



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 06:02 PM UTC

PDB ID : 8OIR / pdb_00008oir
EMDB ID : EMD-16897
Title : 55S human mitochondrial ribosome with mtRF1 and P-site tRNA
Authors : Saurer, M.; Leibundgut, M.; Scaiola, A.; Schoenhut, T.; Ban, N.
Deposited on : 2023-03-23
Resolution : 3.10 Å(reported)
Based on initial models : ., 7QI4

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

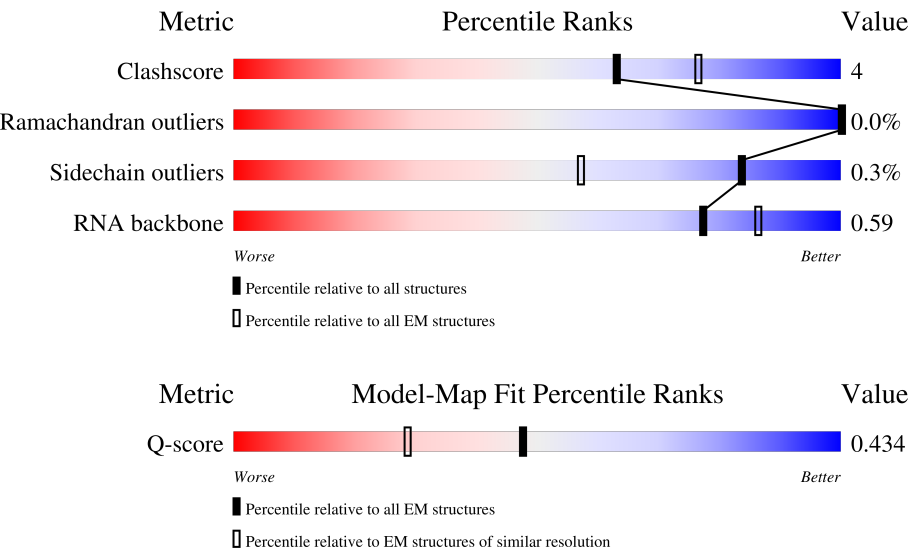
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 3.10 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	14724 (2.60 - 3.60)

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	B1	198	
1	B2	198	
1	B3	198	

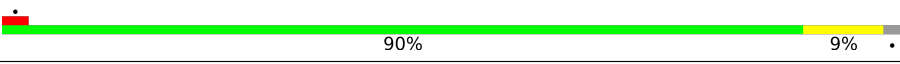
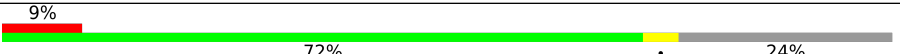
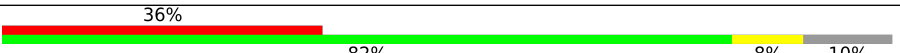
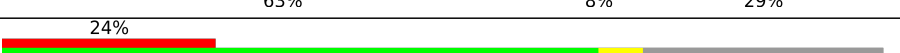
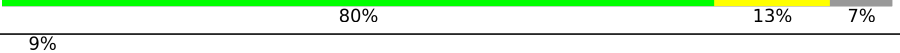
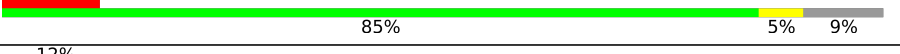
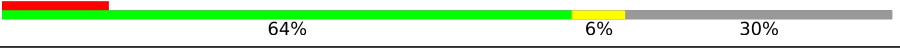
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Mol	Chain	Length	Quality of chain
1	B4	198	
1	B5	198	
1	B6	198	
2	B7	3	
3	B8	1561	
4	B9	72	
5	BA	206	
6	BB	153	
7	BC	216	
8	BD	148	
9	BE	256	
10	BF	250	
11	BG	161	
12	BH	188	
13	BI	65	
14	BJ	92	
15	BK	188	
16	BL	305	
17	BM	348	
18	BN	311	
19	BO	267	
20	BP	261	
21	BQ	192	
22	BR	178	
23	BS	145	

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Mol	Chain	Length	Quality of chain
24	BT	296	
25	BU	251	
26	BV	175	
27	BW	180	
28	BX	292	
29	BY	149	
30	BZ	205	
31	Ba	123	
32	Bb	112	
33	Bc	138	
34	Bd	128	
35	Be	102	
36	Bf	206	
37	Bg	222	
38	Bh	196	
39	Bi	439	
40	Bj	325	
41	Bl	103	
42	Bm	423	
43	Bn	380	
44	Bo	338	
45	Bp	206	
46	Bq	137	
47	Br	142	
48	Bs	215	

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Mol	Chain	Length	Quality of chain
49	Bt	332	
50	Bu	306	
51	Bv	279	
52	Bw	212	
53	Bx	166	
54	By	158	
55	Bz	128	
56	AA	955	
57	AB	323	
58	AC	167	
59	AD	199	
60	AE	125	
61	AF	242	
62	AG	71	
63	AH	201	
64	AI	33	
65	AJ	138	
66	AK	128	
67	AL	257	
68	AM	137	
69	AN	130	
70	AO	258	
71	AP	142	
72	AQ	87	
73	AR	360	

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Mol	Chain	Length	Quality of chain
74	AS	190	
75	AT	173	
76	AU	205	
77	AV	414	
78	AW	187	
79	AX	398	
80	AY	395	
81	AZ	106	
82	Aa	484	
83	Ab	296	
84	Ac	118	
85	Ad	430	
86	Ae	689	
87	Ag	396	
88	Ai	194	
89	Aj	218	

2 Entry composition [i](#)

There are 98 unique types of molecules in this entry. The entry contains 181140 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 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	B1	46	Total	C	N	O	0	0
			354	228	56	70		
1	B2	32	Total	C	N	O	0	0
			257	168	40	49		
1	B3	32	Total	C	N	O	0	0
			257	168	40	49		
1	B4	31	Total	C	N	O	0	0
			245	159	39	47		
1	B5	31	Total	C	N	O	0	0
			245	159	39	47		
1	B6	31	Total	C	N	O	0	0
			245	159	39	47		

- Molecule 2 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B7	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 3 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B8	1558	Total	C	N	O	P	0	0
			33070	14843	5963	10706	1558		

- Molecule 4 is a RNA chain called CP Val-tRNA(Val).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B9	72	Total	C	N	O	P	0	0
			1524	685	269	498	72		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B9	70	C	G	conflict	GB NC_012920.1
B9	72	A	U	conflict	GB NC_012920.1

- Molecule 5 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BA	166	Total	C	N	O	S	0	0
			1369	875	254	233	7		

- Molecule 6 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BB	152	Total	C	N	O	S	0	0
			1251	788	234	226	3		

- Molecule 7 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BC	205	Total	C	N	O	S	0	0
			1676	1068	298	302	8		

- Molecule 8 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BD	116	Total	C	N	O	S	0	0
			904	577	171	153	3		

- Molecule 9 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BE	244	Total	C	N	O	S	0	0
			2044	1322	352	365	5		

- Molecule 10 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BF	181	Total	C	N	O	S	0	0
			1556	995	298	259	4		

- Molecule 11 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BG	122	Total	C	N	O	S	0	0
			996	636	186	171	3		

- Molecule 12 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BH	110	Total	C	N	O	S	0	0
			898	554	176	162	6		

- Molecule 13 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BI	56	Total	C	N	O	S	0	0
			464	296	89	77	2		

- Molecule 14 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BJ	46	Total	C	N	O	S	0	0
			377	233	83	60	1		

- Molecule 15 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BK	95	Total	C	N	O	S	0	0
			832	539	162	128	3		

- Molecule 16 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BL	238	Total	C	N	O	S	0	0
			1859	1157	376	317	9		

- Molecule 17 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BM	305	Total	C	N	O	S	0	0
			2406	1545	418	432	11		

- Molecule 18 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BN	252	Total	C	N	O	S	0	0
			2031	1305	370	350	6		

- Molecule 19 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BO	202	Total	C	N	O	S	0	0
			1661	1067	304	286	4		

- Molecule 20 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BP	212	Total	C	N	O	S	0	0
			1695	1088	304	292	11		

- Molecule 21 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BQ	175	Total	C	N	O	S	0	0
			1330	847	237	244	2		

- Molecule 22 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BR	177	Total	C	N	O	S	0	0
			1455	936	259	253	7		

- Molecule 23 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BS	115	Total	C	N	O	S	0	0
			890	559	171	155	5		

- Molecule 24 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BT	291	Total	C	N	O	S	0	0
			2327	1483	430	408	6		

- Molecule 25 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BU	222	Total	C	N	O	S	0	0
			1786	1143	326	307	10		

- Molecule 26 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BV	154	Total	C	N	O	S	0	0
			1259	792	241	219	7		

- Molecule 27 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BW	144	Total	C	N	O	S	0	0
			1173	733	224	211	5		

- Molecule 28 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BX	238	Total	C	N	O	S	0	0
			1979	1268	352	350	9		

- Molecule 29 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BY	140	Total	C	N	O	S	0	0
			1154	732	231	187	4		

- Molecule 30 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BZ	161	Total	C	N	O	S	0	0
			1293	835	227	227	4		

- Molecule 31 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ba	94	Total	C	N	O	S	0	0
			745	463	144	136	2		

- Molecule 32 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bb	101	Total	C	N	O	S	0	0
			774	479	148	142	5		

- Molecule 33 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bc	82	Total	C	N	O	S	0	0
			688	437	120	128	3		

- Molecule 34 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bd	92	Total	C	N	O	S	0	0
			791	488	159	142	2		

- Molecule 35 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Be	94	Total	C	N	O	S	0	0
			798	501	165	129	3		

- Molecule 36 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Bf	147	Total	C	N	O	S	0	0
			1205	748	228	225	4		

- Molecule 37 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bg	161	Total	C	N	O	S	0	0
			1350	841	260	244	5		

- Molecule 38 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bh	162	Total	C	N	O	S	0	0
			1322	839	252	223	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bi	386	Total	C	N	O	S	0	0
			3155	2023	559	559	14		

- Molecule 40 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bj	164	Total	C	N	O	S	0	0
			1327	856	217	250	4		

- Molecule 41 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bl	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 42 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bm	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 43 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bn	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 44 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bo	294	Total	C	N	O	S	0	0
			2390	1529	405	438	18		

- Molecule 45 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Bp	147	Total	C	N	O	S	0	0
			1243	790	218	233	2		

- Molecule 46 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Bq	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 47 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Br	100	Total	C	N	O	S	0	0
			840	529	152	154	5		

- Molecule 48 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bs	151	Total	C	N	O	S	0	0
			1196	744	231	218	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bs	2	ACE	-	acetylation	UNP Q8N983

- Molecule 49 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Bt	286	Total	C	N	O	S	0	0
			2299	1470	397	423	9		

- Molecule 50 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bu	241	Total	C	N	O	S	0	0
			1985	1273	340	359	13		

- Molecule 51 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Bv	238	Total	C	N	O	S	0	0
			1931	1222	339	364	6		

- Molecule 52 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bw	157	Total	C	N	O	S	0	0
			1252	799	207	242	4		

- Molecule 53 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Bx	134	Total	C	N	O	S	0	0
			1113	719	193	199	2		

- Molecule 54 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	By	110	Total	C	N	O	S	0	0
			895	568	156	168	3		

- Molecule 55 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Bz	97	Total	C	N	O	S	0	0
			828	532	165	127	4		

- Molecule 56 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AA	955	Total	C	N	O	P	0	0
			20283	9098	3652	6578	955		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	62	G	A	conflict	GB OM714795.1

- Molecule 57 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AB	279	Total	C	N	O	S	0	0
			2265	1435	387	432	11		

- Molecule 58 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AC	132	Total	C	N	O	S	0	0
			1083	699	195	185	4		

- Molecule 59 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AD	70	Total	C	N	O	S	0	0
			625	401	134	89	1		

- Molecule 60 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AE	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 61 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AF	208	Total	C	N	O	S	0	0
			1725	1104	312	298	11		

- Molecule 62 is a RNA chain called P-site Met-tRNA(Met).

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AG	71	Total	C	N	O	P	0	0
			1504	674	264	495	71		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	69	C	-	insertion	GB NC_012920.1
AG	70	C	-	insertion	GB NC_012920.1

- Molecule 63 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AH	140	Total	C	N	O	S	0	0
			1152	745	194	210	3		

- Molecule 64 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AI	33	Total	C	N	O	P	0	0
			463	198	29	203	33		

- Molecule 65 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AJ	108	Total	C	N	O	S	0	0
			839	521	169	143	6		

- Molecule 66 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AK	101	Total	C	N	O	S	0	0
			862	537	179	141	5		

- Molecule 67 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AL	174	Total	C	N	O	S	0	0
			1453	925	270	251	7		

- Molecule 68 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AM	119	Total	C	N	O	S	0	0
			942	594	185	157	6		

- Molecule 69 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AN	110	Total	C	N	O	S	0	0
			868	562	156	147	3		

- Molecule 70 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AO	193	Total	C	N	O	S	0	0
			1592	1014	294	277	7		

- Molecule 71 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AP	97	Total	C	N	O	S	0	0
			781	501	134	138	8		

- Molecule 72 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AQ	86	Total	C	N	O	S	0	0
			744	460	150	126	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	50	ARG	CYS	variant	UNP P82921

- Molecule 73 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AR	295	Total	C	N	O	S	0	0
			2409	1533	413	455	8		

- Molecule 74 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AS	135	Total	C	N	O	S	0	0
			1111	716	198	196	1		

- Molecule 75 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AT	168	Total	C	N	O	S	0	0
			1371	877	239	244	11		

- Molecule 76 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	AU	176	Total	C	N	O	S	0	0
			1488	916	301	267	4		

- Molecule 77 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AV	362	Total	C	N	O	S	0	0
			2969	1904	495	558	12		

- Molecule 78 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AW	100	Total	C	N	O	S	0	0
			789	498	141	146	4		

- Molecule 79 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AX	352	Total	C	N	O	S	0	0
			2849	1822	499	517	11		

- Molecule 80 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AY	149	Total	C	N	O	S	0	0
			1246	801	207	234	4		

- Molecule 81 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	AZ	100	Total	C	N	O	S	0	0
			839	534	153	148	4		

- Molecule 82 is a protein called Peptide chain release factor 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Aa	381	Total	C	N	O	S	0	0
			3114	1940	569	592	13		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	311	ALA	GLY	engineered mutation	UNP O75570
Aa	312	ALA	GLY	engineered mutation	UNP O75570
Aa	446	GLY	-	expression tag	UNP O75570
Aa	447	GLY	-	expression tag	UNP O75570
Aa	448	SER	-	expression tag	UNP O75570
Aa	449	GLY	-	expression tag	UNP O75570

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Chain	Residue	Modelled	Actual	Comment	Reference
Aa	450	GLY	-	expression tag	UNP O75570
Aa	451	SER	-	expression tag	UNP O75570
Aa	452	GLY	-	expression tag	UNP O75570
Aa	453	GLY	-	expression tag	UNP O75570
Aa	454	SER	-	expression tag	UNP O75570
Aa	455	GLY	-	expression tag	UNP O75570
Aa	456	GLY	-	expression tag	UNP O75570
Aa	457	SER	-	expression tag	UNP O75570
Aa	458	GLY	-	expression tag	UNP O75570
Aa	459	GLY	-	expression tag	UNP O75570
Aa	460	SER	-	expression tag	UNP O75570
Aa	461	GLY	-	expression tag	UNP O75570
Aa	462	GLY	-	expression tag	UNP O75570
Aa	463	ASP	-	expression tag	UNP O75570
Aa	464	TYR	-	expression tag	UNP O75570
Aa	465	LYS	-	expression tag	UNP O75570
Aa	466	ASP	-	expression tag	UNP O75570
Aa	467	HIS	-	expression tag	UNP O75570
Aa	468	ASP	-	expression tag	UNP O75570
Aa	469	GLY	-	expression tag	UNP O75570
Aa	470	ASP	-	expression tag	UNP O75570
Aa	471	TYR	-	expression tag	UNP O75570
Aa	472	LYS	-	expression tag	UNP O75570
Aa	473	ASP	-	expression tag	UNP O75570
Aa	474	HIS	-	expression tag	UNP O75570
Aa	475	ASP	-	expression tag	UNP O75570
Aa	476	ILE	-	expression tag	UNP O75570
Aa	477	ASP	-	expression tag	UNP O75570
Aa	478	TYR	-	expression tag	UNP O75570
Aa	479	LYS	-	expression tag	UNP O75570
Aa	480	ASP	-	expression tag	UNP O75570
Aa	481	ASP	-	expression tag	UNP O75570
Aa	482	ASP	-	expression tag	UNP O75570
Aa	483	ASP	-	expression tag	UNP O75570
Aa	484	LYS	-	expression tag	UNP O75570

- Molecule 83 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Ab	225	Total	C	N	O	S	0	0
			1828	1164	331	323	10		

- Molecule 84 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein

1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Ac	117	Total	C	N	O	S	0	0
			935	579	182	166	8		

- Molecule 85 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Ad	343	Total	C	N	O	S	0	0
			2731	1713	518	487	13		

- Molecule 86 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Ae	588	Total	C	N	O	S	0	0
			4768	3053	808	879	28		

- Molecule 87 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Ag	327	Total	C	N	O	S	0	0
			2688	1710	477	487	14		

- Molecule 88 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Ai	137	Total	C	N	O	S	0	0
			1020	642	192	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ai	184	5F0	ASN	conflict	UNP P82912

- Molecule 89 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	Aj	215	Total	C	N	O	S	0	0
			1787	1130	339	313	5		

- Molecule 90 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
90	B8	30	Total 30	K 30	0
90	BL	1	Total 1	K 1	0
90	BT	1	Total 1	K 1	0
90	Be	1	Total 1	K 1	0
90	Bn	1	Total 1	K 1	0
90	AA	16	Total 16	K 16	0
90	Ae	1	Total 1	K 1	0

- Molecule 91 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

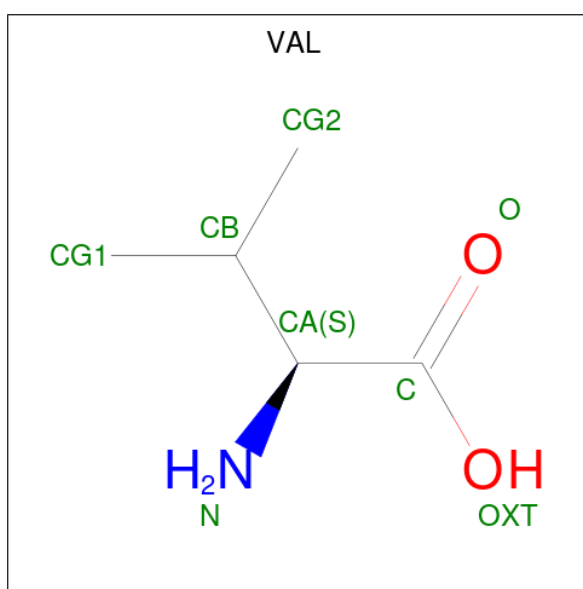
Mol	Chain	Residues	Atoms		AltConf
91	B8	216	Total 216	Mg 216	0
91	BD	1	Total 1	Mg 1	0
91	BL	3	Total 3	Mg 3	0
91	BN	1	Total 1	Mg 1	0
91	BO	1	Total 1	Mg 1	0
91	BR	1	Total 1	Mg 1	0
91	BT	1	Total 1	Mg 1	0
91	BV	1	Total 1	Mg 1	0
91	Bx	1	Total 1	Mg 1	0
91	AA	120	Total 120	Mg 120	0
91	AD	1	Total 1	Mg 1	0
91	AG	2	Total 2	Mg 2	0
91	AU	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
91	AX	1	Total	Mg	0
			1	1	
91	Aa	1	Total	Mg	0
			1	1	
91	Ab	1	Total	Mg	0
			1	1	
91	Ad	1	Total	Mg	0
			1	1	

- Molecule 92 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).

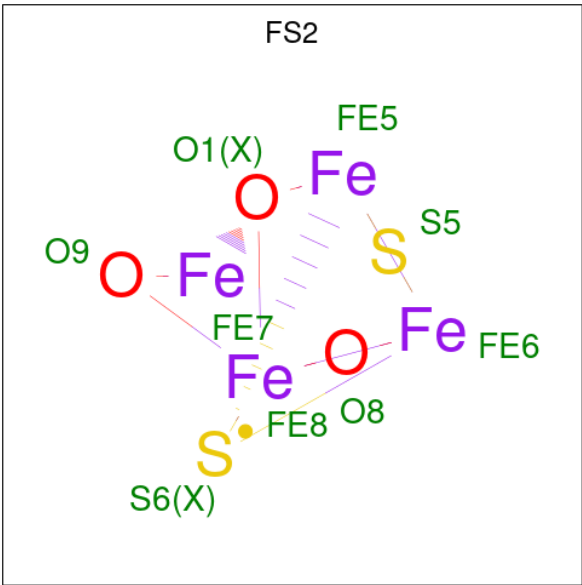


Mol	Chain	Residues	Atoms				AltConf
92	B9	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 93 is ZINC ION (CCD ID: ZN) (formula: Zn).

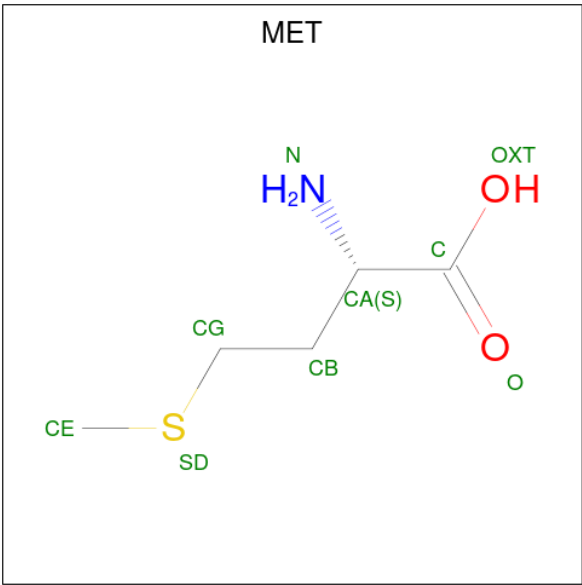
Mol	Chain	Residues	Atoms		AltConf
93	BH	1	Total	Zn	0
			1	1	
93	Bl	1	Total	Zn	0
			1	1	
93	AO	1	Total	Zn	0
			1	1	

- Molecule 94 is FE-S-O HYBRID CLUSTER (CCD ID: FS2) (formula: $Fe_4O_3S_2$).



Mol	Chain	Residues	Atoms			AltConf
94	Bh	1	Total	Fe	S	0
			4	2	2	
94	AP	1	Total	Fe	S	0
			4	2	2	
94	AT	1	Total	Fe	S	0
			4	2	2	

- Molecule 95 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).



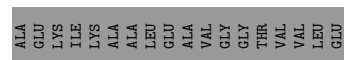
Mol	Chain	Residues	Atoms					AltConf
95	AG	1	Total	C	N	O	S	0
			8	5	1	1	1	

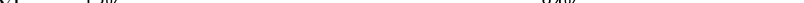
- # ATP

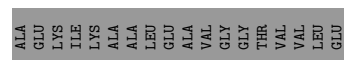
The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine derivative) linked to a ribose sugar, which is in turn linked to two phosphate groups. The guanine base is shown with its characteristic fused ring system, including an amino group at the 2-position. The ribose sugar is a five-membered ring with hydroxyl groups at the 2' and 3' positions. The two phosphate groups are connected by a pyrophosphate linkage, with the second phosphate group being a diphosphate moiety. The structure is labeled with various atoms and bonds, including the guanine base, ribose sugar, and the two phosphate groups.

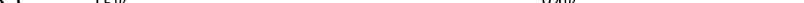


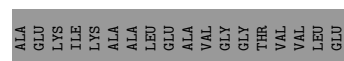
Mol	Chain	Residues	Atoms		AltConf
98	AX	3	Total 3	O 3	0

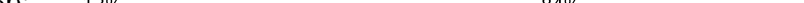


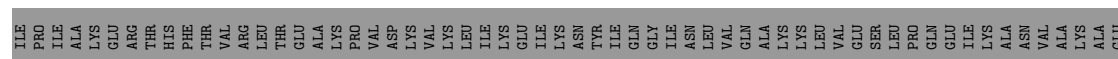
- Chain B4: 



- Chain B5:  16%
15% 84%



- Chain B6: 



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

• Molecule 2: E-site tRNA



C74
C75
A76

• Molecule 3: 16S rRNA



G1
C2
A10
G11
C19
A22
C23
C29
U30
C33
U34
A35
C36
C37
U137
A38
G39
A40
C41
A54
A57
U58
A61
C62
G63
C64
A65
A66
A67
U68
A69
A70
A71
U75
A76
G77
G78
C79
G80
A81
U82
A85
G90
A91
A92
A93
C94
C95
G98

A107
U110
G117
A120
A125
A126
G130
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A135
U136
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C157
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G160
G161
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A166
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C169
A174
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G209
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A329
C330
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A390
C398
U399
U401
A402
A403
A404
U405
C409
U410
U411
G412
U423
G424
U429
A433
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C446
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A511
G512
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C519
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A521
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A553

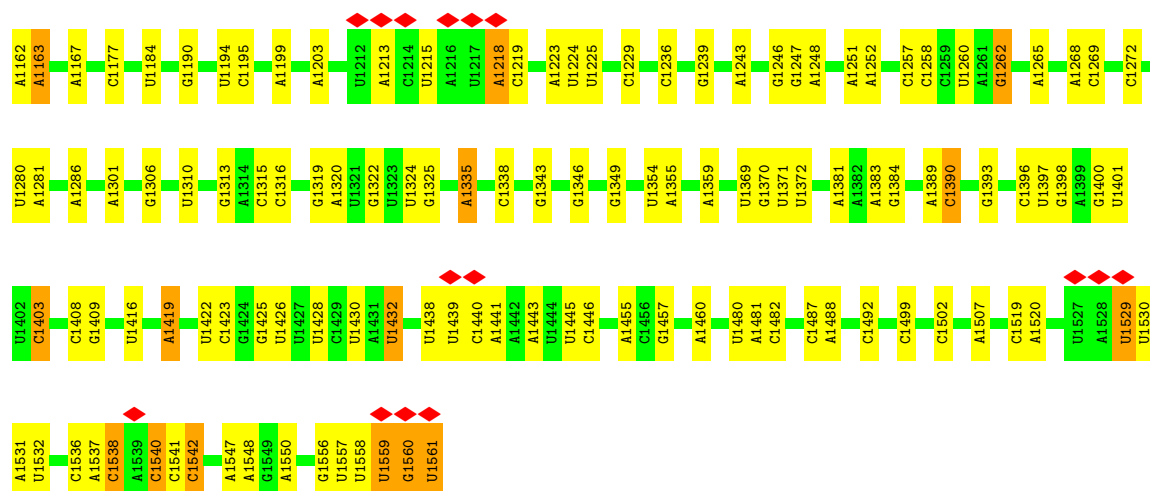
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A560
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A576
C577
U578
A581
C592
C593
A603
U609
C614
U615
G619
A623
A627
A628
U629
G630
G640
A648
A649
A650
A651
C652
U655
C656
U657
C661
C662
A667
A668

G669
G673
C674
G675
U676
G679
A680
U681
U682
A683
A684
C687
A
C
U
G691
A692
A693
A699
U702
A703
A704
A720
A725
U729
G730
A731
U734
C735
A736
U737
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A764
U772
A776

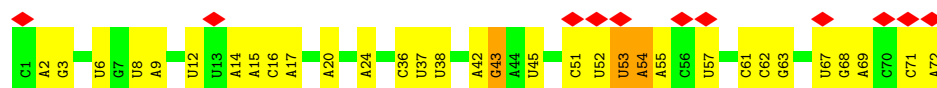
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A789
A793
G801
A802
G808
U813
C814
U815
C823
U829
A830
C831
C832
A833
A834
A842
U845
G849
C850
A851
A857
A860
U861
C870
C871
G872
C873
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U875
G876
A888
U889
C900
C907
C908
A912

C913
U916
G917
G922
G923
U924
A925
G926
C927
U929
A930
A931
U932
C933
A947
U948
G956
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A963
U964
G965
C969
U984
G985
U986
U997
A998
G1005
A1006
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G1048

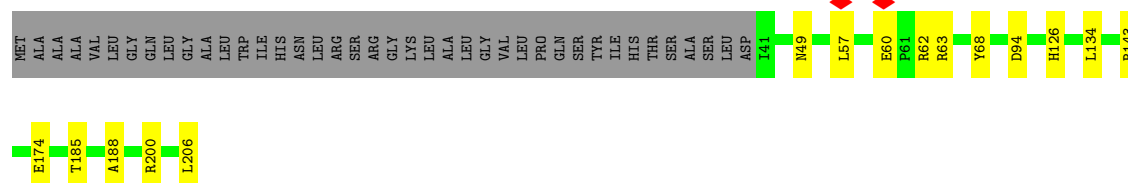
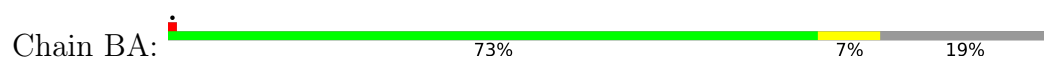
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A1103
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G1106
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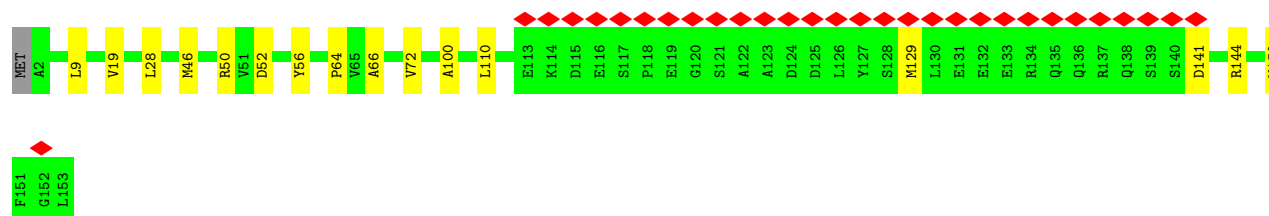
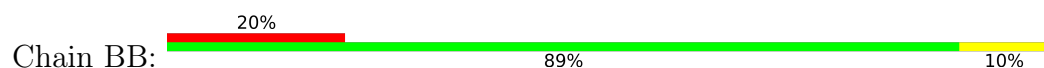
• Molecule 4: CP Val-tRNA(Val)



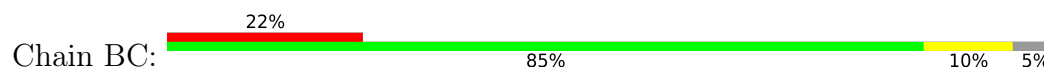
• Molecule 5: 39S ribosomal protein L22, mitochondrial

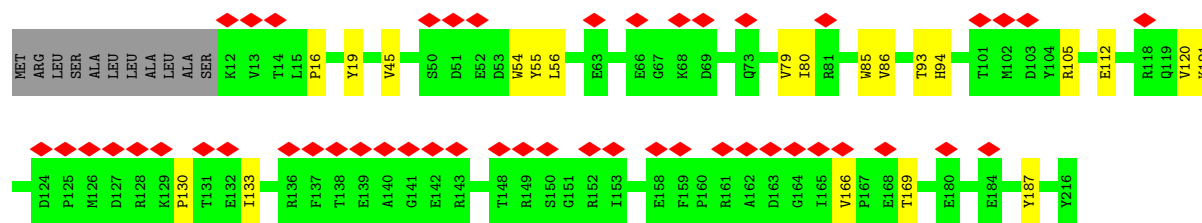


• Molecule 6: 39S ribosomal protein L23, mitochondrial

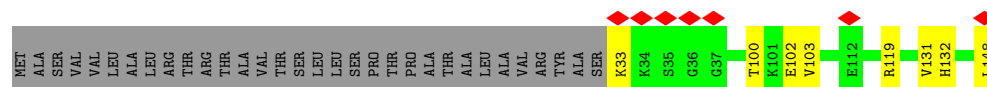
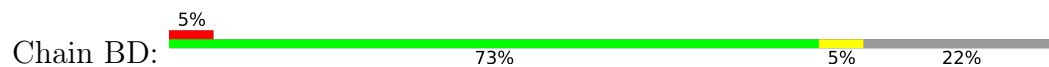


• Molecule 7: 39S ribosomal protein L24, mitochondrial

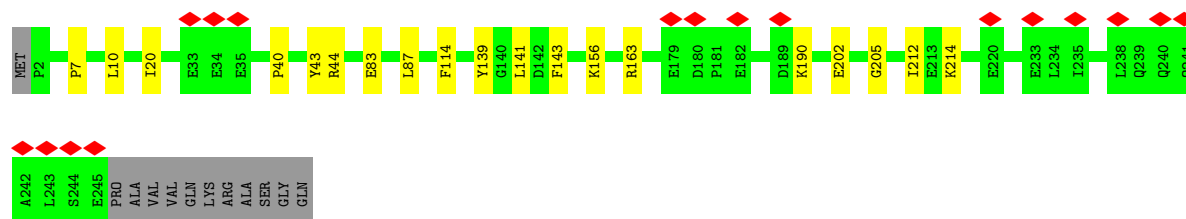
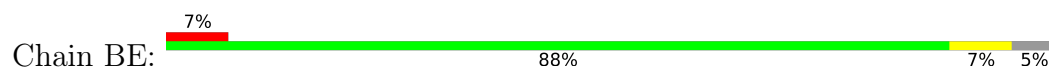




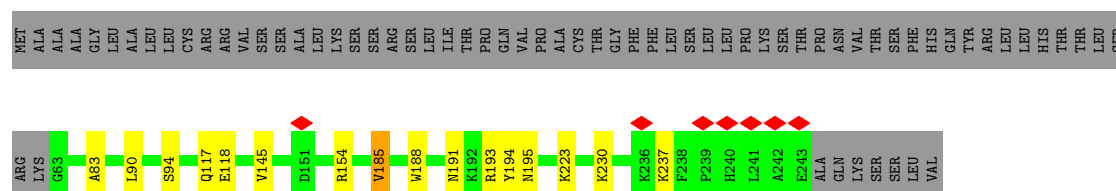
- Molecule 8: 39S ribosomal protein L27, mitochondrial



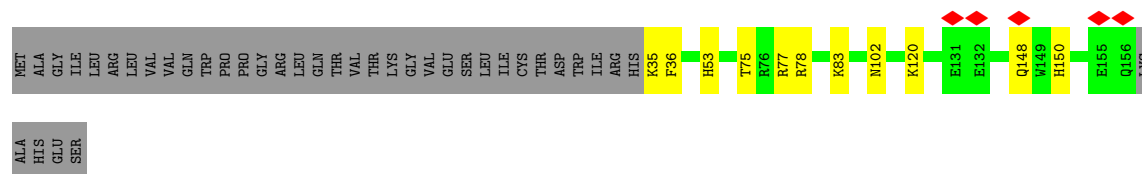
- Molecule 9: 39S ribosomal protein L28, mitochondrial



- Molecule 10: 39S ribosomal protein L47, mitochondrial

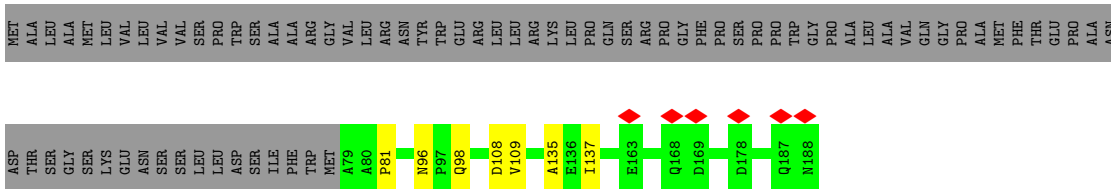


- Molecule 11: 39S ribosomal protein L30, mitochondrial

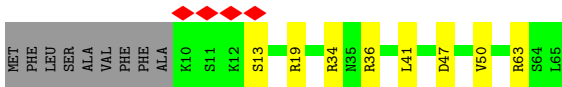
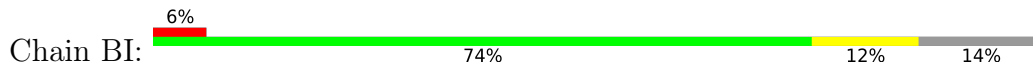


- Molecule 12: 39S ribosomal protein L32, mitochondrial

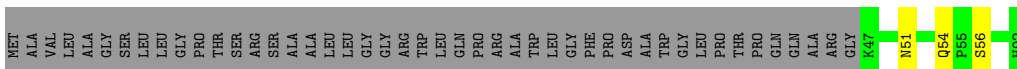




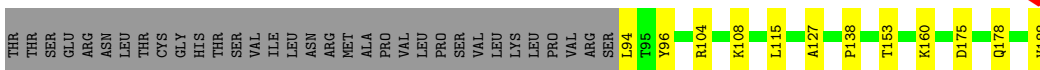
- Molecule 13: 39S ribosomal protein L33, mitochondrial



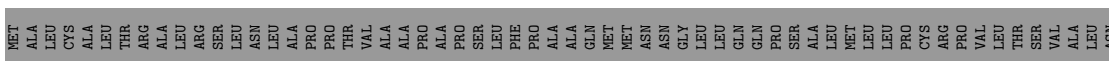
- Molecule 14: 39S ribosomal protein L34, mitochondrial



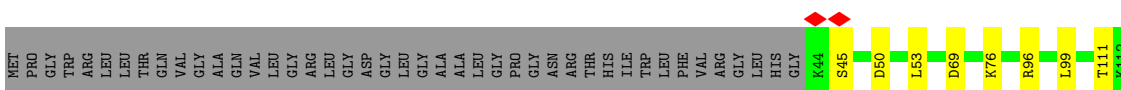
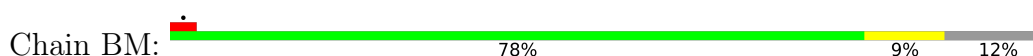
- Molecule 15: 39S ribosomal protein L35, mitochondrial

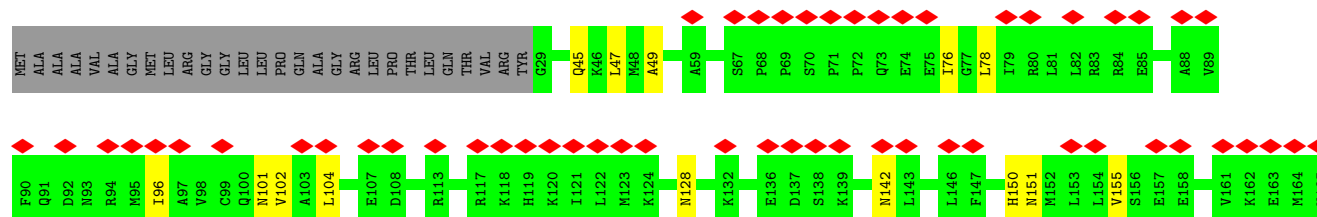


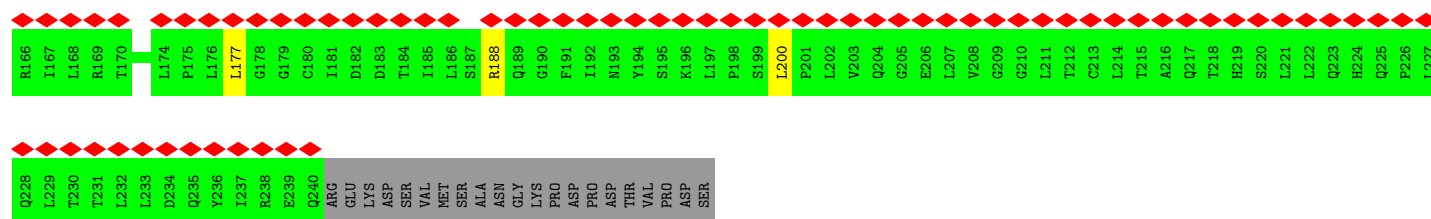
- Molecule 16: 39S ribosomal protein L2, mitochondrial



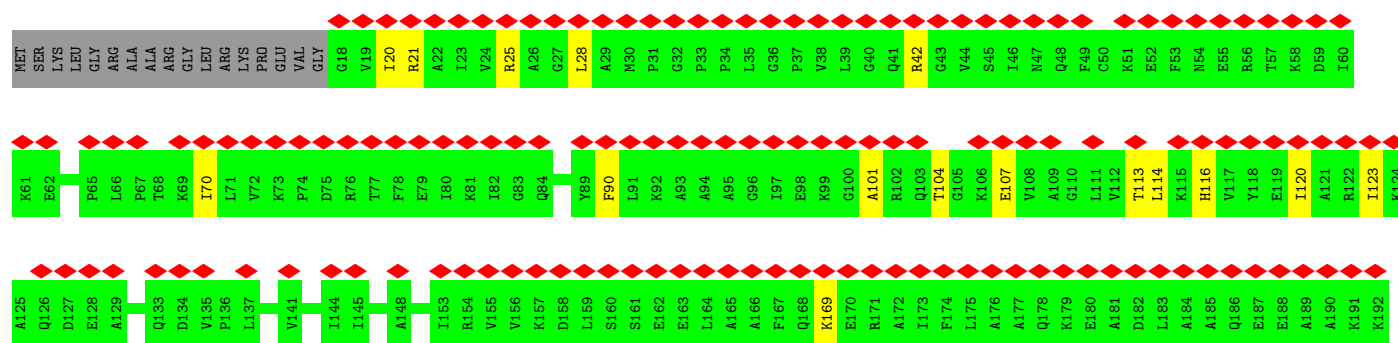
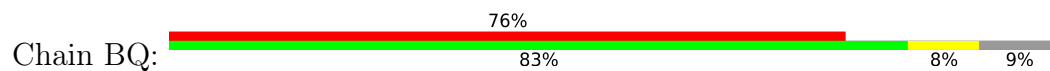
- Molecule 17: 39S ribosomal protein L3, mitochondrial



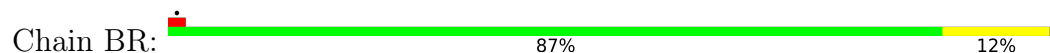




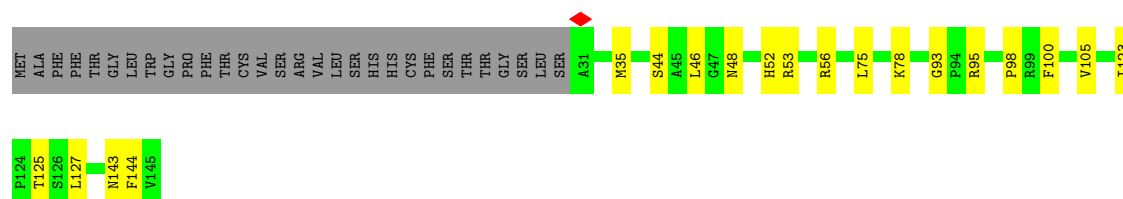
- Molecule 21: 39S ribosomal protein L11, mitochondrial



- Molecule 22: 39S ribosomal protein L13, mitochondrial



- Molecule 23: 39S ribosomal protein L14, mitochondrial



- Molecule 24: 39S ribosomal protein L15, mitochondrial





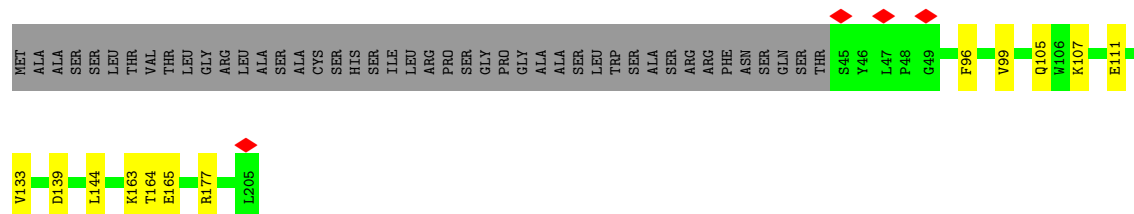
- Molecule 29: 39S ribosomal protein L20, mitochondrial

Chain BY: 85% 9% 6%



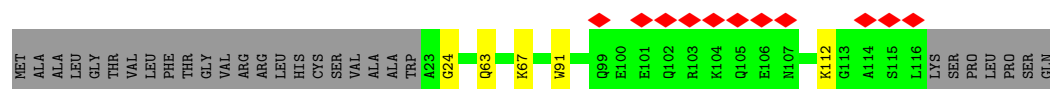
- Molecule 30: 39S ribosomal protein L21, mitochondrial

Chain BZ: 73% 6% 21%



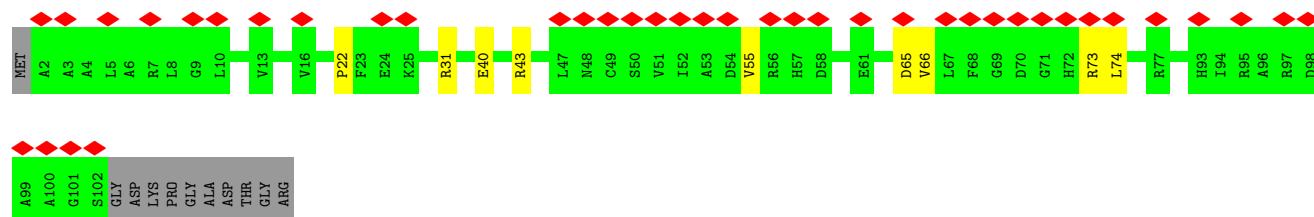
- Molecule 31: 39S ribosomal protein L52, mitochondrial

Chain Ba: 9% 72% 24%



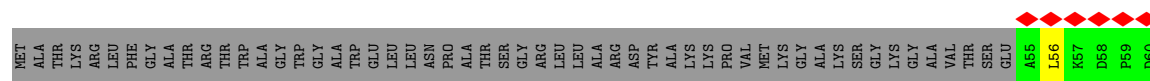
- Molecule 32: 39S ribosomal protein L53, mitochondrial

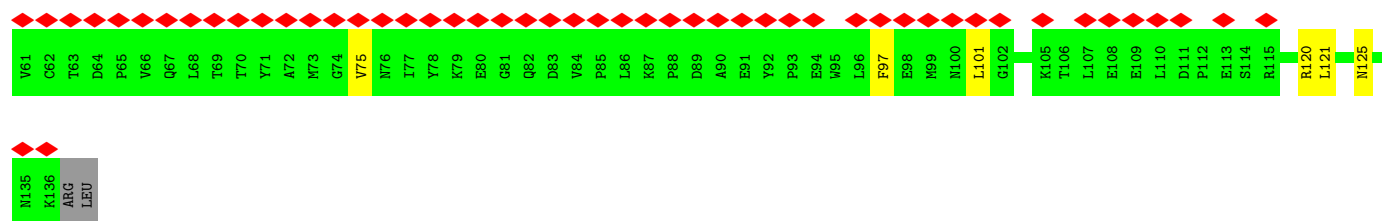
Chain Bb: 36% 82% 8% 10%



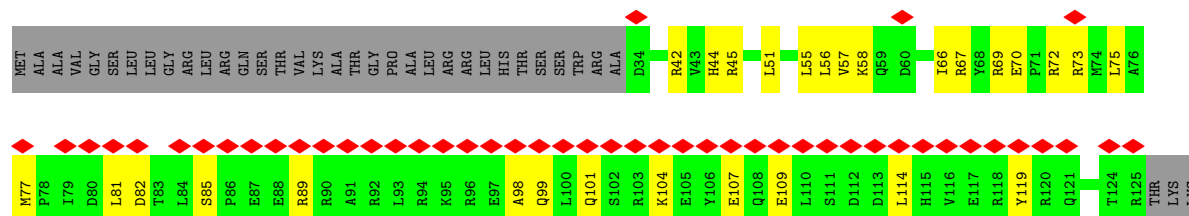
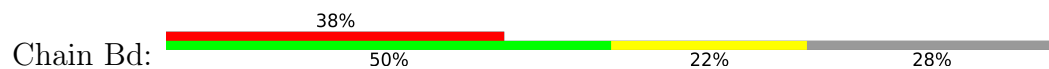
- Molecule 33: 39S ribosomal protein L54, mitochondrial

Chain Bc: 41% 54% 5% 41%

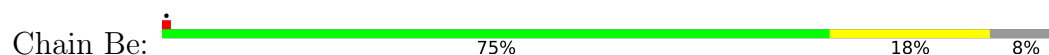




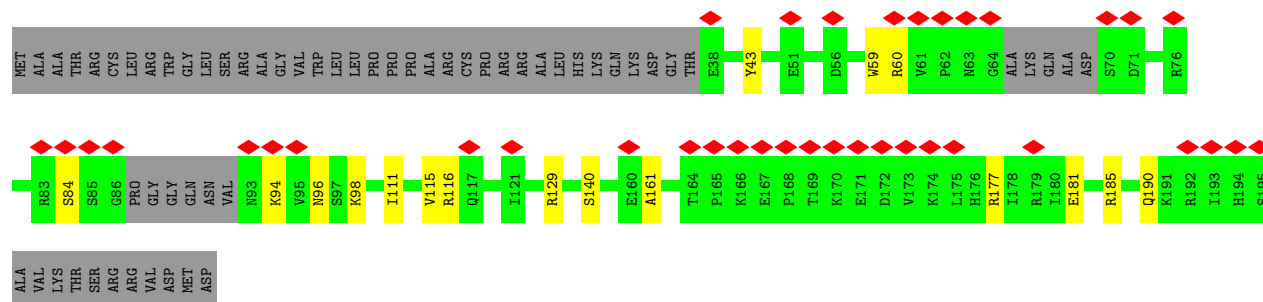
- Molecule 34: 39S ribosomal protein L55, mitochondrial



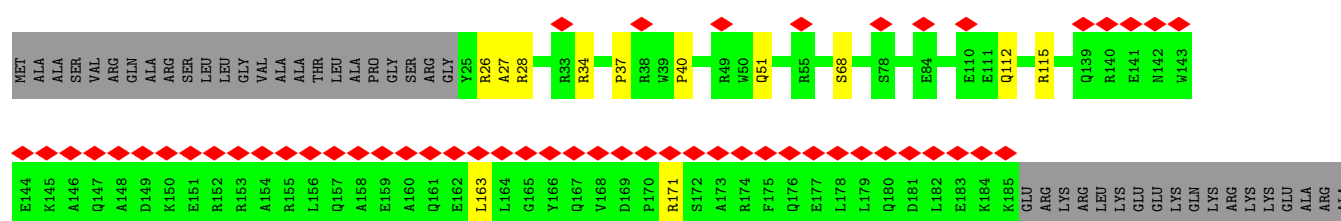
- Molecule 35: Ribosomal protein 63, mitochondrial

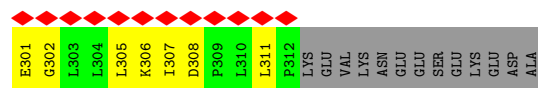


- Molecule 36: Peptidyl-tRNA hydrolase ICT1, mitochondrial



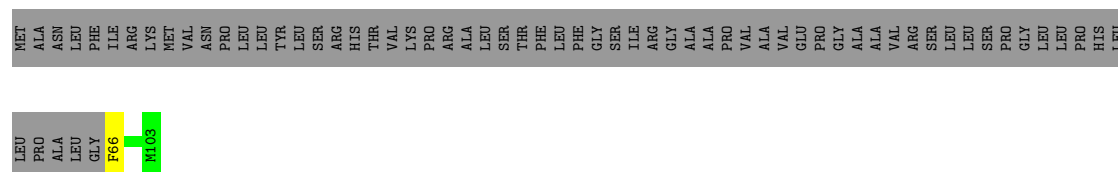
- Molecule 37: Growth arrest and DNA damage-inducible proteins-interacting protein 1





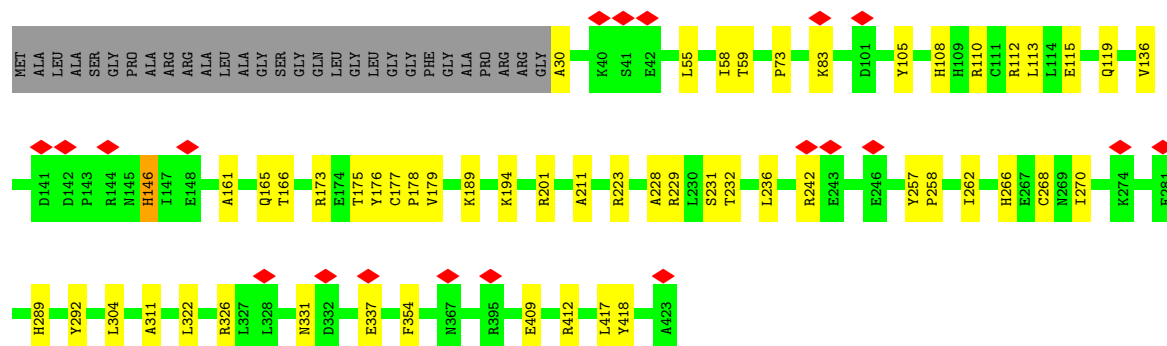
- Molecule 41: 39S ribosomal protein L36, mitochondrial

Chain Bl: 36% 63%



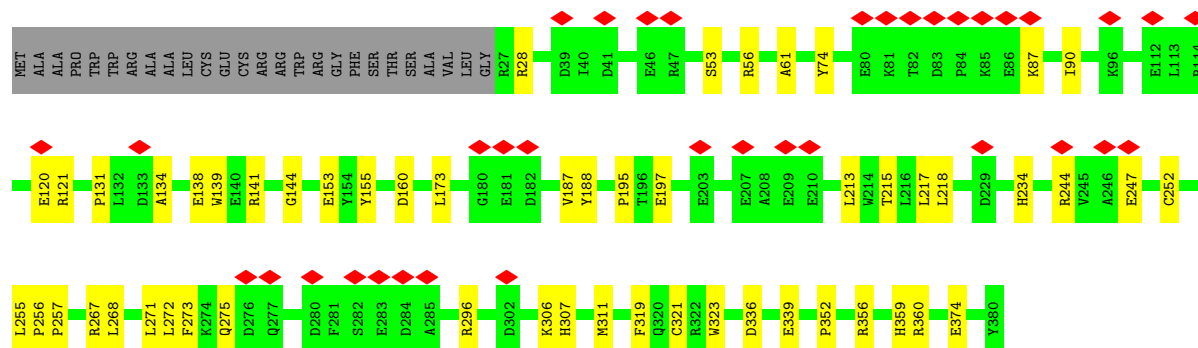
- Molecule 42: 39S ribosomal protein L37, mitochondrial

Chain Bm: 5% 80% 13% 7%



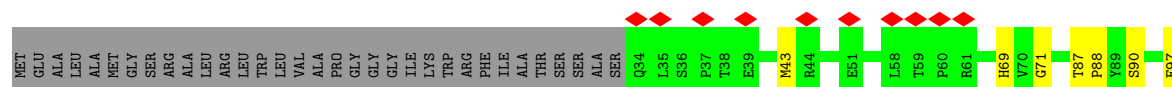
- Molecule 43: 39S ribosomal protein L38, mitochondrial

Chain Bn: 9% 79% 14% 7%

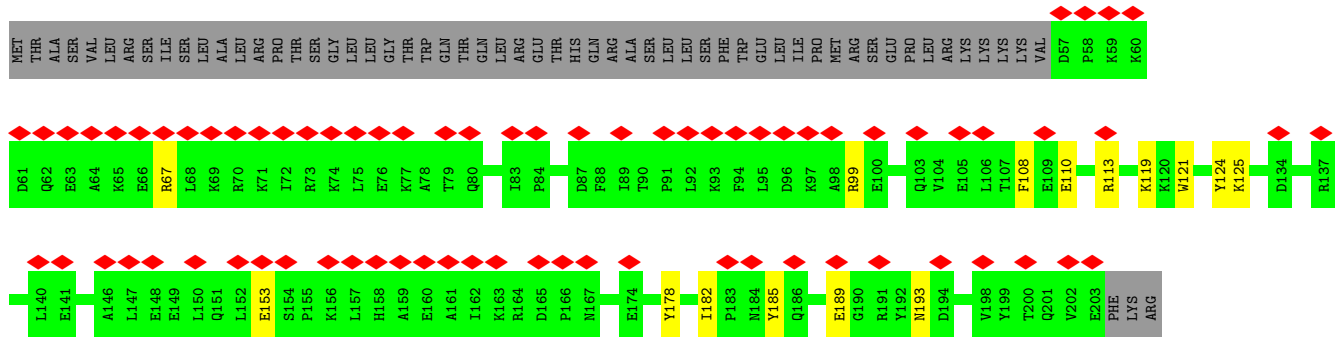


- Molecule 44: 39S ribosomal protein L39, mitochondrial

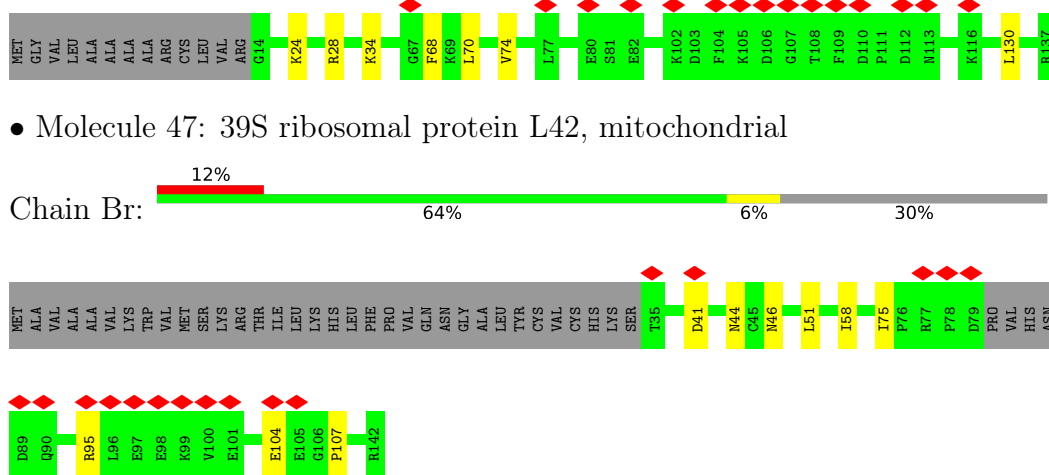
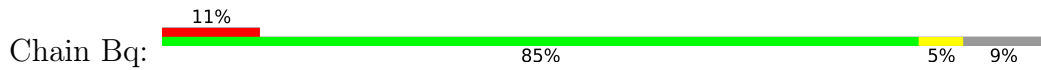
Chain Bo: 15% 74% 13% 13%



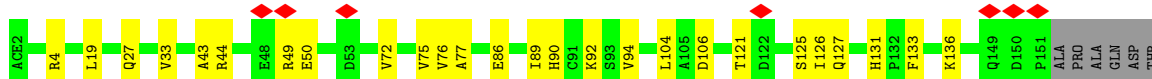
- Molecule 45: 39S ribosomal protein L40, mitochondrial

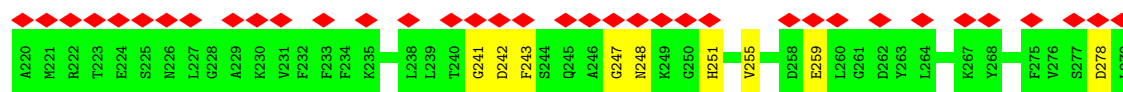


- Molecule 46: 39S ribosomal protein L41, mitochondrial

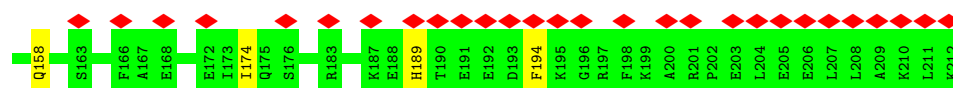
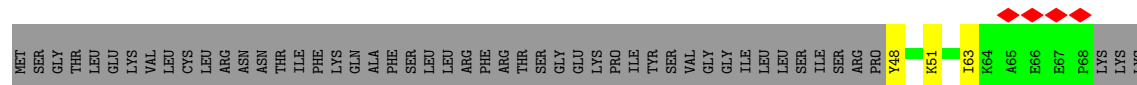


- Molecule 48: Large ribosomal subunit protein mL43

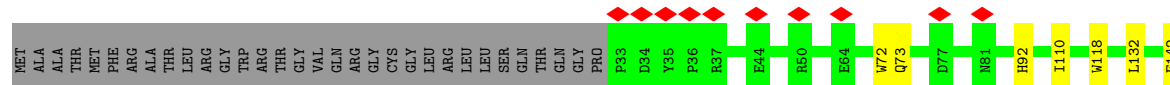
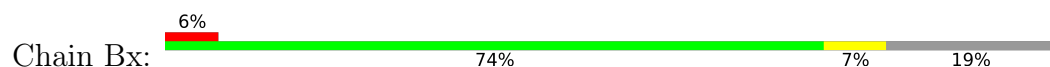




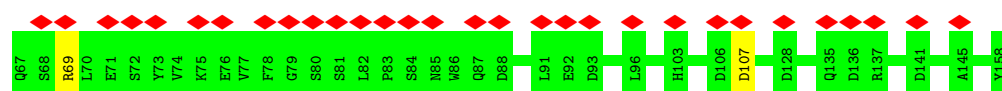
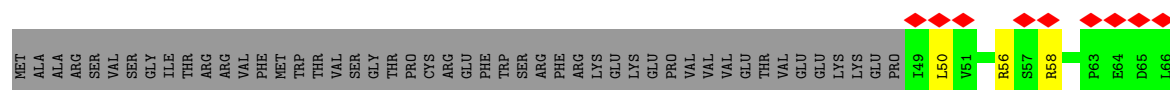
- Molecule 52: 39S ribosomal protein L48, mitochondrial



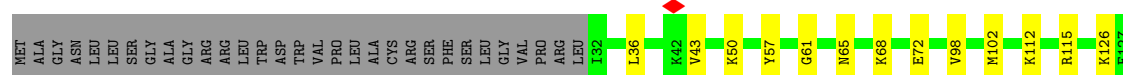
- Molecule 53: 39S ribosomal protein L49, mitochondrial



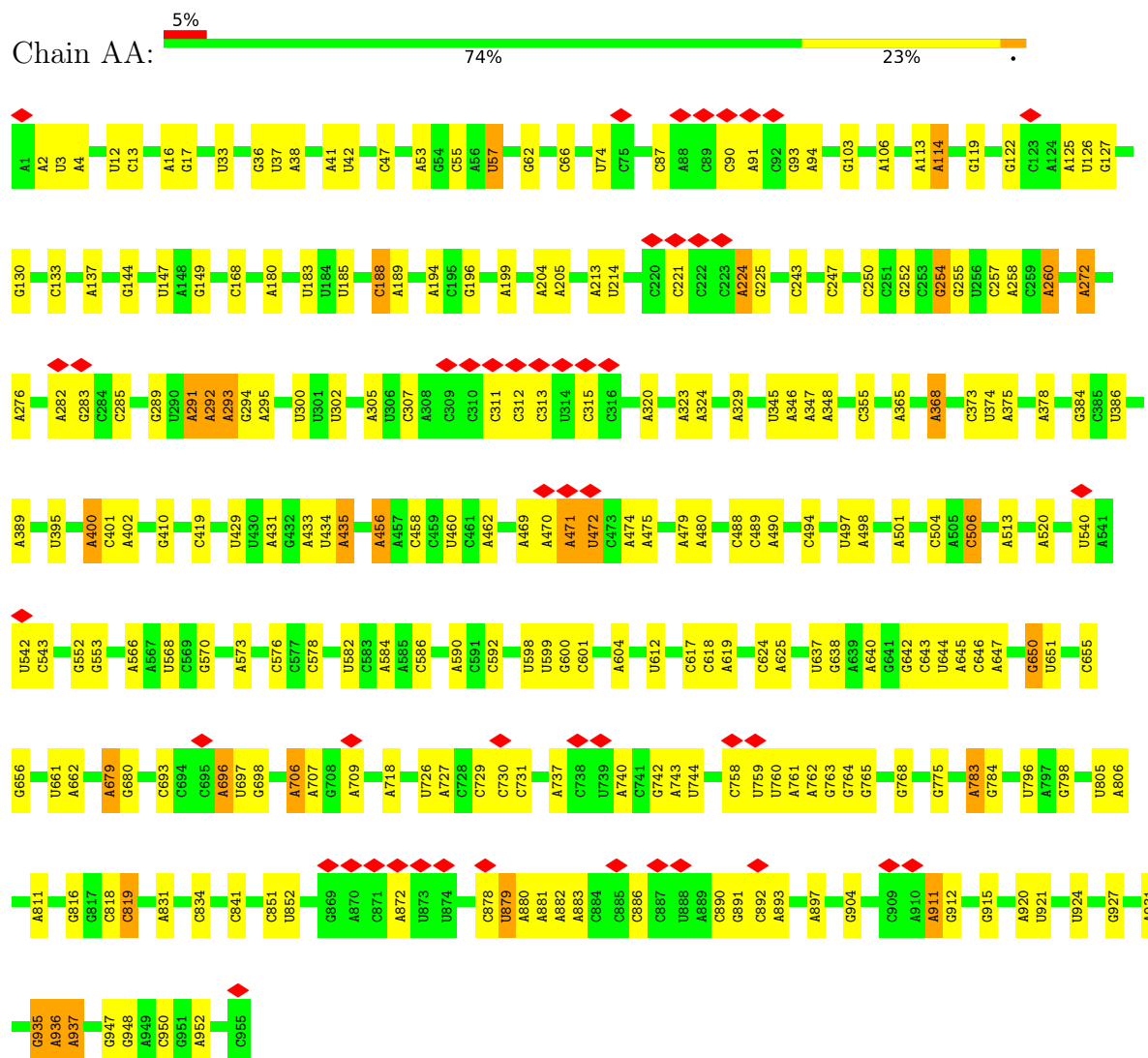
- Molecule 54: 39S ribosomal protein L50, mitochondrial



- Molecule 55: 39S ribosomal protein L51, mitochondrial

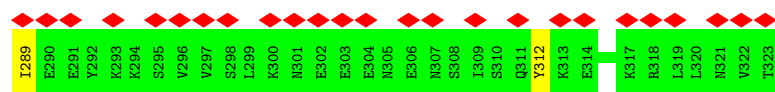


• Molecule 56: 12S rRNA

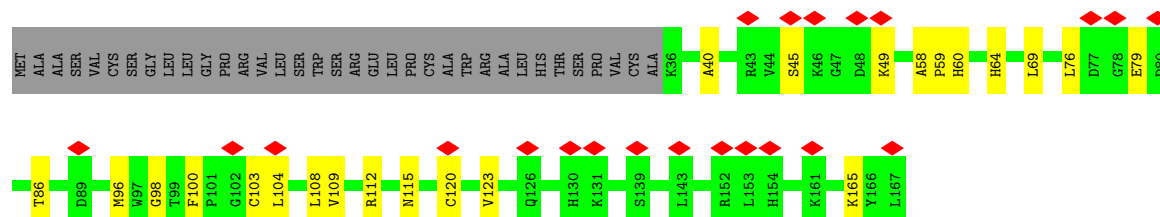


• Molecule 57: 28S ribosomal protein S35, mitochondrial

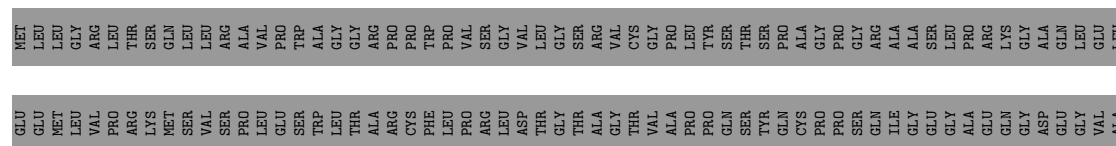




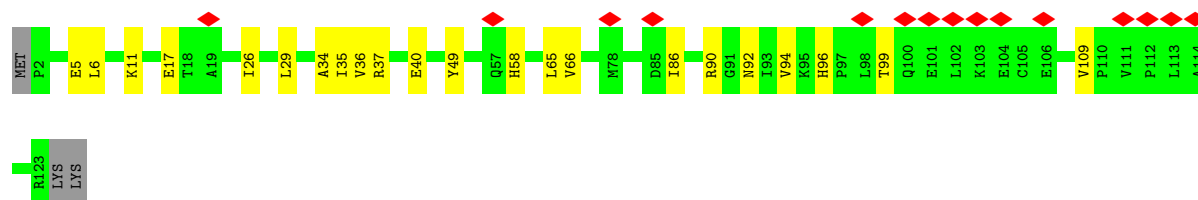
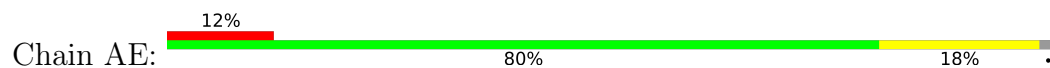
- Molecule 58: 28S ribosomal protein S24, mitochondrial



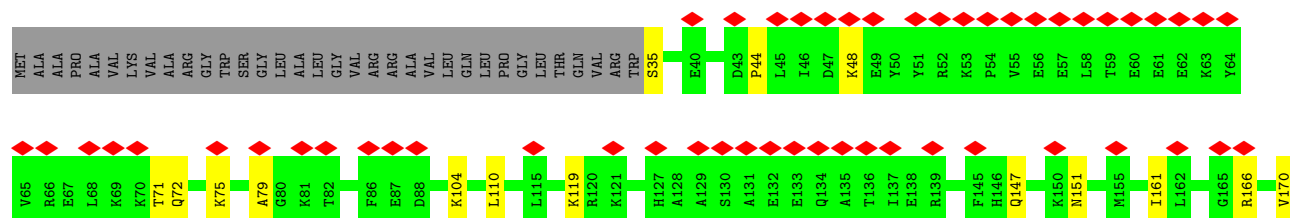
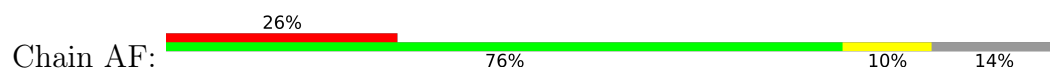
- Molecule 59: Aurora kinase A-interacting protein

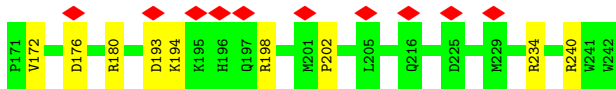


- Molecule 60: 28S ribosomal protein S6, mitochondrial

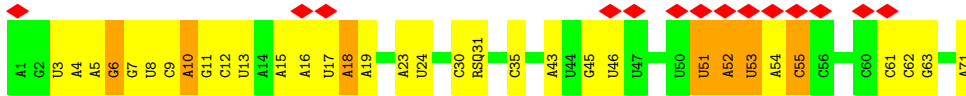


- Molecule 61: 28S ribosomal protein S7, mitochondrial

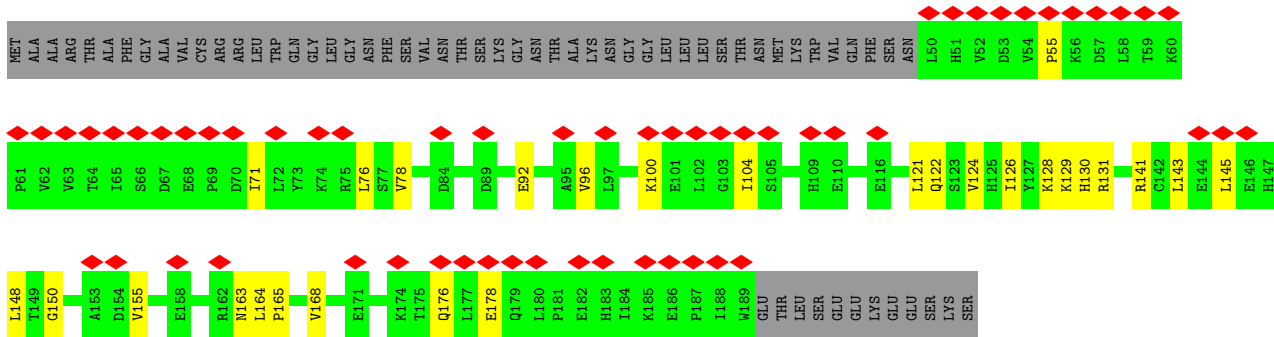




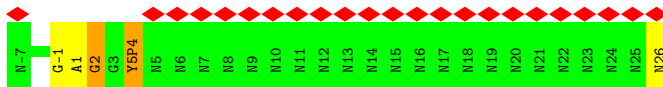
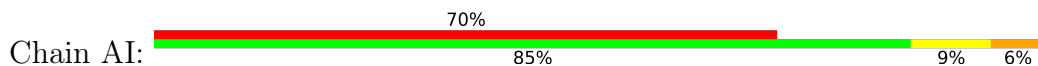
• Molecule 62: P-site Met-tRNA(Met)



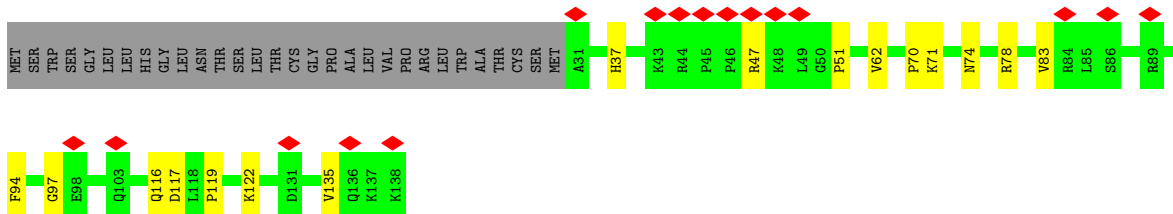
• Molecule 63: 28S ribosomal protein S10, mitochondrial



• Molecule 64: mRNA

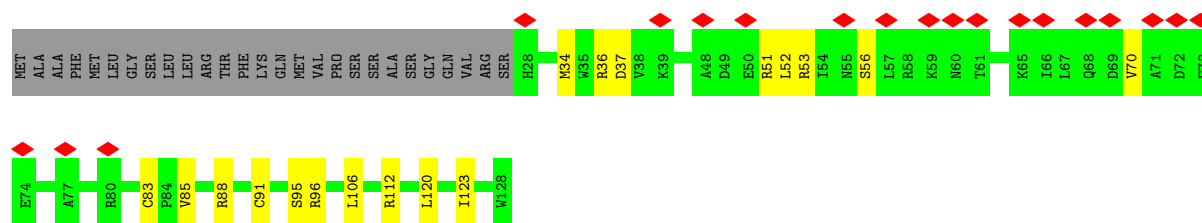


• Molecule 65: 28S ribosomal protein S12, mitochondrial

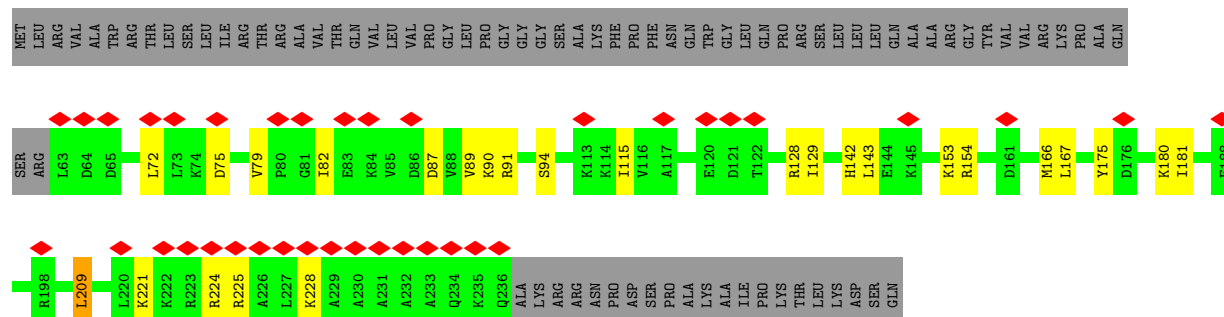


• Molecule 66: 28S ribosomal protein S14, mitochondrial

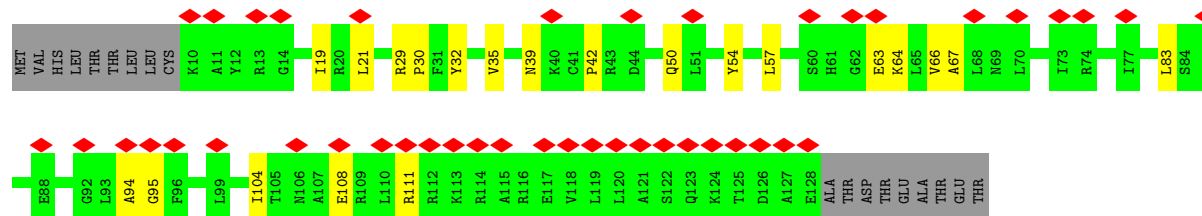
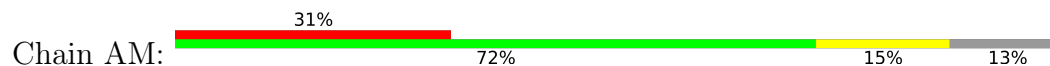




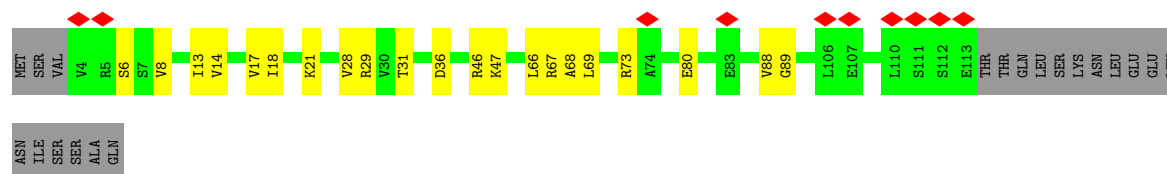
- Molecule 67: 28S ribosomal protein S15, mitochondrial



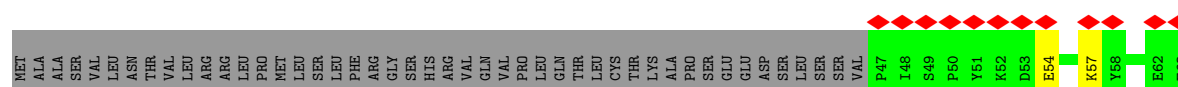
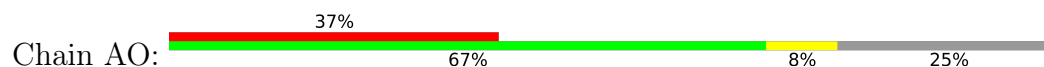
- Molecule 68: 28S ribosomal protein S16, mitochondrial

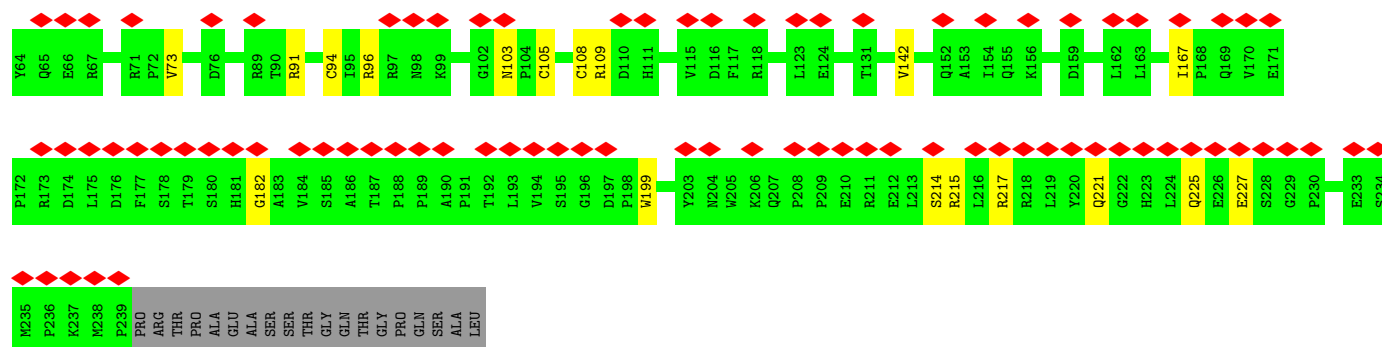


- Molecule 69: 28S ribosomal protein S17, mitochondrial

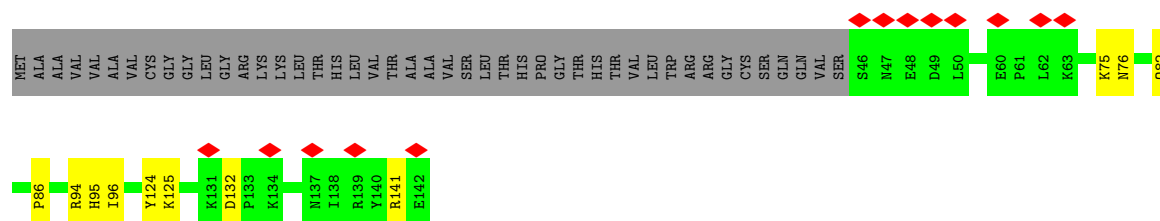


- Molecule 70: 28S ribosomal protein S18b, mitochondrial

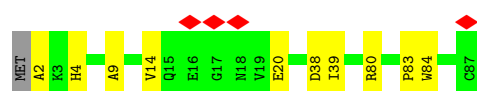
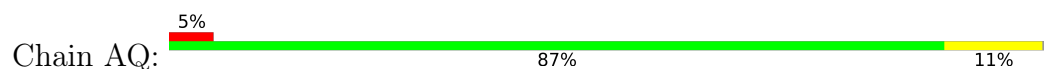




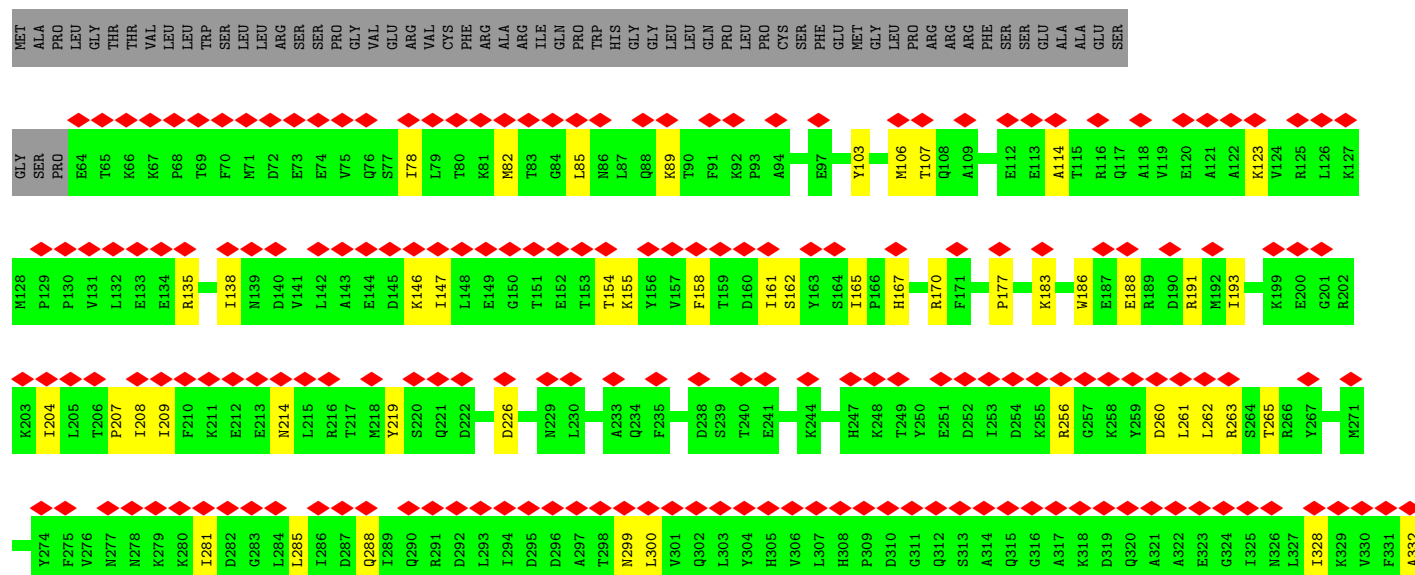
- Molecule 71: 28S ribosomal protein S18c, mitochondrial

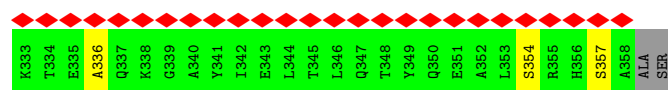


- Molecule 72: 28S ribosomal protein S21, mitochondrial

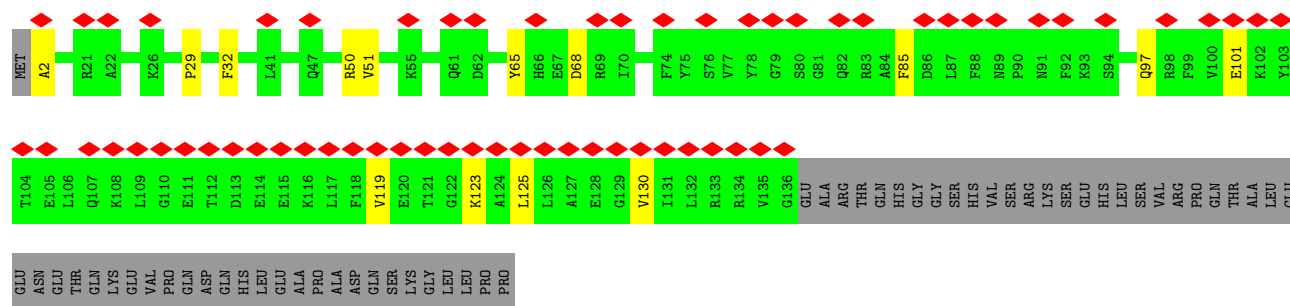


- Molecule 73: 28S ribosomal protein S22, mitochondrial

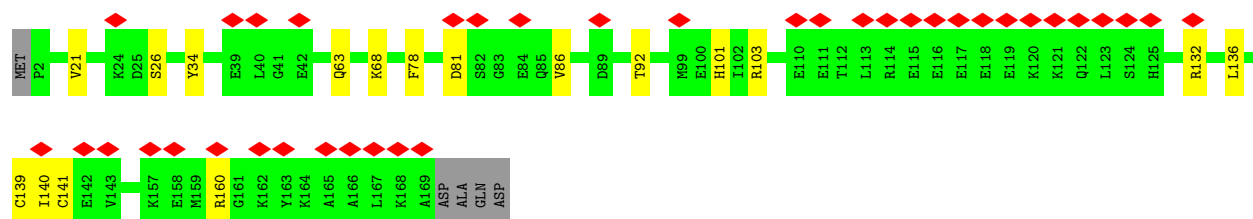
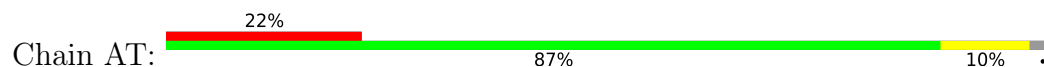




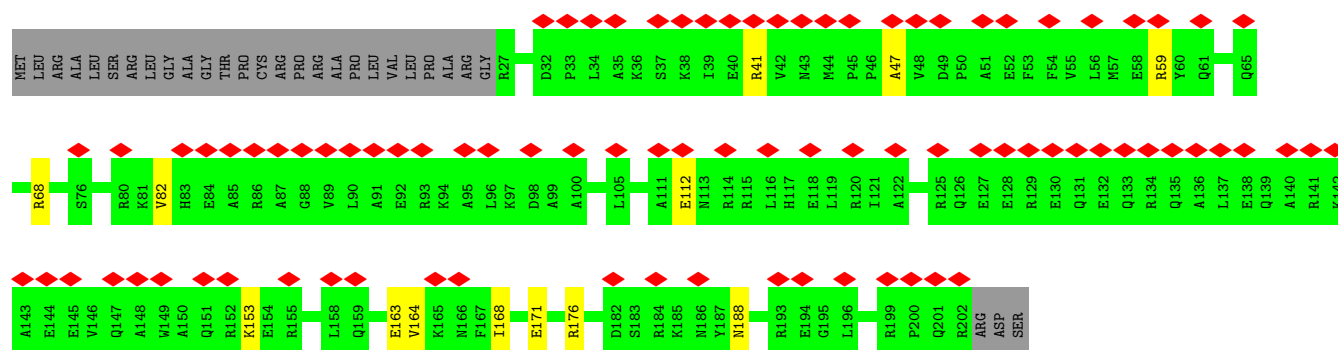
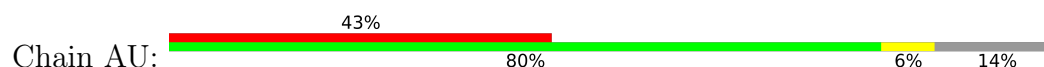
- Molecule 74: 28S ribosomal protein S23, mitochondrial



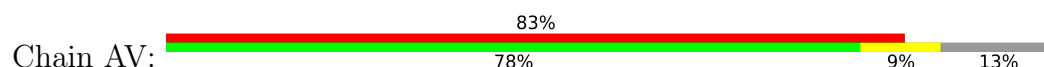
- Molecule 75: 28S ribosomal protein S25, mitochondrial

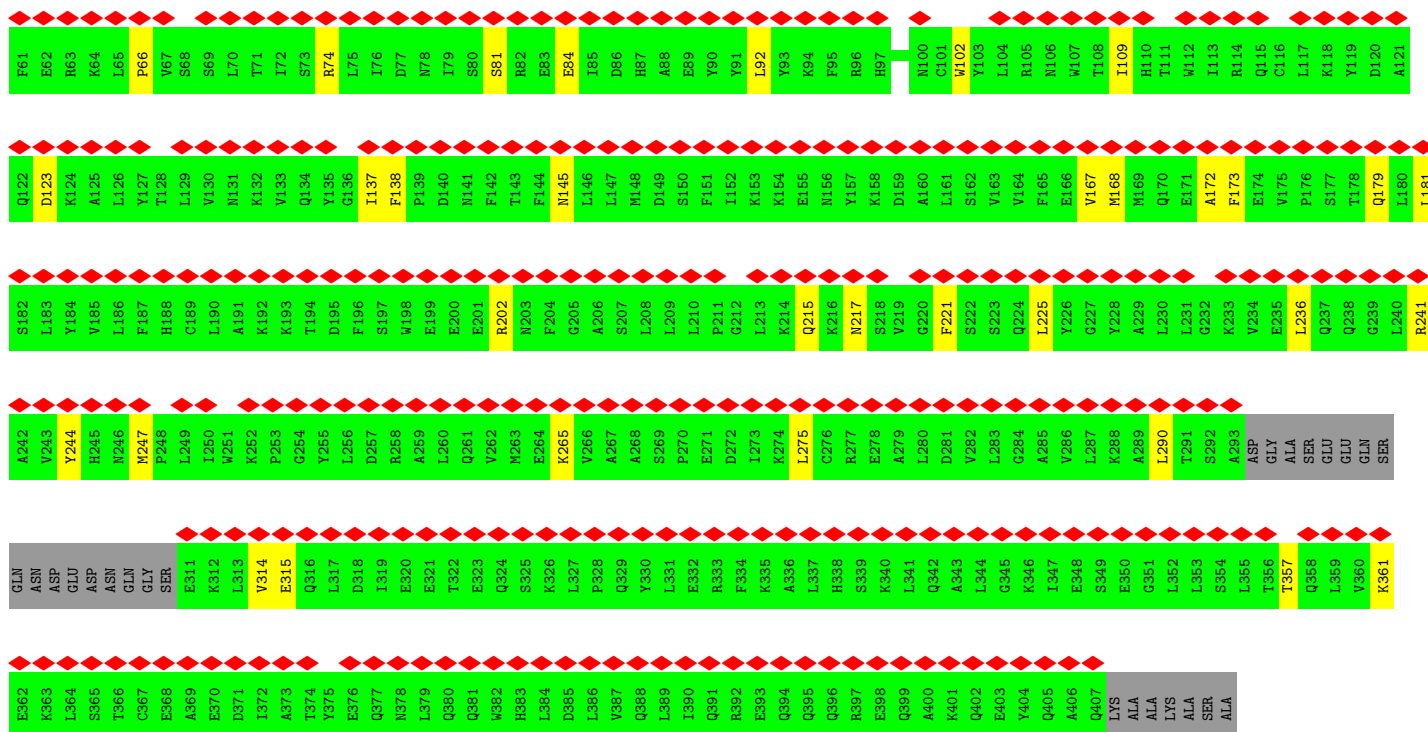


- Molecule 76: 28S ribosomal protein S26, mitochondrial

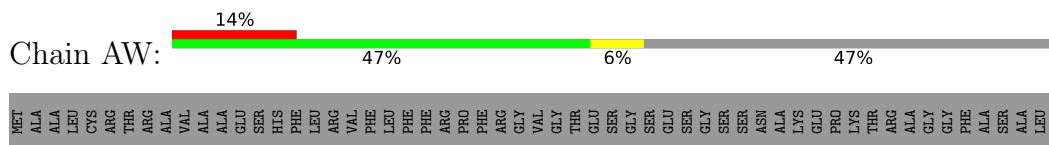


- Molecule 77: 28S ribosomal protein S27, mitochondrial

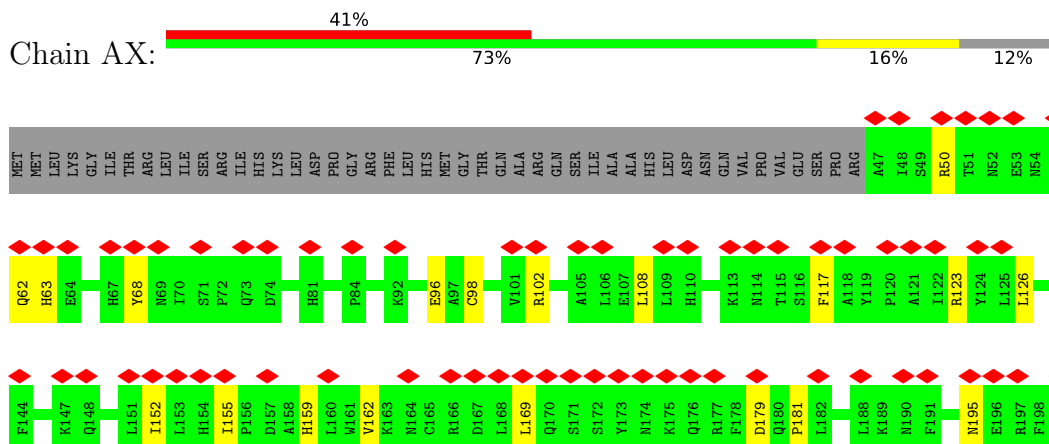


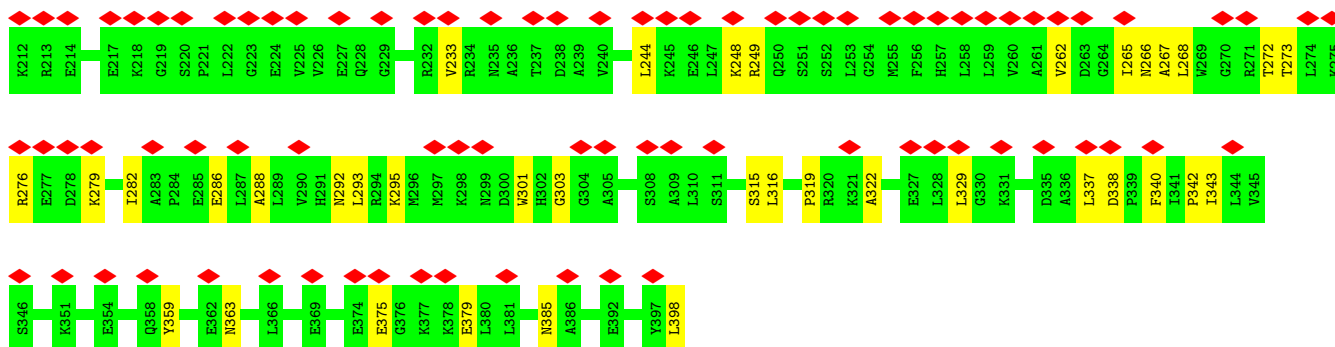


• Molecule 78: 28S ribosomal protein S28, mitochondrial

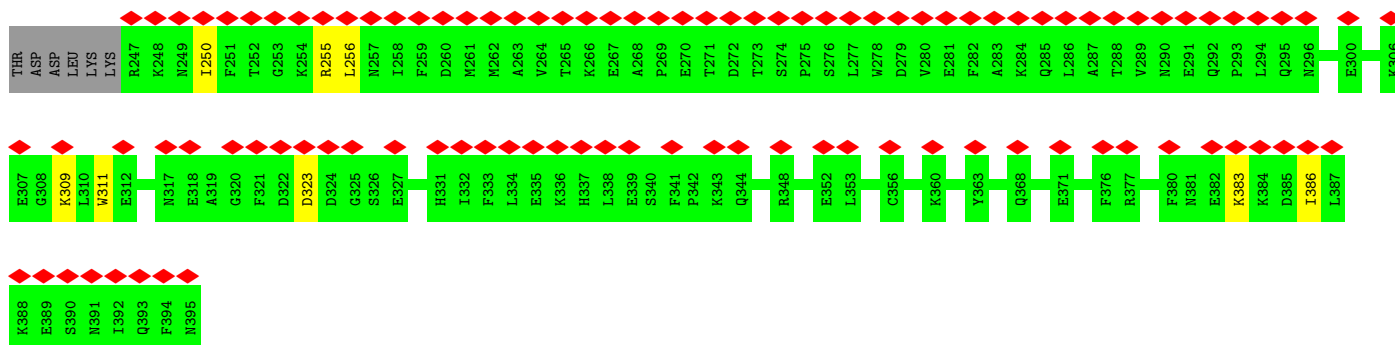
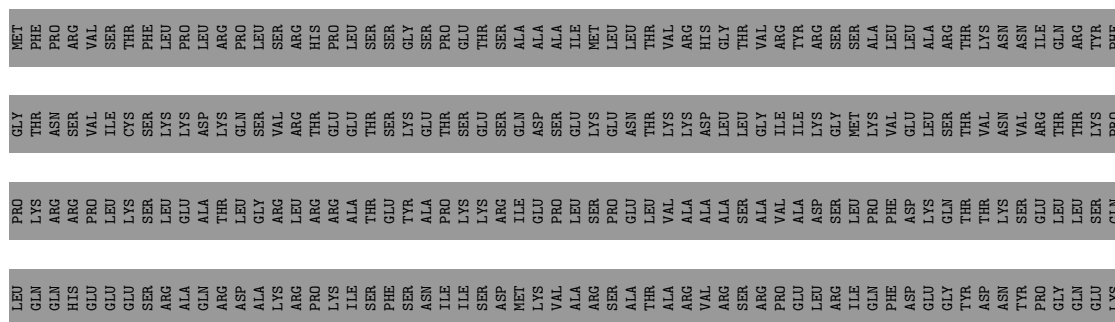


• Molecule 79: 28S ribosomal protein S29, mitochondrial

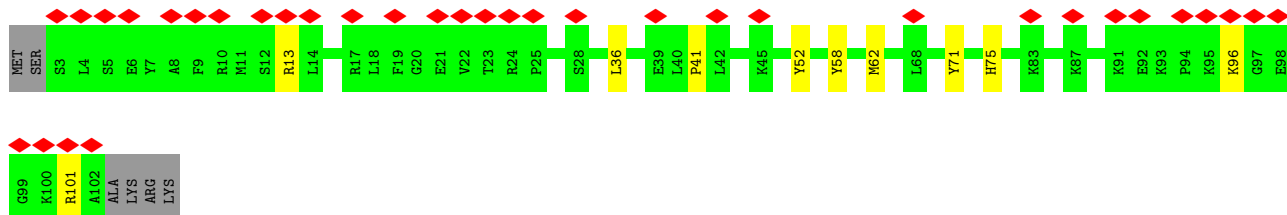
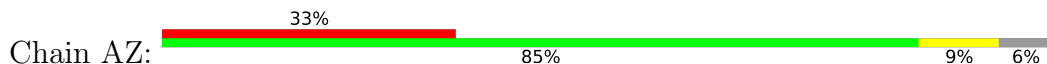




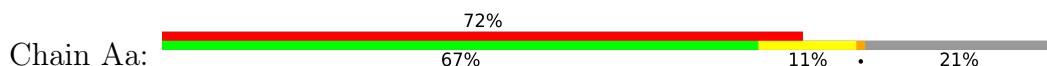
- Molecule 80: 28S ribosomal protein S31, mitochondrial

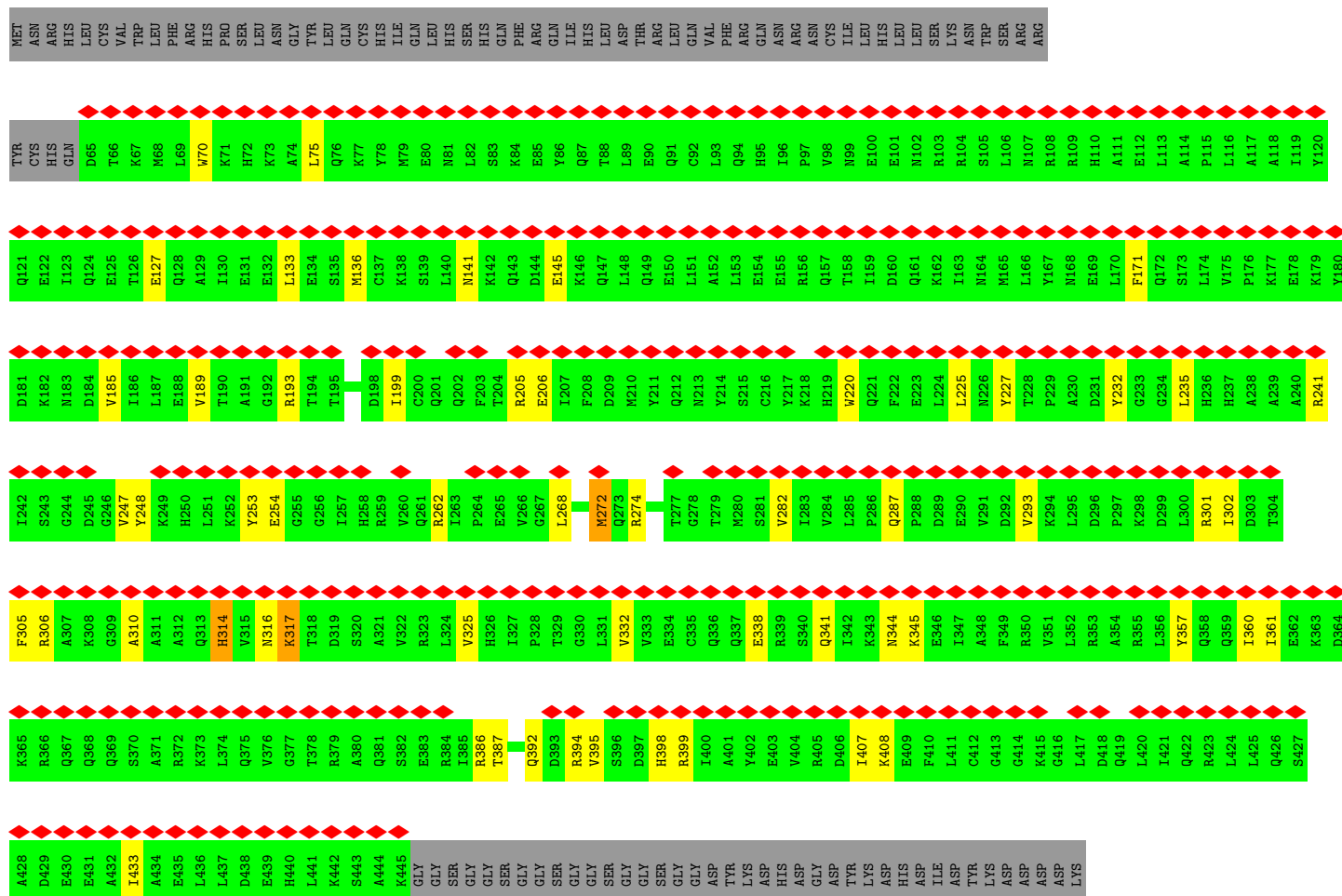


- Molecule 81: 28S ribosomal protein S33, mitochondrial

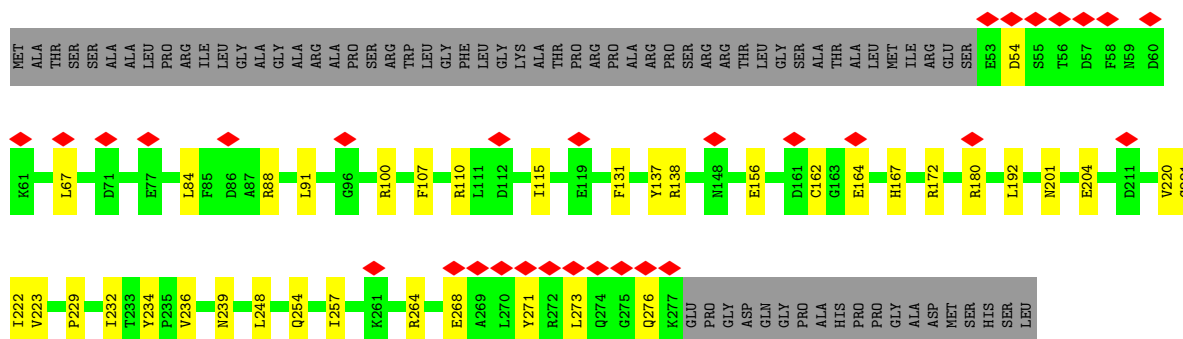


- Molecule 82: Peptide chain release factor 1, mitochondrial

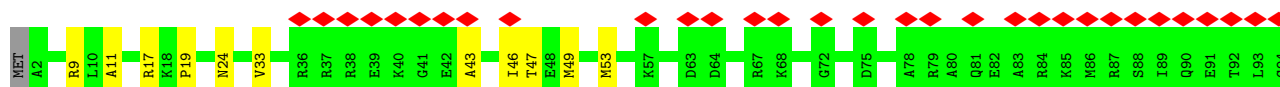
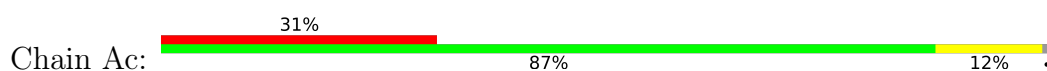


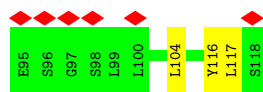


• Molecule 83: 28S ribosomal protein S2, mitochondrial

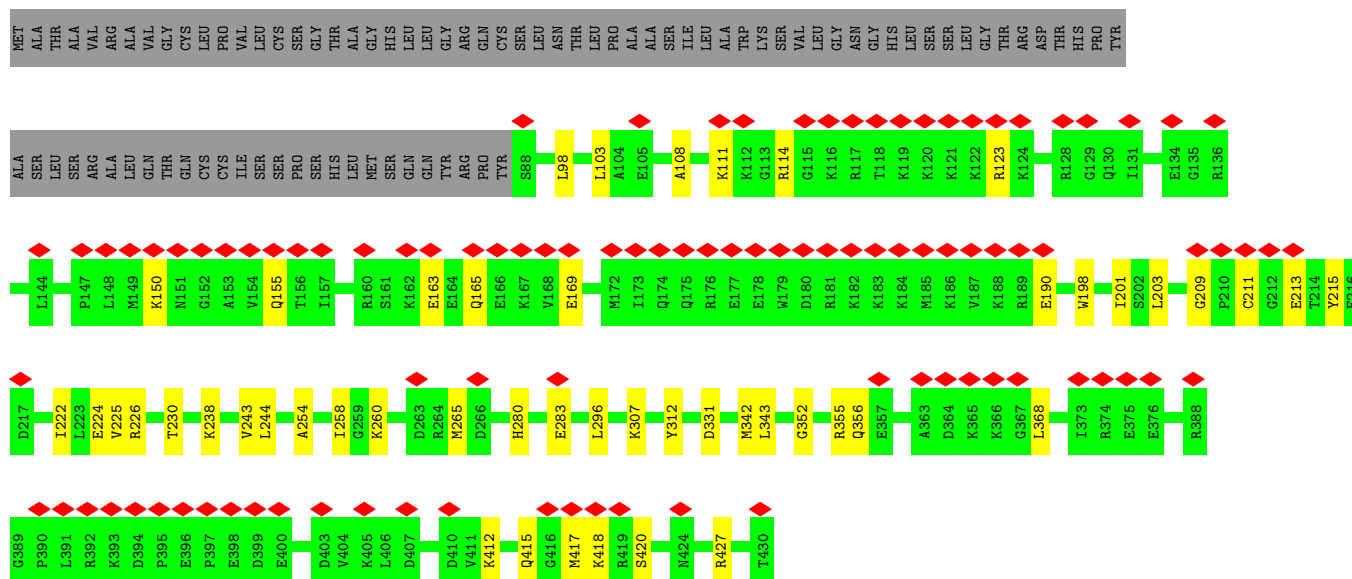


• Molecule 84: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

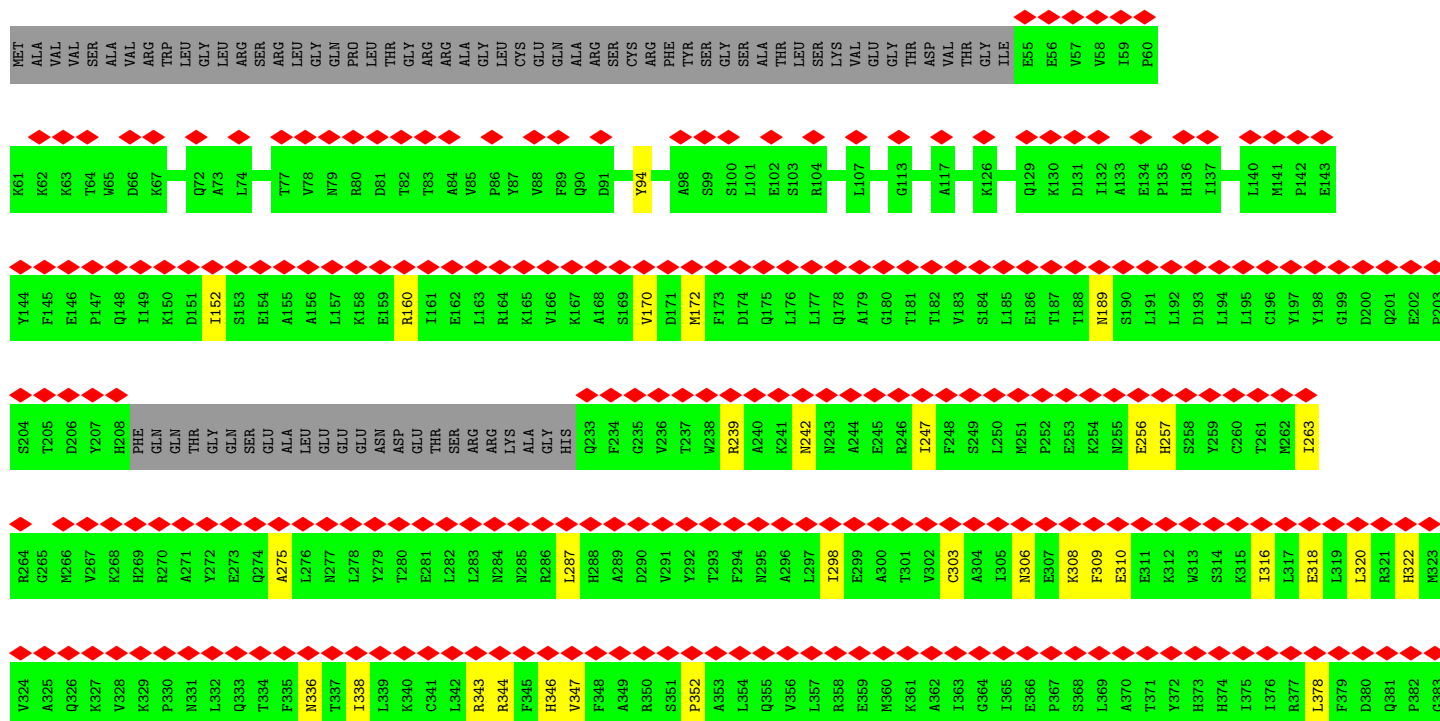
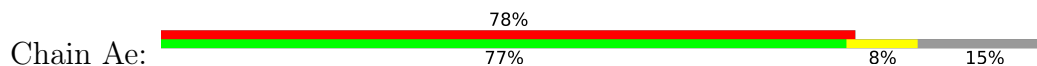


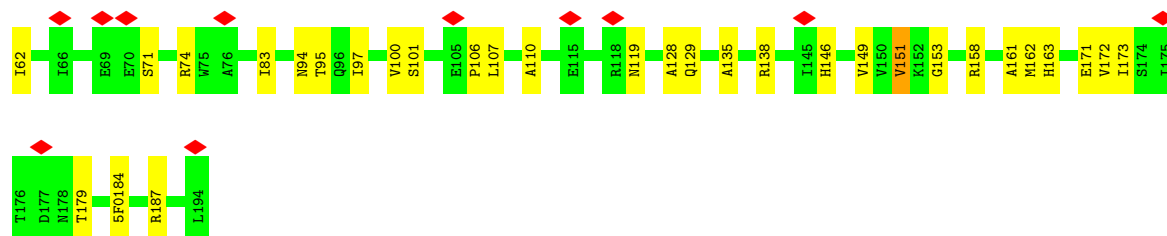


- Molecule 85: 28S ribosomal protein S5, mitochondrial



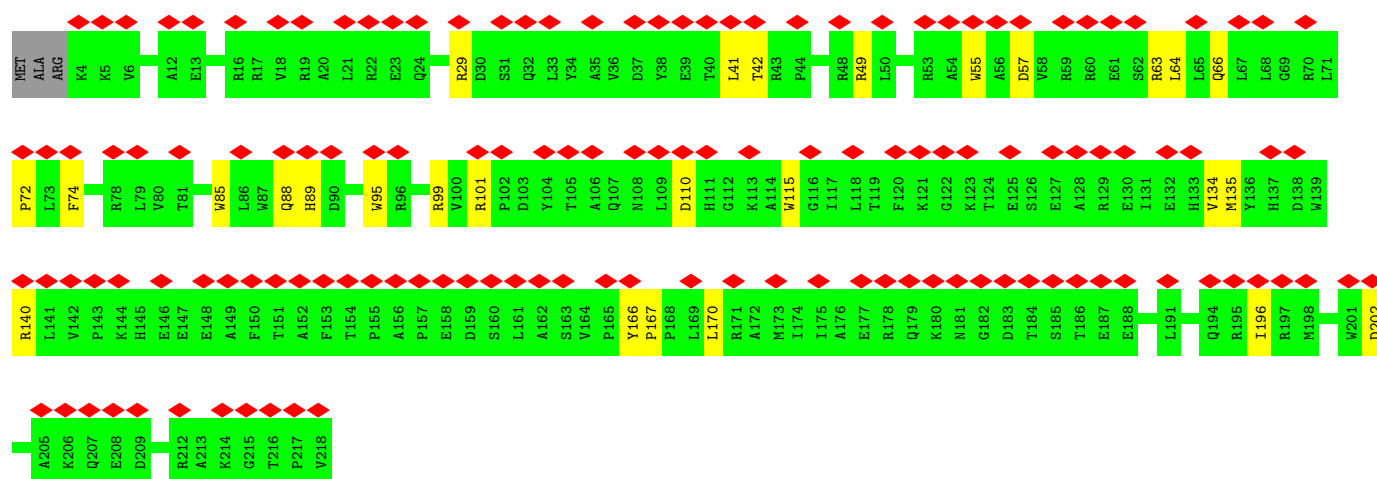
- Molecule 86: Pentatricopeptide repeat domain-containing protein 3, mitochondrial





- Molecule 89: 28S ribosomal protein S34, mitochondrial

Chain Aj: 62% 86% 12% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41288	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.235	Depositor
Minimum map value	-1.433	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.121	Depositor
Recommended contour level	0.6	Depositor
Map size ($\text{\AA}$)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, B8T, PSU, OMU, 5F0, ACE, MG, 2MG, SAC, AYA, 5MC, RSQ, 5MU, ZN, MA6, 1MA, GDP, ATP, Y5P, FS2, K

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	B1	0.08	0/358	0.16	0/486
1	B2	0.09	0/259	0.19	0/350
1	B3	0.08	0/259	0.17	0/350
1	B4	0.06	0/246	0.14	0/331
1	B5	0.06	0/246	0.17	0/331
1	B6	0.06	0/246	0.16	0/331
2	B7	0.06	0/68	0.11	0/103
3	B8	0.10	0/36876	0.15	0/57402
4	B9	0.07	0/1627	0.13	0/2527
5	BA	0.09	0/1403	0.19	0/1886
6	BB	0.09	0/1274	0.20	0/1723
7	BC	0.08	0/1721	0.19	0/2333
8	BD	0.10	0/926	0.20	0/1244
9	BE	0.08	0/2099	0.18	0/2837
10	BF	0.08	0/1593	0.17	0/2136
11	BG	0.10	0/1021	0.22	0/1378
12	BH	0.08	0/913	0.18	0/1224
13	BI	0.09	0/469	0.20	0/621
14	BJ	0.10	0/383	0.20	0/507
15	BK	0.10	0/853	0.21	0/1136
16	BL	0.09	0/1896	0.20	0/2549
17	BM	0.09	0/2475	0.22	0/3355
18	BN	0.10	0/2090	0.21	0/2842
19	BO	0.09	0/1698	0.22	0/2292
20	BP	0.08	0/1731	0.20	0/2345
21	BQ	0.06	0/1348	0.17	0/1813
22	BR	0.10	0/1490	0.21	0/2021
23	BS	0.09	0/905	0.21	0/1218
24	BT	0.09	0/2381	0.21	0/3212
25	BU	0.08	0/1833	0.19	0/2468
26	BV	0.09	0/1283	0.20	0/1727

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	BW	0.09	0/1199	0.20	0/1623
28	BX	0.21	1/2027 (0.0%)	0.31	1/2734 (0.0%)
29	BY	0.10	0/1175	0.18	0/1572
30	BZ	0.10	0/1320	0.23	0/1789
31	Ba	0.08	0/760	0.17	0/1023
32	Bb	0.07	0/777	0.17	0/1048
33	Bc	0.06	0/707	0.17	0/960
34	Bd	0.64	1/805 (0.1%)	0.41	3/1081 (0.3%)
35	Be	0.09	0/819	0.20	0/1097
36	Bf	0.07	0/1223	0.17	0/1641
37	Bg	0.07	0/1384	0.17	0/1869
38	Bh	0.09	0/1362	0.22	0/1846
39	Bi	0.09	0/3239	0.20	0/4400
40	Bj	0.08	0/1354	0.22	0/1831
41	Bl	0.10	0/350	0.21	0/461
42	Bm	0.09	0/3305	0.20	0/4502
43	Bn	0.08	0/3043	0.20	0/4140
44	Bo	0.08	0/2447	0.19	0/3310
45	Bp	0.07	0/1269	0.16	0/1708
46	Bq	0.09	0/1025	0.20	0/1379
47	Br	0.09	0/866	0.24	0/1174
48	Bs	0.10	0/1219	0.22	0/1651
49	Bt	0.08	0/2347	0.19	0/3171
50	Bu	0.08	0/2039	0.20	0/2759
51	Bv	0.06	0/1970	0.17	0/2658
52	Bw	0.07	0/1273	0.18	0/1716
53	Bx	0.10	0/1151	0.21	0/1569
54	By	0.06	0/918	0.16	0/1249
55	Bz	0.10	0/850	0.21	0/1135
56	AA	0.10	0/22563	0.14	0/35124
57	AB	0.09	0/2313	0.20	0/3129
58	AC	0.11	0/1113	0.22	0/1505
59	AD	0.09	0/636	0.20	0/839
60	AE	0.10	0/989	0.21	0/1335
61	AF	0.08	0/1767	0.18	0/2373
62	AG	0.09	0/1588	0.16	0/2466
63	AH	0.10	0/1178	0.22	0/1598
64	AI	0.09	0/149	0.15	0/231
65	AJ	0.09	0/855	0.20	0/1148
66	AK	0.10	0/880	0.21	0/1182
67	AL	0.08	0/1477	0.18	0/1974
68	AM	0.10	0/963	0.21	0/1295
69	AN	0.10	0/886	0.22	0/1199

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
70	AO	0.09	0/1648	0.20	0/2243
71	AP	0.09	0/798	0.21	0/1070
72	AQ	0.09	0/748	0.18	0/994
73	AR	0.08	0/2456	0.18	0/3317
74	AS	0.08	0/1138	0.16	0/1533
75	AT	0.09	0/1402	0.20	0/1883
76	AU	0.08	0/1510	0.19	0/2025
77	AV	0.06	0/3030	0.16	0/4093
78	AW	0.09	0/801	0.19	0/1079
79	AX	0.08	0/2921	0.20	0/3954
80	AY	0.07	0/1280	0.18	0/1725
81	AZ	0.08	0/857	0.18	0/1141
82	Aa	0.18	1/3162 (0.0%)	0.25	0/4253
83	Ab	0.10	0/1871	0.21	0/2531
84	Ac	0.08	0/941	0.19	0/1257
85	Ad	0.10	0/2783	0.22	0/3724
86	Ae	0.07	0/4877	0.18	0/6598
87	Ag	0.08	0/2746	0.19	0/3681
88	Ai	0.09	0/1030	0.23	0/1386
89	Aj	0.09	0/1834	0.22	0/2484
All	All	0.10	3/189383 (0.0%)	0.18	4/268543 (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
28	BX	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	Bd	99	GLN	C-N	18.10	1.58	1.33
28	BX	68	PRO	C-N	-8.62	1.23	1.33
82	Aa	361	ILE	C-N	-6.90	1.25	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BX	68	PRO	O-C-N	-12.01	106.42	122.64
34	Bd	99	GLN	O-C-N	8.05	131.33	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	Bd	99	GLN	CA-C-N	-6.10	114.20	122.86
34	Bd	99	GLN	C-N-CA	-6.10	114.20	122.86

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	BX	68	PRO	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B1	354	0	377	3	0
1	B2	257	0	283	3	0
1	B3	257	0	283	1	0
1	B4	245	0	275	3	0
1	B5	245	0	275	1	0
1	B6	245	0	275	4	0
2	B7	62	0	34	0	0
3	B8	33070	0	16795	240	0
4	B9	1524	0	778	20	0
5	BA	1369	0	1410	11	0
6	BB	1251	0	1232	10	0
7	BC	1676	0	1687	14	0
8	BD	904	0	935	7	0
9	BE	2044	0	2060	14	0
10	BF	1556	0	1597	13	0
11	BG	996	0	1044	9	0
12	BH	898	0	916	5	0
13	BI	464	0	511	6	0
14	BJ	377	0	406	2	0
15	BK	832	0	883	12	0
16	BL	1859	0	1920	18	0
17	BM	2406	0	2415	21	0
18	BN	2031	0	2065	31	0
19	BO	1661	0	1734	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	BP	1695	0	1785	14	0
21	BQ	1330	0	1407	13	0
22	BR	1455	0	1452	15	0
23	BS	890	0	941	12	0
24	BT	2327	0	2395	20	0
25	BU	1786	0	1817	16	0
26	BV	1259	0	1294	18	0
27	BW	1173	0	1165	10	0
28	BX	1979	0	2022	23	0
29	BY	1154	0	1214	13	0
30	BZ	1293	0	1365	10	0
31	Ba	745	0	746	5	0
32	Bb	774	0	784	7	0
33	Bc	688	0	674	7	0
34	Bd	791	0	796	18	0
35	Be	798	0	804	15	0
36	Bf	1205	0	1223	13	0
37	Bg	1350	0	1327	10	0
38	Bh	1322	0	1348	8	0
39	Bi	3155	0	3139	26	0
40	Bj	1327	0	1353	44	0
41	Bl	342	0	361	1	0
42	Bm	3210	0	3206	35	0
43	Bn	2948	0	2841	37	0
44	Bo	2390	0	2397	26	0
45	Bp	1243	0	1265	12	0
46	Bq	997	0	987	6	0
47	Br	840	0	810	7	0
48	Bs	1196	0	1195	19	0
49	Bt	2299	0	2320	17	0
50	Bu	1985	0	1976	16	0
51	Bv	1931	0	1916	24	0
52	Bw	1252	0	1269	14	0
53	Bx	1113	0	1097	7	0
54	By	895	0	881	5	0
55	Bz	828	0	857	11	0
56	AA	20283	0	10300	124	0
57	AB	2265	0	2294	18	0
58	AC	1083	0	1088	16	0
59	AD	625	0	699	15	0
60	AE	972	0	1000	15	0
61	AF	1725	0	1769	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	AG	1504	0	764	25	0
63	AH	1152	0	1183	17	0
64	AI	463	0	286	3	0
65	AJ	839	0	887	12	0
66	AK	862	0	885	15	0
67	AL	1453	0	1540	20	0
68	AM	942	0	965	17	0
69	AN	868	0	928	15	0
70	AO	1592	0	1557	14	0
71	AP	781	0	806	11	0
72	AQ	744	0	758	10	0
73	AR	2409	0	2428	33	0
74	AS	1111	0	1115	10	0
75	AT	1371	0	1393	10	0
76	AU	1488	0	1499	13	0
77	AV	2969	0	2961	26	0
78	AW	789	0	802	9	0
79	AX	2849	0	2843	41	0
80	AY	1246	0	1197	7	0
81	AZ	839	0	858	9	0
82	Aa	3114	0	3115	42	0
83	Ab	1828	0	1815	25	0
84	Ac	935	0	971	11	0
85	Ad	2731	0	2804	35	0
86	Ae	4768	0	4764	33	0
87	Ag	2688	0	2687	26	0
88	Ai	1020	0	1053	20	0
89	Aj	1787	0	1796	23	0
90	AA	16	0	0	0	0
90	Ae	1	0	0	0	0
90	B8	30	0	0	0	0
90	BL	1	0	0	0	0
90	BT	1	0	0	0	0
90	Be	1	0	0	0	0
90	Bn	1	0	0	0	0
91	AA	120	0	0	0	0
91	AD	1	0	0	0	0
91	AG	2	0	0	0	0
91	AU	1	0	0	0	0
91	AX	1	0	0	0	0
91	Aa	1	0	0	0	0
91	Ab	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
91	Ad	1	0	0	0	0
91	B8	216	0	0	0	0
91	BD	1	0	0	0	0
91	BL	3	0	0	0	0
91	BN	1	0	0	0	0
91	BO	1	0	0	0	0
91	BR	1	0	0	0	0
91	BT	1	0	0	0	0
91	BV	1	0	0	0	0
91	Bx	1	0	0	0	0
92	B9	7	0	8	0	0
93	AO	1	0	0	0	0
93	BH	1	0	0	0	0
93	Bl	1	0	0	0	0
94	AP	4	0	0	0	0
94	AT	4	0	0	0	0
94	Bh	4	0	0	1	0
95	AG	8	0	8	0	0
96	AX	31	0	12	0	0
97	AX	28	0	12	2	0
98	AX	3	0	0	0	0
All	All	181140	0	154469	1351	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 (1351) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:1401:U:H5''	82:Aa:310:ALA:HA	1.51	0.93
4:B9:6:U:H3	4:B9:63:G:H1	1.18	0.91
3:B8:926:G:H5'	59:AD:152:PHE:CE1	2.14	0.83
3:B8:1107:G:N3	19:BO:179:ASN:ND2	2.30	0.79
3:B8:969:C:H5''	59:AD:159:GLU:OE2	1.82	0.79
3:B8:1111:U:O2	40:Bj:296:ARG:NH2	2.17	0.78
3:B8:829:U:OP2	3:B8:834:A:N6	2.16	0.78
3:B8:1343:G:HO2'	41:Bl:66:PHE:N	1.82	0.78
3:B8:1109:C:H5'	40:Bj:116:SER:HB3	1.67	0.77
3:B8:107:A:N6	3:B8:110:U:OP2	2.18	0.76
3:B8:912:A:O3'	56:AA:935:G:H1'	1.86	0.76
3:B8:681:U:O4	3:B8:692:A:N6	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AA:679:A:O4'	85:Ad:114:ARG:NH1	2.20	0.74
20:BP:47:LEU:HD22	25:BU:226:ILE:HG12	1.70	0.73
19:BO:163:THR:HG21	40:Bj:87:TYR:HA	1.70	0.73
56:AA:640:A:OP2	85:Ad:260:LYS:NZ	2.23	0.72
3:B8:1184:U:H4'	15:BK:138:PRO:HG2	1.72	0.72
71:AP:82:GLN:HE21	71:AP:132:ASP:HB3	1.54	0.71
88:Ai:97:ILE:HD11	88:Ai:161:ALA:HB1	1.72	0.71
40:Bj:97:TYR:HB3	40:Bj:306:LYS:HB2	1.72	0.71
3:B8:1108:U:OP1	3:B8:1112:A:N6	2.23	0.71
57:AB:152:ASP:OD2	57:AB:174:ARG:NH1	2.24	0.70
82:Aa:70:TRP:HA	82:Aa:75:LEU:HD23	1.73	0.70
30:BZ:144:LEU:HB2	47:Br:58:ILE:HB	1.74	0.69
19:BO:53:THR:N	19:BO:86:THR:HG1	1.91	0.69
28:BX:182:ARG:HG3	28:BX:187:LEU:HD11	1.74	0.69
3:B8:320:G:OP1	16:BL:269:ARG:NH2	2.26	0.69
25:BU:124:VAL:HG12	25:BU:158:ARG:HE	1.58	0.69
1:B3:60:TYR:HB3	1:B3:65:GLN:HE21	1.57	0.68
85:Ad:103:LEU:HD11	85:Ad:123:ARG:HB2	1.75	0.68
3:B8:216:G:H1	55:Bz:61:GLY:HA3	1.58	0.68
74:AS:97:GLN:NE2	74:AS:101:GLU:OE2	2.27	0.68
47:Br:41:ASP:HB3	47:Br:46:ASN:HD22	1.58	0.67
86:Ae:239:ARG:O	86:Ae:242:ASN:ND2	2.23	0.67
85:Ad:244:LEU:HD22	85:Ad:343:LEU:HD23	1.75	0.67
56:AA:122:G:OP2	69:AN:73:ARG:NH2	2.28	0.67
85:Ad:283:GLU:O	85:Ad:356:GLN:NE2	2.28	0.67
3:B8:969:C:C5'	59:AD:159:GLU:OE2	2.43	0.66
18:BN:253:MET:HE3	18:BN:259:LEU:HD22	1.77	0.66
3:B8:433:A:HO2'	11:BG:35:LYS:N	1.94	0.66
3:B8:438:G:N7	25:BU:67:LYS:NZ	2.42	0.66
39:Bi:177:LEU:HD23	39:Bi:238:ASN:HD22	1.59	0.66
56:AA:647:A:OP1	83:Ab:201:ASN:ND2	2.29	0.66
75:AT:21:VAL:HG22	75:AT:103:ARG:HB2	1.76	0.66
9:BE:44:ARG:NH2	19:BO:84:GLU:OE1	2.29	0.66
44:Bo:298:GLN:HE22	44:Bo:323:MET:HA	1.60	0.65
66:AK:51:ARG:NH2	66:AK:83:CYS:SG	2.69	0.65
44:Bo:112:PRO:HB2	44:Bo:267:PRO:HG2	1.78	0.65
49:Bt:215:ILE:HG23	49:Bt:219:LEU:HD12	1.78	0.65
61:AF:79:ALA:O	87:Ag:312:GLN:NE2	2.30	0.65
63:AH:121:LEU:HD21	63:AH:128:LYS:HD2	1.79	0.65
7:BC:79:VAL:HG12	7:BC:86:VAL:HG12	1.77	0.65
42:Bm:115:GLU:HB2	42:Bm:119:GLN:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AA:783:A:OP2	61:AF:35:SER:N	2.30	0.65
60:AE:35:ILE:HD11	67:AL:91:ARG:HD3	1.78	0.65
67:AL:128:ARG:HH21	67:AL:166:MET:HE2	1.62	0.64
79:AX:155:ILE:HB	79:AX:262:VAL:HA	1.79	0.64
62:AG:51:PSU:H3'	62:AG:52:A:H8	1.62	0.64
86:Ae:443:ASP:HB3	86:Ae:446:LYS:HE2	1.79	0.64
4:B9:43:G:O6	27:BW:88:HIS:NE2	2.31	0.64
29:BY:33:GLY:O	29:BY:36:ASN:ND2	2.30	0.64
37:Bg:37:PRO:HG2	37:Bg:68:SER:HA	1.80	0.64
79:AX:288:ALA:O	79:AX:292:ASN:ND2	2.30	0.64
3:B8:1419:A:H62	82:Aa:314:HIS:CD2	2.16	0.64
7:BC:121:LYS:HD3	7:BC:130:PRO:HB2	1.80	0.64
9:BE:163:ARG:HE	42:Bm:55:LEU:HD11	1.63	0.64
56:AA:625:A:N1	56:AA:656:G:O2'	2.29	0.64
40:Bj:245:VAL:HA	40:Bj:253:LEU:HD22	1.79	0.64
79:AX:295:LYS:NZ	97:AX:503:GDP:O1A	2.31	0.64
84:Ac:11:ALA:HB2	84:Ac:19:PRO:HB3	1.80	0.64
3:B8:1540:C:N4	3:B8:1557:U:O4	2.27	0.64
37:Bg:112:GLN:OE1	37:Bg:115:ARG:NH2	2.31	0.64
61:AF:119:LYS:NZ	79:AX:398:LEU:O	2.28	0.64
86:Ae:189:ASN:HB3	86:Ae:257:HIS:HD2	1.63	0.64
3:B8:926:G:C5'	59:AD:152:PHE:CD1	2.81	0.64
51:Bv:255:VAL:HB	51:Bv:259:GLU:HG3	1.78	0.64
43:Bn:255:LEU:HD12	43:Bn:256:PRO:HD2	1.80	0.64
3:B8:1012:A:OP1	29:BY:34:ARG:NH2	2.30	0.63
23:BS:46:LEU:HD12	23:BS:78:LYS:HD3	1.79	0.63
51:Bv:147:THR:HG21	51:Bv:248:ASN:HB3	1.81	0.63
56:AA:292:A:OP1	59:AD:132:LYS:NZ	2.32	0.63
60:AE:49:TYR:OH	60:AE:90:ARG:NH1	2.31	0.63
56:AA:881:A:OP1	89:Aj:101:ARG:NH2	2.31	0.63
25:BU:124:VAL:HA	25:BU:158:ARG:HH21	1.61	0.63
17:BM:244:ALA:HB1	17:BM:248:ILE:HD11	1.80	0.63
34:Bd:81:LEU:HD11	45:Bp:189:GLU:HB3	1.81	0.63
74:AS:51:VAL:HG13	84:Ac:117:LEU:HD11	1.80	0.63
77:AV:36:ASP:OD1	77:AV:38:HIS:ND1	2.32	0.63
16:BL:194:ASN:ND2	16:BL:245:GLY:O	2.32	0.63
43:Bn:155:TYR:O	43:Bn:267:ARG:NH1	2.31	0.63
78:AW:119:LYS:NZ	83:Ab:239:ASN:OD1	2.31	0.63
85:Ad:296:LEU:HD11	85:Ad:352:GLY:HA3	1.81	0.63
56:AA:796:U:O2'	56:AA:798:G:N7	2.28	0.63
62:AG:9:C:O2'	62:AG:10:A:N7	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BL:201:GLY:O	42:Bm:30:ALA:N	2.32	0.62
60:AE:26:ILE:HG23	60:AE:36:VAL:HG21	1.81	0.62
3:B8:82:U:OP1	15:BK:94:LEU:N	2.32	0.62
3:B8:135:A:OP2	7:BC:94:HIS:NE2	2.30	0.62
25:BU:218:ILE:HG23	25:BU:223:MET:HB2	1.81	0.62
65:AJ:37:HIS:ND1	69:AN:36:ASP:OD2	2.33	0.62
57:AB:86:ARG:HB3	57:AB:96:PRO:HB2	1.80	0.62
61:AF:72:GLN:O	87:Ag:365:ARG:NH2	2.33	0.62
73:AR:207:PRO:HB2	73:AR:209:ILE:HG22	1.82	0.62
86:Ae:160:ARG:NH1	86:Ae:172:MET:SD	2.73	0.62
42:Bm:229:ARG:NH1	42:Bm:231:SER:OG	2.33	0.62
58:AC:100:PHE:HB3	58:AC:103:CYS:HB2	1.82	0.62
61:AF:48:LYS:NZ	79:AX:375:GLU:OE2	2.33	0.62
54:By:69:ARG:NH2	54:By:107:ASP:OD2	2.31	0.61
3:B8:346:C:OP2	24:BT:59:ARG:NH1	2.34	0.61
56:AA:882:A:H1'	77:AV:66:PRO:HD3	1.81	0.61
87:Ag:59:LYS:HE2	87:Ag:62:PRO:HA	1.83	0.61
39:Bi:49:ALA:O	39:Bi:61:ARG:NH1	2.34	0.61
39:Bi:287:LYS:NZ	42:Bm:166:THR:O	2.32	0.61
73:AR:85:LEU:HD21	73:AR:123:LYS:HG3	1.82	0.61
49:Bt:151:GLU:O	49:Bt:155:ASN:ND2	2.30	0.61
56:AA:598:U:O2'	81:AZ:96:LYS:NZ	2.31	0.61
19:BO:189:VAL:HG21	19:BO:208:LEU:HD21	1.82	0.61
68:AM:104:ILE:HG23	73:AR:147:ILE:HG12	1.82	0.61
3:B8:219:C:OP1	24:BT:133:LYS:NZ	2.33	0.61
85:Ad:165:GLN:NE2	85:Ad:169:GLU:OE2	2.33	0.61
7:BC:54:TRP:NE1	7:BC:56:LEU:O	2.34	0.61
36:Bf:190:GLN:NE2	43:Bn:188:TYR:OH	2.34	0.61
3:B8:117:G:N2	3:B8:120:A:OP2	2.32	0.60
56:AA:122:G:N2	56:AA:125:A:OP2	2.34	0.60
73:AR:155:LYS:HB3	73:AR:177:PRO:HD3	1.82	0.60
65:AJ:74:ASN:ND2	65:AJ:117:ASP:OD1	2.34	0.60
74:AS:85:PHE:HB2	78:AW:100:VAL:HG12	1.83	0.60
18:BN:114:THR:O	18:BN:156:ARG:NH1	2.34	0.60
39:Bi:204:CYS:SG	39:Bi:240:GLN:NE2	2.74	0.60
56:AA:374:U:OP2	84:Ac:9:ARG:NH2	2.32	0.60
3:B8:1146:G:O6	8:BD:33:LYS:NZ	2.34	0.60
36:Bf:111:ILE:O	36:Bf:116:ARG:NH1	2.34	0.60
49:Bt:161:THR:O	49:Bt:192:GLN:NE2	2.34	0.60
79:AX:276:ARG:NH2	79:AX:286:GLU:OE1	2.34	0.60
83:Ab:180:ARG:NH2	85:Ad:211:CYS:SG	2.73	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:Ag:273:GLU:HG2	87:Ag:282:GLU:HG2	1.81	0.60
3:B8:1561:U:H3	26:BV:53:ARG:HH22	1.50	0.60
56:AA:552:G:N1	56:AA:775:G:OP2	2.32	0.60
79:AX:268:LEU:HD21	79:AX:293:LEU:HD23	1.82	0.60
86:Ae:470:GLN:NE2	86:Ae:472:ASP:OD2	2.34	0.60
3:B8:64:C:OP1	19:BO:72:ARG:NE	2.34	0.60
18:BN:279:ARG:HH12	18:BN:282:PRO:HD3	1.66	0.60
45:Bp:182:ILE:HB	45:Bp:185:TYR:HB2	1.84	0.60
56:AA:247:C:N4	65:AJ:117:ASP:OD2	2.33	0.60
68:AM:108:GLU:OE2	76:AU:59:ARG:NH2	2.29	0.60
53:Bx:110:ILE:HD11	53:Bx:157:LEU:HD13	1.84	0.60
44:Bo:107:LEU:HB3	44:Bo:126:LYS:HB3	1.84	0.60
53:Bx:118:TRP:NE1	53:Bx:142:GLU:OE2	2.28	0.60
5:BA:57:LEU:HB2	5:BA:60:GLU:HG3	1.84	0.60
19:BO:98:LEU:HD23	19:BO:129:ALA:HB2	1.82	0.60
25:BU:123:ARG:NH1	25:BU:162:GLU:OE1	2.35	0.60
50:Bu:98:SER:OG	50:Bu:215:ARG:NH2	2.35	0.60
86:Ae:565:ARG:NH1	86:Ae:569:GLN:OE1	2.35	0.60
8:BD:100:THR:OG1	8:BD:132:HIS:NE2	2.29	0.59
42:Bm:201:ARG:NH1	42:Bm:418:TYR:O	2.33	0.59
69:AN:31:THR:HG22	69:AN:46:ARG:HG2	1.83	0.59
56:AA:472:U:HO2'	56:AA:480:A:HO2'	1.46	0.59
6:BB:110:LEU:HD12	10:BF:118:GLU:HG2	1.85	0.59
24:BT:44:ARG:HG3	24:BT:45:ARG:HG3	1.82	0.59
63:AH:71:ILE:O	63:AH:150:GLY:N	2.35	0.59
3:B8:423:U:H4'	55:Bz:126:LYS:HE2	1.85	0.59
26:BV:16:ARG:NH2	26:BV:50:ASP:OD2	2.35	0.59
44:Bo:148:MET:HE2	44:Bo:257:ILE:HG12	1.85	0.59
62:AG:18:A:H61	62:AG:43:A:H2'	1.66	0.59
70:AO:199:TRP:NE1	89:Aj:166:TYR:O	2.34	0.59
58:AC:45:SER:HB2	58:AC:49:LYS:HE3	1.85	0.59
43:Bn:187:VAL:HG13	43:Bn:319:PHE:HB3	1.83	0.59
51:Bv:164:LYS:HE2	51:Bv:167:ASP:HA	1.85	0.59
82:Aa:205:ARG:HA	82:Aa:235:LEU:HD12	1.83	0.59
3:B8:725:A:OP1	42:Bm:173:ARG:NH2	2.33	0.59
34:Bd:67:ARG:NH1	52:Bw:101:THR:OG1	2.35	0.59
56:AA:590:A:OP1	66:AK:36:ARG:NH2	2.32	0.59
66:AK:34:MET:HE3	66:AK:95:SER:HB2	1.85	0.58
3:B8:283:A:O2'	3:B8:793:A:OP1	2.21	0.58
3:B8:926:G:H5''	59:AD:152:PHE:CD1	2.38	0.58
70:AO:105:CYS:HB2	70:AO:142:VAL:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:674:C:H1'	3:B8:692:A:H4'	1.84	0.58
3:B8:926:G:H5'	59:AD:152:PHE:CD1	2.37	0.58
36:Bf:84:SER:HB3	36:Bf:98:LYS:HB2	1.84	0.58
13:BI:47:ASP:HB3	13:BI:50:VAL:HG22	1.86	0.58
17:BM:69:ASP:OD1	17:BM:154:ARG:NH1	2.36	0.58
51:Bv:58:VAL:HB	51:Bv:153:LEU:HB3	1.84	0.58
74:AS:29:PRO:HG2	74:AS:32:PHE:HB2	1.84	0.58
82:Aa:392:GLN:OE1	82:Aa:394:ARG:NH2	2.36	0.58
72:AQ:14:VAL:HG21	88:Ai:172:VAL:HG12	1.85	0.58
80:AY:255:ARG:NH1	80:AY:256:LEU:O	2.36	0.58
9:BE:7:PRO:HD2	9:BE:10:LEU:HD12	1.85	0.58
37:Bg:163:LEU:HB2	37:Bg:171:ARG:HH12	1.67	0.58
61:AF:176:ASP:OD2	61:AF:180:ARG:NH1	2.35	0.58
86:Ae:318:GLU:OE2	86:Ae:322:HIS:NE2	2.37	0.58
4:B9:68:G:H2'	4:B9:69:A:H8	1.68	0.58
33:Bc:121:LEU:O	33:Bc:125:ASN:ND2	2.34	0.58
79:AX:50:ARG:NH2	79:AX:96:GLU:OE2	2.31	0.58
3:B8:1239:G:OP1	13:BI:63:ARG:NH1	2.31	0.58
6:BB:129:MET:HG3	50:Bu:82:ALA:HB2	1.84	0.58
17:BM:50:ASP:O	26:BV:138:ARG:NH2	2.37	0.58
18:BN:272:LYS:NZ	55:Bz:65:ASN:OD1	2.37	0.58
43:Bn:215:THR:HB	43:Bn:273:PHE:HB2	1.85	0.58
56:AA:291:A:OP1	59:AD:128:LYS:NZ	2.36	0.58
89:Aj:63:ARG:NH2	89:Aj:110:ASP:OD2	2.37	0.58
3:B8:75:U:O4	15:BK:108:LYS:NZ	2.37	0.58
23:BS:93:GLY:O	23:BS:95:ARG:NH2	2.36	0.58
56:AA:329:A:H5''	72:AQ:2:AYA:HM3	1.86	0.58
70:AO:215:ARG:NH1	89:Aj:88:GLN:O	2.36	0.58
87:Ag:378:GLU:OE2	87:Ag:381:LYS:NZ	2.35	0.58
88:Ai:149:VAL:HG11	88:Ai:162:MET:HE2	1.86	0.58
3:B8:578:U:OP1	29:BY:99:ARG:NH2	2.33	0.57
3:B8:1113:A:H4'	40:Bj:302:GLY:H	1.68	0.57
8:BD:148:LEU:OXT	43:Bn:339:GLU:N	2.37	0.57
43:Bn:217:LEU:HD11	43:Bn:271:LEU:HD12	1.86	0.57
85:Ad:412:LYS:HG2	85:Ad:418:LYS:HB2	1.86	0.57
87:Ag:389:ARG:NH1	87:Ag:390:LYS:O	2.38	0.57
3:B8:927:C:OP1	59:AD:156:LYS:NZ	2.23	0.57
29:BY:96:GLU:O	30:BZ:105:GLN:NE2	2.31	0.57
56:AA:283:G:O6	65:AJ:47:ARG:NH2	2.37	0.57
3:B8:77:G:OP2	3:B8:79:C:N4	2.37	0.57
3:B8:788:A:O2'	17:BM:215:PHE:O	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BW:52:ASN:HB3	27:BW:55:ASN:HB2	1.87	0.57
56:AA:378:A:OP1	67:AL:154:ARG:NH2	2.35	0.57
87:Ag:155:LYS:NZ	87:Ag:217:ASP:OD2	2.38	0.57
1:B1:76:LEU:H	1:B4:68:VAL:HG11	1.70	0.57
35:Be:88:ILE:HG13	53:Bx:142:GLU:HB3	1.86	0.57
76:AU:68:ARG:HD2	89:Aj:196:ILE:HG23	1.86	0.57
77:AV:102:TRP:HD1	89:Aj:74:PHE:HD2	1.51	0.57
3:B8:1396:C:O2'	17:BM:233:GLN:OE1	2.20	0.57
13:BI:13:SER:OG	13:BI:36:ARG:NH2	2.38	0.57
52:Bw:127:MET:HE3	52:Bw:128:PRO:HD2	1.86	0.57
63:AH:76:LEU:HB2	63:AH:145:LEU:HB2	1.87	0.57
87:Ag:229:LEU:HD21	87:Ag:241:VAL:HG11	1.85	0.57
3:B8:286:U:O2'	3:B8:1428:U:O2'	2.23	0.57
3:B8:1556:G:O2'	3:B8:1559:U:O4	2.22	0.57
43:Bn:244:ARG:NH1	43:Bn:247:GLU:OE1	2.38	0.57
82:Aa:189:VAL:HG12	82:Aa:282:VAL:HG22	1.86	0.57
17:BM:111:THR:OG1	17:BM:113:ASP:OD1	2.22	0.56
63:AH:104:ILE:HG23	63:AH:148:LEU:HD21	1.86	0.56
3:B8:374:A:OP1	15:BK:153:THR:OG1	2.19	0.56
3:B8:1393:G:O2'	3:B8:1396:C:OP2	2.22	0.56
3:B8:1398:G:N2	3:B8:1398:G:OP2	2.33	0.56
4:B9:42:A:H62	27:BW:120:ARG:HH12	1.53	0.56
16:BL:194:ASN:OD1	16:BL:195:ASN:ND2	2.37	0.56
7:BC:105:ARG:NH2	50:Bu:171:ASP:OD1	2.39	0.56
19:BO:201:VAL:HG13	40:Bj:86:VAL:HG22	1.87	0.56
30:BZ:111:GLU:HG2	48:Bs:19:LEU:HD11	1.87	0.56
31:Ba:112:LYS:NZ	43:Bn:311:MET:O	2.38	0.56
56:AA:194:A:OP1	68:AM:39:ASN:ND2	2.39	0.56
73:AR:167:HIS:HB3	73:AR:193:ILE:HD13	1.86	0.56
3:B8:310:A:OP1	14:BJ:56:SER:OG	2.21	0.56
3:B8:861:U:O4	16:BL:246:ARG:NH2	2.39	0.56
3:B8:1257:C:O2	50:Bu:38:LYS:NZ	2.27	0.56
37:Bg:40:PRO:HG2	37:Bg:51:GLN:HB3	1.88	0.56
80:AY:383:LYS:HD2	80:AY:386:ILE:HD12	1.87	0.56
11:BG:78:ARG:O	11:BG:83:LYS:NZ	2.39	0.56
56:AA:345:U:O2'	56:AA:347:A:OP2	2.19	0.56
82:Aa:293:VAL:HG22	82:Aa:360:ILE:HD12	1.88	0.56
51:Bv:90:ARG:NH2	51:Bv:115:LEU:O	2.38	0.56
3:B8:845:U:OP1	16:BL:284:ARG:NH2	2.36	0.56
4:B9:24:A:N6	27:BW:87:GLN:OE1	2.37	0.56
18:BN:62:VAL:HG23	18:BN:82:LEU:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:AN:67:ARG:NH1	69:AN:80:GLU:OE2	2.38	0.56
7:BC:45:VAL:HG11	10:BF:237:LYS:HG3	1.88	0.56
18:BN:211:ARG:HD3	54:By:58:ARG:HH21	1.71	0.56
39:Bi:66:TRP:O	39:Bi:69:THR:OG1	2.23	0.56
40:Bj:290:VAL:HG11	40:Bj:307:ILE:HD13	1.88	0.56
56:AA:655:C:OP1	58:AC:165:LYS:NZ	2.31	0.56
78:AW:104:ILE:HG12	78:AW:114:ILE:HG12	1.87	0.56
86:Ae:256:GLU:HG2	86:Ae:287:LEU:HB3	1.86	0.56
3:B8:183:A:OP2	30:BZ:177:ARG:NH1	2.33	0.56
6:BB:46:MET:HE1	6:BB:72:VAL:HG13	1.88	0.56
52:Bw:106:TYR:OH	52:Bw:174:ILE:O	2.23	0.56
56:AA:642:G:O2'	56:AA:650:G:OP2	2.20	0.56
56:AA:706:A:H5'	56:AA:707:A:H5'	1.86	0.56
62:AG:6:G:H1	62:AG:62:C:H42	1.53	0.56
83:Ab:162:CYS:HB3	83:Ab:254:GLN:HG3	1.86	0.56
3:B8:161:G:O6	48:Bs:4:ARG:NH2	2.36	0.56
17:BM:45:SER:O	44:Bo:307:ARG:NH2	2.38	0.56
3:B8:347:U:O2'	3:B8:1053:A:N1	2.37	0.55
44:Bo:296:ARG:NH1	44:Bo:324:VAL:O	2.39	0.55
58:AC:115:ASN:ND2	80:AY:309:LYS:O	2.39	0.55
77:AV:167:VAL:HG13	77:AV:172:ALA:HB3	1.86	0.55
5:BA:63:ARG:NH1	50:Bu:228:PHE:O	2.39	0.55
89:Aj:110:ASP:OD1	89:Aj:110:ASP:N	2.35	0.55
3:B8:1306:G:O2'	3:B8:1335:A:N6	2.40	0.55
28:BX:73:ARG:NH1	28:BX:213:GLN:O	2.40	0.55
57:AB:176:LYS:HG2	57:AB:204:VAL:HG22	1.88	0.55
3:B8:916:U:O2'	62:AG:12:C:O2'	2.20	0.55
24:BT:244:LEU:HD12	24:BT:245:PRO:HD2	1.88	0.55
59:AD:173:LEU:HD22	67:AL:209:LEU:HD22	1.89	0.55
3:B8:133:A:H4'	3:B8:134:A:H3'	1.88	0.55
56:AA:729:C:H4'	56:AA:730:C:H5'	1.87	0.55
44:Bo:186:ASP:OD1	44:Bo:187:SER:N	2.40	0.55
75:AT:139:CYS:HB3	75:AT:141:CYS:SG	2.46	0.55
44:Bo:156:ARG:O	47:Br:95:ARG:NH2	2.33	0.55
57:AB:114:LEU:HD11	63:AH:163:ASN:HB3	1.89	0.55
83:Ab:220:VAL:HG22	83:Ab:234:TYR:HB2	1.87	0.55
5:BA:206:LEU:HD11	30:BZ:107:LYS:HD3	1.89	0.55
19:BO:107:VAL:HG22	19:BO:108:ARG:H	1.71	0.55
65:AJ:70:PRO:HB3	65:AJ:117:ASP:HB3	1.87	0.55
72:AQ:20:GLU:OE2	88:Ai:163:HIS:NE2	2.38	0.55
3:B8:1262:G:OP1	18:BN:137:ARG:NH1	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AA:586:C:H42	66:AK:85:VAL:HG12	1.72	0.55
56:AA:768:G:OP2	56:AA:768:G:N2	2.30	0.55
73:AR:188:GLU:HG2	73:AR:191:ARG:HH22	1.72	0.55
18:BN:243:ILE:HG22	37:Bg:27:ALA:HB2	1.89	0.55
15:BK:175:ASP:HB3	15:BK:178:GLN:HB2	1.90	0.54
24:BT:91:ARG:NH1	24:BT:209:GLU:OE2	2.39	0.54
56:AA:196:G:N2	56:AA:199:A:OP2	2.38	0.54
61:AF:44:PRO:HD3	61:AF:75:LYS:HB2	1.89	0.54
73:AR:162:SER:O	73:AR:170:ARG:NH1	2.38	0.54
21:BQ:114:LEU:HD21	33:Bc:101:LEU:HD21	1.89	0.54
86:Ae:170:VAL:HG23	86:Ae:247:ILE:HD11	1.89	0.54
6:BB:64:PRO:HB2	6:BB:100:ALA:HB3	1.89	0.54
40:Bj:128:ASP:N	40:Bj:289:PHE:O	2.41	0.54
40:Bj:295:LEU:HB2	40:Bj:305:LEU:HD11	1.90	0.54
34:Bd:82:ASP:O	34:Bd:89:ARG:NH2	2.41	0.54
35:Be:12:ILE:HG13	35:Be:23:ARG:HB2	1.88	0.54
44:Bo:243:LYS:NZ	44:Bo:265:GLU:OE1	2.33	0.54
48:Bs:136:LYS:O	49:Bt:259:ARG:NH2	2.34	0.54
57:AB:166:PRO:O	57:AB:169:ARG:NH1	2.41	0.54
82:Aa:293:VAL:HG21	82:Aa:357:TYR:HA	1.89	0.54
68:AM:29:ARG:HD2	68:AM:57:LEU:HD12	1.90	0.54
77:AV:236:LEU:HD12	77:AV:290:LEU:HD13	1.88	0.54
20:BP:45:GLN:NE2	35:Be:25:ARG:O	2.39	0.54
71:AP:124:TYR:HB3	72:AQ:9:ALA:HB2	1.90	0.54
83:Ab:223:VAL:HG11	83:Ab:229:PRO:HB3	1.90	0.54
18:BN:184:GLN:HE22	24:BT:22:VAL:HG23	1.73	0.54
49:Bt:105:ARG:HG3	49:Bt:110:ILE:HB	1.90	0.54
3:B8:93:A:H61	37:Bg:51:GLN:HE22	1.56	0.54
31:Ba:112:LYS:HB2	43:Bn:90:ILE:HA	1.89	0.54
42:Bm:105:TYR:CZ	42:Bm:262:ILE:HD12	2.43	0.54
56:AA:494:C:OP1	59:AD:139:ASN:ND2	2.41	0.54
57:AB:155:ASP:OD1	57:AB:215:ARG:NH1	2.35	0.54
77:AV:244:TYR:OH	77:AV:315:GLU:OE2	2.26	0.54
77:AV:357:THR:HG22	77:AV:361:LYS:HE3	1.89	0.54
3:B8:292:A:OP2	3:B8:831:C:N4	2.40	0.53
3:B8:655:U:O2'	26:BV:82:GLU:OE2	2.26	0.53
3:B8:1542:C:H42	3:B8:1560:G:H1	1.53	0.53
28:BX:177:VAL:HG11	28:BX:204:MET:HG3	1.90	0.53
43:Bn:213:LEU:HB2	43:Bn:275:GLN:HB2	1.88	0.53
45:Bp:178:TYR:O	51:Bv:136:ARG:NH1	2.40	0.53
1:B1:48:LEU:O	20:BP:142:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BF:154:ARG:HA	46:Bq:130:LEU:HD13	1.89	0.53
60:AE:5:GLU:OE2	71:AP:75:LYS:NZ	2.30	0.53
73:AR:103:TYR:OH	85:Ad:307:LYS:NZ	2.41	0.53
3:B8:467:C:OP2	11:BG:77:ARG:NH1	2.42	0.53
7:BC:16:PRO:HG2	7:BC:19:TYR:HB2	1.90	0.53
57:AB:169:ARG:O	57:AB:218:ASN:ND2	2.36	0.53
85:Ad:415:GLN:NE2	85:Ad:417:MET:SD	2.80	0.53
3:B8:1114:A:H5''	40:Bj:94:ARG:NH1	2.22	0.53
15:BK:115:LEU:HB2	24:BT:83:PHE:HB3	1.91	0.53
28:BX:153:ASN:OD1	28:BX:154:VAL:N	2.42	0.53
42:Bm:165:GLN:NE2	42:Bm:175:THR:HG22	2.24	0.53
70:AO:221:GLN:NE2	77:AV:314:VAL:O	2.35	0.53
73:AR:106:MET:HE1	73:AR:114:ALA:HB2	1.91	0.53
9:BE:156:LYS:NZ	9:BE:205:GLY:O	2.41	0.53
17:BM:76:LYS:HG3	17:BM:170:LEU:HD21	1.90	0.53
51:Bv:185:ARG:NH1	51:Bv:207:ASN:OD1	2.37	0.53
86:Ae:308:LYS:HE3	86:Ae:310:GLU:HB3	1.90	0.53
18:BN:70:ARG:HA	18:BN:196:PRO:HD3	1.90	0.53
63:AH:92:GLU:OE1	63:AH:141:ARG:NH1	2.41	0.53
63:AH:176:GLN:NE2	63:AH:178:GLU:OE2	2.42	0.53
82:Aa:387:THR:OG1	82:Aa:398:HIS:NE2	2.38	0.53
3:B8:568:A:OP1	38:Bh:165:LYS:NZ	2.42	0.53
3:B8:1338:C:O2'	3:B8:1381:A:N3	2.41	0.53
56:AA:693:C:O3'	81:AZ:101:ARG:NH2	2.42	0.53
3:B8:94:C:OP1	37:Bg:34:ARG:NH2	2.42	0.53
3:B8:1114:A:H2'	3:B8:1115:C:O4'	2.09	0.53
4:B9:12:U:O2'	4:B9:14:A:OP1	2.25	0.53
29:BY:111:LYS:NZ	30:BZ:139:ASP:O	2.41	0.53
43:Bn:252:CYS:SG	43:Bn:296:ARG:NH1	2.82	0.53
56:AA:289:G:O6	56:AA:475:A:N6	2.41	0.53
74:AS:119:VAL:HG12	74:AS:123:LYS:HE3	1.90	0.53
79:AX:206:GLU:HG3	79:AX:249:ARG:HH12	1.74	0.53
47:Br:75:ILE:HD13	49:Bt:255:SER:HB2	1.90	0.53
49:Bt:259:ARG:HB2	49:Bt:271:PHE:HB2	1.90	0.53
68:AM:19:ILE:HB	68:AM:83:LEU:HD23	1.89	0.53
40:Bj:95:GLN:HG3	40:Bj:96:ILE:HG13	1.91	0.52
22:BR:32:ALA:HA	22:BR:108:ILE:HG12	1.90	0.52
35:Be:24:PRO:HG2	38:Bh:169:TRP:HB2	1.91	0.52
58:AC:86:THR:HG21	66:AK:106:LEU:HD11	1.90	0.52
86:Ae:452:GLN:HG2	86:Ae:453:HIS:HD2	1.74	0.52
3:B8:676:U:OP1	39:Bi:223:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Bu:81:THR:HG21	50:Bu:85:PHE:HE1	1.74	0.52
56:AA:113:A:N1	56:AA:133:C:O2'	2.35	0.52
56:AA:586:C:OP1	56:AA:706:A:N6	2.41	0.52
77:AV:315:GLU:OE2	89:Aj:140:ARG:NH2	2.39	0.52
3:B8:169:C:H5''	22:BR:115:ASN:HB2	1.91	0.52
62:AG:15:A:H2	62:AG:18:A:H1'	1.75	0.52
67:AL:75:ASP:HB3	76:AU:153:LYS:HE3	1.90	0.52
82:Aa:395:VAL:HG23	82:Aa:407:ILE:HG12	1.91	0.52
89:Aj:63:ARG:HB2	89:Aj:66:GLN:HG3	1.91	0.52
3:B8:521:A:N6	3:B8:528:A:OP2	2.40	0.52
3:B8:751:G:H5''	46:Bq:24:LYS:HG2	1.92	0.52
3:B8:1040:C:O2'	3:B8:1550:A:N1	2.41	0.52
3:B8:1324:U:O3'	82:Aa:306:ARG:NH1	2.42	0.52
20:BP:96:ILE:HA	20:BP:155:VAL:HG12	1.90	0.52
23:BS:100:PHE:HB3	28:BX:158:GLN:HE21	1.74	0.52
50:Bu:202:MET:HG2	50:Bu:203:MET:HG2	1.92	0.52
68:AM:21:LEU:HB3	68:AM:32:TYR:HB3	1.91	0.52
28:BX:250:THR:H	28:BX:253:GLN:HE21	1.58	0.52
23:BS:52:HIS:CD2	23:BS:53:ARG:HG3	2.45	0.52
40:Bj:130:ALA:O	40:Bj:282:ARG:NH1	2.41	0.52
82:Aa:254:GLU:OE1	82:Aa:386:ARG:NH2	2.43	0.52
89:Aj:135:MET:SD	89:Aj:135:MET:N	2.79	0.52
3:B8:1268:A:H1'	62:AG:71:A:H2'	1.91	0.52
5:BA:185:THR:HG23	5:BA:188:ALA:H	1.75	0.52
29:BY:112:THR:OG1	48:Bs:127:GLN:NE2	2.38	0.52
56:AA:53:A:N1	56:AA:62:G:O2'	2.40	0.52
79:AX:108:LEU:HD23	79:AX:141:VAL:HG21	1.92	0.52
3:B8:699:A:OP1	10:BF:117:GLN:NE2	2.43	0.52
19:BO:244:LYS:HA	19:BO:247:ARG:HH21	1.75	0.52
44:Bo:276:PHE:HB2	44:Bo:304:VAL:HG22	1.91	0.52
48:Bs:72:VAL:HG13	48:Bs:90:HIS:HB2	1.92	0.52
3:B8:130:G:N1	3:B8:133:A:OP2	2.43	0.52
27:BW:104:SER:O	27:BW:135:ARG:NH1	2.43	0.52
56:AA:612:U:O4	82:Aa:274:ARG:HA	2.09	0.52
88:Ai:128:ALA:HB1	88:Ai:161:ALA:HB2	1.92	0.52
3:B8:10:A:OP1	10:BF:230:LYS:NZ	2.43	0.51
6:BB:66:ALA:HB2	6:BB:100:ALA:HA	1.92	0.51
44:Bo:114:ASP:HB2	44:Bo:117:LYS:HB2	1.92	0.51
44:Bo:284:HIS:HB3	44:Bo:323:MET:HE2	1.92	0.51
67:AL:115:ILE:HG23	67:AL:180:LYS:HG2	1.91	0.51
69:AN:29:ARG:HD3	69:AN:46:ARG:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Ad:209:GLY:N	85:Ad:213:GLU:O	2.42	0.51
3:B8:1070:A:N3	3:B8:1251:A:O2'	2.38	0.51
73:AR:219:TYR:O	73:AR:256:ARG:NH2	2.40	0.51
79:AX:319:PRO:HG2	79:AX:322:ALA:HB2	1.93	0.51
3:B8:369:A:N7	3:B8:1059:U:O2'	2.42	0.51
17:BM:345:ILE:HG13	28:BX:169:PRO:HB2	1.92	0.51
43:Bn:173:LEU:HD13	43:Bn:272:LEU:HD22	1.90	0.51
49:Bt:168:HIS:O	49:Bt:172:ASN:ND2	2.33	0.51
51:Bv:155:ARG:NH2	51:Bv:278:ASP:OD2	2.41	0.51
85:Ad:190:GLU:CD	85:Ad:190:GLU:H	2.19	0.51
87:Ag:70:THR:HG23	87:Ag:73:PHE:H	1.75	0.51
3:B8:1109:C:OP1	40:Bj:115:THR:OG1	2.28	0.51
3:B8:1310:U:H4'	82:Aa:341:GLN:HB3	1.92	0.51
4:B9:68:G:H2'	4:B9:69:A:C8	2.44	0.51
7:BC:93:THR:HG22	7:BC:112:GLU:HG3	1.92	0.51
22:BR:78:SER:HB3	22:BR:89:GLN:HG2	1.92	0.51
25:BU:204:GLU:HG3	25:BU:207:ARG:HH21	1.75	0.51
34:Bd:72:ARG:NH1	52:Bw:147:ASP:O	2.43	0.51
56:AA:250:C:OP2	65:AJ:116:GLN:NE2	2.43	0.51
56:AA:302:U:O2'	69:AN:46:ARG:NH1	2.43	0.51
68:AM:64:LYS:HE3	73:AR:154:THR:HB	1.92	0.51
77:AV:109:ILE:HD13	77:AV:138:PHE:H	1.75	0.51
7:BC:80:ILE:HD12	7:BC:85:TRP:HE3	1.74	0.51
17:BM:99:LEU:HD22	17:BM:193:LEU:HB3	1.93	0.51
50:Bu:152:LEU:HD22	50:Bu:176:ILE:HD11	1.91	0.51
56:AA:311:C:H4'	56:AA:312:C:H5'	1.92	0.51
57:AB:129:PHE:HB3	63:AH:155:VAL:HG21	1.92	0.51
68:AM:63:GLU:HG2	73:AR:155:LYS:HE2	1.92	0.51
77:AV:92:LEU:HD21	77:AV:137:ILE:HD11	1.91	0.51
26:BV:142:LEU:HA	26:BV:147:GLN:HE21	1.75	0.51
56:AA:470:A:H2'	56:AA:471:A:H8	1.76	0.51
58:AC:76:LEU:HB2	58:AC:79:GLU:HG3	1.91	0.51
70:AO:225:GLN:NE2	76:AU:47:ALA:O	2.43	0.51
79:AX:272:THR:OG1	79:AX:282:ILE:O	2.28	0.51
86:Ae:556:LYS:NZ	86:Ae:560:GLU:OE2	2.42	0.51
4:B9:67:U:H2'	4:B9:68:G:C8	2.46	0.51
14:BJ:51:ASN:O	14:BJ:54:GLN:NE2	2.44	0.51
21:BQ:20:ILE:HD11	21:BQ:42:ARG:HD3	1.93	0.51
23:BS:125:THR:HG22	23:BS:144:PHE:HB3	1.93	0.51
29:BY:111:LYS:HD3	48:Bs:127:GLN:HB3	1.91	0.51
40:Bj:133:LYS:HG2	40:Bj:134:LYS:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:Bn:215:THR:OG1	43:Bn:275:GLN:OE1	2.28	0.51
70:AO:214:SER:OG	70:AO:217:ARG:NH2	2.43	0.51
85:Ad:203:LEU:HD22	87:Ag:56:ILE:HD11	1.93	0.51
88:Ai:153:GLY:O	88:Ai:158:ARG:NH1	2.41	0.51
3:B8:79:C:OP2	3:B8:1229:C:O2'	2.23	0.51
3:B8:875:U:H5''	3:B8:876:G:H5'	1.93	0.51
4:B9:36:C:OP1	43:Bn:56:ARG:NH2	2.41	0.51
21:BQ:20:ILE:HB	21:BQ:70:ILE:HB	1.92	0.51
34:Bd:51:LEU:HB3	34:Bd:67:ARG:HB3	1.92	0.51
42:Bm:201:ARG:HB3	42:Bm:232:THR:HG22	1.93	0.51
3:B8:1541:C:H4'	3:B8:1542:C:H5	1.76	0.51
32:Bb:65:ASP:OD2	32:Bb:73:ARG:NH2	2.43	0.51
43:Bn:218:LEU:HD11	43:Bn:268:LEU:HB3	1.91	0.51
56:AA:646:C:N4	72:AQ:80:ARG:O	2.43	0.51
75:AT:78:PHE:HB2	75:AT:86:VAL:HB	1.93	0.51
89:Aj:41:LEU:HD13	89:Aj:55:TRP:CG	2.46	0.51
3:B8:739:A:O2'	42:Bm:268:CYS:SG	2.64	0.51
19:BO:201:VAL:HG22	40:Bj:86:VAL:HG13	1.93	0.51
40:Bj:110:GLN:HG2	40:Bj:115:THR:HG23	1.92	0.51
56:AA:293:A:O2'	56:AA:488:C:O2'	2.22	0.51
56:AA:784:G:O6	87:Ag:276:ARG:NH2	2.44	0.51
74:AS:2:ALA:N	85:Ad:213:GLU:OE2	2.44	0.51
83:Ab:273:LEU:HA	83:Ab:276:GLN:HE21	1.76	0.51
3:B8:519:C:O2'	3:B8:528:A:OP1	2.27	0.50
3:B8:1390:C:H6	3:B8:1390:C:O5'	1.94	0.50
85:Ad:203:LEU:HD21	85:Ad:222:ILE:HD11	1.93	0.50
88:Ai:83:ILE:HG21	88:Ai:173:ILE:HD11	1.93	0.50
3:B8:1106:G:N2	19:BO:179:ASN:OD1	2.44	0.50
35:Be:59:GLU:O	35:Be:62:HIS:ND1	2.36	0.50
82:Aa:272:MET:HG3	82:Aa:274:ARG:HG3	1.93	0.50
86:Ae:309:PHE:HZ	86:Ae:352:PRO:HG2	1.76	0.50
39:Bi:178:ASP:HA	39:Bi:239:ASN:HD21	1.77	0.50
39:Bi:271:LEU:HD23	39:Bi:273:LEU:HD13	1.93	0.50
42:Bm:354:PHE:HB3	42:Bm:417:LEU:HD11	1.92	0.50
45:Bp:193:ASN:O	52:Bw:133:GLU:N	2.43	0.50
3:B8:702:U:O4	39:Bi:270:LYS:NZ	2.44	0.50
79:AX:273:THR:HG23	79:AX:316:LEU:HD13	1.94	0.50
3:B8:244:A:N6	3:B8:334:G:O6	2.43	0.50
3:B8:401:U:O2'	43:Bn:28:ARG:NH2	2.44	0.50
8:BD:102:GLU:OE2	43:Bn:74:TYR:N	2.44	0.50
18:BN:103:GLN:O	18:BN:107:LYS:NZ	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Bs:89:ILE:HA	48:Bs:92:LYS:HD2	1.93	0.50
65:Aj:71:LYS:HD3	65:Aj:119:PRO:HG3	1.93	0.50
10:BF:83:ALA:N	46:Bq:74:VAL:O	2.43	0.50
48:Bs:49:ARG:HH21	48:Bs:94:VAL:HG11	1.77	0.50
83:Ab:221:GLY:HA3	83:Ab:232:ILE:HD13	1.92	0.50
3:B8:1301:A:O2'	25:BU:182:LYS:O	2.29	0.50
3:B8:1408:C:H2'	3:B8:1409:G:C8	2.47	0.50
18:BN:49:ARG:NH1	18:BN:81:ASP:O	2.41	0.50
45:Bp:99:ARG:HG2	51:Bv:89:LEU:HD11	1.93	0.50
57:AB:151:ILE:HG13	57:AB:219:TYR:HE1	1.76	0.50
57:AB:264:GLU:HG2	57:AB:268:GLN:HE21	1.76	0.50
65:Aj:78:ARG:HB3	65:Aj:94:PHE:HE1	1.76	0.50
3:B8:913:C:OP1	56:AA:935:G:C8	2.64	0.50
3:B8:1110:C:H5'	40:Bj:120:SER:HB2	1.92	0.50
7:BC:55:TYR:HB2	7:BC:133:ILE:HD11	1.92	0.50
45:Bp:124:TYR:OH	51:Bv:67:GLN:NE2	2.44	0.50
56:AA:42:U:OP1	56:AA:180:A:O2'	2.30	0.50
56:AA:811:A:OP1	61:AF:104:LYS:NZ	2.37	0.50
67:AL:89:VAL:HG22	76:Au:164:VAL:HG21	1.92	0.50
82:Aa:325:VAL:HG22	82:Aa:332:VAL:HG22	1.93	0.50
87:Ag:155:LYS:HB3	87:Ag:158:TYR:HB3	1.92	0.50
3:B8:186:A:OP2	3:B8:1316:C:O2'	2.28	0.50
4:B9:38:U:H5''	27:BW:155:SER:HB3	1.93	0.50
19:BO:53:THR:N	19:BO:86:THR:OG1	2.45	0.50
39:Bi:212:ARG:HD3	39:Bi:379:LEU:HB3	1.92	0.50
46:Bq:68:PHE:CE2	46:Bq:70:LEU:HB2	2.46	0.50
63:AH:164:LEU:HD12	63:AH:165:PRO:HD2	1.94	0.50
75:AT:132:ARG:NH1	75:AT:136:LEU:O	2.44	0.50
83:Ab:131:PHE:HE2	83:Ab:192:LEU:HD13	1.77	0.50
3:B8:457:A:H4'	3:B8:581:A:C5	2.47	0.49
30:BZ:96:PHE:HB3	48:Bs:126:ILE:HD13	1.93	0.49
42:Bm:326:ARG:NH1	42:Bm:331:ASN:OD1	2.45	0.49
43:Bn:87:LYS:NZ	43:Bn:153:GLU:OE2	2.43	0.49
49:Bt:245:LEU:HD12	49:Bt:253:PRO:HD3	1.94	0.49
50:Bu:164:VAL:HG12	50:Bu:261:MET:HB3	1.94	0.49
56:AA:252:G:O2'	56:AA:260:A:N1	2.39	0.49
67:AL:72:LEU:HA	67:AL:94:SER:HA	1.94	0.49
77:AV:202:ARG:HD2	77:AV:247:MET:HG3	1.94	0.49
3:B8:190:A:O2'	3:B8:1012:A:OP1	2.29	0.49
10:BF:90:LEU:HB2	10:BF:145:VAL:HG21	1.94	0.49
42:Bm:113:LEU:HD12	42:Bm:311:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AL:72:LEU:HD13	67:AL:82:ILE:HD13	1.94	0.49
75:AT:101:HIS:HE1	76:AU:112:GLU:HG2	1.77	0.49
79:AX:152:ILE:O	79:AX:195:ASN:ND2	2.41	0.49
84:Ac:33:VAL:HG21	84:Ac:104:LEU:HD23	1.93	0.49
26:BV:67:ASP:OD1	26:BV:67:ASP:N	2.46	0.49
30:BZ:163:LYS:HB2	48:Bs:106:ASP:HB3	1.95	0.49
22:BR:6:ARG:NH2	49:Bt:225:GLY:O	2.44	0.49
51:Bv:178:TRP:NE1	51:Bv:182:GLU:O	2.45	0.49
56:AA:618:C:OP1	66:AK:112:ARG:NH2	2.35	0.49
69:AN:13:ILE:HG13	69:AN:66:LEU:HB2	1.93	0.49
3:B8:1108:U:O2'	40:Bj:116:SER:HB2	2.13	0.49
9:BE:202:GLU:HB3	9:BE:214:LYS:NZ	2.28	0.49
16:BL:111:ARG:NH2	16:BL:165:ASN:OD1	2.43	0.49
23:BS:75:LEU:HD11	23:BS:105:VAL:HG21	1.94	0.49
24:BT:263:ARG:HH21	36:Bf:43:TYR:HE2	1.60	0.49
61:AF:147:GLN:NE2	61:AF:151:ASN:OD1	2.45	0.49
16:BL:109:PHE:HB3	16:BL:204:ALA:HB3	1.95	0.49
39:Bi:332:LEU:HD13	39:Bi:372:TYR:HB2	1.94	0.49
42:Bm:136:VAL:HG11	42:Bm:417:LEU:HD23	1.93	0.49
43:Bn:138:GLU:OE1	43:Bn:141:ARG:NH2	2.39	0.49
70:AO:91:ARG:NH1	70:AO:103:ASN:O	2.45	0.49
86:Ae:343:ARG:HA	86:Ae:378:LEU:HD13	1.95	0.49
3:B8:324:A:H61	3:B8:1066:C:H4'	1.77	0.49
16:BL:172:MET:HE1	60:AE:86:ILE:HG12	1.93	0.49
51:Bv:200:MET:HA	51:Bv:241:GLY:HA3	1.93	0.49
58:AC:96:MET:HB2	58:AC:108:LEU:HD11	1.94	0.49
86:Ae:450:PRO:HD2	86:Ae:453:HIS:CG	2.48	0.49
88:Ai:71:SER:O	88:Ai:74:ARG:NH1	2.36	0.49
4:B9:61:C:H2'	4:B9:62:C:C6	2.47	0.49
20:BP:101:ASN:HB3	20:BP:150:HIS:HB3	1.94	0.49
22:BR:169:LEU:HD22	38:Bh:75:TRP:CD1	2.47	0.49
47:Br:104:GLU:HB2	47:Br:107:PRO:HD2	1.95	0.49
50:Bu:85:PHE:CZ	50:Bu:200:SER:HB3	2.47	0.49
52:Bw:127:MET:HB2	52:Bw:154:GLU:HB3	1.94	0.49
56:AA:66:C:H5''	68:AM:42:PRO:HG3	1.95	0.49
56:AA:375:A:OP2	84:Ac:17:ARG:NE	2.46	0.49
62:AG:13:U:H3	62:AG:19:A:H61	1.59	0.49
20:BP:76:ILE:HG22	20:BP:78:LEU:H	1.78	0.49
36:Bf:140:SER:OG	43:Bn:374:GLU:OE2	2.28	0.49
56:AA:718:A:H4'	56:AA:742:G:H4'	1.94	0.49
57:AB:235:ASN:ND2	57:AB:237:GLU:OE2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:Aa:206:GLU:CD	82:Aa:262:ARG:HH12	2.20	0.49
82:Aa:301:ARG:HH21	82:Aa:325:VAL:HG21	1.78	0.49
86:Ae:336:ASN:ND2	86:Ae:409:ASP:OD2	2.45	0.49
52:Bw:94:HIS:ND1	52:Bw:154:GLU:OE2	2.32	0.49
67:AL:175:TYR:HB2	69:AN:89:GLY:HA3	1.95	0.49
68:AM:95:GLY:O	89:Aj:167:PRO:HB2	2.12	0.49
74:AS:65:TYR:N	74:AS:68:ASP:OD2	2.39	0.49
79:AX:123:ARG:NH2	79:AX:337:LEU:O	2.46	0.49
3:B8:1542:C:N4	3:B8:1560:G:H1	2.10	0.48
16:BL:257:ILE:O	16:BL:262:ARG:NH1	2.36	0.48
40:Bj:62:PRO:HG2	40:Bj:65:LYS:HD2	1.94	0.48
40:Bj:143:VAL:HG22	40:Bj:242:GLU:HA	1.95	0.48
57:AB:181:ASN:O	57:AB:230:TYR:OH	2.27	0.48
60:AE:29:LEU:HB3	60:AE:34:ALA:HB3	1.95	0.48
3:B8:520:C:OP2	33:Bc:120:ARG:NH1	2.33	0.48
50:Bu:188:SER:HA	50:Bu:218:THR:HG22	1.95	0.48
61:AF:71:THR:O	87:Ag:253:LYS:NZ	2.46	0.48
61:AF:161:ILE:HD12	61:AF:170:VAL:HG21	1.96	0.48
26:BV:46:TRP:CD1	26:BV:121:ALA:HB2	2.48	0.48
26:BV:64:LYS:NZ	26:BV:100:GLN:O	2.46	0.48
26:BV:140:SER:O	26:BV:146:ASN:ND2	2.46	0.48
44:Bo:220:GLU:HG2	44:Bo:253:LYS:HG2	1.95	0.48
56:AA:389:A:O2'	67:AL:142:HIS:ND1	2.31	0.48
82:Aa:306:ARG:NH1	82:Aa:316:ASN:O	2.46	0.48
3:B8:517:C:O2'	21:BQ:104:THR:O	2.31	0.48
13:BI:34:ARG:HB3	13:BI:41:LEU:HD11	1.95	0.48
22:BR:27:PRO:HG2	22:BR:30:LYS:HB2	1.94	0.48
78:AW:114:ILE:HD13	78:AW:140:VAL:HG21	1.95	0.48
88:AI:101:SER:HB3	88:AI:107:LEU:HD11	1.94	0.48
3:B8:1531:A:H2'	3:B8:1532:U:O4'	2.12	0.48
31:Ba:91:TRP:CD2	35:Be:58:GLN:HG2	2.48	0.48
56:AA:305:A:N3	56:AA:307:C:N4	2.61	0.48
56:AA:584:A:OP1	66:AK:88:ARG:NH2	2.45	0.48
79:AX:162:VAL:HB	79:AX:272:THR:HG22	1.95	0.48
3:B8:640:G:N2	3:B8:1006:A:OP2	2.43	0.48
25:BU:64:ARG:NH1	25:BU:144:LYS:O	2.46	0.48
56:AA:433:A:O2'	56:AA:435:A:N7	2.41	0.48
86:Ae:593:TRP:HA	86:Ae:596:LEU:HD23	1.95	0.48
3:B8:197:A:N1	3:B8:349:G:O2'	2.45	0.48
20:BP:49:ALA:HB1	35:Be:32:LYS:HE2	1.95	0.48
56:AA:617:C:H1'	63:AH:124:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AB:266:LEU:HD11	57:AB:289:ILE:HD11	1.94	0.48
57:AB:312:TYR:OH	79:AX:338:ASP:OD1	2.23	0.48
86:Ae:152:ILE:HA	86:Ae:172:MET:HE3	1.96	0.48
3:B8:67:A:H61	3:B8:90:G:H1'	1.79	0.48
11:BG:120:LYS:NZ	35:Be:44:GLU:OE2	2.45	0.48
40:Bj:123:LEU:HB2	40:Bj:295:LEU:HD12	1.96	0.48
45:Bp:110:GLU:OE2	45:Bp:113:ARG:NH2	2.37	0.48
79:AX:102:ARG:HH22	79:AX:133:GLY:HA3	1.78	0.48
87:Ag:165:VAL:HA	87:Ag:168:MET:HE2	1.96	0.48
17:BM:50:ASP:HA	17:BM:53:LEU:HG	1.95	0.48
18:BN:231:VAL:HG13	37:Bg:26:ARG:HD2	1.96	0.48
34:Bd:109:GLU:O	81:AZ:13:ARG:NH1	2.47	0.48
70:AO:217:ARG:NH1	70:AO:227:GLU:OE2	2.46	0.48
86:Ae:528:ARG:HH12	86:Ae:562:GLN:HE21	1.60	0.48
3:B8:405:U:O2'	3:B8:1163:A:N7	2.42	0.48
3:B8:547:C:OP1	20:BP:128:ASN:N	2.43	0.48
3:B8:849:G:N7	16:BL:230:SER:OG	2.44	0.48
18:BN:220:ASP:O	18:BN:245:ALA:N	2.46	0.48
43:Bn:131:PRO:HG2	43:Bn:134:ALA:HB3	1.96	0.48
67:AL:87:ASP:HA	67:AL:90:LYS:HE3	1.96	0.48
73:AR:191:ARG:HG3	73:AR:204:ILE:HG23	1.96	0.48
4:B9:6:U:O2	4:B9:63:G:N2	2.38	0.47
42:Bm:228:ALA:HB3	42:Bm:292:TYR:HB2	1.96	0.47
56:AA:258:A:O2'	56:AA:260:A:OP1	2.31	0.47
63:AH:128:LYS:HE2	63:AH:131:ARG:NH2	2.29	0.47
72:AQ:39:ILE:HD13	88:Ai:179:THR:HG21	1.96	0.47
3:B8:801:G:O2'	3:B8:984:U:O4	2.30	0.47
22:BR:140:ASN:HB2	49:Bt:262:GLY:HA2	1.96	0.47
23:BS:98:PRO:HA	28:BX:162:ILE:HG12	1.96	0.47
60:AE:37:ARG:NH2	76:AU:163:GLU:OE1	2.47	0.47
82:Aa:227:TYR:CZ	82:Aa:235:LEU:HD21	2.48	0.47
84:Ac:47:THR:HG23	88:Ai:129:GLN:HE22	1.79	0.47
3:B8:33:C:OP1	46:Bq:34:LYS:NZ	2.46	0.47
12:BH:108:ASP:OD1	12:BH:109:VAL:N	2.44	0.47
48:Bs:27:GLN:NE2	49:Bt:177:GLN:OE1	2.47	0.47
53:Bx:154:ASP:OD1	53:Bx:154:ASP:N	2.47	0.47
56:AA:292:A:N3	56:AA:489:C:O2'	2.44	0.47
77:AV:81:SER:HB3	77:AV:84:GLU:HG3	1.96	0.47
79:AX:50:ARG:NH1	79:AX:98:CYS:SG	2.87	0.47
3:B8:332:G:N3	3:B8:1065:G:O2'	2.36	0.47
3:B8:703:A:OP1	6:BB:50:ARG:NH2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:1269:C:H5''	82:Aa:317:LYS:HD2	1.96	0.47
5:BA:49:ASN:ND2	5:BA:68:TYR:O	2.35	0.47
57:AB:50:ARG:NH1	86:Ae:94:TYR:O	2.47	0.47
62:AG:16:A:O2'	62:AG:54:A:O2'	2.29	0.47
62:AG:18:A:H2'	62:AG:43:A:N6	2.30	0.47
73:AR:89:LYS:NZ	73:AR:261:LEU:O	2.44	0.47
75:AT:34:TYR:CZ	75:AT:68:LYS:HG2	2.48	0.47
88:Ai:151:VAL:HG21	88:Ai:158:ARG:HG3	1.96	0.47
3:B8:1024:A:N3	3:B8:1272:C:O2'	2.45	0.47
40:Bj:79:GLU:HG2	40:Bj:97:TYR:HE2	1.78	0.47
60:AE:6:LEU:HB3	60:AE:66:VAL:HB	1.96	0.47
5:BA:94:ASP:OD2	44:Bo:97:GLU:N	2.46	0.47
23:BS:143:ASN:ND2	28:BX:156:GLU:HG3	2.30	0.47
39:Bi:239:ASN:HB2	39:Bi:299:PHE:HB2	1.97	0.47
56:AA:497:U:H2'	56:AA:498:A:H8	1.78	0.47
60:AE:40:GLU:HB2	60:AE:65:LEU:HB2	1.97	0.47
63:AH:55:PRO:HA	86:Ae:440:LYS:HB3	1.95	0.47
66:AK:52:LEU:HD11	81:AZ:36:LEU:HB3	1.96	0.47
73:AR:82:MET:HE3	73:AR:288:GLN:HE22	1.78	0.47
87:Ag:59:LYS:HE2	87:Ag:63:THR:H	1.80	0.47
3:B8:98:G:OP1	55:Bz:50:LYS:NZ	2.46	0.47
3:B8:216:G:N7	18:BN:170:ARG:NH2	2.61	0.47
3:B8:1236:C:N3	13:BI:19:ARG:NH2	2.59	0.47
19:BO:156:GLN:OE1	19:BO:226:ASN:ND2	2.48	0.47
36:Bf:185:ARG:NH1	43:Bn:197:GLU:OE2	2.47	0.47
37:Bg:28:ARG:O	55:Bz:57:TYR:OH	2.27	0.47
42:Bm:211:ALA:HB1	42:Bm:322:LEU:HD23	1.97	0.47
43:Bn:359:HIS:CD2	43:Bn:360:ARG:HG3	2.50	0.47
44:Bo:195:THR:H	44:Bo:198:ASN:HD22	1.62	0.47
61:AF:110:LEU:HD22	61:AF:202:PRO:HD3	1.96	0.47
62:AG:30:C:OP2	87:Ag:396:ARG:NH1	2.45	0.47
62:AG:51:PSU:H3'	62:AG:52:A:C8	2.44	0.47
66:AK:52:LEU:HD22	81:AZ:41:PRO:HG3	1.96	0.47
75:AT:26:SER:O	75:AT:81:ASP:N	2.47	0.47
88:Ai:110:ALA:HB2	88:Ai:138:ARG:HH21	1.80	0.47
3:B8:1457:G:N2	3:B8:1460:A:OP2	2.47	0.47
83:Ab:264:ARG:NE	83:Ab:268:GLU:OE2	2.48	0.47
3:B8:36:C:OP1	10:BF:193:ARG:NH2	2.44	0.47
3:B8:1093:U:H4'	19:BO:247:ARG:HD2	1.97	0.47
38:Bh:71:PRO:HD2	38:Bh:107:LEU:HD23	1.96	0.47
39:Bi:191:HIS:O	39:Bi:428:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:Bn:120:GLU:OE2	45:Bp:119:LYS:NZ	2.30	0.47
56:AA:419:C:O2'	88:Ai:187:ARG:O	2.32	0.47
56:AA:431:A:OP1	62:AG:35:C:O2'	2.23	0.47
3:B8:492:C:N4	3:B8:552:U:O2	2.48	0.47
19:BO:193:PHE:O	19:BO:198:GLY:N	2.48	0.47
19:BO:242:LYS:HB2	19:BO:245:THR:HG23	1.96	0.47
44:Bo:163:MET:H	44:Bo:186:ASP:HB2	1.79	0.47
65:AJ:62:VAL:HA	65:AJ:83:VAL:HG12	1.97	0.47
3:B8:739:A:O2'	42:Bm:270:ILE:O	2.33	0.46
3:B8:1110:C:OP2	40:Bj:119:GLN:HA	2.16	0.46
3:B8:1114:A:H5''	40:Bj:94:ARG:HH12	1.79	0.46
19:BO:190:ALA:HA	19:BO:193:PHE:HD2	1.80	0.46
40:Bj:257:ILE:HD12	40:Bj:274:VAL:HG21	1.97	0.46
69:AN:18:ILE:HD13	69:AN:29:ARG:HB2	1.97	0.46
3:B8:402:A:H2'	3:B8:403:A:C8	2.50	0.46
3:B8:1354:U:H2'	3:B8:1355:A:H8	1.80	0.46
3:B8:1432:U:C2	12:BH:81:PRO:HA	2.50	0.46
5:BA:134:LEU:HD23	5:BA:174:GLU:HA	1.97	0.46
19:BO:163:THR:HG22	40:Bj:88:LEU:HG	1.97	0.46
39:Bi:89:MET:HE3	39:Bi:275:LYS:HB3	1.97	0.46
42:Bm:161:ALA:HB1	42:Bm:176:TYR:HB2	1.97	0.46
57:AB:159:SER:HB2	58:AC:112:ARG:HB3	1.97	0.46
79:AX:181:PRO:HB2	79:AX:233:VAL:HG12	1.97	0.46
3:B8:107:A:H4'	18:BN:115:LYS:NZ	2.30	0.46
3:B8:1097:A:O2'	3:B8:1099:A:N7	2.49	0.46
20:BP:102:VAL:HG23	20:BP:104:LEU:HG	1.97	0.46
21:BQ:25:ARG:HD2	33:Bc:56:LEU:HB3	1.95	0.46
21:BQ:113:THR:OG1	21:BQ:116:HIS:ND1	2.35	0.46
24:BT:62:ARG:O	55:Bz:128:ARG:NH2	2.46	0.46
26:BV:150:GLN:HE21	26:BV:154:GLN:HE21	1.63	0.46
56:AA:347:A:O2'	61:AF:166:ARG:NH1	2.48	0.46
64:AI:1:A:N3	64:AI:2:G:N1	2.59	0.46
70:AO:94:CYS:HB2	70:AO:108:CYS:SG	2.55	0.46
72:AQ:83:PRO:HA	78:AW:108:VAL:HG21	1.98	0.46
77:AV:30:LEU:HD21	77:AV:181:LEU:HD11	1.97	0.46
82:Aa:241:ARG:NE	82:Aa:287:GLN:OE1	2.37	0.46
3:B8:575:A:H4'	3:B8:576:A:OP1	2.15	0.46
61:AF:172:VAL:HG12	61:AF:240:ARG:HD2	1.97	0.46
79:AX:265:ILE:HD13	79:AX:337:LEU:HD11	1.96	0.46
82:Aa:253:TYR:O	82:Aa:399:ARG:NH1	2.33	0.46
85:Ad:312:TYR:N	85:Ad:331:ASP:OD2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:411:U:H2'	3:B8:412:G:C8	2.50	0.46
3:B8:526:A:O2'	3:B8:543:A:N1	2.49	0.46
3:B8:640:G:O2'	3:B8:1005:G:O6	2.30	0.46
4:B9:62:C:H2'	4:B9:63:G:C8	2.51	0.46
9:BE:87:LEU:O	19:BO:78:ARG:NH1	2.47	0.46
22:BR:25:MET:O	22:BR:149:ARG:NH1	2.48	0.46
32:Bb:40:GLU:OE1	32:Bb:43:ARG:NH2	2.47	0.46
56:AA:651:U:H4'	83:Ab:172:ARG:HH21	1.80	0.46
62:AG:61:C:H2'	62:AG:62:C:C6	2.50	0.46
3:B8:499:A:OP1	21:BQ:21:ARG:NH2	2.49	0.46
48:Bs:76:VAL:HG22	48:Bs:86:GLU:HG3	1.98	0.46
68:AM:30:PRO:HD2	68:AM:57:LEU:HD11	1.97	0.46
3:B8:2:C:O2'	5:BA:143:ARG:O	2.27	0.46
3:B8:181:G:H2'	3:B8:1023:A:N7	2.30	0.46
3:B8:201:A:N3	15:BK:104:ARG:NH2	2.64	0.46
13:BI:34:ARG:HD3	13:BI:41:LEU:HG	1.98	0.46
25:BU:73:ARG:O	25:BU:155:LYS:NZ	2.45	0.46
51:Bv:177:GLU:O	51:Bv:190:ARG:NH2	2.49	0.46
67:AL:221:LYS:O	67:AL:225:ARG:HG2	2.16	0.46
3:B8:1532:U:O2	17:BM:303:LYS:NZ	2.46	0.46
42:Bm:112:ARG:HG2	42:Bm:304:LEU:HD22	1.98	0.46
44:Bo:139:ASN:HB3	44:Bo:174:VAL:HG21	1.98	0.46
56:AA:348:A:H5'	88:Ai:119:ASN:HD22	1.80	0.46
56:AA:472:U:O2'	56:AA:480:A:O2'	2.23	0.46
62:AG:62:C:H2'	62:AG:63:G:C8	2.51	0.46
66:AK:53:ARG:O	66:AK:56:SER:OG	2.33	0.46
68:AM:54:TYR:HD1	68:AM:66:VAL:HG22	1.80	0.46
3:B8:609:U:OP1	18:BN:255:LYS:NZ	2.40	0.46
3:B8:813:U:H2'	3:B8:814:C:O4'	2.15	0.46
3:B8:1349:G:O2'	3:B8:1455:A:N1	2.49	0.46
15:BK:96:TYR:OH	55:Bz:128:ARG:O	2.30	0.46
15:BK:188:VAL:O	43:Bn:356:ARG:NH2	2.49	0.46
56:AA:47:C:H2'	56:AA:168:C:H41	1.81	0.46
3:B8:282:U:H2'	3:B8:283:A:C8	2.51	0.46
3:B8:789:A:N6	3:B8:998:A:O2'	2.48	0.46
3:B8:1403:C:OP2	3:B8:1425:G:N2	2.45	0.46
16:BL:235:GLN:HB3	16:BL:294:SER:HA	1.98	0.46
17:BM:345:ILE:O	28:BX:172:GLN:NE2	2.49	0.46
28:BX:210:GLU:HB2	28:BX:213:GLN:HG3	1.97	0.46
34:Bd:98:ALA:HB1	34:Bd:101:GLN:HE21	1.81	0.46
44:Bo:195:THR:H	44:Bo:198:ASN:ND2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:AO:54:GLU:OE1	70:AO:57:LYS:NZ	2.38	0.46
80:AY:250:ILE:HG21	86:Ae:392:ILE:HD13	1.98	0.46
86:Ae:559:TYR:HA	86:Ae:562:GLN:HG3	1.97	0.46
3:B8:198:G:H2'	24:BT:40:PRO:HG3	1.98	0.45
28:BX:183:LEU:HD21	28:BX:219:GLU:HG2	1.97	0.45
56:AA:389:A:HO2'	67:AL:142:HIS:HD1	1.36	0.45
85:Ad:224:GLU:HB2	85:Ad:342:MET:HG2	1.98	0.45
22:BR:5:SER:HB2	22:BR:8:PRO:HD2	1.98	0.45
28:BX:121:THR:HG22	28:BX:171:VAL:HA	1.98	0.45
56:AA:87:C:O2	56:AA:93:G:N1	2.48	0.45
56:AA:879:U:H2'	89:Aj:99:ARG:HD3	1.97	0.45
67:AL:143:LEU:HD11	67:AL:153:LYS:HA	1.99	0.45
77:AV:138:PHE:HB3	89:Aj:72:PRO:HG3	1.98	0.45
9:BE:139:TYR:HD1	19:BO:131:TYR:HB3	1.80	0.45
16:BL:213:CYS:HB3	16:BL:246:ARG:HG2	1.98	0.45
26:BV:62:TYR:OH	28:BX:272:GLU:OE2	2.34	0.45
38:Bh:70:CYS:HB3	94:Bh:201:FS2:S6	2.56	0.45
39:Bi:358:GLN:NE2	39:Bi:427:ASN:HD22	2.14	0.45
42:Bm:108:HIS:CE1	42:Bm:110:ARG:HB3	2.52	0.45
49:Bt:72:ILE:HD13	49:Bt:178:LEU:HD13	1.97	0.45
56:AA:566:A:N3	56:AA:592:C:O2'	2.46	0.45
63:AH:78:VAL:HB	63:AH:143:LEU:HB2	1.98	0.45
82:Aa:272:MET:HE3	82:Aa:272:MET:HB2	1.77	0.45
87:Ag:200:LEU:O	87:Ag:218:TYR:OH	2.31	0.45
28:BX:122:ALA:HB2	28:BX:172:GLN:HE21	1.81	0.45
39:Bi:316:CYS:HB3	39:Bi:319:GLN:HB2	1.99	0.45
42:Bm:409:GLU:HG2	42:Bm:412:ARG:HH21	1.81	0.45
56:AA:126:U:OP2	67:AL:225:ARG:NH2	2.48	0.45
68:AM:67:ALA:HB1	73:AR:161:ILE:HD13	1.98	0.45
88:Ai:146:HIS:NE2	88:Ai:171:GLU:OE1	2.49	0.45
1:B6:84:GLU:HG3	1:B6:88:LYS:HD2	1.97	0.45
3:B8:93:A:N6	37:Bg:51:GLN:HE22	2.14	0.45
3:B8:1119:C:H2'	3:B8:1120:A:H5''	1.97	0.45
3:B8:1144:G:O2'	3:B8:1313:G:OP1	2.35	0.45
9:BE:114:PHE:HB3	9:BE:141:LEU:HD22	1.98	0.45
34:Bd:55:LEU:HD12	51:Bv:128:PHE:HE1	1.82	0.45
34:Bd:57:VAL:N	34:Bd:75:LEU:O	2.37	0.45
56:AA:13:C:OP2	85:Ad:226:ARG:NH1	2.50	0.45
66:AK:91:CYS:HB3	66:AK:96:ARG:H	1.80	0.45
83:Ab:167:HIS:CD2	87:Ag:153:THR:HA	2.52	0.45
85:Ad:254:ALA:O	85:Ad:280:HIS:N	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:912:A:O2'	56:AA:935:G:N3	2.45	0.45
26:BV:108:LEU:HD11	26:BV:135:LEU:HD23	1.99	0.45
49:Bt:42:GLN:NE2	55:Bz:36:LEU:O	2.50	0.45
53:Bx:72:TRP:NE1	53:Bx:92:HIS:O	2.44	0.45
56:AA:456:A:N7	56:AA:927:G:O2'	2.48	0.45
60:AE:96:HIS:HB3	60:AE:99:THR:HG23	1.98	0.45
89:Aj:85:TRP:HH2	89:Aj:95:TRP:HE1	1.63	0.45
3:B8:738:U:O2'	42:Bm:266:HIS:ND1	2.49	0.45
3:B8:873:C:O2'	59:AD:155:ARG:NH2	2.49	0.45
3:B8:1481:A:H4'	28:BX:146:GLY:O	2.17	0.45
4:B9:71:C:N4	51:Bv:216:LYS:HB2	2.32	0.45
7:BC:80:ILE:HB	7:BC:85:TRP:HB2	1.98	0.45
18:BN:223:HIS:HA	18:BN:226:MET:HE3	1.98	0.45
31:Ba:63:GLN:HE21	31:Ba:67:LYS:HE2	1.82	0.45
38:Bh:72:ILE:HD11	38:Bh:115:ILE:HD11	1.99	0.45
56:AA:737:A:OP2	61:AF:198:ARG:NH1	2.50	0.45
73:AR:208:ILE:O	73:AR:214:ASN:ND2	2.50	0.45
3:B8:484:A:OP2	35:Be:28:SER:OG	2.28	0.45
3:B8:1269:C:H4'	82:Aa:317:LYS:HD2	1.98	0.45
34:Bd:104:LYS:HB2	34:Bd:107:GLU:HG3	1.98	0.45
42:Bm:146:HIS:O	42:Bm:194:LYS:NZ	2.49	0.45
48:Bs:133:PHE:HE2	49:Bt:269:LEU:HD23	1.82	0.45
65:AJ:51:PRO:HG3	65:AJ:122:LYS:HB3	1.98	0.45
3:B8:383:U:HO2'	3:B8:384:U:H6	1.62	0.45
3:B8:740:U:P	42:Bm:223:ARG:HH12	2.40	0.45
4:B9:53:U:H5''	4:B9:54:A:C8	2.52	0.45
7:BC:86:VAL:HG21	7:BC:120:VAL:HG21	1.98	0.45
10:BF:191:ASN:HB3	10:BF:194:TYR:HB3	1.98	0.45
17:BM:334:ASP:HB3	17:BM:337:VAL:HG23	1.99	0.45
19:BO:177:LYS:HD2	40:Bj:114:PHE:O	2.17	0.45
51:Bv:60:SER:O	51:Bv:136:ARG:NH2	2.37	0.45
56:AA:188:C:N4	56:AA:204:A:OP2	2.42	0.45
56:AA:570:G:OP1	82:Aa:408:LYS:NZ	2.50	0.45
86:Ae:298:ILE:HG21	86:Ae:338:ILE:HG12	1.99	0.45
3:B8:144:A:N3	3:B8:192:U:O2'	2.45	0.45
3:B8:1354:U:H2'	3:B8:1355:A:C8	2.51	0.45
21:BQ:28:LEU:HD13	33:Bc:56:LEU:HD22	1.99	0.45
62:AG:5:A:H2	62:AG:63:G:H1	1.64	0.45
88:Ai:100:VAL:HG12	88:Ai:106:PRO:HA	1.99	0.45
9:BE:20:ILE:HD13	9:BE:212:ILE:HG23	2.00	0.44
32:Bb:66:VAL:HB	32:Bb:74:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:AJ:97:GLY:HA3	65:AJ:135:VAL:HG11	1.99	0.44
71:AP:141:ARG:HD2	88:Ai:62:ILE:HD13	1.99	0.44
73:AR:332:ALA:HA	73:AR:336:ALA:HB3	1.99	0.44
79:AX:117:PHE:HB3	79:AX:303:GLY:HA2	1.99	0.44
3:B8:743:C:OP1	42:Bm:83:LYS:NZ	2.36	0.44
24:BT:127:VAL:HG21	24:BT:138:VAL:HG11	1.99	0.44
34:Bd:56:LEU:HD22	34:Bd:66:ILE:HD13	1.99	0.44
39:Bi:105:TRP:CG	39:Bi:271:LEU:HD13	2.52	0.44
44:Bo:87:THR:O	44:Bo:90:SER:OG	2.27	0.44
3:B8:662:C:H41	3:B8:772:U:H3	1.64	0.44
8:BD:33:LYS:HE3	25:BU:139:ARG:HD2	1.99	0.44
17:BM:150:LYS:HD2	17:BM:296:LEU:HD21	1.99	0.44
19:BO:154:LYS:HA	19:BO:228:LEU:HD13	1.98	0.44
22:BR:7:ALA:HB3	22:BR:8:PRO:HD3	1.99	0.44
35:Be:15:ARG:HB3	35:Be:18:ILE:HG12	1.99	0.44
56:AA:293:A:HO2'	56:AA:488:C:HO2'	1.60	0.44
56:AA:400:A:OP2	56:AA:402:A:N6	2.39	0.44
56:AA:410:G:H4'	56:AA:931:A:H4'	1.99	0.44
79:AX:385:ASN:ND2	87:Ag:301:GLN:OE1	2.36	0.44
82:Aa:133:LEU:HA	82:Aa:136:MET:HE2	1.99	0.44
82:Aa:220:TRP:CH2	82:Aa:247:VAL:HA	2.53	0.44
9:BE:40:PRO:HB3	9:BE:43:TYR:CZ	2.53	0.44
18:BN:211:ARG:HD3	54:By:58:ARG:HE	1.83	0.44
21:BQ:90:PHE:HB3	21:BQ:120:ILE:HD13	2.00	0.44
24:BT:28:LYS:HD3	35:Be:94:HIS:CD2	2.52	0.44
25:BU:67:LYS:HE3	25:BU:67:LYS:HB2	1.86	0.44
27:BW:60:SER:HB3	36:Bf:177:ARG:HH11	1.81	0.44
56:AA:94:A:H4'	76:AU:82:VAL:HG21	2.00	0.44
56:AA:950:C:OP2	84:Ac:24:ASN:ND2	2.50	0.44
60:AE:90:ARG:HG2	60:AE:92:ASN:HD21	1.83	0.44
62:AG:3:U:H2'	62:AG:4:A:C8	2.53	0.44
77:AV:215:GLN:HB3	77:AV:217:ASN:HD21	1.81	0.44
79:AX:266:ASN:HA	79:AX:329:LEU:HD23	1.99	0.44
3:B8:1199:A:OP1	15:BK:127:ALA:N	2.37	0.44
7:BC:187:TYR:HD1	10:BF:94:SER:HA	1.82	0.44
36:Bf:115:VAL:HG13	36:Bf:161:ALA:HB3	1.99	0.44
40:Bj:139:PRO:HB3	40:Bj:245:VAL:HG21	2.00	0.44
45:Bp:153:GLU:HG2	51:Bv:47:LEU:HD21	2.00	0.44
53:Bx:73:GLN:HB3	53:Bx:162:LEU:HD11	2.00	0.44
57:AB:152:ASP:HB2	57:AB:172:VAL:HB	2.00	0.44
73:AR:138:ILE:HG13	73:AR:186:TRP:NE1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BO:98:LEU:HD11	19:BO:105:VAL:HG12	2.00	0.44
42:Bm:59:THR:HB	42:Bm:73:PRO:HG3	1.99	0.44
56:AA:66:C:O2'	56:AA:205:A:O2'	2.32	0.44
86:Ae:517:LYS:HG2	86:Ae:522:THR:HG23	2.00	0.44
3:B8:189:A:OP1	3:B8:629:U:O2'	2.32	0.44
8:BD:119:ARG:HH12	52:Bw:63:ILE:HG23	1.82	0.44
70:AO:73:VAL:O	70:AO:109:ARG:NH2	2.51	0.44
73:AR:135:ARG:CZ	73:AR:186:TRP:HB3	2.48	0.44
1:B4:75:THR:O	1:B4:79:ILE:HG13	2.18	0.44
18:BN:82:LEU:HB3	18:BN:87:PHE:CD1	2.53	0.44
19:BO:159:ALA:O	19:BO:163:THR:HG23	2.18	0.44
27:BW:142:ASN:HD22	36:Bf:181:GLU:HG2	1.81	0.44
36:Bf:94:LYS:HE2	36:Bf:96:ASN:HB2	2.00	0.44
56:AA:55:C:OP1	76:AU:41:ARG:NH2	2.38	0.44
73:AR:354:SER:O	73:AR:357:SER:OG	2.31	0.44
79:AX:62:GLN:HG2	79:AX:63:HIS:CD2	2.53	0.44
79:AX:244:LEU:HD12	79:AX:292:ASN:HB3	2.00	0.44
3:B8:648:A:H2'	3:B8:649:A:C8	2.53	0.44
20:BP:188:ARG:HD2	32:Bb:55:VAL:HB	2.00	0.44
34:Bd:73:ARG:HH12	51:Bv:121:GLU:HB3	1.82	0.44
39:Bi:91:TYR:HE2	39:Bi:229:LEU:HD22	1.82	0.44
40:Bj:77:TYR:HB2	40:Bj:97:TYR:OH	2.18	0.44
53:Bx:132:LEU:HD11	53:Bx:153:PHE:CZ	2.53	0.44
56:AA:805:U:H2'	56:AA:806:A:C8	2.52	0.44
79:AX:159:HIS:CD2	79:AX:267:ALA:HB2	2.53	0.44
3:B8:1118:C:H2'	3:B8:1119:C:C6	2.53	0.43
18:BN:123:GLY:HA2	18:BN:141:ILE:HG12	1.99	0.43
20:BP:151:ASN:HD21	32:Bb:31:ARG:HH22	1.65	0.43
39:Bi:332:LEU:HD21	39:Bi:359:ALA:HB2	1.99	0.43
69:AN:6:SER:OG	69:AN:69:LEU:O	2.33	0.43
70:AO:167:ILE:HD12	73:AR:226:ASP:HB3	1.99	0.43
1:B5:64:ILE:HD13	1:B6:82:LEU:HD13	1.99	0.43
18:BN:67:GLU:HB2	18:BN:190:MET:SD	2.58	0.43
28:BX:227:LYS:HE3	28:BX:249:LEU:HD21	2.00	0.43
56:AA:471:A:H4'	85:Ad:355:ARG:NH1	2.33	0.43
62:AG:31:RSQ:HN4	64:AI:-1:G:H1	1.66	0.43
66:AK:120:LEU:HB3	66:AK:123:ILE:HD12	2.00	0.43
67:AL:129:ILE:HD13	67:AL:167:LEU:HD23	2.00	0.43
84:Ac:49:MET:HG2	84:Ac:53:MET:HE2	2.00	0.43
86:Ae:650:MET:HE3	86:Ae:659:GLN:HB3	1.99	0.43
3:B8:71:A:N1	3:B8:85:A:H5''	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:360:U:H1'	3:B8:376:C:H1'	2.01	0.43
4:B9:2:A:H2'	4:B9:3:G:C8	2.52	0.43
18:BN:211:ARG:NH2	54:By:56:ARG:O	2.38	0.43
26:BV:57:GLU:OE2	26:BV:105:THR:OG1	2.29	0.43
39:Bi:174:LEU:HB3	39:Bi:175:PRO:HD3	1.99	0.43
56:AA:936:MA6:O5'	56:AA:936:MA6:H8	2.18	0.43
71:AP:95:HIS:CD2	71:AP:96:ILE:HG13	2.53	0.43
71:AP:124:TYR:HE2	72:AQ:4:HIS:HB3	1.83	0.43
73:AR:260:ASP:HA	73:AR:263:ARG:HG3	1.98	0.43
73:AR:281:ILE:HB	73:AR:300:LEU:HD21	2.01	0.43
82:Aa:241:ARG:HE	82:Aa:287:GLN:CD	2.26	0.43
3:B8:1529:U:H1'	22:BR:98:ARG:HA	2.00	0.43
16:BL:110:LEU:HD22	42:Bm:30:ALA:HB2	2.00	0.43
16:BL:210:ALA:HB1	16:BL:249:ASN:HB2	2.01	0.43
17:BM:251:VAL:HG11	17:BM:257:MET:HE3	2.00	0.43
25:BU:191:SER:H	25:BU:194:THR:HG1	1.64	0.43
27:BW:152:GLU:O	27:BW:155:SER:OG	2.27	0.43
28:BX:233:TRP:HB3	28:BX:240:ILE:HD12	2.00	0.43
39:Bi:246:GLN:NE2	39:Bi:354:PRO:O	2.52	0.43
48:Bs:49:ARG:HG3	48:Bs:50:GLU:HG2	1.99	0.43
58:AC:40:ALA:HB3	58:AC:59:PRO:HG3	2.01	0.43
78:AW:110:ASN:HB2	78:AW:125:ARG:HH21	1.83	0.43
78:AW:143:ARG:HH12	78:AW:170:LEU:HD21	1.83	0.43
86:Ae:303:CYS:SG	86:Ae:344:ARG:NH2	2.91	0.43
87:Ag:309:ASP:OD1	87:Ag:337:ARG:NH1	2.51	0.43
3:B8:457:A:H2'	3:B8:458:G:H8	1.83	0.43
3:B8:842:A:O2'	3:B8:871:C:OP1	2.25	0.43
4:B9:15:A:HO2'	4:B9:17:A:H62	1.58	0.43
18:BN:212:TRP:O	18:BN:258:THR:OG1	2.20	0.43
42:Bm:236:LEU:HD21	42:Bm:289:HIS:CD2	2.54	0.43
42:Bm:242:ARG:NH2	42:Bm:337:GLU:O	2.51	0.43
43:Bn:195:PRO:HG3	43:Bn:321:CYS:SG	2.58	0.43
44:Bo:154:ILE:HD13	44:Bo:183:VAL:HG21	1.99	0.43
49:Bt:79:LEU:HD13	49:Bt:214:PHE:HE1	1.84	0.43
56:AA:12:U:OP1	85:Ad:226:ARG:HD3	2.18	0.43
56:AA:501:A:P	59:AD:165:LYS:HE3	2.58	0.43
67:AL:224:ARG:O	67:AL:228:LYS:HG2	2.18	0.43
69:AN:8:VAL:HB	69:AN:68:ALA:HB1	1.98	0.43
84:Ac:43:ALA:HB1	84:Ac:46:ILE:HD11	2.00	0.43
3:B8:307:U:H2'	3:B8:308:A:H8	1.83	0.43
3:B8:357:A:O2'	3:B8:378:U:OP1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:Bn:121:ARG:HD2	45:Bp:108:PHE:HZ	1.83	0.43
50:Bu:209:TYR:HE1	50:Bu:251:GLN:HG3	1.83	0.43
52:Bw:189:HIS:HE1	52:Bw:194:PHE:HB2	1.83	0.43
55:Bz:112:LYS:HG2	55:Bz:115:ARG:HH21	1.83	0.43
60:AE:11:LYS:HD3	60:AE:58:HIS:HE1	1.83	0.43
3:B8:474:A:OP1	29:BY:57:ARG:NH1	2.42	0.43
3:B8:1203:A:H3'	3:B8:1218:A:H62	1.83	0.43
4:B9:53:U:H5''	4:B9:54:A:N7	2.32	0.43
21:BQ:101:ALA:HB1	21:BQ:107:GLU:HG3	2.00	0.43
24:BT:261:ASP:HB3	24:BT:264:GLN:HB2	2.00	0.43
29:BY:141:ILE:HG22	47:Br:51:LEU:HD12	1.99	0.43
43:Bn:139:TRP:O	43:Bn:144:GLY:N	2.52	0.43
83:Ab:88:ARG:HB3	83:Ab:91:LEU:HD12	2.01	0.43
86:Ae:346:HIS:CD2	86:Ae:347:VAL:HG23	2.54	0.43
19:BO:144:LYS:HA	19:BO:147:ARG:HE	1.84	0.43
39:Bi:142:LEU:HD13	39:Bi:422:VAL:HG21	2.01	0.43
40:Bj:115:THR:OG1	40:Bj:116:SER:N	2.52	0.43
56:AA:765:G:OP1	79:AX:279:LYS:NZ	2.30	0.43
56:AA:911:A:O2'	82:Aa:193:ARG:HB3	2.18	0.43
79:AX:68:TYR:HH	79:AX:140:HIS:CE1	2.33	0.43
82:Aa:232:TYR:CZ	82:Aa:268:LEU:HD22	2.54	0.43
82:Aa:394:ARG:H	82:Aa:407:ILE:HD11	1.84	0.43
85:Ad:244:LEU:HD23	85:Ad:342:MET:HG3	1.99	0.43
3:B8:283:A:OP1	17:BM:232:GLY:HA2	2.19	0.43
3:B8:375:A:N6	3:B8:424:G:O6	2.51	0.43
4:B9:36:C:H5''	43:Bn:53:SER:HB3	2.00	0.43
11:BG:53:HIS:ND1	35:Be:47:TYR:OH	2.50	0.43
11:BG:102:ASN:ND2	35:Be:51:MET:O	2.46	0.43
12:BH:96:ASN:ND2	12:BH:98:GLN:H	2.17	0.43
21:BQ:114:LEU:HD13	33:Bc:97:PHE:HA	2.00	0.43
23:BS:35:MET:O	23:BS:56:ARG:NH1	2.52	0.43
34:Bd:69:ARG:HG3	34:Bd:70:GLU:HG3	2.00	0.43
48:Bs:33:VAL:HG12	48:Bs:43:ALA:HB1	2.00	0.43
55:Bz:68:LYS:NZ	55:Bz:72:GLU:OE1	2.39	0.43
56:AA:130:G:H5''	69:AN:21:LYS:HB3	2.01	0.43
73:AR:285:LEU:HD21	73:AR:328:ILE:HG23	2.01	0.43
74:AS:50:ARG:O	83:Ab:100:ARG:NH1	2.44	0.43
83:Ab:84:LEU:HD23	83:Ab:248:LEU:HD21	2.01	0.43
1:B4:84:GLU:HG3	1:B4:88:LYS:HD2	2.01	0.43
3:B8:1445:U:H2'	3:B8:1446:C:C6	2.54	0.43
3:B8:1482:C:OP1	28:BX:141:SER:OG	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BU:61:LYS:NZ	25:BU:65:GLU:OE2	2.40	0.43
28:BX:77:SER:HB2	28:BX:80:PHE:HD1	1.84	0.43
43:Bn:323:TRP:NE1	43:Bn:339:GLU:OE2	2.48	0.43
62:AG:52:A:H2'	62:AG:53:U:O4'	2.18	0.43
73:AR:107:THR:HG22	85:Ad:368:LEU:HD22	2.01	0.43
79:AX:126:LEU:HD23	79:AX:343:ILE:HB	2.00	0.43
81:AZ:58:TYR:O	81:AZ:62:MET:HG2	2.19	0.43
1:B2:60:TYR:HB2	1:B2:61:PRO:HD3	2.00	0.42
18:BN:254:LEU:HD13	24:BT:27:LEU:HD11	2.01	0.42
44:Bo:227:LEU:HD22	44:Bo:237:VAL:HG13	2.01	0.42
56:AA:373:C:H4'	71:AP:94:ARG:NH1	2.33	0.42
56:AA:805:U:H2'	56:AA:806:A:H8	1.84	0.42
82:Aa:70:TRP:NE1	82:Aa:127:GLU:OE2	2.51	0.42
3:B8:567:A:OP1	38:Bh:171:ARG:NH2	2.48	0.42
3:B8:1325:G:H4'	3:B8:1372:U:H5'	2.01	0.42
17:BM:274:TRP:HE1	17:BM:286:ASN:HB2	1.85	0.42
18:BN:72:PHE:HE2	54:By:50:LEU:HB3	1.83	0.42
28:BX:148:THR:HG22	28:BX:165:GLU:HG2	2.01	0.42
56:AA:16:A:H2'	56:AA:17:G:C8	2.54	0.42
58:AC:58:ALA:HB3	58:AC:60:HIS:CE1	2.54	0.42
70:AO:182:GLY:O	73:AR:183:LYS:NZ	2.46	0.42
71:AP:86:PRO:HA	71:AP:125:LYS:HB3	2.01	0.42
77:AV:173:PHE:O	77:AV:179:GLN:NE2	2.45	0.42
77:AV:241:ARG:HA	77:AV:244:TYR:CE1	2.54	0.42
79:AX:295:LYS:NZ	97:AX:503:GDP:O1B	2.50	0.42
87:Ag:263:ASP:OD1	87:Ag:267:MET:N	2.51	0.42
3:B8:449:U:O2'	11:BG:36:PHE:O	2.31	0.42
16:BL:281:TRP:O	16:BL:285:LYS:NZ	2.53	0.42
17:BM:330:GLU:OE2	28:BX:97:LYS:NZ	2.53	0.42
44:Bo:88:PRO:HB3	44:Bo:125:ILE:HD11	2.01	0.42
52:Bw:122:GLU:N	52:Bw:158:GLN:O	2.51	0.42
52:Bw:135:LEU:HG	52:Bw:146:LEU:HA	2.00	0.42
72:AQ:83:PRO:HG2	72:AQ:84:TRP:CD1	2.54	0.42
83:Ab:164:GLU:HG3	83:Ab:257:ILE:HD13	2.01	0.42
88:Ai:110:ALA:HB3	88:Ai:135:ALA:HB2	2.00	0.42
1:B6:70:ASP:O	1:B6:74:LEU:HG	2.19	0.42
1:B6:74:LEU:HD22	1:B6:78:GLU:HG2	2.01	0.42
3:B8:209:G:OP1	18:BN:92:ARG:NH1	2.41	0.42
3:B8:1012:A:H4'	29:BY:41:LEU:HD13	2.00	0.42
5:BA:62:ARG:NE	50:Bu:230:ARG:HD2	2.34	0.42
7:BC:166:VAL:HG12	7:BC:169:THR:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BG:75:THR:HB	11:BG:83:LYS:HG2	2.01	0.42
43:Bn:160:ASP:OD2	43:Bn:267:ARG:NH2	2.43	0.42
55:Bz:98:VAL:O	55:Bz:102:MET:HG3	2.20	0.42
56:AA:619:A:H5''	63:AH:130:HIS:CE1	2.55	0.42
62:AG:3:U:H2'	62:AG:4:A:H8	1.84	0.42
71:AP:76:ASN:OD1	76:AU:188:ASN:HA	2.19	0.42
3:B8:61:A:OP1	19:BO:74:HIS:NE2	2.52	0.42
3:B8:669:G:N2	3:B8:756:C:O2'	2.53	0.42
9:BE:214:LYS:HB2	42:Bm:58:ILE:HD13	2.02	0.42
51:Bv:58:VAL:N	51:Bv:153:LEU:O	2.52	0.42
51:Bv:247:GLY:HA3	51:Bv:251:HIS:CE1	2.53	0.42
56:AA:36:G:OP1	75:AT:160:ARG:NH2	2.49	0.42
69:AN:17:VAL:HG22	69:AN:28:VAL:HG22	2.01	0.42
85:Ad:108:ALA:HA	85:Ad:111:LYS:HE3	2.01	0.42
85:Ad:198:TRP:HA	85:Ad:201:ILE:HD12	2.02	0.42
3:B8:603:A:N1	3:B8:623:A:O2'	2.49	0.42
28:BX:110:GLU:OE2	28:BX:112:TYR:OH	2.28	0.42
76:AU:168:ILE:HG12	76:AU:176:ARG:HG2	2.01	0.42
3:B8:438:G:H2'	3:B8:439:A:H2'	2.02	0.42
50:Bu:122:ILE:HD13	50:Bu:134:ILE:HG13	2.00	0.42
76:AU:171:GLU:OE1	76:AU:171:GLU:N	2.52	0.42
79:AX:169:LEU:O	79:AX:179:ASP:N	2.35	0.42
82:Aa:302:ILE:HD13	82:Aa:345:LYS:HE3	2.02	0.42
3:B8:1024:A:C6	3:B8:1315:C:H1'	2.55	0.42
24:BT:55:GLY:O	24:BT:59:ARG:HD2	2.20	0.42
34:Bd:45:ARG:NH2	52:Bw:104:GLU:OE2	2.51	0.42
40:Bj:243:ILE:HG23	40:Bj:255:THR:HG21	2.01	0.42
43:Bn:306:LYS:HG3	43:Bn:307:HIS:CD2	2.55	0.42
51:Bv:187:THR:HG23	51:Bv:190:ARG:HH21	1.84	0.42
56:AA:386:U:H4'	60:AE:94:VAL:HG12	2.02	0.42
63:AH:122:GLN:O	66:AK:112:ARG:NH1	2.53	0.42
68:AM:29:ARG:HH22	75:AT:140:ILE:HG23	1.83	0.42
69:AN:14:VAL:O	75:AT:63:GLN:NE2	2.49	0.42
83:Ab:107:PHE:N	83:Ab:115:ILE:O	2.51	0.42
83:Ab:156:GLU:OE1	87:Ag:163:HIS:ND1	2.52	0.42
83:Ab:222:ILE:HD13	83:Ab:236:VAL:HB	2.01	0.42
3:B8:1324:U:H4'	82:Aa:316:ASN:O	2.20	0.42
3:B8:1390:C:O2	82:Aa:306:ARG:NH2	2.53	0.42
39:Bi:207:HIS:ND1	39:Bi:234:ASP:OD1	2.41	0.42
40:Bj:124:ASP:HB2	40:Bj:296:ARG:NH1	2.35	0.42
42:Bm:165:GLN:NE2	42:Bm:179:VAL:HG21	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Bo:69:HIS:CD2	44:Bo:71:GLY:H	2.37	0.42
51:Bv:242:ASP:OD1	51:Bv:243:PHE:N	2.50	0.42
56:AA:3:U:C4	85:Ad:427:ARG:HD3	2.55	0.42
56:AA:469:A:P	83:Ab:100:ARG:HH22	2.42	0.42
82:Aa:185:VAL:HG22	82:Aa:248:TYR:HD1	1.85	0.42
85:Ad:258:ILE:HD11	85:Ad:343:LEU:HD22	2.01	0.42
3:B8:328:U:OP1	3:B8:331:C:N4	2.34	0.42
3:B8:366:C:N4	3:B8:1248:A:N7	2.68	0.42
3:B8:761:C:OP2	3:B8:763:C:N4	2.41	0.42
3:B8:1190:G:H5''	43:Bn:352:PRO:HD3	2.02	0.42
24:BT:95:PRO:HA	24:BT:139:GLN:HG3	2.02	0.42
24:BT:230:PRO:HB3	36:Bf:60:ARG:O	2.19	0.42
48:Bs:77:ALA:HB2	48:Bs:104:LEU:HD13	2.02	0.42
56:AA:103:G:H5''	69:AN:47:LYS:NZ	2.35	0.42
56:AA:661:U:O2'	58:AC:64:HIS:ND1	2.50	0.42
56:AA:818:C:H4'	56:AA:819:C:H5'	2.01	0.42
82:Aa:338:GLU:O	82:Aa:344:ASN:ND2	2.46	0.42
86:Ae:573:ALA:HB2	86:Ae:604:LYS:HD2	2.00	0.42
3:B8:443:G:H22	3:B8:1023:A:P	2.42	0.41
3:B8:1032:G:H5'	22:BR:114:LYS:HE2	2.01	0.41
3:B8:1224:U:H5''	3:B8:1225:U:O4'	2.20	0.41
23:BS:44:SER:O	23:BS:48:ASN:ND2	2.35	0.41
39:Bi:152:GLN:HE22	39:Bi:179:GLN:HE22	1.67	0.41
56:AA:57:U:N3	89:Aj:57:ASP:OD2	2.39	0.41
56:AA:126:U:H2'	56:AA:127:G:C8	2.55	0.41
56:AA:696:A:O2'	56:AA:698:G:N7	2.38	0.41
56:AA:883:A:OP1	89:Aj:29:ARG:NH2	2.51	0.41
73:AR:162:SER:HB2	73:AR:165:ILE:HD12	2.02	0.41
77:AV:123:ASP:OD1	77:AV:123:ASP:N	2.53	0.41
81:AZ:75:HIS:ND1	85:Ad:98:LEU:HD11	2.35	0.41
82:Aa:171:PHE:HB3	82:Aa:433:ILE:HD13	2.01	0.41
3:B8:125:A:N6	3:B8:126:A:N1	2.68	0.41
3:B8:577:C:OP1	31:Ba:24:GLY:N	2.53	0.41
29:BY:83:TYR:CZ	29:BY:87:ILE:HG13	2.55	0.41
30:BZ:164:THR:OG1	30:BZ:165:GLU:N	2.53	0.41
56:AA:761:A:H2'	56:AA:762:A:C8	2.55	0.41
79:AX:159:HIS:CD2	79:AX:315:SER:HA	2.55	0.41
79:AX:248:LYS:HE3	79:AX:301:TRP:CD1	2.55	0.41
85:Ad:265:MET:HE1	87:Ag:54:PHE:HZ	1.85	0.41
85:Ad:418:LYS:NZ	85:Ad:420:SER:HB2	2.35	0.41
87:Ag:315:PHE:CD2	87:Ag:369:LEU:HD21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:667:A:H5'	46:Bq:28:ARG:HD3	2.02	0.41
8:BD:103:VAL:HG11	43:Bn:61:ALA:HB1	2.01	0.41
10:BF:188:TRP:O	10:BF:195:ASN:ND2	2.45	0.41
38:Bh:136:PRO:HG2	38:Bh:139:VAL:HG21	2.02	0.41
44:Bo:43:MET:HE1	44:Bo:232:HIS:CD2	2.55	0.41
45:Bp:121:TRP:CZ2	45:Bp:125:LYS:HD3	2.55	0.41
56:AA:726:U:H2'	56:AA:727:A:H8	1.85	0.41
58:AC:98:GLY:HA3	81:AZ:71:TYR:CE1	2.56	0.41
61:AF:193:ASP:OD1	61:AF:194:LYS:N	2.53	0.41
68:AM:35:VAL:HA	68:AM:50:GLN:HA	2.03	0.41
79:AX:206:GLU:OE2	79:AX:249:ARG:NH2	2.52	0.41
3:B8:356:A:H2'	3:B8:357:A:C8	2.55	0.41
25:BU:96:TYR:OH	25:BU:129:LYS:NZ	2.52	0.41
56:AA:254:G:H5'	56:AA:255:G:OP2	2.21	0.41
62:AG:10:A:C2	62:AG:23:A:H1'	2.55	0.41
83:Ab:204:GLU:OE2	84:Ac:116:TYR:OH	2.28	0.41
1:B2:76:LEU:HD13	20:BP:200:LEU:HA	2.03	0.41
3:B8:656:C:OP2	39:Bi:55:SER:OG	2.25	0.41
3:B8:673:G:H3'	3:B8:673:G:N3	2.35	0.41
3:B8:964:U:OP1	16:BL:278:LYS:NZ	2.41	0.41
3:B8:1007:A:H2'	3:B8:1008:A:C8	2.55	0.41
3:B8:1113:A:H4'	40:Bj:301:GLU:HA	2.01	0.41
6:BB:141:ASP:HB3	6:BB:144:ARG:HG2	2.03	0.41
29:BY:108:TYR:HD1	48:Bs:125:SER:HB2	1.85	0.41
56:AA:506:C:N4	59:AD:197:ARG:HG2	2.36	0.41
56:AA:851:C:H2'	56:AA:852:U:C6	2.56	0.41
68:AM:111:ARG:NH2	73:AR:146:LYS:O	2.53	0.41
73:AR:78:ILE:HG23	73:AR:299:ASN:HB3	2.03	0.41
76:AU:188:ASN:OD1	76:AU:188:ASN:N	2.53	0.41
89:Aj:64:LEU:HD23	89:Aj:134:VAL:HG13	2.01	0.41
3:B8:69:A:O2'	3:B8:218:G:H1'	2.21	0.41
3:B8:91:A:H2'	3:B8:92:A:C8	2.56	0.41
3:B8:191:U:H2'	3:B8:192:U:C6	2.56	0.41
3:B8:315:G:OP1	3:B8:317:G:O2'	2.36	0.41
27:BW:83:VAL:HG11	27:BW:158:MET:HE1	2.01	0.41
34:Bd:58:LYS:HG2	34:Bd:77:MET:HE2	2.02	0.41
40:Bj:308:ASP:HA	40:Bj:311:LEU:HG	2.01	0.41
56:AA:726:U:H2'	56:AA:727:A:C8	2.55	0.41
59:AD:145:LYS:HB3	59:AD:145:LYS:HE2	1.88	0.41
63:AH:165:PRO:HG2	63:AH:168:VAL:HG21	2.02	0.41
68:AM:94:ALA:HB2	73:AR:158:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:AR:262:LEU:O	73:AR:265:THR:OG1	2.29	0.41
77:AV:225:LEU:HD22	77:AV:275:LEU:HD13	2.01	0.41
80:AY:323:ASP:OD1	80:AY:323:ASP:N	2.51	0.41
86:Ae:316:ILE:O	86:Ae:320:LEU:HG	2.21	0.41
86:Ae:470:GLN:HG2	86:Ae:472:ASP:H	1.86	0.41
3:B8:266:A:H4'	3:B8:267:A:C8	2.56	0.41
3:B8:1115:C:H4'	40:Bj:75:TYR:CE2	2.56	0.41
3:B8:1280:U:H2'	3:B8:1281:A:C8	2.55	0.41
5:BA:126:HIS:HD2	50:Bu:227:ARG:HH21	1.69	0.41
9:BE:44:ARG:HG3	19:BO:55:ILE:HG21	2.02	0.41
56:AA:224:A:H4'	56:AA:225:G:H5'	2.02	0.41
62:AG:31:RSQ:O2	62:AG:31:RSQ:H2'	2.21	0.41
79:AX:136:LEU:HD23	79:AX:136:LEU:HA	1.93	0.41
79:AX:379:GLU:OE2	87:Ag:318:HIS:NE2	2.53	0.41
3:B8:657:U:H4'	26:BV:30:ARG:HH21	1.86	0.41
3:B8:1113:A:H2'	3:B8:1114:A:O4'	2.21	0.41
18:BN:187:LEU:HD13	18:BN:259:LEU:HD23	2.02	0.41
19:BO:185:ASN:OD1	19:BO:188:ILE:HG13	2.21	0.41
20:BP:151:ASN:ND2	32:Bb:31:ARG:HH22	2.17	0.41
21:BQ:169:LYS:HE3	21:BQ:169:LYS:HB2	1.92	0.41
26:BV:144:LEU:HD12	44:Bo:174:VAL:HG11	2.03	0.41
34:Bd:42:ARG:O	34:Bd:44:HIS:ND1	2.53	0.41
39:Bi:182:SER:O	42:Bm:189:LYS:NZ	2.46	0.41
40:Bj:72:ILE:HA	40:Bj:75:TYR:CE2	2.55	0.41
43:Bn:234:HIS:CE1	43:Bn:257:PRO:HA	2.56	0.41
61:AF:234:ARG:HB2	84:Ac:53:MET:HE1	2.02	0.41
63:AH:96:VAL:O	63:AH:100:LYS:HG2	2.21	0.41
64:AI:26:N:OP1	86:Ae:306:ASN:ND2	2.54	0.41
82:Aa:141:ASN:O	82:Aa:145:GLU:HG3	2.20	0.41
89:Aj:99:ARG:HB3	89:Aj:115:TRP:HB2	2.03	0.41
89:Aj:167:PRO:HG2	89:Aj:170:LEU:HB2	2.03	0.41
1:B1:85:LEU:HD23	1:B2:68:VAL:HG21	2.03	0.41
3:B8:916:U:H2'	3:B8:917:G:C8	2.56	0.41
3:B8:1372:U:H3	82:Aa:305:PHE:HB2	1.86	0.41
6:BB:52:ASP:O	6:BB:56:TYR:N	2.51	0.41
6:BB:150:TRP:CE2	50:Bu:172:MET:HG2	2.55	0.41
11:BG:148:GLN:HB3	11:BG:150:HIS:CE1	2.56	0.41
15:BK:104:ARG:NH1	15:BK:160:LYS:O	2.53	0.41
18:BN:94:ASP:OD1	18:BN:94:ASP:N	2.53	0.41
21:BQ:123:ILE:HG13	33:Bc:75:VAL:HG13	2.02	0.41
22:BR:37:ILE:HG23	22:BR:42:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BU:104:MET:HE3	25:BU:104:MET:HB3	1.94	0.41
42:Bm:177:CYS:HB3	42:Bm:178:PRO:HD3	2.02	0.41
45:Bp:67:ARG:NH1	62:AG:43:A:H5''	2.36	0.41
51:Bv:109:GLU:HB2	51:Bv:112:GLN:NE2	2.36	0.41
52:Bw:104:GLU:HG2	52:Bw:155:ARG:HE	1.85	0.41
56:AA:37:U:H2'	56:AA:38:A:H8	1.86	0.41
56:AA:323:A:H2'	56:AA:324:A:C8	2.56	0.41
58:AC:104:LEU:HD23	58:AC:123:VAL:HG12	2.01	0.41
62:AG:54:A:H2'	62:AG:55:C:H5''	2.03	0.41
73:AR:281:ILE:HD12	73:AR:300:LEU:HG	2.03	0.41
74:AS:125:LEU:HB3	74:AS:130:VAL:HB	2.01	0.41
77:AV:221:PHE:HE2	77:AV:265:LYS:HD3	1.85	0.41
79:AX:359:TYR:O	79:AX:363:ASN:ND2	2.47	0.41
82:Aa:225:LEU:HD11	82:Aa:241:ARG:HB2	2.03	0.41
83:Ab:137:TYR:O	83:Ab:264:ARG:NH1	2.46	0.41
85:Ad:225:VAL:HG22	85:Ad:243:VAL:HG22	2.03	0.41
86:Ae:263:ILE:HG23	86:Ae:275:ALA:HB1	2.02	0.41
89:Aj:64:LEU:HB3	89:Aj:134:VAL:HG13	2.03	0.41
3:B8:444:C:H4'	3:B8:1313:G:O2'	2.21	0.41
3:B8:468:U:O2'	3:B8:481:A:N3	2.52	0.41
3:B8:619:G:OP1	24:BT:34:LYS:NZ	2.50	0.41
3:B8:860:A:H5''	16:BL:212:THR:HG21	2.02	0.41
3:B8:1110:C:OP1	40:Bj:120:SER:OG	2.24	0.41
3:B8:1422:U:H2'	3:B8:1423:C:C6	2.56	0.41
34:Bd:114:LEU:HD12	34:Bd:119:TYR:CE2	2.55	0.41
36:Bf:129:ARG:NH2	43:Bn:336:ASP:OD1	2.48	0.41
42:Bm:257:TYR:CD2	42:Bm:258:PRO:HA	2.56	0.41
56:AA:250:C:P	65:AJ:116:GLN:HE21	2.43	0.41
66:AK:37:ASP:OD2	81:AZ:52:TYR:OH	2.28	0.41
71:AP:75:LYS:HE3	71:AP:75:LYS:HB2	1.83	0.41
77:AV:168:MET:HE3	77:AV:168:MET:HB3	2.01	0.41
79:AX:102:ARG:NH1	79:AX:132:THR:O	2.51	0.41
3:B8:237:A:N3	3:B8:1260:U:O2'	2.49	0.40
3:B8:651:A:H5'	12:BH:135:ALA:HA	2.03	0.40
3:B8:802:A:H5''	23:BS:35:MET:HE2	2.03	0.40
3:B8:997:U:H2'	3:B8:998:A:O4'	2.20	0.40
3:B8:1093:U:O2'	19:BO:247:ARG:HB3	2.21	0.40
4:B9:72:A:H5'	51:Bv:170:VAL:HG21	2.01	0.40
9:BE:143:PHE:HE2	9:BE:190:LYS:HE2	1.86	0.40
17:BM:311:GLY:HA2	17:BM:314:LEU:HD12	2.03	0.40
26:BV:30:ARG:HD2	26:BV:78:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BZ:99:VAL:HG12	30:BZ:133:VAL:HG22	2.02	0.40
40:Bj:127:LEU:O	40:Bj:251:ASN:HB3	2.21	0.40
48:Bs:131:HIS:HD2	48:Bs:133:PHE:H	1.67	0.40
60:AE:17:GLU:OE1	60:AE:17:GLU:N	2.54	0.40
74:AS:2:ALA:HB2	85:Ad:215:TYR:HE1	1.86	0.40
78:AW:90:THR:O	83:Ab:110:ARG:NH2	2.49	0.40
79:AX:102:ARG:HH12	79:AX:133:GLY:HA3	1.86	0.40
83:Ab:67:LEU:HD11	83:Ab:138:ARG:HH21	1.84	0.40
3:B8:785:U:H2'	3:B8:786:U:C6	2.57	0.40
3:B8:1088:G:H2'	3:B8:1089:U:C6	2.56	0.40
12:BH:137:ILE:HD12	26:BV:131:PRO:HD3	2.03	0.40
15:BK:127:ALA:HA	24:BT:79:PRO:HD3	2.03	0.40
20:BP:177:LEU:HD22	32:Bb:22:PRO:HB3	2.03	0.40
23:BS:123:ILE:HD12	23:BS:127:LEU:HD12	2.04	0.40
40:Bj:72:ILE:HA	40:Bj:75:TYR:CD2	2.56	0.40
49:Bt:148:MET:SD	49:Bt:149:PRO:HD2	2.61	0.40
52:Bw:48:TYR:HB3	52:Bw:51:LYS:HG2	2.04	0.40
56:AA:368:A:O2'	72:AQ:38:ASP:OD2	2.37	0.40
57:AB:107:LYS:HD3	58:AC:69:LEU:HD23	2.02	0.40
62:AG:5:A:H2'	62:AG:6:G:C8	2.56	0.40
67:AL:115:ILE:HG21	67:AL:181:ILE:HD13	2.03	0.40
77:AV:30:LEU:HD13	77:AV:34:TYR:CD1	2.56	0.40
5:BA:200:ARG:NH1	22:BR:52:ASP:O	2.49	0.40
6:BB:9:LEU:HD21	10:BF:185:VAL:HG22	2.03	0.40
24:BT:257:CYS:SG	36:Bf:59:TRP:NE1	2.94	0.40
29:BY:114:LYS:HD2	47:Br:44:ASN:HB3	2.03	0.40
34:Bd:85:SER:O	34:Bd:89:ARG:HG3	2.22	0.40
56:AA:661:U:H2'	56:AA:662:A:H8	1.85	0.40
56:AA:763:G:H2'	56:AA:764:G:H8	1.86	0.40
67:AL:79:VAL:HG23	67:AL:82:ILE:HB	2.02	0.40
77:AV:46:GLU:OE2	77:AV:74:ARG:NE	2.55	0.40
79:AX:340:PHE:CE2	79:AX:342:PRO:HG3	2.56	0.40
85:Ad:150:LYS:HB2	85:Ad:155:GLN:NE2	2.37	0.40
85:Ad:230:THR:HG23	85:Ad:238:LYS:HB3	2.03	0.40
89:Aj:42:THR:HG22	89:Aj:49:ARG:HG2	2.03	0.40
3:B8:66:A:H2	3:B8:91:A:N7	2.19	0.40
3:B8:81:A:C5	3:B8:82:U:H1'	2.56	0.40
3:B8:249:C:O2'	3:B8:830:A:N1	2.50	0.40
3:B8:442:A:H5''	35:Be:20:LYS:HB2	2.04	0.40
3:B8:1537:A:O2'	3:B8:1538:C:O4'	2.39	0.40
9:BE:83:GLU:OE2	19:BO:53:THR:OG1	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BF:223:LYS:HE2	10:BF:223:LYS:HB3	1.93	0.40
19:BO:173:GLU:OE1	19:BO:246:LYS:NZ	2.52	0.40
19:BO:191:ARG:NH2	40:Bj:301:GLU:OE1	2.52	0.40
26:BV:46:TRP:HD1	26:BV:121:ALA:HB2	1.87	0.40
40:Bj:123:LEU:HD21	40:Bj:125:LEU:HD21	2.03	0.40
58:AC:115:ASN:HB2	80:AY:311:TRP:CG	2.57	0.40
60:AE:65:LEU:HD11	71:AP:75:LYS:HD2	2.04	0.40
66:AK:70:VAL:HG21	80:AY:386:ILE:HD13	2.04	0.40
83:Ab:54:ASP:OD1	83:Ab:271:TYR:OH	2.38	0.40
87:Ag:143:ASP:N	87:Ag:143:ASP:OD1	2.54	0.40
3:B8:446:C:O2'	3:B8:1167:A:N3	2.54	0.40
17:BM:96:ARG:HH21	17:BM:202:GLN:HE22	1.69	0.40
18:BN:61:PRO:HA	18:BN:84:PRO:HD3	2.02	0.40
18:BN:218:LEU:HD23	18:BN:260:VAL:HB	2.04	0.40
19:BO:188:ILE:HG12	40:Bj:112:LEU:HA	2.03	0.40
22:BR:119:ARG:HA	22:BR:119:ARG:HD3	1.81	0.40
35:Be:99:LYS:O	48:Bs:44:ARG:NH2	2.54	0.40
40:Bj:291:VAL:HG12	40:Bj:292:ARG:HG3	2.04	0.40
44:Bo:226:ALA:HB1	44:Bo:240:ILE:HD13	2.02	0.40
56:AA:114:A:O2'	56:AA:137:A:N1	2.43	0.40
56:AA:272:A:OP2	70:AO:96:ARG:NH2	2.45	0.40
58:AC:109:VAL:HB	58:AC:120:CYS:HB2	2.03	0.40
77:AV:30:LEU:HD11	77:AV:145:ASN:HB3	2.04	0.40
77:AV:202:ARG:HG2	77:AV:247:MET:HE2	2.03	0.40
78:AW:143:ARG:NH1	78:AW:170:LEU:HD21	2.36	0.40
88:Ai:94:ASN:OD1	88:Ai:95:THR:N	2.55	0.40
89:Aj:89:HIS:NE2	89:Aj:202:ASP:OD2	2.49	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	B1	44/198 (22%)	44 (100%)	0	0	100	100
1	B2	30/198 (15%)	30 (100%)	0	0	100	100
1	B3	30/198 (15%)	29 (97%)	1 (3%)	0	100	100
1	B4	29/198 (15%)	29 (100%)	0	0	100	100
1	B5	29/198 (15%)	29 (100%)	0	0	100	100
1	B6	29/198 (15%)	29 (100%)	0	0	100	100
5	BA	164/206 (80%)	162 (99%)	2 (1%)	0	100	100
6	BB	150/153 (98%)	148 (99%)	2 (1%)	0	100	100
7	BC	203/216 (94%)	201 (99%)	2 (1%)	0	100	100
8	BD	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
9	BE	242/256 (94%)	240 (99%)	2 (1%)	0	100	100
10	BF	179/250 (72%)	178 (99%)	1 (1%)	0	100	100
11	BG	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
12	BH	108/188 (57%)	108 (100%)	0	0	100	100
13	BI	54/65 (83%)	53 (98%)	1 (2%)	0	100	100
14	BJ	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
15	BK	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
16	BL	236/305 (77%)	230 (98%)	6 (2%)	0	100	100
17	BM	303/348 (87%)	300 (99%)	3 (1%)	0	100	100
18	BN	250/311 (80%)	246 (98%)	4 (2%)	0	100	100
19	BO	200/267 (75%)	193 (96%)	7 (4%)	0	100	100
20	BP	210/261 (80%)	205 (98%)	5 (2%)	0	100	100
21	BQ	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
22	BR	175/178 (98%)	174 (99%)	1 (1%)	0	100	100
23	BS	113/145 (78%)	113 (100%)	0	0	100	100
24	BT	289/296 (98%)	285 (99%)	4 (1%)	0	100	100
25	BU	220/251 (88%)	219 (100%)	1 (0%)	0	100	100
26	BV	152/175 (87%)	149 (98%)	3 (2%)	0	100	100
27	BW	142/180 (79%)	139 (98%)	3 (2%)	0	100	100
28	BX	236/292 (81%)	233 (99%)	3 (1%)	0	100	100
29	BY	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
30	BZ	159/205 (78%)	158 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	Ba	92/123 (75%)	91 (99%)	1 (1%)	0	100	100
32	Bb	99/112 (88%)	99 (100%)	0	0	100	100
33	Bc	80/138 (58%)	80 (100%)	0	0	100	100
34	Bd	90/128 (70%)	90 (100%)	0	0	100	100
35	Be	92/102 (90%)	92 (100%)	0	0	100	100
36	Bf	141/206 (68%)	140 (99%)	1 (1%)	0	100	100
37	Bg	159/222 (72%)	158 (99%)	1 (1%)	0	100	100
38	Bh	160/196 (82%)	158 (99%)	2 (1%)	0	100	100
39	Bi	382/439 (87%)	377 (99%)	5 (1%)	0	100	100
40	Bj	160/325 (49%)	156 (98%)	4 (2%)	0	100	100
41	Bl	36/103 (35%)	36 (100%)	0	0	100	100
42	Bm	392/423 (93%)	388 (99%)	4 (1%)	0	100	100
43	Bn	352/380 (93%)	343 (97%)	9 (3%)	0	100	100
44	Bo	292/338 (86%)	285 (98%)	7 (2%)	0	100	100
45	Bp	145/206 (70%)	145 (100%)	0	0	100	100
46	Bq	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
47	Br	96/142 (68%)	96 (100%)	0	0	100	100
48	Bs	149/215 (69%)	146 (98%)	3 (2%)	0	100	100
49	Bt	282/332 (85%)	278 (99%)	4 (1%)	0	100	100
50	Bu	235/306 (77%)	233 (99%)	2 (1%)	0	100	100
51	Bv	236/279 (85%)	230 (98%)	6 (2%)	0	100	100
52	Bw	153/212 (72%)	151 (99%)	2 (1%)	0	100	100
53	Bx	132/166 (80%)	129 (98%)	3 (2%)	0	100	100
54	By	108/158 (68%)	107 (99%)	1 (1%)	0	100	100
55	Bz	95/128 (74%)	95 (100%)	0	0	100	100
57	AB	277/323 (86%)	274 (99%)	3 (1%)	0	100	100
58	AC	130/167 (78%)	129 (99%)	1 (1%)	0	100	100
59	AD	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
60	AE	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
61	AF	206/242 (85%)	206 (100%)	0	0	100	100
63	AH	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	18	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	AJ	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
66	AK	99/128 (77%)	99 (100%)	0	0	100	100
67	AL	172/257 (67%)	171 (99%)	1 (1%)	0	100	100
68	AM	117/137 (85%)	115 (98%)	2 (2%)	0	100	100
69	AN	108/130 (83%)	107 (99%)	1 (1%)	0	100	100
70	AO	191/258 (74%)	190 (100%)	1 (0%)	0	100	100
71	AP	95/142 (67%)	95 (100%)	0	0	100	100
72	AQ	84/87 (97%)	84 (100%)	0	0	100	100
73	AR	293/360 (81%)	290 (99%)	3 (1%)	0	100	100
74	AS	133/190 (70%)	132 (99%)	1 (1%)	0	100	100
75	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
76	AU	174/205 (85%)	174 (100%)	0	0	100	100
77	AV	358/414 (86%)	354 (99%)	4 (1%)	0	100	100
78	AW	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
79	AX	350/398 (88%)	349 (100%)	1 (0%)	0	100	100
80	AY	147/395 (37%)	147 (100%)	0	0	100	100
81	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
82	Aa	379/484 (78%)	376 (99%)	3 (1%)	0	100	100
83	Ab	223/296 (75%)	220 (99%)	3 (1%)	0	100	100
84	Ac	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
85	Ad	341/430 (79%)	335 (98%)	6 (2%)	0	100	100
86	Ae	584/689 (85%)	582 (100%)	2 (0%)	0	100	100
87	Ag	323/396 (82%)	318 (98%)	5 (2%)	0	100	100
88	Ai	134/194 (69%)	132 (98%)	2 (2%)	0	100	100
89	Aj	213/218 (98%)	212 (100%)	1 (0%)	0	100	100
All	All	14978/19969 (75%)	14810 (99%)	167 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
63	AH	126	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	B1	40/158 (25%)	40 (100%)	0	100	100
1	B2	31/158 (20%)	31 (100%)	0	100	100
1	B3	31/158 (20%)	31 (100%)	0	100	100
1	B4	30/158 (19%)	30 (100%)	0	100	100
1	B5	30/158 (19%)	30 (100%)	0	100	100
1	B6	30/158 (19%)	30 (100%)	0	100	100
5	BA	146/176 (83%)	146 (100%)	0	100	100
6	BB	134/135 (99%)	132 (98%)	2 (2%)	57	75
7	BC	183/191 (96%)	183 (100%)	0	100	100
8	BD	94/119 (79%)	93 (99%)	1 (1%)	65	78
9	BE	220/229 (96%)	220 (100%)	0	100	100
10	BF	163/223 (73%)	162 (99%)	1 (1%)	78	83
11	BG	113/147 (77%)	113 (100%)	0	100	100
12	BH	99/164 (60%)	99 (100%)	0	100	100
13	BI	53/60 (88%)	53 (100%)	0	100	100
14	BJ	40/72 (56%)	40 (100%)	0	100	100
15	BK	88/166 (53%)	88 (100%)	0	100	100
16	BL	192/245 (78%)	191 (100%)	1 (0%)	81	85
17	BM	260/290 (90%)	259 (100%)	1 (0%)	84	86
18	BN	219/262 (84%)	219 (100%)	0	100	100
19	BO	182/228 (80%)	181 (100%)	1 (0%)	81	85
20	BP	194/232 (84%)	194 (100%)	0	100	100
21	BQ	138/150 (92%)	138 (100%)	0	100	100
22	BR	154/155 (99%)	154 (100%)	0	100	100
23	BS	98/124 (79%)	98 (100%)	0	100	100
24	BT	246/249 (99%)	246 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	BU	189/211 (90%)	188 (100%)	1 (0%)	81	85
26	BV	134/150 (89%)	134 (100%)	0	100	100
27	BW	126/155 (81%)	126 (100%)	0	100	100
28	BX	220/256 (86%)	220 (100%)	0	100	100
29	BY	118/126 (94%)	118 (100%)	0	100	100
30	BZ	146/180 (81%)	146 (100%)	0	100	100
31	Ba	74/97 (76%)	74 (100%)	0	100	100
32	Bb	83/90 (92%)	83 (100%)	0	100	100
33	Bc	76/116 (66%)	76 (100%)	0	100	100
34	Bd	85/113 (75%)	85 (100%)	0	100	100
35	Be	80/87 (92%)	80 (100%)	0	100	100
36	Bf	135/181 (75%)	135 (100%)	0	100	100
37	Bg	138/178 (78%)	138 (100%)	0	100	100
38	Bh	147/169 (87%)	146 (99%)	1 (1%)	76	82
39	Bi	340/381 (89%)	339 (100%)	1 (0%)	86	87
40	Bj	150/287 (52%)	150 (100%)	0	100	100
41	Bl	37/89 (42%)	37 (100%)	0	100	100
42	Bm	353/368 (96%)	352 (100%)	1 (0%)	86	87
43	Bn	313/332 (94%)	313 (100%)	0	100	100
44	Bo	270/303 (89%)	269 (100%)	1 (0%)	84	86
45	Bp	136/190 (72%)	136 (100%)	0	100	100
46	Bq	104/112 (93%)	104 (100%)	0	100	100
47	Br	96/133 (72%)	96 (100%)	0	100	100
48	Bs	132/185 (71%)	130 (98%)	2 (2%)	57	75
49	Bt	251/288 (87%)	251 (100%)	0	100	100
50	Bu	223/274 (81%)	221 (99%)	2 (1%)	70	80
51	Bv	207/236 (88%)	207 (100%)	0	100	100
52	Bw	139/188 (74%)	139 (100%)	0	100	100
53	Bx	124/148 (84%)	124 (100%)	0	100	100
54	By	104/148 (70%)	104 (100%)	0	100	100
55	Bz	86/110 (78%)	85 (99%)	1 (1%)	63	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	AB	257/291 (88%)	257 (100%)	0	100	100
58	AC	115/143 (80%)	115 (100%)	0	100	100
59	AD	65/166 (39%)	64 (98%)	1 (2%)	57	75
60	AE	104/107 (97%)	103 (99%)	1 (1%)	68	79
61	AF	185/209 (88%)	185 (100%)	0	100	100
63	AH	130/180 (72%)	129 (99%)	1 (1%)	73	81
65	AJ	93/118 (79%)	93 (100%)	0	100	100
66	AK	91/113 (80%)	91 (100%)	0	100	100
67	AL	158/226 (70%)	157 (99%)	1 (1%)	78	83
68	AM	97/113 (86%)	97 (100%)	0	100	100
69	AN	96/115 (84%)	95 (99%)	1 (1%)	68	79
70	AO	174/230 (76%)	174 (100%)	0	100	100
71	AP	88/123 (72%)	88 (100%)	0	100	100
72	AQ	78/79 (99%)	78 (100%)	0	100	100
73	AR	264/318 (83%)	264 (100%)	0	100	100
74	AS	116/164 (71%)	116 (100%)	0	100	100
75	AT	153/157 (98%)	152 (99%)	1 (1%)	76	82
76	AU	152/174 (87%)	152 (100%)	0	100	100
77	AV	325/364 (89%)	324 (100%)	1 (0%)	86	87
78	AW	87/158 (55%)	86 (99%)	1 (1%)	65	78
79	AX	311/351 (89%)	311 (100%)	0	100	100
80	AY	137/357 (38%)	137 (100%)	0	100	100
81	AZ	90/95 (95%)	90 (100%)	0	100	100
82	Aa	338/427 (79%)	334 (99%)	4 (1%)	63	78
83	Ab	198/249 (80%)	198 (100%)	0	100	100
84	Ac	100/101 (99%)	100 (100%)	0	100	100
85	Ad	286/357 (80%)	285 (100%)	1 (0%)	86	87
86	Ae	526/609 (86%)	525 (100%)	1 (0%)	87	89
87	Ag	285/342 (83%)	284 (100%)	1 (0%)	84	86
88	Ai	104/146 (71%)	103 (99%)	1 (1%)	68	79
89	Aj	188/190 (99%)	188 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	13415/17218 (78%)	13382 (100%)	33 (0%)	84 89

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	BB	19	VAL
6	BB	28	LEU
8	BD	131	VAL
10	BF	185	VAL
16	BL	215	VAL
17	BM	151	THR
19	BO	102	VAL
25	BU	59	VAL
38	Bh	70	CYS
39	Bi	157	LEU
42	Bm	146	HIS
44	Bo	143	TRP
48	Bs	75	VAL
48	Bs	121	THR
50	Bu	81	THR
50	Bu	89	VAL
55	Bz	43	VAL
59	AD	155	ARG
60	AE	109	VAL
63	AH	129	LYS
67	AL	209	LEU
69	AN	88	VAL
75	AT	92	THR
77	AV	35	VAL
78	AW	162	VAL
82	Aa	199	ILE
82	Aa	272	MET
82	Aa	314	HIS
82	Aa	317	LYS
85	Ad	163	GLU
86	Ae	508	VAL
87	Ag	210	VAL
88	Ai	151	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165) such sidechains are listed below:

Mol	Chain	Res	Type
1	B1	69	GLN
1	B3	65	GLN
5	BA	126	HIS
5	BA	204	HIS
6	BB	27	GLN
6	BB	77	ASN
9	BE	89	GLN
9	BE	172	GLN
10	BF	110	ASN
10	BF	179	HIS
10	BF	225	ASN
11	BG	64	HIS
11	BG	150	HIS
12	BH	83	ASN
15	BK	170	ASN
17	BM	52	HIS
17	BM	63	GLN
17	BM	88	HIS
17	BM	125	GLN
17	BM	137	ASN
17	BM	280	HIS
18	BN	103	GLN
18	BN	208	HIS
19	BO	192	HIS
19	BO	196	ASN
20	BP	93	ASN
20	BP	151	ASN
21	BQ	84	GLN
22	BR	9	GLN
22	BR	56	HIS
22	BR	94	GLN
23	BS	59	HIS
23	BS	143	ASN
24	BT	84	ASN
25	BU	237	HIS
26	BV	100	GLN
26	BV	147	GLN
26	BV	154	GLN
27	BW	142	ASN
28	BX	158	GLN
28	BX	172	GLN
28	BX	253	GLN
29	BY	149	HIS

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Mol	Chain	Res	Type
30	BZ	84	ASN
30	BZ	118	ASN
30	BZ	140	ASN
33	Bc	82	GLN
33	Bc	135	ASN
34	Bd	65	HIS
34	Bd	101	GLN
35	Be	94	HIS
36	Bf	176	HIS
36	Bf	190	GLN
37	Bg	51	GLN
37	Bg	120	HIS
38	Bh	79	HIS
38	Bh	96	HIS
38	Bh	130	ASN
39	Bi	152	GLN
39	Bi	238	ASN
39	Bi	240	GLN
39	Bi	314	GLN
39	Bi	343	GLN
39	Bi	358	GLN
39	Bi	386	ASN
39	Bi	387	ASN
40	Bj	241	HIS
40	Bj	266	GLN
42	Bm	160	HIS
42	Bm	165	GLN
42	Bm	221	GLN
42	Bm	353	HIS
42	Bm	384	GLN
43	Bn	308	GLN
44	Bo	69	HIS
44	Bo	198	ASN
44	Bo	247	ASN
44	Bo	298	GLN
47	Br	46	ASN
47	Br	90	GLN
47	Br	111	GLN
48	Bs	66	ASN
48	Bs	129	GLN
48	Bs	131	HIS
49	Bt	73	GLN

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Mol	Chain	Res	Type
49	Bt	80	GLN
49	Bt	118	ASN
49	Bt	168	HIS
49	Bt	193	GLN
49	Bt	204	GLN
50	Bu	167	HIS
51	Bv	67	GLN
51	Bv	75	GLN
51	Bv	212	HIS
51	Bv	251	HIS
51	Bv	252	HIS
52	Bw	61	HIS
52	Bw	92	ASN
52	Bw	189	HIS
53	Bx	93	ASN
53	Bx	141	ASN
54	By	135	GLN
57	AB	110	ASN
57	AB	268	GLN
59	AD	166	GLN
60	AE	58	HIS
60	AE	92	ASN
61	AF	147	GLN
61	AF	151	ASN
63	AH	83	HIS
63	AH	109	HIS
63	AH	125	HIS
65	AJ	105	HIS
67	AL	118	ASN
67	AL	162	GLN
68	AM	50	GLN
68	AM	75	HIS
70	AO	169	GLN
73	AR	277	ASN
73	AR	288	GLN
75	AT	14	GLN
75	AT	33	ASN
75	AT	56	GLN
76	AU	109	ASN
76	AU	117	HIS
77	AV	122	GLN
77	AV	134	GLN

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Mol	Chain	Res	Type
77	AV	380	GLN
77	AV	396	GLN
79	AX	110	HIS
79	AX	180	GLN
79	AX	211	ASN
79	AX	326	GLN
80	AY	285	GLN
80	AY	316	ASN
81	AZ	56	HIS
81	AZ	76	GLN
81	AZ	82	GLN
82	Aa	107	ASN
82	Aa	124	GLN
82	Aa	261	GLN
82	Aa	314	HIS
82	Aa	341	GLN
82	Aa	368	GLN
83	Ab	134	HIS
83	Ab	265	GLN
83	Ab	276	GLN
85	Ad	155	GLN
85	Ad	415	GLN
86	Ae	257	HIS
86	Ae	306	ASN
86	Ae	453	HIS
86	Ae	504	ASN
86	Ae	540	HIS
86	Ae	562	GLN
86	Ae	603	ASN
86	Ae	626	GLN
87	Ag	77	GLN
87	Ag	135	GLN
87	Ag	261	GLN
87	Ag	384	GLN
88	Ai	129	GLN
89	Aj	108	ASN
89	Aj	111	HIS
89	Aj	207	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B7	2/3 (66%)	1 (50%)	0
3	B8	1556/1561 (99%)	236 (15%)	1 (0%)
4	B9	71/72 (98%)	11 (15%)	0
56	AA	954/955 (99%)	122 (12%)	1 (0%)
62	AG	70/71 (98%)	11 (15%)	0
64	AI	6/33 (18%)	2 (33%)	0
All	All	2659/2695 (98%)	383 (14%)	2 (0%)

All (383) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B7	76	A
3	B8	2	C
3	B8	11	G
3	B8	19	C
3	B8	22	A
3	B8	23	C
3	B8	29	C
3	B8	30	U
3	B8	34	U
3	B8	38	A
3	B8	39	G
3	B8	41	C
3	B8	54	A
3	B8	57	A
3	B8	58	U
3	B8	62	C
3	B8	65	A
3	B8	78	G
3	B8	95	C
3	B8	107	A
3	B8	135	A
3	B8	137	U
3	B8	138	A
3	B8	147	C
3	B8	151	A
3	B8	157	C
3	B8	158	A
3	B8	159	A
3	B8	162	A
3	B8	166	A
3	B8	174	A
3	B8	184	U

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Mol	Chain	Res	Type
3	B8	186	A
3	B8	199	A
3	B8	203	A
3	B8	212	A
3	B8	217	A
3	B8	223	A
3	B8	231	C
3	B8	233	C
3	B8	248	G
3	B8	267	A
3	B8	270	A
3	B8	304	A
3	B8	315	G
3	B8	322	C
3	B8	324	A
3	B8	330	C
3	B8	332	G
3	B8	333	A
3	B8	345	G
3	B8	352	G
3	B8	359	A
3	B8	360	U
3	B8	362	G
3	B8	366	C
3	B8	367	U
3	B8	369	A
3	B8	384	U
3	B8	390	A
3	B8	401	U
3	B8	409	C
3	B8	429	U
3	B8	443	G
3	B8	455	C
3	B8	456	U
3	B8	462	A
3	B8	477	G
3	B8	490	A
3	B8	493	A
3	B8	498	U
3	B8	511	A
3	B8	512	G
3	B8	522	A

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Mol	Chain	Res	Type
3	B8	528	A
3	B8	530	A
3	B8	544	A
3	B8	549	C
3	B8	550	A
3	B8	551	C
3	B8	553	A
3	B8	554	C
3	B8	555	C
3	B8	556	U
3	B8	558	A
3	B8	560	A
3	B8	563	U
3	B8	567	A
3	B8	571	A
3	B8	573	A
3	B8	575	A
3	B8	576	A
3	B8	592	C
3	B8	593	C
3	B8	614	C
3	B8	615	U
3	B8	627	A
3	B8	630	G
3	B8	652	C
3	B8	661	C
3	B8	662	C
3	B8	675	G
3	B8	679	G
3	B8	680	A
3	B8	683	A
3	B8	687	C
3	B8	693	A
3	B8	702	U
3	B8	704	A
3	B8	720	A
3	B8	729	A
3	B8	731	A
3	B8	734	U
3	B8	737	U
3	B8	745	C
3	B8	763	C

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Mol	Chain	Res	Type
3	B8	764	A
3	B8	776	A
3	B8	781	A
3	B8	782	A
3	B8	808	G
3	B8	814	C
3	B8	815	U
3	B8	823	C
3	B8	832	C
3	B8	850	C
3	B8	851	A
3	B8	857	A
3	B8	870	C
3	B8	900	C
3	B8	912	A
3	B8	922	G
3	B8	923	G
3	B8	924	U
3	B8	929	U
3	B8	930	A
3	B8	931	A
3	B8	933	C
3	B8	948	U
3	B8	956	U
3	B8	957	G
3	B8	958	U
3	B8	963	A
3	B8	965	G
3	B8	984	U
3	B8	986	U
3	B8	1013	C
3	B8	1016	G
3	B8	1024	A
3	B8	1026	A
3	B8	1036	A
3	B8	1048	C
3	B8	1049	G
3	B8	1053	A
3	B8	1054	G
3	B8	1055	A
3	B8	1056	C
3	B8	1062	G

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Mol	Chain	Res	Type
3	B8	1075	A
3	B8	1088	G
3	B8	1092	C
3	B8	1093	U
3	B8	1094	A
3	B8	1095	A
3	B8	1097	A
3	B8	1098	A
3	B8	1103	A
3	B8	1105	A
3	B8	1111	U
3	B8	1112	A
3	B8	1113	A
3	B8	1119	C
3	B8	1120	A
3	B8	1122	A
3	B8	1140	G
3	B8	1162	A
3	B8	1163	A
3	B8	1177	C
3	B8	1194	U
3	B8	1195	C
3	B8	1213	A
3	B8	1215	U
3	B8	1218	A
3	B8	1219	C
3	B8	1223	A
3	B8	1243	A
3	B8	1246	G
3	B8	1247	G
3	B8	1252	A
3	B8	1258	C
3	B8	1262	G
3	B8	1265	A
3	B8	1286	A
3	B8	1319	G
3	B8	1320	A
3	B8	1322	G
3	B8	1335	A
3	B8	1346	G
3	B8	1359	A
3	B8	1371	U

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Mol	Chain	Res	Type
3	B8	1383	A
3	B8	1384	G
3	B8	1389	A
3	B8	1390	C
3	B8	1400	G
3	B8	1403	C
3	B8	1416	U
3	B8	1419	A
3	B8	1426	U
3	B8	1430	U
3	B8	1432	U
3	B8	1438	U
3	B8	1439	U
3	B8	1440	C
3	B8	1441	A
3	B8	1443	A
3	B8	1480	U
3	B8	1487	C
3	B8	1488	A
3	B8	1492	C
3	B8	1499	C
3	B8	1502	C
3	B8	1507	A
3	B8	1519	C
3	B8	1520	A
3	B8	1529	U
3	B8	1530	U
3	B8	1536	C
3	B8	1538	C
3	B8	1540	C
3	B8	1542	C
3	B8	1547	A
3	B8	1548	A
3	B8	1558	U
3	B8	1559	U
3	B8	1560	G
3	B8	1561	U
4	B9	8	U
4	B9	16	C
4	B9	20	A
4	B9	43	G
4	B9	45	U

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Mol	Chain	Res	Type
4	B9	51	C
4	B9	52	U
4	B9	53	U
4	B9	54	A
4	B9	55	A
4	B9	57	U
56	AA	2	A
56	AA	4	A
56	AA	33	U
56	AA	41	A
56	AA	57	U
56	AA	74	U
56	AA	90	C
56	AA	91	A
56	AA	106	A
56	AA	114	A
56	AA	119	G
56	AA	144	G
56	AA	147	U
56	AA	149	G
56	AA	183	U
56	AA	185	U
56	AA	188	C
56	AA	189	A
56	AA	213	A
56	AA	214	U
56	AA	221	C
56	AA	224	A
56	AA	243	C
56	AA	254	G
56	AA	257	C
56	AA	260	A
56	AA	272	A
56	AA	276	A
56	AA	282	A
56	AA	285	C
56	AA	291	A
56	AA	292	A
56	AA	293	A
56	AA	294	G
56	AA	295	A
56	AA	300	U

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Mol	Chain	Res	Type
56	AA	313	C
56	AA	315	C
56	AA	320	A
56	AA	346	A
56	AA	355	C
56	AA	365	A
56	AA	368	A
56	AA	384	G
56	AA	395	U
56	AA	400	A
56	AA	401	C
56	AA	434	U
56	AA	435	A
56	AA	456	A
56	AA	458	C
56	AA	460	U
56	AA	462	A
56	AA	471	A
56	AA	472	U
56	AA	474	A
56	AA	479	A
56	AA	490	A
56	AA	504	C
56	AA	506	C
56	AA	513	A
56	AA	520	A
56	AA	540	U
56	AA	542	U
56	AA	543	C
56	AA	553	G
56	AA	568	U
56	AA	573	A
56	AA	576	C
56	AA	578	C
56	AA	582	U
56	AA	599	U
56	AA	600	G
56	AA	601	C
56	AA	604	A
56	AA	624	C
56	AA	637	U
56	AA	638	G

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Mol	Chain	Res	Type
56	AA	643	C
56	AA	644	U
56	AA	645	A
56	AA	650	G
56	AA	679	A
56	AA	680	G
56	AA	696	A
56	AA	697	U
56	AA	706	A
56	AA	709	A
56	AA	731	C
56	AA	740	A
56	AA	743	A
56	AA	744	U
56	AA	758	C
56	AA	759	U
56	AA	760	U
56	AA	783	A
56	AA	816	G
56	AA	819	C
56	AA	831	A
56	AA	834	C
56	AA	872	A
56	AA	878	C
56	AA	879	U
56	AA	880	A
56	AA	886	C
56	AA	890	C
56	AA	891	G
56	AA	892	C
56	AA	893	A
56	AA	897	A
56	AA	904	G
56	AA	911	A
56	AA	912	G
56	AA	915	G
56	AA	920	A
56	AA	921	U
56	AA	924	U
56	AA	935	G
56	AA	937	MA6
56	AA	947	G

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Mol	Chain	Res	Type
56	AA	948	G
56	AA	952	A
62	AG	6	G
62	AG	7	G
62	AG	8	U
62	AG	10	A
62	AG	11	G
62	AG	17	U
62	AG	18	A
62	AG	45	G
62	AG	52	A
62	AG	53	U
62	AG	55	C
64	AI	2	G
64	AI	4	Y5P

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	B8	575	A
56	AA	400	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMU	B8	1369	3,90	19,22,23	1.21	3 (15%)	25,31,34	1.79	5 (20%)
4	2MG	B9	10	4	23,26,27	0.45	0	33,38,41	0.52	0
64	Y5P	AI	4	64	14,19,20	2.24	1 (7%)	18,26,29	0.50	0
88	5F0	Ai	184	88	8,8,9	1.44	2 (25%)	8,9,11	1.60	1 (12%)
3	OMG	B8	1370	3	23,26,27	1.17	3 (13%)	32,38,41	1.93	6 (18%)
4	PSU	B9	37	4	18,21,22	1.36	2 (11%)	21,30,33	1.97	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	PSU	AG	51	62	18,21,22	1.38	2 (11%)	21,30,33	1.94	3 (14%)
4	1MA	B9	9	4	21,25,26	0.47	0	30,37,40	0.77	1 (3%)
84	AYA	Ac	2	84	6,7,8	0.76	0	6,8,10	0.64	0
72	AYA	AQ	2	72	6,7,8	0.78	0	6,8,10	0.61	0
3	OMG	B8	1145	3,90,62	23,26,27	1.17	3 (13%)	32,38,41	1.92	6 (18%)
56	5MC	AA	841	56	19,22,23	1.56	3 (15%)	26,32,35	1.09	2 (7%)
56	MA6	AA	936	56	23,26,27	2.36	5 (21%)	33,38,41	3.77	13 (39%)
56	5MU	AA	429	56	19,22,23	1.38	6 (31%)	27,32,35	2.06	6 (22%)
3	PSU	B8	1397	3	18,21,22	1.40	2 (11%)	21,30,33	2.00	3 (14%)
62	RSQ	AG	31	64,62	19,23,24	0.36	0	25,33,36	0.46	0
3	1MA	B8	947	3	21,25,26	0.43	0	30,37,40	0.73	1 (3%)
6	AYA	BB	2	6	6,7,8	0.81	0	6,8,10	0.62	0
62	PSU	AG	46	62	18,21,22	1.38	2 (11%)	21,30,33	1.96	3 (14%)
22	SAC	BR	2	22	7,8,9	0.57	0	7,9,11	1.03	1 (14%)
32	AYA	Bb	2	32	6,7,8	0.69	0	6,8,10	0.70	0
56	B8T	AA	839	90,56	19,22,23	0.37	0	25,31,34	0.35	0
56	MA6	AA	937	56	23,26,27	2.37	5 (21%)	33,38,41	3.78	13 (39%)
62	PSU	AG	24	62	18,21,22	1.35	2 (11%)	21,30,33	2.06	4 (19%)

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
3	OMU	B8	1369	3,90	-	0/9/27/28	0/2/2/2
4	2MG	B9	10	4	-	0/9/27/28	0/3/3/3
64	Y5P	AI	4	64	-	5/7/33/34	0/2/2/2
88	5F0	Ai	184	88	-	4/9/9/10	-
3	OMG	B8	1370	3	-	0/9/27/28	0/3/3/3
4	PSU	B9	37	4	-	0/7/25/26	0/2/2/2
62	PSU	AG	51	62	-	3/7/25/26	0/2/2/2
4	1MA	B9	9	4	-	0/7/25/26	0/3/3/3
84	AYA	Ac	2	84	-	2/5/6/8	-
72	AYA	AQ	2	72	-	0/5/6/8	-
3	OMG	B8	1145	3,90,62	-	0/9/27/28	0/3/3/3
56	5MC	AA	841	56	-	0/7/25/26	0/2/2/2
56	MA6	AA	936	56	-	0/11/29/30	0/3/3/3
56	5MU	AA	429	56	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	B8	1397	3	-	0/7/25/26	0/2/2/2
62	RSQ	AG	31	64,62	-	1/9/27/28	0/2/2/2
3	1MA	B8	947	3	-	0/7/25/26	0/3/3/3
6	AYA	BB	2	6	-	1/5/6/8	-
62	PSU	AG	46	62	-	0/7/25/26	0/2/2/2
22	SAC	BR	2	22	-	0/7/8/10	-
32	AYA	Bb	2	32	-	3/5/6/8	-
56	B8T	AA	839	90,56	-	0/7/27/28	0/2/2/2
56	MA6	AA	937	56	-	2/11/29/30	0/3/3/3
62	PSU	AG	24	62	-	0/7/25/26	0/2/2/2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	AI	4	Y5P	C2-N3	8.27	1.33	1.27
56	AA	936	MA6	C5-N7	6.97	1.51	1.39
56	AA	937	MA6	C5-N7	6.96	1.51	1.39
56	AA	937	MA6	C8-N9	-5.80	1.27	1.37
56	AA	936	MA6	C8-N9	-5.75	1.27	1.37
56	AA	841	5MC	C5-C4	5.57	1.48	1.44
56	AA	937	MA6	C4-N9	-4.00	1.29	1.37
56	AA	936	MA6	C4-N9	-3.95	1.29	1.37
62	AG	51	PSU	C6-C5	3.50	1.39	1.35
62	AG	46	PSU	C6-C5	3.49	1.39	1.35
56	AA	936	MA6	C5-C4	3.39	1.45	1.39
4	B9	37	PSU	C6-C5	3.36	1.39	1.35
56	AA	937	MA6	C5-C4	3.32	1.45	1.39
56	AA	937	MA6	C6-N6	3.30	1.45	1.36
3	B8	1397	PSU	C6-C5	3.29	1.38	1.35
62	AG	24	PSU	C6-C5	3.27	1.38	1.35
56	AA	936	MA6	C6-N6	3.26	1.45	1.36
3	B8	1370	OMG	C5-C4	3.09	1.47	1.38
3	B8	1145	OMG	C5-C4	3.01	1.47	1.38
88	Ai	184	5F0	OD1-C1	2.84	1.40	1.33
3	B8	1397	PSU	C4-N3	-2.73	1.33	1.38
56	AA	429	5MU	C4-N3	-2.64	1.33	1.38
56	AA	429	5MU	C6-C5	2.64	1.38	1.34
3	B8	1369	OMU	C4-N3	-2.64	1.34	1.38
62	AG	24	PSU	C4-N3	-2.64	1.33	1.38
4	B9	37	PSU	C4-N3	-2.62	1.33	1.38
56	AA	841	5MC	C6-C5	2.62	1.38	1.34
62	AG	46	PSU	C4-N3	-2.59	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B8	1145	OMG	C6-N1	-2.53	1.34	1.38
62	AG	51	PSU	C4-N3	-2.48	1.34	1.38
3	B8	1370	OMG	C6-N1	-2.42	1.34	1.38
56	AA	429	5MU	C6-N1	-2.26	1.34	1.38
56	AA	429	5MU	C4-C5	2.25	1.48	1.44
3	B8	1369	OMU	C2-N3	-2.24	1.34	1.38
88	Ai	184	5F0	OD1-CXT	-2.22	1.40	1.45
56	AA	841	5MC	C6-N1	-2.20	1.34	1.38
3	B8	1145	OMG	C5-N7	-2.13	1.34	1.39
56	AA	429	5MU	C2-N1	2.09	1.41	1.38
56	AA	429	5MU	C2-N3	-2.08	1.34	1.38
3	B8	1370	OMG	C5-N7	-2.07	1.34	1.39
3	B8	1369	OMU	C5-C4	-2.03	1.39	1.43

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	AA	937	MA6	C4-N9-C8	15.14	121.63	105.74
56	AA	936	MA6	C4-N9-C8	14.95	121.43	105.74
62	AG	24	PSU	N1-C2-N3	6.41	121.93	115.17
56	AA	936	MA6	N3-C4-N9	6.37	138.00	127.17
56	AA	936	MA6	C4-C5-N7	-6.34	103.34	110.58
56	AA	937	MA6	N3-C4-N9	6.34	137.94	127.17
3	B8	1397	PSU	N1-C2-N3	6.34	121.85	115.17
56	AA	937	MA6	C4-C5-N7	-6.27	103.42	110.58
62	AG	46	PSU	N1-C2-N3	6.15	121.66	115.17
4	B9	37	PSU	N1-C2-N3	6.13	121.63	115.17
62	AG	51	PSU	N1-C2-N3	6.05	121.55	115.17
3	B8	1145	OMG	C5-C4-N3	-5.94	118.94	128.39
3	B8	1370	OMG	C5-C4-N3	-5.94	118.94	128.39
56	AA	937	MA6	N9-C8-N7	-5.74	105.79	113.94
56	AA	936	MA6	N9-C8-N7	-5.68	105.88	113.94
56	AA	936	MA6	C5-C4-N3	-5.40	119.28	126.72
56	AA	937	MA6	C5-C4-N3	-5.23	119.52	126.72
56	AA	429	5MU	C4-N3-C2	-5.03	120.75	127.34
56	AA	429	5MU	N3-C2-N1	4.95	121.34	114.89
3	B8	1370	OMG	C2-N3-C4	4.86	120.67	112.30
3	B8	1145	OMG	C2-N3-C4	4.80	120.57	112.30
3	B8	1369	OMU	C4-N3-C2	-4.70	120.78	126.61
3	B8	1370	OMG	N9-C4-N3	4.47	134.90	125.95
3	B8	1145	OMG	N9-C4-N3	4.43	134.82	125.95
56	AA	429	5MU	C5-C4-N3	4.28	119.05	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	AA	936	MA6	N1-C2-N3	-4.28	122.11	128.58
3	B8	1369	OMU	N3-C2-N1	4.22	120.38	114.89
62	AG	24	PSU	C4-N3-C2	-4.18	120.62	126.37
56	AA	937	MA6	N1-C2-N3	-4.17	122.27	128.58
56	AA	429	5MU	O4-C4-C5	-4.06	120.27	124.92
4	B9	37	PSU	C4-N3-C2	-3.99	120.88	126.37
56	AA	936	MA6	C2-N1-C6	3.98	121.56	111.83
56	AA	937	MA6	C2-N1-C6	3.97	121.52	111.83
3	B8	1397	PSU	C4-N3-C2	-3.94	120.94	126.37
62	AG	46	PSU	C4-N3-C2	-3.91	120.98	126.37
3	B8	1369	OMU	C5-C4-N3	3.80	120.12	114.80
62	AG	51	PSU	C4-N3-C2	-3.74	121.21	126.37
62	AG	24	PSU	O2-C2-N1	-3.63	119.04	122.79
3	B8	1397	PSU	O2-C2-N1	-3.57	119.10	122.79
56	AA	936	MA6	C6-C5-N7	3.56	139.12	133.43
56	AA	937	MA6	C6-C5-N7	3.55	139.10	133.43
62	AG	51	PSU	O2-C2-N1	-3.50	119.18	122.79
56	AA	936	MA6	C4-N9-C1'	-3.47	118.51	126.63
56	AA	937	MA6	C1'-N9-C8	-3.46	119.42	127.09
56	AA	429	5MU	C5-C6-N1	-3.45	119.57	123.31
4	B9	37	PSU	O2-C2-N1	-3.42	119.26	122.79
62	AG	46	PSU	O2-C2-N1	-3.39	119.30	122.79
88	Ai	184	5F0	OD1-C1-CA	3.36	120.04	111.50
56	AA	937	MA6	C4-N9-C1'	-3.28	118.95	126.63
56	AA	936	MA6	C2-N3-C4	3.26	119.80	111.83
56	AA	841	5MC	C5-C6-N1	-3.20	119.84	123.31
56	AA	937	MA6	C2-N3-C4	3.17	119.58	111.83
56	AA	936	MA6	C1'-N9-C8	-3.17	120.06	127.09
3	B8	1370	OMG	C6-C5-N7	3.10	135.93	130.29
3	B8	1145	OMG	C6-C5-N7	3.02	135.79	130.29
56	AA	937	MA6	C5-C4-N9	-3.00	102.54	105.81
3	B8	1369	OMU	O4-C4-C5	-2.97	120.04	125.16
56	AA	936	MA6	C5-C4-N9	-2.84	102.72	105.81
56	AA	841	5MC	C5-C4-N3	-2.81	118.87	121.75
22	BR	2	SAC	O-C-CA	-2.59	118.11	124.77
3	B8	1370	OMG	C4-C5-N7	-2.47	106.75	110.67
3	B8	1145	OMG	C4-C5-N7	-2.43	106.81	110.67
56	AA	429	5MU	O2-C2-N1	-2.43	119.64	122.80
3	B8	1369	OMU	O2-C2-N1	-2.30	119.81	122.80
4	B9	9	1MA	N1-C6-N6	2.23	125.31	119.71
62	AG	24	PSU	C5-C6-N1	-2.20	119.09	122.14
3	B8	947	1MA	N1-C6-N6	2.17	125.16	119.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B8	1145	OMG	O6-C6-C5	-2.13	120.91	126.53
3	B8	1370	OMG	O6-C6-C5	-2.12	120.92	126.53
56	AA	936	MA6	C5-N7-C8	2.03	106.64	103.45
56	AA	937	MA6	C5-N7-C8	2.02	106.62	103.45

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	AG	51	PSU	O4'-C1'-C5-C4
62	AG	51	PSU	O4'-C1'-C5-C6
32	Bb	2	AYA	OT-CT-N-CA
32	Bb	2	AYA	CM-CT-N-CA
88	Ai	184	5F0	CA-C1-OD1-CXT
88	Ai	184	5F0	O1-C1-OD1-CXT
88	Ai	184	5F0	O1-C1-CA-CB
6	BB	2	AYA	C-CA-N-CT
32	Bb	2	AYA	C-CA-N-CT
88	Ai	184	5F0	OD1-C1-CA-CB
64	AI	4	Y5P	C2'-C1'-N1-C6
64	AI	4	Y5P	C2'-C1'-N1-C2
56	AA	937	MA6	C3'-C4'-C5'-O5'
84	Ac	2	AYA	CM-CT-N-CA
64	AI	4	Y5P	O4'-C1'-N1-C2
64	AI	4	Y5P	O4'-C1'-N1-C6
56	AA	937	MA6	C4'-C5'-O5'-P
84	Ac	2	AYA	OT-CT-N-CA
64	AI	4	Y5P	O4'-C4'-C5'-O5'
62	AG	51	PSU	C2'-C1'-C5-C6
62	AG	31	RSQ	C2'-C1'-N1-C2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	AG	51	PSU	2	0
72	AQ	2	AYA	1	0
56	AA	936	MA6	1	0
62	AG	31	RSQ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 415 ligands modelled in this entry, 408 are monoatomic - leaving 7 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	$\# Z > 2$
94	FS2	AT	201	68,75	0,5,14	-	-	-		
97	GDP	AX	503	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
94	FS2	AP	201	60,71	0,5,14	-	-	-		
94	FS2	Bh	201	20,38	0,5,14	-	-	-		
92	VAL	B9	101	4	4,6,7	0.54	0	6,7,9	0.87	0
95	MET	AG	101	62	6,7,8	0.47	0	2,7,9	0.14	0
96	ATP	AX	501	91	32,33,33	0.29	0	48,52,52	0.30	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
94	FS2	AT	201	68,75	-	-	0/2/2/6
97	GDP	AX	503	-	-	4/16/32/32	0/3/3/3
94	FS2	AP	201	60,71	-	-	0/2/2/6
94	FS2	Bh	201	20,38	-	-	0/2/2/6
92	VAL	B9	101	4	-	3/5/6/8	-
95	MET	AG	101	62	-	1/5/6/8	-
96	ATP	AX	501	91	-	1/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	AX	503	GDP	C5-C4	3.16	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	AX	503	GDP	C6-N1	-2.44	1.34	1.38
97	AX	503	GDP	C5-N7	-2.04	1.35	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	AX	503	GDP	C5-C4-N3	-6.19	118.53	128.39
97	AX	503	GDP	C2-N3-C4	5.01	120.93	112.30
97	AX	503	GDP	N9-C4-N3	4.60	135.14	125.95
97	AX	503	GDP	C6-C5-N7	3.14	136.01	130.29
97	AX	503	GDP	C4-C5-N7	-2.57	106.60	110.67
97	AX	503	GDP	C3'-C2'-C1'	2.21	105.64	101.46
97	AX	503	GDP	O6-C6-C5	-2.10	120.99	126.53

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	B9	101	VAL	N-CA-CB-CG2
92	B9	101	VAL	C-CA-CB-CG1
92	B9	101	VAL	C-CA-CB-CG2
95	AG	101	MET	O-C-CA-CB
97	AX	503	GDP	C5'-O5'-PA-O3A
97	AX	503	GDP	C5'-O5'-PA-O2A
97	AX	503	GDP	C3'-C4'-C5'-O5'
96	AX	501	ATP	PA-O3A-PB-O2B
97	AX	503	GDP	O4'-C4'-C5'-O5'

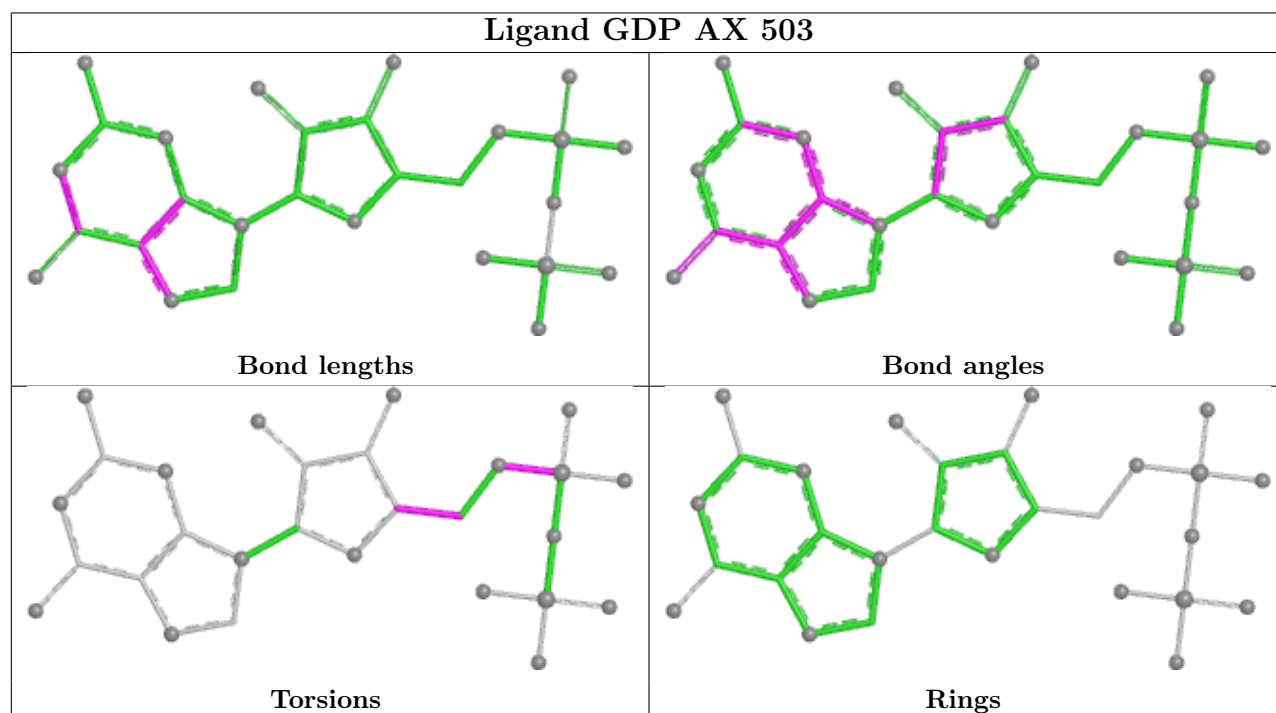
There are no ring outliers.

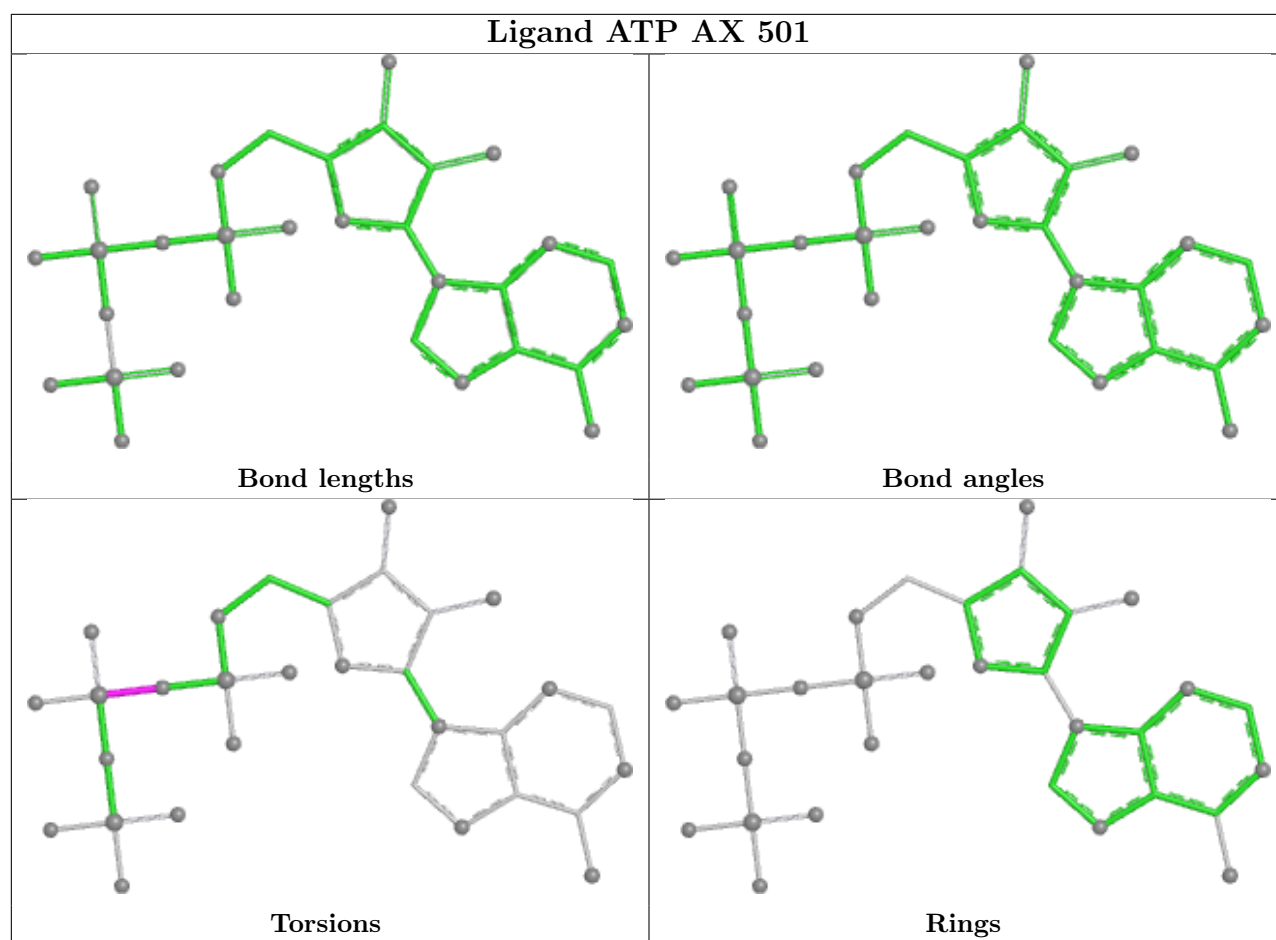
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
97	AX	503	GDP	2	0
94	Bh	201	FS2	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

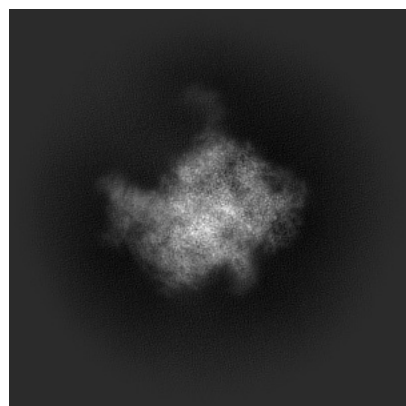
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16897. These allow visual inspection of the internal detail of the map and identification of artifacts.

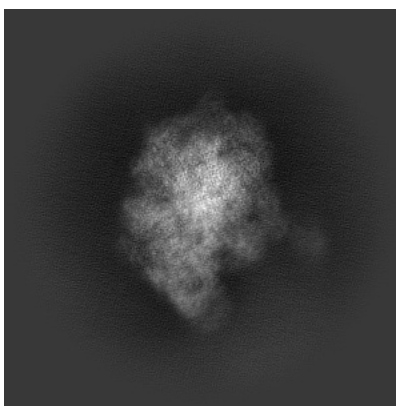
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

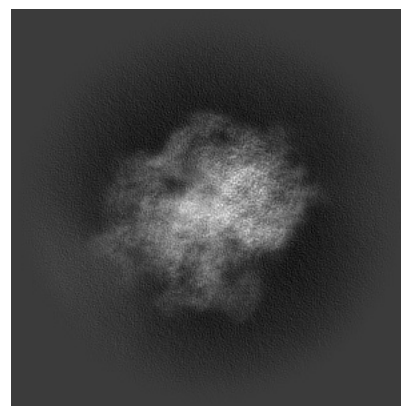
6.1.1 Primary map



X

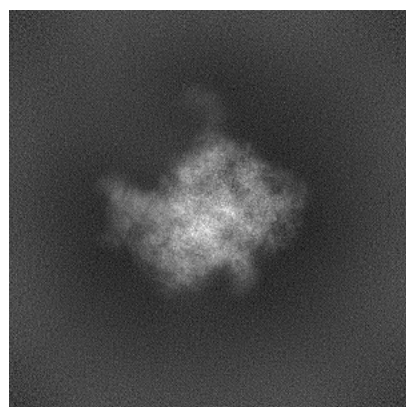


Y

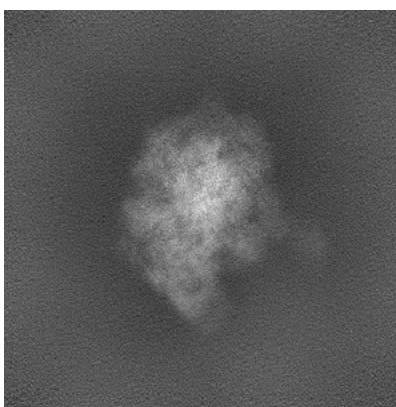


Z

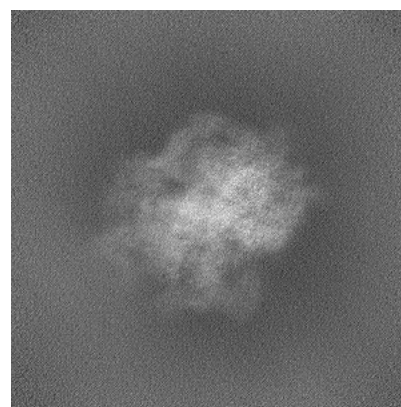
6.1.2 Raw map



X



Y

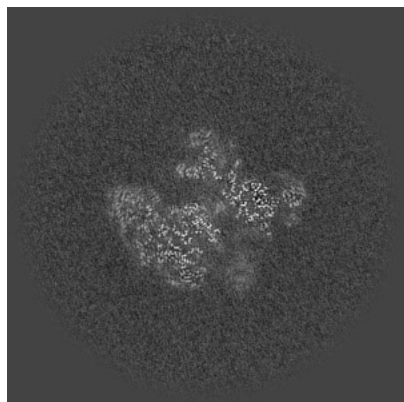


Z

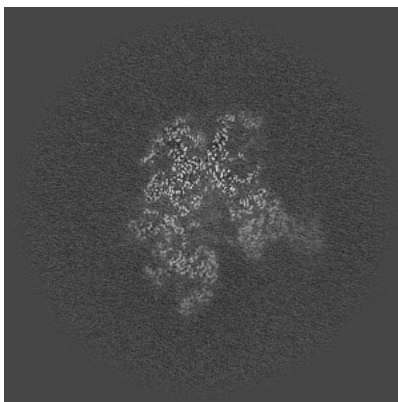
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

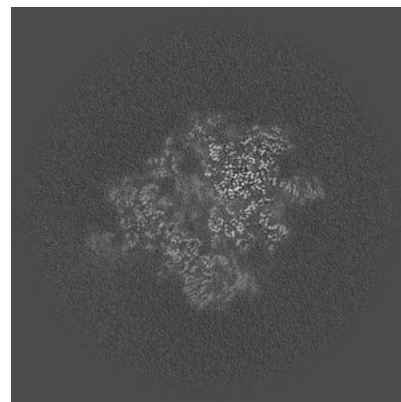
6.2.1 Primary map



X Index: 256

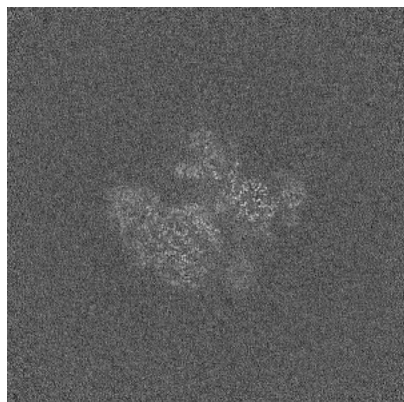


Y Index: 256

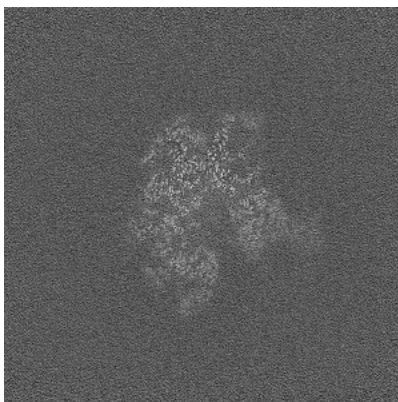


Z Index: 256

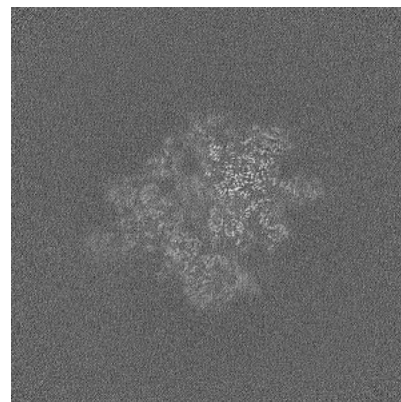
6.2.2 Raw map



X Index: 256



Y Index: 256

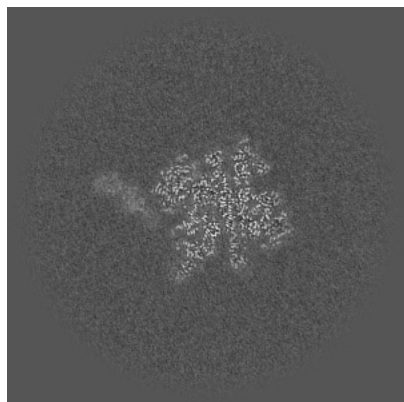


Z Index: 256

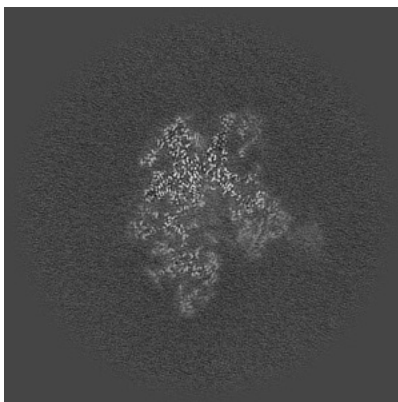
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

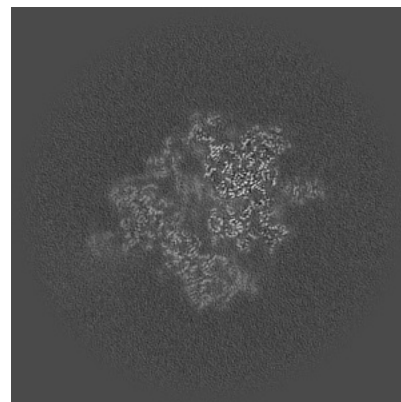
6.3.1 Primary map



X Index: 297

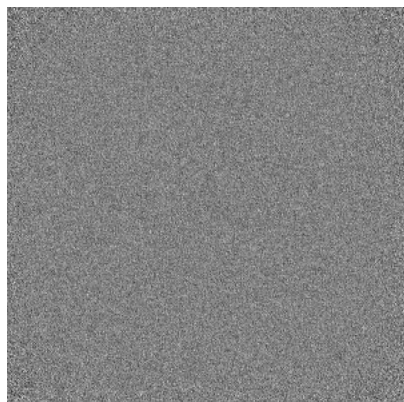


Y Index: 254

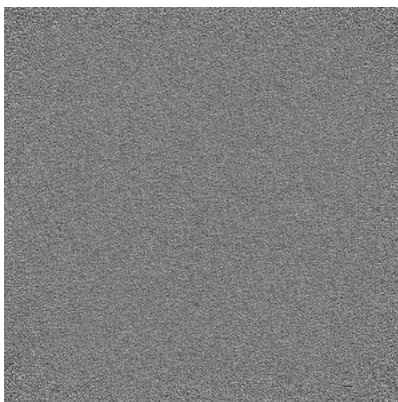


Z Index: 257

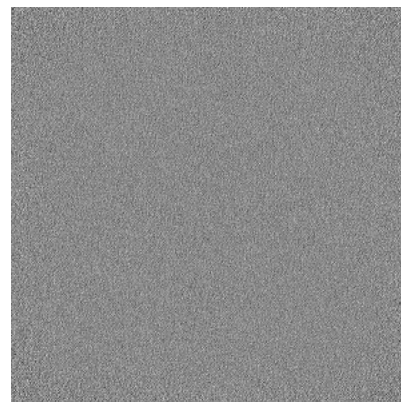
6.3.2 Raw map



X Index: 0



Y Index: 0

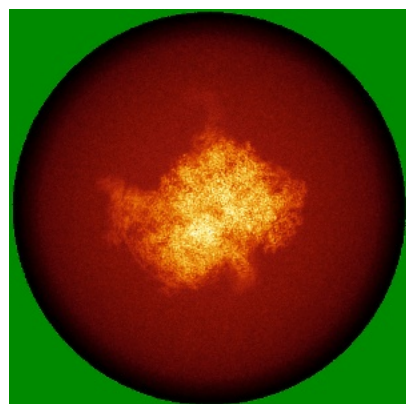


Z Index: 0

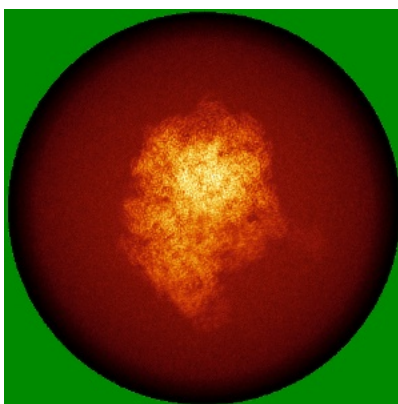
The images above show the largest variance slices of the map in three orthogonal directions.

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

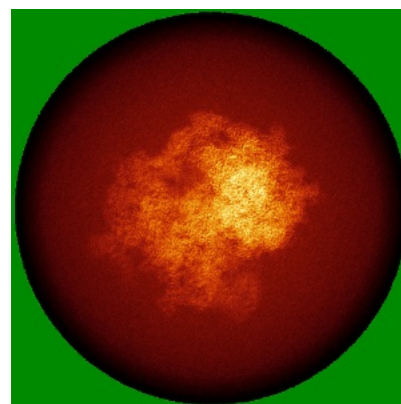
6.4.1 Primary map



X

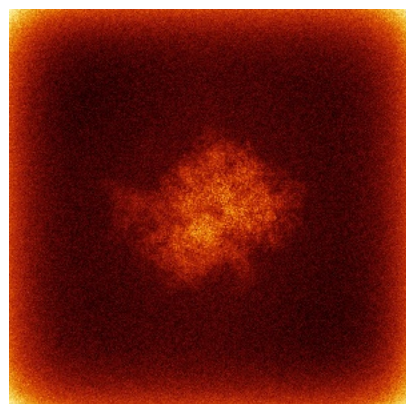


Y

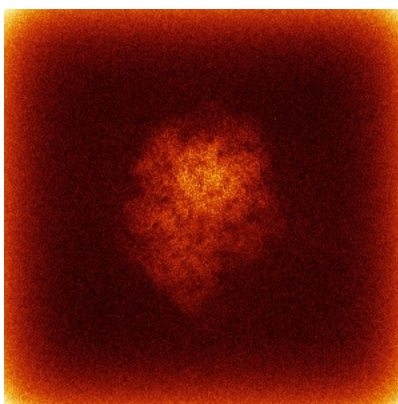


Z

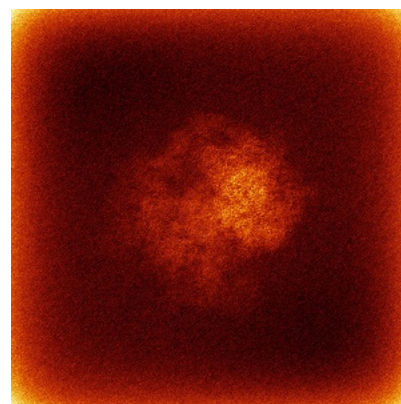
6.4.2 Raw map



X



Y

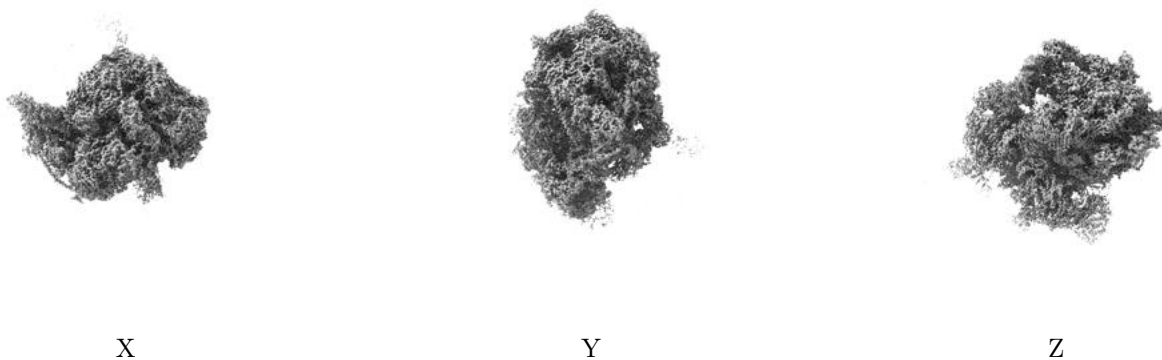


Z

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.

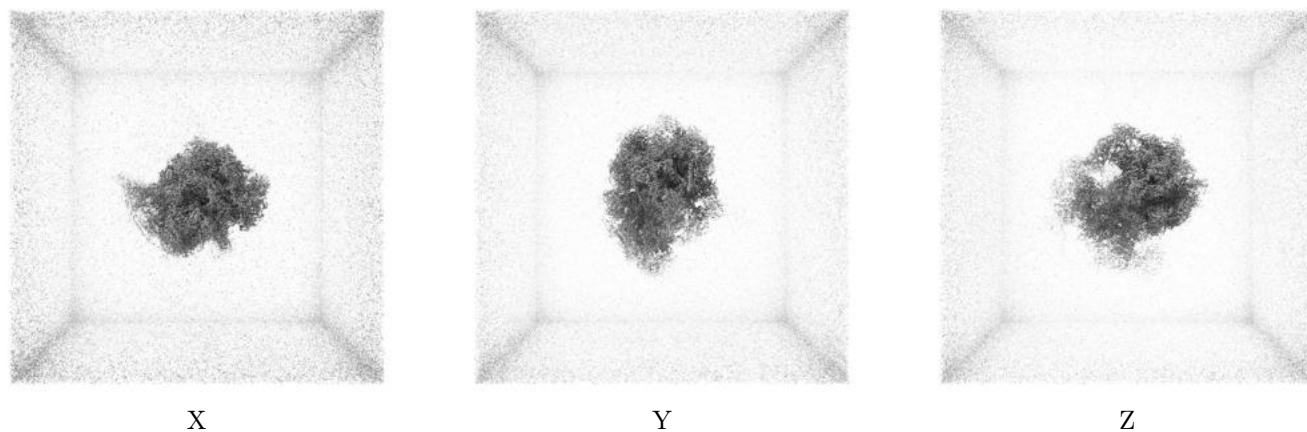
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. 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.

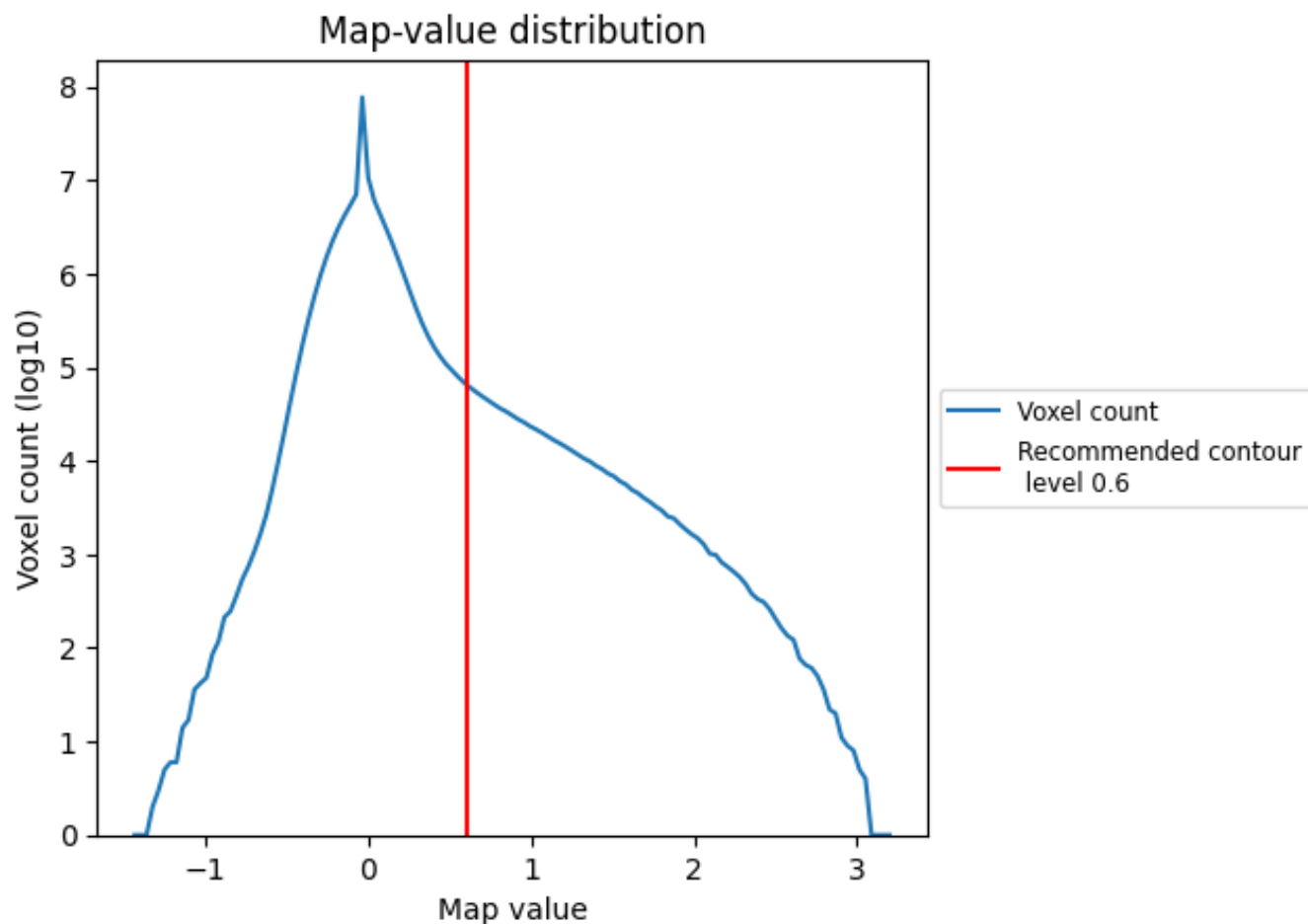
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

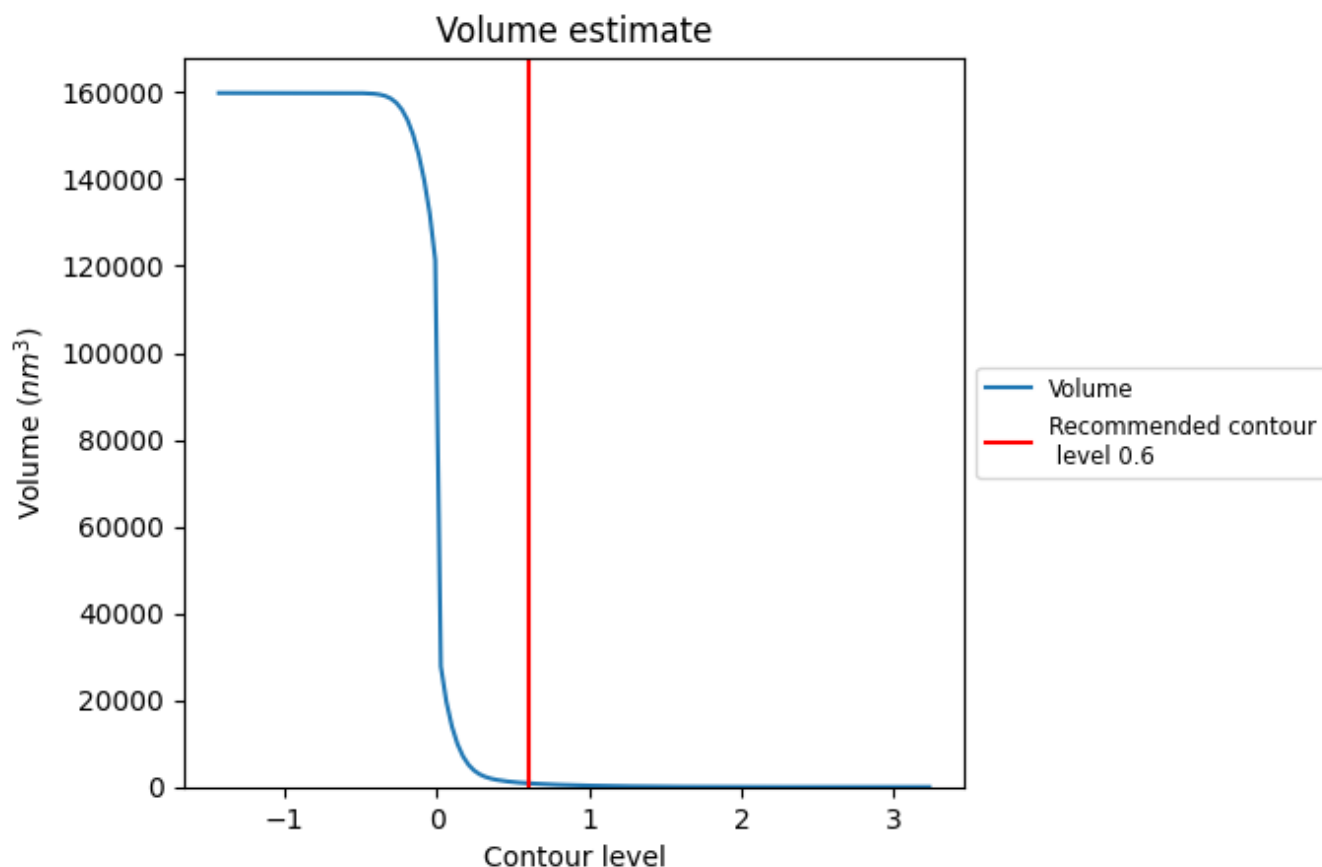
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

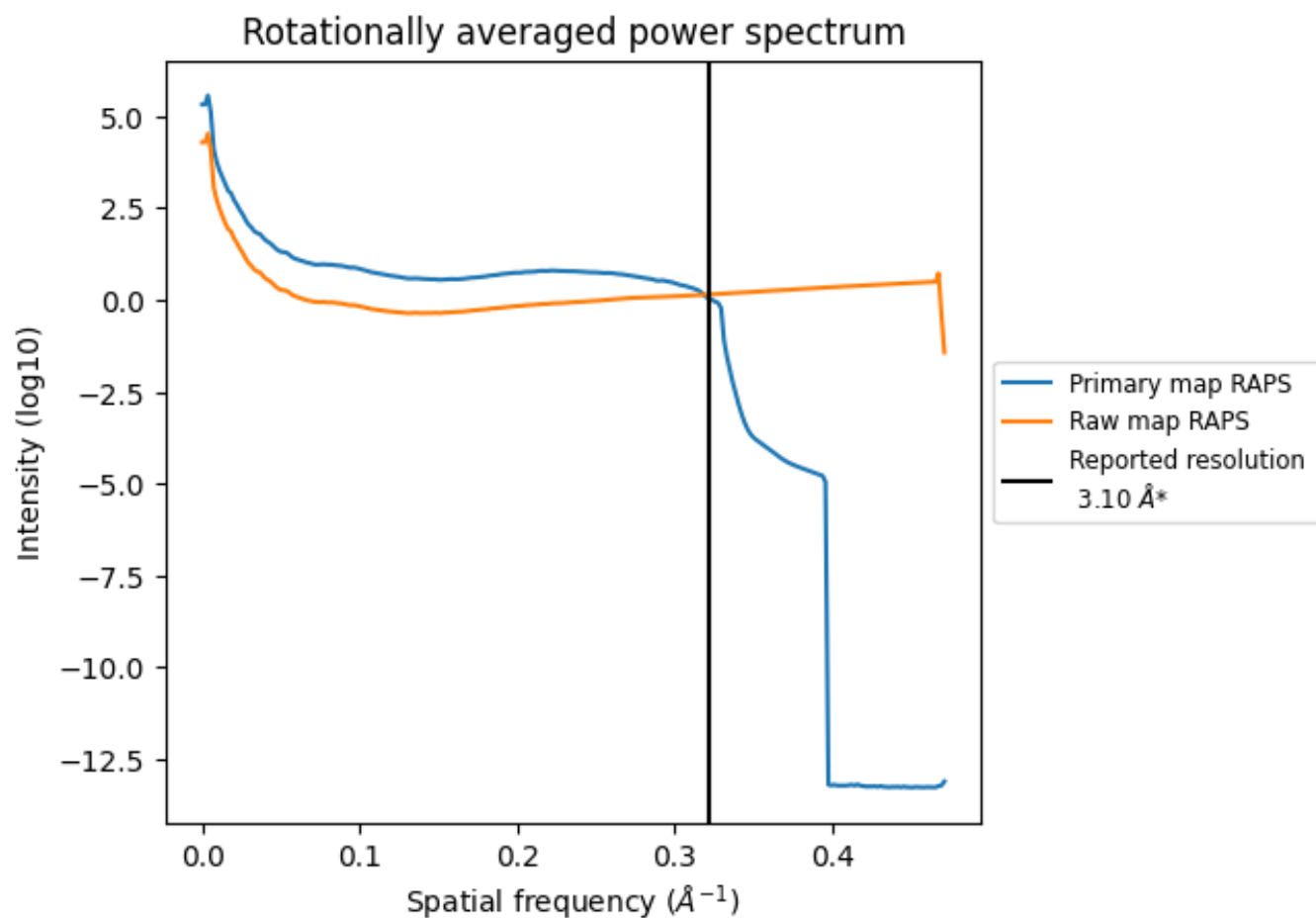
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 850 nm³; this corresponds to an approximate mass of 768 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 ⓘ

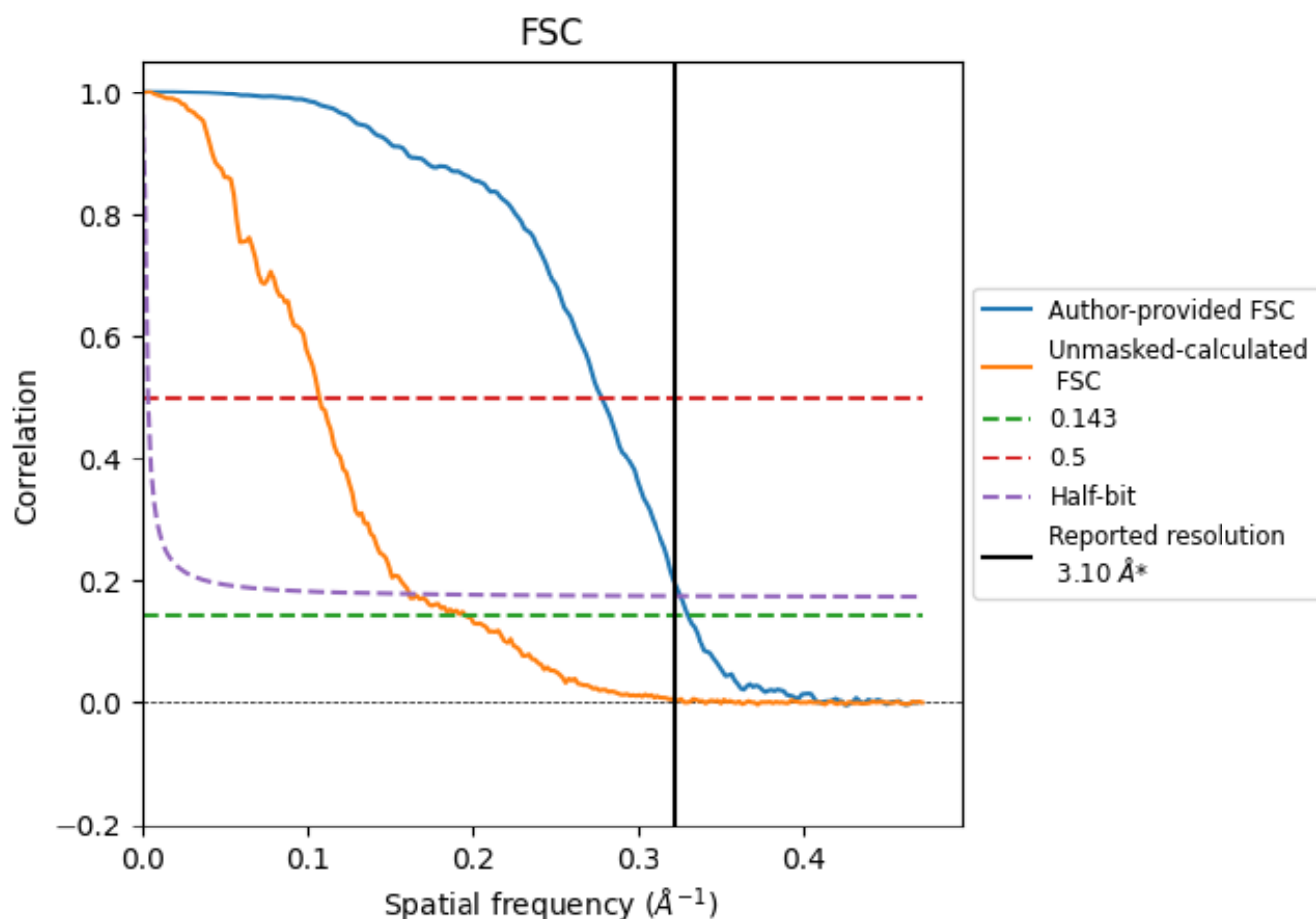


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

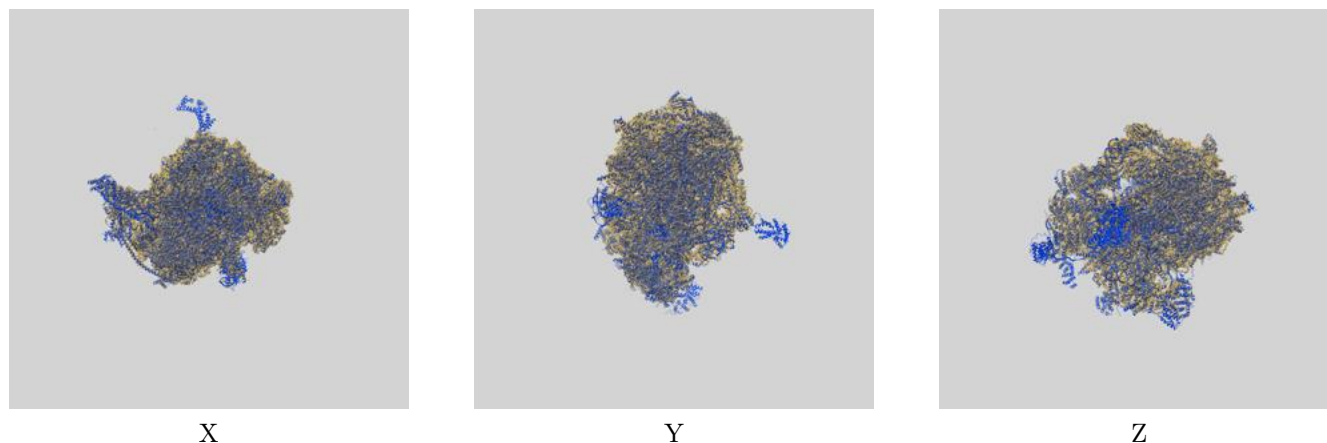
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.03	3.60	3.07
Unmasked-calculated*	5.12	9.33	6.20

*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 5.12 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

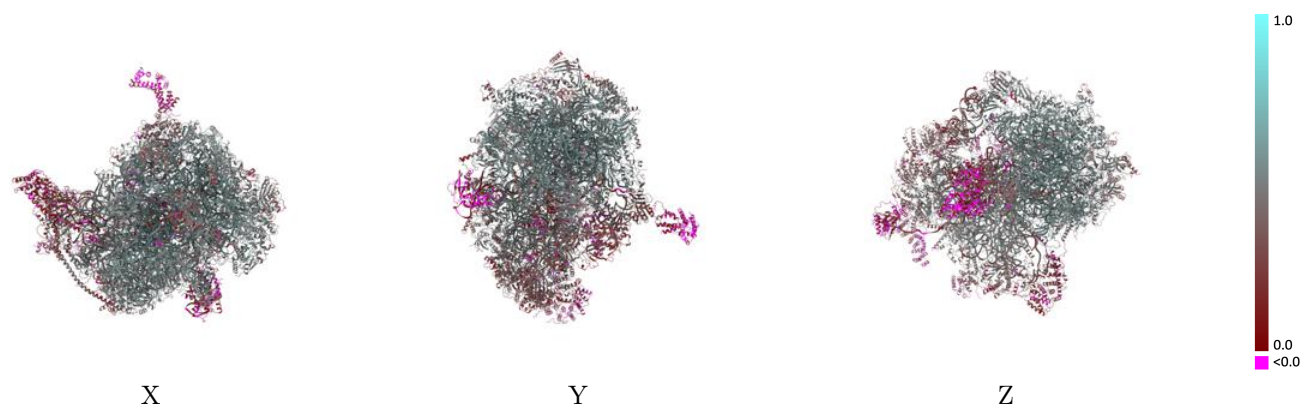
This section contains information regarding the fit between EMDB map EMD-16897 and PDB model 8OIR. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



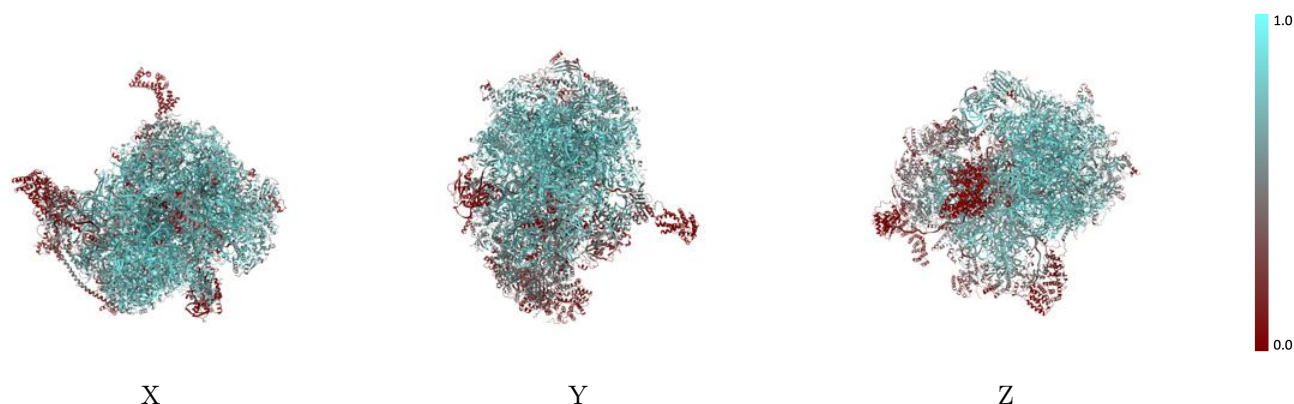
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



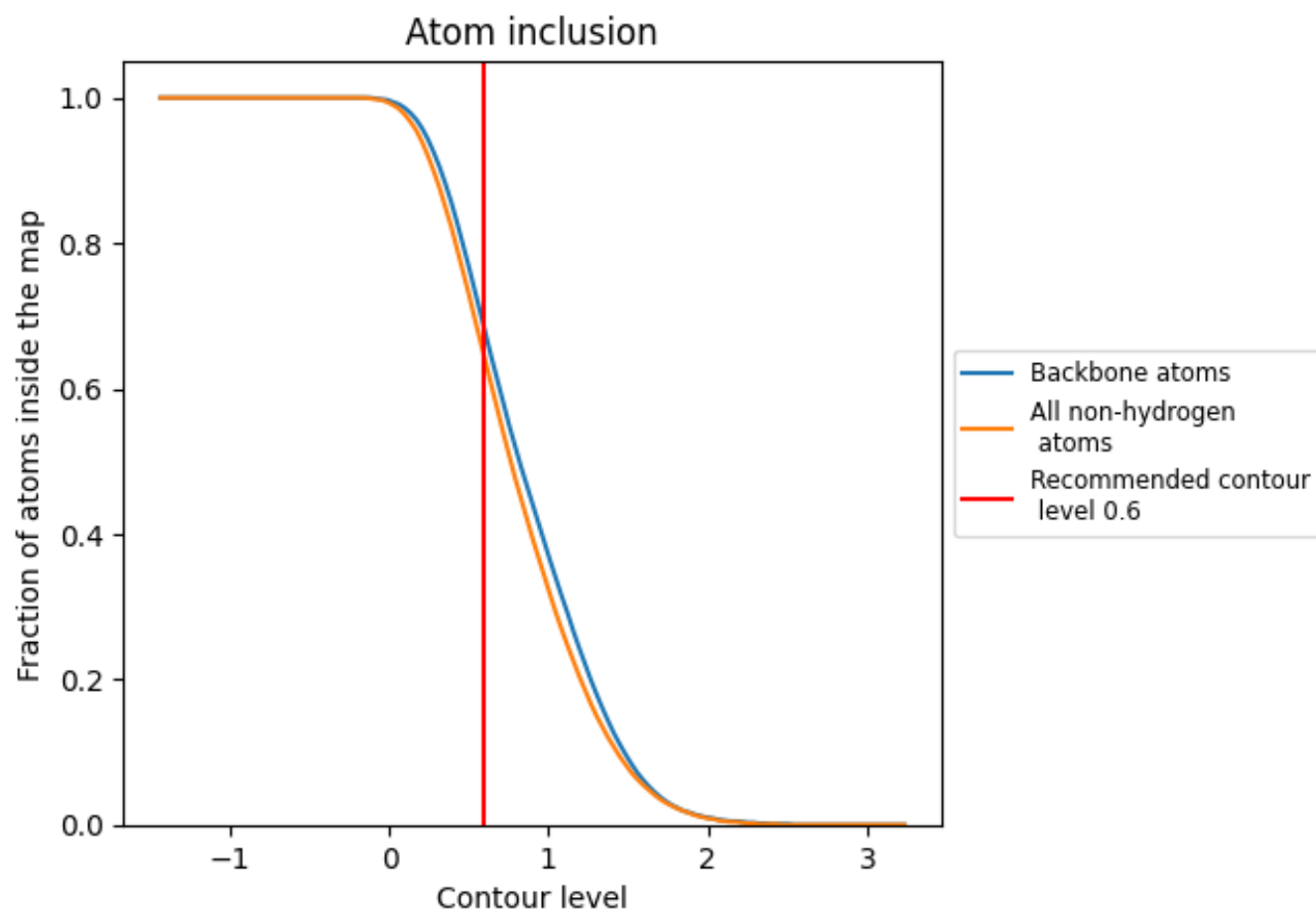
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6420	 0.4340
AA	 0.8150	 0.4790
AB	 0.3570	 0.3290
AC	 0.5900	 0.4550
AD	 0.7380	 0.4870
AE	 0.6540	 0.4620
AF	 0.5200	 0.3960
AG	 0.5960	 0.3520
AH	 0.4660	 0.3820
AI	 0.2980	 0.2680
AJ	 0.6150	 0.4720
AK	 0.6460	 0.4420
AL	 0.5800	 0.4160
AM	 0.4750	 0.3660
AN	 0.6290	 0.4660
AO	 0.4210	 0.3620
AP	 0.6890	 0.4560
AQ	 0.7250	 0.4960
AR	 0.2830	 0.3010
AS	 0.4320	 0.3820
AT	 0.5770	 0.4360
AU	 0.4320	 0.3210
AV	 0.1230	 0.1670
AW	 0.5510	 0.4450
AX	 0.4170	 0.3270
AY	 0.2770	 0.2700
AZ	 0.4770	 0.3850
Aa	 0.1040	 0.1450
Ab	 0.6440	 0.4560
Ac	 0.5410	 0.4080
Ad	 0.5540	 0.4430
Ae	 0.0870	 0.1490
Ag	 0.4860	 0.3980
Ai	 0.6660	 0.4600
Aj	 0.3440	 0.2900



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Chain	Atom inclusion	Q-score
B1	0.0250	0.0860
B2	0.0120	0.0790
B3	0.0000	0.0200
B4	0.0000	-0.0130
B5	0.0000	-0.0520
B6	0.0000	-0.0490
B7	0.1940	0.3470
B8	0.8840	0.5250
B9	0.6940	0.3640
BA	0.7960	0.5460
BB	0.6990	0.4820
BC	0.5560	0.4450
BD	0.8260	0.5500
BE	0.7320	0.5060
BF	0.7670	0.5230
BG	0.7950	0.5420
BH	0.7290	0.5250
BI	0.6870	0.4900
BJ	0.8970	0.5870
BK	0.8660	0.5720
BL	0.8430	0.5530
BM	0.7980	0.5260
BN	0.7950	0.5390
BO	0.3140	0.2410
BP	0.3560	0.2890
BQ	0.2080	0.2080
BR	0.8320	0.5450
BS	0.7970	0.5290
BT	0.7920	0.5350
BU	0.7690	0.5050
BV	0.7910	0.5360
BW	0.7820	0.5100
BX	0.7020	0.4810
BY	0.8200	0.5480
BZ	0.7750	0.5280
Ba	0.6910	0.4730
Bb	0.4760	0.3690
Bc	0.3090	0.2860
Bd	0.3770	0.2790
Be	0.8470	0.5590
Bf	0.5530	0.4140
Bg	0.4910	0.3460

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Chain	Atom inclusion	Q-score
Bh	 0.7670	 0.5090
Bi	 0.7620	 0.5130
Bj	 0.0160	 0.0330
Bl	 0.8440	 0.5380
Bm	 0.7600	 0.5120
Bn	 0.7000	 0.4620
Bo	 0.6140	 0.4520
Bp	 0.3970	 0.3110
Bq	 0.6910	 0.4910
Br	 0.6560	 0.4670
Bs	 0.7900	 0.5450
Bt	 0.6770	 0.4880
Bu	 0.5010	 0.4150
Bv	 0.3390	 0.2660
Bw	 0.4740	 0.3670
Bx	 0.7450	 0.5160
By	 0.5060	 0.4300
Bz	 0.8460	 0.5650