mL64

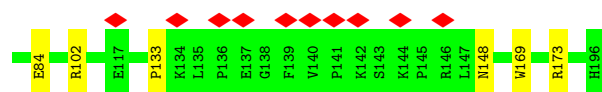


• Molecule 46: 39S ribosomal protein S30, mitochondrial

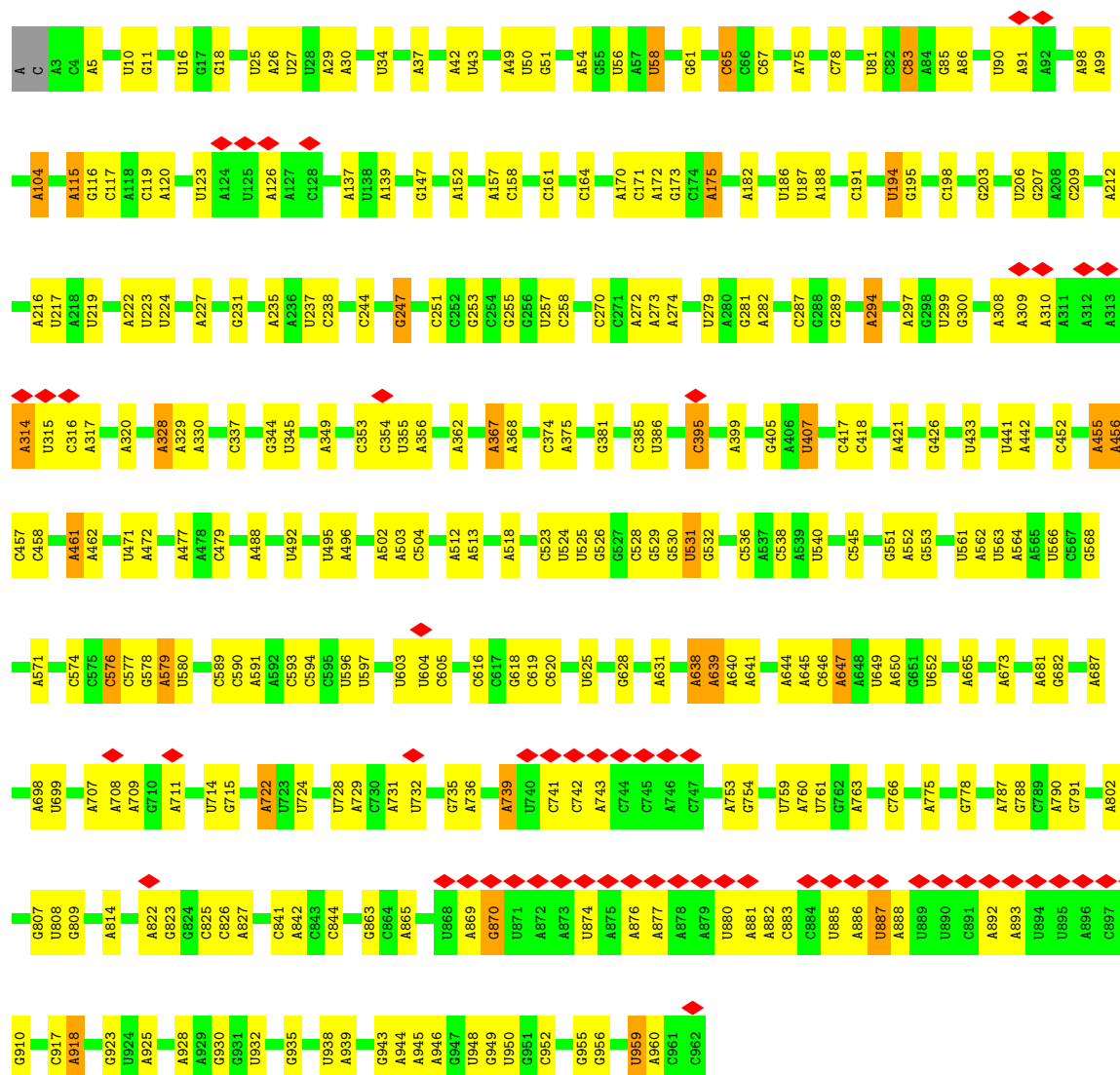


• Molecule 47: Mitochondrial ribosomal protein S18A

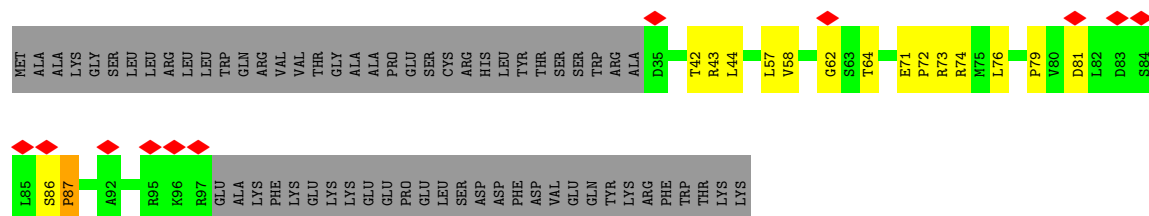
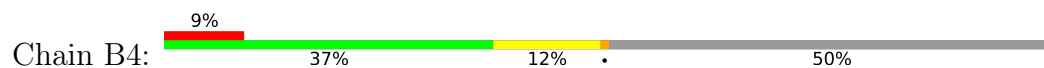


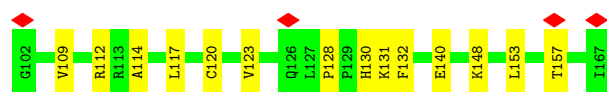


• Molecule 48: 12S rRNA

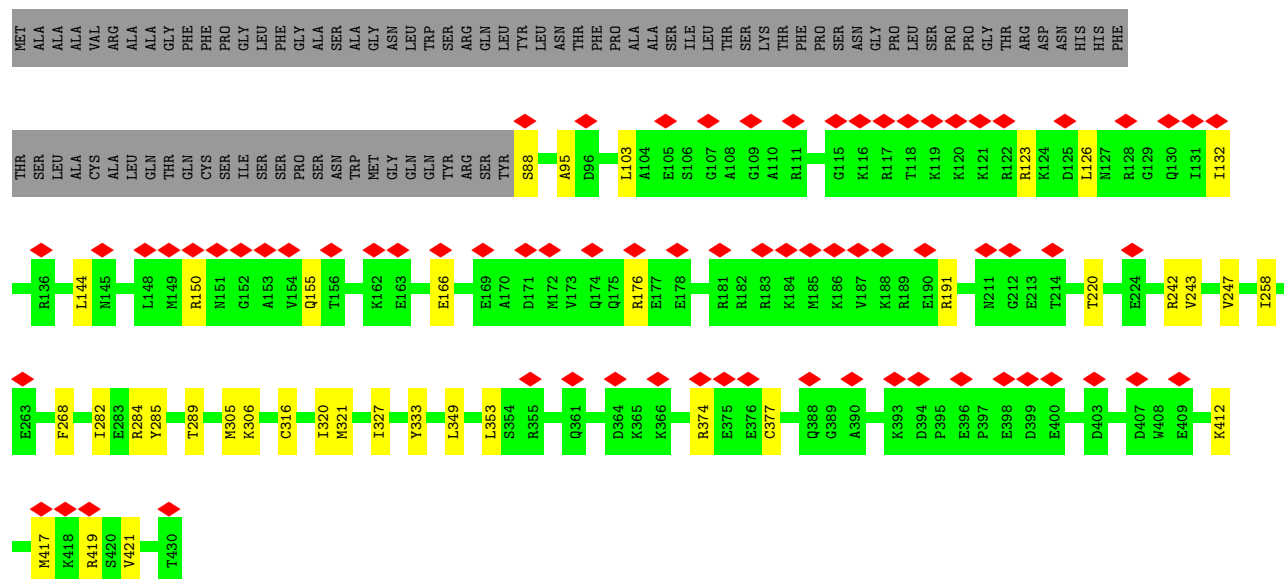
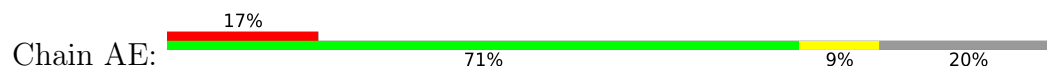


• Molecule 49: bL31m

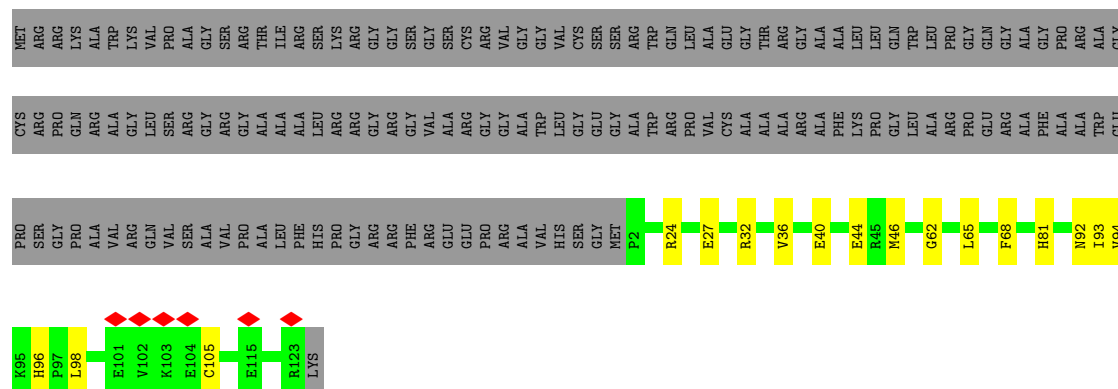
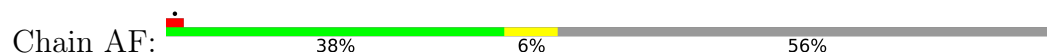




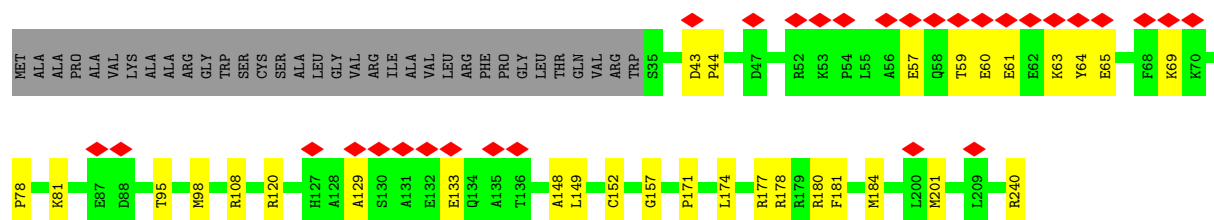
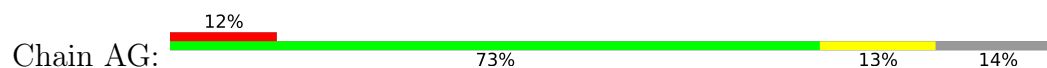
- Molecule 55: Mitochondrial ribosomal protein S5



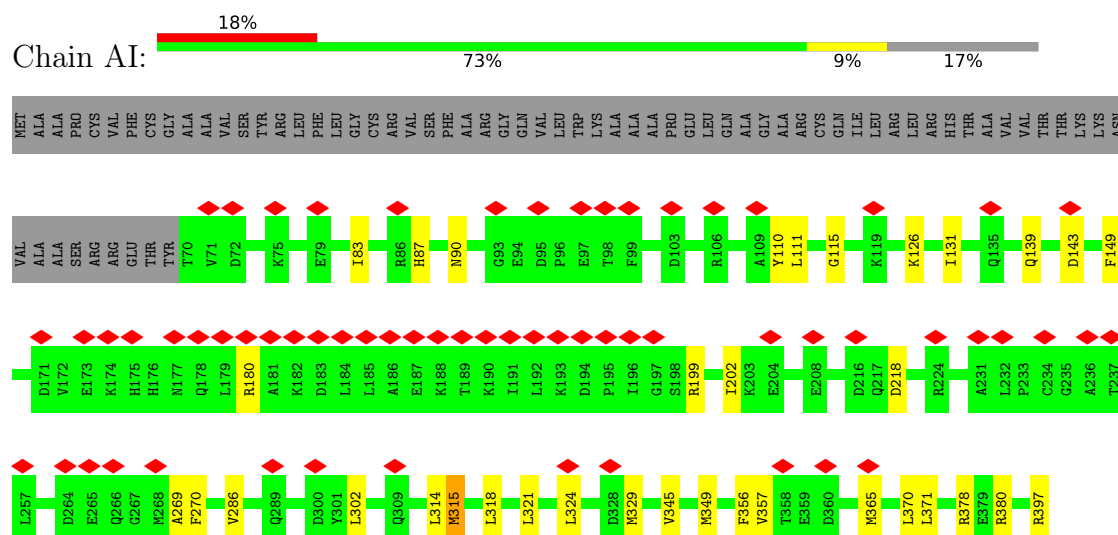
- Molecule 56: bS6m



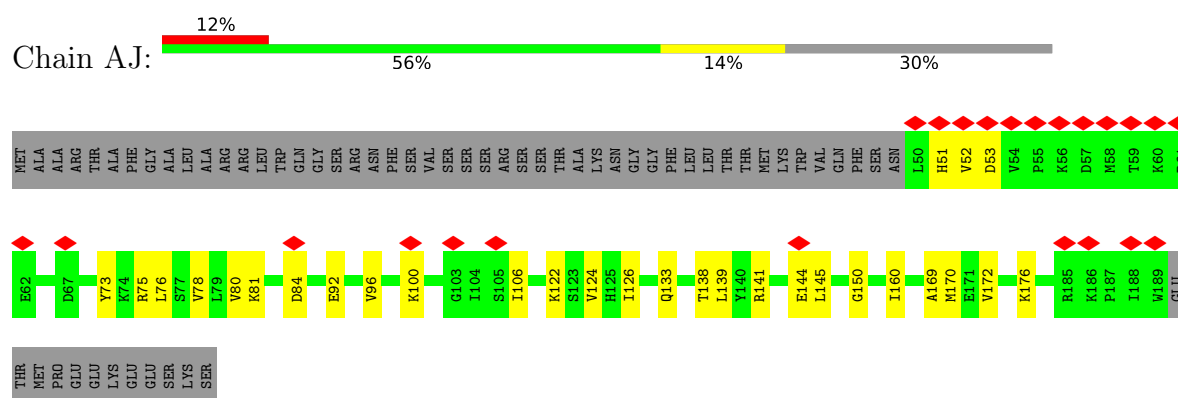
- Molecule 57: 28S ribosomal protein S7, mitochondrial



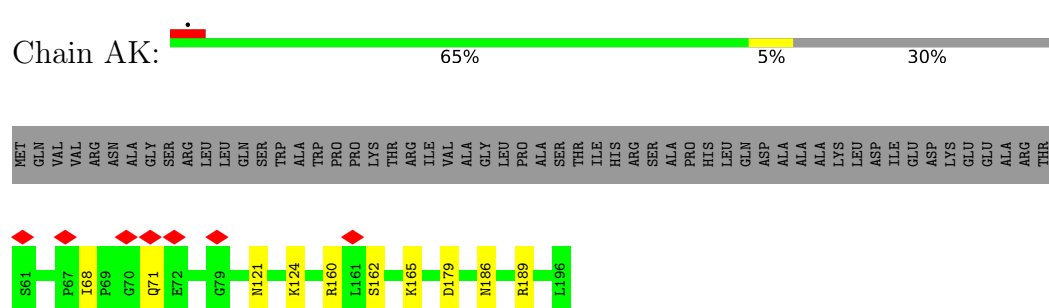
- Molecule 58: uS9m



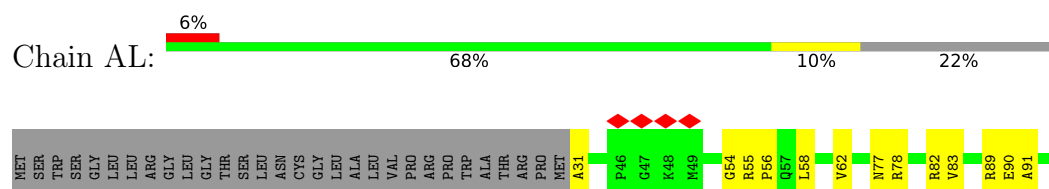
- Molecule 59: Mitochondrial ribosomal protein S10



- Molecule 60: uS11m



- Molecule 61: Mitochondrial ribosomal protein S12





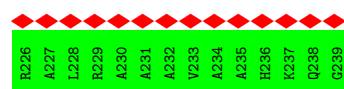
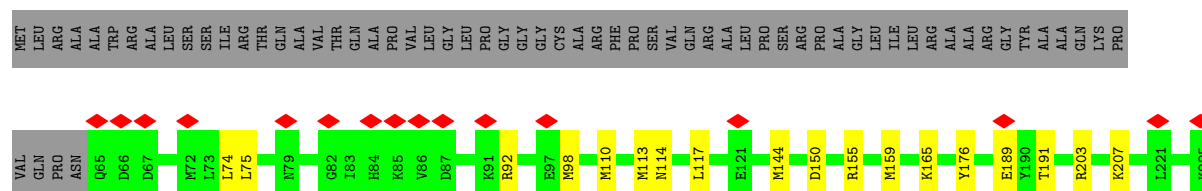
- Molecule 62: Mitochondrial ribosomal protein S14

Chain AN: 65% 14% 21%



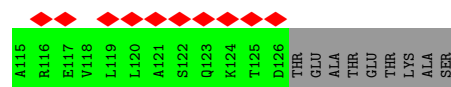
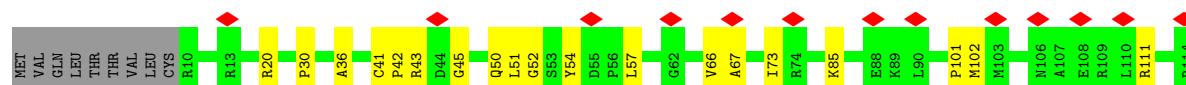
- Molecule 63: uS15m

Chain AO: 13% 66% 8% 27%



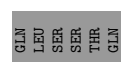
- Molecule 64: 28S ribosomal protein S16, mitochondrial

Chain AP: 17% 73% 14% 13%

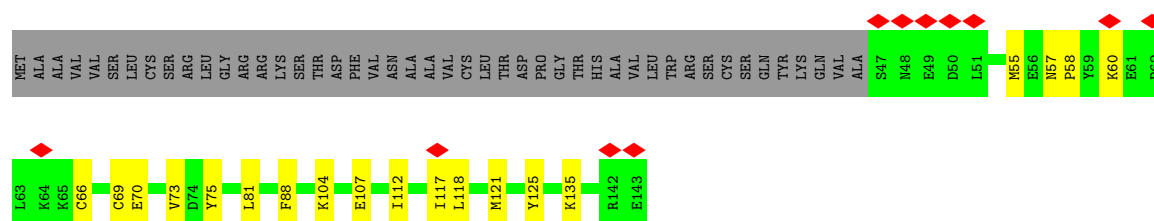


- Molecule 65: uS17m

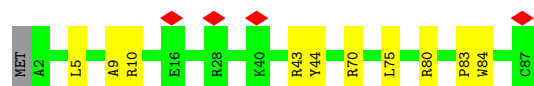
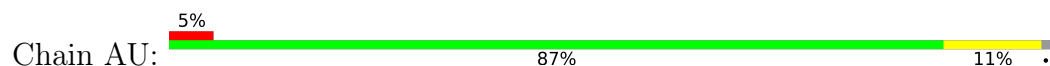
Chain AQ: 7% 71% 15% 14%



- Molecule 66: Mitochondrial ribosomal protein S18C



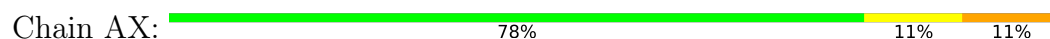
- Molecule 67: bS21m



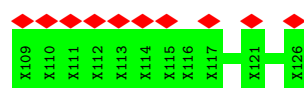
- Molecule 68: tRNAMet



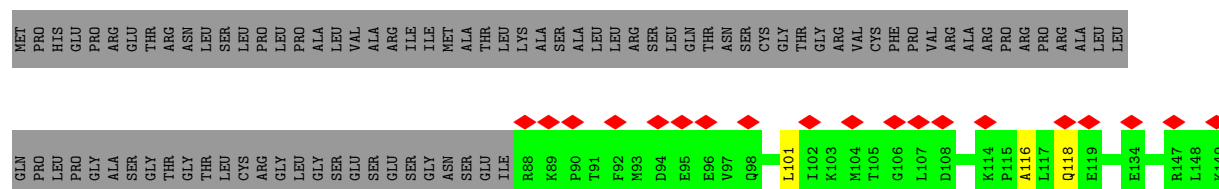
- Molecule 69: mRNA

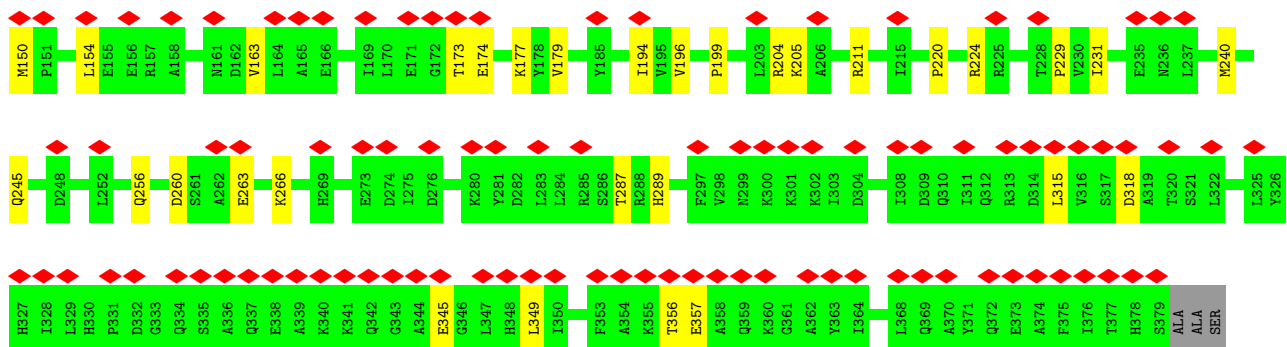


- Molecule 70: unknown

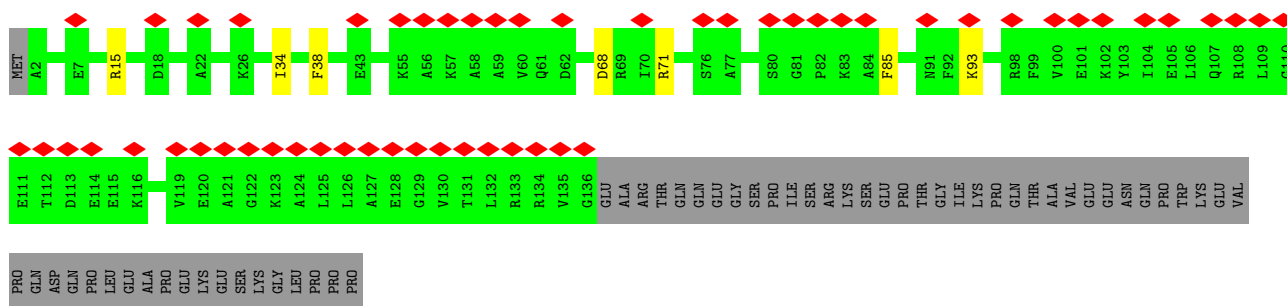


- Molecule 71: Mitochondrial ribosomal protein S22

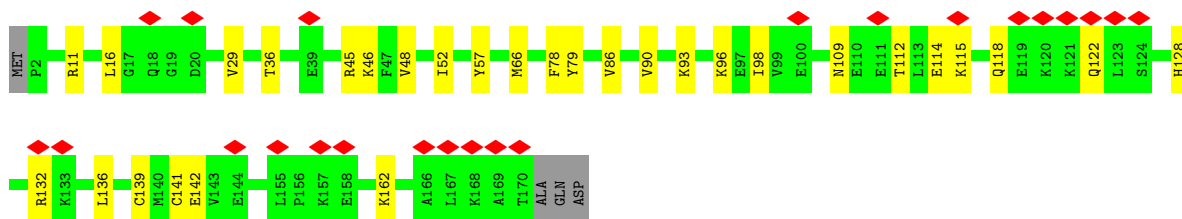
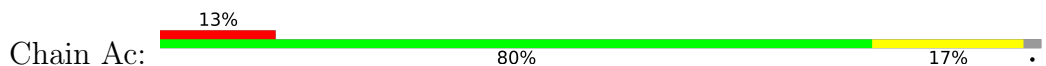




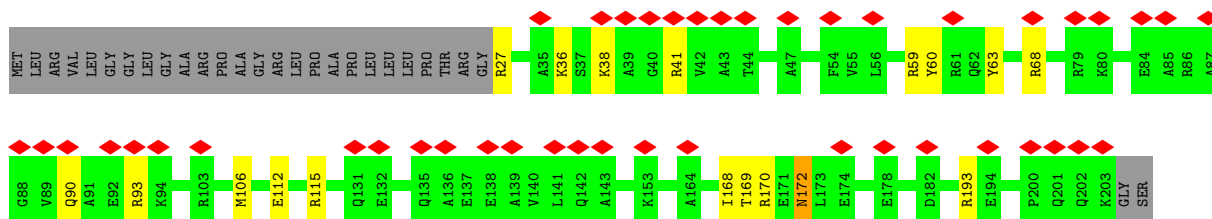
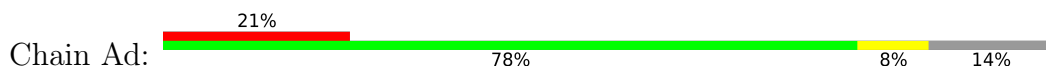
• Molecule 72: mS23



• Molecule 73: Mitochondrial ribosomal protein S25

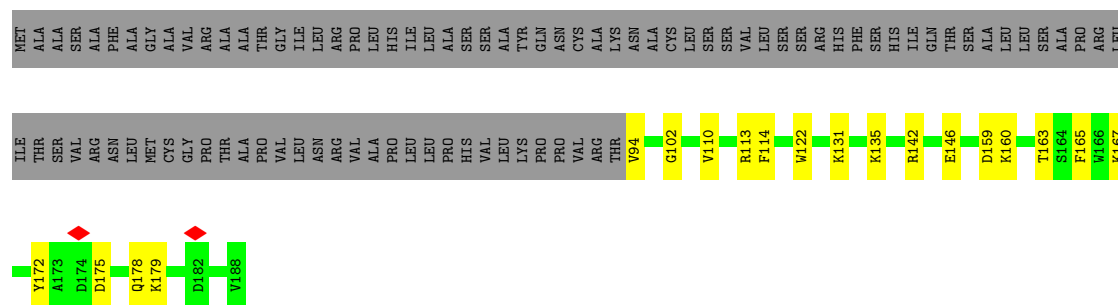


• Molecule 74: Mitochondrial ribosomal protein S26

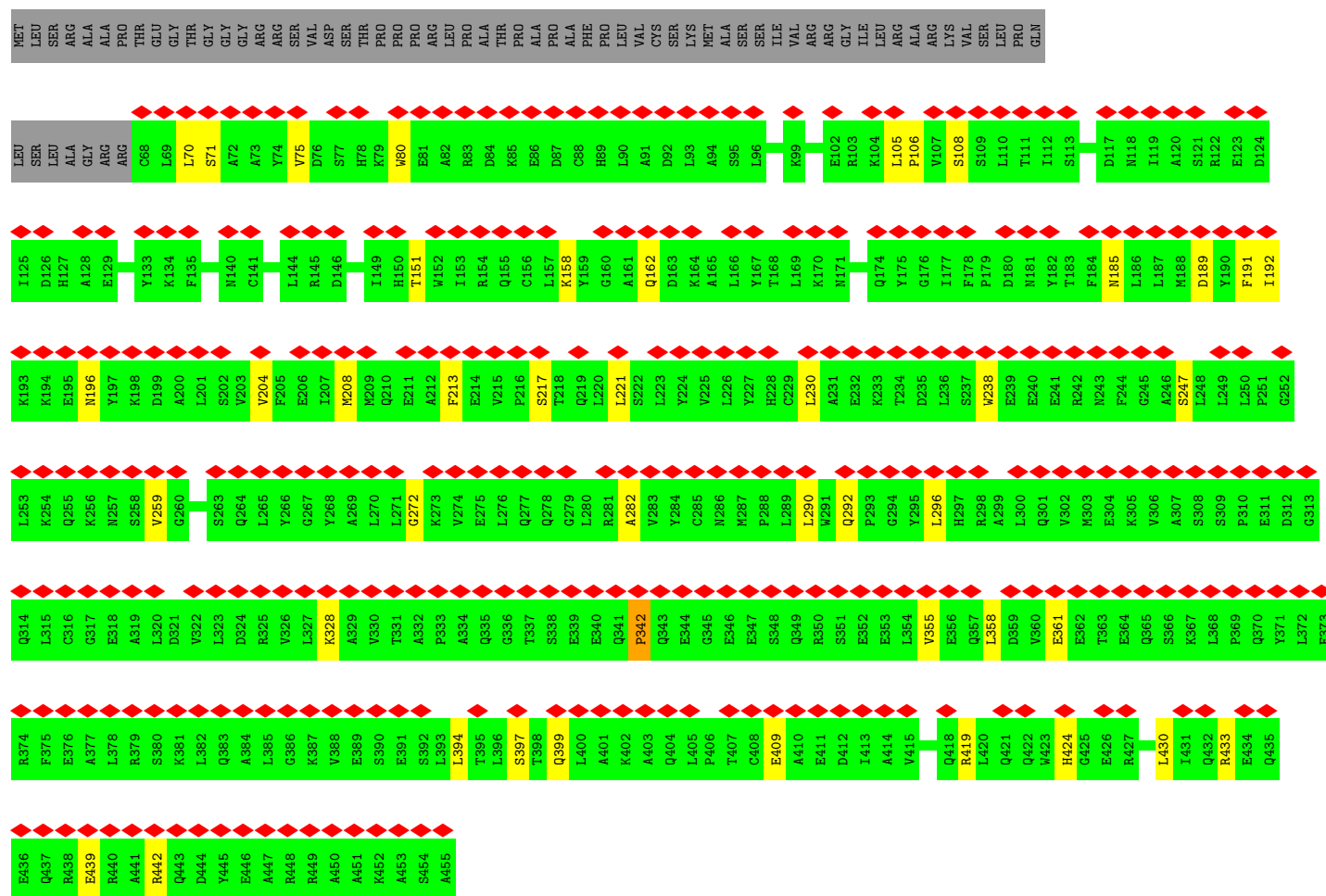
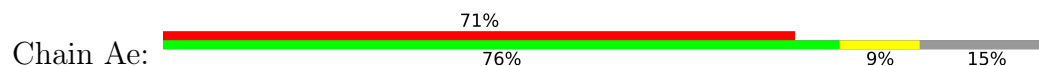


• Molecule 75: Mitochondrial ribosomal protein L35

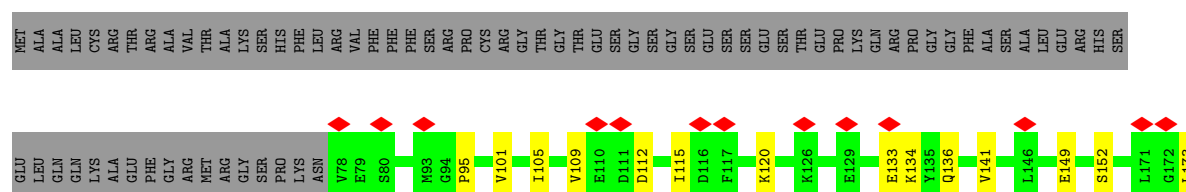




• Molecule 76: Mitochondrial ribosomal protein S27

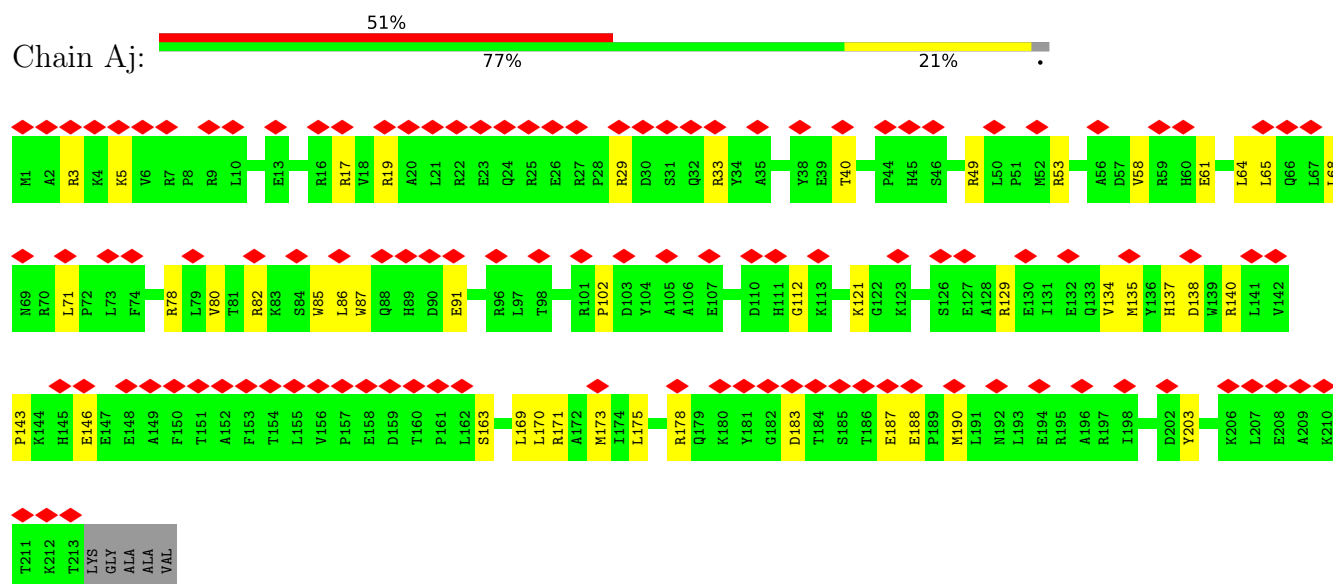


• Molecule 77: Mitoribosomal protein ms28, mrps28

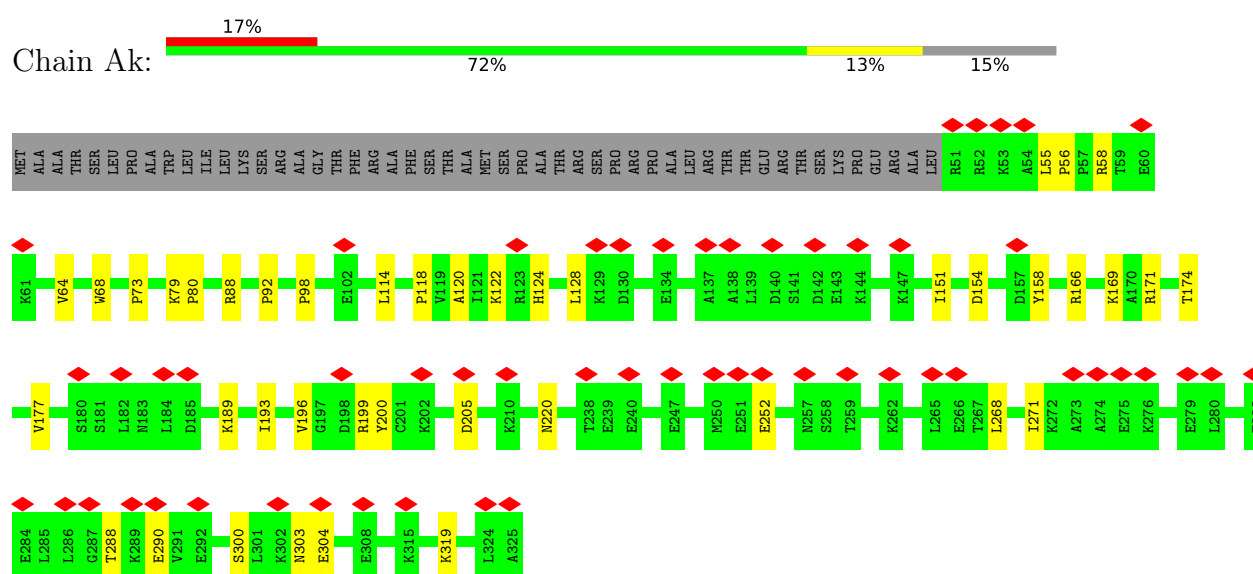




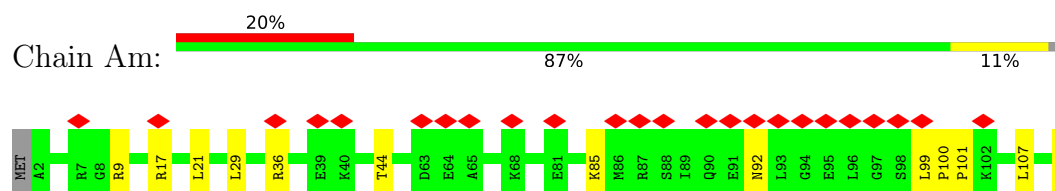
- Molecule 81: mS34



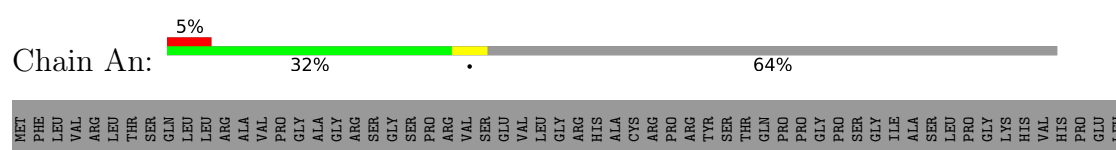
- Molecule 82: Mitochondrial ribosomal protein S35

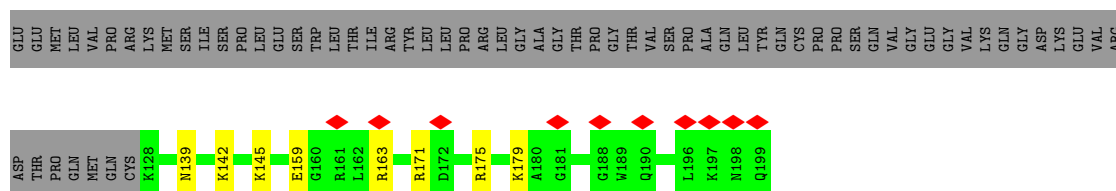


- Molecule 83: mS37

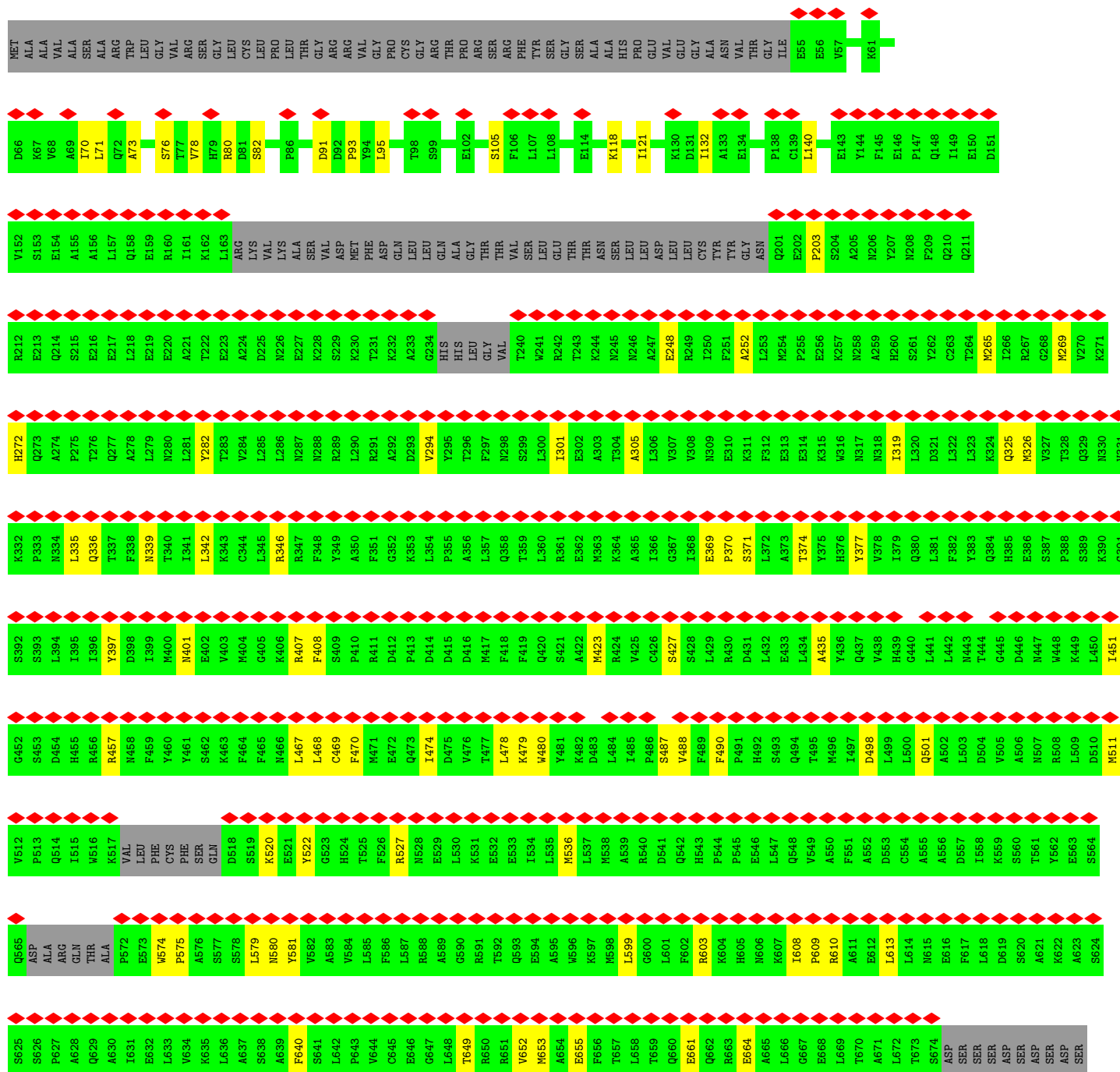
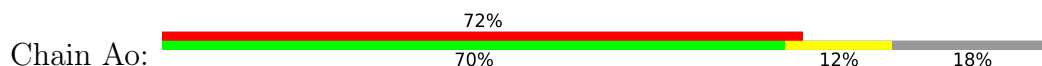


- Molecule 84: Aurora kinase A interacting protein 1





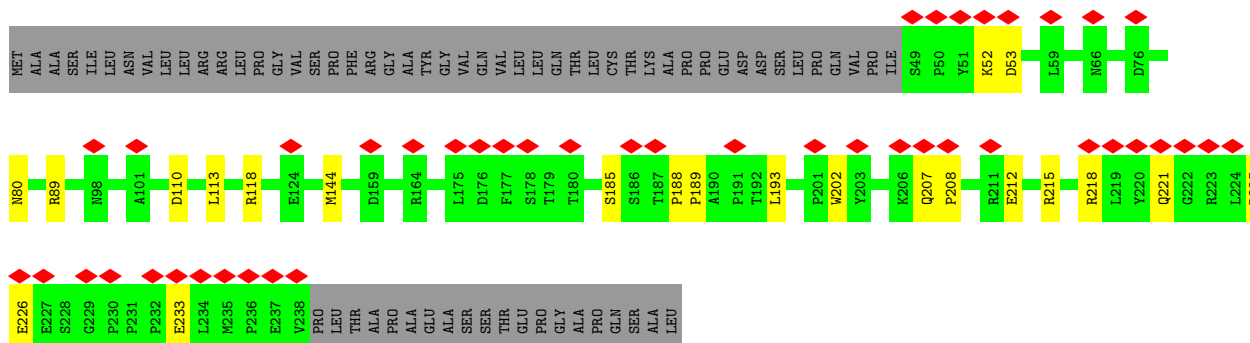
● Molecule 85: Pentatricopeptide repeat domain 3



ASP
SER
ALA
ILE
SER
GLU
GLY
LYS

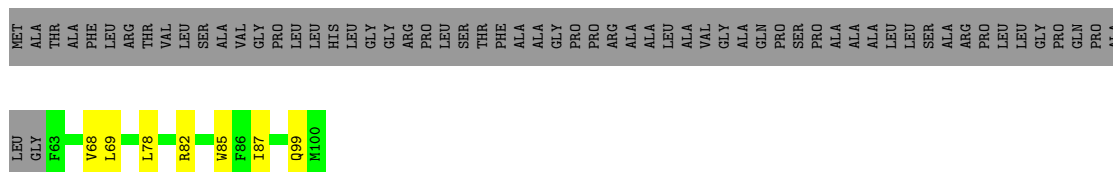
- Molecule 86: 28S ribosomal protein S18b, mitochondrial

Chain Ap: 



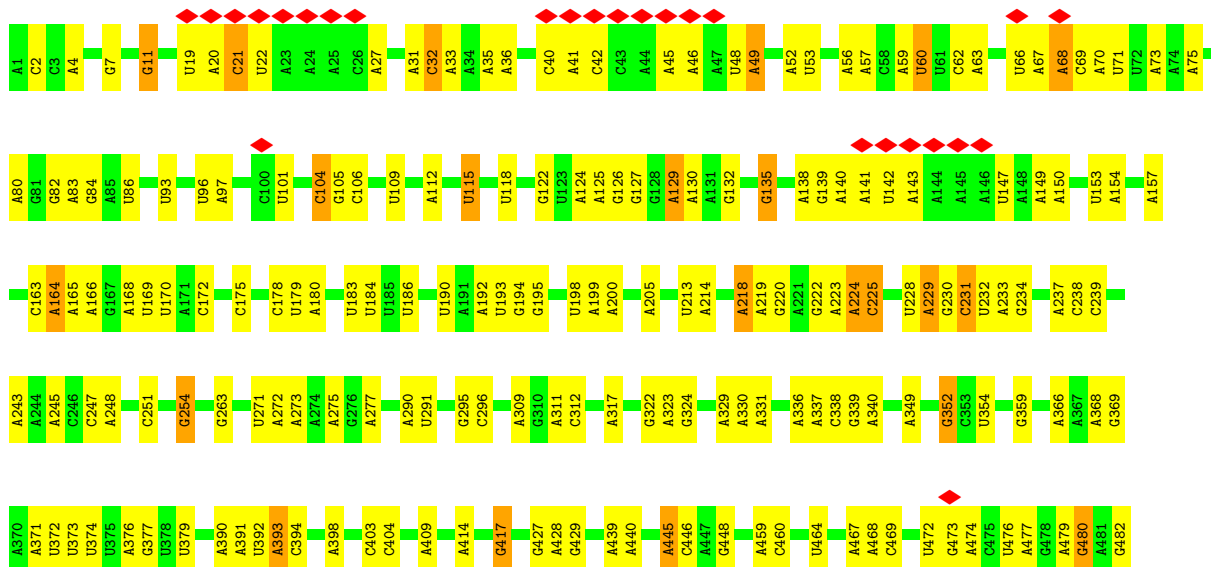
- Molecule 87: Ribosomal protein

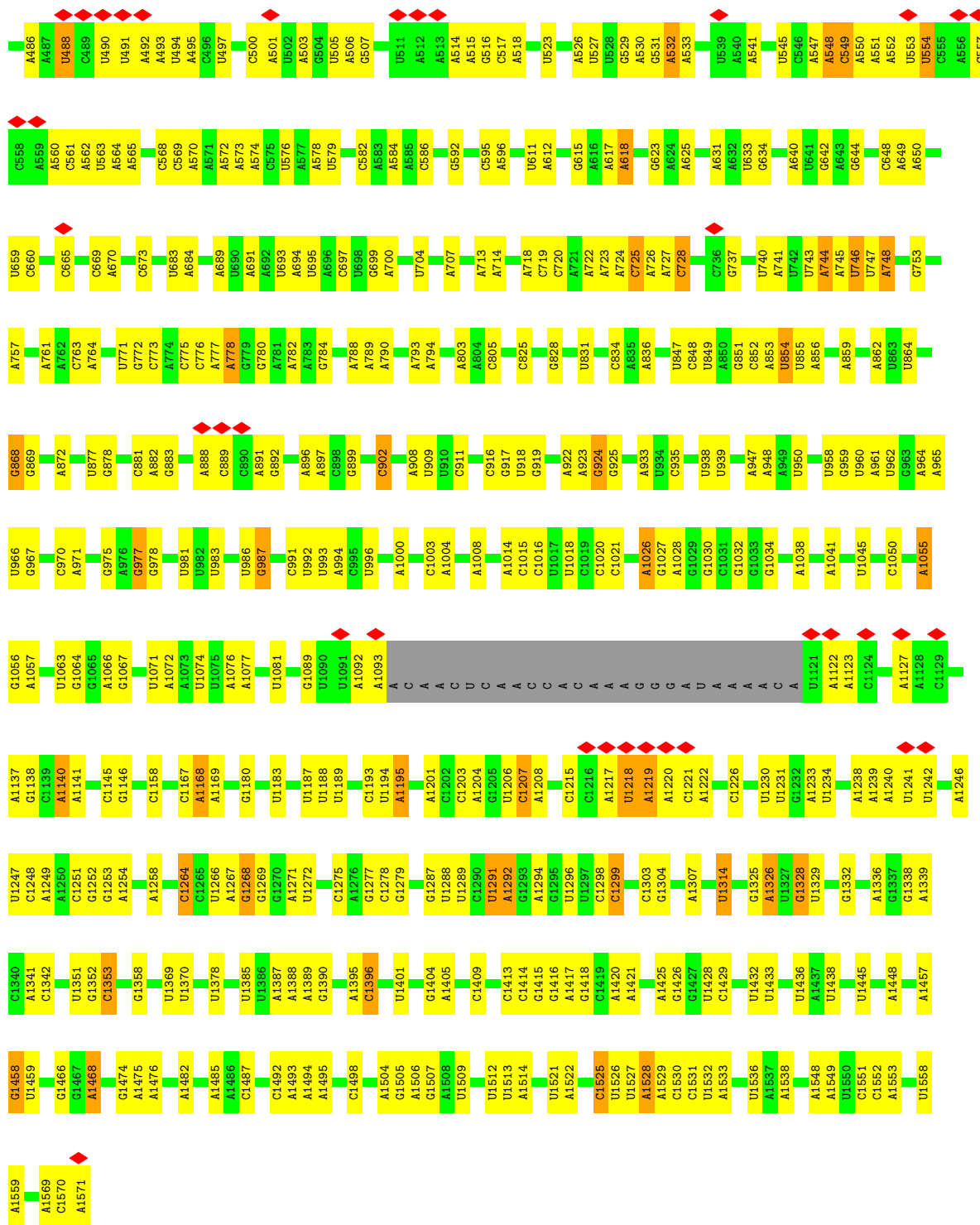
Chain B9: 



- Molecule 88: 16S rRNA

Chain BA: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47048	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.933	Depositor
Minimum map value	-0.616	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, 5GP, SPM, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	CL	0.18	0/319	0.47	0/435
1	DL	0.16	0/212	0.46	0/286
1	EL	0.16	0/221	0.45	0/297
1	FL	0.15	0/212	0.44	0/286
1	GL	0.14	0/212	0.38	0/286
1	HL	0.18	0/204	0.55	0/275
2	B0	0.21	0/880	0.51	0/1189
3	B1	0.18	0/2093	0.52	0/2835
4	B2	0.22	0/1586	0.51	0/2123
5	BB	0.16	0/1595	0.36	0/2475
6	BD	0.20	0/1658	0.52	0/2234
7	BE	0.22	0/2255	0.59	2/3057 (0.1%)
8	BF	0.21	0/1843	0.54	1/2505 (0.0%)
9	BI	0.18	0/819	0.52	0/1101
10	BJ	0.28	0/1742	0.70	1/2358 (0.0%)
11	BK	0.20	0/1323	0.52	0/1785
12	BL	0.26	0/2038	0.69	0/2744
13	BN	0.19	0/1487	0.50	0/2017
14	BO	0.17	0/912	0.50	0/1231
15	BP	0.22	0/2368	0.57	0/3198
16	BQ	0.19	0/1850	0.52	0/2491
17	BR	0.21	0/1262	0.53	0/1700
18	BS	0.24	0/1197	0.65	0/1624
19	BT	0.26	0/2002	0.60	3/2708 (0.1%)
20	BU	0.21	0/1179	0.49	0/1578
21	BV	0.24	0/1256	0.64	0/1706
22	BW	0.20	0/1407	0.49	0/1891
23	BX	0.19	0/1211	0.52	0/1646
24	BY	0.21	0/1719	0.55	0/2329
25	Ba	0.24	0/3267	0.60	2/4455 (0.0%)
26	Bb	0.22	0/3047	0.56	2/4139 (0.0%)
27	B3	0.18	0/993	0.48	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	Bc	0.21	0/2464	0.55	0/3330
29	Bd	0.27	0/1183	0.58	0/1594
30	Be	0.19	0/1000	0.47	0/1345
31	Bf	0.22	0/851	0.64	2/1159 (0.2%)
32	Bg	0.23	0/1191	0.55	0/1614
33	Bh	0.22	0/2372	0.59	0/3211
34	Bi	0.21	0/2199	0.59	0/2980
35	Bj	0.28	0/1811	0.61	0/2436
36	Bk	0.27	0/1270	0.77	3/1714 (0.2%)
37	Bl	0.23	0/1135	0.56	0/1549
38	Bm	0.19	0/917	0.49	0/1248
39	Bn	0.22	0/860	0.55	0/1150
40	Bo	0.23	0/787	0.61	0/1056
41	Bp	0.19	0/752	0.57	0/1013
42	Bq	0.24	0/558	0.68	3/756 (0.4%)
43	Bt	0.22	0/798	0.53	0/1073
44	Bu	0.24	0/1214	0.63	1/1630 (0.1%)
45	Bv	0.21	0/1157	0.43	0/1560
46	Bw	0.23	0/3206	0.55	0/4354
47	Bx	0.24	0/1364	0.66	2/1849 (0.1%)
48	AA	0.15	0/22852	0.32	0/35580
49	B4	0.24	0/486	0.67	1/660 (0.2%)
50	B5	0.20	0/917	0.50	0/1227
51	B6	0.24	0/430	0.63	0/570
52	B7	0.17	0/395	0.43	0/524
53	AB	0.24	0/1804	0.58	0/2445
54	AC	0.26	0/1105	0.72	2/1496 (0.1%)
55	AE	0.21	0/2785	0.57	1/3735 (0.0%)
56	AF	0.21	0/999	0.58	0/1347
57	AG	0.22	0/1731	0.64	0/2322
58	AI	0.21	0/2707	0.56	2/3636 (0.1%)
59	AJ	0.26	0/1181	0.61	0/1597
60	AK	0.21	0/1027	0.60	1/1389 (0.1%)
61	AL	0.22	0/858	0.62	0/1152
62	AN	0.21	0/874	0.58	1/1171 (0.1%)
63	AO	0.23	0/1473	0.58	2/1970 (0.1%)
64	AP	0.23	0/954	0.58	0/1284
65	AQ	0.19	0/894	0.50	0/1213
66	AR	0.23	0/802	0.56	0/1079
67	AU	0.19	0/745	0.47	0/993
68	AV	0.19	0/1673	0.42	0/2602
69	AX	0.11	0/210	0.25	0/325
71	Aa	0.24	0/2428	0.60	1/3279 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
72	Ab	0.23	0/1126	0.51	0/1514
73	Ac	0.24	0/1399	0.64	1/1881 (0.1%)
74	Ad	0.26	0/1490	0.58	0/2005
75	B8	0.16	0/853	0.46	0/1136
76	Ae	0.25	0/3171	0.67	1/4292 (0.0%)
77	Af	0.26	0/790	0.74	1/1064 (0.1%)
78	Ag	0.24	0/2945	0.62	1/3984 (0.0%)
79	Ah	0.23	0/1045	0.53	0/1409
80	Ai	0.21	0/841	0.59	1/1121 (0.1%)
81	Aj	0.23	0/1835	0.60	0/2484
82	Ak	0.22	0/2268	0.57	0/3069
83	Am	0.21	0/947	0.62	0/1268
84	An	0.22	0/650	0.56	0/858
85	Ao	0.24	0/4626	0.64	4/6269 (0.1%)
86	Ap	0.21	0/1616	0.54	0/2195
87	B9	0.22	0/342	0.53	0/450
88	BA	0.16	0/36784	0.37	0/57270
All	All	0.20	0/183516	0.51	42/260811 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	BE	0	1
10	BJ	0	1
32	Bg	0	1
36	Bk	0	1
39	Bn	0	1
43	Bt	0	1
All	All	0	6

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	Af	95	PRO	CA-N-CD	-11.10	96.45	112.00
54	AC	114	ALA	CA-C-N	8.88	138.51	121.54
54	AC	114	ALA	C-N-CA	8.88	138.51	121.54
47	Bx	69	GLN	CA-C-N	8.56	132.29	120.39
47	Bx	69	GLN	C-N-CA	8.56	132.29	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	Bu	167	PRO	N-CA-CB	7.82	111.46	103.25
31	Bf	80	PRO	N-CA-CB	7.72	111.36	103.25
42	Bq	88	PRO	CA-N-CD	-7.51	101.49	112.00
31	Bf	78	PRO	N-CA-CB	7.47	111.10	103.25
36	Bk	168	GLU	N-CA-CB	7.35	120.93	110.12
76	Ae	342	PRO	N-CA-CB	7.30	110.91	103.25
36	Bk	127	MET	CB-CG-SD	6.77	133.00	112.70
49	B4	87	PRO	N-CA-CB	6.67	110.25	103.25
19	BT	68	PRO	N-CA-CB	6.35	109.91	103.25
73	Ac	114	GLU	N-CA-CB	6.19	119.88	110.28
71	Aa	220	PRO	CA-N-CD	-6.17	103.37	112.00
80	Ai	36	LEU	CA-CB-CG	6.06	137.53	116.30
36	Bk	168	GLU	CA-CB-CG	6.06	126.22	114.10
85	Ao	203	PRO	N-CA-CB	5.88	110.02	103.44
19	BT	268	ASP	CA-C-N	5.86	132.73	121.54
19	BT	268	ASP	C-N-CA	5.86	132.73	121.54
25	Ba	205	GLN	CA-C-N	5.80	130.64	122.46
25	Ba	205	GLN	C-N-CA	5.80	130.64	122.46
78	Ag	337	ASP	CB-CA-C	5.72	121.44	110.17
42	Bq	91	GLU	CA-C-N	5.67	129.30	120.68
42	Bq	91	GLU	C-N-CA	5.67	129.30	120.68
62	AN	74	GLU	CA-CB-CG	5.66	125.42	114.10
85	Ao	132	ILE	N-CA-C	-5.63	107.34	111.90
8	BF	289	PRO	CA-N-CD	-5.51	104.28	112.00
60	AK	121	ASN	N-CA-C	5.42	117.63	111.02
26	Bb	193	VAL	CA-C-N	5.38	128.13	120.49
26	Bb	193	VAL	C-N-CA	5.38	128.13	120.49
63	AO	74	LEU	CA-C-N	5.37	127.79	120.54
63	AO	74	LEU	C-N-CA	5.37	127.79	120.54
85	Ao	511	MET	CA-C-N	5.30	124.57	120.33
85	Ao	511	MET	C-N-CA	5.30	124.57	120.33
7	BE	317	PRO	CA-C-N	5.25	131.57	121.54
7	BE	317	PRO	C-N-CA	5.25	131.57	121.54
58	AI	315	MET	CA-C-N	5.13	129.68	121.62
58	AI	315	MET	C-N-CA	5.13	129.68	121.62
10	BJ	127	PRO	CA-N-CD	-5.12	104.83	112.00
55	AE	166	GLU	N-CA-CB	5.11	118.88	110.39

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	BE	316	PHE	Peptide
10	BJ	156	SER	Peptide
32	Bg	49	ARG	Peptide
36	Bk	197	ARG	Sidechain
39	Bn	65	ASN	Peptide
43	Bt	18	ILE	Peptide

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	CL	317	0	309	5	0
1	DL	213	0	234	3	0
1	EL	222	0	247	4	0
1	FL	213	0	234	2	0
1	GL	213	0	234	0	0
1	HL	205	0	223	3	0
2	B0	857	0	878	7	0
3	B1	2036	0	2058	20	0
4	B2	1548	0	1583	15	0
5	BB	1427	0	726	8	0
6	BD	1625	0	1678	16	0
7	BE	2192	0	2195	25	0
8	BF	1792	0	1843	19	0
9	BI	805	0	845	9	0
10	BJ	1705	0	1804	23	0
11	BK	1303	0	1343	10	0
12	BL	2003	0	2000	28	0
13	BN	1444	0	1437	20	0
14	BO	896	0	946	13	0
15	BP	2312	0	2373	34	0
16	BQ	1803	0	1841	16	0
17	BR	1240	0	1260	13	0
18	BS	1168	0	1159	14	0
19	BT	1954	0	1943	20	0
20	BU	1159	0	1228	13	0
21	BV	1231	0	1278	21	0
22	BW	1374	0	1405	18	0
23	BX	1181	0	1139	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	BY	1678	0	1683	20	0
25	Ba	3173	0	3153	39	0
26	Bb	2952	0	2840	34	0
27	B3	968	0	1018	10	0
28	Bc	2408	0	2415	24	0
29	Bd	1158	0	1166	20	0
30	Be	972	0	971	12	0
31	Bf	827	0	736	6	0
32	Bg	1167	0	1173	22	0
33	Bh	2319	0	2332	19	0
34	Bi	2138	0	2139	29	0
35	Bj	1775	0	1797	33	0
36	Bk	1246	0	1251	19	0
37	Bl	1097	0	1080	11	0
38	Bm	893	0	878	7	0
39	Bn	837	0	860	11	0
40	Bo	772	0	773	5	0
41	Bp	742	0	749	6	0
42	Bq	542	0	485	3	0
43	Bt	780	0	792	14	0
44	Bu	1198	0	1192	13	0
45	Bv	1131	0	1093	5	0
46	Bw	3126	0	3153	39	0
47	Bx	1325	0	1354	10	0
48	AA	20411	0	10344	109	0
49	B4	479	0	456	12	0
50	B5	902	0	916	9	0
51	B6	425	0	471	8	0
52	B7	387	0	413	7	0
53	AB	1762	0	1774	19	0
54	AC	1075	0	1087	19	0
55	AE	2732	0	2774	23	0
56	AF	981	0	1012	14	0
57	AG	1693	0	1727	19	0
58	AI	2650	0	2613	27	0
59	AJ	1155	0	1193	21	0
60	AK	1007	0	1042	6	0
61	AL	840	0	890	11	0
62	AN	858	0	883	12	0
63	AO	1448	0	1536	13	0
64	AP	932	0	951	15	0
65	AQ	875	0	931	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	AR	784	0	813	14	0
67	AU	734	0	745	8	0
68	AV	1498	0	766	5	0
69	AX	188	0	99	3	0
70	AZ	90	0	20	0	0
71	Aa	2378	0	2392	17	0
72	Ab	1101	0	1118	6	0
73	Ac	1367	0	1385	20	0
74	Ad	1467	0	1466	15	0
75	B8	833	0	883	16	0
76	Ae	3109	0	3029	25	0
77	Af	778	0	791	11	0
78	Ag	2875	0	2885	39	0
79	Ah	1015	0	969	6	0
80	Ai	824	0	842	8	0
81	Aj	1788	0	1799	29	0
82	Ak	2222	0	2270	26	0
83	Am	930	0	959	10	0
84	An	639	0	709	8	0
85	Ao	4526	0	4434	51	0
86	Ap	1564	0	1531	14	0
87	B9	335	0	359	5	0
88	BA	32844	0	16617	192	0
89	AA	104	0	0	0	0
89	AB	1	0	0	0	0
89	AL	2	0	0	0	0
89	Ag	1	0	0	0	0
89	Am	1	0	0	0	0
89	An	1	0	0	0	0
89	B0	1	0	0	0	0
89	B3	2	0	0	0	0
89	BA	197	0	0	0	0
89	BB	1	0	0	0	0
89	BD	3	0	0	0	0
89	BE	1	0	0	0	0
89	BP	3	0	0	0	0
89	BR	1	0	0	0	0
89	Be	1	0	0	0	0
89	Bl	1	0	0	0	0
89	Bt	2	0	0	0	0
90	AR	1	0	0	0	0
90	Ac	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	Ap	1	0	0	0	0
90	B5	1	0	0	0	0
90	B9	1	0	0	0	0
90	Bx	1	0	0	0	0
91	AA	14	0	26	0	0
91	BA	28	0	52	2	0
92	Ag	32	0	12	3	0
93	BA	48	0	23	0	0
94	Ag	3	0	0	0	0
All	All	174617	0	147533	1347	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 (1347) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B0:86:ASN:C	2:B0:86:ASN:HD22	1.95	0.75
33:Bh:158:ASP:O	33:Bh:162:SER:HB3	1.88	0.73
10:BJ:64:CYS:SG	47:Bx:70:CYS:HB2	2.30	0.70
88:BA:486:A:H61	88:BA:582:C:H42	1.39	0.70
25:Ba:126:THR:HG22	25:Ba:372:ASN:HB2	1.73	0.70
29:Bd:164:ARG:HE	29:Bd:168:LEU:HD22	1.57	0.69
21:BV:111:LYS:HD2	22:BW:210:LEU:HD11	1.74	0.69
50:B5:179:ARG:HH12	50:B5:182:PRO:HG3	1.58	0.68
63:AO:113:MET:O	63:AO:117:LEU:HB2	1.93	0.68
71:Aa:345:GLU:O	71:Aa:349:LEU:HB2	1.94	0.67
36:Bk:127:MET:HE3	36:Bk:128:PRO:HD2	1.77	0.66
59:AJ:73:TYR:HA	59:AJ:176:LYS:HA	1.76	0.66
74:Ad:59:ARG:O	74:Ad:63:TYR:HB2	1.96	0.66
7:BE:62:LYS:HG2	88:BA:1569:A:H4'	1.79	0.65
7:BE:151:THR:HG22	88:BA:1569:A:H61	1.61	0.65
57:AG:120:ARG:NH1	78:Ag:88:MET:SD	2.69	0.65
15:BP:117:ASP:OD1	15:BP:120:GLN:NE2	2.30	0.65
35:Bj:256:SER:O	35:Bj:260:LEU:HB2	1.96	0.64
58:AI:111:LEU:HD12	82:Ak:114:LEU:HD23	1.79	0.64
75:B8:172:TYR:HB2	75:B8:175:ASP:HB2	1.79	0.64
18:BS:44:VAL:HG23	26:Bb:225:LEU:HB3	1.79	0.64
8:BF:262:THR:HG22	8:BF:264:PRO:HD2	1.80	0.64
78:Ag:259:VAL:HB	78:Ag:305:ILE:HG22	1.80	0.64
28:Bc:76:PHE:HB3	28:Bc:78:MET:HE3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Bn:99:GLY:HA2	39:Bn:102:MET:HE2	1.80	0.64
24:BY:126:THR:OG1	24:BY:152:ARG:NH1	2.31	0.64
27:B3:74:SER:HB3	88:BA:472:U:H5''	1.79	0.63
56:AF:96:HIS:HE1	56:AF:98:LEU:HG	1.61	0.63
73:Ac:29:VAL:HB	73:Ac:79:TYR:HB2	1.78	0.63
76:Ae:430:LEU:HD23	76:Ae:433:ARG:HH12	1.64	0.63
10:BJ:95:MET:HB2	10:BJ:159:PRO:HB3	1.79	0.63
74:Ad:38:LYS:HG3	74:Ad:41:ARG:HD3	1.81	0.63
73:Ac:139:CYS:HB2	73:Ac:142:GLU:HG3	1.79	0.63
77:Af:105:ILE:HG12	77:Af:115:ILE:HG12	1.80	0.63
12:BL:308:ARG:HG3	12:BL:319:HIS:CE1	2.34	0.62
27:B3:88:MET:SD	88:BA:417:G:N2	2.69	0.62
88:BA:392:U:H2'	88:BA:393:A:H8	1.64	0.62
56:AF:96:HIS:CE1	56:AF:98:LEU:HG	2.34	0.62
13:BN:27:PRO:HG2	13:BN:30:LYS:HB2	1.81	0.62
12:BL:270:LEU:O	12:BL:274:HIS:ND1	2.27	0.62
35:Bj:179:GLN:HE21	35:Bj:182:GLU:HG3	1.64	0.62
34:Bi:152:LEU:HD11	34:Bi:172:MET:HB2	1.82	0.62
34:Bi:267:PRO:HG2	34:Bi:270:ALA:HB2	1.82	0.62
35:Bj:157:LEU:HD23	35:Bj:254:TRP:HB3	1.82	0.62
13:BN:25:MET:SD	47:Bx:148:ASN:ND2	2.73	0.61
28:Bc:48:GLU:HG3	28:Bc:216:LEU:HD21	1.80	0.61
73:Ac:90:VAL:HG23	73:Ac:93:LYS:HB2	1.83	0.61
46:Bw:81:ARG:O	46:Bw:85:LYS:HB3	2.00	0.61
88:BA:112:A:N6	88:BA:115:U:OP2	2.34	0.61
88:BA:877:U:H5''	88:BA:878:G:H5'	1.82	0.61
38:Bm:75:VAL:O	38:Bm:79:PHE:HB2	2.00	0.61
73:Ac:48:VAL:HA	73:Ac:52:ILE:HD12	1.83	0.61
58:AI:321:LEU:HD11	58:AI:365:MET:HE1	1.82	0.61
48:AA:188:A:N7	48:AA:207:G:N2	2.48	0.61
48:AA:90:U:OP1	74:Ad:68:ARG:NH1	2.34	0.60
28:Bc:41:GLN:HB3	28:Bc:258:ILE:HD12	1.83	0.60
85:Ao:603:ARG:HH21	85:Ao:609:PRO:HG2	1.66	0.60
54:AC:109:VAL:HB	54:AC:120:CYS:HB2	1.83	0.60
82:Ak:73:PRO:HB3	85:Ao:78:VAL:HG11	1.82	0.60
53:AB:134:VAL:HG11	53:AB:191:LEU:HD13	1.82	0.60
25:Ba:160:HIS:HA	25:Ba:164:TRP:HB2	1.84	0.60
12:BL:187:GLY:O	69:AX:7:C:N4	2.34	0.60
37:Bl:89:SER:HB3	37:Bl:93:ASN:H	1.67	0.60
55:AE:150:ARG:HB2	55:AE:155:GLN:HE21	1.65	0.60
81:Aj:68:LEU:HD12	81:Aj:71:LEU:HD12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B1:24:LEU:HD12	3:B1:25:PRO:HD2	1.84	0.59
10:BJ:97:ALA:HB3	10:BJ:154:LEU:HB2	1.84	0.59
34:Bi:192:PRO:HB3	34:Bi:216:MET:HG2	1.84	0.59
24:BY:80:ILE:HB	24:BY:85:TRP:HB2	1.83	0.59
63:AO:110:MET:SD	63:AO:114:ASN:ND2	2.75	0.59
83:Am:99:LEU:HD12	83:Am:100:PRO:HD2	1.84	0.59
11:BK:17:SER:N	11:BK:72:VAL:O	2.35	0.59
85:Ao:427:SER:HA	85:Ao:467:LEU:HD21	1.83	0.59
36:Bk:201:ARG:HB3	36:Bk:204:LEU:HB2	1.85	0.59
12:BL:239:VAL:HG12	12:BL:246:VAL:HG12	1.84	0.59
74:Ad:169:THR:H	74:Ad:172:ASN:HB3	1.68	0.59
6:BD:213:THR:HG21	88:BA:862:A:H5''	1.83	0.59
13:BN:8:PRO:HB2	33:Bh:285:PRO:HG2	1.84	0.59
48:AA:562:A:O2'	48:AA:708:A:N6	2.36	0.59
78:Ag:122:ARG:HG2	78:Ag:305:ILE:HD11	1.84	0.58
3:B1:133:ASP:OD1	9:BI:120:ARG:NH2	2.36	0.58
78:Ag:137:LEU:HD11	78:Ag:260:ALA:HB1	1.85	0.58
6:BD:113:ARG:O	6:BD:148:ARG:NH2	2.36	0.58
11:BK:87:VAL:HG22	11:BK:124:LYS:HE3	1.86	0.58
46:Bw:147:GLU:HG2	46:Bw:169:PRO:HG2	1.86	0.58
58:AI:397:ARG:NH2	68:AV:30:C:OP2	2.36	0.58
12:BL:253:ARG:NH2	68:AV:70:C:OP2	2.36	0.58
32:Bg:85:ARG:NH1	32:Bg:107:GLN:OE1	2.36	0.58
64:AP:51:LEU:HD13	64:AP:73:ILE:HG12	1.84	0.58
79:Ah:330:LEU:O	79:Ah:340:ARG:NH2	2.36	0.58
88:BA:220:G:N3	88:BA:231:C:O2'	2.36	0.58
76:Ae:162:GLN:OE1	76:Ae:196:ASN:ND2	2.37	0.58
18:BS:173:ARG:NH2	88:BA:1219:A:OP1	2.36	0.58
82:Ak:154:ASP:HB2	82:Ak:174:THR:HB	1.85	0.58
27:B3:77:ARG:NH1	88:BA:469:C:OP2	2.36	0.58
46:Bw:237:ILE:HG22	46:Bw:239:ARG:H	1.69	0.58
46:Bw:397:GLU:HG2	46:Bw:398:THR:HG22	1.86	0.58
75:B8:175:ASP:HB3	75:B8:178:GLN:HB2	1.86	0.58
88:BA:529:G:H1'	88:BA:549:C:H1'	1.86	0.58
88:BA:569:C:N4	88:BA:1020:C:O2	2.37	0.58
82:Ak:128:LEU:HG	85:Ao:70:ILE:HD11	1.85	0.57
36:Bk:175:HIS:HA	36:Bk:178:LEU:HG	1.85	0.57
48:AA:50:U:H2'	48:AA:51:G:H8	1.70	0.57
37:Bl:118:TRP:NE1	37:Bl:142:GLU:OE2	2.37	0.57
63:AO:113:MET:HB2	63:AO:117:LEU:HD12	1.86	0.57
85:Ao:469:CYS:SG	85:Ao:470:PHE:N	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Ap:89:ARG:HG3	86:Ap:144:MET:HE3	1.86	0.57
41:Bp:14:LYS:HG2	41:Bp:68:PHE:HA	1.87	0.57
74:Ad:90:GLN:HA	74:Ad:93:ARG:HD2	1.86	0.57
76:Ae:80:TRP:HE1	76:Ae:158:LYS:HD2	1.68	0.57
12:BL:106:LEU:O	12:BL:156:SER:HA	2.04	0.57
25:Ba:123:LEU:HD22	25:Ba:220:LEU:HD21	1.87	0.57
36:Bk:127:MET:HB2	36:Bk:154:GLU:HB3	1.86	0.57
46:Bw:243:GLU:HA	46:Bw:350:VAL:HG21	1.86	0.57
46:Bw:308:GLN:HG3	88:BA:748:A:H8	1.69	0.57
26:Bb:90:ILE:HA	40:Bo:113:LYS:HB2	1.86	0.57
10:BJ:128:ASN:ND2	88:BA:551:A:OP1	2.38	0.57
14:BO:118:ARG:HH21	14:BO:142:GLN:HG3	1.68	0.57
26:Bb:360:ARG:NH2	88:BA:1203:C:OP2	2.37	0.57
48:AA:948:U:H2'	48:AA:949:G:H8	1.69	0.57
78:Ag:99:MET:H	92:Ag:500:GTP:HN1	1.53	0.57
46:Bw:53:ALA:O	46:Bw:62:ARG:NH2	2.38	0.57
82:Ak:151:ILE:HG12	82:Ak:177:VAL:HG22	1.86	0.57
24:BY:146:VAL:HG22	24:BY:153:ILE:HG22	1.86	0.56
25:Ba:125:LYS:HG3	25:Ba:253:LEU:HD11	1.87	0.56
35:Bj:257:LYS:HE2	35:Bj:273:ARG:HE	1.69	0.56
74:Ad:59:ARG:NH1	86:Ap:202:TRP:O	2.38	0.56
87:B9:68:VAL:HG12	88:BA:1289:U:H5''	1.86	0.56
87:B9:78:LEU:HD12	88:BA:495:A:H5''	1.87	0.56
57:AG:60:GLU:HA	57:AG:63:LYS:HD2	1.87	0.56
64:AP:111:ARG:NH2	86:Ap:233:GLU:O	2.36	0.56
4:B2:127:PRO:HB3	34:Bi:67:ILE:HD11	1.88	0.56
5:BB:41:G:OP1	18:BS:85:ARG:NH2	2.39	0.56
5:BB:44:U:H5''	29:Bd:119:LYS:HD2	1.88	0.56
11:BK:156:VAL:HG11	11:BK:159:LEU:HD13	1.86	0.56
14:BO:145:VAL:HG11	19:BT:160:VAL:HG11	1.87	0.56
21:BV:176:MET:HA	21:BV:186:ARG:O	2.05	0.56
25:Ba:200:ARG:HE	25:Ba:233:LYS:HD2	1.69	0.56
26:Bb:93:PRO:HB3	40:Bo:118:GLN:HB3	1.86	0.56
46:Bw:370:THR:HG22	46:Bw:383:ARG:HG3	1.85	0.56
48:AA:11:G:H1	48:AA:524:U:H3	1.53	0.56
54:AC:148:LYS:HD2	85:Ao:140:LEU:HB3	1.88	0.56
58:AI:115:GLY:HA3	59:AJ:84:ASP:HB2	1.86	0.56
66:AR:66:CYS:SG	66:AR:69:CYS:HB2	2.45	0.56
39:Bn:35:ARG:NH1	39:Bn:37:THR:O	2.38	0.56
28:Bc:113:TYR:OH	28:Bc:268:ARG:NH2	2.39	0.56
45:Bv:40:PRO:HG3	45:Bv:51:GLN:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:BA:53:U:O4	88:BA:62:C:N3	2.39	0.56
78:Ag:80:HIS:HB3	78:Ag:155:PRO:HG3	1.87	0.56
8:BF:142:ARG:NH2	88:BA:129:A:OP1	2.38	0.56
26:Bb:45:LEU:O	26:Bb:50:LYS:NZ	2.39	0.56
54:AC:92:LEU:HD11	54:AC:117:LEU:HD21	1.87	0.56
82:Ak:58:ARG:NH2	85:Ao:91:ASP:OD2	2.38	0.56
25:Ba:113:LEU:HD12	25:Ba:311:ALA:HB1	1.88	0.56
50:B5:91:ARG:NH1	88:BA:154:A:OP2	2.39	0.56
43:Bt:24:PRO:HD2	47:Bx:169:TRP:HB2	1.87	0.56
46:Bw:49:ALA:O	46:Bw:61:ARG:NH1	2.39	0.56
72:Ab:68:ASP:OD1	72:Ab:71:ARG:NH1	2.39	0.56
7:BE:97:VAL:O	7:BE:197:HIS:NE2	2.39	0.56
63:AO:92:ARG:HG2	63:AO:98:MET:HE1	1.86	0.56
82:Ak:171:ARG:O	82:Ak:220:ASN:ND2	2.38	0.56
48:AA:349:A:N3	48:AA:426:G:O2'	2.37	0.55
85:Ao:520:LYS:O	85:Ao:527:ARG:NH2	2.39	0.55
18:BS:104:SER:O	18:BS:135:ARG:NH1	2.39	0.55
27:B3:134:MET:HE1	40:Bo:78:VAL:HG21	1.87	0.55
29:Bd:114:ARG:HG2	35:Bj:73:LEU:HD13	1.88	0.55
22:BW:105:GLU:OE1	22:BW:116:LYS:NZ	2.39	0.55
48:AA:194:U:O2	64:AP:43:ARG:NH1	2.39	0.55
52:B7:82:ILE:HG22	52:B7:86:MET:HE2	1.87	0.55
48:AA:822:A:N7	57:AG:177:ARG:NH1	2.55	0.55
57:AG:65:GLU:O	57:AG:69:LYS:HB2	2.06	0.55
4:B2:145:ASP:OD2	23:BX:21:ARG:NH1	2.38	0.55
12:BL:107:GLU:HB2	12:BL:197:ALA:HB3	1.87	0.55
15:BP:164:ILE:HG12	15:BP:174:VAL:HG11	1.87	0.55
35:Bj:198:ASN:C	35:Bj:198:ASN:HD22	2.13	0.55
29:Bd:75:LEU:HD13	36:Bk:203:GLU:HG3	1.87	0.55
34:Bi:240:ARG:HH12	34:Bi:274:GLN:HB3	1.72	0.55
48:AA:673:A:H1'	62:AN:127:MET:HE3	1.89	0.55
10:BJ:95:MET:HB3	10:BJ:156:SER:HB2	1.88	0.55
35:Bj:52:CYS:HB3	35:Bj:234:PHE:O	2.07	0.55
64:AP:20:ARG:NH2	64:AP:41:CYS:SG	2.79	0.55
73:Ac:132:ARG:NH1	73:Ac:136:LEU:O	2.40	0.55
15:BP:119:THR:O	15:BP:123:ASN:ND2	2.36	0.55
18:BS:51:ARG:NH1	26:Bb:228:PRO:O	2.40	0.55
28:Bc:141:ARG:HH21	28:Bc:262:GLU:HG2	1.72	0.55
32:Bg:27:GLN:HE21	32:Bg:80:LEU:HD23	1.71	0.55
32:Bg:36:ASP:HB3	88:BA:615:G:H5''	1.89	0.55
59:AJ:78:VAL:HG22	59:AJ:172:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:Ak:88:ARG:NH1	82:Ak:98:PRO:O	2.39	0.55
83:Am:29:LEU:HB2	83:Am:113:ASN:HD22	1.72	0.55
6:BD:127:VAL:HG22	6:BD:143:VAL:HG22	1.89	0.55
43:Bt:78:GLN:OE1	88:BA:391:A:N6	2.40	0.55
50:B5:169:ASP:HA	50:B5:172:LYS:HE3	1.90	0.55
54:AC:123:VAL:O	54:AC:157:THR:HA	2.07	0.55
78:Ag:160:TRP:O	78:Ag:179:GLN:NE2	2.39	0.55
29:Bd:80:GLN:OE1	36:Bk:201:ARG:NH2	2.38	0.54
30:Be:127:GLN:HB3	30:Be:130:PRO:HD2	1.89	0.54
48:AA:328:A:H2'	48:AA:329:A:H8	1.72	0.54
59:AJ:160:ILE:HG22	59:AJ:170:MET:HE1	1.88	0.54
62:AN:41:ARG:NH1	80:Ai:48:THR:O	2.40	0.54
77:Af:134:LYS:HG3	77:Af:173:LEU:HD11	1.88	0.54
15:BP:72:THR:OG1	15:BP:77:ARG:NH2	2.41	0.54
25:Ba:106:VAL:HA	25:Ba:221:GLN:O	2.07	0.54
34:Bi:125:ILE:HG12	34:Bi:252:LEU:HD11	1.89	0.54
43:Bt:9:ARG:NH2	88:BA:564:A:OP1	2.38	0.54
7:BE:50:ASP:OD1	17:BR:139:ARG:NH2	2.40	0.54
9:BI:78:ARG:NH1	88:BA:49:A:OP1	2.40	0.54
15:BP:133:LYS:HE2	88:BA:225:C:H5'	1.87	0.54
22:BW:77:GLN:H	22:BW:171:HIS:HD2	1.56	0.54
27:B3:110:LEU:O	27:B3:114:LYS:HB3	2.07	0.54
33:Bh:33:LYS:NZ	88:BA:106:C:OP1	2.40	0.54
48:AA:492:U:OP1	84:An:139:ASN:ND2	2.37	0.54
50:B5:90:ASN:OD1	50:B5:93:ARG:NH2	2.41	0.54
83:Am:36:ARG:NH2	83:Am:92:ASN:OD1	2.40	0.54
15:BP:30:ASN:ND2	88:BA:213:U:O2'	2.35	0.54
20:BU:34:ARG:NH2	88:BA:1014:A:OP1	2.39	0.54
32:Bg:133:PHE:HZ	33:Bh:261:SER:HB2	1.73	0.54
33:Bh:151:GLU:HG2	33:Bh:232:TRP:HE1	1.72	0.54
48:AA:115:A:OP1	63:AO:203:ARG:NH2	2.41	0.54
71:Aa:224:ARG:NH1	71:Aa:256:GLN:O	2.41	0.54
73:Ac:78:PHE:HB2	73:Ac:86:VAL:HB	1.89	0.54
16:BQ:67:LYS:NZ	88:BA:445:A:OP2	2.40	0.54
21:BV:198:ARG:NH2	32:Bg:13:SER:OG	2.40	0.54
27:B3:133:ASP:OD2	27:B3:148:ARG:NH1	2.41	0.54
29:Bd:146:ALA:HB1	35:Bj:212:HIS:CE1	2.43	0.54
37:Bl:143:VAL:HG12	43:Bt:88:LEU:HD23	1.90	0.54
48:AA:619:C:H1'	59:AJ:124:VAL:HG23	1.88	0.54
85:Ao:305:ALA:HB2	85:Ao:319:ILE:HD11	1.90	0.54
23:BX:79:ARG:NH2	88:BA:700:A:OP2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AA:618:G:H21	48:AA:687:A:H62	1.56	0.54
54:AC:132:PHE:HD2	85:Ao:95:LEU:HD21	1.73	0.54
76:Ae:355:VAL:H	86:Ap:221:GLN:HE22	1.55	0.54
22:BW:82:LYS:HD3	22:BW:147:ARG:HB3	1.89	0.54
13:BN:71:LYS:NZ	88:BA:573:A:OP2	2.40	0.54
19:BT:121:THR:HG22	19:BT:171:ILE:HG12	1.90	0.54
26:Bb:364:ARG:NH1	75:B8:146:GLU:OE2	2.40	0.54
27:B3:75:THR:HB	27:B3:83:LYS:HG2	1.89	0.54
35:Bj:78:GLU:O	35:Bj:82:SER:HB3	2.08	0.54
48:AA:551:G:N2	48:AA:778:G:O2'	2.41	0.54
88:BA:978:G:H4'	88:BA:1429:C:H4'	1.89	0.54
33:Bh:97:TYR:HB2	33:Bh:181:SER:HA	1.90	0.54
35:Bj:47:LEU:HA	35:Bj:230:LYS:HE3	1.90	0.54
55:AE:88:SER:N	62:AN:28:TYR:O	2.41	0.54
86:Ap:53:ASP:O	86:Ap:118:ARG:NH1	2.40	0.54
7:BE:201:GLY:H	7:BE:273:VAL:HG13	1.72	0.53
8:BF:249:ASN:ND2	39:Bn:55:GLY:O	2.40	0.53
78:Ag:162:LYS:HD3	78:Ag:315:LEU:HD21	1.90	0.53
3:B1:213:GLU:OE1	25:Ba:63:LYS:NZ	2.40	0.53
10:BJ:94:ARG:HE	10:BJ:158:GLU:H	1.55	0.53
26:Bb:330:VAL:HA	26:Bb:334:LEU:HD13	1.90	0.53
27:B3:104:PRO:HA	27:B3:107:ASN:HB2	1.89	0.53
88:BA:869:G:O2'	88:BA:966:U:OP2	2.26	0.53
5:BB:23:A:OP2	26:Bb:106:ARG:NH1	2.41	0.53
7:BE:133:THR:HB	7:BE:144:ALA:HB3	1.90	0.53
48:AA:405:G:N1	48:AA:452:C:O2'	2.38	0.53
68:AV:6:G:H1	68:AV:62:C:H42	1.54	0.53
71:Aa:229:PRO:HB2	71:Aa:231:ILE:HG22	1.90	0.53
1:CL:40:LEU:HB3	1:FL:72:ALA:HA	1.90	0.53
16:BQ:118:MET:HE1	16:BQ:167:CYS:HB2	1.91	0.53
18:BS:112:ILE:HG22	18:BS:116:LEU:HD22	1.90	0.53
20:BU:52:LYS:NZ	88:BA:164:A:OP1	2.38	0.53
21:BV:115:GLU:HG2	32:Bg:19:LEU:HD11	1.90	0.53
25:Ba:240:ALA:H	25:Ba:358:GLN:HE22	1.56	0.53
45:Bv:117:ARG:NH2	51:B6:25:GLY:O	2.41	0.53
55:AE:306:LYS:HB2	55:AE:333:TYR:HB3	1.89	0.53
88:BA:198:U:H2'	88:BA:199:A:H8	1.73	0.53
88:BA:296:C:OP2	91:BA:1793:SPM:N1	2.41	0.53
3:B1:167:LEU:HD21	3:B1:202:GLU:HB3	1.90	0.53
23:BX:68:VAL:HG22	23:BX:97:VAL:HG12	1.90	0.53
32:Bg:37:ALA:O	32:Bg:44:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:AE:95:ALA:HB2	80:Ai:74:GLU:HB3	1.90	0.53
76:Ae:439:GLU:HG3	76:Ae:442:ARG:HH12	1.72	0.53
81:Aj:129:ARG:NH2	81:Aj:203:TYR:OH	2.40	0.53
12:BL:108:VAL:HG12	12:BL:196:VAL:HG22	1.91	0.53
26:Bb:87:ARG:NH2	26:Bb:153:GLU:OE2	2.42	0.53
84:An:163:ARG:HH22	88:BA:971:A:H4'	1.74	0.53
85:Ao:423:MET:HE1	85:Ao:435:ALA:HA	1.90	0.53
88:BA:789:A:N6	88:BA:1000:A:O2'	2.42	0.53
88:BA:1140:A:H2'	88:BA:1141:A:H8	1.74	0.53
35:Bj:50:ALA:HA	35:Bj:175:GLN:HA	1.89	0.53
78:Ag:101:ARG:HG2	78:Ag:103:PRO:HD2	1.90	0.53
85:Ao:608:ILE:HD13	85:Ao:640:PHE:HB3	1.90	0.53
13:BN:115:ASN:HB2	88:BA:175:C:H5''	1.90	0.53
19:BT:122:ALA:O	19:BT:170:ARG:NH1	2.42	0.53
35:Bj:185:ARG:NH2	35:Bj:189:GLU:OE2	2.40	0.53
35:Bj:211:GLY:HA3	35:Bj:233:PHE:HB2	1.91	0.53
59:AJ:92:GLU:OE2	59:AJ:141:ARG:NH1	2.40	0.53
76:Ae:272:GLY:HA3	76:Ae:296:LEU:HD21	1.91	0.53
81:Aj:64:LEU:HD23	81:Aj:134:VAL:HG13	1.90	0.53
6:BD:142:LEU:HD21	6:BD:149:LYS:HD3	1.89	0.53
52:B7:60:ASN:OD1	52:B7:63:ARG:NH1	2.42	0.53
56:AF:27:GLU:OE2	74:Ad:170:ARG:NH1	2.41	0.53
19:BT:252:GLU:OE1	19:BT:255:ARG:NH2	2.41	0.53
30:Be:32:LYS:NZ	88:BA:35:A:OP1	2.41	0.53
85:Ao:580:ASN:HA	85:Ao:613:LEU:HD13	1.90	0.53
26:Bb:175:VAL:HB	26:Bb:187:VAL:HB	1.90	0.52
63:AO:144:MET:HE1	63:AO:150:ASP:HB3	1.91	0.52
2:B0:88:CYS:SG	88:BA:1207:C:O2'	2.67	0.52
13:BN:28:PRO:HB3	13:BN:65:ILE:HD11	1.92	0.52
15:BP:284:LYS:NZ	37:Bl:41:SER:OG	2.42	0.52
19:BT:181:LYS:HD2	19:BT:217:VAL:HG22	1.91	0.52
48:AA:117:C:OP1	84:An:175:ARG:NH2	2.41	0.52
73:Ac:139:CYS:HB3	73:Ac:141:CYS:H	1.74	0.52
13:BN:75:LYS:NZ	88:BA:572:A:OP2	2.42	0.52
21:BV:166:GLU:HB3	21:BV:196:VAL:HB	1.92	0.52
36:Bk:94:HIS:ND1	36:Bk:154:GLU:OE2	2.40	0.52
48:AA:714:U:H2'	48:AA:715:G:H8	1.74	0.52
81:Aj:65:LEU:HD13	81:Aj:68:LEU:HD23	1.91	0.52
82:Ak:120:ALA:O	82:Ak:124:HIS:ND1	2.34	0.52
88:BA:1158:C:O2'	88:BA:1251:C:OP2	2.27	0.52
7:BE:206:VAL:O	7:BE:267:THR:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BL:311:ASP:O	12:BL:315:ASN:HA	2.09	0.52
16:BQ:73:ARG:NH1	88:BA:439:A:OP1	2.38	0.52
23:BX:71:ARG:NH1	23:BX:73:GLN:OE1	2.40	0.52
58:AI:110:TYR:HD2	58:AI:111:LEU:HD22	1.75	0.52
59:AJ:75:ARG:NH1	59:AJ:144:GLU:OE1	2.43	0.52
85:Ao:579:LEU:HD12	85:Ao:599:LEU:HD23	1.91	0.52
19:BT:262:GLN:HB3	19:BT:265:LEU:HD23	1.91	0.52
48:AA:37:A:OP1	73:Ac:162:LYS:NZ	2.42	0.52
51:B6:50:VAL:HG12	51:B6:52:LYS:HG2	1.92	0.52
58:AI:365:MET:HG3	58:AI:370:LEU:HB2	1.91	0.52
86:Ap:225:ARG:NH2	86:Ap:226:GLU:O	2.43	0.52
88:BA:790:A:N6	88:BA:1000:A:O2'	2.42	0.52
11:BK:85:PRO:O	11:BK:124:LYS:NZ	2.43	0.52
13:BN:10:GLN:NE2	22:BW:201:LEU:O	2.42	0.52
18:BS:91:GLU:HG3	18:BS:106:SER:HB3	1.92	0.52
27:B3:59:ASP:O	43:Bt:51:ARG:NH2	2.42	0.52
64:AP:54:TYR:HD1	64:AP:66:VAL:HG22	1.74	0.52
10:BJ:140:TYR:HB3	10:BJ:143:LEU:HD12	1.91	0.52
13:BN:112:LEU:HD13	13:BN:121:MET:HG3	1.91	0.52
21:BV:76:GLU:OE2	21:BV:80:HIS:NE2	2.42	0.52
26:Bb:308:GLN:O	40:Bo:113:LYS:NZ	2.42	0.52
48:AA:164:C:OP1	81:Aj:19:ARG:NH2	2.43	0.52
58:AI:155:LYS:NZ	58:AI:218:ASP:OD2	2.43	0.52
59:AJ:96:VAL:HG22	59:AJ:106:ILE:HD11	1.92	0.52
76:Ae:208:MET:HG3	76:Ae:247:SER:HA	1.92	0.52
88:BA:52:A:O2'	88:BA:349:A:N3	2.42	0.52
88:BA:1292:A:N6	88:BA:1304:G:O2'	2.43	0.52
17:BR:10:SER:HB3	88:BA:788:A:H3'	1.92	0.52
28:Bc:177:CYS:HA	28:Bc:293:PHE:O	2.09	0.52
34:Bi:88:TYR:OH	34:Bi:108:ARG:NH1	2.38	0.52
44:Bu:71:ILE:HG21	44:Bu:150:LEU:HD22	1.91	0.52
48:AA:289:G:O6	61:AL:31:ALA:N	2.43	0.52
8:BF:147:ARG:NH2	88:BA:130:A:OP1	2.43	0.52
24:BY:49:ILE:O	24:BY:81:ARG:NH2	2.43	0.52
30:Be:21:TRP:O	30:Be:32:LYS:NZ	2.42	0.52
32:Bg:74:ARG:NH2	88:BA:618:A:OP2	2.42	0.52
71:Aa:154:LEU:HD12	71:Aa:260:ASP:HB3	1.91	0.52
82:Ak:55:LEU:HD12	82:Ak:56:PRO:HD2	1.92	0.52
43:Bt:9:ARG:HD2	88:BA:568:C:H5''	1.90	0.52
78:Ag:161:VAL:HG21	78:Ag:266:ALA:HB1	1.91	0.52
4:B2:92:LEU:HB3	4:B2:147:VAL:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BD:290:LEU:HD12	6:BD:291:PRO:HD2	1.91	0.51
25:Ba:380:GLN:HB3	25:Ba:410:THR:HG22	1.91	0.51
64:AP:102:MET:SD	74:Ad:60:TYR:OH	2.61	0.51
74:Ad:112:GLU:OE2	74:Ad:115:ARG:NH2	2.43	0.51
85:Ao:407:ARG:NH1	85:Ao:408:PHE:O	2.43	0.51
14:BO:55:PRO:HB3	14:BO:77:ILE:HG12	1.93	0.51
26:Bb:367:ASP:OD1	75:B8:179:LYS:NZ	2.42	0.51
58:AI:256:GLN:HE22	58:AI:371:LEU:HB3	1.76	0.51
88:BA:73:A:HO2'	88:BA:224:A:HO2'	1.58	0.51
88:BA:220:G:H1'	88:BA:231:C:H1'	1.91	0.51
3:B1:168:ARG:HH22	25:Ba:53:PRO:HB2	1.75	0.51
4:B2:93:ARG:HH21	4:B2:150:GLU:HG3	1.76	0.51
20:BU:105:LEU:HD13	20:BU:109:GLU:HG3	1.92	0.51
26:Bb:214:TRP:HB2	26:Bb:240:ILE:HB	1.91	0.51
46:Bw:86:MET:O	46:Bw:274:ASN:ND2	2.43	0.51
76:Ae:204:VAL:HG13	76:Ae:221:LEU:HD23	1.93	0.51
6:BD:133:ASP:OD2	6:BD:136:ARG:NH1	2.43	0.51
46:Bw:291:THR:HG22	46:Bw:352:GLN:HB2	1.92	0.51
48:AA:386:U:O2'	56:AF:93:ILE:O	2.28	0.51
81:Aj:171:ARG:HD2	81:Aj:175:LEU:HD13	1.91	0.51
87:B9:69:LEU:HD22	87:B9:87:ILE:HG12	1.93	0.51
5:BB:73:A:N3	35:Bj:268:TYR:OH	2.44	0.51
15:BP:33:SER:O	88:BA:234:G:N2	2.42	0.51
25:Ba:209:LEU:O	25:Ba:223:HIS:HA	2.10	0.51
50:B5:93:ARG:NH2	88:BA:642:G:OP1	2.42	0.51
57:AG:157:GLY:O	57:AG:171:PRO:HA	2.09	0.51
59:AJ:76:LEU:HD22	59:AJ:145:LEU:HD12	1.91	0.51
73:Ac:36:THR:HA	73:Ac:45:ARG:HD3	1.91	0.51
88:BA:993:U:H2'	88:BA:994:A:H8	1.76	0.51
13:BN:71:LYS:O	13:BN:75:LYS:HB3	2.11	0.51
41:Bp:18:VAL:HG22	41:Bp:64:VAL:HG23	1.93	0.51
49:B4:58:VAL:HG12	49:B4:64:THR:HG22	1.93	0.51
51:B6:40:LYS:NZ	51:B6:42:THR:OG1	2.43	0.51
53:AB:93:LYS:HE2	77:Af:149:GLU:HB3	1.91	0.51
54:AC:73:THR:HG22	54:AC:79:GLU:HG2	1.92	0.51
58:AI:286:VAL:HG23	58:AI:329:MET:HG2	1.91	0.51
63:AO:176:TYR:HB2	65:AQ:89:GLY:HA3	1.92	0.51
85:Ao:282:TYR:OH	85:Ao:325:GLN:OE1	2.28	0.51
88:BA:975:G:O2'	88:BA:977:G:OP2	2.29	0.51
24:BY:25:ARG:HB3	24:BY:28:SER:HB3	1.93	0.51
41:Bp:16:VAL:HB	41:Bp:51:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AA:640:A:OP1	55:AE:242:ARG:NH1	2.44	0.51
53:AB:133:HIS:HB3	72:Ab:34:ILE:HD13	1.91	0.51
53:AB:196:HIS:NE2	53:AB:239:ASP:O	2.43	0.51
55:AE:103:LEU:HD11	55:AE:123:ARG:HB2	1.93	0.51
88:BA:987:G:N2	88:BA:991:C:O2'	2.43	0.51
48:AA:814:A:OP2	58:AI:378:ARG:NH1	2.44	0.51
10:BJ:113:ARG:HH11	10:BJ:123:MET:HG3	1.76	0.51
11:BK:20:ILE:HB	11:BK:70:ILE:HB	1.93	0.51
17:BR:41:ARG:HG3	17:BR:125:GLU:HB3	1.92	0.51
25:Ba:229:ARG:HH21	25:Ba:288:PRO:HG2	1.75	0.51
29:Bd:136:ILE:HD12	36:Bk:173:ILE:HG13	1.92	0.51
1:HL:76:LEU:HA	1:HL:79:ILE:HG12	1.92	0.51
35:Bj:152:LYS:HB2	35:Bj:157:LEU:HD11	1.92	0.51
50:B5:95:ARG:NH1	88:BA:157:A:OP2	2.43	0.51
78:Ag:260:ALA:HA	78:Ag:306:VAL:O	2.11	0.51
86:Ap:110:ASP:HB3	86:Ap:113:LEU:HD13	1.92	0.51
7:BE:244:SER:HB2	7:BE:251:VAL:HG23	1.93	0.50
38:Bm:74:HIS:HA	38:Bm:77:GLU:HG2	1.93	0.50
46:Bw:195:ASP:HB2	46:Bw:234:GLN:HB2	1.93	0.50
56:AF:40:GLU:HB3	56:AF:65:LEU:HB3	1.92	0.50
88:BA:150:A:N3	88:BA:198:U:O2'	2.38	0.50
46:Bw:221:ASP:OD2	46:Bw:224:ARG:NH2	2.44	0.50
53:AB:220:GLY:HA3	53:AB:231:ILE:HD13	1.93	0.50
55:AE:242:ARG:HD2	55:AE:258:ILE:HD11	1.92	0.50
81:Aj:64:LEU:HD13	81:Aj:80:VAL:HG11	1.93	0.50
88:BA:164:A:N1	88:BA:1030:G:N2	2.59	0.50
15:BP:56:GLU:OE1	88:BA:377:G:O2'	2.30	0.50
22:BW:151:LEU:HB2	22:BW:167:LYS:HB2	1.93	0.50
23:BX:86:ARG:HH12	30:Be:18:MET:HB2	1.77	0.50
28:Bc:175:ALA:HB2	28:Bc:316:SER:HB2	1.92	0.50
76:Ae:204:VAL:HG22	76:Ae:221:LEU:HG	1.93	0.50
88:BA:1418:G:N2	88:BA:1421:A:OP2	2.39	0.50
5:BB:35:G:N2	36:Bk:124:SER:O	2.44	0.50
15:BP:202:LYS:HD2	15:BP:263:ARG:HD2	1.93	0.50
16:BQ:124:VAL:HG12	16:BQ:158:ARG:HE	1.76	0.50
78:Ag:283:PRO:HB2	78:Ag:293:ARG:HH22	1.77	0.50
8:BF:255:LYS:NZ	39:Bn:51:ARG:O	2.44	0.50
17:BR:88:LYS:O	17:BR:92:VAL:HB	2.12	0.50
24:BY:41:ARG:NH1	88:BA:135:G:O6	2.43	0.50
48:AA:407:U:O2'	48:AA:950:U:O2	2.28	0.50
52:B7:59:SER:OG	88:BA:317:A:OP1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Aj:143:PRO:HD2	81:Aj:146:GLU:HB2	1.93	0.50
7:BE:175:LYS:HB2	7:BE:296:LEU:HD12	1.93	0.50
8:BF:279:ARG:NH1	8:BF:280:TYR:O	2.44	0.50
35:Bj:145:ASP:OD1	35:Bj:145:ASP:N	2.44	0.50
11:BK:32:GLY:O	11:BK:36:GLY:N	2.45	0.50
48:AA:29:A:H2'	48:AA:30:A:H8	1.77	0.50
48:AA:65:C:O2'	48:AA:157:A:N6	2.45	0.50
51:B6:21:MET:HE1	51:B6:27:GLY:HA2	1.92	0.50
56:AF:36:VAL:HG23	74:Ad:168:ILE:HB	1.92	0.50
71:Aa:205:LYS:NZ	86:Ap:185:SER:O	2.45	0.50
76:Ae:290:LEU:HG	76:Ae:292:GLN:H	1.77	0.50
5:BB:32:A:OP1	49:B4:43:ARG:NE	2.42	0.50
15:BP:55:GLY:O	15:BP:59:ARG:NH1	2.44	0.50
39:Bn:94:LYS:NZ	39:Bn:102:MET:SD	2.85	0.50
42:Bq:123:LYS:HG3	88:BA:531:G:H5''	1.92	0.50
53:AB:164:TYR:HD2	58:AI:149:PHE:HA	1.76	0.50
88:BA:53:U:N3	88:BA:62:C:O2	2.41	0.50
88:BA:218:A:N6	88:BA:229:A:O4'	2.44	0.50
88:BA:1351:U:H2'	88:BA:1353:C:H5''	1.94	0.50
1:DL:90:LEU:HD22	10:BJ:214:LEU:HD13	1.92	0.50
12:BL:219:LYS:HB2	88:BA:1378:U:H3	1.77	0.50
24:BY:41:ARG:NH2	88:BA:135:G:N7	2.45	0.50
48:AA:736:A:O3'	78:Ag:165:ARG:NH2	2.45	0.50
78:Ag:187:LEU:HD22	78:Ag:225:VAL:HG23	1.93	0.50
88:BA:1026:A:O2'	88:BA:1277:G:N2	2.40	0.50
25:Ba:135:LYS:HD3	25:Ba:239:VAL:HG23	1.94	0.49
32:Bg:26:LEU:HD22	32:Bg:105:ALA:HA	1.92	0.49
32:Bg:73:PRO:HB2	32:Bg:89:ILE:HG13	1.94	0.49
48:AA:56:U:O2	48:AA:198:C:O2'	2.30	0.49
48:AA:83:C:O2'	48:AA:99:A:N6	2.45	0.49
57:AG:148:ALA:O	57:AG:152:CYS:HB2	2.12	0.49
61:AL:62:VAL:HA	61:AL:83:VAL:HG12	1.94	0.49
76:Ae:238:TRP:HZ2	76:Ae:282:ALA:HB3	1.77	0.49
88:BA:565:A:N6	88:BA:1314:U:OP1	2.45	0.49
39:Bn:97:MET:HE3	88:BA:71:U:H5'	1.93	0.49
3:B1:6:VAL:HG12	88:BA:21:C:H41	1.76	0.49
33:Bh:245:LEU:HD22	33:Bh:250:ILE:HB	1.93	0.49
35:Bj:51:LEU:HD12	35:Bj:188:ALA:HB1	1.94	0.49
47:Bx:69:GLN:O	47:Bx:74:ARG:NH1	2.46	0.49
54:AC:77:ASP:HB2	59:AJ:138:THR:HG21	1.92	0.49
67:AU:43:ARG:NH2	67:AU:44:TYR:OH	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:BA:776:C:O2'	88:BA:778:A:N7	2.45	0.49
88:BA:1187:U:O2'	88:BA:1189:U:OP2	2.29	0.49
88:BA:1291:U:OP2	88:BA:1299:C:N4	2.45	0.49
16:BQ:81:GLU:O	16:BQ:123:ARG:NH2	2.43	0.49
22:BW:81:SER:O	22:BW:85:MET:HB2	2.12	0.49
34:Bi:181:VAL:HG12	34:Bi:224:ILE:HA	1.95	0.49
48:AA:386:U:H4'	56:AF:94:VAL:HG12	1.95	0.49
56:AF:92:ASN:HD22	66:AR:118:LEU:HG	1.77	0.49
66:AR:73:VAL:HG21	66:AR:107:GLU:HB3	1.93	0.49
67:AU:75:LEU:HB3	83:Am:107:LEU:HD11	1.95	0.49
71:Aa:179:VAL:HG22	71:Aa:196:VAL:HG22	1.93	0.49
5:BB:9:A:OP1	5:BB:47:A:O2'	2.30	0.49
18:BS:80:ARG:NH2	18:BS:95:GLU:OE2	2.45	0.49
25:Ba:166:SER:O	46:Bw:281:LYS:NZ	2.37	0.49
40:Bo:23:ALA:N	88:BA:482:G:OP1	2.45	0.49
48:AA:495:U:H2'	48:AA:496:A:H8	1.78	0.49
81:Aj:170:LEU:HA	81:Aj:173:MET:HE2	1.94	0.49
22:BW:92:ILE:HA	22:BW:95:MET:HE2	1.95	0.49
48:AA:882:A:H5'	76:Ae:108:SER:HB3	1.94	0.49
55:AE:374:ARG:HB2	55:AE:377:CYS:HB2	1.93	0.49
12:BL:116:GLU:OE2	12:BL:179:ARG:NE	2.45	0.49
13:BN:109:TYR:O	13:BN:118:ARG:NH1	2.46	0.49
39:Bn:89:GLN:NE2	75:B8:102:GLY:O	2.45	0.49
58:AI:90:ASN:ND2	82:Ak:64:VAL:O	2.45	0.49
85:Ao:294:VAL:HA	85:Ao:326:MET:HE1	1.95	0.49
9:BI:55:ILE:HB	9:BI:84:GLU:HB3	1.94	0.49
16:BQ:101:HIS:NE2	88:BA:1307:A:O3'	2.46	0.49
25:Ba:174:GLU:HA	25:Ba:296:SER:HB2	1.94	0.49
25:Ba:299:LEU:HB2	25:Ba:302:ARG:HG2	1.93	0.49
31:Bf:128:GLN:OE1	31:Bf:132:ARG:NH1	2.46	0.49
35:Bj:74:LEU:HD22	49:B4:43:ARG:HB3	1.93	0.49
36:Bk:119:ILE:HD11	36:Bk:166:PHE:HE2	1.77	0.49
44:Bu:110:ILE:O	44:Bu:115:ARG:NH2	2.46	0.49
82:Ak:158:TYR:HE1	82:Ak:169:LYS:HB2	1.78	0.49
48:AA:826:C:H2'	48:AA:827:A:H8	1.77	0.49
65:AQ:75:LYS:O	65:AQ:78:LYS:NZ	2.46	0.49
24:BY:79:VAL:HG12	24:BY:86:VAL:HG12	1.95	0.49
44:Bu:175:ARG:NH1	88:BA:1218:U:OP2	2.46	0.49
55:AE:305:MET:HA	55:AE:333:TYR:O	2.13	0.49
7:BE:105:GLY:HA3	19:BT:91:LYS:HD2	1.95	0.48
7:BE:175:LYS:HD3	7:BE:296:LEU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BF:241:ASN:OD1	45:Bv:25:TYR:N	2.46	0.48
15:BP:65:LEU:HD21	75:B8:160:LYS:HB3	1.94	0.48
48:AA:51:G:OP1	74:Ad:36:LYS:NZ	2.45	0.48
57:AG:240:ARG:NH2	83:Am:44:THR:O	2.45	0.48
64:AP:30:PRO:HD2	64:AP:57:LEU:HD11	1.94	0.48
73:Ac:52:ILE:HD13	73:Ac:66:MET:HE1	1.93	0.48
75:B8:122:TRP:NE1	75:B8:159:ASP:OD1	2.45	0.48
81:Aj:82:ARG:HB3	81:Aj:85:TRP:HE3	1.77	0.48
25:Ba:233:LYS:HA	25:Ba:286:PRO:HD2	1.96	0.48
28:Bc:218:VAL:HG21	28:Bc:251:LEU:HD12	1.95	0.48
35:Bj:162:ARG:HB3	35:Bj:251:HIS:HB2	1.95	0.48
46:Bw:99:ALA:HB3	46:Bw:102:ALA:HB2	1.94	0.48
71:Aa:116:ALA:HB3	71:Aa:118:GLN:HE22	1.78	0.48
10:BJ:95:MET:HG3	10:BJ:181:ILE:HG12	1.94	0.48
15:BP:47:ARG:NH1	88:BA:183:U:OP1	2.45	0.48
19:BT:118:ARG:HB2	19:BT:134:LEU:HD12	1.95	0.48
25:Ba:125:LYS:HG2	25:Ba:371:LYS:HG3	1.94	0.48
34:Bi:138:PRO:HB2	34:Bi:192:PRO:HG2	1.95	0.48
36:Bk:136:GLN:HG2	49:B4:79:PRO:HG3	1.96	0.48
56:AF:44:GLU:HA	56:AF:62:GLY:HA2	1.96	0.48
76:Ae:162:GLN:HA	76:Ae:191:PHE:HE1	1.78	0.48
88:BA:1195:A:N6	88:BA:1208:A:O2'	2.47	0.48
15:BP:284:LYS:NZ	37:Bl:44:GLU:OE2	2.37	0.48
25:Ba:115:GLU:HB3	25:Ba:118:LYS:HE2	1.96	0.48
34:Bi:90:PRO:HB2	34:Bi:269:TRP:HH2	1.79	0.48
48:AA:385:C:H1'	66:AR:117:ILE:HG21	1.94	0.48
68:AV:9:C:O2	68:AV:10:A:N6	2.46	0.48
71:Aa:177:LYS:HB3	71:Aa:199:PRO:HD3	1.95	0.48
21:BV:121:GLU:OE1	21:BV:192:ASN:ND2	2.46	0.48
28:Bc:80:LYS:NZ	28:Bc:117:THR:O	2.44	0.48
28:Bc:211:LEU:O	28:Bc:269:THR:OG1	2.26	0.48
48:AA:405:G:H1	48:AA:452:C:HO2'	1.59	0.48
48:AA:763:A:OP1	62:AN:51:ARG:NH1	2.45	0.48
71:Aa:356:THR:HG22	71:Aa:357:GLU:HG3	1.96	0.48
85:Ao:118:LYS:HA	85:Ao:121:ILE:HD12	1.95	0.48
1:CL:40:LEU:HD21	1:EL:90:LEU:HD11	1.95	0.48
29:Bd:142:ALA:O	29:Bd:146:ALA:HB2	2.13	0.48
32:Bg:114:ARG:NH2	88:BA:169:U:OP2	2.47	0.48
34:Bi:108:ARG:HG3	34:Bi:193:GLN:HG2	1.94	0.48
44:Bu:141:TYR:HB2	44:Bu:144:ARG:HG3	1.96	0.48
86:Ap:189:PRO:HB3	86:Ap:193:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:BA:644:G:N2	88:BA:1008:A:OP2	2.41	0.48
1:EL:76:LEU:HA	1:EL:79:ILE:HD12	1.94	0.48
25:Ba:193:LEU:HA	46:Bw:184:VAL:HG12	1.96	0.48
26:Bb:236:LEU:HB3	26:Bb:252:CYS:HB3	1.95	0.48
48:AA:272:A:H4'	48:AA:274:A:H4'	1.96	0.48
65:AQ:28:VAL:HG21	65:AQ:66:LEU:HD21	1.96	0.48
78:Ag:328:LEU:HB3	78:Ag:332:GLY:HA3	1.95	0.48
80:Ai:13:ARG:HG2	80:Ai:23:ALA:HB1	1.95	0.48
88:BA:1230:U:H5'	88:BA:1231:U:H5'	1.96	0.48
3:B1:55:LYS:NZ	88:BA:80:A:OP2	2.46	0.48
24:BY:64:ILE:HD11	24:BY:88:VAL:HG21	1.96	0.48
46:Bw:211:ILE:HD11	46:Bw:221:ASP:HB3	1.96	0.48
48:AA:158:C:O3'	48:AA:172:A:N6	2.47	0.48
48:AA:512:A:H2'	48:AA:513:A:H8	1.77	0.48
12:BL:112:VAL:HB	12:BL:193:THR:HB	1.96	0.48
25:Ba:145:ASN:O	25:Ba:191:GLN:NE2	2.47	0.48
54:AC:73:THR:HG23	59:AJ:169:ALA:HB2	1.95	0.48
56:AF:36:VAL:HG12	56:AF:68:PHE:HB3	1.96	0.48
58:AI:345:VAL:HG12	58:AI:349:MET:HE2	1.95	0.48
84:An:159:GLU:OE1	84:An:163:ARG:NH2	2.47	0.48
7:BE:310:PHE:HE1	7:BE:313:ASN:HD21	1.62	0.48
15:BP:196:ARG:HD3	88:BA:93:U:H5'	1.96	0.48
24:BY:65:LEU:HD11	24:BY:121:LYS:HE2	1.96	0.48
26:Bb:27:ARG:N	88:BA:1168:A:N1	2.62	0.48
33:Bh:94:ASN:HD22	33:Bh:181:SER:HB2	1.79	0.48
36:Bk:125:TYR:HB2	36:Bk:197:ARG:HH12	1.79	0.48
48:AA:552:A:H2'	48:AA:553:G:H8	1.78	0.48
53:AB:78:PHE:HB3	53:AB:251:LEU:HD21	1.95	0.48
64:AP:36:ALA:HB2	64:AP:51:LEU:HD11	1.96	0.48
75:B8:142:ARG:NH1	88:BA:1193:C:OP2	2.46	0.48
81:Aj:87:TRP:O	86:Ap:218:ARG:NH2	2.46	0.48
82:Ak:55:LEU:HB3	85:Ao:93:PRO:HB3	1.95	0.48
88:BA:1278:C:H2'	88:BA:1279:G:H8	1.79	0.48
21:BV:108:HIS:ND1	88:BA:480:G:OP2	2.42	0.47
78:Ag:347:TYR:HB2	78:Ag:385:ARG:HB2	1.96	0.47
6:BD:178:ARG:NH1	6:BD:181:ASP:OD1	2.47	0.47
14:BO:43:ASN:HD21	14:BO:117:THR:HB	1.79	0.47
14:BO:86:ILE:HA	14:BO:105:VAL:HG12	1.95	0.47
15:BP:54:LYS:HD2	88:BA:184:U:H5''	1.95	0.47
21:BV:160:VAL:HG22	21:BV:199:ILE:HD11	1.95	0.47
24:BY:134:GLU:OE1	24:BY:148:THR:OG1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Bc:96:TYR:O	28:Bc:100:SER:HB3	2.13	0.47
32:Bg:65:VAL:HB	38:Bm:155:ILE:HG23	1.96	0.47
9:Bl:65:ALA:HB1	9:Bl:69:ARG:HB2	1.96	0.47
20:BU:85:ALA:O	20:BU:89:ASN:ND2	2.47	0.47
26:Bb:237:VAL:HG13	26:Bb:240:ILE:HD11	1.97	0.47
28:Bc:151:ILE:HG21	28:Bc:180:VAL:HG21	1.96	0.47
39:Bn:57:TYR:OH	45:Bv:28:ARG:O	2.30	0.47
48:AA:67:C:H5'	64:AP:42:PRO:HD3	1.97	0.47
75:B8:94:VAL:N	88:BA:86:U:OP1	2.47	0.47
78:Ag:364:TRP:NE1	78:Ag:394:CYS:O	2.46	0.47
88:BA:611:U:H2'	88:BA:612:A:H8	1.79	0.47
88:BA:669:C:H2'	88:BA:670:A:H8	1.79	0.47
8:BF:123:GLY:HA3	8:BF:142:ARG:HG2	1.96	0.47
25:Ba:272:ASP:OD1	25:Ba:272:ASP:N	2.47	0.47
37:Bl:110:ILE:HD12	37:Bl:147:LEU:HD23	1.97	0.47
46:Bw:91:TYR:HE2	46:Bw:223:LEU:HD22	1.77	0.47
48:AA:552:A:H2'	48:AA:553:G:C8	2.50	0.47
49:B4:57:LEU:HD12	49:B4:76:LEU:HD23	1.95	0.47
61:AL:55:ARG:HE	61:AL:58:LEU:HD21	1.80	0.47
85:Ao:536:MET:SD	85:Ao:581:TYR:OH	2.72	0.47
13:BN:122:MET:HE3	13:BN:122:MET:HB3	1.81	0.47
23:BX:16:GLN:NE2	23:BX:17:LEU:O	2.46	0.47
46:Bw:145:LEU:HD22	46:Bw:402:ASN:HA	1.96	0.47
12:BL:231:THR:O	88:BA:1396:C:N4	2.48	0.47
28:Bc:147:MET:HE2	28:Bc:277:VAL:HG22	1.94	0.47
34:Bi:94:ASP:HB2	34:Bi:269:TRP:HZ2	1.79	0.47
15:BP:115:PRO:HD3	15:BP:255:MET:HG2	1.97	0.47
28:Bc:111:ASP:OD2	28:Bc:215:THR:OG1	2.30	0.47
34:Bi:244:GLU:HG2	34:Bi:264:LYS:HE2	1.97	0.47
41:Bp:84:GLN:OE1	41:Bp:88:THR:OG1	2.32	0.47
48:AA:56:U:O2'	48:AA:198:C:O2	2.31	0.47
48:AA:568:G:H21	59:AJ:126:ILE:HD13	1.80	0.47
55:AE:191:ARG:NH2	86:Ap:80:ASN:OD1	2.48	0.47
58:AI:199:ARG:HH21	58:AI:202:ILE:HG12	1.80	0.47
59:AJ:80:VAL:HG12	59:AJ:170:MET:HB3	1.96	0.47
66:AR:75:TYR:HA	66:AR:81:LEU:HD11	1.95	0.47
67:AU:70:ARG:NH2	77:Af:152:SER:OG	2.48	0.47
82:Ak:252:GLU:HB2	82:Ak:303:ASN:HD21	1.80	0.47
88:BA:290:A:O2'	88:BA:794:A:OP1	2.33	0.47
88:BA:1404:G:OP2	88:BA:1404:G:N2	2.40	0.47
6:BD:95:GLY:HA2	6:BD:270:ARG:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BD:173:MET:SD	56:AF:24:ARG:NH1	2.88	0.47
10:BJ:51:THR:OG1	16:BQ:250:ARG:NH2	2.43	0.47
25:Ba:125:LYS:HE2	25:Ba:364:LEU:HD22	1.97	0.47
54:AC:72:HIS:HB3	54:AC:112:ARG:HG3	1.97	0.47
57:AG:174:LEU:HD22	57:AG:178:ARG:HG2	1.97	0.47
2:B0:86:ASN:C	2:B0:86:ASN:ND2	2.70	0.47
4:B2:185:GLN:NE2	23:BX:7:TYR:O	2.48	0.47
18:BS:115:HIS:CE1	26:Bb:131:PRO:HG2	2.50	0.47
25:Ba:210:SER:HB2	25:Ba:276:ASP:HB3	1.96	0.47
48:AA:728:U:H2'	48:AA:729:A:C8	2.50	0.47
60:AK:162:SER:HA	60:AK:165:LYS:HE2	1.96	0.47
88:BA:529:G:O2'	88:BA:548:A:N3	2.48	0.47
16:BQ:124:VAL:HA	16:BQ:158:ARG:HH21	1.80	0.47
41:Bp:8:LEU:HD13	41:Bp:95:GLN:HG3	1.97	0.47
66:AR:81:LEU:HB3	66:AR:112:ILE:HG12	1.97	0.47
78:Ag:133:LYS:NZ	92:Ag:500:GTP:O3G	2.46	0.47
88:BA:831:U:OP2	88:BA:836:A:N6	2.33	0.47
3:B1:173:ASP:HB3	3:B1:175:GLN:HG2	1.96	0.46
6:BD:149:LYS:HE2	25:Ba:114:LEU:HD21	1.97	0.46
46:Bw:55:SER:HB2	88:BA:659:U:H5''	1.97	0.46
46:Bw:236:ARG:HA	46:Bw:289:GLY:HA2	1.97	0.46
48:AA:545:C:H5''	57:AG:181:PHE:HE1	1.80	0.46
48:AA:647:A:N6	67:Au:80:ARG:O	2.47	0.46
85:Ao:248:GLU:O	85:Ao:252:ALA:HB3	2.15	0.46
3:B1:96:LYS:O	88:BA:60:U:O2'	2.31	0.46
30:Be:51:ILE:HG22	30:Be:53:GLU:H	1.80	0.46
46:Bw:335:MET:HE3	46:Bw:371:LEU:HD11	1.97	0.46
47:Bx:133:PRO:HD2	88:BA:1530:C:H1'	1.98	0.46
62:AN:126:ALA:HB1	62:AN:128:TRP:HZ3	1.80	0.46
6:BD:258:ILE:HG23	6:BD:263:ARG:HB3	1.97	0.46
7:BE:221:ARG:NH1	7:BE:257:MET:O	2.48	0.46
14:BO:34:LYS:HG2	14:BO:35:MET:HG2	1.97	0.46
16:BQ:223:MET:HE2	43:Bt:39:LEU:HD22	1.97	0.46
22:BW:155:ARG:HH11	22:BW:165:MET:HE2	1.80	0.46
26:Bb:179:VAL:HG21	44:Bu:188:ARG:HH12	1.80	0.46
38:Bm:114:PRO:HG2	38:Bm:117:ARG:HG3	1.95	0.46
73:Ac:86:VAL:HG22	74:Ad:106:MET:HE1	1.96	0.46
73:Ac:90:VAL:HG21	73:Ac:98:ILE:HD11	1.97	0.46
1:CL:54:LEU:HD13	10:BJ:204:GLN:HB3	1.97	0.46
7:BE:218:VAL:HB	7:BE:258:PRO:HG3	1.96	0.46
7:BE:221:ARG:HG3	7:BE:261:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BJ:47:LEU:O	10:BJ:51:THR:OG1	2.30	0.46
29:Bd:101:ARG:NH2	35:Bj:79:ILE:O	2.48	0.46
34:Bi:211:GLN:HA	34:Bi:248:PHE:O	2.15	0.46
48:AA:590:C:H2'	48:AA:591:A:H8	1.80	0.46
58:AI:270:PHE:HA	58:AI:286:VAL:O	2.14	0.46
58:AI:321:LEU:HD13	58:AI:357:VAL:HG21	1.97	0.46
4:B2:212:ARG:O	4:B2:216:GLU:HG2	2.14	0.46
26:Bb:121:ARG:NH2	29:Bd:112:GLU:OE1	2.42	0.46
38:Bm:143:GLU:O	38:Bm:147:SER:OG	2.29	0.46
58:AI:380:ARG:NH2	59:AJ:133:GLN:OE1	2.48	0.46
85:Ao:661:GLU:HG3	85:Ao:664:GLU:HB2	1.97	0.46
87:B9:85:TRP:H	87:B9:99:GLN:HG2	1.81	0.46
1:EL:76:LEU:HD11	1:HL:79:ILE:HG21	1.98	0.46
3:B1:10:LEU:HD21	88:BA:68:A:H62	1.80	0.46
21:BV:99:LEU:HD23	21:BV:142:ALA:HB2	1.98	0.46
25:Ba:163:LEU:O	46:Bw:281:LYS:NZ	2.42	0.46
56:AF:46:MET:HE2	67:AU:5:LEU:HD21	1.98	0.46
62:AN:92:VAL:HG23	62:AN:93:MET:HE2	1.97	0.46
88:BA:803:A:N3	88:BA:805:C:N4	2.62	0.46
88:BA:1266:U:H2'	88:BA:1267:A:H8	1.80	0.46
4:B2:175:PHE:O	4:B2:214:ARG:NH2	2.35	0.46
31:Bf:129:TYR:OH	31:Bf:133:ARG:NH1	2.49	0.46
35:Bj:202:ALA:HB2	35:Bj:238:LEU:HD23	1.97	0.46
35:Bj:216:LYS:HA	35:Bj:228:GLY:HA2	1.98	0.46
48:AA:314:A:O3'	48:AA:395:C:N4	2.49	0.46
48:AA:579:A:OP1	62:AN:96:ARG:NH1	2.49	0.46
53:AB:58:ARG:HA	53:AB:61:ILE:HG22	1.97	0.46
76:Ae:358:LEU:HB2	76:Ae:361:GLU:HG3	1.97	0.46
78:Ag:312:THR:OG1	92:Ag:500:GTP:O2G	2.31	0.46
12:BL:214:LEU:HD21	12:BL:263:MET:HE1	1.98	0.46
15:BP:282:ILE:HG13	37:Bl:44:GLU:HG2	1.97	0.46
20:BU:54:THR:HG21	21:BV:176:MET:H	1.79	0.46
26:Bb:239:ASN:OD1	26:Bb:275:GLN:NE2	2.42	0.46
28:Bc:156:LYS:HD2	28:Bc:159:TYR:HE1	1.81	0.46
31:Bf:49:LEU:HD23	31:Bf:60:CYS:HB3	1.97	0.46
33:Bh:73:GLN:O	33:Bh:77:HIS:ND1	2.38	0.46
36:Bk:101:ALA:HB1	49:B4:42:THR:HG23	1.98	0.46
53:AB:218:THR:HG23	53:AB:231:ILE:HG23	1.97	0.46
55:AE:132:ILE:HG22	55:AE:144:LEU:HD13	1.97	0.46
56:AF:105:CYS:HB2	66:AR:70:GLU:H	1.80	0.46
62:AN:66:ASP:HB3	79:Ah:378:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AR:57:ASN:HB3	66:AR:60:LYS:HG3	1.97	0.46
67:AU:83:PRO:HG2	67:AU:84:TRP:CD1	2.51	0.46
82:Ak:68:TRP:HE1	82:Ak:114:LEU:HB3	1.81	0.46
88:BA:771:U:H2'	88:BA:772:G:H8	1.81	0.46
88:BA:1003:C:H2'	88:BA:1004:A:H8	1.80	0.46
22:BW:77:GLN:H	22:BW:171:HIS:CD2	2.34	0.46
25:Ba:193:LEU:HD12	25:Ba:194:LYS:HG3	1.97	0.46
32:Bg:146:ARG:HA	32:Bg:146:ARG:HD3	1.67	0.46
54:AC:128:PRO:HD2	54:AC:131:LYS:HD2	1.97	0.46
59:AJ:73:TYR:HE2	59:AJ:150:GLY:HA2	1.81	0.46
71:Aa:287:THR:HG22	71:Aa:289:HIS:H	1.81	0.46
88:BA:881:C:H4'	88:BA:882:A:H5'	1.96	0.46
88:BA:902:C:O5'	88:BA:924:G:O2'	2.32	0.46
10:BJ:118:LYS:HA	10:BJ:118:LYS:HD3	1.73	0.46
15:BP:225:ASP:HB3	15:BP:228:ARG:HG3	1.98	0.46
37:Bl:76:ARG:HD2	37:Bl:165:GLY:HA3	1.97	0.46
43:Bt:9:ARG:N	88:BA:1021:C:O3'	2.49	0.46
48:AA:251:C:OP1	61:AL:114:ARG:NH1	2.49	0.46
53:AB:233:TYR:OH	72:Ab:38:PHE:O	2.34	0.46
88:BA:193:U:H2'	88:BA:194:G:C8	2.51	0.46
88:BA:916:C:H2'	88:BA:917:G:H8	1.81	0.46
14:BO:77:ILE:HD12	14:BO:107:LEU:HD11	1.98	0.45
15:BP:79:PRO:HB3	88:BA:1234:U:H5'	1.98	0.45
15:BP:234:LEU:HD23	44:Bu:66:LYS:HE3	1.98	0.45
20:BU:57:ARG:HH12	21:BV:173:LYS:HB3	1.79	0.45
34:Bi:164:VAL:HG12	34:Bi:261:MET:HB3	1.98	0.45
48:AA:344:G:O6	60:AK:124:LYS:NZ	2.45	0.45
71:Aa:101:LEU:HB3	71:Aa:150:MET:HE1	1.97	0.45
81:Aj:171:ARG:NH1	81:Aj:188:GLU:OE2	2.49	0.45
12:BL:306:GLN:OE1	12:BL:308:ARG:NH2	2.47	0.45
17:BR:119:ALA:HB3	17:BR:121:MET:HE2	1.98	0.45
28:Bc:182:LEU:HD12	28:Bc:291:ARG:HG3	1.97	0.45
33:Bh:216:ARG:HA	33:Bh:220:ILE:HD12	1.98	0.45
34:Bi:202:LEU:HD12	34:Bi:209:TYR:HE1	1.81	0.45
35:Bj:102:LYS:HB3	78:Ag:230:MET:HE1	1.98	0.45
48:AA:25:U:H2'	48:AA:26:A:H8	1.82	0.45
48:AA:901:A:O2'	84:An:171:ARG:NH1	2.49	0.45
81:Aj:178:ARG:HB2	81:Aj:183:ASP:HB3	1.99	0.45
85:Ao:73:ALA:O	85:Ao:76:SER:OG	2.35	0.45
85:Ao:336:GLN:HA	85:Ao:339:ASN:HB3	1.97	0.45
88:BA:135:G:N1	88:BA:138:A:OP2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:BA:1416:G:H2'	88:BA:1417:A:H8	1.81	0.45
12:BL:124:ILE:HG23	12:BL:127:MET:HE3	1.98	0.45
19:BT:178:LYS:HG3	19:BT:207:ILE:HD12	1.97	0.45
21:BV:112:VAL:HG13	21:BV:199:ILE:HG21	1.99	0.45
34:Bi:82:ALA:O	34:Bi:167:ASN:ND2	2.49	0.45
52:B7:85:ARG:NH1	88:BA:125:A:OP1	2.50	0.45
78:Ag:267:LEU:O	78:Ag:293:ARG:NH1	2.49	0.45
82:Ak:288:THR:HG22	82:Ak:290:GLU:H	1.81	0.45
88:BA:1066:A:H2'	88:BA:1067:G:H8	1.81	0.45
88:BA:1338:G:H2'	88:BA:1339:A:H8	1.80	0.45
9:BI:134:PRO:HA	9:BI:137:LYS:HB2	1.98	0.45
15:BP:47:ARG:HD3	21:BV:183:ASN:HD22	1.82	0.45
24:BY:124:ASP:OD1	24:BY:124:ASP:N	2.49	0.45
28:Bc:65:LYS:HB3	28:Bc:121:GLU:HG2	1.97	0.45
31:Bf:105:GLN:O	31:Bf:109:ILE:HG12	2.17	0.45
32:Bg:133:PHE:HB3	33:Bh:259:ARG:HD3	1.98	0.45
34:Bi:161:HIS:O	34:Bi:260:ARG:NH2	2.49	0.45
39:Bn:61:GLY:HA3	88:BA:222:G:H1	1.80	0.45
47:Bx:72:ILE:HG23	47:Bx:77:LEU:HB2	1.98	0.45
48:AA:16:U:O2'	48:AA:294:A:N6	2.49	0.45
48:AA:194:U:H2'	48:AA:195:G:H8	1.81	0.45
48:AA:195:G:H5''	64:AP:20:ARG:HB2	1.98	0.45
48:AA:374:C:OP2	83:Am:9:ARG:NH2	2.47	0.45
55:AE:243:VAL:HG11	55:AE:268:PHE:HE1	1.81	0.45
55:AE:412:LYS:HG2	55:AE:417:MET:HB2	1.98	0.45
82:Ak:79:LYS:HA	82:Ak:80:PRO:HD3	1.85	0.45
83:Am:100:PRO:HA	83:Am:101:PRO:HD3	1.86	0.45
88:BA:888:A:O2'	88:BA:891:A:N6	2.43	0.45
88:BA:1458:G:N2	88:BA:1468:A:OP2	2.46	0.45
13:BN:21:LEU:HD13	13:BN:145:LEU:HB2	1.98	0.45
14:BO:58:ILE:HD11	14:BO:76:ALA:HB2	1.98	0.45
15:BP:88:SER:HB2	15:BP:134:ARG:HH12	1.82	0.45
26:Bb:214:TRP:HB3	26:Bb:272:LEU:HD11	1.97	0.45
28:Bc:141:ARG:NH2	28:Bc:262:GLU:O	2.49	0.45
34:Bi:251:HIS:HE1	34:Bi:253:VAL:HB	1.81	0.45
36:Bk:94:HIS:HB2	36:Bk:185:SER:HB3	1.98	0.45
53:AB:205:HIS:HB3	53:AB:208:VAL:HG23	1.99	0.45
81:Aj:3:ARG:HG3	81:Aj:5:LYS:H	1.81	0.45
88:BA:229:A:H4'	88:BA:230:G:H5'	1.98	0.45
3:B1:41:VAL:HG11	3:B1:83:GLU:HB3	1.97	0.45
15:BP:162:LEU:HD22	44:Bu:144:ARG:HE	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AA:631:A:H4'	54:AC:46:LYS:HE3	1.99	0.45
81:Aj:82:ARG:HB3	81:Aj:85:TRP:CE3	2.52	0.45
88:BA:918:U:H2'	88:BA:919:G:H8	1.81	0.45
3:B1:99:LYS:HB2	3:B1:99:LYS:HE2	1.75	0.45
23:BX:38:ASP:O	23:BX:98:GLN:HA	2.17	0.45
26:Bb:110:LEU:O	26:Bb:114:ARG:HG2	2.17	0.45
46:Bw:146:GLN:HA	46:Bw:150:PHE:HB2	1.99	0.45
57:AG:78:PRO:HG2	57:AG:81:LYS:HB2	1.99	0.45
88:BA:550:A:N6	88:BA:551:A:N1	2.64	0.45
48:AA:722:A:OP2	48:AA:739:A:N6	2.50	0.45
58:AI:83:ILE:HG22	58:AI:87:HIS:CE1	2.52	0.45
71:Aa:263:GLU:HA	71:Aa:266:LYS:HG2	1.99	0.45
73:Ac:118:GLN:HE22	73:Ac:122:GLN:HE21	1.64	0.45
76:Ae:259:VAL:HG21	76:Ae:397:SER:HB3	1.98	0.45
85:Ao:346:ARG:HE	85:Ao:377:TYR:HB3	1.82	0.45
88:BA:291:U:H4'	88:BA:793:A:H4'	1.99	0.45
4:B2:240:PHE:HD1	24:BY:47:GLU:HB2	1.82	0.45
9:BI:126:GLN:HB3	9:BI:128:LEU:HD23	1.99	0.45
51:B6:20:MET:O	51:B6:29:SER:HA	2.17	0.45
58:AI:139:GLN:OE1	58:AI:156:GLN:NE2	2.49	0.45
58:AI:315:MET:HE2	78:Ag:381:PHE:HB3	1.99	0.45
65:AQ:16:LYS:O	65:AQ:29:ARG:N	2.47	0.45
78:Ag:173:ASN:HB2	78:Ag:176:ARG:HB2	1.99	0.45
85:Ao:342:LEU:HD12	85:Ao:374:THR:HG23	1.98	0.45
88:BA:354:U:O2'	88:BA:1055:A:N1	2.45	0.45
15:BP:80:LYS:HA	75:B8:113:ARG:HB3	1.97	0.45
52:B7:88:LYS:NZ	88:BA:127:G:OP2	2.41	0.45
10:BJ:101:HIS:HB3	10:BJ:150:HIS:ND1	2.33	0.44
16:BQ:224:LEU:HD21	43:Bt:38:ARG:HB3	1.98	0.44
17:BR:97:PHE:HE1	17:BR:127:LYS:HB2	1.81	0.44
21:BV:167:LYS:HB2	32:Bg:106:ASP:HB3	1.99	0.44
47:Bx:102:ARG:NH2	88:BA:554:U:O2'	2.50	0.44
48:AA:525:U:H2'	48:AA:526:G:H8	1.82	0.44
61:AL:89:ARG:HH21	61:AL:91:ALA:HB2	1.83	0.44
62:AN:44:ALA:O	62:AN:48:ALA:HB2	2.17	0.44
75:B8:113:ARG:NH2	88:BA:84:G:OP2	2.51	0.44
78:Ag:264:VAL:HG21	78:Ag:307:LEU:HB3	1.98	0.44
6:BD:155:THR:HG22	6:BD:156:GLU:H	1.82	0.44
10:BJ:62:PRO:HA	10:BJ:65:LEU:HD12	1.98	0.44
15:BP:140:LEU:HG	15:BP:156:VAL:HG11	1.99	0.44
25:Ba:210:SER:OG	25:Ba:223:HIS:ND1	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Bi:159:ARG:HE	34:Bi:159:ARG:HB3	1.68	0.44
34:Bi:230:ARG:H	34:Bi:230:ARG:HG2	1.59	0.44
35:Bj:52:CYS:HB3	35:Bj:235:LYS:HA	1.99	0.44
48:AA:590:C:H2'	48:AA:591:A:C8	2.52	0.44
55:AE:320:ILE:HG23	55:AE:349:LEU:HD11	1.98	0.44
57:AG:149:LEU:HA	57:AG:152:CYS:HB3	1.99	0.44
77:Af:141:VAL:HA	77:Af:173:LEU:HA	1.98	0.44
86:Ap:212:GLU:OE1	86:Ap:215:ARG:NH1	2.50	0.44
9:BI:122:ARG:O	9:BI:126:GLN:HB2	2.18	0.44
17:BR:65:LEU:HB3	17:BR:69:ASN:HD22	1.82	0.44
20:BU:99:ARG:NH2	88:BA:582:C:OP1	2.50	0.44
64:AP:50:GLN:HB3	73:Ac:128:HIS:HD2	1.82	0.44
78:Ag:210:ASN:ND2	78:Ag:213:GLU:OE2	2.50	0.44
88:BA:726:A:O2'	88:BA:728:C:N4	2.49	0.44
88:BA:1326:A:O2'	88:BA:1328:G:OP2	2.32	0.44
14:BO:75:LEU:HD23	14:BO:77:ILE:HD11	2.00	0.44
26:Bb:179:VAL:HG11	44:Bu:188:ARG:HH22	1.82	0.44
28:Bc:47:LYS:HE2	28:Bc:47:LYS:HB2	1.85	0.44
49:B4:71:GLU:O	49:B4:73:ARG:N	2.47	0.44
55:AE:176:ARG:HD3	80:Ai:84:ARG:HH22	1.83	0.44
55:AE:417:MET:HA	55:AE:419:ARG:HH11	1.82	0.44
60:AK:68:ILE:HB	60:AK:71:GLN:HB2	1.98	0.44
66:AR:135:LYS:O	74:Ad:193:ARG:NE	2.50	0.44
88:BA:1369:U:H5''	88:BA:1370:U:H5'	1.99	0.44
7:BE:129:VAL:HG23	7:BE:189:PRO:HA	1.98	0.44
10:BJ:49:ALA:HB1	43:Bt:32:LYS:HE3	1.99	0.44
28:Bc:136:ASN:HB3	28:Bc:171:VAL:HG11	1.98	0.44
28:Bc:145:MET:HE1	28:Bc:252:HIS:HB2	2.00	0.44
29:Bd:146:ALA:HB1	35:Bj:212:HIS:ND1	2.32	0.44
35:Bj:261:GLY:HA3	35:Bj:273:ARG:HH22	1.82	0.44
48:AA:279:U:O2'	61:AL:54:GLY:O	2.35	0.44
60:AK:160:ARG:NH2	60:AK:179:ASP:OD1	2.47	0.44
75:B8:131:LYS:NZ	88:BA:1234:U:OP2	2.51	0.44
77:Af:133:GLU:O	77:Af:136:GLN:NE2	2.51	0.44
79:Ah:289:GLY:O	79:Ah:293:MET:HG2	2.18	0.44
81:Aj:58:VAL:HA	81:Aj:137:HIS:HD1	1.82	0.44
88:BA:476:U:H2'	88:BA:477:A:H8	1.82	0.44
8:BF:249:ASN:ND2	39:Bn:56:VAL:O	2.50	0.44
11:BK:42:ARG:HG3	11:BK:72:VAL:HG21	1.97	0.44
29:Bd:83:ILE:HD12	29:Bd:84:PRO:HD2	1.99	0.44
48:AA:532:G:O2'	48:AA:959:U:N3	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AA:576:C:HO2'	48:AA:809:G:HO2'	1.59	0.44
79:Ah:284:ARG:NH2	85:Ao:451:ILE:O	2.44	0.44
85:Ao:82:SER:O	85:Ao:487:SER:OG	2.34	0.44
85:Ao:490:PHE:HB3	85:Ao:522:TYR:HB3	1.99	0.44
88:BA:1264:C:OP2	88:BA:1409:C:O2'	2.36	0.44
11:BK:159:LEU:O	11:BK:163:GLU:N	2.46	0.44
23:BX:141:ARG:HD2	23:BX:141:ARG:HA	1.74	0.44
24:BY:60:ASP:HB3	24:BY:157:PRO:HB3	1.99	0.44
27:B3:71:ARG:NH1	27:B3:73:LYS:O	2.50	0.44
54:AC:43:ARG:HA	54:AC:43:ARG:HD3	1.73	0.44
57:AG:57:GLU:OE2	57:AG:59:THR:OG1	2.32	0.44
82:Ak:92:PRO:HB3	82:Ak:98:PRO:HD3	2.00	0.44
85:Ao:468:LEU:HD21	85:Ao:480:TRP:HE3	1.82	0.44
3:B1:24:LEU:HD11	3:B1:211:ALA:HB1	2.00	0.44
4:B2:165:ALA:HB1	30:Be:131:LYS:HD3	1.99	0.44
7:BE:210:THR:OG1	7:BE:262:GLY:O	2.30	0.44
10:BJ:110:LEU:HG	11:BK:132:LEU:HG	2.00	0.44
25:Ba:213:TRP:HH2	25:Ba:315:LEU:HD11	1.82	0.44
26:Bb:161:LEU:HD21	26:Bb:221:LEU:HD22	2.00	0.44
34:Bi:80:CYS:SG	34:Bi:165:THR:OG1	2.64	0.44
48:AA:418:C:O2'	60:AK:189:ARG:O	2.35	0.44
57:AG:129:ALA:HB1	57:AG:133:GLU:HB2	2.00	0.44
4:B2:195:LYS:NZ	88:BA:32:C:OP1	2.45	0.44
43:Bt:32:LYS:O	43:Bt:36:ILE:HG13	2.18	0.44
48:AA:456:A:OP2	48:AA:952:C:O2'	2.35	0.44
53:AB:212:ALA:O	72:Ab:15:ARG:NH2	2.51	0.44
81:Aj:102:PRO:HA	81:Aj:112:GLY:HA3	2.00	0.44
85:Ao:346:ARG:NE	85:Ao:377:TYR:HB3	2.33	0.44
8:BF:53:LEU:HD11	8:BF:271:GLU:HA	1.99	0.43
11:BK:91:LEU:HD12	11:BK:151:LEU:HD23	2.01	0.43
19:BT:97:LYS:HE2	19:BT:97:LYS:HB3	1.85	0.43
24:BY:108:MET:HG2	34:Bi:166:GLU:HB3	1.99	0.43
25:Ba:140:ALA:HB1	25:Ba:412:ARG:HG2	1.99	0.43
48:AA:461:A:H2'	48:AA:462:A:H8	1.82	0.43
48:AA:822:A:OP2	57:AG:177:ARG:NH2	2.51	0.43
55:AE:285:TYR:N	55:AE:289:THR:O	2.49	0.43
61:AL:82:ARG:NH1	61:AL:90:GLU:OE2	2.43	0.43
64:AP:42:PRO:HG2	64:AP:45:GLY:HA3	1.99	0.43
2:B0:125:VAL:HG21	26:Bb:64:GLU:HG2	2.00	0.43
33:Bh:79:LEU:HD11	33:Bh:173:LEU:HD21	1.99	0.43
35:Bj:271:GLN:HB3	35:Bj:274:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Bl:139:GLN:HB2	43:Bt:82:PHE:HE2	1.83	0.43
48:AA:29:A:H2'	48:AA:30:A:C8	2.54	0.43
48:AA:58:U:OP1	81:Aj:53:ARG:NH1	2.47	0.43
76:Ae:189:ASP:HA	76:Ae:192:ILE:HD12	2.00	0.43
78:Ag:250:SER:HA	78:Ag:255:PHE:HD2	1.83	0.43
79:Ah:291:GLU:HA	79:Ah:294:ILE:HG12	2.00	0.43
85:Ao:498:ASP:HA	85:Ao:501:GLN:HG2	2.00	0.43
2:B0:77:PRO:HG3	2:B0:83:LEU:HD12	2.01	0.43
3:B1:163:ARG:HD3	3:B1:205:GLY:H	1.84	0.43
6:BD:256:ARG:HE	6:BD:256:ARG:HB3	1.64	0.43
15:BP:62:ARG:NH1	88:BA:379:U:OP1	2.48	0.43
18:BS:109:GLU:O	18:BS:113:LYS:HB2	2.19	0.43
32:Bg:35:ARG:HB2	43:Bt:101:TRP:HB2	2.01	0.43
48:AA:56:U:H1'	48:AA:198:C:H1'	2.00	0.43
48:AA:104:A:OP2	65:AQ:49:TYR:OH	2.29	0.43
55:AE:282:ILE:HD12	55:AE:353:LEU:HB3	2.00	0.43
73:Ac:96:LYS:HD2	73:Ac:96:LYS:HA	1.88	0.43
8:BF:270:GLU:O	8:BF:274:LEU:HB2	2.18	0.43
12:BL:270:LEU:HA	12:BL:273:MET:HG2	2.00	0.43
15:BP:56:GLU:HG3	88:BA:352:G:H5'	1.99	0.43
17:BR:32:LEU:HB3	17:BR:52:LEU:HD22	2.00	0.43
28:Bc:162:SER:HB2	28:Bc:181:VAL:HB	2.01	0.43
35:Bj:52:CYS:CB	35:Bj:234:PHE:O	2.66	0.43
79:Ah:309:ASN:O	82:Ak:166:ARG:NH1	2.51	0.43
81:Aj:135:MET:SD	81:Aj:135:MET:N	2.92	0.43
85:Ao:342:LEU:O	85:Ao:346:ARG:HG2	2.17	0.43
9:BI:120:ARG:HA	9:BI:124:LEU:HD12	1.99	0.43
14:BO:81:LYS:HE2	88:BA:947:A:H1'	2.01	0.43
15:BP:211:VAL:O	15:BP:215:THR:OG1	2.34	0.43
50:B5:132:LYS:HB2	50:B5:132:LYS:HE2	1.80	0.43
58:AI:314:LEU:HA	58:AI:349:MET:HE1	1.99	0.43
62:AN:72:ASP:HA	62:AN:75:ILE:HG22	2.00	0.43
64:AP:52:GLY:HA3	64:AP:67:ALA:O	2.18	0.43
80:Ai:66:ARG:NH2	80:Ai:80:ASP:OD2	2.50	0.43
82:Ak:196:VAL:HG22	82:Ak:199:ARG:HB2	2.01	0.43
7:BE:312:LYS:HD3	7:BE:312:LYS:HA	1.79	0.43
12:BL:311:ASP:O	12:BL:315:ASN:CA	2.66	0.43
46:Bw:93:VAL:HB	46:Bw:227:ILE:HG12	1.99	0.43
48:AA:206:U:H1'	74:Ad:27:ARG:HH12	1.83	0.43
48:AA:441:U:H2'	48:AA:442:A:H8	1.84	0.43
48:AA:870:G:O2'	84:An:179:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AG:180:ARG:HG2	57:AG:184:MET:HE3	2.00	0.43
65:AQ:98:LYS:HB2	65:AQ:98:LYS:HE2	1.87	0.43
71:Aa:173:THR:OG1	71:Aa:174:GLU:OE1	2.31	0.43
78:Ag:83:PRO:HA	78:Ag:84:PRO:HD3	1.88	0.43
78:Ag:204:GLN:HA	78:Ag:217:LYS:HB2	2.01	0.43
88:BA:165:A:H2'	88:BA:166:A:C8	2.54	0.43
88:BA:247:C:H2'	88:BA:248:A:H8	1.83	0.43
88:BA:1328:G:N2	88:BA:1329:U:O4	2.41	0.43
3:B1:227:PHE:HD1	4:B2:158:LEU:HD12	1.83	0.43
19:BT:141:SER:OG	88:BA:1487:C:OP1	2.29	0.43
21:BV:143:ASP:HA	32:Bg:127:GLN:HB3	1.99	0.43
21:BV:168:THR:OG1	21:BV:169:GLU:N	2.52	0.43
23:BX:39:THR:HA	23:BX:97:VAL:O	2.18	0.43
46:Bw:145:LEU:HD23	46:Bw:399:ILE:HD11	2.01	0.43
51:B6:34:ARG:NH2	51:B6:38:ARG:O	2.51	0.43
53:AB:195:LEU:HA	53:AB:221:ILE:HD13	2.01	0.43
78:Ag:365:LEU:HD23	78:Ag:370:ALA:HB1	2.00	0.43
84:An:142:LYS:HD3	84:An:142:LYS:HA	1.77	0.43
85:Ao:269:MET:HA	85:Ao:272:HIS:HB2	2.01	0.43
85:Ao:346:ARG:HA	85:Ao:346:ARG:HD3	1.79	0.43
26:Bb:72:ARG:HA	26:Bb:72:ARG:HD3	1.84	0.43
26:Bb:218:LEU:HD11	26:Bb:268:PHE:HB3	2.01	0.43
28:Bc:231:LYS:HD2	28:Bc:234:LEU:HD12	2.01	0.43
48:AA:761:U:O2'	48:AA:804:A:N3	2.46	0.43
52:B7:66:LYS:NZ	88:BA:254:G:O5'	2.51	0.43
54:AC:140:GLU:OE2	54:AC:153:LEU:N	2.51	0.43
85:Ao:574:TRP:HA	85:Ao:575:PRO:HD3	1.89	0.43
3:B1:222:ASP:N	3:B1:222:ASP:OD1	2.52	0.43
7:BE:119:VAL:HA	7:BE:285:VAL:O	2.19	0.43
8:BF:132:GLY:HA3	34:Bi:42:THR:HG21	1.99	0.43
12:BL:259:LYS:HB2	12:BL:259:LYS:HE3	1.84	0.43
21:BV:148:LEU:HB2	31:Bf:58:ILE:HB	2.00	0.43
29:Bd:63:ALA:HB1	29:Bd:67:ARG:HH21	1.84	0.43
48:AA:182:A:H62	61:AL:55:ARG:HG2	1.84	0.43
53:AB:81:ARG:HA	53:AB:81:ARG:HD3	1.90	0.43
56:AF:32:ARG:HH12	56:AF:81:HIS:HB2	1.84	0.43
72:Ab:85:PHE:HB2	77:Af:101:VAL:HG22	2.01	0.43
4:B2:95:LYS:NZ	24:BY:181:ASP:O	2.52	0.43
7:BE:215:PHE:O	88:BA:789:A:O2'	2.29	0.43
16:BQ:36:VAL:HG11	42:Bq:124:HIS:HB3	1.99	0.43
17:BR:150:LEU:HD23	17:BR:150:LEU:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Bw:369:ASN:ND2	46:Bw:384:LYS:O	2.49	0.43
51:B6:16:ILE:HG21	51:B6:34:ARG:HH11	1.84	0.43
53:AB:117:LEU:HA	53:AB:120:THR:HB	2.01	0.43
54:AC:76:LEU:HD13	59:AJ:81:LYS:HG3	2.00	0.43
59:AJ:96:VAL:HG12	59:AJ:100:LYS:HD2	2.00	0.43
65:AQ:52:HIS:HB3	65:AQ:80:GLU:HG3	2.01	0.43
77:Af:109:VAL:HB	77:Af:112:ASP:HB2	2.01	0.43
85:Ao:610:ARG:HA	85:Ao:610:ARG:HD3	1.74	0.43
13:BN:62:THR:HG21	13:BN:101:VAL:HA	2.00	0.42
18:BS:151:TRP:HH2	26:Bb:54:PHE:HB3	1.84	0.42
32:Bg:14:VAL:HG13	32:Bg:25:GLN:HE22	1.84	0.42
37:Bl:60:PRO:HA	37:Bl:61:PRO:HD3	1.93	0.42
41:Bp:10:LEU:HD13	41:Bp:42:VAL:HG13	2.02	0.42
72:Ab:93:LYS:HB3	72:Ab:93:LYS:HE3	1.72	0.42
76:Ae:328:LYS:HA	76:Ae:328:LYS:HD3	1.81	0.42
85:Ao:474:ILE:HG22	85:Ao:478:LEU:HD23	2.01	0.42
88:BA:1528:A:H2'	88:BA:1529:A:H8	1.84	0.42
1:CL:50:LEU:HD23	1:CL:50:LEU:HA	1.92	0.42
7:BE:206:VAL:HG11	7:BE:289:VAL:HG13	2.00	0.42
22:BW:48:LYS:N	88:BA:2:C:OP1	2.51	0.42
24:BY:95:TYR:HB3	24:BY:108:MET:HE3	2.00	0.42
46:Bw:227:ILE:HD12	46:Bw:328:ALA:HB2	2.01	0.42
53:AB:67:LYS:HB2	53:AB:67:LYS:HE3	1.75	0.42
54:AC:95:PHE:O	54:AC:99:THR:OG1	2.31	0.42
59:AJ:51:HIS:NE2	59:AJ:53:ASP:O	2.53	0.42
71:Aa:194:ILE:HG13	71:Aa:211:ARG:HG3	2.01	0.42
73:Ac:46:LYS:HB2	73:Ac:46:LYS:HE3	1.83	0.42
77:Af:115:ILE:HD13	77:Af:141:VAL:HG21	2.01	0.42
78:Ag:54:ASP:HB3	78:Ag:57:LYS:HG2	2.01	0.42
80:Ai:41:PRO:HG2	80:Ai:44:LYS:HG3	2.02	0.42
81:Aj:29:ARG:O	81:Aj:33:ARG:HB2	2.18	0.42
81:Aj:61:GLU:HG2	81:Aj:138:ASP:HA	2.00	0.42
81:Aj:178:ARG:NH2	81:Aj:187:GLU:O	2.52	0.42
86:Ap:207:GLN:HA	86:Ap:208:PRO:HD3	1.92	0.42
87:B9:82:ARG:NH1	88:BA:1512:U:OP2	2.52	0.42
88:BA:232:U:H2'	88:BA:233:A:H8	1.85	0.42
15:BP:287:ASP:HB3	15:BP:290:LEU:HB2	2.00	0.42
30:Be:44:ARG:HG2	88:BA:744:A:C6	2.54	0.42
38:Bm:88:GLN:HA	38:Bm:124:VAL:HB	2.01	0.42
48:AA:227:A:H61	48:AA:270:C:H42	1.66	0.42
49:B4:72:PRO:O	49:B4:74:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:Ae:105:LEU:HD12	76:Ae:106:PRO:HD2	2.01	0.42
85:Ao:652:VAL:HA	85:Ao:655:GLU:HB3	2.01	0.42
8:BF:160:SER:HB3	39:Bn:80:LEU:HD13	2.02	0.42
14:BO:96:MET:HE3	19:BT:168:ASN:HD22	1.83	0.42
25:Ba:36:ARG:HH21	88:BA:854:U:H5'	1.83	0.42
33:Bh:121:ASP:N	33:Bh:121:ASP:OD1	2.52	0.42
33:Bh:145:PHE:HB3	33:Bh:148:LEU:HD23	2.02	0.42
35:Bj:162:ARG:HD3	35:Bj:171:TRP:HE3	1.84	0.42
46:Bw:115:LEU:HD11	46:Bw:251:ILE:HD13	2.01	0.42
46:Bw:310:CYS:HB3	46:Bw:313:GLN:HB2	2.00	0.42
48:AA:355:U:H2'	48:AA:356:A:H8	1.83	0.42
48:AA:759:U:H2'	48:AA:760:A:H8	1.85	0.42
50:B5:116:LEU:HD23	50:B5:116:LEU:HA	1.91	0.42
59:Aj:122:LYS:O	62:AN:112:ARG:NH1	2.53	0.42
81:Aj:163:SER:HB3	81:Aj:190:MET:HB3	2.01	0.42
82:Ak:189:LYS:O	82:Ak:193:ILE:HG13	2.19	0.42
7:BE:239:ARG:NH2	88:BA:1401:U:OP2	2.53	0.42
17:BR:144:THR:HB	17:BR:147:ASN:HD22	1.84	0.42
19:BT:152:ARG:NH2	19:BT:190:LEU:O	2.52	0.42
29:Bd:182:ILE:HG12	49:B4:62:GLY:HA3	2.01	0.42
33:Bh:60:ARG:NH1	33:Bh:65:ASN:O	2.53	0.42
47:Bx:173:ARG:NH1	88:BA:488:U:O2'	2.53	0.42
48:AA:175:A:N3	48:AA:187:U:O2'	2.48	0.42
73:Ac:109:ASN:O	73:Ac:112:THR:OG1	2.29	0.42
73:Ac:112:THR:HA	73:Ac:115:LYS:HG2	2.00	0.42
76:Ae:71:SER:OG	76:Ae:189:ASP:OD1	2.32	0.42
1:HL:76:LEU:O	1:HL:80:SER:OG	2.30	0.42
2:B0:92:LEU:HD13	18:BS:66:ARG:HB2	2.02	0.42
8:BF:252:SER:O	8:BF:256:HIS:ND1	2.45	0.42
12:BL:178:GLN:OE1	69:AX:6:A:N6	2.52	0.42
12:BL:296:SER:O	61:AL:77:ASN:ND2	2.53	0.42
15:BP:264:GLN:NE2	15:BP:269:LEU:O	2.52	0.42
18:BS:39:VAL:HG12	18:BS:41:ASN:H	1.84	0.42
18:BS:85:ARG:HG2	18:BS:90:ILE:HD12	2.01	0.42
36:Bk:93:ILE:O	36:Bk:156:VAL:HA	2.20	0.42
46:Bw:292:GLN:OE1	46:Bw:294:HIS:NE2	2.52	0.42
62:AN:53:ARG:O	62:AN:56:SER:OG	2.35	0.42
76:Ae:213:PHE:HE2	76:Ae:221:LEU:HD22	1.84	0.42
88:BA:165:A:H2'	88:BA:166:A:H8	1.84	0.42
5:BB:40:U:H2'	5:BB:41:G:C8	2.55	0.42
13:BN:171:SER:HB3	47:Bx:59:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BQ:89:ILE:HD11	16:BQ:176:LEU:HD22	2.02	0.42
20:BU:105:LEU:O	20:BU:109:GLU:HB2	2.19	0.42
30:Be:58:LEU:HD23	30:Be:58:LEU:HA	1.88	0.42
31:Bf:52:THR:HG22	31:Bf:54:ASP:H	1.85	0.42
33:Bh:79:LEU:HD12	33:Bh:214:PHE:HE1	1.85	0.42
46:Bw:107:GLN:HG2	46:Bw:112:THR:HG23	2.02	0.42
58:AI:302:LEU:HD22	78:Ag:384:ASN:HB3	2.02	0.42
66:AR:121:MET:HE3	66:AR:121:MET:HB2	1.91	0.42
75:B8:135:LYS:HD3	88:BA:1231:U:H5''	2.01	0.42
78:Ag:278:LYS:HE3	78:Ag:278:LYS:HB2	1.74	0.42
81:Aj:91:GLU:HG3	81:Aj:121:LYS:HA	2.01	0.42
82:Ak:300:SER:O	82:Ak:304:GLU:HB3	2.19	0.42
85:Ao:335:LEU:HD21	85:Ao:371:SER:HB3	2.02	0.42
3:B1:167:LEU:HD23	3:B1:167:LEU:HA	1.86	0.42
4:B2:230:ARG:NH2	88:BA:101:U:O3'	2.53	0.42
6:BD:277:GLN:NE2	88:BA:868:G:OP1	2.53	0.42
7:BE:308:LYS:HA	7:BE:308:LYS:HD2	1.90	0.42
19:BT:77:SER:HB2	19:BT:80:PHE:HD2	1.84	0.42
34:Bi:111:ARG:O	34:Bi:115:ASN:ND2	2.52	0.42
54:AC:95:PHE:HD2	80:Ai:62:MET:HE1	1.85	0.42
57:AG:61:GLU:HA	57:AG:64:TYR:CE1	2.54	0.42
68:AV:40:A:H2'	68:AV:41:A:C8	2.55	0.42
88:BA:69:C:H4'	88:BA:70:A:H5'	2.02	0.42
10:BJ:163:GLU:OE2	10:BJ:166:ARG:NH2	2.53	0.42
17:BR:113:ARG:HE	17:BR:115:GLU:HB2	1.85	0.42
22:BW:210:LEU:HB3	32:Bg:119:PHE:CE2	2.54	0.42
22:BW:210:LEU:HD23	32:Bg:121:THR:HG21	2.02	0.42
76:Ae:230:LEU:HD22	76:Ae:394:LEU:HD22	2.00	0.42
81:Aj:86:LEU:HD12	81:Aj:140:ARG:HH11	1.84	0.42
82:Ak:319:LYS:HZ2	82:Ak:319:LYS:HG3	1.71	0.42
88:BA:994:A:OP1	88:BA:1495:A:O2'	2.36	0.42
12:BL:231:THR:HG21	88:BA:1275:C:H4'	2.02	0.42
16:BQ:96:TYR:OH	16:BQ:129:LYS:NZ	2.47	0.42
20:BU:71:ARG:HD3	20:BU:107:ILE:HD11	2.01	0.42
25:Ba:389:LEU:H	88:BA:725:C:H5	1.68	0.42
29:Bd:150:LEU:HD13	35:Bj:209:PRO:HG3	2.01	0.42
55:AE:126:LEU:HD21	80:Ai:81:GLU:HG3	2.02	0.42
71:Aa:163:VAL:HG22	71:Aa:204:ARG:HB3	2.02	0.42
78:Ag:156:ASP:HB2	78:Ag:159:ILE:HD12	2.02	0.42
85:Ao:80:ARG:HH21	85:Ao:82:SER:HA	1.85	0.42
85:Ao:301:ILE:HG23	85:Ao:319:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:BA:247:C:H2'	88:BA:248:A:C8	2.55	0.42
1:EL:82:LEU:HB3	1:FL:64:ILE:HG23	2.02	0.41
13:BN:91:THR:HB	13:BN:94:GLN:HG3	2.02	0.41
25:Ba:201:ARG:HH22	25:Ba:421:GLY:HA3	1.85	0.41
29:Bd:115:ALA:O	29:Bd:119:LYS:HG2	2.20	0.41
44:Bu:107:ALA:O	44:Bu:115:ARG:NH2	2.46	0.41
65:AQ:98:LYS:HE3	65:AQ:109:PRO:HA	2.02	0.41
76:Ae:185:ASN:OD1	76:Ae:217:SER:OG	2.38	0.41
85:Ao:71:LEU:HD23	85:Ao:71:LEU:HA	1.89	0.41
91:BA:1793:SPM:H62	91:BA:1793:SPM:H91	1.83	0.41
10:BJ:128:ASN:HA	10:BJ:131:LEU:HB3	2.01	0.41
26:Bb:184:LEU:HD23	44:Bu:190:LYS:HE2	2.01	0.41
30:Be:49:VAL:HG21	88:BA:746:U:H3	1.86	0.41
46:Bw:43:ARG:HA	46:Bw:43:ARG:HD2	1.85	0.41
53:AB:145:SER:HB2	53:AB:195:LEU:HB2	2.01	0.41
58:AI:269:ALA:HB1	58:AI:356:PHE:HE1	1.85	0.41
75:B8:163:THR:O	75:B8:167:LYS:NZ	2.54	0.41
85:Ao:369:GLU:HA	85:Ao:370:PRO:HD3	1.93	0.41
88:BA:784:G:O6	88:BA:1004:A:N6	2.53	0.41
88:BA:1513:U:OP2	88:BA:1525:C:N4	2.52	0.41
19:BT:100:LEU:HD21	19:BT:286:ILE:HG12	2.02	0.41
22:BW:96:SER:H	22:BW:99:GLN:HE21	1.69	0.41
22:BW:189:THR:HG23	22:BW:192:ALA:H	1.84	0.41
25:Ba:212:THR:HG23	25:Ba:221:GLN:HB2	2.03	0.41
44:Bu:177:SER:O	44:Bu:181:ASN:HB2	2.21	0.41
46:Bw:80:LEU:O	46:Bw:84:THR:OG1	2.33	0.41
65:AQ:69:LEU:HD12	65:AQ:70:PRO:HD2	2.01	0.41
71:Aa:315:LEU:HG	71:Aa:318:ASP:HB2	2.01	0.41
78:Ag:161:VAL:HG22	78:Ag:289:ILE:HD11	2.02	0.41
7:BE:218:VAL:HG23	7:BE:222:TRP:HD1	1.85	0.41
8:BF:103:GLN:HE21	8:BF:103:GLN:HB3	1.72	0.41
8:BF:262:THR:O	8:BF:265:THR:OG1	2.30	0.41
36:Bk:148:ALA:HB2	49:B4:76:LEU:HD11	2.01	0.41
43:Bt:81:ARG:HE	43:Bt:81:ARG:HB3	1.73	0.41
46:Bw:215:HIS:ND1	88:BA:757:A:OP1	2.54	0.41
58:AI:180:ARG:NH1	77:Af:136:GLN:OE1	2.53	0.41
65:AQ:72:PRO:HB3	65:AQ:78:LYS:HG2	2.03	0.41
66:AR:55:MET:HE2	66:AR:58:PRO:HG3	2.01	0.41
75:B8:110:VAL:O	75:B8:114:PHE:HB2	2.19	0.41
83:Am:9:ARG:HB3	83:Am:21:LEU:HD13	2.01	0.41
12:BL:163:GLU:HA	12:BL:166:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BL:213:ASP:HB3	12:BL:242:PRO:HD3	2.03	0.41
13:BN:30:LYS:HG3	88:BA:573:A:H4'	2.01	0.41
13:BN:62:THR:HB	13:BN:129:PRO:HA	2.02	0.41
15:BP:30:ASN:ND2	88:BA:214:A:H5'	2.35	0.41
25:Ba:310:ARG:O	25:Ba:314:ILE:HG12	2.20	0.41
29:Bd:165:ASP:N	29:Bd:165:ASP:OD1	2.53	0.41
33:Bh:166:VAL:HG11	33:Bh:192:ARG:HG3	2.03	0.41
44:Bu:146:LEU:HD12	44:Bu:146:LEU:HA	1.93	0.41
48:AA:638:A:H1'	48:AA:639:A:H2'	2.02	0.41
48:AA:887:U:H2'	48:AA:888:A:H8	1.84	0.41
58:AI:126:LYS:HB2	58:AI:131:ILE:HD11	2.02	0.41
59:AJ:81:LYS:HA	59:AJ:139:LEU:O	2.21	0.41
63:AO:165:LYS:NZ	63:AO:191:THR:H	2.19	0.41
66:AR:125:TYR:HB3	67:AU:9:ALA:HB2	2.02	0.41
73:Ac:16:LEU:HD12	73:Ac:57:TYR:HB2	2.03	0.41
81:Aj:169:LEU:HD23	81:Aj:173:MET:HE1	2.02	0.41
85:Ao:649:THR:HG22	85:Ao:653:MET:HE1	2.02	0.41
88:BA:523:U:O2'	88:BA:532:A:OP1	2.38	0.41
88:BA:1076:A:H2'	88:BA:1077:A:H8	1.85	0.41
3:B1:145:ILE:HG13	3:B1:161:LEU:HD23	2.02	0.41
3:B1:162:LYS:O	3:B1:166:LEU:HB2	2.20	0.41
9:BI:123:LEU:HA	9:BI:128:LEU:HB2	2.02	0.41
12:BL:191:THR:O	12:BL:295:ARG:NH2	2.44	0.41
12:BL:233:ASP:OD1	12:BL:233:ASP:N	2.50	0.41
13:BN:45:PRO:HB3	20:BU:75:ALA:HB2	2.02	0.41
16:BQ:204:GLU:HA	16:BQ:207:ARG:HG2	2.02	0.41
19:BT:108:ILE:HD13	19:BT:166:LEU:HD22	2.02	0.41
19:BT:114:GLY:HA3	19:BT:182:ARG:HG3	2.03	0.41
22:BW:205:THR:OG1	88:BA:170:U:O2	2.31	0.41
28:Bc:138:ALA:O	28:Bc:142:SER:OG	2.33	0.41
30:Be:20:LYS:HB2	30:Be:20:LYS:HE2	1.84	0.41
36:Bk:158:GLN:OE1	36:Bk:189:HIS:CE1	2.73	0.41
48:AA:787:A:H2'	48:AA:788:G:C8	2.55	0.41
51:B6:59:GLN:HG2	51:B6:60:LYS:HG3	2.02	0.41
53:AB:238:ASN:OD1	77:Af:120:LYS:NZ	2.53	0.41
63:AO:189:GLU:OE1	63:AO:191:THR:OG1	2.39	0.41
76:Ae:80:TRP:HZ3	76:Ae:151:THR:HG22	1.84	0.41
78:Ag:310:SER:O	78:Ag:314:SER:OG	2.39	0.41
85:Ao:397:TYR:O	85:Ao:401:ASN:ND2	2.48	0.41
85:Ao:457:ARG:HH22	85:Ao:488:VAL:HG13	1.86	0.41
86:Ap:188:PRO:HA	86:Ap:189:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:BA:195:G:OP1	88:BA:633:U:O2'	2.36	0.41
6:BD:199:SER:HB2	6:BD:207:TYR:HE1	1.86	0.41
13:BN:152:PRO:HB3	47:Bx:84:GLU:HG2	2.01	0.41
20:BU:51:VAL:HG21	21:BV:178:PHE:HB3	2.02	0.41
22:BW:57:TYR:HD1	34:Bi:228:PHE:HA	1.86	0.41
45:Bv:147:GLN:NE2	45:Bv:151:ASP:OD2	2.54	0.41
48:AA:367:A:H4'	60:AK:186:ASN:HD22	1.85	0.41
48:AA:735:G:N3	78:Ag:163:ASN:ND2	2.69	0.41
57:AG:98:MET:HE1	57:AG:201:MET:HE3	2.03	0.41
65:AQ:63:ILE:HD13	65:AQ:86:PHE:HB2	2.03	0.41
66:AR:104:LYS:HA	66:AR:104:LYS:HD3	1.86	0.41
82:Ak:200:TYR:OH	82:Ak:205:ASP:OD1	2.36	0.41
88:BA:464:U:O2	88:BA:1032:G:O2'	2.33	0.41
88:BA:699:G:H2'	88:BA:700:A:C8	2.56	0.41
88:BA:1269:G:N2	88:BA:1272:U:O2	2.47	0.41
1:CL:31:LEU:HD22	1:DL:67:LEU:HD12	2.02	0.41
1:DL:77:LEU:HD11	10:BJ:186:LEU:HD21	2.02	0.41
2:B0:122:GLN:HA	26:Bb:51:TYR:HD1	1.84	0.41
12:BL:176:ARG:HD3	12:BL:298:LYS:HD3	2.02	0.41
14:BO:73:ILE:HG23	14:BO:84:ALA:HB3	2.02	0.41
17:BR:17:ARG:NH2	88:BA:996:U:OP2	2.44	0.41
19:BT:59:LYS:HA	19:BT:60:PRO:HD3	1.90	0.41
24:BY:78:GLN:HB2	34:Bi:74:ARG:HD3	2.02	0.41
24:BY:192:LYS:HD3	24:BY:192:LYS:HA	1.85	0.41
48:AA:50:U:H2'	48:AA:51:G:C8	2.53	0.41
48:AA:247:G:N7	61:AL:78:ARG:NH1	2.67	0.41
48:AA:299:U:H2'	48:AA:300:G:C8	2.55	0.41
48:AA:528:C:H2'	48:AA:529:G:C8	2.56	0.41
48:AA:531:U:H2'	48:AA:532:G:H8	1.85	0.41
49:B4:43:ARG:NH1	49:B4:44:LEU:O	2.54	0.41
52:B7:50:LYS:HB3	52:B7:51:ALA:H	1.66	0.41
55:AE:284:ARG:HD3	55:AE:327:ILE:HG22	2.03	0.41
65:AQ:29:ARG:HH11	65:AQ:46:ARG:HD2	1.85	0.41
76:Ae:70:LEU:HA	76:Ae:409:GLU:HG3	2.02	0.41
78:Ag:46:ALA:HB3	78:Ag:357:GLN:HG3	2.02	0.41
8:BF:137:ARG:NH1	88:BA:1268:G:OP1	2.37	0.41
19:BT:152:ARG:HH12	19:BT:191:ARG:HA	1.86	0.41
20:BU:25:LEU:HB3	20:BU:29:ARG:HH12	1.86	0.41
26:Bb:157:LEU:HD11	26:Bb:318:PHE:CG	2.56	0.41
29:Bd:121:TRP:CE2	35:Bj:70:MET:HE2	2.56	0.41
34:Bi:135:LYS:HA	34:Bi:135:LYS:HD2	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Bw:298:ASP:HA	46:Bw:301:LYS:HE3	2.02	0.41
48:AA:116:G:OP1	63:AO:207:LYS:NZ	2.42	0.41
48:AA:375:A:OP2	83:Am:17:ARG:NE	2.49	0.41
48:AA:455:A:N7	48:AA:935:G:O2'	2.43	0.41
48:AA:880:U:H2'	48:AA:881:A:C8	2.56	0.41
48:AA:938:U:H2'	48:AA:939:A:C8	2.55	0.41
48:AA:944:A:H5''	84:An:145:LYS:HZ1	1.85	0.41
64:AP:85:LYS:H	64:AP:85:LYS:HG2	1.73	0.41
65:AQ:16:LYS:HE2	65:AQ:16:LYS:HB3	1.91	0.41
65:AQ:69:LEU:HD23	65:AQ:72:PRO:HA	2.03	0.41
75:B8:163:THR:HG23	75:B8:165:PHE:H	1.86	0.41
81:Aj:40:THR:O	81:Aj:49:ARG:NH1	2.54	0.41
85:Ao:451:ILE:HG21	85:Ao:457:ARG:HG3	2.02	0.41
88:BA:104:C:H6	88:BA:623:G:H21	1.68	0.41
88:BA:1122:A:H2'	88:BA:1123:A:H8	1.85	0.41
88:BA:1414:C:H2'	88:BA:1415:G:C8	2.55	0.41
4:B2:158:LEU:HD11	30:Be:90:PHE:HB2	2.03	0.41
25:Ba:163:LEU:HD23	46:Bw:281:LYS:HD2	2.03	0.41
30:Be:34:ARG:HA	30:Be:34:ARG:HD2	1.79	0.41
38:Bm:89:ASP:OD1	38:Bm:125:ARG:NH1	2.54	0.41
48:AA:892:A:N3	81:Aj:17:ARG:NH2	2.52	0.41
54:AC:88:GLU:HB2	54:AC:112:ARG:HH22	1.84	0.41
58:AI:318:LEU:HB2	58:AI:324:LEU:HD23	2.03	0.41
63:AO:117:LEU:HD23	63:AO:117:LEU:HA	1.90	0.41
78:Ag:65:GLN:O	78:Ag:99:MET:HA	2.21	0.41
88:BA:1506:A:H2'	88:BA:1507:G:C8	2.55	0.41
10:BJ:86:ILE:HA	10:BJ:89:VAL:HG12	2.03	0.40
21:BV:164:VAL:HA	21:BV:197:LEU:HD23	2.03	0.40
23:BX:18:ARG:NH2	24:BY:206:GLU:OE2	2.45	0.40
26:Bb:233:VAL:O	26:Bb:296:ARG:NH2	2.47	0.40
29:Bd:100:GLN:HG3	35:Bj:84:TYR:HE2	1.85	0.40
34:Bi:271:PRO:HA	34:Bi:272:PRO:HD3	1.96	0.40
48:AA:85:G:H2'	48:AA:86:A:H8	1.85	0.40
48:AA:182:A:C6	61:AL:56:PRO:HD2	2.55	0.40
55:AE:316:CYS:HB2	55:AE:321:MET:HG3	2.03	0.40
63:AO:155:ARG:O	63:AO:159:MET:HG3	2.21	0.40
82:Ak:118:PRO:O	82:Ak:122:LYS:HG2	2.22	0.40
88:BA:740:U:H2'	88:BA:741:A:H8	1.86	0.40
17:BR:117:ASP:OD2	88:BA:784:G:O2'	2.29	0.40
22:BW:79:LYS:HA	22:BW:79:LYS:HD2	1.88	0.40
25:Ba:231:ASN:HA	25:Ba:288:PRO:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Bh:258:THR:HG22	33:Bh:259:ARG:HG3	2.02	0.40
36:Bk:96:ILE:HB	36:Bk:183:LYS:HB2	2.03	0.40
48:AA:123:U:OP2	65:AQ:73:ARG:NH2	2.52	0.40
58:AI:143:ASP:OD1	58:AI:143:ASP:N	2.52	0.40
59:AJ:52:VAL:HG21	85:Ao:479:LYS:HB3	2.02	0.40
66:AR:88:PHE:O	67:AU:10:ARG:N	2.53	0.40
76:Ae:419:ARG:HA	76:Ae:419:ARG:HD2	1.95	0.40
82:Ak:268:LEU:HD23	82:Ak:271:ILE:HD12	2.04	0.40
6:BD:202:GLY:O	25:Ba:30:ALA:N	2.54	0.40
8:BF:156:ARG:HD2	8:BF:156:ARG:HA	1.99	0.40
14:BO:99:ARG:NH1	19:BT:161:GLU:OE1	2.55	0.40
15:BP:149:LYS:HD2	15:BP:149:LYS:HA	1.81	0.40
37:Bl:41:SER:OG	37:Bl:44:GLU:OE2	2.38	0.40
46:Bw:397:GLU:HB3	46:Bw:406:GLY:HA3	2.04	0.40
48:AA:282:A:H2	55:AE:421:VAL:HG21	1.86	0.40
63:AO:75:LEU:HD11	63:AO:110:MET:HG3	2.03	0.40
64:AP:101:PRO:HB3	74:Ad:59:ARG:HB3	2.02	0.40
65:AQ:41:LYS:HB2	73:Ac:11:ARG:HD2	2.03	0.40
78:Ag:205:GLU:HG2	78:Ag:248:ARG:HH22	1.86	0.40
83:Am:85:LYS:HB2	83:Am:85:LYS:HE3	1.84	0.40
88:BA:124:A:N3	88:BA:251:C:O2'	2.43	0.40
7:BE:275:ARG:HB3	7:BE:284:TYR:CD2	2.56	0.40
10:BJ:54:ILE:HG13	16:BQ:210:GLN:HB2	2.04	0.40
12:BL:185:LYS:HD2	48:AA:844:C:H1'	2.04	0.40
20:BU:57:ARG:NH1	21:BV:173:LYS:HB3	2.37	0.40
26:Bb:179:VAL:HG21	44:Bu:188:ARG:HH22	1.86	0.40
29:Bd:192:TYR:HE2	49:B4:81:ASP:HB2	1.87	0.40
35:Bj:256:SER:O	35:Bj:260:LEU:CB	2.68	0.40
42:Bq:114:THR:HG22	42:Bq:116:GLU:H	1.87	0.40
46:Bw:103:ASP:OD1	46:Bw:103:ASP:N	2.53	0.40
48:AA:603:U:H2'	48:AA:605:C:H4'	2.03	0.40
48:AA:918:A:H2	69:AX:6:A:H5''	1.86	0.40
53:AB:241:SER:HA	53:AB:242:PRO:HD3	1.94	0.40
54:AC:48:ASP:OD1	54:AC:48:ASP:N	2.54	0.40
57:AG:43:ASP:HA	57:AG:44:PRO:HD3	1.98	0.40
57:AG:95:THR:HG21	57:AG:108:ARG:HG2	2.03	0.40
81:Aj:78:ARG:HE	81:Aj:78:ARG:HB3	1.59	0.40
3:B1:12:LYS:HE2	3:B1:12:LYS:HB2	1.85	0.40
4:B2:228:LEU:HD11	88:BA:11:G:H5'	2.04	0.40
8:BF:220:ASP:O	8:BF:245:ALA:N	2.54	0.40
15:BP:92:GLN:HB2	15:BP:135:ASP:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BQ:72:ILE:HD11	16:BQ:96:TYR:CZ	2.57	0.40
32:Bg:26:LEU:HD21	32:Bg:29:LEU:HD11	2.04	0.40
32:Bg:35:ARG:O	32:Bg:44:ARG:NH1	2.55	0.40
33:Bh:56:PRO:HA	33:Bh:57:PRO:HD3	1.91	0.40
36:Bk:122:GLU:HG2	36:Bk:160:SER:HB2	2.03	0.40
50:B5:108:ASP:OD1	50:B5:109:VAL:N	2.54	0.40
54:AC:130:HIS:NE2	85:Ao:105:SER:OG	2.47	0.40
55:AE:220:THR:HB	55:AE:247:VAL:HG12	2.04	0.40
71:Aa:240:MET:HB3	71:Aa:245:GLN:HB2	2.02	0.40
85:Ao:265:MET:HB3	85:Ao:269:MET:HE1	2.02	0.40
88:BA:199:A:H2'	88:BA:200:A:C8	2.56	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	CL	43/198 (22%)	39 (91%)	4 (9%)	0	100	100
1	DL	25/198 (13%)	25 (100%)	0	0	100	100
1	EL	26/198 (13%)	26 (100%)	0	0	100	100
1	FL	25/198 (13%)	24 (96%)	1 (4%)	0	100	100
1	GL	25/198 (13%)	25 (100%)	0	0	100	100
1	HL	24/198 (12%)	24 (100%)	0	0	100	100
2	B0	108/148 (73%)	107 (99%)	1 (1%)	0	100	100
3	B1	242/256 (94%)	241 (100%)	1 (0%)	0	100	100
4	B2	177/252 (70%)	175 (99%)	2 (1%)	0	100	100
6	BD	208/306 (68%)	202 (97%)	5 (2%)	1 (0%)	24	57
7	BE	275/399 (69%)	259 (94%)	15 (6%)	1 (0%)	30	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	BF	219/294 (74%)	214 (98%)	5 (2%)	0	100	100
9	BI	96/268 (36%)	92 (96%)	4 (4%)	0	100	100
10	BJ	210/262 (80%)	203 (97%)	7 (3%)	0	100	100
11	BK	174/192 (91%)	171 (98%)	3 (2%)	0	100	100
12	BL	248/362 (68%)	233 (94%)	14 (6%)	1 (0%)	30	62
13	BN	175/178 (98%)	171 (98%)	4 (2%)	0	100	100
14	BO	113/145 (78%)	110 (97%)	3 (3%)	0	100	100
15	BP	286/296 (97%)	277 (97%)	9 (3%)	0	100	100
16	BQ	220/251 (88%)	216 (98%)	4 (2%)	0	100	100
17	BR	151/169 (89%)	147 (97%)	4 (3%)	0	100	100
18	BS	141/180 (78%)	133 (94%)	8 (6%)	0	100	100
19	BT	238/292 (82%)	229 (96%)	8 (3%)	1 (0%)	30	62
20	BU	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
21	BV	153/209 (73%)	148 (97%)	5 (3%)	0	100	100
22	BW	164/210 (78%)	161 (98%)	3 (2%)	0	100	100
23	BX	147/150 (98%)	144 (98%)	3 (2%)	0	100	100
24	BY	204/216 (94%)	198 (97%)	6 (3%)	0	100	100
25	Ba	391/423 (92%)	375 (96%)	16 (4%)	0	100	100
26	Bb	352/380 (93%)	337 (96%)	15 (4%)	0	100	100
27	B3	116/161 (72%)	114 (98%)	2 (2%)	0	100	100
28	Bc	293/334 (88%)	282 (96%)	11 (4%)	0	100	100
29	Bd	136/206 (66%)	132 (97%)	4 (3%)	0	100	100
30	Be	120/135 (89%)	113 (94%)	7 (6%)	0	100	100
31	Bf	106/142 (75%)	102 (96%)	2 (2%)	2 (2%)	6	33
32	Bg	146/159 (92%)	139 (95%)	7 (5%)	0	100	100
33	Bh	287/332 (86%)	277 (96%)	10 (4%)	0	100	100
34	Bi	258/306 (84%)	247 (96%)	11 (4%)	0	100	100
35	Bj	211/279 (76%)	199 (94%)	12 (6%)	0	100	100
36	Bk	151/269 (56%)	142 (94%)	8 (5%)	1 (1%)	18	51
37	Bl	131/166 (79%)	129 (98%)	2 (2%)	0	100	100
38	Bm	107/198 (54%)	103 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	Bn	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
40	Bo	95/124 (77%)	95 (100%)	0	0	100	100
41	Bp	95/112 (85%)	92 (97%)	3 (3%)	0	100	100
42	Bq	66/138 (48%)	62 (94%)	4 (6%)	0	100	100
43	Bt	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
44	Bu	147/205 (72%)	141 (96%)	5 (3%)	1 (1%)	18	51
45	Bv	133/222 (60%)	132 (99%)	1 (1%)	0	100	100
46	Bw	385/433 (89%)	362 (94%)	22 (6%)	1 (0%)	36	67
47	Bx	160/196 (82%)	152 (95%)	8 (5%)	0	100	100
49	B4	61/126 (48%)	51 (84%)	8 (13%)	2 (3%)	3	23
50	B5	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
51	B6	50/65 (77%)	50 (100%)	0	0	100	100
52	B7	44/95 (46%)	43 (98%)	1 (2%)	0	100	100
53	AB	218/289 (75%)	209 (96%)	9 (4%)	0	100	100
54	AC	130/167 (78%)	125 (96%)	5 (4%)	0	100	100
55	AE	341/430 (79%)	324 (95%)	17 (5%)	0	100	100
56	AF	120/276 (44%)	115 (96%)	5 (4%)	0	100	100
57	AG	204/240 (85%)	200 (98%)	4 (2%)	0	100	100
58	AI	326/397 (82%)	318 (98%)	8 (2%)	0	100	100
59	AJ	138/200 (69%)	129 (94%)	9 (6%)	0	100	100
60	AK	135/196 (69%)	125 (93%)	10 (7%)	0	100	100
61	AL	107/139 (77%)	101 (94%)	6 (6%)	0	100	100
62	AN	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
63	AO	173/239 (72%)	166 (96%)	7 (4%)	0	100	100
64	AP	115/135 (85%)	113 (98%)	2 (2%)	0	100	100
65	AQ	110/130 (85%)	108 (98%)	2 (2%)	0	100	100
66	AR	95/143 (66%)	93 (98%)	2 (2%)	0	100	100
67	AU	84/87 (97%)	84 (100%)	0	0	100	100
71	Aa	290/382 (76%)	282 (97%)	8 (3%)	0	100	100
72	Ab	133/190 (70%)	129 (97%)	4 (3%)	0	100	100
73	Ac	167/173 (96%)	163 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	Ad	175/205 (85%)	174 (99%)	1 (1%)	0	100	100
75	B8	93/188 (50%)	88 (95%)	5 (5%)	0	100	100
76	Ae	386/455 (85%)	354 (92%)	30 (8%)	2 (0%)	24	57
77	Af	97/188 (52%)	94 (97%)	3 (3%)	0	100	100
78	Ag	351/410 (86%)	338 (96%)	12 (3%)	1 (0%)	36	67
79	Ah	118/387 (30%)	117 (99%)	1 (1%)	0	100	100
80	Ai	97/106 (92%)	96 (99%)	1 (1%)	0	100	100
81	Aj	211/218 (97%)	206 (98%)	5 (2%)	0	100	100
82	Ak	273/325 (84%)	264 (97%)	9 (3%)	0	100	100
83	Am	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
84	An	70/199 (35%)	67 (96%)	3 (4%)	0	100	100
85	Ao	564/699 (81%)	540 (96%)	24 (4%)	0	100	100
86	Ap	188/258 (73%)	184 (98%)	3 (2%)	1 (0%)	24	57
87	B9	36/100 (36%)	36 (100%)	0	0	100	100
All	All	14349/19793 (72%)	13839 (96%)	495 (3%)	15 (0%)	49	79

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	BT	68	PRO
31	Bf	78	PRO
31	Bf	80	PRO
36	Bk	90	VAL
44	Bu	167	PRO
46	Bw	159	VAL
78	Ag	337	ASP
7	BE	317	PRO
76	Ae	342	PRO
86	Ap	52	LYS
49	B4	87	PRO
76	Ae	75	VAL
49	B4	86	SER
6	BD	208	ILE
12	BL	209	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	CL	30/157 (19%)	30 (100%)	0	100	100
1	DL	26/157 (17%)	26 (100%)	0	100	100
1	EL	27/157 (17%)	27 (100%)	0	100	100
1	FL	26/157 (17%)	26 (100%)	0	100	100
1	GL	26/157 (17%)	26 (100%)	0	100	100
1	HL	25/157 (16%)	25 (100%)	0	100	100
2	B0	90/115 (78%)	89 (99%)	1 (1%)	65	74
3	B1	219/229 (96%)	219 (100%)	0	100	100
4	B2	164/228 (72%)	164 (100%)	0	100	100
6	BD	167/248 (67%)	167 (100%)	0	100	100
7	BE	237/320 (74%)	237 (100%)	0	100	100
8	BF	194/251 (77%)	194 (100%)	0	100	100
9	BI	88/228 (39%)	88 (100%)	0	100	100
10	BJ	192/230 (84%)	191 (100%)	1 (0%)	81	80
11	BK	129/151 (85%)	129 (100%)	0	100	100
12	BL	218/318 (69%)	218 (100%)	0	100	100
13	BN	156/157 (99%)	155 (99%)	1 (1%)	78	79
14	BO	99/123 (80%)	99 (100%)	0	100	100
15	BP	245/249 (98%)	245 (100%)	0	100	100
16	BQ	190/210 (90%)	190 (100%)	0	100	100
17	BR	132/143 (92%)	132 (100%)	0	100	100
18	BS	123/153 (80%)	123 (100%)	0	100	100
19	BT	212/258 (82%)	212 (100%)	0	100	100
20	BU	118/127 (93%)	118 (100%)	0	100	100
21	BV	136/178 (76%)	136 (100%)	0	100	100
22	BW	144/180 (80%)	144 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	BX	116/134 (87%)	116 (100%)	0	100	100
24	BY	185/192 (96%)	185 (100%)	0	100	100
25	Ba	348/365 (95%)	348 (100%)	0	100	100
26	Bb	310/328 (94%)	310 (100%)	0	100	100
27	B3	110/150 (73%)	110 (100%)	0	100	100
28	Bc	271/299 (91%)	271 (100%)	0	100	100
29	Bd	127/181 (70%)	127 (100%)	0	100	100
30	Be	100/108 (93%)	100 (100%)	0	100	100
31	Bf	80/133 (60%)	80 (100%)	0	100	100
32	Bg	128/136 (94%)	128 (100%)	0	100	100
33	Bh	251/284 (88%)	251 (100%)	0	100	100
34	Bi	236/275 (86%)	236 (100%)	0	100	100
35	Bj	190/242 (78%)	189 (100%)	1 (0%)	81	80
36	Bk	135/226 (60%)	135 (100%)	0	100	100
37	Bl	122/147 (83%)	122 (100%)	0	100	100
38	Bm	103/178 (58%)	103 (100%)	0	100	100
39	Bn	88/113 (78%)	88 (100%)	0	100	100
40	Bo	77/97 (79%)	77 (100%)	0	100	100
41	Bp	79/88 (90%)	79 (100%)	0	100	100
42	Bq	50/114 (44%)	50 (100%)	0	100	100
43	Bt	75/82 (92%)	75 (100%)	0	100	100
44	Bu	126/177 (71%)	125 (99%)	1 (1%)	73	77
45	Bv	115/183 (63%)	115 (100%)	0	100	100
46	Bw	340/373 (91%)	340 (100%)	0	100	100
47	Bx	149/173 (86%)	149 (100%)	0	100	100
49	B4	45/114 (40%)	45 (100%)	0	100	100
50	B5	99/163 (61%)	99 (100%)	0	100	100
51	B6	49/60 (82%)	49 (100%)	0	100	100
52	B7	41/78 (53%)	41 (100%)	0	100	100
53	AB	187/233 (80%)	187 (100%)	0	100	100
54	AC	115/142 (81%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	AE	282/351 (80%)	282 (100%)	0	100	100
56	AF	107/210 (51%)	107 (100%)	0	100	100
57	AG	179/203 (88%)	179 (100%)	0	100	100
58	AI	273/333 (82%)	273 (100%)	0	100	100
59	AJ	130/180 (72%)	130 (100%)	0	100	100
60	AK	103/151 (68%)	103 (100%)	0	100	100
61	AL	92/116 (79%)	92 (100%)	0	100	100
62	AN	92/114 (81%)	92 (100%)	0	100	100
63	AO	159/205 (78%)	159 (100%)	0	100	100
64	AP	97/113 (86%)	97 (100%)	0	100	100
65	AQ	97/114 (85%)	97 (100%)	0	100	100
66	AR	89/127 (70%)	89 (100%)	0	100	100
67	AU	77/78 (99%)	77 (100%)	0	100	100
71	Aa	258/330 (78%)	258 (100%)	0	100	100
72	Ab	113/162 (70%)	113 (100%)	0	100	100
73	Ac	152/155 (98%)	152 (100%)	0	100	100
74	Ad	149/168 (89%)	148 (99%)	1 (1%)	76	78
75	B8	87/162 (54%)	87 (100%)	0	100	100
76	Ae	325/393 (83%)	323 (99%)	2 (1%)	78	79
77	Af	86/160 (54%)	86 (100%)	0	100	100
78	Ag	312/361 (86%)	312 (100%)	0	100	100
79	Ah	109/346 (32%)	109 (100%)	0	100	100
80	Ai	86/93 (92%)	86 (100%)	0	100	100
81	Aj	188/190 (99%)	188 (100%)	0	100	100
82	Ak	249/289 (86%)	249 (100%)	0	100	100
83	Am	100/102 (98%)	100 (100%)	0	100	100
84	An	66/174 (38%)	66 (100%)	0	100	100
85	Ao	478/611 (78%)	478 (100%)	0	100	100
86	Ap	170/225 (76%)	170 (100%)	0	100	100
87	B9	36/77 (47%)	36 (100%)	0	100	100
All	All	12601/16899 (75%)	12593 (100%)	8 (0%)	87	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B0	86	ASN
10	BJ	115	GLN
13	BN	40	GLN
35	Bj	198	ASN
44	Bu	159	GLU
74	Ad	172	ASN
76	Ae	399	GLN
76	Ae	424	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
2	B0	86	ASN
3	B1	27	HIS
3	B1	70	HIS
3	B1	93	ASN
4	B2	90	GLN
4	B2	159	GLN
4	B2	197	ASN
6	BD	116	HIS
6	BD	147	ASN
6	BD	183	HIS
6	BD	253	HIS
7	BE	139	ASN
7	BE	156	HIS
7	BE	277	ASN
7	BE	313	ASN
8	BF	241	ASN
9	BI	126	GLN
10	BJ	128	ASN
10	BJ	151	ASN
10	BJ	189	GLN
10	BJ	235	GLN
11	BK	28	GLN
11	BK	84	GLN
11	BK	116	HIS
12	BL	130	GLN
12	BL	190	HIS
12	BL	201	GLN
12	BL	230	ASN
13	BN	97	GLN

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Mol	Chain	Res	Type
14	BO	103	ASN
15	BP	120	GLN
15	BP	264	GLN
17	BR	69	ASN
17	BR	91	GLN
17	BR	98	GLN
18	BS	41	ASN
18	BS	55	ASN
18	BS	115	HIS
19	BT	107	HIS
19	BT	172	GLN
19	BT	175	GLN
20	BU	70	ASN
20	BU	77	GLN
20	BU	89	ASN
21	BV	179	GLN
22	BW	199	GLN
23	BX	11	GLN
25	Ba	119	GLN
25	Ba	186	GLN
25	Ba	343	GLN
25	Ba	358	GLN
25	Ba	360	ASN
26	Bb	266	HIS
26	Bb	307	HIS
26	Bb	354	GLN
27	B3	102	ASN
27	B3	115	HIS
28	Bc	46	ASN
28	Bc	228	GLN
28	Bc	294	GLN
30	Be	132	ASN
31	Bf	44	ASN
31	Bf	130	HIS
32	Bg	24	GLN
32	Bg	25	GLN
33	Bh	73	GLN
33	Bh	94	ASN
34	Bi	167	ASN
36	Bk	111	HIS
36	Bk	189	HIS
38	Bm	68	GLN

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Mol	Chain	Res	Type
38	Bm	111	HIS
38	Bm	120	GLN
39	Bn	120	HIS
40	Bo	108	ASN
43	Bt	30	GLN
44	Bu	145	ASN
45	Bv	51	GLN
46	Bw	71	HIS
46	Bw	101	ASN
46	Bw	104	ASN
46	Bw	107	GLN
46	Bw	173	GLN
46	Bw	379	GLN
46	Bw	381	ASN
46	Bw	403	ASN
47	Bx	58	GLN
47	Bx	69	GLN
49	B4	66	HIS
50	B5	83	ASN
50	B5	120	HIS
52	B7	57	GLN
53	AB	152	HIS
53	AB	265	GLN
54	AC	75	ASN
55	AE	137	HIS
55	AE	155	GLN
55	AE	211	ASN
55	AE	277	HIS
55	AE	344	ASN
55	AE	360	GLN
55	AE	415	GLN
57	AG	113	GLN
58	AI	87	HIS
58	AI	163	HIS
58	AI	175	HIS
58	AI	256	GLN
59	AJ	130	HIS
60	AK	89	HIS
60	AK	98	GLN
60	AK	148	HIS
62	AN	68	GLN
63	AO	213	GLN

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Mol	Chain	Res	Type
64	AP	123	GLN
71	Aa	132	GLN
71	Aa	161	ASN
71	Aa	216	GLN
72	Ab	36	ASN
73	Ac	122	GLN
74	Ad	155	GLN
74	Ad	159	GLN
75	B8	154	GLN
75	B8	181	GLN
77	Af	104	GLN
78	Ag	89	GLN
78	Ag	115	ASN
78	Ag	325	GLN
79	Ah	353	ASN
79	Ah	370	ASN
81	Aj	60	HIS
84	An	129	ASN
84	An	140	HIS
84	An	166	GLN
85	Ao	287	ASN
85	Ao	288	ASN
85	Ao	329	GLN
85	Ao	339	ASN
85	Ao	439	HIS
85	Ao	507	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
48	AA	959/962 (99%)	192 (20%)	1 (0%)
5	BB	64/73 (87%)	14 (21%)	0
68	AV	70/71 (98%)	26 (37%)	0
69	AX	8/9 (88%)	1 (12%)	0
88	BA	1542/1571 (98%)	418 (27%)	5 (0%)
All	All	2643/2686 (98%)	651 (24%)	6 (0%)

All (651) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	BB	3	U

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Mol	Chain	Res	Type
5	BB	5	A
5	BB	7	G
5	BB	8	U
5	BB	13	U
5	BB	21	C
5	BB	34	U
5	BB	43	C
5	BB	44	U
5	BB	46	G
5	BB	47	A
5	BB	48	U
5	BB	69	C
5	BB	70	A
48	AA	5	A
48	AA	10	U
48	AA	18	G
48	AA	27	U
48	AA	34	U
48	AA	42	A
48	AA	43	U
48	AA	49	A
48	AA	54	A
48	AA	58	U
48	AA	61	G
48	AA	65	C
48	AA	75	A
48	AA	78	C
48	AA	81	U
48	AA	83	C
48	AA	91	A
48	AA	98	A
48	AA	104	A
48	AA	115	A
48	AA	119	C
48	AA	120	A
48	AA	126	A
48	AA	137	A
48	AA	139	A
48	AA	147	G
48	AA	152	A
48	AA	161	C
48	AA	170	A

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Mol	Chain	Res	Type
48	AA	171	C
48	AA	173	G
48	AA	175	A
48	AA	186	U
48	AA	191	C
48	AA	194	U
48	AA	203	G
48	AA	209	C
48	AA	212	A
48	AA	216	A
48	AA	217	U
48	AA	219	U
48	AA	222	A
48	AA	223	U
48	AA	224	U
48	AA	231	G
48	AA	235	A
48	AA	237	U
48	AA	238	C
48	AA	244	C
48	AA	247	G
48	AA	253	G
48	AA	255	G
48	AA	257	U
48	AA	258	C
48	AA	273	A
48	AA	281	G
48	AA	287	C
48	AA	294	A
48	AA	297	A
48	AA	308	A
48	AA	309	A
48	AA	310	A
48	AA	314	A
48	AA	315	U
48	AA	316	C
48	AA	317	A
48	AA	320	A
48	AA	328	A
48	AA	330	A
48	AA	337	C
48	AA	345	U

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Mol	Chain	Res	Type
48	AA	353	C
48	AA	354	C
48	AA	362	A
48	AA	367	A
48	AA	368	A
48	AA	381	G
48	AA	395	C
48	AA	399	A
48	AA	407	U
48	AA	417	C
48	AA	421	A
48	AA	433	U
48	AA	455	A
48	AA	456	A
48	AA	457	C
48	AA	458	C
48	AA	461	A
48	AA	471	U
48	AA	472	A
48	AA	477	A
48	AA	479	C
48	AA	488	A
48	AA	502	A
48	AA	503	A
48	AA	504	C
48	AA	518	A
48	AA	523	C
48	AA	530	G
48	AA	531	U
48	AA	536	C
48	AA	538	C
48	AA	540	U
48	AA	561	U
48	AA	563	U
48	AA	564	A
48	AA	566	U
48	AA	571	A
48	AA	574	C
48	AA	576	C
48	AA	577	C
48	AA	578	G
48	AA	579	A

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Mol	Chain	Res	Type
48	AA	580	U
48	AA	589	C
48	AA	593	C
48	AA	594	C
48	AA	596	U
48	AA	597	U
48	AA	604	U
48	AA	616	C
48	AA	620	C
48	AA	625	U
48	AA	628	G
48	AA	638	A
48	AA	639	A
48	AA	641	A
48	AA	644	A
48	AA	645	A
48	AA	646	C
48	AA	647	A
48	AA	649	U
48	AA	650	A
48	AA	652	U
48	AA	665	A
48	AA	681	A
48	AA	682	G
48	AA	698	A
48	AA	699	U
48	AA	707	A
48	AA	709	A
48	AA	711	A
48	AA	722	A
48	AA	724	U
48	AA	731	A
48	AA	732	U
48	AA	739	A
48	AA	741	C
48	AA	742	C
48	AA	743	A
48	AA	753	A
48	AA	754	G
48	AA	766	C
48	AA	775	A
48	AA	790	A

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Mol	Chain	Res	Type
48	AA	791	G
48	AA	802	A
48	AA	807	G
48	AA	808	U
48	AA	823	G
48	AA	825	C
48	AA	841	C
48	AA	842	A
48	AA	863	G
48	AA	865	A
48	AA	869	A
48	AA	870	G
48	AA	874	U
48	AA	876	A
48	AA	877	A
48	AA	883	C
48	AA	885	U
48	AA	886	A
48	AA	887	U
48	AA	893	A
48	AA	899	C
48	AA	900	A
48	AA	903	C
48	AA	910	G
48	AA	918	A
48	AA	923	G
48	AA	925	A
48	AA	928	A
48	AA	930	G
48	AA	932	U
48	AA	943	G
48	AA	945	A
48	AA	946	A
48	AA	955	G
48	AA	956	G
48	AA	959	U
48	AA	960	A
68	AV	2	G
68	AV	4	A
68	AV	6	G
68	AV	8	U
68	AV	9	C

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Mol	Chain	Res	Type
68	AV	13	U
68	AV	14	A
68	AV	15	A
68	AV	16	A
68	AV	17	U
68	AV	18	A
68	AV	43	A
68	AV	44	U
68	AV	45	G
68	AV	46	U
68	AV	51	U
68	AV	52	A
68	AV	53	U
68	AV	54	A
68	AV	56	C
68	AV	63	G
68	AV	64	U
68	AV	65	A
68	AV	68	A
68	AV	69	C
68	AV	71	A
69	AX	7	C
88	BA	4	A
88	BA	7	G
88	BA	11	G
88	BA	19	U
88	BA	20	A
88	BA	21	C
88	BA	22	U
88	BA	27	A
88	BA	31	A
88	BA	32	C
88	BA	33	A
88	BA	36	A
88	BA	40	C
88	BA	41	A
88	BA	42	C
88	BA	45	A
88	BA	46	A
88	BA	49	A
88	BA	56	A
88	BA	57	A

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Mol	Chain	Res	Type
88	BA	59	A
88	BA	60	U
88	BA	63	A
88	BA	66	U
88	BA	67	A
88	BA	68	A
88	BA	75	A
88	BA	82	G
88	BA	83	A
88	BA	96	U
88	BA	97	A
88	BA	104	C
88	BA	105	G
88	BA	109	U
88	BA	115	U
88	BA	118	U
88	BA	122	G
88	BA	126	G
88	BA	129	A
88	BA	132	G
88	BA	135	G
88	BA	139	G
88	BA	140	A
88	BA	141	A
88	BA	142	U
88	BA	143	A
88	BA	147	U
88	BA	149	A
88	BA	153	U
88	BA	163	C
88	BA	164	A
88	BA	168	A
88	BA	172	C
88	BA	178	C
88	BA	179	U
88	BA	180	A
88	BA	186	U
88	BA	190	U
88	BA	192	A
88	BA	205	A
88	BA	218	A
88	BA	219	A

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Mol	Chain	Res	Type
88	BA	223	A
88	BA	224	A
88	BA	225	C
88	BA	228	U
88	BA	229	A
88	BA	231	C
88	BA	237	A
88	BA	238	C
88	BA	239	C
88	BA	243	A
88	BA	245	A
88	BA	254	G
88	BA	263	G
88	BA	271	U
88	BA	272	A
88	BA	273	A
88	BA	275	A
88	BA	277	A
88	BA	295	G
88	BA	309	A
88	BA	311	A
88	BA	312	C
88	BA	322	G
88	BA	323	A
88	BA	324	G
88	BA	329	A
88	BA	330	A
88	BA	331	A
88	BA	336	A
88	BA	337	A
88	BA	338	C
88	BA	339	G
88	BA	340	A
88	BA	352	G
88	BA	359	G
88	BA	366	A
88	BA	368	A
88	BA	369	G
88	BA	371	A
88	BA	372	U
88	BA	373	U
88	BA	374	U

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Mol	Chain	Res	Type
88	BA	376	A
88	BA	390	A
88	BA	393	A
88	BA	394	C
88	BA	398	A
88	BA	403	C
88	BA	404	C
88	BA	409	A
88	BA	414	A
88	BA	417	G
88	BA	427	G
88	BA	428	A
88	BA	429	G
88	BA	440	A
88	BA	445	A
88	BA	446	C
88	BA	448	G
88	BA	459	A
88	BA	460	C
88	BA	467	A
88	BA	468	A
88	BA	473	G
88	BA	474	A
88	BA	479	A
88	BA	480	G
88	BA	488	U
88	BA	490	U
88	BA	491	U
88	BA	492	A
88	BA	493	A
88	BA	494	U
88	BA	497	U
88	BA	500	C
88	BA	501	A
88	BA	503	A
88	BA	505	U
88	BA	506	A
88	BA	507	G
88	BA	514	A
88	BA	515	A
88	BA	516	G
88	BA	517	C

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Mol	Chain	Res	Type
88	BA	518	A
88	BA	526	A
88	BA	527	U
88	BA	530	A
88	BA	532	A
88	BA	533	A
88	BA	541	A
88	BA	545	U
88	BA	547	A
88	BA	548	A
88	BA	549	C
88	BA	552	A
88	BA	553	U
88	BA	554	U
88	BA	557	C
88	BA	560	A
88	BA	561	C
88	BA	562	A
88	BA	563	U
88	BA	570	A
88	BA	574	A
88	BA	576	U
88	BA	578	A
88	BA	579	U
88	BA	584	A
88	BA	586	C
88	BA	592	G
88	BA	595	C
88	BA	596	A
88	BA	617	A
88	BA	618	A
88	BA	625	A
88	BA	631	A
88	BA	634	G
88	BA	640	A
88	BA	648	C
88	BA	649	A
88	BA	650	A
88	BA	660	C
88	BA	665	C
88	BA	673	C
88	BA	683	U

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Mol	Chain	Res	Type
88	BA	684	A
88	BA	689	A
88	BA	691	A
88	BA	693	U
88	BA	694	A
88	BA	695	U
88	BA	697	C
88	BA	704	U
88	BA	707	A
88	BA	713	A
88	BA	714	A
88	BA	718	A
88	BA	719	C
88	BA	720	C
88	BA	722	A
88	BA	723	A
88	BA	724	A
88	BA	725	C
88	BA	727	A
88	BA	728	C
88	BA	737	G
88	BA	743	U
88	BA	744	A
88	BA	745	A
88	BA	746	U
88	BA	747	U
88	BA	748	A
88	BA	753	G
88	BA	761	A
88	BA	763	C
88	BA	764	A
88	BA	773	C
88	BA	775	C
88	BA	777	A
88	BA	778	A
88	BA	780	G
88	BA	782	A
88	BA	825	C
88	BA	828	G
88	BA	834	C
88	BA	847	U
88	BA	848	C

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Mol	Chain	Res	Type
88	BA	849	U
88	BA	851	G
88	BA	852	C
88	BA	853	A
88	BA	854	U
88	BA	855	U
88	BA	856	A
88	BA	859	A
88	BA	864	U
88	BA	868	G
88	BA	872	A
88	BA	883	G
88	BA	889	C
88	BA	892	G
88	BA	896	A
88	BA	897	A
88	BA	899	G
88	BA	902	C
88	BA	908	A
88	BA	909	U
88	BA	911	C
88	BA	922	A
88	BA	923	A
88	BA	924	G
88	BA	925	G
88	BA	933	A
88	BA	935	C
88	BA	938	U
88	BA	939	U
88	BA	948	A
88	BA	950	U
88	BA	958	U
88	BA	959	G
88	BA	960	U
88	BA	961	A
88	BA	962	U
88	BA	964	A
88	BA	965	A
88	BA	967	G
88	BA	970	C
88	BA	977	G
88	BA	981	U

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Mol	Chain	Res	Type
88	BA	983	U
88	BA	986	U
88	BA	987	G
88	BA	992	U
88	BA	1015	C
88	BA	1016	C
88	BA	1018	U
88	BA	1026	A
88	BA	1027	G
88	BA	1028	A
88	BA	1034	G
88	BA	1038	A
88	BA	1041	A
88	BA	1045	U
88	BA	1050	C
88	BA	1055	A
88	BA	1056	G
88	BA	1057	A
88	BA	1063	U
88	BA	1064	G
88	BA	1071	U
88	BA	1072	A
88	BA	1074	U
88	BA	1081	U
88	BA	1089	G
88	BA	1092	A
88	BA	1093	A
88	BA	1127	A
88	BA	1137	A
88	BA	1138	G
88	BA	1140	A
88	BA	1146	G
88	BA	1167	C
88	BA	1168	A
88	BA	1169	A
88	BA	1180	G
88	BA	1183	U
88	BA	1188	U
88	BA	1194	U
88	BA	1195	A
88	BA	1201	A
88	BA	1204	A

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Mol	Chain	Res	Type
88	BA	1206	U
88	BA	1207	C
88	BA	1215	C
88	BA	1217	A
88	BA	1218	U
88	BA	1219	A
88	BA	1220	A
88	BA	1221	C
88	BA	1222	A
88	BA	1226	C
88	BA	1233	A
88	BA	1238	A
88	BA	1239	A
88	BA	1240	A
88	BA	1241	U
88	BA	1242	U
88	BA	1246	A
88	BA	1247	U
88	BA	1248	C
88	BA	1249	A
88	BA	1252	G
88	BA	1253	G
88	BA	1254	A
88	BA	1258	A
88	BA	1264	C
88	BA	1268	G
88	BA	1271	A
88	BA	1287	G
88	BA	1288	U
88	BA	1291	U
88	BA	1292	A
88	BA	1294	A
88	BA	1296	U
88	BA	1298	C
88	BA	1299	C
88	BA	1303	C
88	BA	1314	U
88	BA	1325	G
88	BA	1326	A
88	BA	1328	G
88	BA	1332	G
88	BA	1336	A

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Mol	Chain	Res	Type
88	BA	1341	A
88	BA	1342	C
88	BA	1352	G
88	BA	1353	C
88	BA	1358	G
88	BA	1385	U
88	BA	1387	A
88	BA	1388	A
88	BA	1389	A
88	BA	1390	G
88	BA	1395	A
88	BA	1396	C
88	BA	1405	A
88	BA	1413	C
88	BA	1420	A
88	BA	1425	A
88	BA	1426	G
88	BA	1428	U
88	BA	1432	U
88	BA	1433	U
88	BA	1436	U
88	BA	1438	U
88	BA	1445	U
88	BA	1448	A
88	BA	1457	A
88	BA	1458	G
88	BA	1459	U
88	BA	1466	G
88	BA	1468	A
88	BA	1474	G
88	BA	1475	A
88	BA	1476	A
88	BA	1482	A
88	BA	1485	A
88	BA	1492	C
88	BA	1493	A
88	BA	1494	A
88	BA	1498	C
88	BA	1504	A
88	BA	1505	G
88	BA	1509	U
88	BA	1514	A

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Mol	Chain	Res	Type
88	BA	1521	U
88	BA	1522	A
88	BA	1525	C
88	BA	1526	U
88	BA	1527	U
88	BA	1528	A
88	BA	1531	C
88	BA	1532	U
88	BA	1533	A
88	BA	1536	U
88	BA	1538	A
88	BA	1548	A
88	BA	1549	A
88	BA	1551	C
88	BA	1552	C
88	BA	1553	A
88	BA	1558	U
88	BA	1559	A
88	BA	1570	C
88	BA	1571	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	AA	917	C
88	BA	48	U
88	BA	1145	C
88	BA	1219	A
88	BA	1220	A
88	BA	1241	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 335 ligands modelled in this entry, 329 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	GTP	Ag	500	89	30,34,34	0.86	2 (6%)	46,54,54	1.78	11 (23%)
93	5GP	BA	1791	-	26,26,26	0.98	2 (7%)	40,40,40	1.77	8 (20%)
93	5GP	BA	1792	89	26,26,26	0.99	2 (7%)	40,40,40	1.69	8 (20%)
91	SPM	AA	3001	-	13,13,13	0.33	0	12,12,12	0.77	0
91	SPM	BA	1793	-	13,13,13	0.32	0	12,12,12	0.79	0
91	SPM	BA	1794	-	13,13,13	0.34	0	12,12,12	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	GTP	Ag	500	89	-	2/22/38/38	0/3/3/3
93	5GP	BA	1791	-	-	2/10/26/26	0/3/3/3
93	5GP	BA	1792	89	-	0/10/26/26	0/3/3/3
91	SPM	AA	3001	-	-	3/11/11/11	-
91	SPM	BA	1793	-	-	3/11/11/11	-
91	SPM	BA	1794	-	-	3/11/11/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
93	BA	1791	5GP	C6-N1	-2.57	1.34	1.38
93	BA	1792	5GP	C6-N1	-2.54	1.34	1.38
92	Ag	500	GTP	C2-N3	2.23	1.38	1.33
92	Ag	500	GTP	C5-N7	-2.05	1.35	1.39
93	BA	1791	5GP	C5-N7	-2.04	1.35	1.39
93	BA	1792	5GP	C5-N7	-2.01	1.35	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
93	BA	1791	5GP	C5-C4-N3	-6.06	118.62	128.46
93	BA	1792	5GP	C5-C4-N3	-5.67	119.27	128.46
92	Ag	500	GTP	C5-C4-N3	-5.34	119.79	128.46
93	BA	1791	5GP	C2-N3-C4	4.65	120.58	112.30
92	Ag	500	GTP	C2-N3-C4	4.55	120.41	112.30
93	BA	1792	5GP	C2-N3-C4	4.36	120.07	112.30
93	BA	1791	5GP	N9-C4-N3	3.92	133.81	125.94
92	Ag	500	GTP	N9-C4-N3	3.67	133.32	125.94
93	BA	1792	5GP	N9-C4-N3	3.53	133.03	125.94
92	Ag	500	GTP	PA-O3A-PB	-3.44	121.03	132.83
92	Ag	500	GTP	PB-O3B-PG	-3.21	121.82	132.83
92	Ag	500	GTP	C2-N1-C6	-2.97	119.68	125.10
92	Ag	500	GTP	O6-C6-C5	-2.64	119.61	126.60
92	Ag	500	GTP	C5-C6-N1	2.53	119.60	113.19
93	BA	1791	5GP	C5-C6-N1	2.52	119.60	113.19
93	BA	1792	5GP	C5-C6-N1	2.50	119.55	113.19
93	BA	1792	5GP	O6-C6-C5	-2.44	120.13	126.60
93	BA	1791	5GP	C2-N1-C6	-2.40	120.72	125.10
93	BA	1792	5GP	C2-N1-C6	-2.33	120.85	125.10
93	BA	1791	5GP	O6-C6-C5	-2.33	120.42	126.60
92	Ag	500	GTP	C8-N7-C5	2.28	108.37	104.24
92	Ag	500	GTP	N9-C8-N7	-2.24	109.17	113.39
93	BA	1792	5GP	N9-C8-N7	-2.21	109.22	113.39
93	BA	1791	5GP	N9-C8-N7	-2.17	109.31	113.39
92	Ag	500	GTP	C3'-C2'-C1'	2.07	105.36	101.43
93	BA	1791	5GP	C4-C5-N7	-2.04	107.49	110.72
93	BA	1792	5GP	C4-C5-N7	-2.04	107.50	110.72

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
93	BA	1791	5GP	O4'-C4'-C5'-O5'
91	BA	1794	SPM	C12-C11-N10-C9
91	AA	3001	SPM	C7-C8-C9-N10
91	BA	1794	SPM	C6-C7-C8-C9
93	BA	1791	5GP	C3'-C4'-C5'-O5'
91	AA	3001	SPM	C6-C7-C8-C9
92	Ag	500	GTP	O4'-C4'-C5'-O5'
91	BA	1793	SPM	C7-C8-C9-N10
91	BA	1793	SPM	N5-C6-C7-C8

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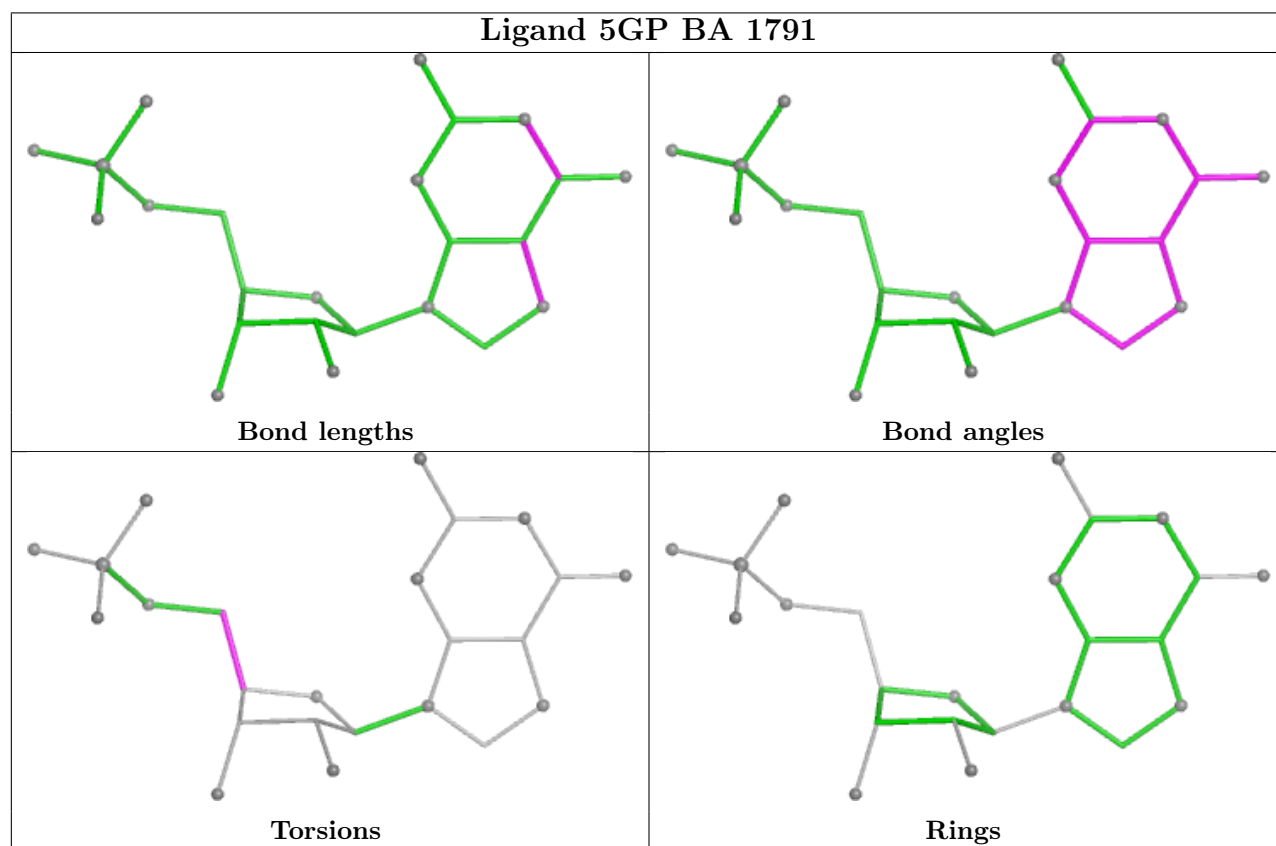
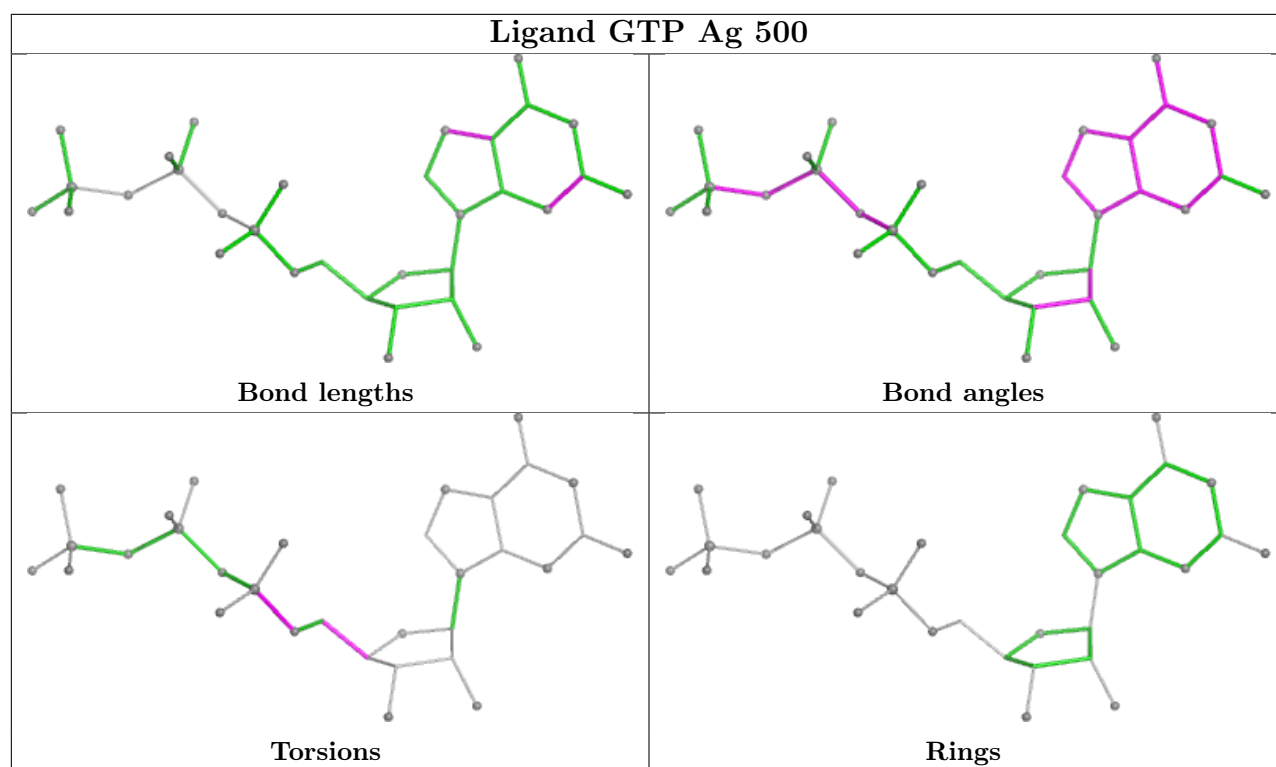
Mol	Chain	Res	Type	Atoms
91	BA	1793	SPM	C7-C6-N5-C4
91	AA	3001	SPM	C7-C6-N5-C4
92	Ag	500	GTP	C5'-O5'-PA-O1A
91	BA	1794	SPM	C8-C9-N10-C11

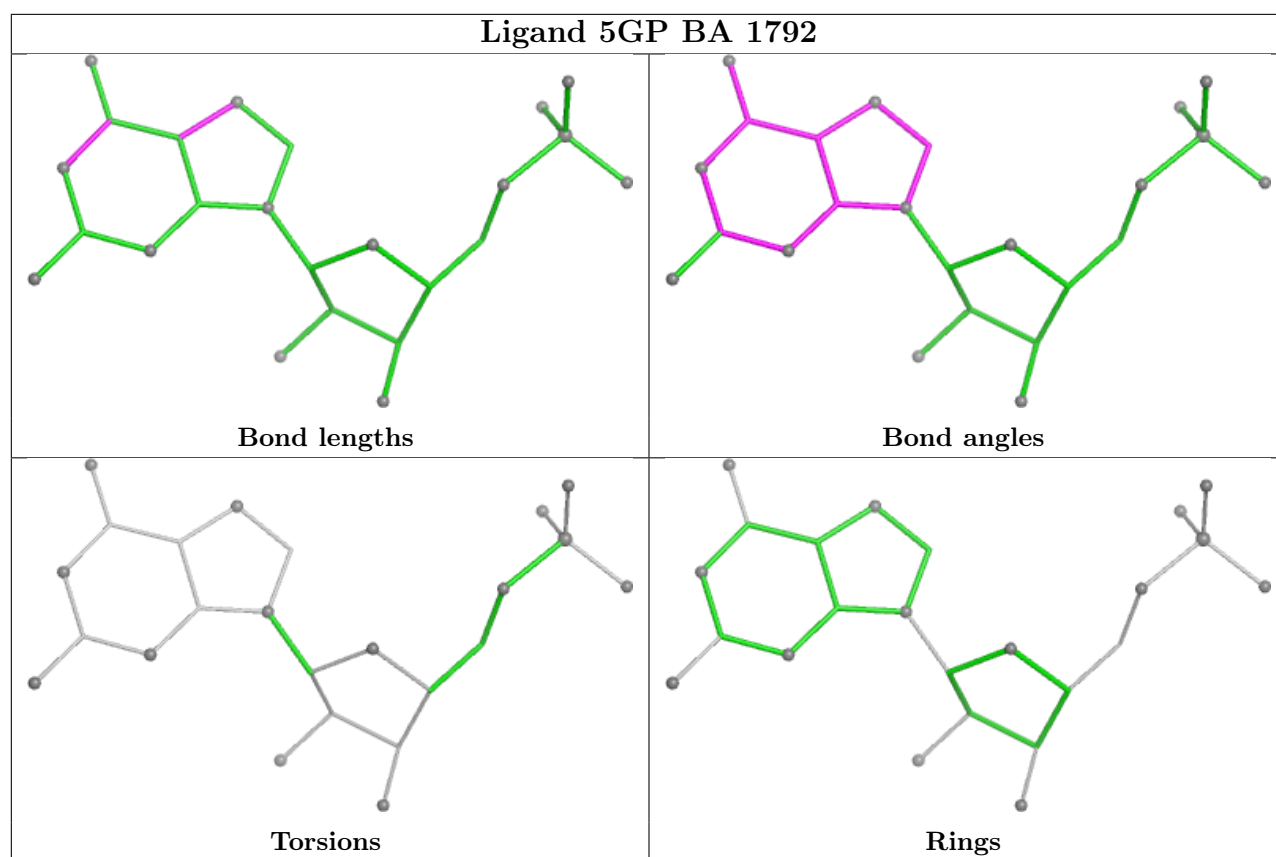
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	Ag	500	GTP	3	0
91	BA	1793	SPM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

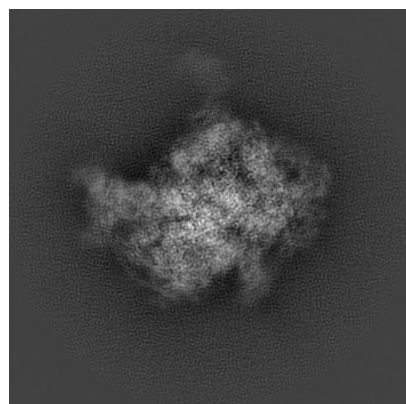
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12527. These allow visual inspection of the internal detail of the map and identification of artifacts.

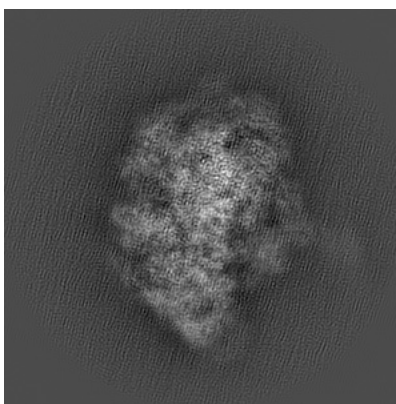
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

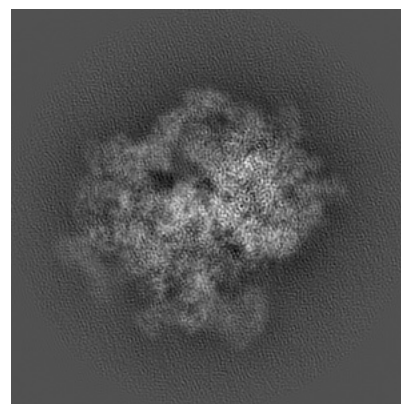
6.1.1 Primary map



X

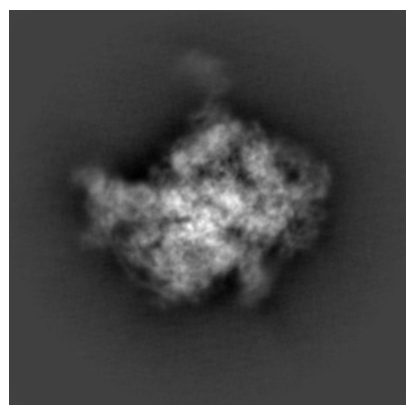


Y

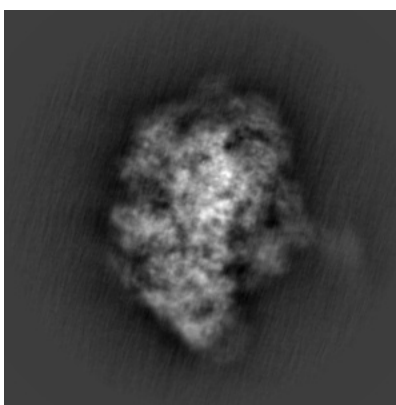


Z

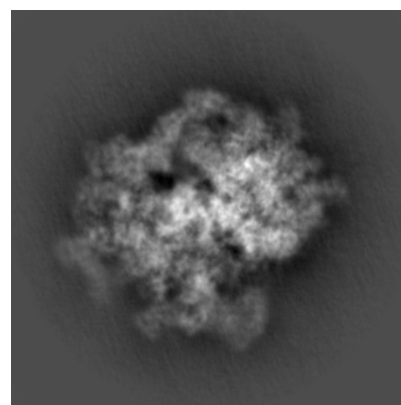
6.1.2 Raw map



X



Y

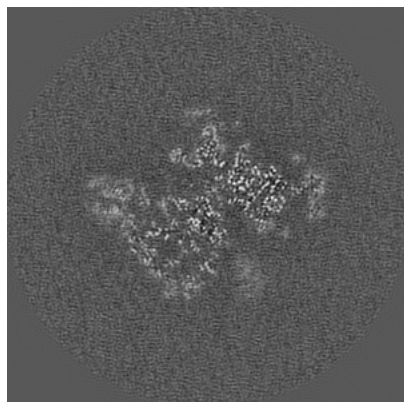


Z

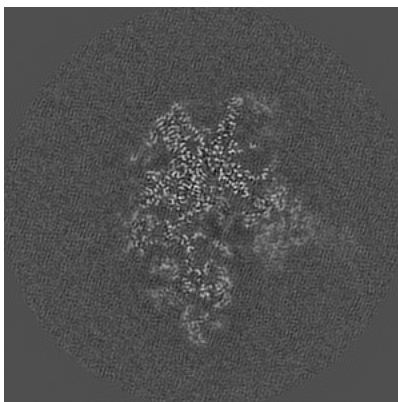
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

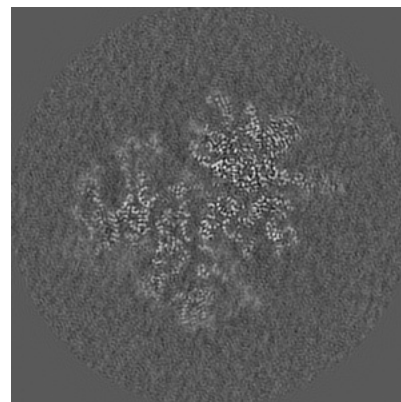
6.2.1 Primary map



X Index: 160

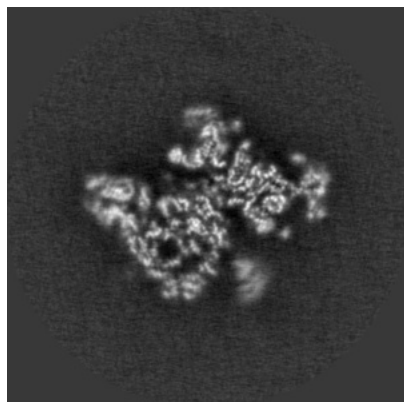


Y Index: 160

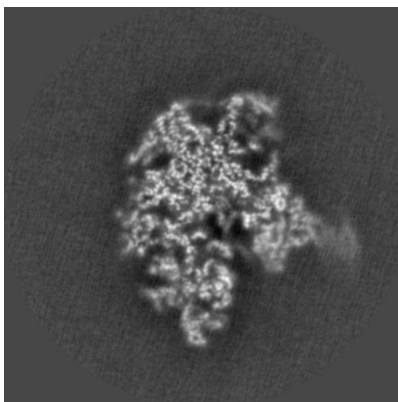


Z Index: 160

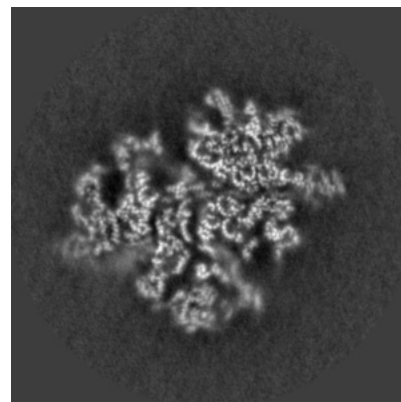
6.2.2 Raw map



X Index: 160



Y Index: 160

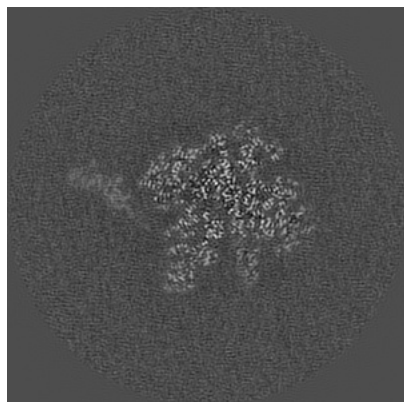


Z Index: 160

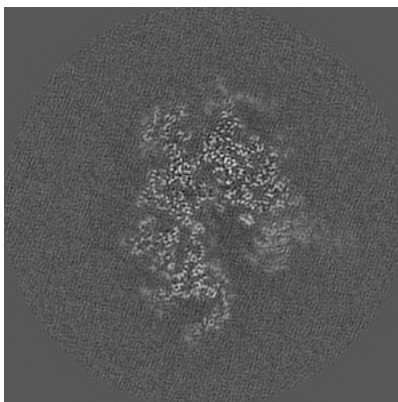
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

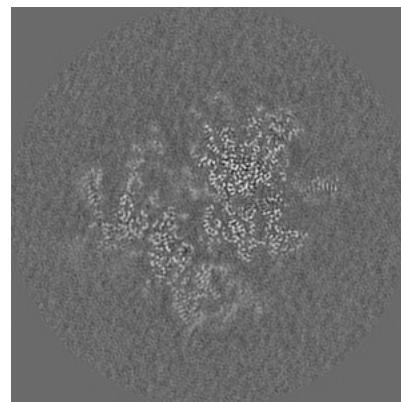
6.3.1 Primary map



X Index: 187

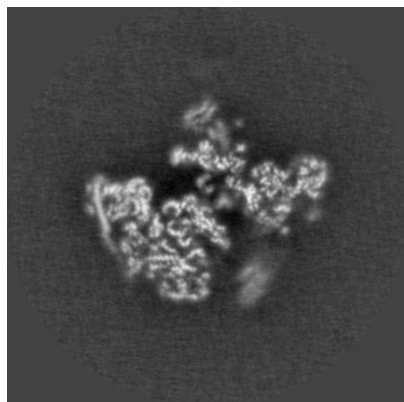


Y Index: 165

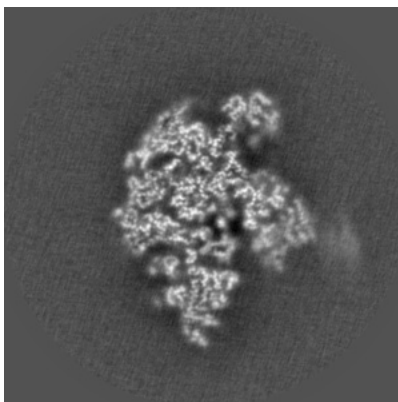


Z Index: 165

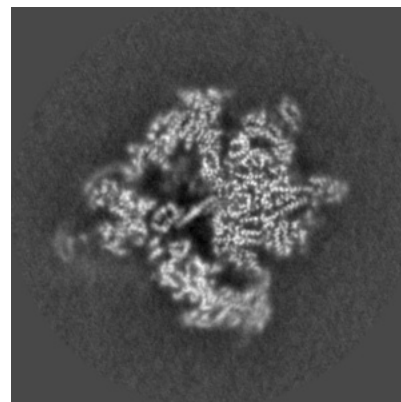
6.3.2 Raw map



X Index: 154



Y Index: 156

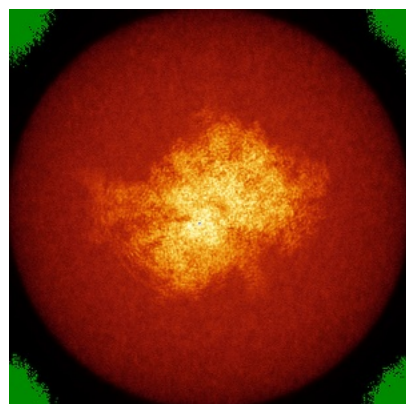


Z Index: 174

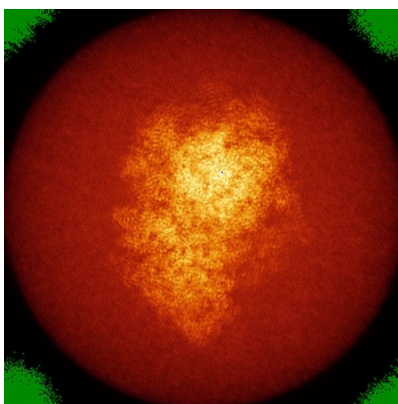
The images above show the largest variance slices of the map in three orthogonal directions.

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

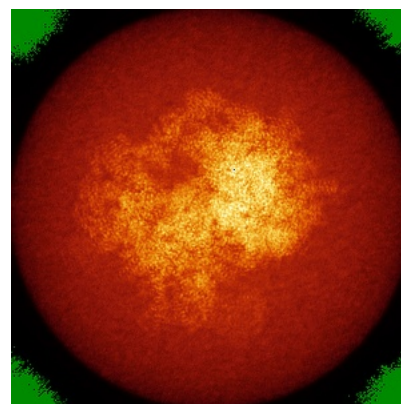
6.4.1 Primary map



X

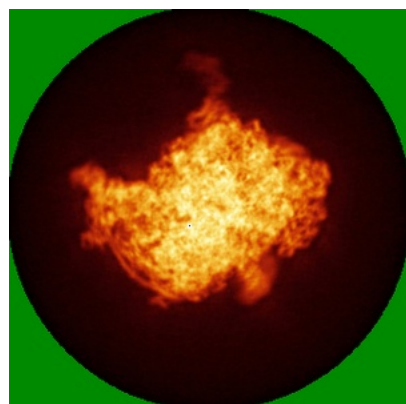


Y

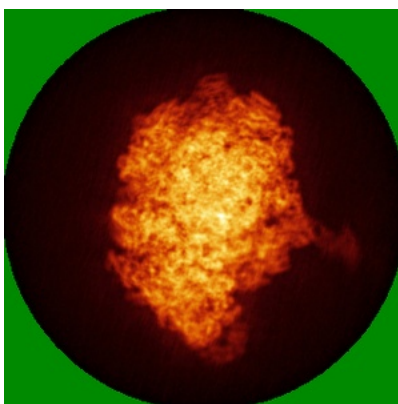


Z

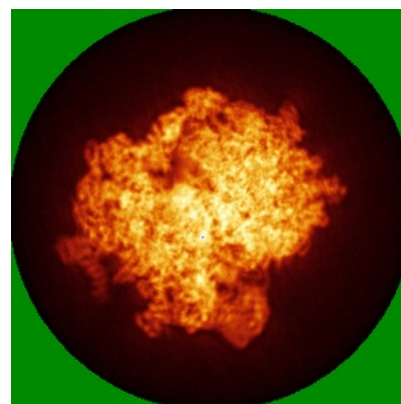
6.4.2 Raw map



X



Y

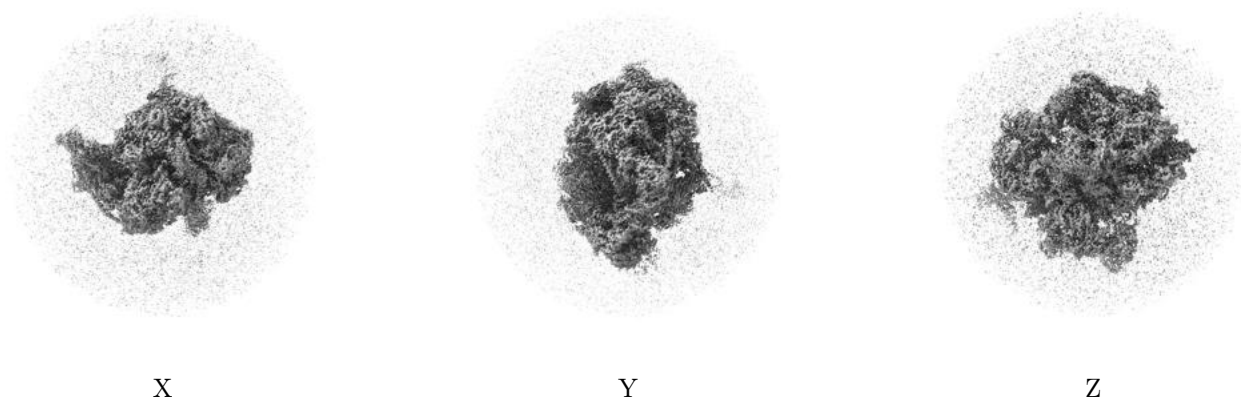


Z

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

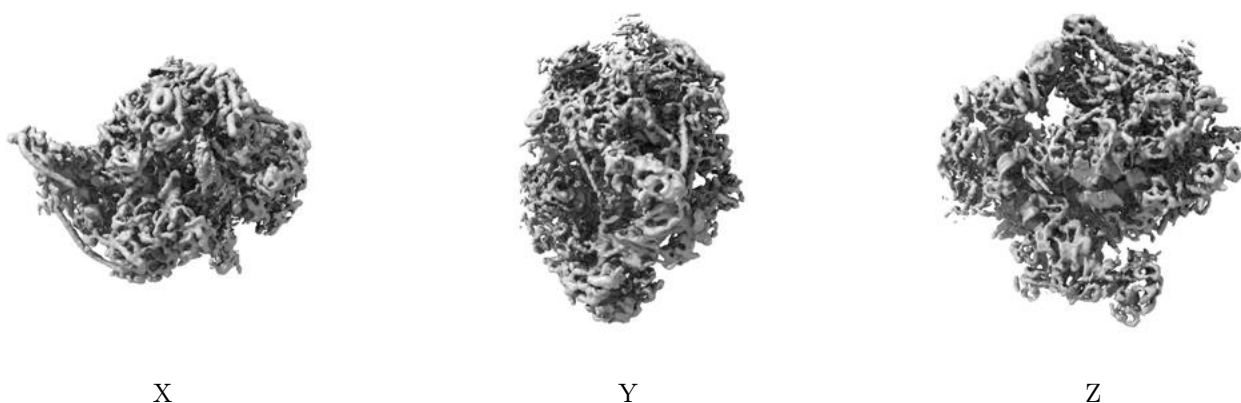
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

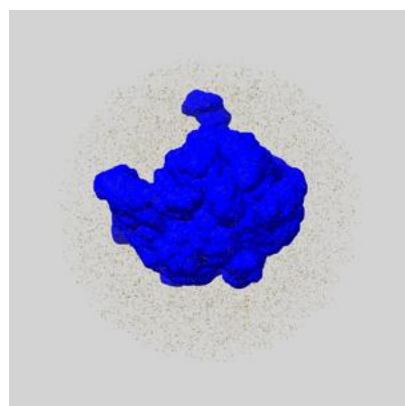
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

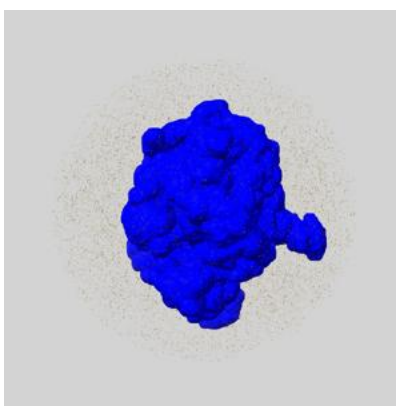
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

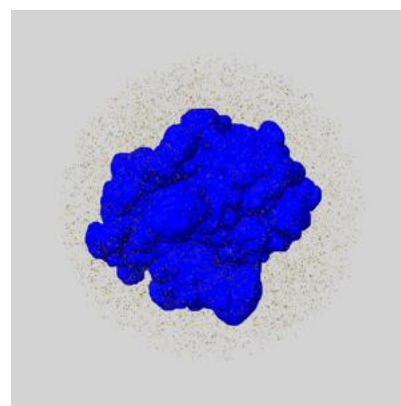
6.6.1 emd_12527_msk_1.map [i](#)



X



Y

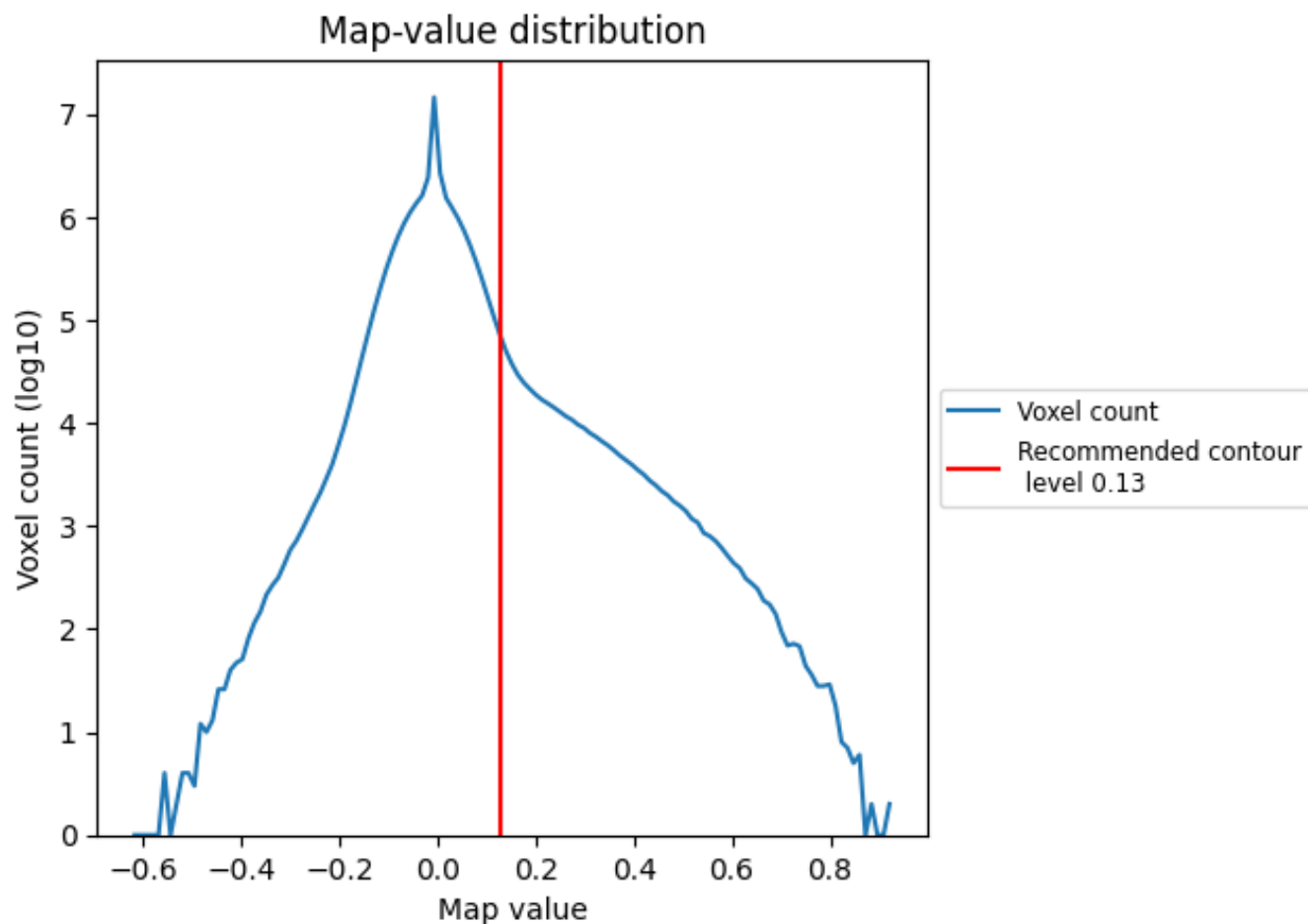


Z

7 Map analysis [i](#)

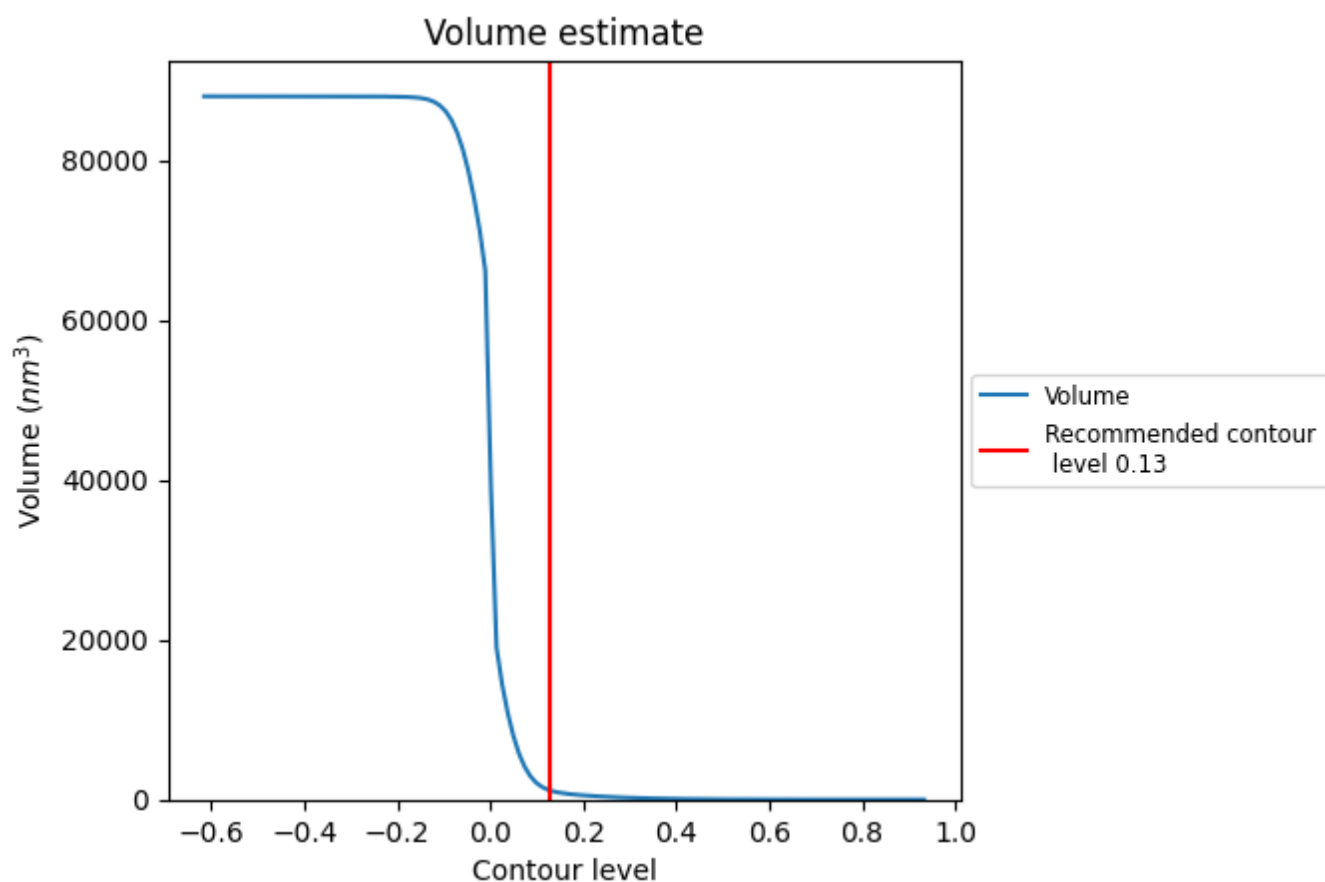
This section contains the results of statistical analysis of the map.

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.

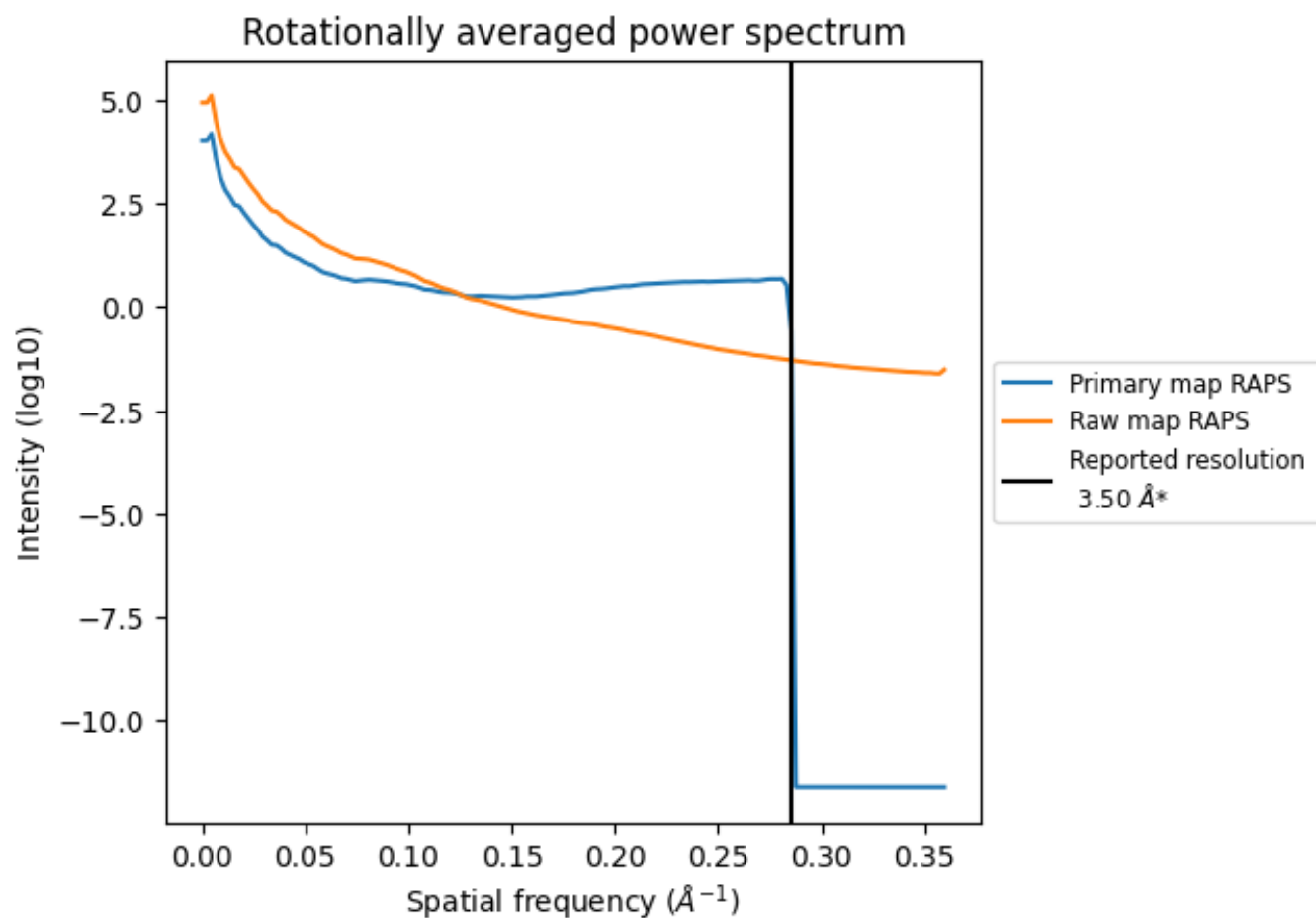
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1125 nm³; this corresponds to an approximate mass of 1016 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 ⓘ

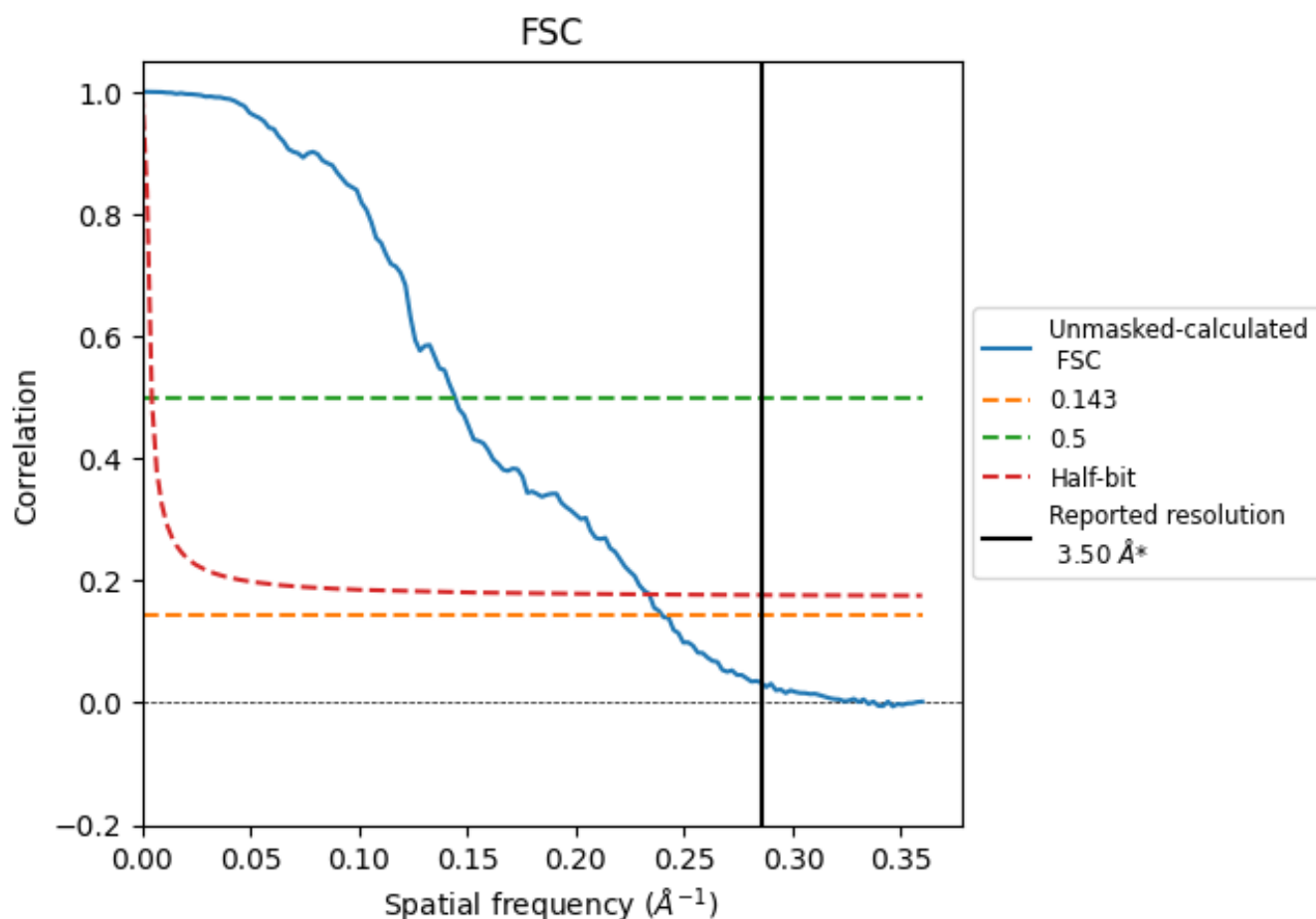


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

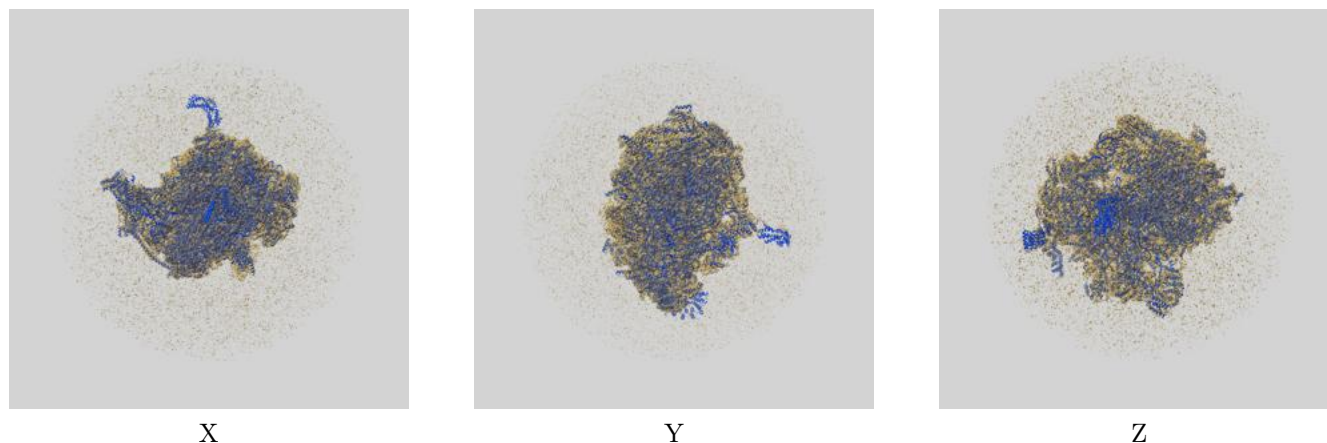
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.17	6.93	4.28

*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 4.17 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

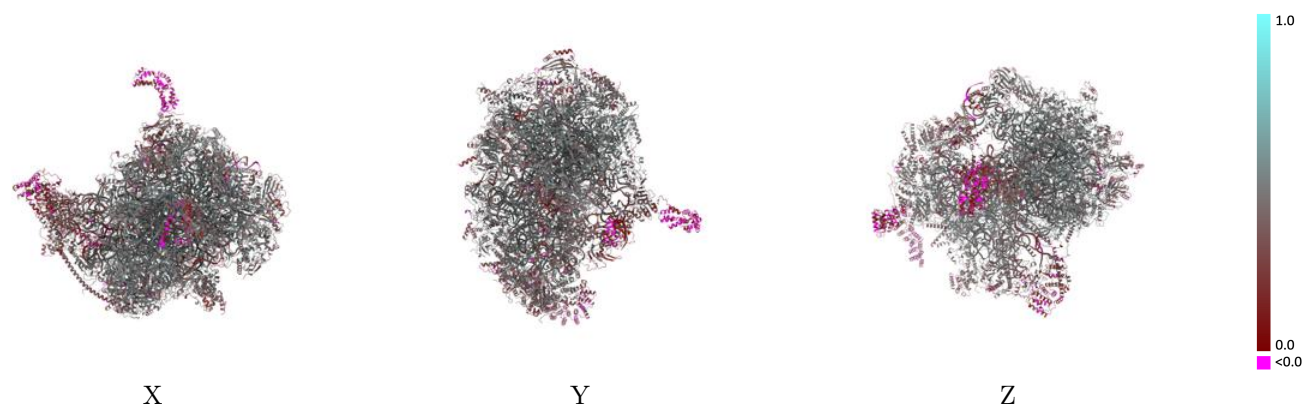
This section contains information regarding the fit between EMDB map EMD-12527 and PDB model 7NQH. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



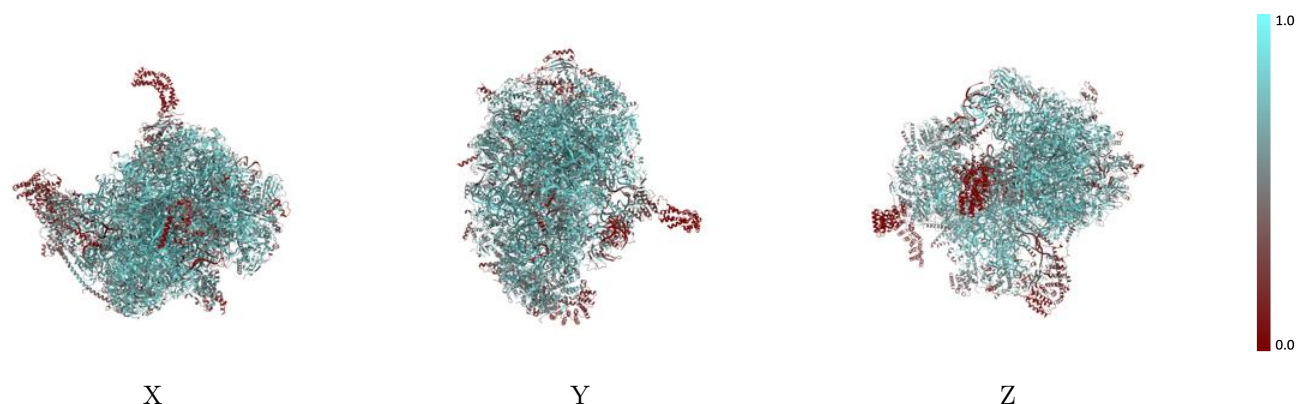
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



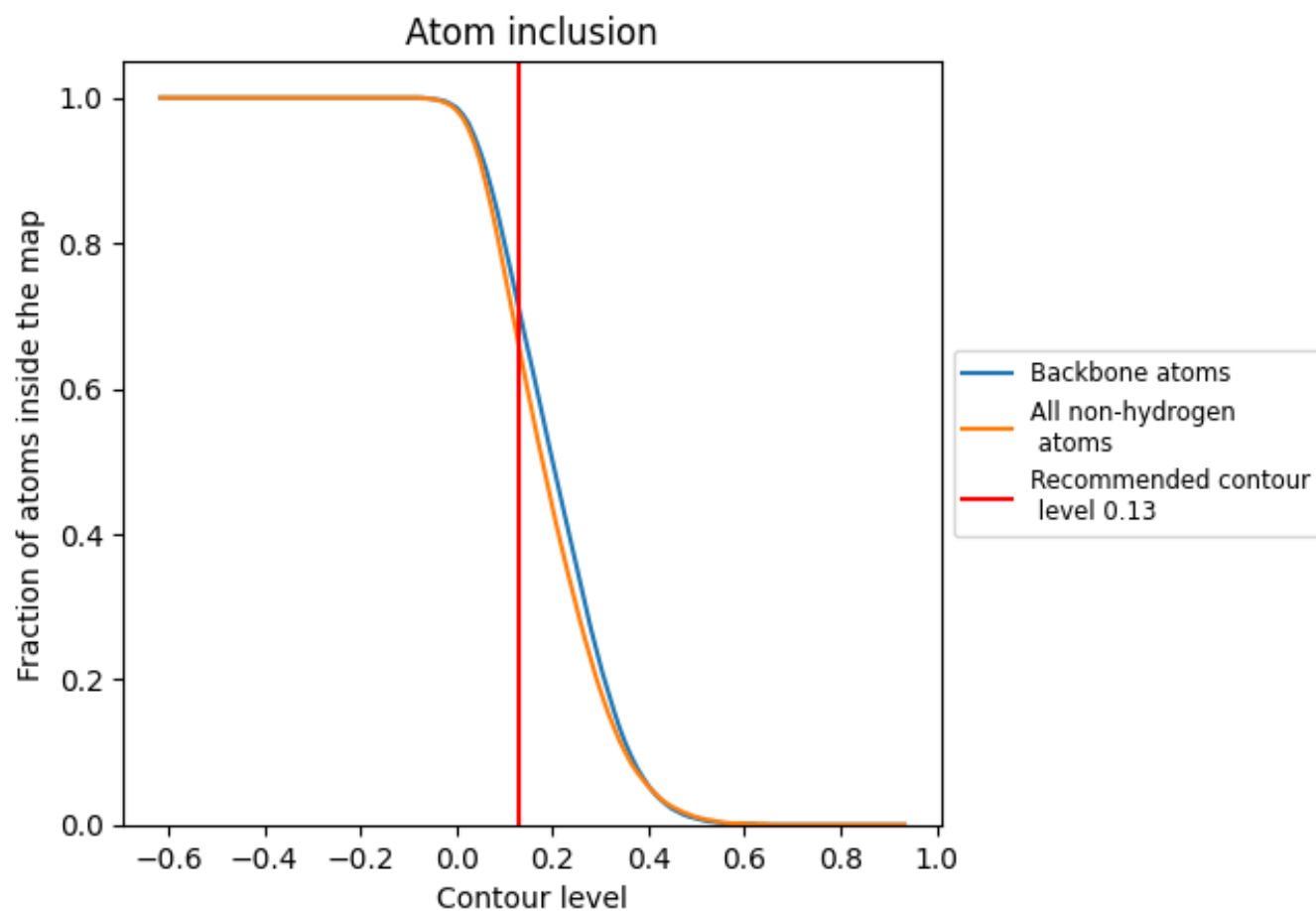
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6580	 0.4210
AA	 0.8040	 0.4400
AB	 0.6810	 0.4490
AC	 0.6630	 0.4700
AE	 0.6060	 0.4490
AF	 0.6660	 0.4600
AG	 0.6420	 0.4280
AI	 0.6020	 0.4120
AJ	 0.6050	 0.4060
AK	 0.6800	 0.4510
AL	 0.7170	 0.4850
AN	 0.7280	 0.4830
AO	 0.5940	 0.4180
AP	 0.5850	 0.4010
AQ	 0.6460	 0.4440
AR	 0.6730	 0.4640
AU	 0.7220	 0.4760
AV	 0.6400	 0.3540
AX	 0.8030	 0.4770
AZ	 0.4890	 0.2550
Aa	 0.4690	 0.3540
Ab	 0.5090	 0.3780
Ac	 0.6380	 0.4300
Ad	 0.5410	 0.3620
Ae	 0.2310	 0.1960
Af	 0.6020	 0.4340
Ag	 0.6050	 0.3830
Ah	 0.5420	 0.3590
Ai	 0.6280	 0.4340
Aj	 0.4020	 0.3200
Ak	 0.5700	 0.3960
Am	 0.5990	 0.4200
An	 0.6790	 0.4730
Ao	 0.1210	 0.1730
Ap	 0.5870	 0.4050



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Chain	Atom inclusion	Q-score
B0	 0.7780	 0.5170
B1	 0.5980	 0.4480
B2	 0.6950	 0.4680
B3	 0.7570	 0.5040
B4	 0.6200	 0.3890
B5	 0.7160	 0.4780
B6	 0.4420	 0.4050
B7	 0.8210	 0.5380
B8	 0.7890	 0.5150
B9	 0.8220	 0.5150
BA	 0.8230	 0.4640
BB	 0.5380	 0.2700
BD	 0.7460	 0.4970
BE	 0.7430	 0.4830
BF	 0.7560	 0.4890
BI	 0.5350	 0.4050
BJ	 0.3540	 0.3030
BK	 0.1990	 0.2230
BL	 0.5050	 0.3960
BN	 0.7710	 0.5030
BO	 0.7240	 0.4860
BP	 0.7290	 0.4800
BQ	 0.7250	 0.4780
BR	 0.7500	 0.4890
BS	 0.7440	 0.4790
BT	 0.6620	 0.4460
BU	 0.7580	 0.4980
BV	 0.7350	 0.4920
BW	 0.7490	 0.5070
BX	 0.6600	 0.4470
BY	 0.4730	 0.3890
Ba	 0.7030	 0.4580
Bb	 0.6970	 0.4330
Bc	 0.6260	 0.4140
Bd	 0.5540	 0.3790
Be	 0.5920	 0.4160
Bf	 0.6750	 0.4500
Bg	 0.7470	 0.4940
Bh	 0.6810	 0.4430
Bi	 0.4040	 0.3380
Bj	 0.4730	 0.3060
Bk	 0.5670	 0.3950

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Chain	Atom inclusion	Q-score
Bl	 0.7340	 0.4650
Bm	 0.3950	 0.3760
Bn	 0.7720	 0.4990
Bo	 0.6910	 0.4400
Bp	 0.4020	 0.3190
Bq	 0.4060	 0.3030
Bt	 0.7670	 0.4970
Bu	 0.4990	 0.3670
Bv	 0.4970	 0.3860
Bw	 0.7000	 0.4570
Bx	 0.6900	 0.4400
CL	 0.0160	 0.0630
DL	 0.0000	 -0.0080
EL	 0.0090	 0.0110
FL	 0.0050	 0.0280
GL	 0.0090	 0.0450
HL	 0.0000	 0.0150