



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 07:39 AM UTC

PDB ID : 8OIN / pdb_00008oin
EMDB ID : EMD-16894
Title : 55S mammalian 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 : 3.60 Å(reported)
Based on initial models : ., 7NQH, 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:

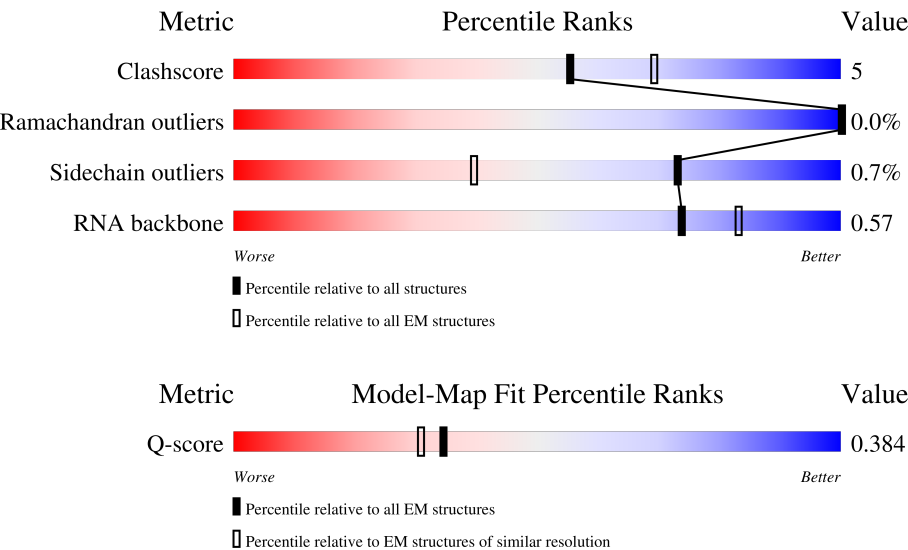
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	23% 22% 77%
1	B2	198	14% 11% 86%
1	B3	198	14% 12% 86%

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Mol	Chain	Length	Quality of chain
1	B4	198	
1	B5	198	
1	B6	198	
2	B7	3	
3	B8	1571	
4	B9	73	
5	BA	210	
6	BB	150	
7	BC	216	
8	BD	148	
9	BE	256	
10	BF	250	
11	BG	161	
12	BH	207	
13	BI	65	
14	BJ	95	
15	BK	188	
16	BL	306	
17	BM	399	
18	BN	294	
19	BO	268	
20	BP	257	
21	BQ	192	
22	BR	197	
23	BS	325	

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Mol	Chain	Length	Quality of chain
24	BT	296	
25	BU	251	
26	BV	169	
27	BW	188	
28	BX	303	
29	BY	149	
30	BZ	209	
31	Ba	160	
32	Bb	112	
33	Bc	138	
34	Bd	126	
35	Be	102	
36	Bf	205	
37	Bg	222	
38	Bh	196	
39	Bi	433	
40	Bj	304	
41	Bl	100	
42	Bm	423	
43	Bn	380	
44	Bo	334	
45	Bp	162	
46	Bq	135	
47	Br	142	
48	Bs	159	

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Mol	Chain	Length	Quality of chain
49	Bt	332	
50	Bu	306	
51	Bv	279	
52	Bw	269	
53	Bx	166	
54	By	198	
55	Bz	128	
56	AA	960	
57	AB	366	
58	AC	167	
59	AD	199	
60	AE	124	
61	AF	242	
62	AG	71	
63	AH	200	
64	AI	9	
65	AJ	139	
66	AK	128	
67	AL	259	
68	AM	135	
69	AN	130	
70	AO	258	
71	AP	143	
72	AQ	87	
73	AR	382	

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Mol	Chain	Length	Quality of chain
74	AS	190	
75	AT	173	
76	AU	205	
77	AV	395	
78	AW	188	
79	AX	410	
80	AY	381	
81	AZ	148	
82	Aa	474	
83	Ab	289	
84	Ac	118	
85	Ad	430	
86	Ae	692	
87	Ag	397	
88	Ai	196	
89	Aj	505	

2 Entry composition [i](#)

There are 100 unique types of molecules in this entry. The entry contains 180624 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mitochondrial ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	B1	45	Total	C	N	O	0	0
			317	203	52	62		
1	B2	27	Total	C	N	O	0	0
			213	137	33	43		
1	B3	28	Total	C	N	O	0	0
			222	143	35	44		
1	B4	27	Total	C	N	O	0	0
			213	137	33	43		
1	B5	27	Total	C	N	O	0	0
			213	137	33	43		
1	B6	26	Total	C	N	O	0	0
			205	131	32	42		

- 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	1571	Total	C	N	O	P	0	0
			33427	15015	6087	10754	1571		

- Molecule 4 is a RNA chain called CP Phe-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	B9	73	Total	C	N	O	P	S	0	0
			1560	703	283	500	73	1		

- Molecule 5 is a protein called Large ribosomal subunit protein uL22m.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BB	149	Total	C	N	O	S	0	0
			1184	754	227	201	2		

- Molecule 7 is a protein called uL24m.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BD	112	Total	C	N	O	S	0	0
			867	558	158	148	3		

- Molecule 9 is a protein called Mitochondrial ribosomal protein L28.

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

- Molecule 10 is a protein called Mitochondrial ribosomal protein L47.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BG	107	Total	C	N	O	S	0	0
			874	562	159	150	3		

- Molecule 12 is a protein called Mitochondrial ribosomal protein L32.

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

- Molecule 13 is a protein called Large ribosomal subunit protein bL33m.

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

- Molecule 14 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BJ	46	Total	C	N	O	S	0	0
			387	239	89	58	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
			833	539	163	129	2		

- Molecule 16 is a protein called Mitochondrial ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BL	240	Total	C	N	O	S	0	0
			1860	1160	371	319	10		

- Molecule 17 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BM	307	Total	C	N	O	S	0	0
			2420	1554	426	430	10		

- Molecule 18 is a protein called Mitochondrial ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BN	250	Total	C	N	O	S	1	0
			2019	1299	370	344	6		

- Molecule 19 is a protein called Mitochondrial ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BO	202	Total	C	N	O	S	0	0
			1660	1059	311	286	4		

- Molecule 20 is a protein called Mitochondrial ribosomal protein L10.

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

- Molecule 21 is a protein called Mitochondrial ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BQ	176	Total	C	N	O	S	0	0
			1339	851	243	243	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
			1447	928	258	254	7		

- Molecule 23 is a protein called Mitochondrial ribosomal protein L14.

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

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

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

- Molecule 25 is a protein called uL16m.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 26 is a protein called bL17m.

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

- Molecule 27 is a protein called Mitochondrial ribosomal protein L18.

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

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

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

- Molecule 29 is a protein called Mitochondrial ribosomal protein L20.

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

- Molecule 30 is a protein called Mitochondrial ribosomal protein L21.

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

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

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

- Molecule 32 is a protein called Mitochondrial ribosomal protein L53.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bb	97	Total	C	N	O	S	0	0
			745	461	143	135	6		

- Molecule 33 is a protein called mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bc	84	Total	C	N	O	S	0	0
			716	458	128	127	3		

- Molecule 34 is a protein called Mitochondrial ribosomal protein L55.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bd	92	Total	C	N	O	S	0	0
			763	477	148	135	3		

- Molecule 35 is a protein called Mitochondrial ribosomal protein L57.

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

- Molecule 36 is a protein called mL62 (ICT1).

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

- Molecule 37 is a protein called mL64.

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

- Molecule 38 is a protein called Mitochondrial ribosomal protein S18A.

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

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

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

- 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
			1325	853	217	251	4		

- Molecule 41 is a protein called Ribosomal protein.

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

- Molecule 42 is a protein called Mitochondrial ribosomal protein L37.

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

- Molecule 43 is a protein called Mitochondrial ribosomal protein L38.

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

- Molecule 44 is a protein called Mitochondrial ribosomal protein L39.

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

- Molecule 45 is a protein called Mitochondrial ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Bp	143	Total	C	N	O	S	0	0
			1202	757	217	227	1		

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

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

- Molecule 47 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Br	108	Total	C	N	O	S	0	0
			906	570	167	165	4		

- 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
			1185	738	227	217	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bs	2	ACE	-	acetylation	UNP F1S8U4

- Molecule 49 is a protein called mL44.

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

- Molecule 50 is a protein called Mitochondrial ribosomal protein L45.

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

- Molecule 51 is a protein called Mitochondrial ribosomal protein L46.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Bv	238	Total	C	N	O	S	0	0
			1948	1240	338	363	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bw	165	Total	C	N	O	S	0	0
			1295	825	224	241	5		

- Molecule 53 is a protein called Mrpl34.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 54 is a protein called Mitochondrial ribosomal protein L50.

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

- Molecule 55 is a protein called Large ribosomal subunit protein mL51.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AA	960	Total	C	N	O	P	0	0
			20418	9169	3708	6581	960		

- Molecule 57 is a protein called 28S ribosomal protein S35, mitochondrial isoform 1.

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

- Molecule 58 is a protein called Mitochondrial ribosomal protein S24.

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

- Molecule 59 is a protein called Small ribosomal subunit protein mS38.

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

- Molecule 60 is a protein called Mitoribosomal protein bs6m, mrps6.

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

- Molecule 61 is a protein called Mitochondrial ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AF	208	Total	C	N	O	S	0	0
			1722	1097	314	300	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AG	71	Total	C	N	O	P	0	0
			1502	673	264	494	71		

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 63 is a protein called Mitochondrial ribosomal protein S10.

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

- Molecule 64 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AI	9	Total	C	N	O	P	0	0
			193	88	40	57	8		

- Molecule 65 is a protein called Mitochondrial ribosomal protein S12.

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

- Molecule 66 is a protein called Mitochondrial ribosomal protein S14.

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

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

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

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

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

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

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

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

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

- Molecule 71 is a protein called Mitochondrial ribosomal protein S18C.

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

- 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
			737	455	148	126	8		

- Molecule 73 is a protein called Mitochondrial ribosomal protein S22.

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

- Molecule 74 is a protein called mS23.

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

- Molecule 75 is a protein called Mitochondrial ribosomal protein S25.

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

- Molecule 76 is a protein called Mitochondrial ribosomal protein S26.

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

- Molecule 77 is a protein called Mitochondrial ribosomal protein S27.

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

- Molecule 78 is a protein called Mitoribosomal protein ms28, mrps28.

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

- Molecule 79 is a protein called Small ribosomal subunit protein mS29.

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

- 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
			1250	807	211	229	3		

- Molecule 81 is a protein called Mitochondrial ribosomal protein S33.

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

- 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	1	0
			3120	1943	572	592	13		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
Aa	450	GLY	-	expression tag	UNP O75570
Aa	451	SER	-	expression tag	UNP O75570
Aa	452	GLY	-	expression tag	UNP O75570
Aa	453	ASP	-	expression tag	UNP O75570
Aa	454	TYR	-	expression tag	UNP O75570
Aa	455	LYS	-	expression tag	UNP O75570
Aa	456	ASP	-	expression tag	UNP O75570
Aa	457	HIS	-	expression tag	UNP O75570

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Chain	Residue	Modelled	Actual	Comment	Reference
Aa	458	ASP	-	expression tag	UNP O75570
Aa	459	GLY	-	expression tag	UNP O75570
Aa	460	ASP	-	expression tag	UNP O75570
Aa	461	TYR	-	expression tag	UNP O75570
Aa	462	LYS	-	expression tag	UNP O75570
Aa	463	ASP	-	expression tag	UNP O75570
Aa	464	HIS	-	expression tag	UNP O75570
Aa	465	ASP	-	expression tag	UNP O75570
Aa	466	ILE	-	expression tag	UNP O75570
Aa	467	ASP	-	expression tag	UNP O75570
Aa	468	TYR	-	expression tag	UNP O75570
Aa	469	LYS	-	expression tag	UNP O75570
Aa	470	ASP	-	expression tag	UNP O75570
Aa	471	ASP	-	expression tag	UNP O75570
Aa	472	ASP	-	expression tag	UNP O75570
Aa	473	ASP	-	expression tag	UNP O75570
Aa	474	LYS	-	expression tag	UNP O75570

- Molecule 83 is a protein called Mitochondrial ribosomal protein S2.

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

- Molecule 84 is a protein called Coiled-coil-helix-coiled-coil-helix domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Ac	116	Total	C	N	O	S	0	0
			933	579	185	161	8		

- Molecule 85 is a protein called 28S ribosomal protein S5, mitochondrial isoform X2.

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

- Molecule 86 is a protein called mS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Ae	588	Total	C	N	O	S	0	0
			4748	3039	804	879	26		

- Molecule 87 is a protein called uS9m.

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

- Molecule 88 is a protein called Mitochondrial ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Ai	137	Total	C	N	O	S	0	0
			1008	632	192	181	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ai	186	5F0	ASN	variant	UNP A0A286ZJJ6

- Molecule 89 is a protein called Mitochondrial ribosomal protein S34.

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

- Molecule 90 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	B8	192	Total	Mg	0
			192	192	
90	B9	1	Total	Mg	0
			1	1	
90	BL	2	Total	Mg	0
			2	2	
90	BM	2	Total	Mg	0
			2	2	
90	BT	1	Total	Mg	0
			1	1	
90	BV	3	Total	Mg	0
			3	3	
90	BY	1	Total	Mg	0
			1	1	
90	Be	1	Total	Mg	0
			1	1	
90	Bq	1	Total	Mg	0
			1	1	

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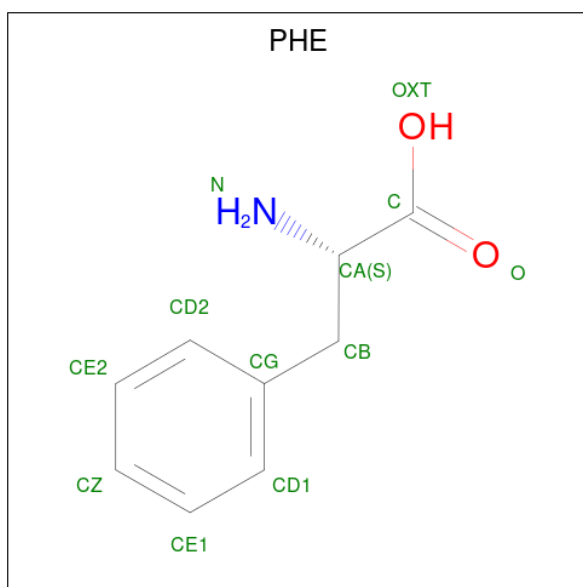
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Mol	Chain	Residues	Atoms		AltConf
90	Bx	1	Total 1	Mg 1	0
90	AA	121	Total 121	Mg 121	0
90	AD	1	Total 1	Mg 1	0
90	AG	1	Total 1	Mg 1	0
90	AI	1	Total 1	Mg 1	0
90	AJ	1	Total 1	Mg 1	0
90	AX	1	Total 1	Mg 1	0
90	Ab	1	Total 1	Mg 1	0

- Molecule 91 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
91	B8	25	Total 25	K 25	0
91	BL	1	Total 1	K 1	0
91	BU	1	Total 1	K 1	0
91	BW	1	Total 1	K 1	0
91	Be	1	Total 1	K 1	0
91	Bz	1	Total 1	K 1	0
91	AA	11	Total 11	K 11	0

- Molecule 92 is PHENYLALANINE (CCD ID: PHE) (formula: C₉H₁₁NO₂).

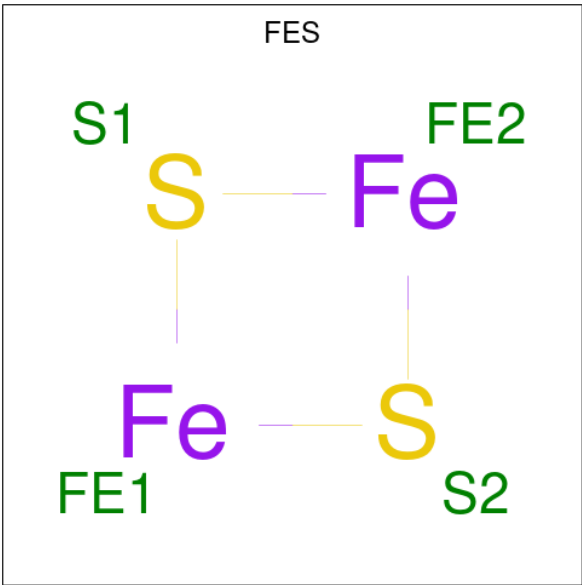


Mol	Chain	Residues	Atoms				AltConf
92	B9	1	Total	C	N	O	0
			11	9	1	1	

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

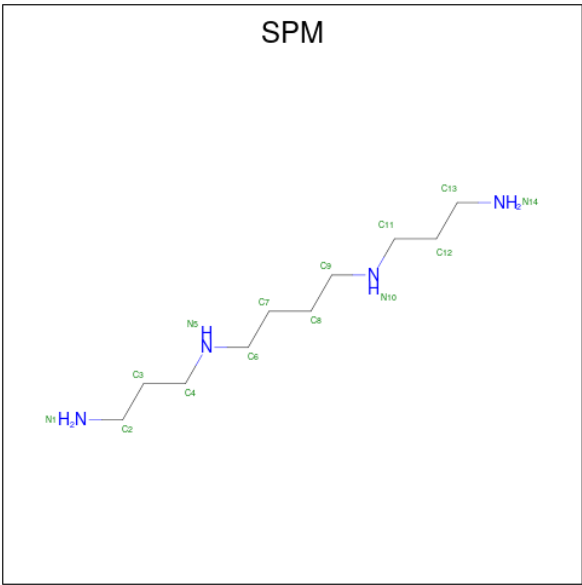
Mol	Chain	Residues	Atoms		AltConf
93	BH	1	Total	Zn	0
			1	1	
93	Bl	1	Total	Zn	0
			1	1	
93	AO	1	Total	Zn	0
			1	1	

- Molecule 94 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



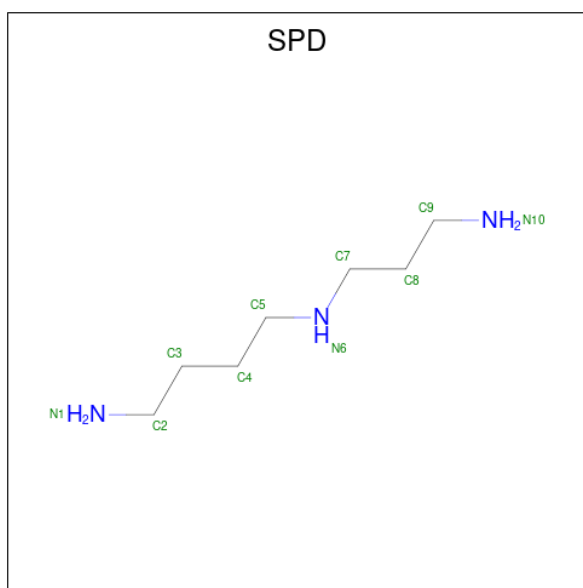
Mol	Chain	Residues	Atoms			AltConf
94	Bh	1	Total	Fe	S	0
			4	2	2	
94	AP	1	Total	Fe	S	0
			4	2	2	
94	AT	1	Total	Fe	S	0
			4	2	2	

- Molecule 95 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



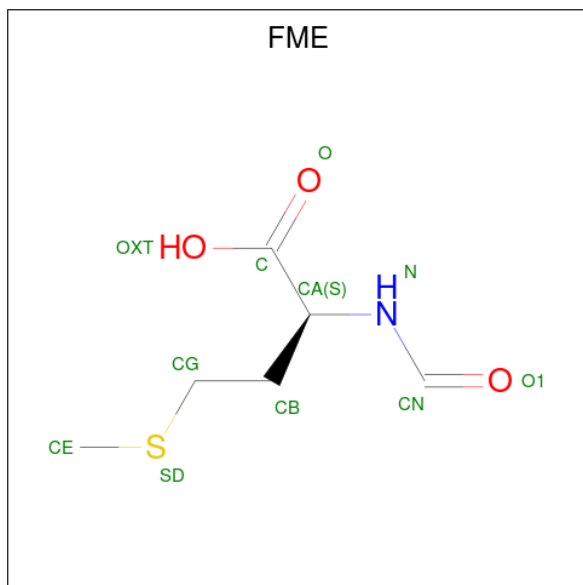
Mol	Chain	Residues	Atoms			AltConf
95	AA	1	Total	C	N	0
			14	10	4	

- Molecule 96 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



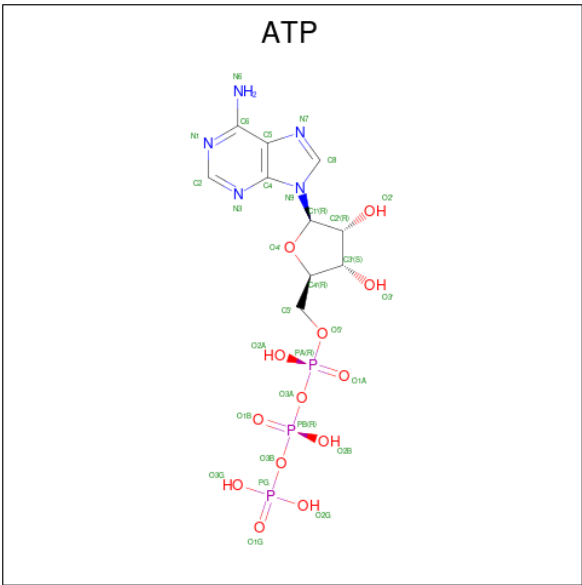
Mol	Chain	Residues	Atoms			AltConf
96	AA	1	Total	C	N	0
			10	7	3	

- Molecule 97 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



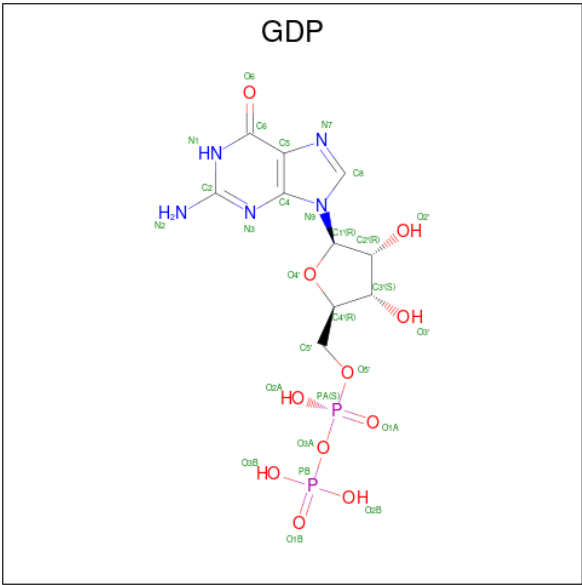
Mol	Chain	Residues	Atoms					AltConf
97	AG	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 98 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

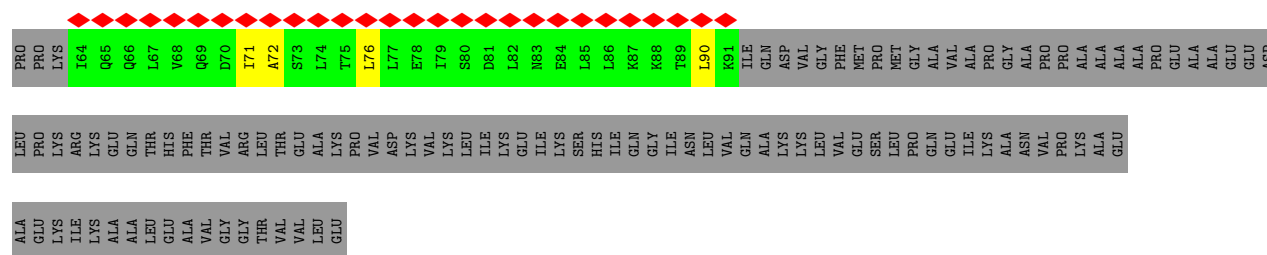
- Molecule 99 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



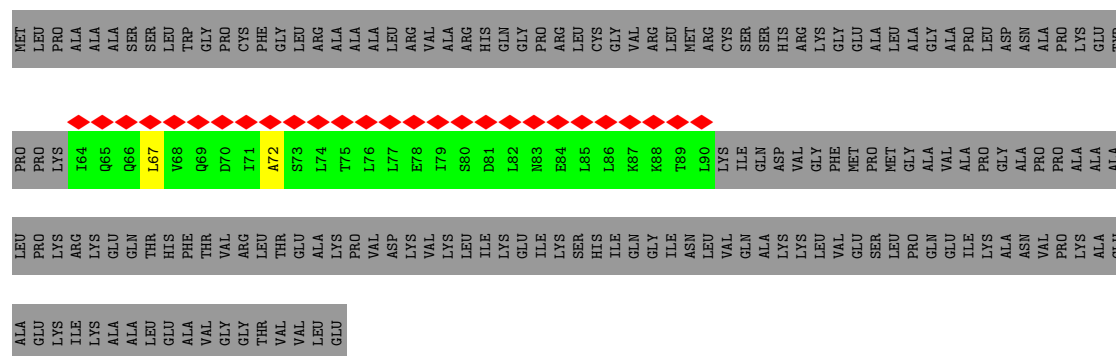
Mol	Chain	Residues	Atoms					AltConf
99	AX	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 100 is water.

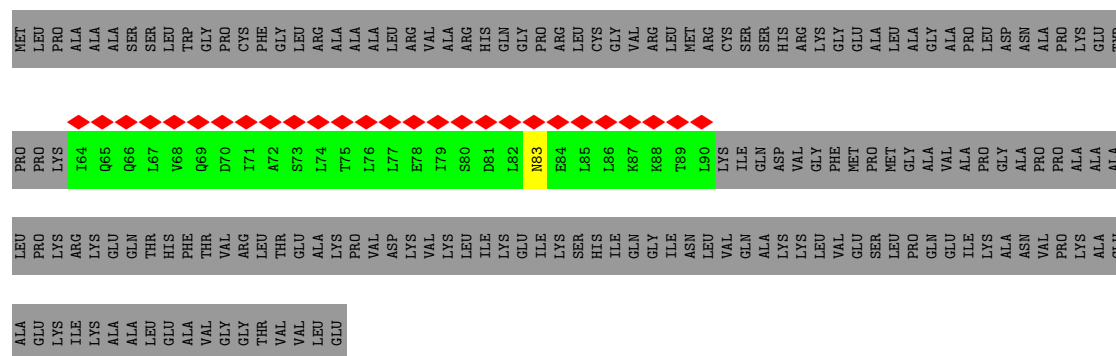
Mol	Chain	Residues	Atoms		AltConf
100	AX	3	Total 3	O 3	0



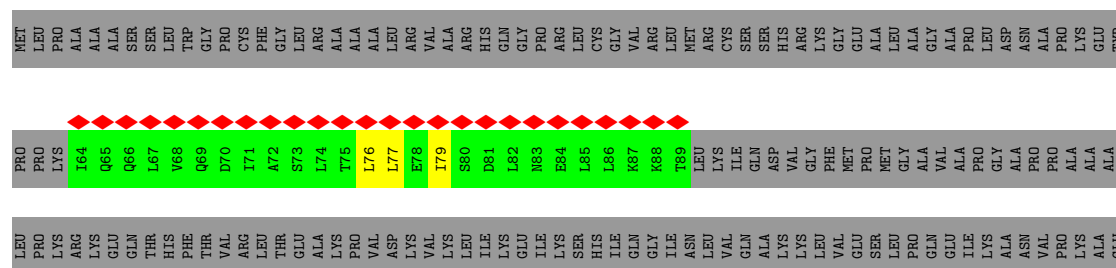
- Molecule 1: Mitochondrial ribosomal protein L12



- Molecule 1: Mitochondrial ribosomal protein L12



- Molecule 1: Mitochondrial ribosomal protein L12

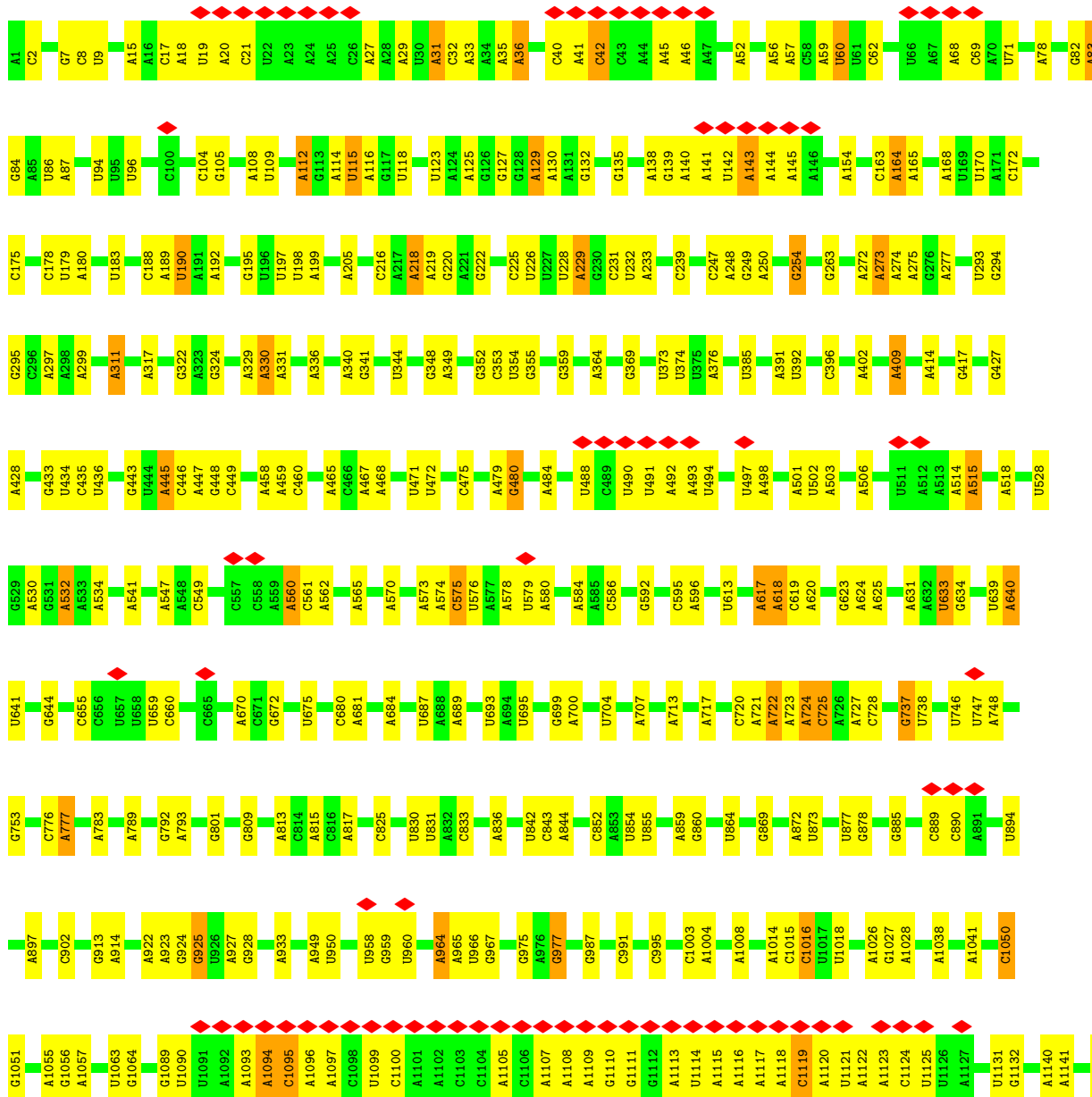


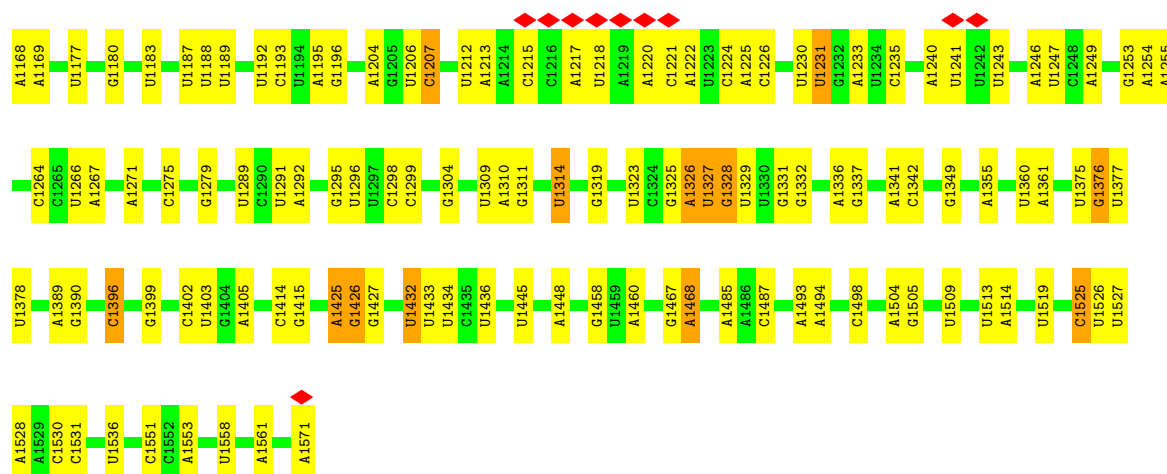
ALA	GLU
LYS	ILE
LYS	LYS
ALA	ALA
LEU	LEU
VAL	VAL
GLY	GLY
THR	THR
VAL	VAL
LEU	LEU
GLU	GLU

• Molecule 2: E-site tRNA

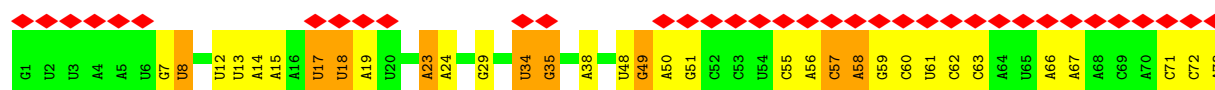


• Molecule 3: 16S rRNA

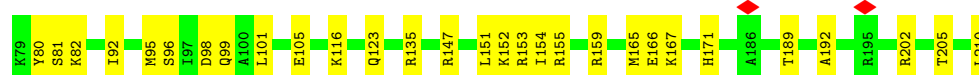
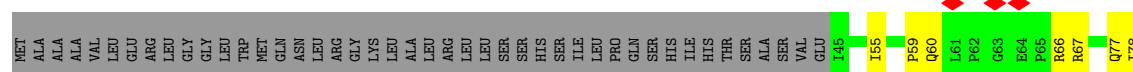




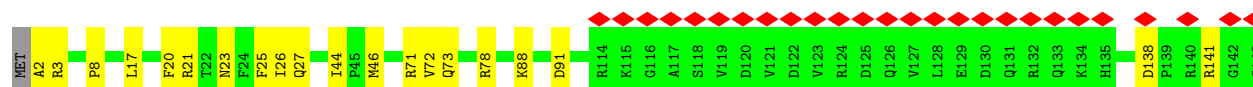
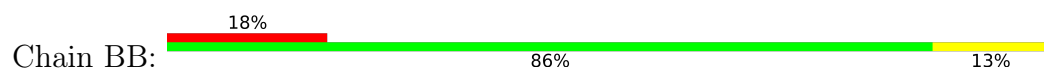
- Molecule 4: CP Phe-tRNA



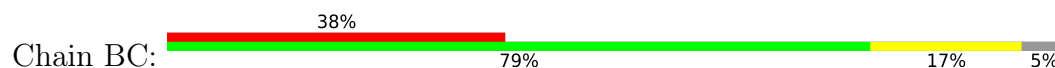
- Molecule 5: Large ribosomal subunit protein uL22m

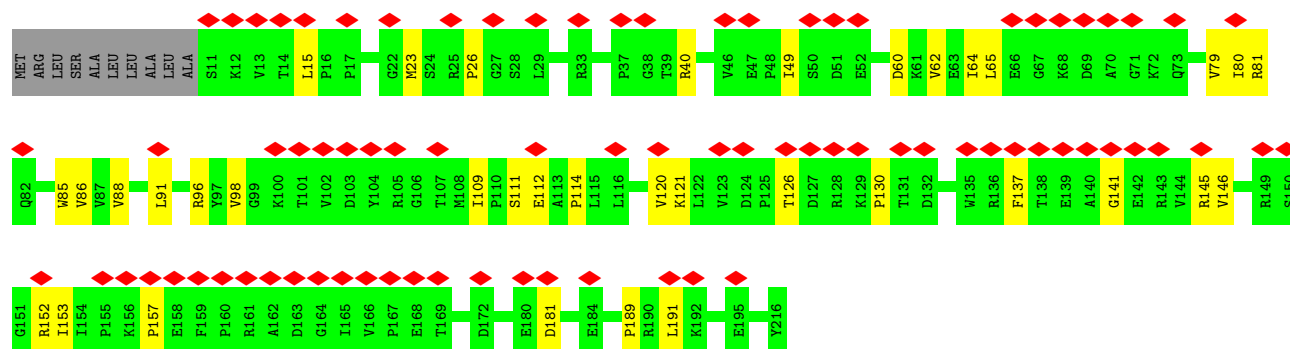


- Molecule 6: 39S ribosomal protein L23, mitochondrial

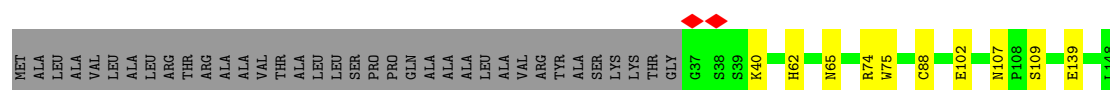


- Molecule 7: uL24m

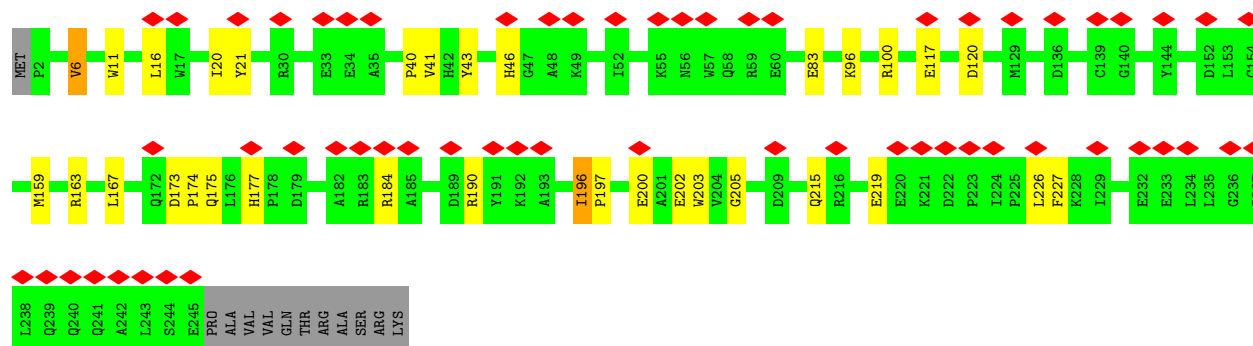
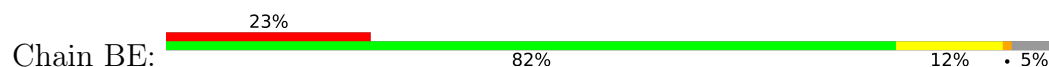




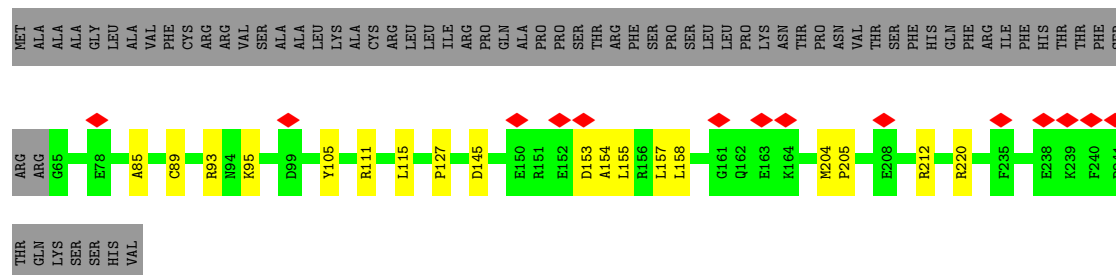
- Molecule 8: 39S ribosomal protein L27, mitochondrial



- Molecule 9: Mitochondrial ribosomal protein L28

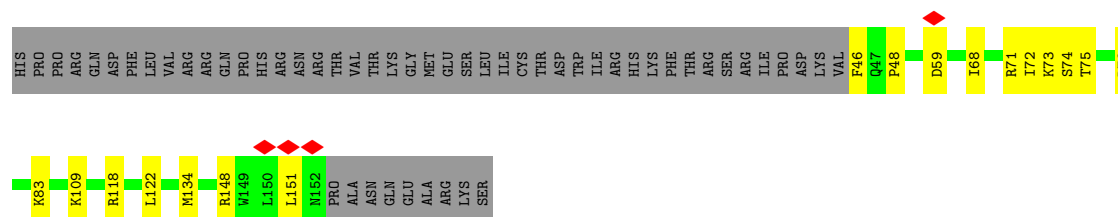


- Molecule 10: Mitochondrial ribosomal protein L47

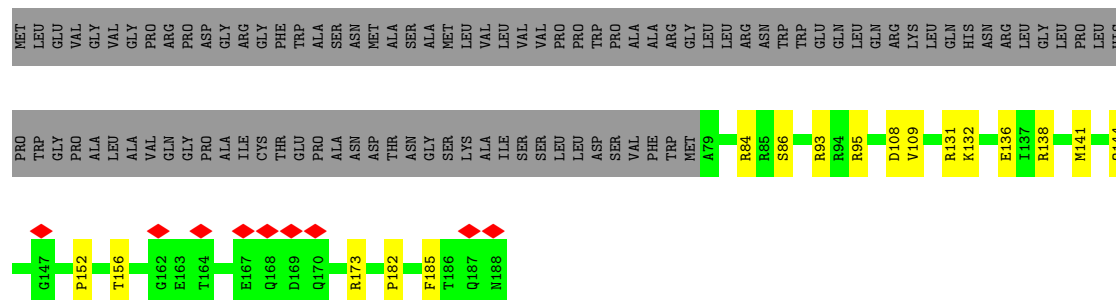


- Molecule 11: Large ribosomal subunit protein uL30m





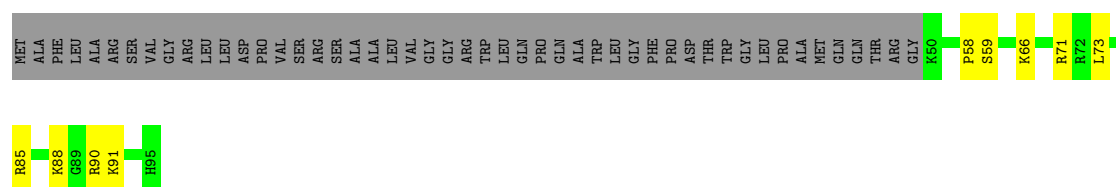
• Molecule 12: Mitochondrial ribosomal protein L32



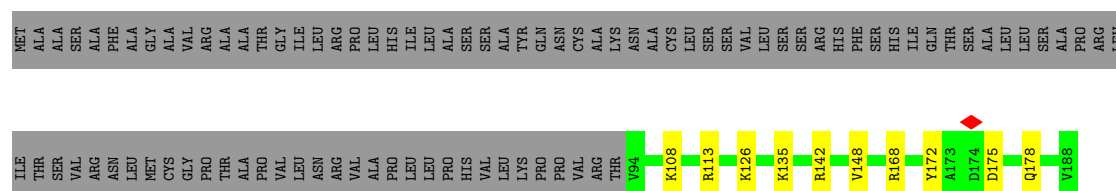
• Molecule 13: Large ribosomal subunit protein bL33m



• Molecule 14: Large ribosomal subunit protein bL34m

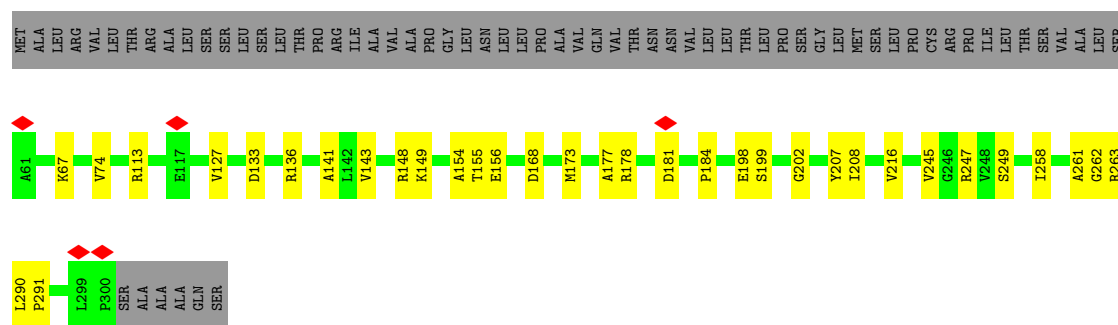


• Molecule 15: 39S ribosomal protein L35, mitochondrial



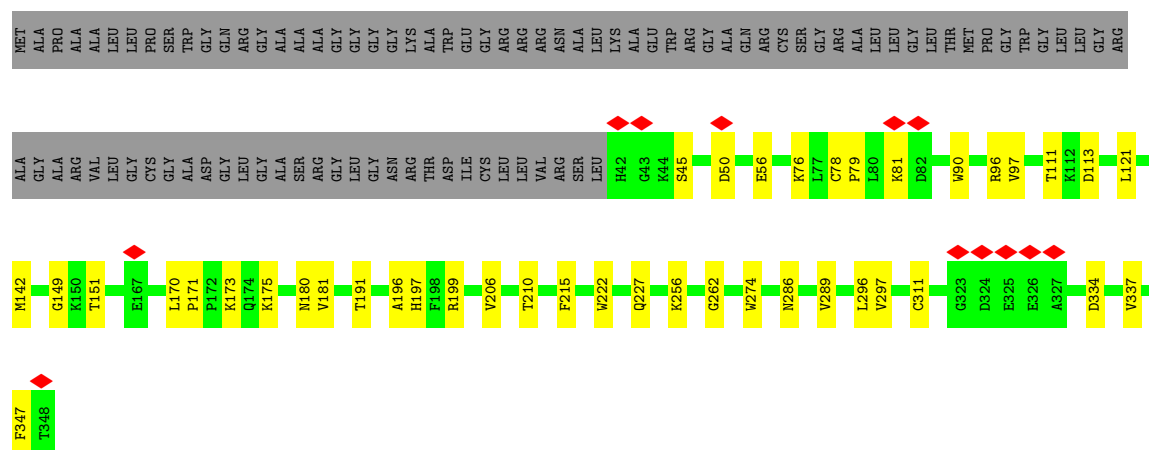
• Molecule 16: Mitochondrial ribosomal protein L2

Chain BL: 



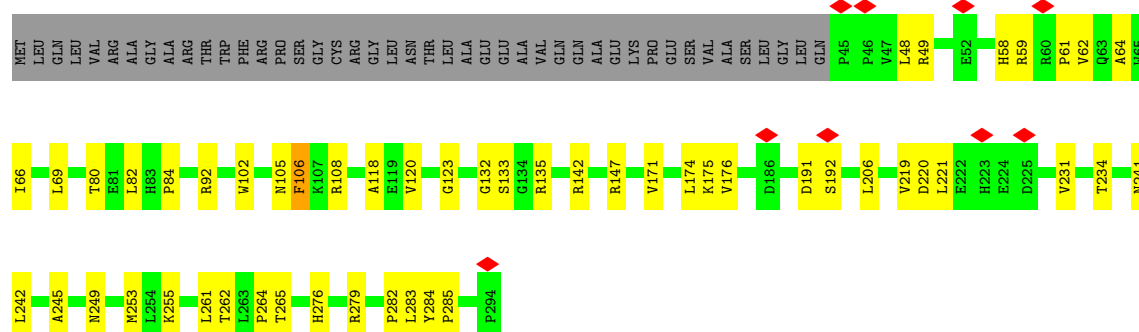
• Molecule 17: ICT1

Chain BM: 



• Molecule 18: Mitochondrial ribosomal protein L4

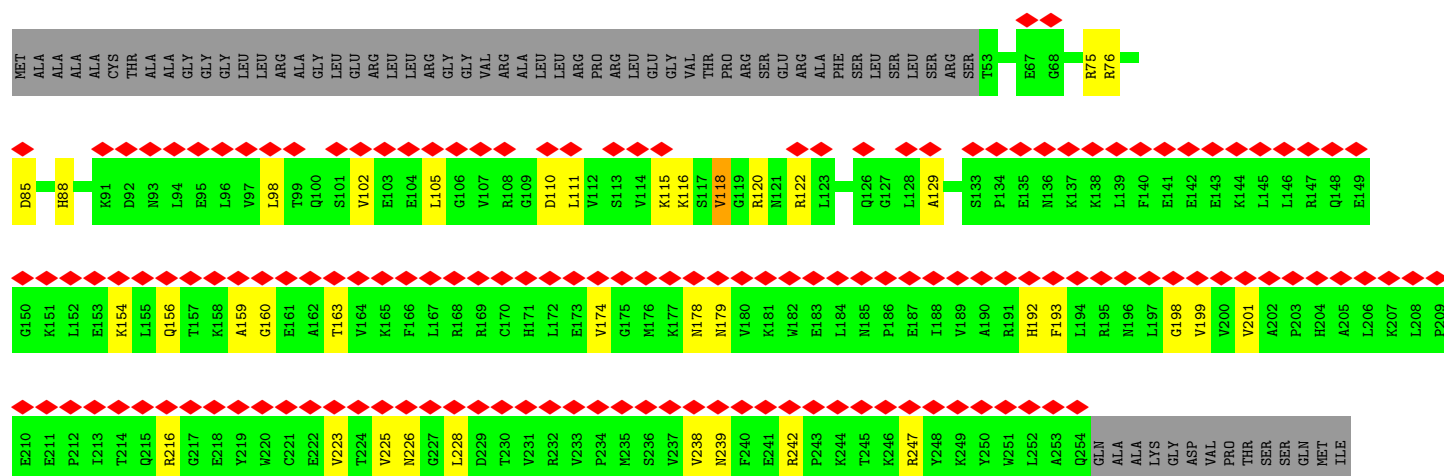
Chain BN: 



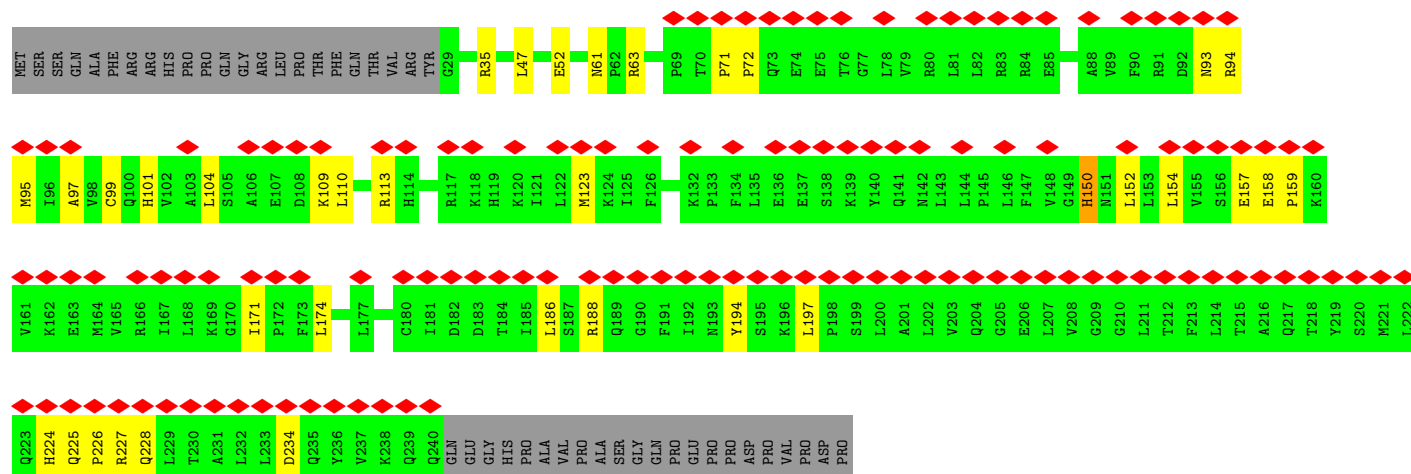
• Molecule 19: Mitochondrial ribosomal protein L9

Chain BO: 

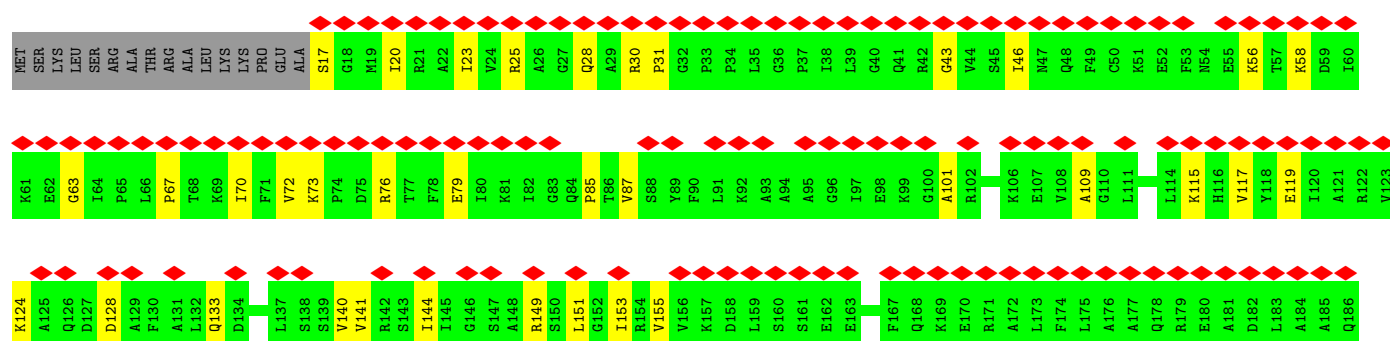
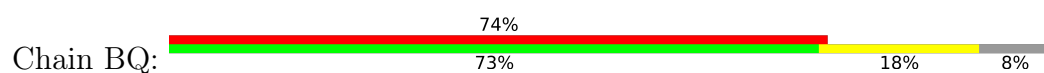


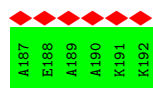


• Molecule 20: Mitochondrial ribosomal protein L10



• Molecule 21: Mitochondrial ribosomal protein L11





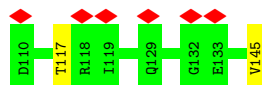
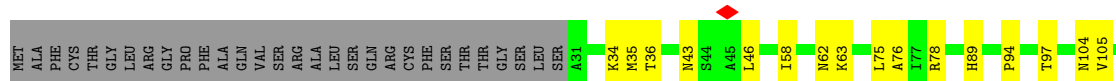
- Molecule 22: 39S ribosomal protein L13, mitochondrial

Chain BR: 80% 9% 10%



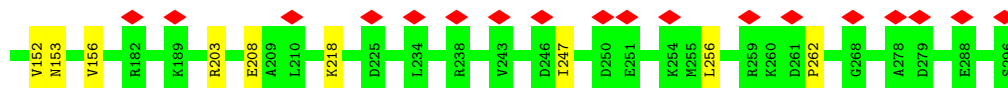
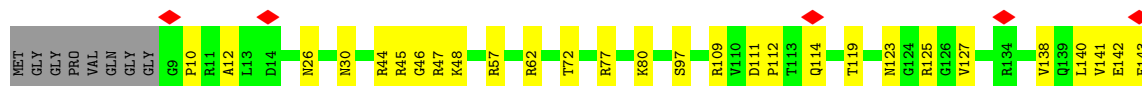
- Molecule 23: Mitochondrial ribosomal protein L14

Chain BS: 30% 6% 65%



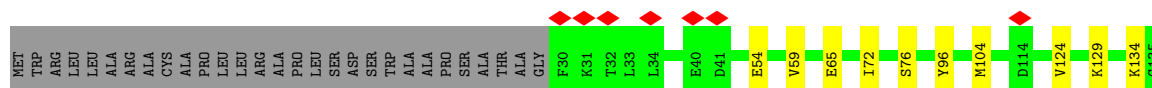
- Molecule 24: 39S ribosomal protein L15, mitochondrial

Chain BT: 8% 85% 12%



- Molecule 25: uL16m

Chain BU: 80% 8% 12%





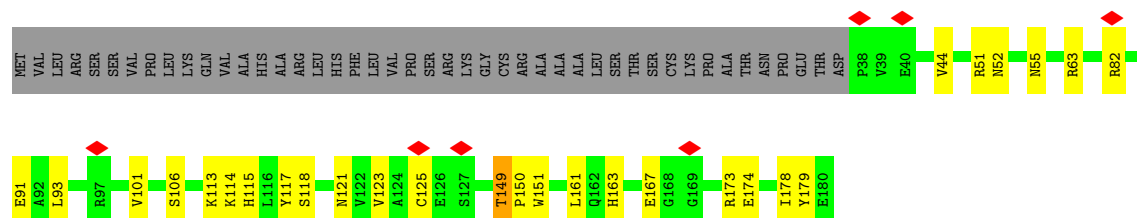
- Molecule 26: bL17m

Chain BV: 77% 14% 9%



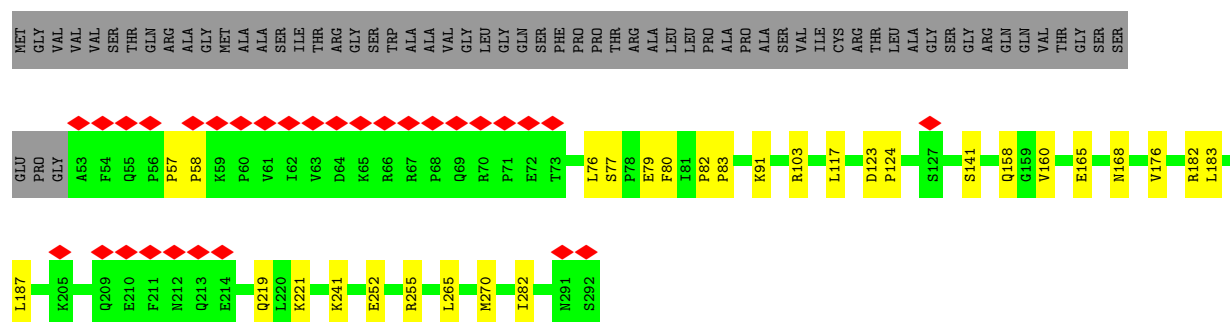
- Molecule 27: Mitochondrial ribosomal protein L18

Chain BW: 61% 14% 24%



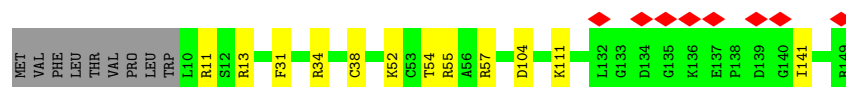
- Molecule 28: 39S ribosomal protein L19, mitochondrial

Chain BX: 10% 69% 10% 21%



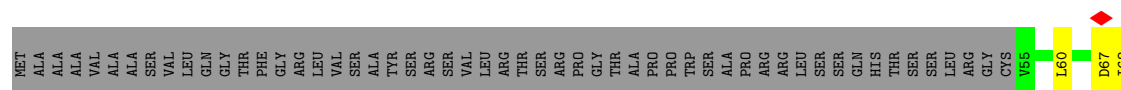
- Molecule 29: Mitochondrial ribosomal protein L20

Chain BY: 5% 86% 8% 6%

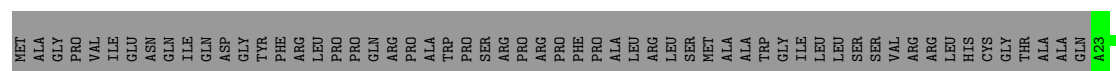


- Molecule 30: Mitochondrial ribosomal protein L21

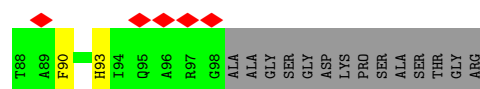
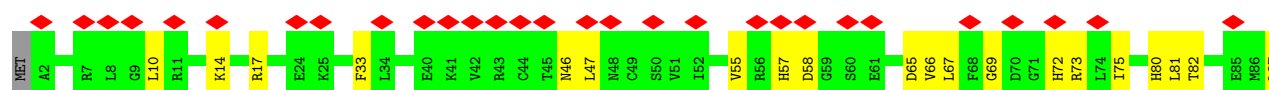
Chain BZ: 61% 13% 26%



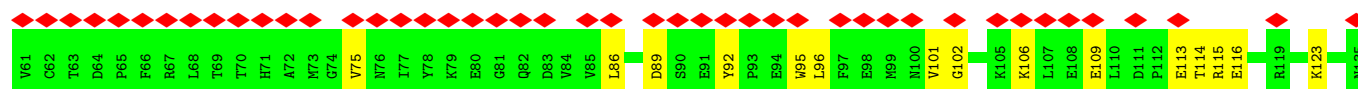
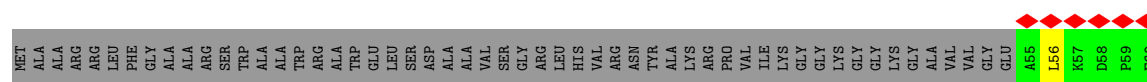
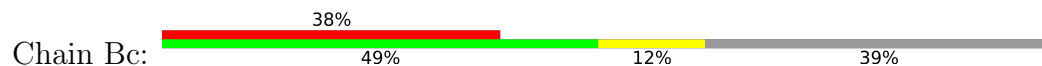
- Molecule 31: 39S ribosomal protein L52, mitochondrial



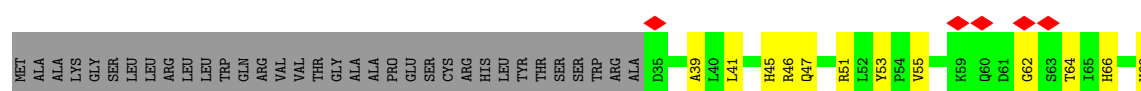
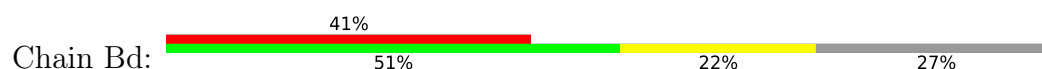
- Molecule 32: Mitochondrial ribosomal protein L53

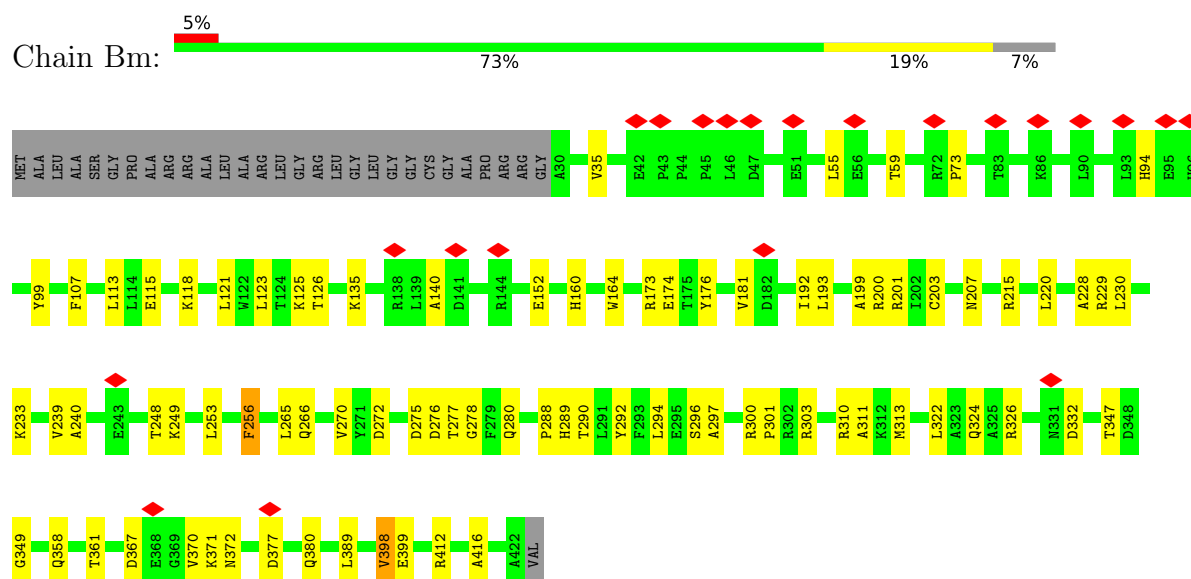


- Molecule 33: mL54

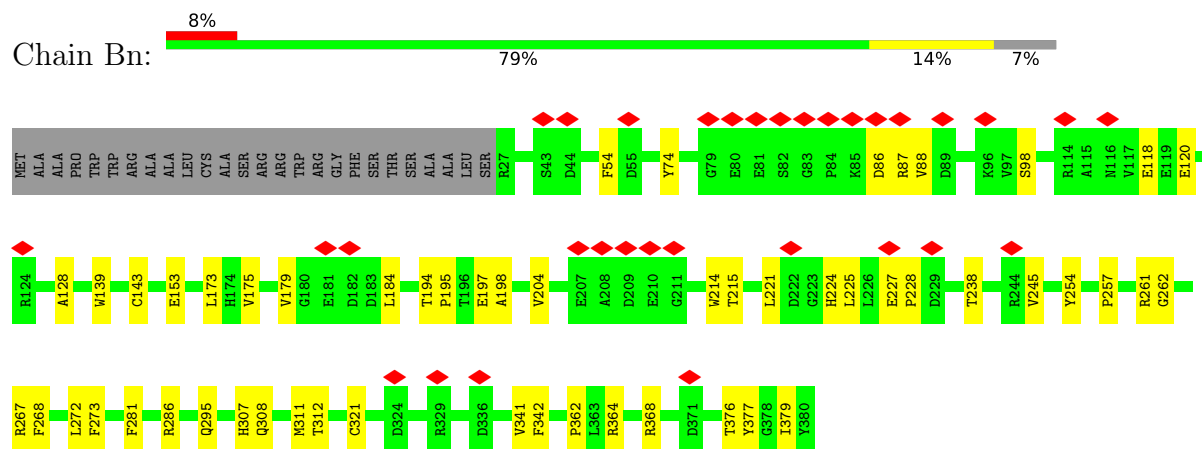


- Molecule 34: Mitochondrial ribosomal protein L55

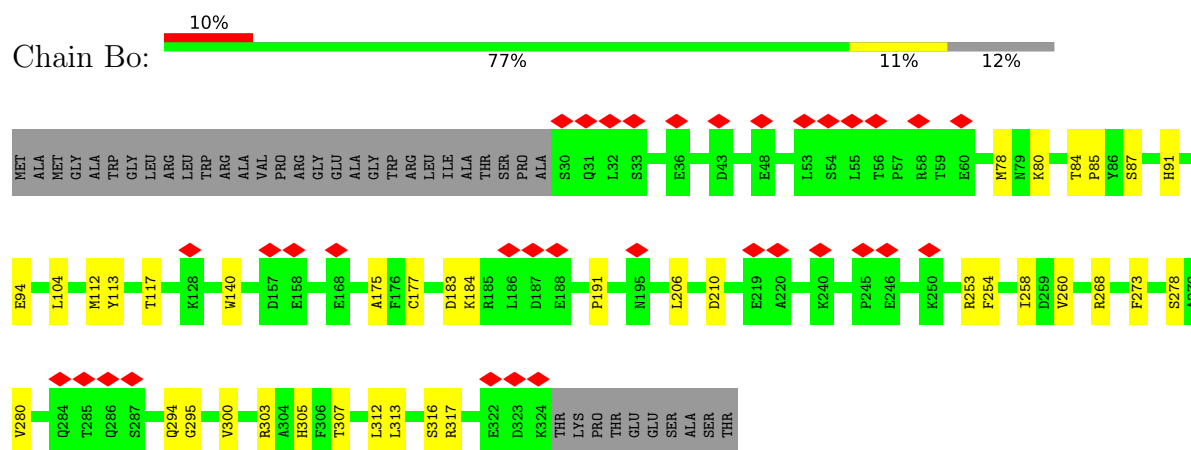




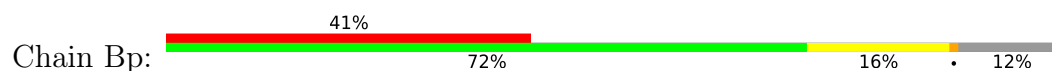
• Molecule 43: Mitochondrial ribosomal protein L38

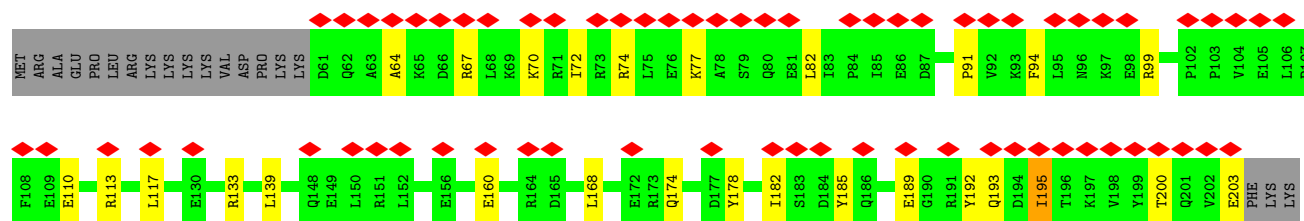


• Molecule 44: Mitochondrial ribosomal protein L39

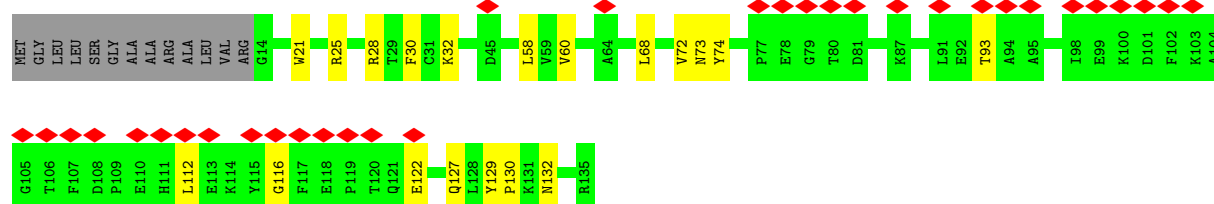
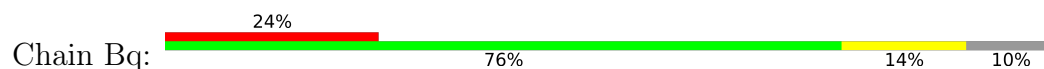


• Molecule 45: Mitochondrial ribosomal protein L40

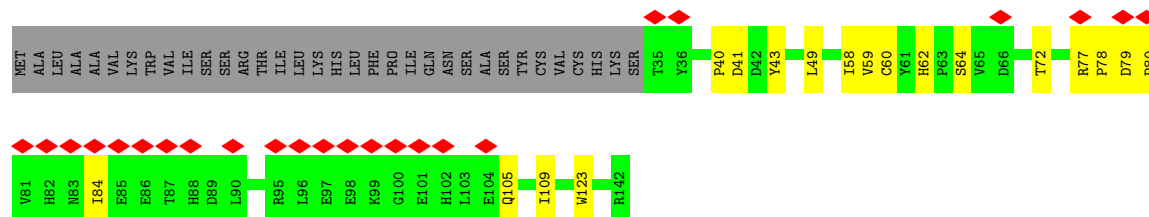




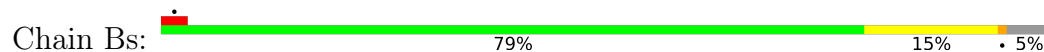
- Molecule 46: 39S ribosomal protein L41, mitochondrial



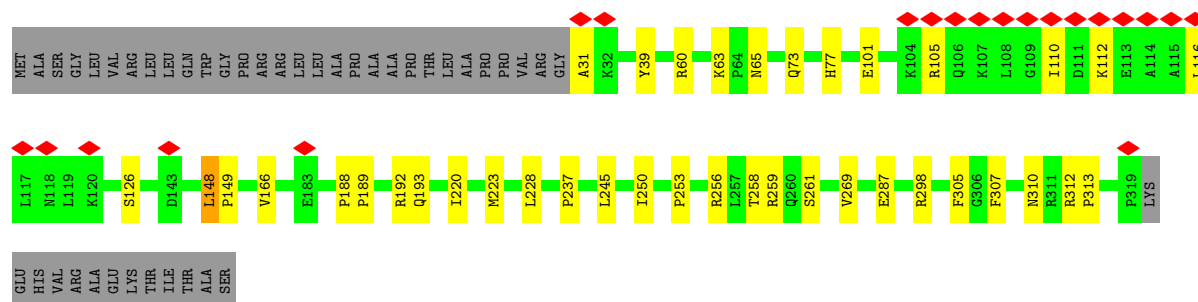
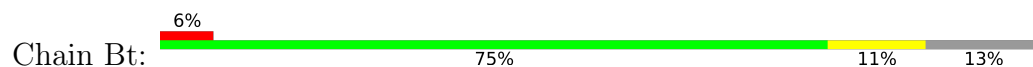
- Molecule 47: mL42



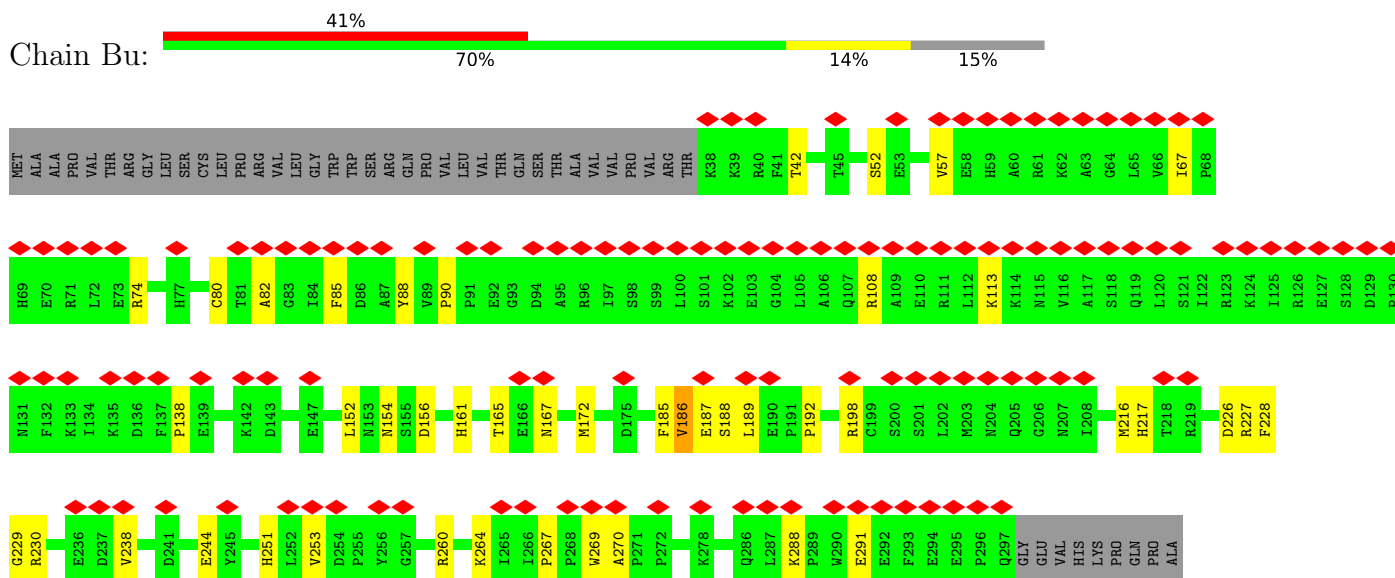
- Molecule 48: Large ribosomal subunit protein mL43



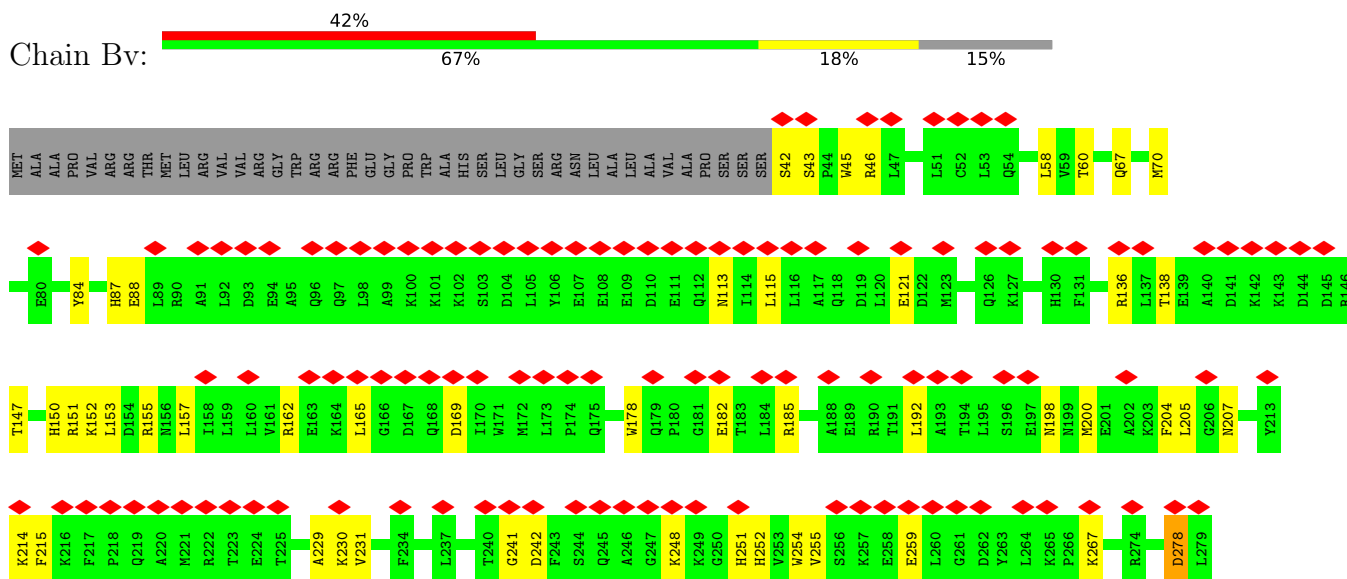
- Molecule 49: mL44



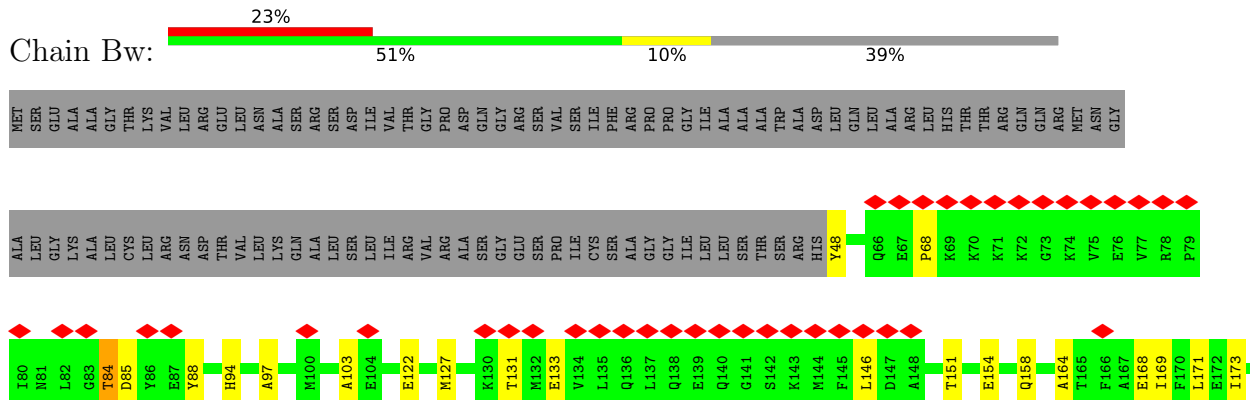
Chain Bu:

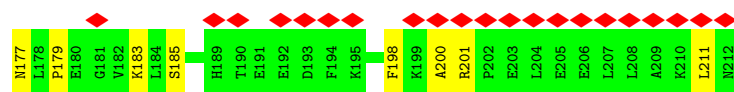


Chain Bv:

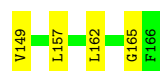
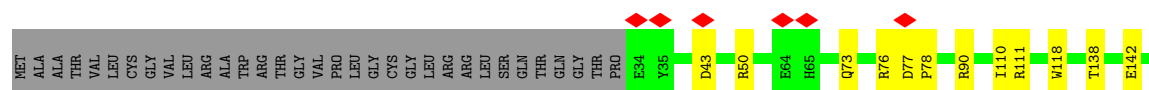


Chain Bw:

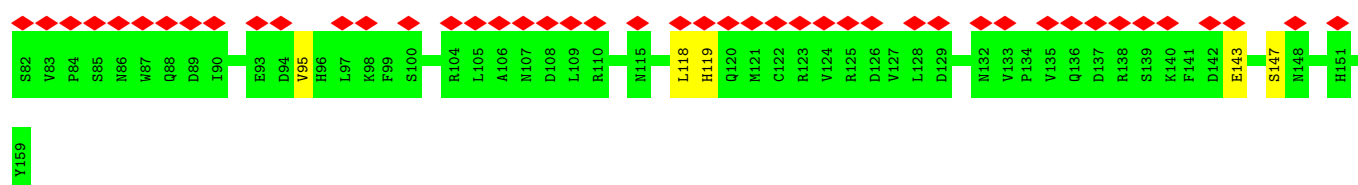
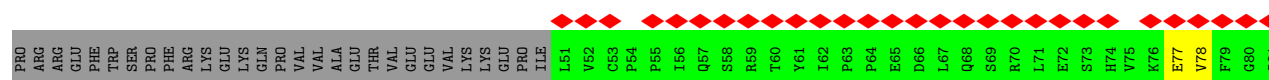
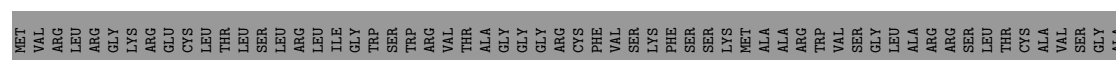
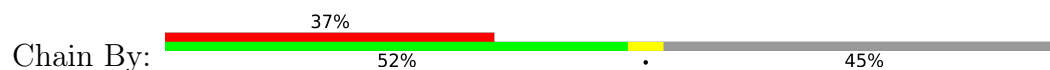




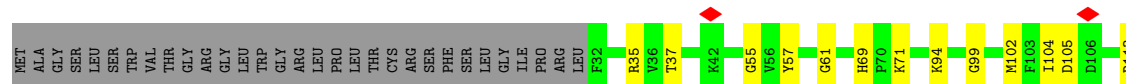
• Molecule 53: Mrpl34



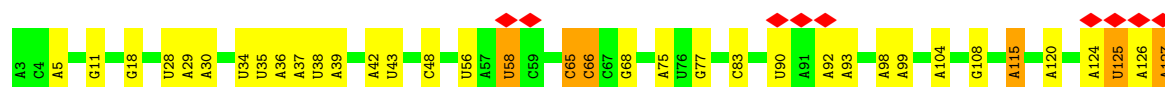
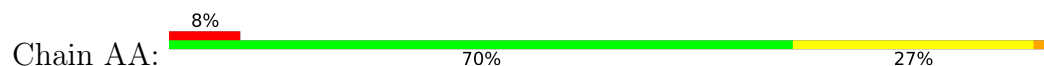
• Molecule 54: Mitochondrial ribosomal protein L50

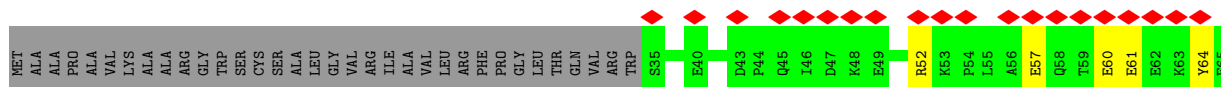


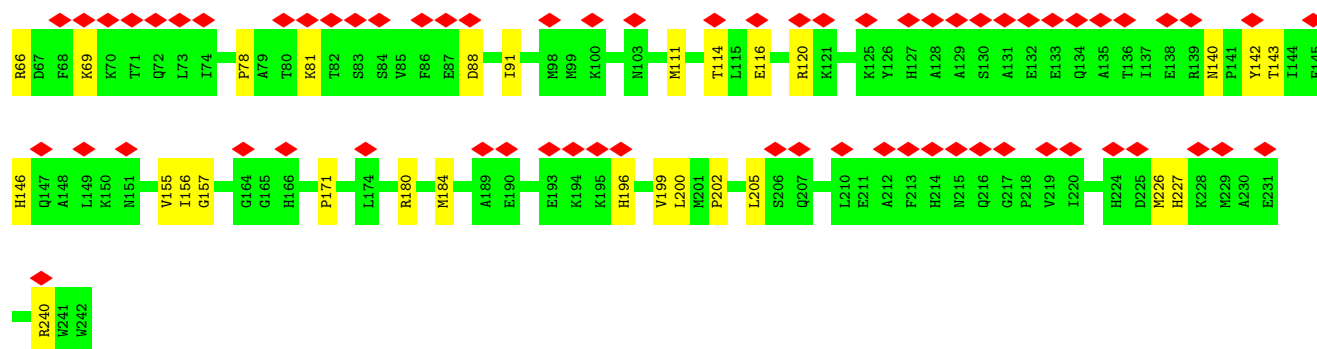
• Molecule 55: Large ribosomal subunit protein mL51



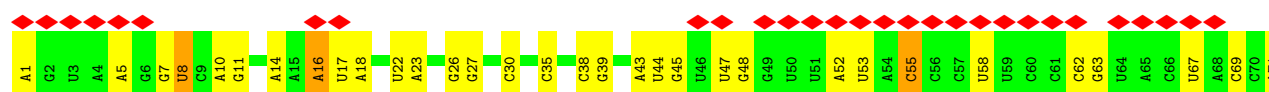
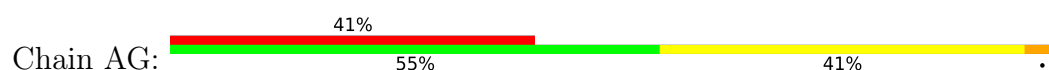
• Molecule 56: 12S rRNA



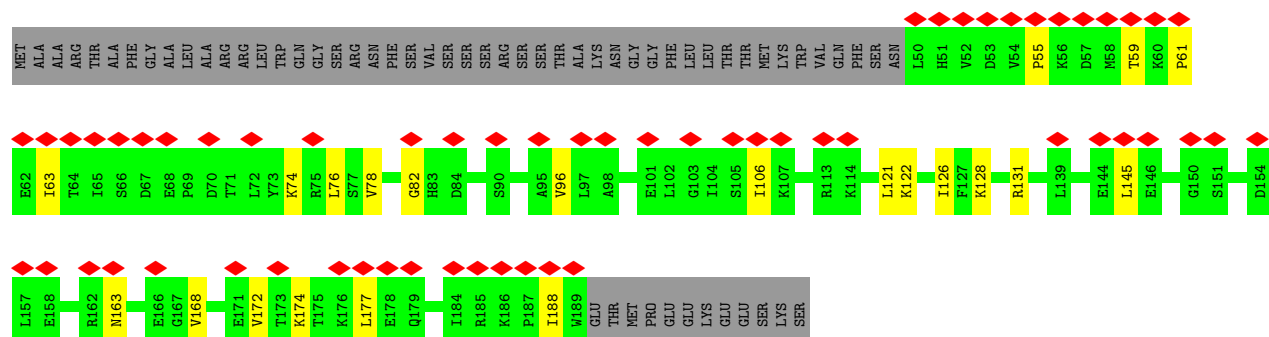




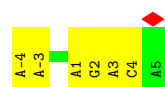
- Molecule 62: P-site Met-tRNA(fMet)



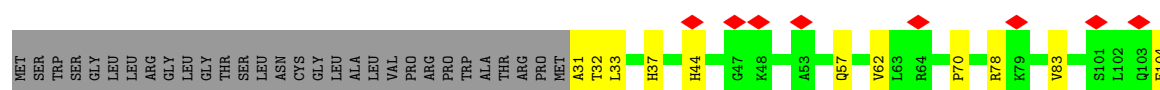
- Molecule 63: Mitochondrial ribosomal protein S10

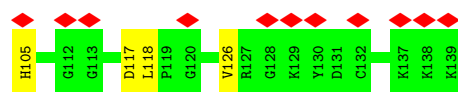


- Molecule 64: mRNA

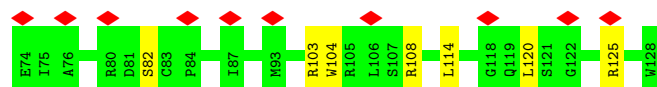
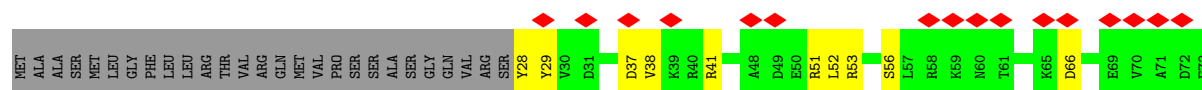


- Molecule 65: Mitochondrial ribosomal protein S12

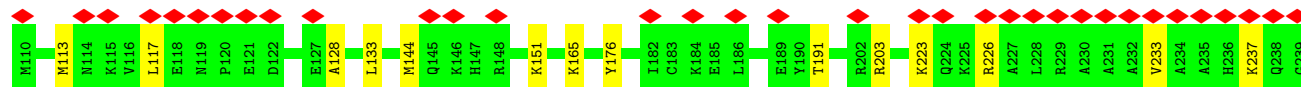
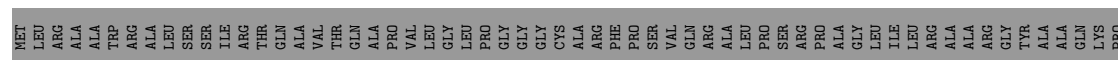




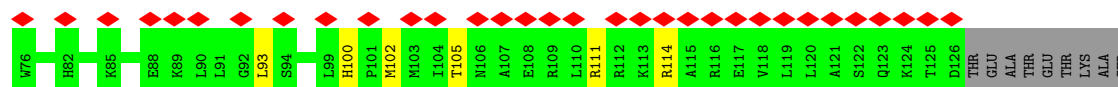
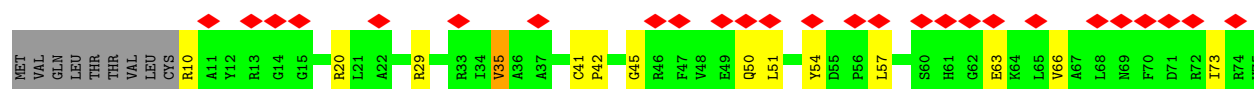
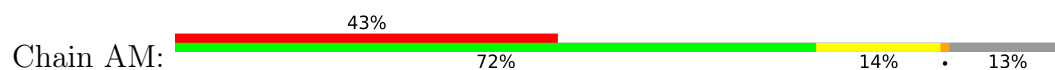
- Molecule 66: Mitochondrial ribosomal protein S14



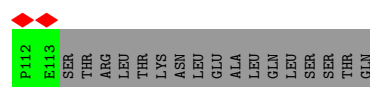
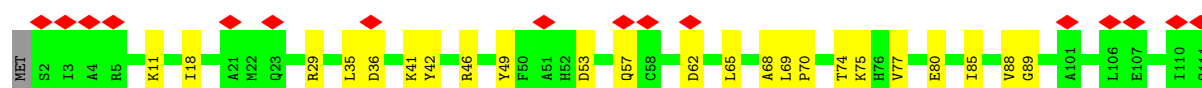
- Molecule 67: 28S ribosomal protein S15, mitochondrial



- Molecule 68: 28S ribosomal protein S16, mitochondrial

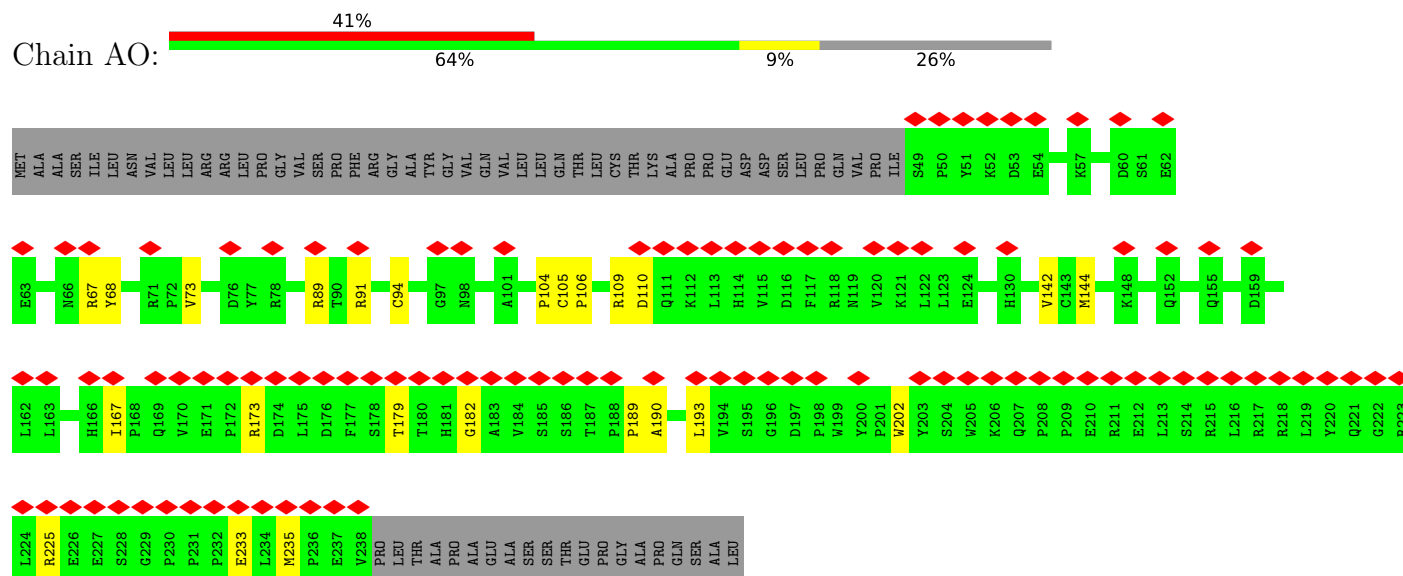


- Molecule 69: 28S ribosomal protein S17, mitochondrial



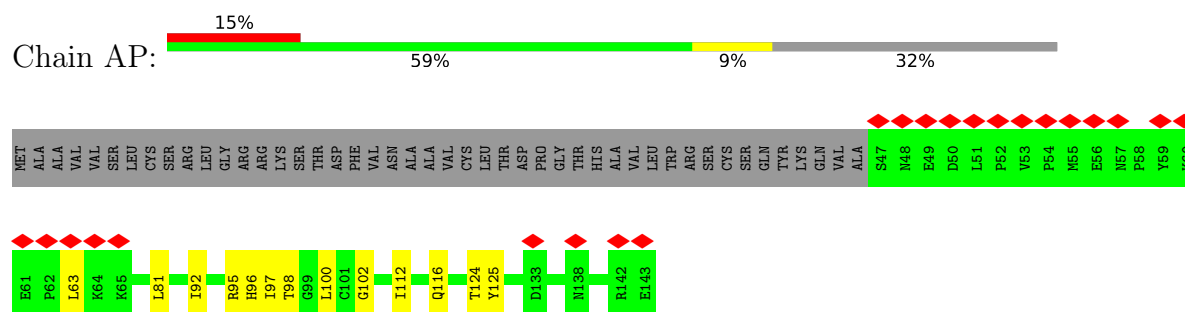
- Molecule 70: 28S ribosomal protein S18b, mitochondrial

Chain AO:



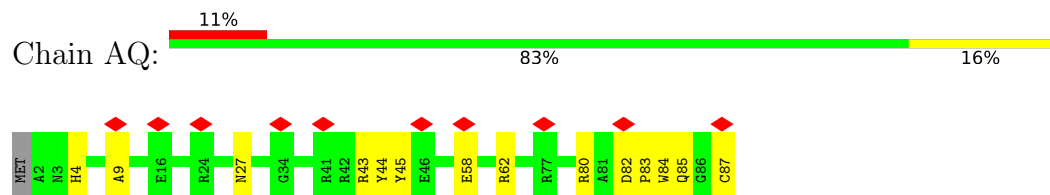
- Molecule 71: Mitochondrial ribosomal protein S18C

Chain AP:



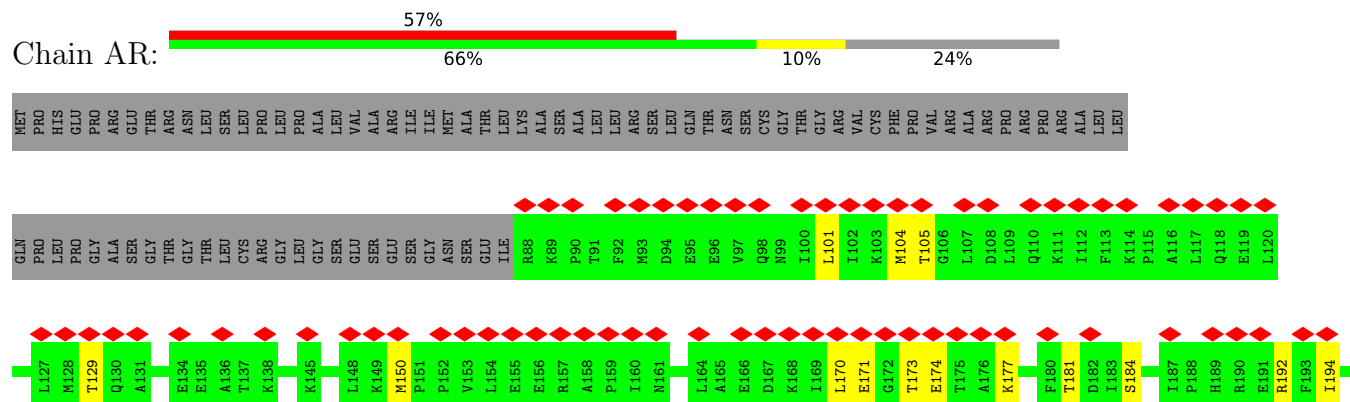
- Molecule 72: 28S ribosomal protein S21, mitochondrial

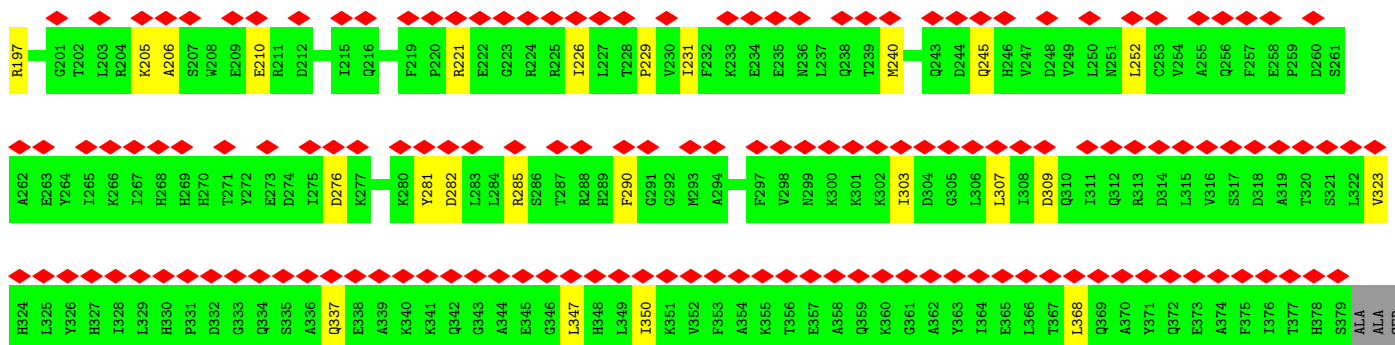
Chain AQ:



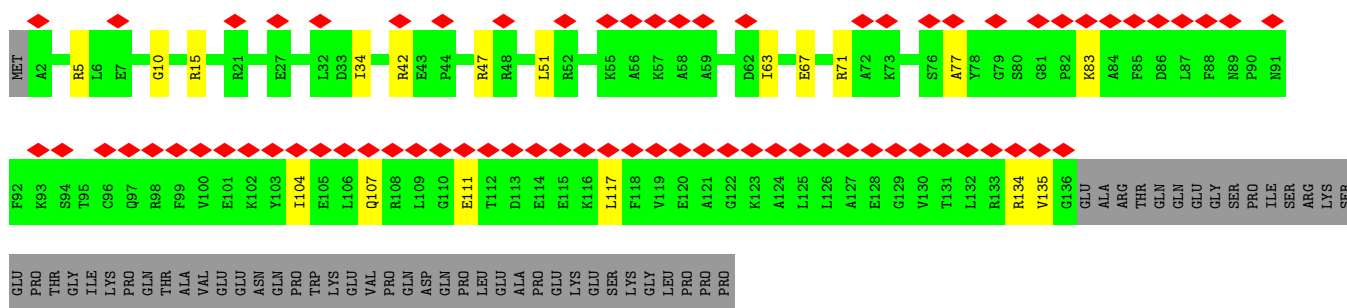
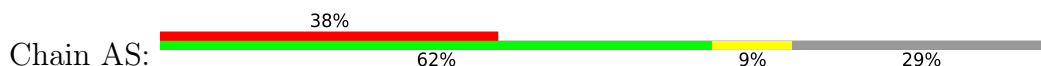
- Molecule 73: Mitochondrial ribosomal protein S22

Chain AR:

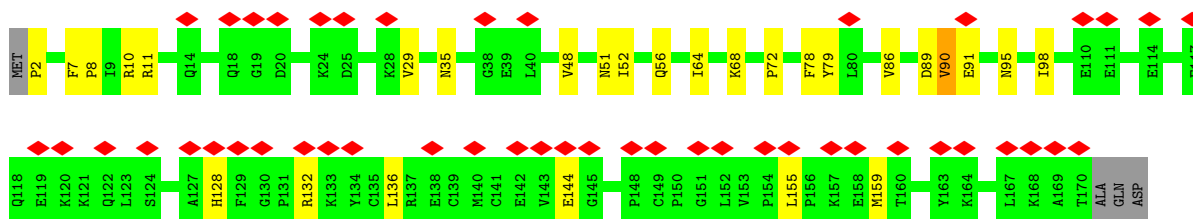
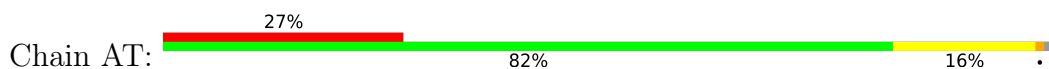




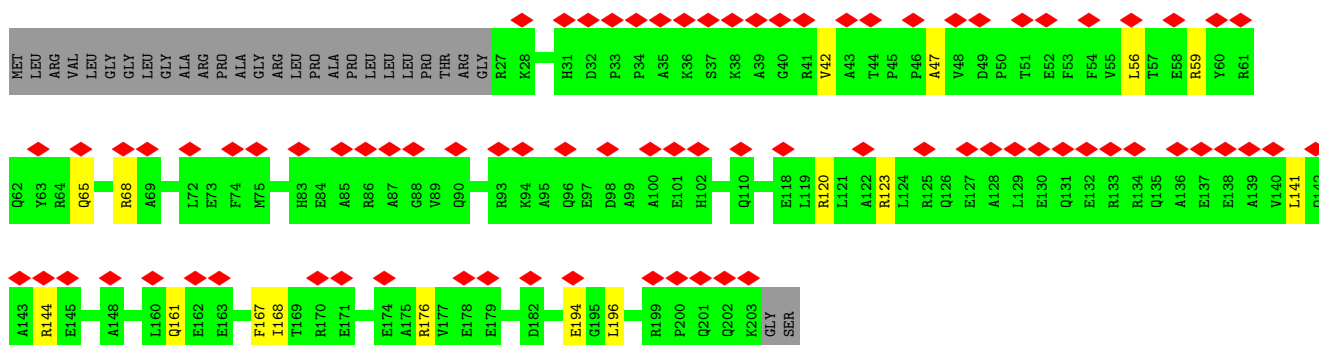
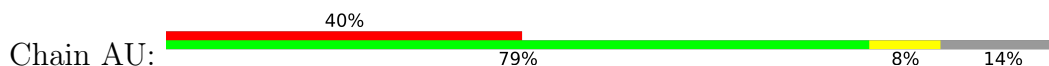
• Molecule 74: mS23



• Molecule 75: Mitochondrial ribosomal protein S25



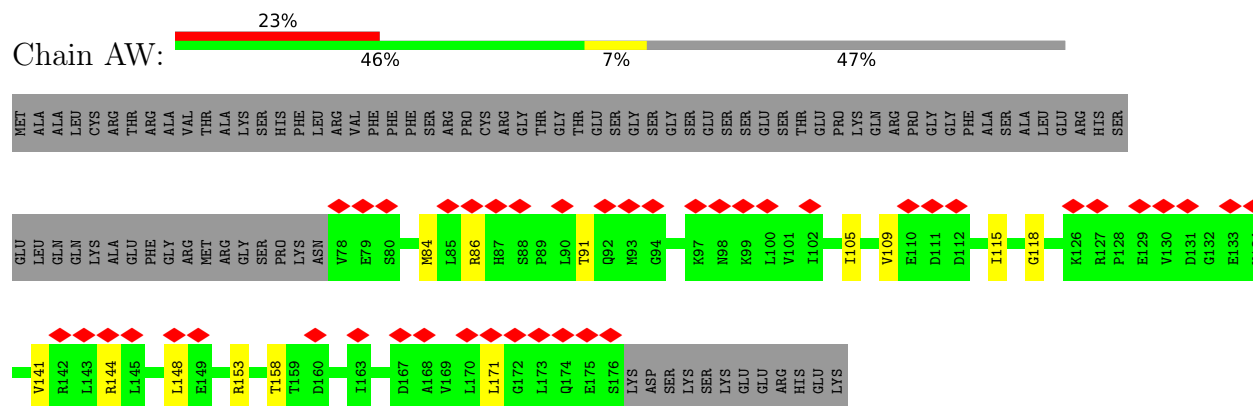
• Molecule 76: Mitochondrial ribosomal protein S26



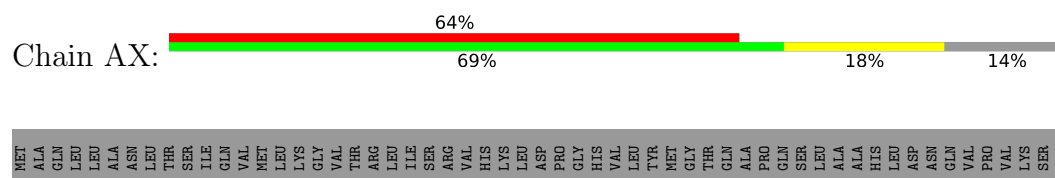
Chain AV:

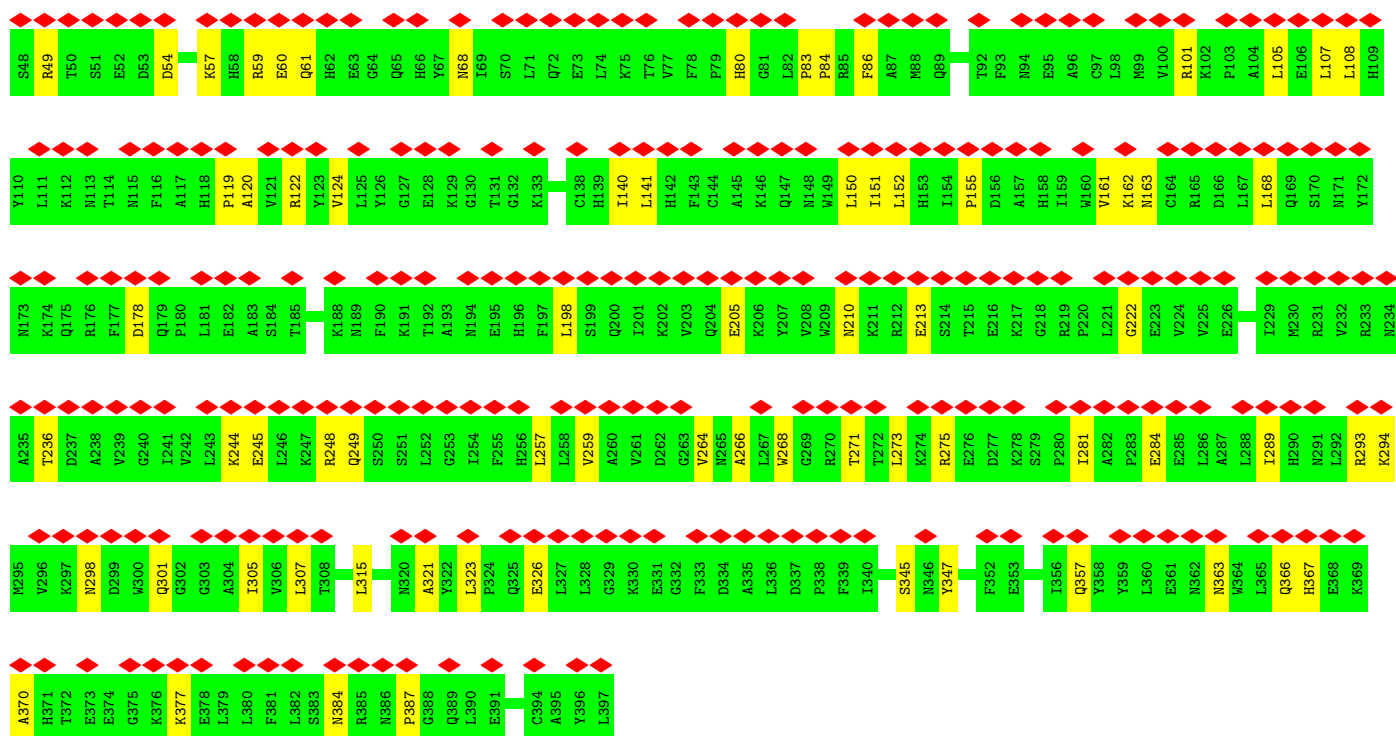


Chain AW:



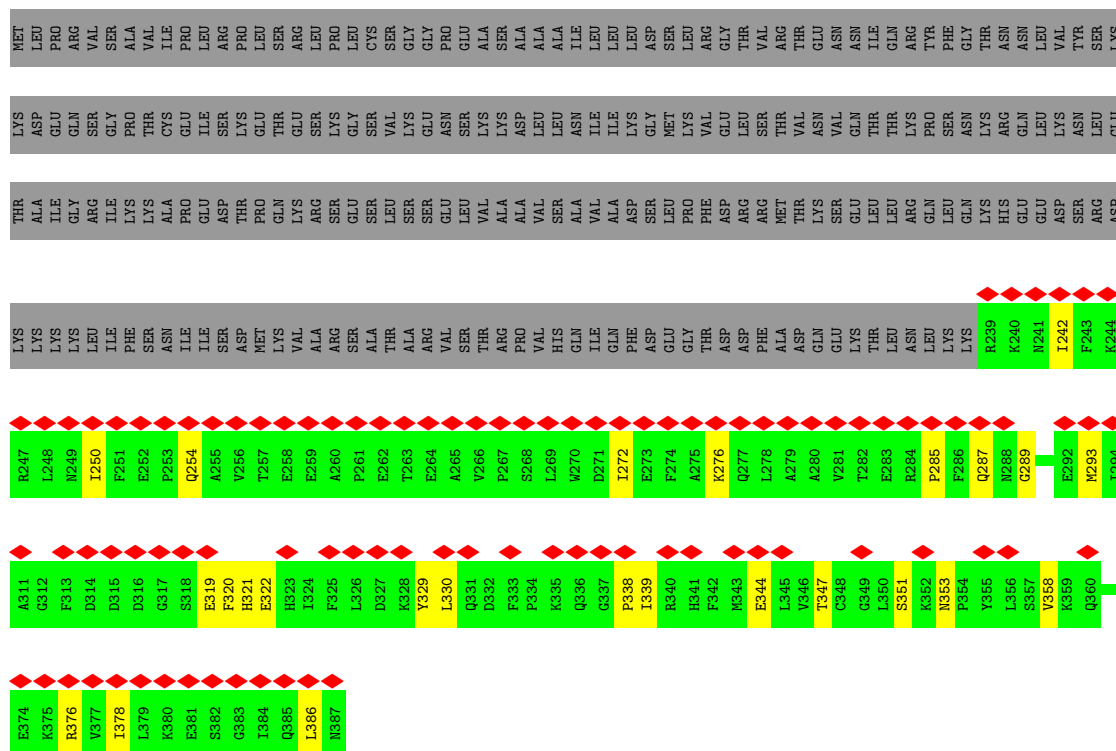
Chain AX:



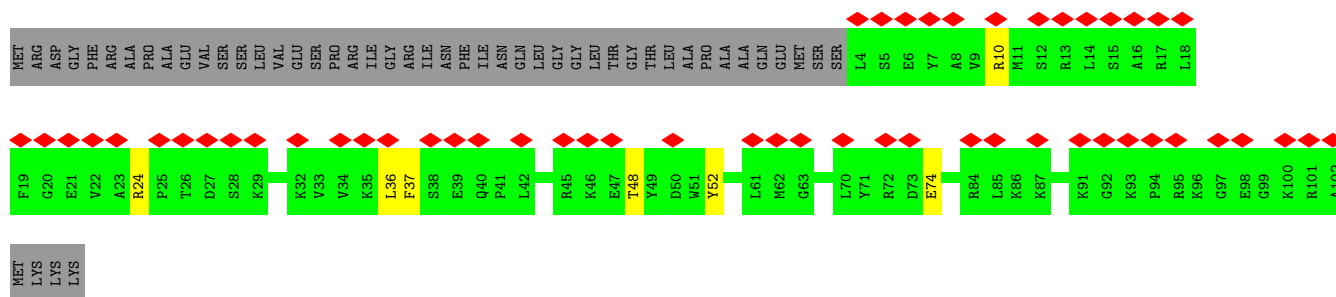


• Molecule 80: 28S ribosomal protein S31, mitochondrial

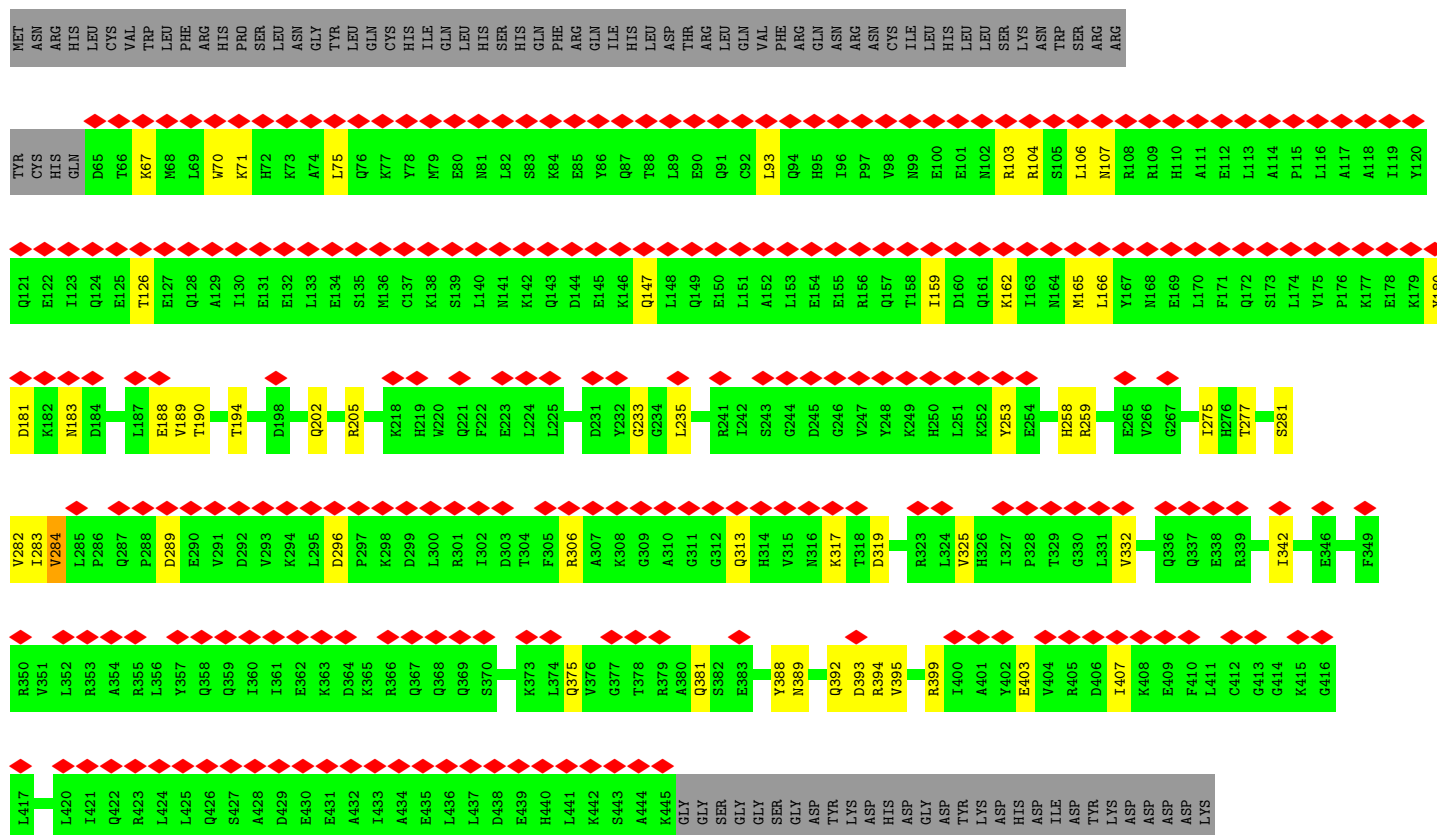
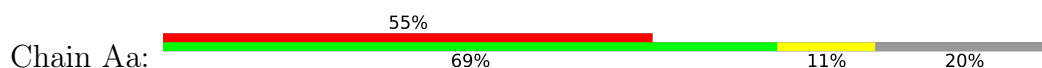
Chain AY: 29% 32% 7% 61%



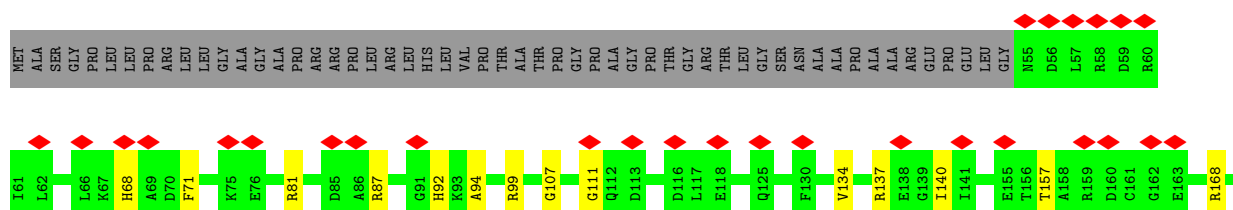
• Molecule 81: Mitochondrial ribosomal protein S33

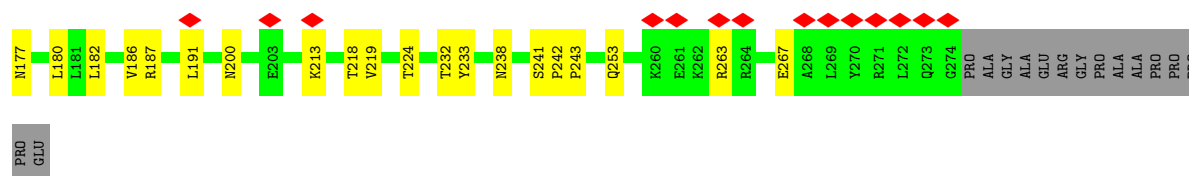


• Molecule 82: Peptide chain release factor 1, mitochondrial

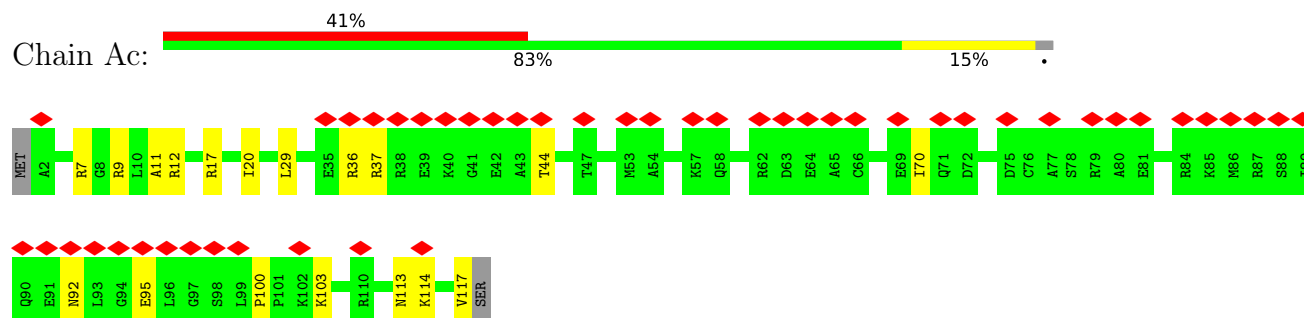


• Molecule 83: Mitochondrial ribosomal protein S2

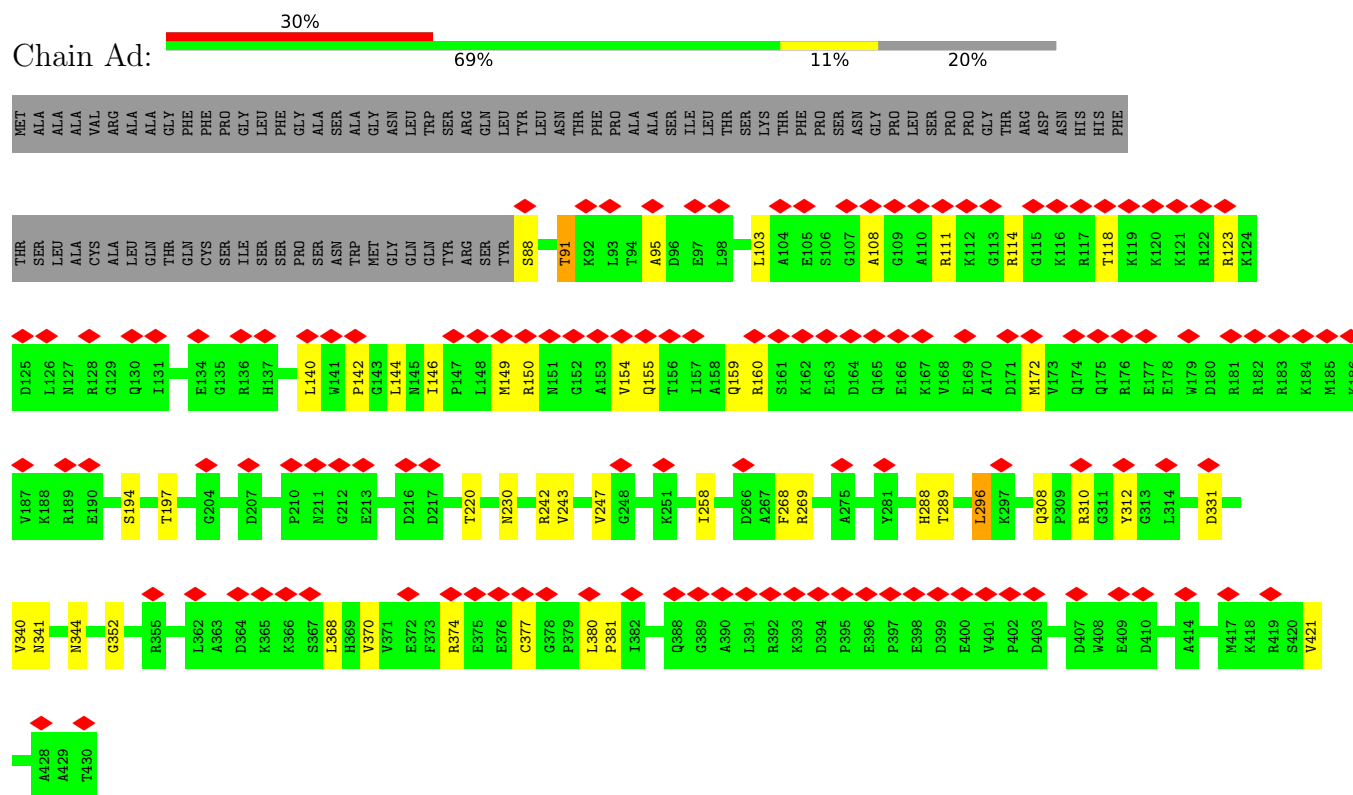




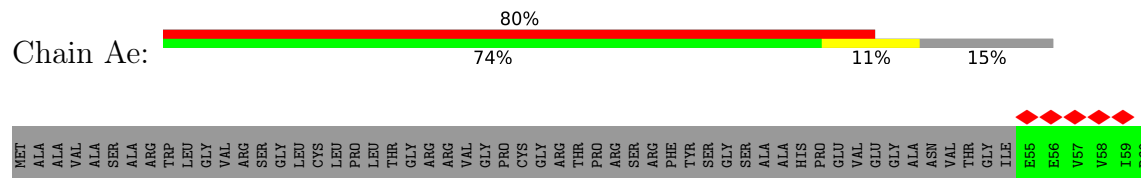
- Molecule 84: Coiled-coil-helix-coiled-coil-helix domain containing 1

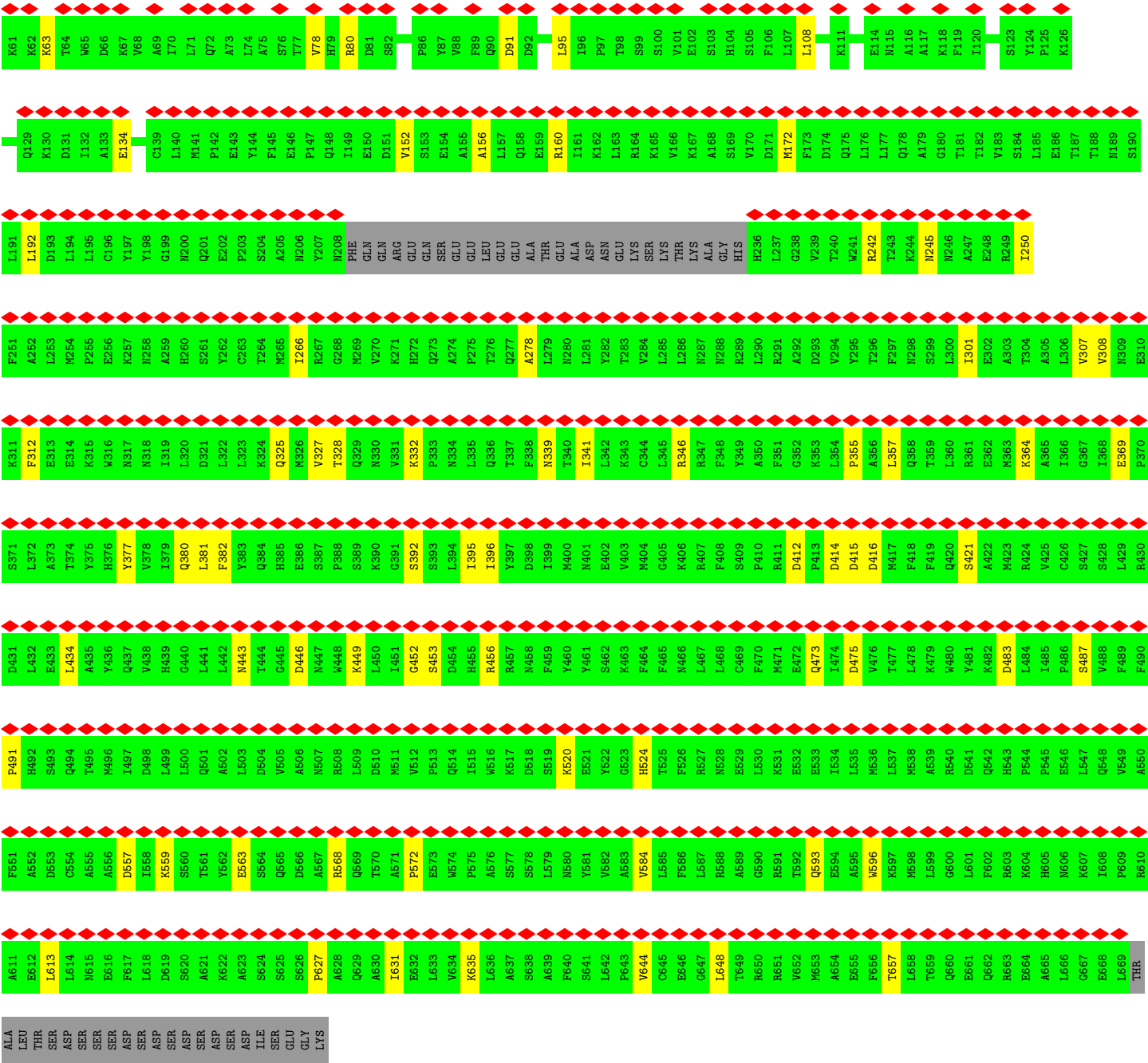


- Molecule 85: 28S ribosomal protein S5, mitochondrial isoform X2

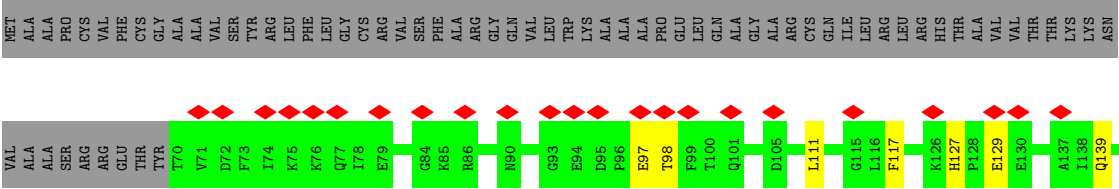
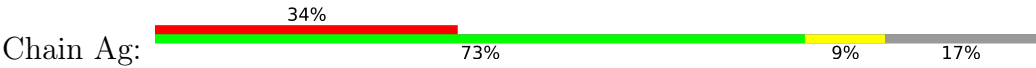


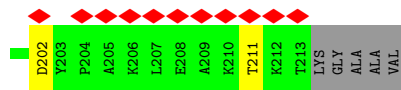
- Molecule 86: mS39





• Molecule 87: uS9m





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50622	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 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.040	Depositor
Minimum map value	-1.903	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.108	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	532.5, 532.5, 532.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.06	0/319	0.17	0/435
1	B2	0.05	0/212	0.16	0/286
1	B3	0.06	0/221	0.18	0/297
1	B4	0.05	0/212	0.13	0/286
1	B5	0.05	0/212	0.12	0/286
1	B6	0.06	0/204	0.19	0/275
2	B7	0.05	0/68	0.10	0/103
3	B8	0.09	0/37315	0.14	0/58099
4	B9	0.07	0/1712	0.14	0/2659
5	BA	0.09	0/1407	0.22	0/1891
6	BB	0.09	0/1206	0.23	0/1639
7	BC	0.08	0/1719	0.23	0/2329
8	BD	0.10	0/890	0.22	0/1202
9	BE	0.07	0/2093	0.19	0/2835
10	BF	0.08	0/1586	0.19	0/2123
11	BG	0.09	0/897	0.22	0/1213
12	BH	0.08	0/917	0.19	0/1227
13	BI	0.07	0/430	0.20	0/570
14	BJ	0.09	0/395	0.19	0/524
15	BK	0.09	0/853	0.20	0/1136
16	BL	0.11	0/1898	0.23	0/2555
17	BM	0.09	0/2493	0.23	0/3387
18	BN	0.11	0/2080	0.25	0/2830
19	BO	0.07	0/1695	0.21	0/2288
20	BP	0.08	0/1742	0.22	0/2358
21	BQ	0.07	0/1359	0.20	0/1828
22	BR	0.24	1/1481 (0.1%)	0.22	0/2009
23	BS	0.09	0/912	0.22	0/1231
24	BT	0.09	0/2368	0.24	0/3198
25	BU	0.09	0/1850	0.23	0/2491
26	BV	0.09	0/1262	0.21	0/1700

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	BW	0.08	0/1197	0.21	0/1624
28	BX	0.11	0/2002	0.23	0/2708
29	BY	0.09	0/1179	0.19	0/1578
30	BZ	0.10	0/1256	0.24	0/1706
31	Ba	0.08	0/787	0.22	0/1056
32	Bb	0.10	0/747	0.23	0/1006
33	Bc	0.06	0/737	0.19	0/997
34	Bd	0.09	0/778	0.26	0/1048
35	Be	0.10	0/798	0.22	0/1073
36	Bf	0.06	0/1214	0.20	0/1630
37	Bg	0.06	0/1157	0.17	0/1560
38	Bh	0.10	0/1364	0.24	0/1849
39	Bi	0.10	0/3206	0.23	0/4354
40	Bj	0.07	0/1350	0.22	0/1823
41	Bl	0.09	0/342	0.18	0/450
42	Bm	0.09	0/3267	0.24	0/4455
43	Bn	0.09	0/3047	0.23	0/4139
44	Bo	0.08	0/2464	0.20	0/3330
45	Bp	0.09	0/1228	0.22	0/1656
46	Bq	0.08	0/1000	0.21	0/1345
47	Br	0.11	0/934	0.26	0/1267
48	Bs	0.11	0/1208	0.24	0/1639
49	Bt	0.09	0/2372	0.22	0/3211
50	Bu	0.08	0/2199	0.22	0/2980
51	Bv	0.06	0/1988	0.19	0/2678
52	Bw	0.10	0/1320	0.29	1/1785 (0.1%)
53	Bx	0.09	0/1135	0.22	0/1549
54	By	0.09	0/917	0.21	0/1248
55	Bz	0.10	0/860	0.21	0/1150
56	AA	0.07	0/22734	0.12	0/35392
57	AB	0.08	0/2268	0.22	0/3069
58	AC	0.09	0/1105	0.25	0/1496
59	AD	0.07	0/650	0.20	0/858
60	AE	0.10	0/999	0.23	0/1347
61	AF	0.07	0/1764	0.20	0/2368
62	AG	0.07	0/1677	0.15	0/2606
63	AH	0.10	0/1181	0.26	0/1597
64	AI	0.07	0/217	0.13	0/337
65	AJ	0.08	0/858	0.21	0/1152
66	AK	0.07	0/874	0.20	0/1171
67	AL	0.07	0/1473	0.18	0/1970
68	AM	0.08	0/954	0.22	0/1284
69	AN	0.08	0/894	0.22	0/1213

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
70	AO	0.08	0/1616	0.22	0/2195
71	AP	0.08	0/802	0.21	0/1079
72	AQ	0.08	0/740	0.21	0/986
73	AR	0.07	0/2428	0.21	0/3279
74	AS	0.07	0/1126	0.19	0/1514
75	AT	0.08	0/1399	0.20	0/1881
76	AU	0.06	0/1490	0.17	0/2005
77	AV	0.08	0/3171	0.23	0/4292
78	AW	0.07	0/790	0.20	0/1064
79	AX	0.07	0/2945	0.21	0/3984
80	AY	0.07	0/1285	0.19	0/1734
81	AZ	0.07	0/841	0.19	0/1121
82	Aa	0.07	0/3171	0.18	0/4263
83	Ab	0.08	0/1804	0.23	0/2445
84	Ac	0.08	0/942	0.28	0/1261
85	Ad	0.08	0/2785	0.20	0/3735
86	Ae	0.07	0/4856	0.18	0/6579
87	Ag	0.07	0/2707	0.21	0/3636
88	Ai	0.09	0/1018	0.27	1/1375 (0.1%)
89	Aj	0.07	0/1835	0.21	0/2484
All	All	0.08	1/189460 (0.0%)	0.19	2/268956 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BR	4	PHE	C-N	-8.51	1.22	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	Bw	68	PRO	N-CA-CB	7.91	110.68	103.33
88	Ai	121	ASN	CB-CA-C	-5.03	110.80	116.63

There are no chirality outliers.

There are no planarity outliers.

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	317	0	309	3	0
1	B2	213	0	234	5	0
1	B3	222	0	247	5	0
1	B4	213	0	234	2	0
1	B5	213	0	234	1	0
1	B6	205	0	223	4	0
2	B7	62	0	34	2	0
3	B8	33427	0	16915	219	0
4	B9	1560	0	798	21	0
5	BA	1374	0	1405	30	0
6	BB	1184	0	1143	14	0
7	BC	1678	0	1683	22	0
8	BD	867	0	886	7	0
9	BE	2036	0	2058	22	0
10	BF	1548	0	1583	15	0
11	BG	874	0	914	12	0
12	BH	902	0	916	16	0
13	BI	425	0	471	4	0
14	BJ	387	0	413	8	0
15	BK	833	0	883	10	0
16	BL	1860	0	1923	19	0
17	BM	2420	0	2418	27	0
18	BN	2019	0	2062	40	0
19	BO	1660	0	1730	29	0
20	BP	1705	0	1804	27	0
21	BQ	1339	0	1407	25	0
22	BR	1447	0	1441	13	0
23	BS	896	0	946	10	0
24	BT	2312	0	2373	29	0
25	BU	1803	0	1841	16	0
26	BV	1240	0	1260	18	0
27	BW	1168	0	1159	19	0
28	BX	1954	0	1943	19	0
29	BY	1159	0	1228	13	0
30	BZ	1231	0	1278	21	0
31	Ba	772	0	773	10	0
32	Bb	745	0	753	13	0
33	Bc	716	0	706	14	0
34	Bd	763	0	747	24	0
35	Be	780	0	792	14	0
36	Bf	1198	0	1192	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	Bg	1131	0	1093	9	0
38	Bh	1325	0	1354	25	0
39	Bi	3126	0	3153	30	0
40	Bj	1325	0	1351	25	0
41	Bl	335	0	359	2	0
42	Bm	3173	0	3153	51	0
43	Bn	2952	0	2839	40	0
44	Bo	2408	0	2415	20	0
45	Bp	1202	0	1205	30	0
46	Bq	972	0	971	16	0
47	Br	906	0	886	13	0
48	Bs	1185	0	1188	17	0
49	Bt	2319	0	2332	28	0
50	Bu	2138	0	2139	27	0
51	Bv	1948	0	1955	35	0
52	Bw	1295	0	1272	20	0
53	Bx	1097	0	1080	11	0
54	By	893	0	878	5	0
55	Bz	837	0	860	12	0
56	AA	20418	0	10343	128	0
57	AB	2222	0	2270	38	0
58	AC	1075	0	1087	27	0
59	AD	639	0	709	5	0
60	AE	981	0	1012	16	0
61	AF	1722	0	1747	20	0
62	AG	1502	0	764	21	0
63	AH	1155	0	1193	15	0
64	AI	193	0	100	3	0
65	AJ	840	0	890	10	0
66	AK	858	0	883	14	0
67	AL	1448	0	1536	18	0
68	AM	932	0	951	14	0
69	AN	875	0	931	15	0
70	AO	1564	0	1531	21	0
71	AP	784	0	813	11	0
72	AQ	737	0	749	10	0
73	AR	2378	0	2392	23	0
74	AS	1101	0	1118	11	0
75	AT	1367	0	1385	19	0
76	AU	1467	0	1466	13	0
77	AV	3109	0	3029	44	0
78	AW	778	0	791	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
79	AX	2875	0	2885	44	0
80	AY	1250	0	1206	26	0
81	AZ	824	0	842	7	0
82	Aa	3120	0	3124	35	0
83	Ab	1762	0	1774	21	0
84	Ac	933	0	963	11	0
85	Ad	2732	0	2774	29	0
86	Ae	4748	0	4733	48	0
87	Ag	2650	0	2613	24	0
88	Ai	1008	0	1036	13	0
89	Aj	1788	0	1799	29	0
90	AA	121	0	0	0	0
90	AD	1	0	0	0	0
90	AG	1	0	0	0	0
90	AI	1	0	0	0	0
90	AJ	1	0	0	0	0
90	AX	1	0	0	0	0
90	Ab	1	0	0	0	0
90	B8	192	0	0	0	0
90	B9	1	0	0	0	0
90	BL	2	0	0	0	0
90	BM	2	0	0	0	0
90	BT	1	0	0	0	0
90	BV	3	0	0	0	0
90	BY	1	0	0	0	0
90	Be	1	0	0	0	0
90	Bq	1	0	0	0	0
90	Bx	1	0	0	0	0
91	AA	11	0	0	0	0
91	B8	25	0	0	0	0
91	BL	1	0	0	0	0
91	BU	1	0	0	0	0
91	BW	1	0	0	0	0
91	Be	1	0	0	0	0
91	Bz	1	0	0	0	0
92	B9	11	0	8	1	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	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
95	AA	14	0	26	3	0
96	AA	10	0	19	0	0
97	AG	10	0	10	0	0
98	AX	31	0	12	0	0
99	AX	28	0	12	3	0
100	AX	3	0	0	0	0
All	All	180624	0	153368	1621	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 5.

All (1621) 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)
18:BN:66:ILE:HD11	18:BN:80:THR:HB	1.43	0.97
27:BW:52:ASN:HD22	43:Bn:267:ARG:HD3	1.44	0.81
22:BR:2:SAC:H2A3	49:Bt:310:ASN:HD21	1.45	0.80
24:BT:47:ARG:HD3	30:BZ:183:ASN:HD22	1.47	0.80
42:Bm:126:THR:HG22	42:Bm:372:ASN:HB2	1.65	0.78
42:Bm:200:ARG:HE	42:Bm:233:LYS:HD2	1.49	0.78
18:BN:249:ASN:ND2	55:Bz:55:GLY:O	2.16	0.77
34:Bd:45:HIS:O	34:Bd:46:ARG:NH1	2.17	0.77
12:BH:144:GLN:HE21	12:BH:173:ARG:HH21	1.32	0.76
45:Bp:67:ARG:NH2	62:AG:10:A:OP2	2.18	0.76
45:Bp:64:ALA:HA	45:Bp:67:ARG:HD2	1.67	0.76
20:BP:95:MET:HB2	20:BP:159:PRO:HB3	1.68	0.74
39:Bi:152:ARG:HH21	42:Bm:280:GLN:HG2	1.52	0.74
31:Ba:113:LYS:NZ	43:Bn:311:MET:O	2.20	0.74
42:Bm:140:ALA:HB2	42:Bm:416:ALA:HB2	1.68	0.73
34:Bd:123:TRP:HE1	80:AY:321:HIS:HB3	1.53	0.73
34:Bd:119:TYR:OH	57:AB:234:GLU:OE1	2.06	0.73
51:Bv:67:GLN:HA	51:Bv:70:MET:HE2	1.71	0.72
17:BM:210:THR:OG1	17:BM:262:GLY:O	2.08	0.72
55:Bz:94:LYS:NZ	55:Bz:102:MET:SD	2.63	0.72
3:B8:831:U:OP2	3:B8:836:A:N6	2.22	0.71
18:BN:283:LEU:HB2	24:BT:125:ARG:HH12	1.54	0.71
56:AA:65:C:N4	56:AA:157:A:O2'	2.23	0.71
56:AA:328:A:OP1	60:AE:90:ARG:NH2	2.19	0.71
24:BT:57:ARG:HG2	24:BT:62:ARG:HH21	1.56	0.71
39:Bi:237:ILE:HG22	39:Bi:239:ARG:H	1.56	0.71
17:BM:206:VAL:HG11	17:BM:289:VAL:HB	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BP:110:LEU:HD11	21:BQ:133:GLN:HG2	1.71	0.70
32:Bb:82:THR:HG23	38:Bh:36:ARG:HH12	1.57	0.70
49:Bt:105:ARG:HH21	49:Bt:112:LYS:HB2	1.56	0.70
7:BC:80:ILE:HB	7:BC:85:TRP:HB2	1.73	0.70
16:BL:74:VAL:HG11	16:BL:149:LYS:HB2	1.74	0.70
35:Be:24:PRO:HD2	38:Bh:169:TRP:HB2	1.73	0.70
20:BP:104:LEU:H	20:BP:109:LYS:HE3	1.55	0.69
79:AX:80:HIS:HB3	79:AX:155:PRO:HG3	1.72	0.69
79:AX:264:VAL:HG21	79:AX:307:LEU:HB3	1.73	0.69
45:Bp:117:LEU:HD21	51:Bv:70:MET:HG2	1.75	0.69
89:Aj:178:ARG:HB2	89:Aj:183:ASP:HB3	1.75	0.69
65:AJ:78:ARG:HG3	65:AJ:118:LEU:HD11	1.74	0.68
1:B1:40:LEU:HB3	1:B4:72:ALA:HA	1.75	0.68
53:Bx:118:TRP:NE1	53:Bx:142:GLU:OE2	2.25	0.68
29:BY:54:THR:HG21	30:BZ:176:MET:H	1.57	0.68
39:Bi:397:GLU:HG2	39:Bi:398:THR:HG22	1.75	0.68
39:Bi:53:ALA:O	39:Bi:62:ARG:NH2	2.26	0.67
71:AP:125:TYR:HB3	72:AQ:9:ALA:HB2	1.75	0.67
17:BM:175:LYS:HD3	17:BM:296:LEU:HB2	1.76	0.67
38:Bh:149:ARG:HD3	38:Bh:152:THR:HG21	1.75	0.67
63:AH:59:THR:HG22	63:AH:61:PRO:HD3	1.76	0.67
82:Aa:189:VAL:HG12	82:Aa:282:VAL:HG22	1.74	0.67
49:Bt:258:THR:HG22	49:Bt:259:ARG:HG3	1.76	0.67
47:Br:80:PRO:HB2	47:Br:84:ILE:HG12	1.74	0.67
55:Bz:35:ARG:NH1	55:Bz:37:THR:O	2.27	0.67
3:B8:175:C:H5''	22:BR:115:ASN:HB2	1.77	0.67
3:B8:417:G:N3	11:BG:109:LYS:NZ	2.43	0.67
40:Bj:97:TYR:HB3	40:Bj:306:LYS:HB2	1.75	0.67
3:B8:129:A:OP1	18:BN:142:ARG:NH2	2.28	0.67
3:B8:565:A:N6	3:B8:1314:U:OP1	2.27	0.67
3:B8:1207:C:O2'	8:BD:88:CYS:SG	2.53	0.67
5:BA:105:GLU:OE1	5:BA:116:LYS:NZ	2.28	0.67
58:AC:60:HIS:HA	66:AK:125:ARG:HG3	1.75	0.67
3:B8:1396:C:N3	82:Aa:306:ARG:NH2	2.43	0.66
24:BT:119:THR:O	24:BT:123:ASN:ND2	2.29	0.66
34:Bd:74:ARG:HH22	51:Bv:121:GLU:HB3	1.60	0.66
82:Aa:183:ASN:ND2	82:Aa:289:ASP:OD1	2.29	0.66
79:AX:259:VAL:HB	79:AX:305:ILE:HG22	1.77	0.66
3:B8:639:U:H5'	5:BA:147:ARG:HH12	1.60	0.66
25:BU:136:MET:HG3	82:Aa:342:ILE:HD13	1.78	0.66
24:BT:109:ARG:HH21	24:BT:125:ARG:HB2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Bo:85:PRO:HG2	44:Bo:112:MET:HA	1.76	0.66
38:Bh:71:PRO:HD2	38:Bh:107:LEU:HD23	1.79	0.65
3:B8:644:G:N2	3:B8:1008:A:OP2	2.29	0.65
56:AA:468:A:OP2	83:Ab:99:ARG:NH2	2.29	0.65
3:B8:1014:A:H5''	29:BY:34:ARG:HH21	1.60	0.65
18:BN:59:ARG:HH12	24:BT:10:PRO:HD3	1.61	0.65
3:B8:458:A:O2'	3:B8:467:A:O2'	2.14	0.65
27:BW:149:THR:HG22	27:BW:150:PRO:HD2	1.77	0.65
77:AV:86:GLU:HG3	77:AV:114:ARG:HG2	1.79	0.65
7:BC:126:THR:OG1	7:BC:152:ARG:NH1	2.30	0.65
56:AA:328:A:N6	56:AA:366:A:N1	2.45	0.65
21:BQ:31:PRO:HA	21:BQ:46:ILE:HG21	1.79	0.64
77:AV:258:SER:HB3	77:AV:311:GLU:HB3	1.79	0.64
3:B8:125:A:OP1	14:BJ:85:ARG:NH1	2.30	0.64
50:Bu:90:PRO:HB2	50:Bu:269:TRP:HH2	1.62	0.64
50:Bu:267:PRO:HG2	50:Bu:270:ALA:HB2	1.78	0.64
27:BW:51:ARG:NH1	43:Bn:228:PRO:O	2.29	0.64
56:AA:648:A:OP1	83:Ab:200:ASN:ND2	2.29	0.64
86:Ae:242:ARG:O	86:Ae:245:ASN:ND2	2.29	0.64
9:BE:16:LEU:HD12	9:BE:21:TYR:HB3	1.78	0.64
61:AF:240:ARG:NH2	84:Ac:44:THR:O	2.31	0.64
23:BS:34:LYS:HG2	23:BS:35:MET:HG2	1.79	0.64
3:B8:62:C:OP1	19:BO:76:ARG:NH1	2.31	0.64
9:BE:196:ILE:HG12	9:BE:197:PRO:HD2	1.80	0.64
11:BG:68:ILE:HD11	11:BG:122:LEU:HD13	1.80	0.64
28:BX:76:LEU:HD21	28:BX:282:ILE:HD11	1.79	0.64
45:Bp:67:ARG:CZ	62:AG:43:A:H4'	2.28	0.64
17:BM:90:TRP:NE1	17:BM:311:CYS:SG	2.70	0.64
25:BU:124:VAL:HG12	25:BU:158:ARG:HE	1.62	0.64
3:B8:493:A:O2'	3:B8:494:U:O2	2.14	0.64
56:AA:306:G:H2'	56:AA:307:A:H8	1.61	0.63
77:AV:405:LEU:O	77:AV:409:GLU:N	2.25	0.63
50:Bu:192:PRO:HB3	50:Bu:216:MET:HG2	1.80	0.63
3:B8:530:A:O2'	3:B8:547:A:N1	2.30	0.63
56:AA:375:A:H62	84:Ac:17:ARG:HH22	1.46	0.63
73:AR:285:ARG:NH2	73:AR:309:ASP:OD2	2.31	0.63
13:BI:59:GLN:HG2	13:BI:60:LYS:HG3	1.80	0.63
20:BP:93:ASN:ND2	20:BP:157:GLU:OE2	2.32	0.63
56:AA:869:A:N6	56:AA:899:C:O2'	2.31	0.63
79:AX:284:GLU:OE2	79:AX:293:ARG:NH2	2.32	0.63
19:BO:193:PHE:HB3	19:BO:199:VAL:HB	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BS:43:ASN:HD21	23:BS:117:THR:HB	1.63	0.63
5:BA:152:LYS:NZ	5:BA:166:GLU:OE2	2.31	0.63
10:BF:204:MET:HE3	10:BF:205:PRO:HD2	1.81	0.63
20:BP:224:HIS:HA	20:BP:227:ARG:HE	1.63	0.63
42:Bm:201:ARG:HB3	42:Bm:230:LEU:HD11	1.81	0.63
56:AA:83:C:O2'	56:AA:99:A:N6	2.32	0.63
62:AG:30:C:OP2	87:Ag:397:ARG:NH2	2.32	0.62
3:B8:396:C:O2'	3:B8:414:A:N6	2.27	0.62
17:BM:50:ASP:OD1	26:BV:139:ARG:NH2	2.32	0.62
68:AM:114:ARG:HD3	70:AO:235:MET:HB3	1.82	0.62
80:AY:330:LEU:HD11	80:AY:347:THR:HG21	1.79	0.62
3:B8:1349:G:HO2'	41:Bl:63:PHE:N	1.98	0.62
24:BT:114:GLN:OE1	53:Bx:50:ARG:NH1	2.32	0.62
79:AX:107:LEU:HD23	79:AX:140:ILE:HG13	1.82	0.62
31:Ba:63:GLN:OE1	31:Ba:66:ARG:NH1	2.33	0.62
70:AO:190:ALA:HB2	89:Aj:171:ARG:HH22	1.63	0.62
79:AX:294:LYS:NZ	99:AX:503:GDP:O1A	2.33	0.62
85:Ad:140:LEU:HB3	85:Ad:146:ILE:HD13	1.82	0.62
16:BL:113:ARG:O	16:BL:148:ARG:NH2	2.32	0.62
5:BA:82:LYS:HD3	5:BA:147:ARG:HB3	1.82	0.62
77:AV:80:TRP:HA	77:AV:83:ARG:HG3	1.82	0.62
19:BO:118:VAL:HG13	19:BO:122:ARG:HE	1.65	0.62
57:AB:154:ASP:HB2	57:AB:174:THR:HB	1.81	0.62
5:BA:92:ILE:HA	5:BA:95:MET:HE2	1.81	0.62
40:Bj:118:ASN:OD1	40:Bj:261:ASN:ND2	2.33	0.62
51:Bv:113:ASN:ND2	51:Bv:115:LEU:O	2.33	0.62
45:Bp:193:GLN:HB2	52:Bw:133:GLU:HB3	1.82	0.62
60:AE:37:ARG:NH2	60:AE:69:TYR:OH	2.32	0.62
3:B8:293:U:O2'	3:B8:1434:U:O2'	2.16	0.61
17:BM:196:ALA:O	17:BM:199:ARG:NH1	2.32	0.61
25:BU:96:TYR:OH	25:BU:129:LYS:NZ	2.31	0.61
3:B8:877:U:H5''	3:B8:878:G:H5'	1.82	0.61
18:BN:262:THR:HG22	18:BN:264:PRO:HD2	1.82	0.61
60:AE:51:ILE:HB	60:AE:89:ILE:HD11	1.82	0.61
70:AO:89:ARG:HG3	70:AO:144:MET:HE3	1.83	0.61
77:AV:83:ARG:HH12	77:AV:154:ARG:HG3	1.65	0.61
80:AY:254:GLN:HE22	86:Ae:332:LYS:HB3	1.64	0.61
65:AJ:62:VAL:HA	65:AJ:83:VAL:HG12	1.82	0.61
89:Aj:135:MET:SD	89:Aj:135:MET:N	2.73	0.61
25:BU:211:ASN:ND2	25:BU:213:TRP:O	2.33	0.61
34:Bd:51:ARG:NH1	51:Bv:88:GLU:OE2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Ab:238:ASN:ND2	83:Ab:241:SER:OG	2.34	0.61
3:B8:112:A:N6	3:B8:115:U:OP2	2.32	0.61
69:AN:29:ARG:HD3	69:AN:46:ARG:HD2	1.82	0.61
79:AX:363:ASN:O	79:AX:366:GLN:NE2	2.33	0.61
10:BF:127:PRO:HB3	50:Bu:67:ILE:HD11	1.82	0.61
30:BZ:150:LYS:HE3	47:Br:58:ILE:HD11	1.82	0.61
67:AL:176:TYR:HB2	69:AN:89:GLY:HA3	1.82	0.61
48:Bs:45:GLU:OE1	48:Bs:49:ARG:NH1	2.34	0.61
48:Bs:85:ARG:NH1	48:Bs:107:GLN:OE1	2.34	0.61
72:AQ:43:ARG:NH2	72:AQ:44:TYR:OH	2.33	0.61
42:Bm:275:ASP:OD2	42:Bm:326:ARG:NH1	2.34	0.61
57:AB:73:PRO:HB3	86:Ae:78:VAL:HG11	1.83	0.61
77:AV:74:TYR:HD2	77:AV:409:GLU:HG2	1.66	0.61
77:AV:189:ASP:HA	77:AV:192:ILE:HD12	1.83	0.61
79:AX:122:ARG:HG2	79:AX:305:ILE:HD11	1.82	0.61
82:Aa:394[B]:ARG:NH1	82:Aa:403:GLU:OE1	2.34	0.61
3:B8:216:C:OP2	53:Bx:111:ARG:NH2	2.34	0.60
36:Bf:96:SER:O	36:Bf:145:ASN:ND2	2.34	0.60
84:Ac:36:ARG:NH2	84:Ac:92:ASN:OD1	2.35	0.60
3:B8:62:C:OP2	19:BO:75:ARG:NH2	2.34	0.60
3:B8:1275:C:H4'	82:Aa:317:LYS:HG3	1.82	0.60
3:B8:1399:G:O2'	3:B8:1402:C:OP2	2.19	0.60
23:BS:46:LEU:HD12	23:BS:78:ARG:HD3	1.83	0.60
56:AA:115:A:OP1	67:AL:203:ARG:NH2	2.33	0.60
3:B8:640:A:OP1	5:BA:147:ARG:NH1	2.34	0.60
3:B8:1289:U:H5''	41:Bl:68:VAL:HG12	1.83	0.60
50:Bu:244:GLU:HG2	50:Bu:264:LYS:HE2	1.83	0.60
56:AA:90:U:OP1	76:AU:68:ARG:NH1	2.34	0.60
3:B8:188:C:O2'	3:B8:190:U:OP2	2.20	0.60
3:B8:472:U:H5''	11:BG:74:SER:HB3	1.83	0.60
5:BA:96:SER:H	5:BA:99:GLN:HE21	1.49	0.60
7:BC:146:VAL:HG22	7:BC:153:ILE:HG22	1.83	0.60
26:BV:77:ASP:OD1	26:BV:83:LYS:NZ	2.33	0.60
26:BV:113:ARG:NH2	26:BV:117:ASP:OD2	2.31	0.60
45:Bp:193:GLN:O	52:Bw:133:GLU:N	2.27	0.60
9:BE:120:ASP:OD2	9:BE:177:HIS:NE2	2.35	0.59
46:Bq:127:GLN:HB3	46:Bq:130:PRO:HD2	1.83	0.59
50:Bu:80:CYS:SG	50:Bu:165:THR:OG1	2.60	0.59
77:AV:157:LEU:HA	77:AV:161:ALA:HB2	1.84	0.59
82:Aa:194:THR:HG21	82:Aa:381:GLN:HG3	1.84	0.59
3:B8:1230:U:H5'	3:B8:1231:U:H5'	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BF:220:ARG:NH2	55:Bz:105:ASP:OD2	2.35	0.59
70:AO:235:MET:SD	70:AO:235:MET:N	2.74	0.59
28:BX:252:GLU:OE1	28:BX:255:ARG:NH2	2.35	0.59
39:Bi:152:ARG:NH1	42:Bm:276:ASP:OD1	2.36	0.59
42:Bm:140:ALA:HB1	42:Bm:412:ARG:HG2	1.84	0.59
47:Br:79:ASP:HB3	47:Br:80:PRO:HD3	1.84	0.59
56:AA:722:A:N6	56:AA:738:U:O2'	2.35	0.59
87:Ag:97:GLU:HG3	87:Ag:98:THR:HG23	1.84	0.59
18:BN:69:LEU:HD22	18:BN:206:LEU:HD21	1.85	0.59
42:Bm:59:THR:HB	42:Bm:73:PRO:HG3	1.83	0.59
42:Bm:215:ARG:NH1	42:Bm:367:ASP:OD1	2.33	0.59
3:B8:1095:C:H4'	19:BO:247:ARG:HD2	1.84	0.59
24:BT:203:ARG:HH21	24:BT:262:PRO:HA	1.67	0.59
40:Bj:290:VAL:HG11	40:Bj:307:ILE:HD13	1.84	0.59
66:AK:66:ASP:HB3	80:AY:378:ILE:HD11	1.84	0.59
3:B8:528:U:O3'	33:Bc:115:ARG:NH2	2.36	0.59
3:B8:995:C:H5''	26:BV:13:ARG:HH12	1.68	0.59
19:BO:225:VAL:HG22	40:Bj:86:VAL:HB	1.83	0.59
49:Bt:105:ARG:HH12	49:Bt:110:ILE:HB	1.68	0.59
79:AX:120:ALA:O	79:AX:298:ASN:ND2	2.35	0.59
6:BB:26:ILE:HD12	6:BB:44:ILE:HG22	1.83	0.59
56:AA:568:G:N2	56:AA:577:C:O2	2.36	0.59
3:B8:127:G:OP2	14:BJ:88:LYS:NZ	2.34	0.59
3:B8:183:U:OP1	24:BT:47:ARG:NH1	2.31	0.59
3:B8:869:G:O2'	3:B8:966:U:OP2	2.19	0.59
38:Bh:35:PHE:N	38:Bh:56:THR:OG1	2.35	0.59
21:BQ:87:VAL:HG22	21:BQ:124:LYS:HE3	1.85	0.59
68:AM:51:LEU:HD13	68:AM:73:ILE:HG12	1.84	0.59
56:AA:689:G:H5'	85:Ad:91:THR:HG22	1.85	0.59
69:AN:65:LEU:HB2	69:AN:85:ILE:HD11	1.84	0.59
77:AV:125:ILE:HG21	77:AV:164:LYS:HD3	1.85	0.59
79:AX:124:VAL:HG12	79:AX:307:LEU:HB2	1.85	0.59
62:AG:8:U:H3	62:AG:14:A:H62	1.49	0.58
70:AO:68:TYR:OH	70:AO:110:ASP:OD2	2.20	0.58
77:AV:298:ARG:NH2	89:Aj:146:GLU:OE2	2.36	0.58
86:Ae:446:ASP:HB3	86:Ae:449:LYS:HE2	1.84	0.58
3:B8:164:A:OP1	29:BY:52:LYS:NZ	2.36	0.58
47:Br:72:THR:O	49:Bt:256:ARG:NH2	2.37	0.58
86:Ae:266:ILE:HG23	86:Ae:278:ALA:HB1	1.84	0.58
83:Ab:177:ASN:HD21	83:Ab:180:LEU:HD22	1.69	0.58
21:BQ:149:ARG:NH2	33:Bc:102:GLY:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BZ:198:ARG:NH2	48:Bs:13:SER:OG	2.36	0.58
42:Bm:160:HIS:HA	42:Bm:164:TRP:HB2	1.85	0.58
51:Bv:178:TRP:NE1	51:Bv:182:GLU:O	2.37	0.58
3:B8:195:G:OP1	3:B8:633:U:O2'	2.21	0.58
51:Bv:60:THR:O	51:Bv:136:ARG:NH2	2.31	0.58
80:AY:329:TYR:O	80:AY:369:ARG:NH2	2.36	0.58
87:Ag:203:LYS:NZ	87:Ag:216:ASP:OD1	2.34	0.58
1:B5:83:ASN:ND2	20:BP:234:ASP:OD1	2.36	0.58
8:BD:107:ASN:ND2	8:BD:109:SER:OG	2.37	0.58
32:Bb:14:LYS:HE3	32:Bb:69:GLY:HA2	1.86	0.58
33:Bc:114:THR:HG22	33:Bc:116:GLU:H	1.69	0.58
82:Aa:306:ARG:NH1	82:Aa:319:ASP:OD1	2.37	0.58
56:AA:29:A:H1'	65:AJ:57:GLN:HE22	1.69	0.58
28:BX:183:LEU:HD21	28:BX:219:GLN:HG3	1.85	0.58
32:Bb:80:HIS:O	38:Bh:36:ARG:NH1	2.33	0.58
50:Bu:82:ALA:O	50:Bu:167:ASN:ND2	2.37	0.58
50:Bu:189:LEU:HB2	50:Bu:217:HIS:HD2	1.69	0.58
51:Bv:185:ARG:HH21	51:Bv:204:PHE:HB2	1.69	0.58
57:AB:120:ALA:O	57:AB:124:HIS:ND1	2.35	0.58
58:AC:38:ARG:HG2	58:AC:43:ARG:HH21	1.69	0.58
63:AH:74:LYS:HB2	63:AH:177:LEU:HD23	1.86	0.58
69:AN:18:ILE:HD11	69:AN:29:ARG:HB2	1.86	0.58
78:AW:105:ILE:HG12	78:AW:115:ILE:HG12	1.86	0.58
80:AY:344:GLU:OE2	81:AZ:24:ARG:NE	2.34	0.58
3:B8:60:U:O2'	9:BE:96:LYS:O	2.21	0.57
3:B8:987:G:N2	3:B8:991:C:O2'	2.37	0.57
21:BQ:17:SER:N	21:BQ:72:VAL:O	2.37	0.57
50:Bu:161:HIS:O	50:Bu:260:ARG:NH2	2.37	0.57
60:AE:24:ARG:NH1	60:AE:85:ASP:OD2	2.36	0.57
71:AP:125:TYR:HE1	72:AQ:4:HIS:HB3	1.67	0.57
3:B8:130:A:OP1	18:BN:147:ARG:NH2	2.37	0.57
22:BR:26:GLN:NE2	22:BR:147:GLN:OE1	2.37	0.57
24:BT:12:ALA:HB2	35:Be:88:LEU:HD13	1.86	0.57
53:Bx:110:ILE:HD11	53:Bx:157:LEU:HD13	1.87	0.57
62:AG:5:A:H2	62:AG:63:G:H1	1.52	0.57
76:AU:168:ILE:HG12	76:AU:176:ARG:HG3	1.86	0.57
77:AV:238:TRP:HZ2	77:AV:282:ALA:HB3	1.69	0.57
86:Ae:416:ASP:HB2	86:Ae:452:GLY:HA2	1.86	0.57
66:AK:28:TYR:O	85:Ad:88:SER:N	2.37	0.57
68:AM:100:HIS:HD2	68:AM:102:MET:HB2	1.70	0.57
7:BC:64:ILE:HD11	7:BC:88:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BF:89:CYS:SG	10:BF:93:ARG:NH1	2.78	0.57
15:BK:175:ASP:HB3	15:BK:178:GLN:HB2	1.86	0.57
45:Bp:203:GLU:OE1	52:Bw:201:ARG:NH1	2.37	0.57
56:AA:199:G:N2	56:AA:202:A:OP2	2.37	0.57
70:AO:167:ILE:HD12	73:AR:252:LEU:HD21	1.86	0.57
86:Ae:307:VAL:HG12	86:Ae:308:VAL:HG13	1.86	0.57
3:B8:123:U:O2	3:B8:254:G:N2	2.37	0.57
6:BB:46:MET:HE1	6:BB:72:VAL:HG13	1.87	0.57
42:Bm:228:ALA:HB3	42:Bm:292:TYR:HB2	1.87	0.57
89:Aj:194:GLU:OE2	89:Aj:197:ARG:NH2	2.36	0.57
5:BA:67:ARG:HD2	50:Bu:228:PHE:HB3	1.86	0.57
27:BW:173:ARG:NH1	27:BW:174:GLU:O	2.38	0.57
36:Bf:188:ARG:HH12	43:Bn:179:VAL:HG11	1.69	0.57
48:Bs:133:PHE:HZ	49:Bt:261:SER:HB2	1.70	0.57
3:B8:96:U:N3	37:Bg:34:SER:O	2.38	0.57
21:BQ:101:ALA:HB2	21:BQ:109:ALA:HB2	1.87	0.57
21:BQ:155:VAL:HG23	33:Bc:101:VAL:HG13	1.87	0.57
34:Bd:39:ALA:HB3	52:Bw:179:PRO:HG3	1.87	0.57
56:AA:532:G:O2'	56:AA:959:U:N3	2.38	0.57
57:AB:70:SER:HA	86:Ae:78:VAL:HG13	1.87	0.57
72:AQ:87:CYS:O	83:Ab:168:ARG:NH1	2.36	0.57
74:AS:10:GLY:O	74:AS:15:ARG:NH1	2.37	0.57
89:Aj:43:ARG:HH21	89:Aj:50:LEU:HD21	1.69	0.57
2:B7:76:A:O2'	3:B8:1235:C:N3	2.36	0.57
3:B8:573:A:H5'	22:BR:29:GLY:HA3	1.86	0.57
77:AV:147:TRP:HB3	77:AV:423:TRP:CD2	2.40	0.57
13:BI:16:ILE:HD12	13:BI:64:SER:HA	1.87	0.56
74:AS:134:ARG:NH1	74:AS:135:VAL:O	2.38	0.56
34:Bd:123:TRP:NE1	80:AY:321:HIS:HB3	2.20	0.56
42:Bm:248:THR:HG22	42:Bm:371:LYS:HB2	1.86	0.56
50:Bu:186:VAL:HG22	50:Bu:187:GLU:HG3	1.87	0.56
89:Aj:68:LEU:HD12	89:Aj:71:LEU:HD12	1.87	0.56
3:B8:843:C:O2'	16:BL:258:ILE:O	2.14	0.56
19:BO:154:LYS:HA	19:BO:228:LEU:HD13	1.86	0.56
40:Bj:128:ASP:N	40:Bj:289:PHE:O	2.37	0.56
44:Bo:80:LYS:NZ	44:Bo:117:THR:O	2.38	0.56
44:Bo:191:PRO:HD2	44:Bo:280:VAL:HG21	1.87	0.56
48:Bs:26:LEU:HD21	48:Bs:29:LEU:HD11	1.86	0.56
58:AC:113:ARG:NH1	58:AC:118:GLU:OE2	2.30	0.56
65:AJ:70:PRO:HB3	65:AJ:117:ASP:HB3	1.88	0.56
71:AP:95:ARG:HH12	71:AP:102:GLY:HA2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:AT:91:GLU:OE2	76:AU:123:ARG:NH2	2.37	0.56
3:B8:885:G:H1	3:B8:894:U:H3	1.54	0.56
34:Bd:62:GLY:HA3	45:Bp:182:ILE:HG12	1.87	0.56
49:Bt:60:ARG:NH1	49:Bt:65:ASN:O	2.39	0.56
52:Bw:122:GLU:OE1	52:Bw:158:GLN:NE2	2.38	0.56
70:AO:202:TRP:O	76:AU:59:ARG:NH1	2.38	0.56
73:AR:129:THR:HG22	85:Ad:368:LEU:HD22	1.88	0.56
77:AV:154:ARG:NH2	77:AV:416:TYR:OH	2.38	0.56
48:Bs:73:PRO:HB2	48:Bs:89:ILE:HG13	1.87	0.56
67:AL:74:LEU:HD12	67:AL:76:ASP:H	1.69	0.56
82:Aa:395:VAL:HG23	82:Aa:407:ILE:HG12	1.88	0.56
3:B8:52:A:O2'	3:B8:349:A:N3	2.38	0.56
51:Bv:46:ARG:H	51:Bv:229:ALA:HA	1.71	0.56
82:Aa:188:GLU:HB2	82:Aa:283:ILE:HB	1.88	0.56
86:Ae:80:ARG:NH2	86:Ae:483:ASP:O	2.35	0.56
32:Bb:66:VAL:HG11	32:Bb:90:PHE:HE1	1.71	0.56
16:BL:199:SER:HB3	16:BL:207:TYR:HE1	1.71	0.56
40:Bj:108:LYS:HE2	40:Bj:112:LEU:HD11	1.88	0.56
88:Ai:73:ASN:O	88:Ai:76:ARG:NH1	2.39	0.56
11:BG:78:ARG:O	11:BG:83:LYS:NZ	2.39	0.56
87:Ag:366:ARG:HG3	87:Ag:371:LEU:HD12	1.87	0.56
9:BE:174:PRO:O	9:BE:184:ARG:NH2	2.36	0.55
20:BP:47:LEU:HD22	25:BU:226:ILE:HG12	1.87	0.55
28:BX:182:ARG:HD3	28:BX:187:LEU:HD11	1.87	0.55
42:Bm:201:ARG:HD3	42:Bm:230:LEU:HD21	1.87	0.55
42:Bm:377:ASP:HB3	42:Bm:380:GLN:HE21	1.71	0.55
56:AA:869:A:OP2	56:AA:900:A:N6	2.34	0.55
28:BX:165:GLU:HB2	28:BX:168:ASN:HB2	1.88	0.55
54:By:77:GLU:HG3	54:By:78:VAL:HG13	1.88	0.55
56:AA:353:C:H5''	56:AA:354:C:H5''	1.87	0.55
89:Aj:29:ARG:H	89:Aj:32:GLN:HE21	1.53	0.55
51:Bv:87:HIS:NE2	51:Bv:121:GLU:OE2	2.39	0.55
58:AC:163:VAL:HG21	58:AC:167:ILE:HD12	1.87	0.55
89:Aj:88:GLN:NE2	89:Aj:202:ASP:OD2	2.39	0.55
3:B8:218:A:N6	3:B8:229:A:O4'	2.40	0.55
48:Bs:144:ARG:HB2	48:Bs:147:GLU:HB2	1.89	0.55
82:Aa:70:TRP:HA	82:Aa:75:LEU:HD23	1.87	0.55
32:Bb:73:ARG:HB3	38:Bh:46:THR:HG22	1.89	0.55
20:BP:99:CYS:O	20:BP:152:LEU:N	2.37	0.55
24:BT:140:LEU:HG	24:BT:156:VAL:HG11	1.88	0.55
35:Be:102:SER:O	48:Bs:35:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AA:386:U:O2'	60:AE:93:ILE:O	2.23	0.55
57:AB:196:VAL:HG21	57:AB:207:LEU:HD11	1.88	0.55
68:AM:105:THR:HG21	76:AU:56:LEU:HD13	1.89	0.55
73:AR:303:ILE:HG22	73:AR:307:LEU:HG	1.88	0.55
82:Aa:202:GLN:NE2	82:Aa:233:GLY:O	2.40	0.55
56:AA:386:U:H4'	60:AE:94:VAL:HG12	1.88	0.55
87:Ag:161:LEU:HD22	87:Ag:210:LEU:HD21	1.88	0.55
3:B8:222:G:H1	55:Bz:61:GLY:HA3	1.71	0.55
14:BJ:66:LYS:HA	14:BJ:71:ARG:HH11	1.72	0.55
46:Bq:122:GLU:HA	46:Bq:127:GLN:HE21	1.72	0.55
61:AF:155:VAL:HG11	84:Ac:70:ILE:HD12	1.89	0.55
86:Ae:346:ARG:HA	86:Ae:381:LEU:HD13	1.89	0.55
3:B8:7:G:OP2	3:B8:7:G:N2	2.39	0.55
79:AX:60:GLU:HA	79:AX:105:LEU:HD13	1.89	0.55
17:BM:111:THR:OG1	17:BM:113:ASP:OD1	2.24	0.54
61:AF:142:TYR:O	61:AF:146:HIS:ND1	2.41	0.54
64:AI:3:A:N7	82:Aa:277:THR:OG1	2.36	0.54
40:Bj:245:VAL:HA	40:Bj:253:LEU:HD22	1.88	0.54
44:Bo:278:SER:O	44:Bo:317:ARG:NH1	2.40	0.54
80:AY:250:ILE:HG22	86:Ae:327:VAL:HG21	1.88	0.54
3:B8:317:A:OP1	14:BJ:59:SER:OG	2.26	0.54
5:BA:155:ARG:HH11	5:BA:165:MET:HE2	1.71	0.54
7:BC:65:LEU:HD11	7:BC:121:LYS:HE2	1.88	0.54
7:BC:79:VAL:HG12	7:BC:86:VAL:HG12	1.90	0.54
21:BQ:30:ARG:HE	33:Bc:56:LEU:HD21	1.71	0.54
36:Bf:71:ILE:HG21	36:Bf:150:LEU:HD22	1.89	0.54
56:AA:289:G:O6	65:AJ:31:ALA:N	2.41	0.54
70:AO:105:CYS:HB2	70:AO:142:VAL:HA	1.89	0.54
3:B8:1487:C:OP1	28:BX:141:SER:OG	2.21	0.54
7:BC:96:ARG:NH1	7:BC:111:SER:OG	2.40	0.54
38:Bh:43:ASP:O	38:Bh:46:THR:OG1	2.23	0.54
39:Bi:184:VAL:HG12	42:Bm:193:LEU:HA	1.90	0.54
39:Bi:370:THR:HG22	39:Bi:383:ARG:HG3	1.89	0.54
3:B8:672:G:H4'	14:BJ:58:PRO:HB2	1.88	0.54
56:AA:632:A:OP1	85:Ad:269:ARG:NH2	2.40	0.54
57:AB:151:ILE:HG12	57:AB:177:VAL:HG22	1.88	0.54
3:B8:1108:A:O2'	19:BO:239:ASN:ND2	2.40	0.54
33:Bc:89:ASP:HA	33:Bc:92:TYR:HD2	1.70	0.54
70:AO:189:PRO:HB3	70:AO:193:LEU:HD22	1.89	0.54
72:AQ:45:TYR:HB2	88:Ai:190:PRO:HG2	1.88	0.54
85:Ad:380:LEU:HD12	85:Ad:381:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BE:167:LEU:HD21	9:BE:202:GLU:HB3	1.88	0.54
13:BI:34:ARG:NH1	13:BI:38:ARG:O	2.40	0.54
21:BQ:115:LYS:HD2	33:Bc:86:LEU:HD13	1.88	0.54
42:Bm:135:LYS:HD3	42:Bm:239:VAL:HG23	1.88	0.54
56:AA:259:A:O2'	56:AA:261:A:OP1	2.25	0.54
73:AR:206:ALA:HB1	73:AR:210:GLU:HG3	1.90	0.54
89:Aj:167:PRO:HG2	89:Aj:170:LEU:HB3	1.88	0.54
3:B8:1192:U:OP2	15:BK:142:ARG:NH2	2.40	0.54
87:Ag:139:GLN:OE1	87:Ag:156:GLN:NE2	2.39	0.54
87:Ag:256:GLN:HE22	87:Ag:371:LEU:HB3	1.72	0.54
87:Ag:296:VAL:HG22	87:Ag:331:CYS:HB2	1.89	0.54
79:AX:162:LYS:HD3	79:AX:315:LEU:HD21	1.90	0.54
3:B8:975:G:O2'	3:B8:977:G:OP2	2.21	0.54
7:BC:145:ARG:HH22	7:BC:157:PRO:HD3	1.73	0.54
25:BU:124:VAL:HA	25:BU:158:ARG:HH21	1.72	0.54
27:BW:163:HIS:NE2	27:BW:167:GLU:OE2	2.41	0.54
57:AB:103:GLY:H	58:AC:156:GLN:HE22	1.56	0.54
61:AF:156:ILE:HD11	61:AF:171:PRO:HB2	1.89	0.54
3:B8:29:A:N3	3:B8:35:A:O2'	2.38	0.53
16:BL:198:GLU:OE2	16:BL:202:GLY:N	2.38	0.53
30:BZ:135:GLU:N	30:BZ:135:GLU:OE1	2.41	0.53
89:Aj:82:ARG:NH1	89:Aj:133:GLN:OE1	2.36	0.53
15:BK:126:LYS:HE2	15:BK:148:VAL:HG11	1.89	0.53
16:BL:168:ASP:HA	16:BL:184:PRO:HD3	1.90	0.53
39:Bi:86:MET:O	39:Bi:274:ASN:ND2	2.41	0.53
56:AA:405:G:N1	56:AA:452:C:O2'	2.40	0.53
67:AL:104:LYS:HE2	67:AL:108:LYS:HE3	1.90	0.53
85:Ad:308:GLN:NE2	85:Ad:312:TYR:O	2.40	0.53
21:BQ:20:ILE:HB	21:BQ:70:ILE:HB	1.89	0.53
22:BR:37:VAL:HG13	22:BR:42:LEU:HB2	1.91	0.53
55:Bz:69:HIS:HD2	55:Bz:71:LYS:H	1.56	0.53
67:AL:80:VAL:HG23	67:AL:83:ILE:HD11	1.90	0.53
79:AX:161:VAL:HG22	79:AX:289:ILE:HD11	1.89	0.53
79:AX:198:LEU:HD12	79:AX:222:GLY:HA2	1.89	0.53
42:Bm:123:LEU:HD22	42:Bm:220:LEU:HD21	1.90	0.53
42:Bm:398:VAL:HG22	42:Bm:399:GLU:HG3	1.89	0.53
45:Bp:77:LYS:NZ	62:AG:48:G:OP2	2.32	0.53
45:Bp:160:GLU:O	51:Bv:207:ASN:ND2	2.42	0.53
51:Bv:255:VAL:HB	51:Bv:259:GLU:HG3	1.91	0.53
70:AO:104:PRO:HB2	70:AO:109:ARG:HB3	1.90	0.53
3:B8:216:C:O3'	53:Bx:90:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BE:173:ASP:HB3	9:BE:175:GLN:HG2	1.90	0.53
21:BQ:25:ARG:NH1	21:BQ:63:GLY:O	2.41	0.53
44:Bo:183:ASP:OD1	44:Bo:184:LYS:N	2.41	0.53
56:AA:290:C:OP1	95:AA:1120:SPM:N1	2.42	0.53
67:AL:69:PRO:HB2	67:AL:72:MET:HG3	1.90	0.53
75:AT:56:GLN:HB2	75:AT:64:ILE:HD12	1.91	0.53
77:AV:363:THR:HG22	77:AV:365:GLN:H	1.73	0.53
3:B8:1089:G:N2	3:B8:1124:C:O2	2.40	0.53
3:B8:1131:U:H2'	3:B8:1132:G:H8	1.73	0.53
4:B9:18:U:H5'	4:B9:57:C:H5	1.73	0.53
4:B9:34:U:N3	4:B9:35:G:N7	2.56	0.53
37:Bg:28:ARG:O	55:Bz:57:TYR:OH	2.17	0.53
42:Bm:115:GLU:HB3	42:Bm:118:LYS:HE2	1.91	0.53
50:Bu:154:ASN:ND2	50:Bu:156:ASP:OD2	2.41	0.53
3:B8:9:U:O2	3:B8:132:G:N2	2.42	0.53
11:BG:71:ARG:NH1	11:BG:73:LYS:O	2.42	0.53
19:BO:98:LEU:HD23	19:BO:129:ALA:HB2	1.90	0.53
20:BP:113:ARG:HH11	20:BP:123:MET:HG3	1.74	0.53
27:BW:44:VAL:HG22	43:Bn:225:LEU:HD13	1.90	0.53
40:Bj:61:ALA:N	40:Bj:134:LYS:O	2.41	0.53
56:AA:66:C:OP2	68:AM:10:ARG:NH2	2.42	0.53
77:AV:230:LEU:HD22	77:AV:394:LEU:HD13	1.90	0.53
82:Aa:67:LYS:HG2	82:Aa:71:LYS:HE3	1.91	0.53
86:Ae:396:ILE:HG12	86:Ae:434:LEU:HD21	1.90	0.53
3:B8:1131:U:H2'	3:B8:1132:G:C8	2.44	0.53
17:BM:56:GLU:HG2	26:BV:154:ARG:HH12	1.74	0.53
56:AA:306:G:H2'	56:AA:307:A:C8	2.44	0.53
79:AX:49:ARG:HH21	79:AX:68:ASN:HB2	1.72	0.53
87:Ag:284:VAL:HG11	87:Ag:349:MET:HG2	1.91	0.53
3:B8:86:U:H2'	3:B8:87:A:H8	1.73	0.53
3:B8:135:G:N1	3:B8:138:A:OP2	2.42	0.53
4:B9:66:A:H2'	4:B9:67:A:C8	2.44	0.53
7:BC:98:VAL:HG21	7:BC:109:ILE:HD12	1.91	0.53
34:Bd:126:LYS:H	34:Bd:126:LYS:HD2	1.74	0.53
51:Bv:192:LEU:O	51:Bv:198:ASN:ND2	2.41	0.53
56:AA:296:G:O2'	56:AA:461:A:OP2	2.24	0.53
75:AT:155:LEU:HD13	75:AT:159:MET:HE3	1.91	0.53
82:Aa:190:THR:OG1	82:Aa:281:SER:OG	2.27	0.53
4:B9:18:U:H5'	4:B9:57:C:C5	2.44	0.52
3:B8:31:A:H1'	14:BJ:73:LEU:HD12	1.90	0.52
3:B8:353:C:O2	3:B8:1267:A:O2'	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Bf:107:ALA:O	36:Bf:115:ARG:NH2	2.28	0.52
55:Bz:99:GLY:HA2	55:Bz:102:MET:HE2	1.90	0.52
56:AA:443:U:H2'	56:AA:444:G:H8	1.75	0.52
56:AA:962:C:O2	84:Ac:37:ARG:NH1	2.43	0.52
58:AC:73:THR:HG22	58:AC:79:GLU:HG2	1.90	0.52
83:Ab:140:ILE:HG13	83:Ab:187:ARG:HH21	1.73	0.52
86:Ae:80:ARG:NH2	86:Ae:487:SER:OG	2.41	0.52
3:B8:1193:C:OP2	15:BK:142:ARG:NH1	2.43	0.52
17:BM:227:GLN:OE1	17:BM:227:GLN:N	2.42	0.52
57:AB:306:ASP:HB2	79:AX:323:LEU:HD13	1.91	0.52
86:Ae:380:GLN:HE21	86:Ae:421:SER:HB3	1.74	0.52
9:BE:159:MET:HB3	9:BE:205:GLY:HA2	1.92	0.52
15:BK:172:TYR:HB2	15:BK:175:ASP:HB2	1.90	0.52
18:BN:133:SER:HB2	18:BN:135[B]:ARG:HH21	1.74	0.52
34:Bd:83:ASP:HA	34:Bd:90:ARG:HH21	1.74	0.52
39:Bi:173:GLN:HE22	42:Bm:203:CYS:HB3	1.75	0.52
5:BA:210:LEU:HB3	48:Bs:119:PHE:CE1	2.45	0.52
31:Ba:47:PRO:HA	31:Ba:60:MET:HE3	1.92	0.52
34:Bd:55:VAL:HG21	34:Bd:69:TYR:HB3	1.90	0.52
56:AA:844:C:O2'	64:Al:1:A:N6	2.33	0.52
3:B8:41:A:H2'	3:B8:42:C:H4'	1.91	0.52
11:BG:134:MET:HE1	31:Ba:78:VAL:HG21	1.91	0.52
58:AC:128:PRO:HD2	58:AC:131:LYS:HD2	1.91	0.52
73:AR:184:SER:H	73:AR:192:ARG:HH12	1.57	0.52
77:AV:306:VAL:HB	77:AV:382:LEU:HD22	1.91	0.52
84:Ac:11:ALA:O	84:Ac:12:ARG:NH1	2.35	0.52
84:Ac:17:ARG:HE	84:Ac:20:ILE:HD11	1.74	0.52
9:BE:100:ARG:HH12	19:BO:75:ARG:HE	1.58	0.52
16:BL:133:ASP:OD2	16:BL:136:ARG:NH1	2.43	0.52
19:BO:156:GLN:OE1	19:BO:226:ASN:ND2	2.37	0.52
27:BW:51:ARG:NH2	43:Bn:221:LEU:O	2.43	0.52
31:Ba:45:GLU:HG3	31:Ba:63:GLN:HE22	1.75	0.52
51:Bv:157:LEU:HB3	51:Bv:254:TRP:HB3	1.92	0.52
56:AA:56:U:O2'	56:AA:198:C:O2	2.27	0.52
66:AK:52:LEU:HD11	81:AZ:36:LEU:HB3	1.92	0.52
77:AV:191:PHE:HA	77:AV:196:ASN:HD22	1.75	0.52
92:B9:101:PHE:HB2	51:Bv:165:LEU:HG	1.92	0.52
21:BQ:128:ASP:OD1	21:BQ:128:ASP:N	2.43	0.52
22:BR:27:PRO:HG2	22:BR:30:LYS:HB2	1.90	0.52
28:BX:79:GLU:OE2	28:BX:103:ARG:NH2	2.42	0.52
57:AB:114:LEU:HD23	87:Ag:111:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:AV:157:LEU:HD22	77:AV:190:TYR:HD2	1.75	0.52
85:Ad:154:VAL:HG21	86:Ae:108:LEU:HD13	1.90	0.52
9:BE:202:GLU:HG3	9:BE:203:TRP:CD1	2.44	0.52
24:BT:141:VAL:HG21	43:Bn:377:TYR:CE1	2.45	0.52
60:AE:36:VAL:HG23	76:Au:168:ILE:HB	1.91	0.52
75:AT:78:PHE:HB2	75:AT:86:VAL:HB	1.91	0.52
73:AR:173:THR:OG1	73:AR:174:GLU:OE1	2.23	0.52
85:Ad:194:SER:HB2	85:Ad:197:THR:HG22	1.92	0.52
86:Ae:339:ASN:ND2	86:Ae:412:ASP:OD2	2.42	0.52
86:Ae:520:LYS:NZ	86:Ae:557:ASP:OD2	2.43	0.52
5:BA:98:ASP:OD2	44:Bo:94:GLU:N	2.41	0.51
56:AA:876:A:H4'	56:AA:877:A:C5	2.45	0.51
66:AK:29:TYR:CZ	66:AK:38:VAL:HG21	2.46	0.51
73:AR:276:ASP:OD1	73:AR:281:TYR:OH	2.27	0.51
83:Ab:263:ARG:NH1	83:Ab:267:GLU:OE2	2.43	0.51
86:Ae:325:GLN:O	86:Ae:328:THR:OG1	2.28	0.51
26:BV:33:LEU:HD21	26:BV:59:LEU:HD22	1.91	0.51
30:BZ:148:LEU:HB2	47:Br:58:ILE:HB	1.92	0.51
39:Bi:198:ARG:HD3	39:Bi:199:PRO:HD2	1.92	0.51
42:Bm:240:ALA:H	42:Bm:358:GLN:HE22	1.59	0.51
56:AA:643:G:O2'	56:AA:651:G:OP2	2.20	0.51
57:AB:217:LYS:NZ	80:AY:310:GLU:OE1	2.41	0.51
61:AF:155:VAL:H	61:AF:227:HIS:HE1	1.58	0.51
67:AL:223:LYS:HA	67:AL:226:ARG:HE	1.75	0.51
79:AX:245:GLU:OE2	79:AX:249:GLN:NE2	2.44	0.51
89:Aj:85:TRP:HD1	89:Aj:89:HIS:HD2	1.57	0.51
3:B8:1110:G:OP2	19:BO:242:ARG:NE	2.44	0.51
9:BE:41:VAL:HG11	9:BE:83:GLU:HB3	1.91	0.51
3:B8:471:U:O2'	3:B8:484:A:N3	2.41	0.51
5:BA:123:GLN:NE2	5:BA:135:ARG:O	2.43	0.51
22:BR:15:ALA:HB1	49:Bt:269:VAL:HG21	1.91	0.51
6:BB:138:ASP:HB3	6:BB:141:ARG:HG2	1.91	0.51
18:BN:62:VAL:HG23	54:By:119:HIS:HB3	1.92	0.51
50:Bu:152:LEU:HD11	50:Bu:172:MET:HB2	1.93	0.51
56:AA:654:A:H5'	57:AB:95:ARG:HH12	1.75	0.51
78:AW:84:MET:HE1	83:Ab:81:ARG:HA	1.92	0.51
83:Ab:134:VAL:HG11	83:Ab:191:LEU:HD13	1.92	0.51
86:Ae:593:GLN:HA	86:Ae:596:TRP:HD1	1.75	0.51
25:BU:134:LYS:HB3	25:BU:138:GLN:HE21	1.75	0.51
45:Bp:99:ARG:HB2	51:Bv:84:TYR:H	1.75	0.51
77:AV:259:VAL:HG21	77:AV:397:SER:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Bi:100:LEU:O	39:Bi:313:GLN:NE2	2.38	0.51
56:AA:230:U:H2'	56:AA:237:U:H5	1.75	0.51
3:B8:445:A:OP1	20:BP:35:ARG:NH2	2.43	0.51
3:B8:644:G:OP1	12:BH:93:ARG:NH1	2.43	0.51
60:AE:13:MET:HE3	60:AE:18:THR:HA	1.93	0.51
77:AV:286:ASN:HA	89:Aj:70:ARG:HH22	1.76	0.51
1:B2:77:LEU:HD11	20:BP:186:LEU:HD21	1.93	0.51
3:B8:1329:U:O2	82:Aa:313:GLN:NE2	2.43	0.51
53:Bx:43:ASP:OD1	53:Bx:43:ASP:N	2.42	0.51
66:AK:114:LEU:HB3	66:AK:120:LEU:HD13	1.93	0.51
70:AO:182:GLY:O	73:AR:205:LYS:NZ	2.43	0.51
56:AA:728:U:H2'	56:AA:729:A:C8	2.45	0.51
68:AM:100:HIS:CD2	68:AM:102:MET:HB2	2.46	0.51
76:AU:65:GLN:HG2	89:Aj:193:LEU:HD22	1.94	0.51
84:Ac:100:PRO:HD2	84:Ac:103:LYS:HD2	1.92	0.51
85:Ad:140:LEU:HD11	85:Ad:160:ARG:HE	1.76	0.51
3:B8:613:U:H5'	18:BN:255:LYS:HE3	1.93	0.50
3:B8:659:U:H5''	39:Bi:55:SER:HB2	1.93	0.50
4:B9:29:G:OP1	45:Bp:133:ARG:NH2	2.44	0.50
77:AV:238:TRP:CZ3	77:AV:278:GLN:HB2	2.46	0.50
11:BG:46:PHE:O	35:Be:50:SER:OG	2.23	0.50
16:BL:258:ILE:HG23	16:BL:263:ARG:HB3	1.92	0.50
51:Bv:138:THR:OG1	51:Bv:150:HIS:O	2.29	0.50
56:AA:287:C:N3	75:AT:11:ARG:NH2	2.60	0.50
6:BB:20:PHE:O	10:BF:105:TYR:OH	2.27	0.50
9:BE:117:GLU:OE1	9:BE:190:ARG:NH2	2.42	0.50
10:BF:85:ALA:N	46:Bq:72:VAL:O	2.43	0.50
39:Bi:146:GLN:HA	39:Bi:150:PHE:HB2	1.92	0.50
47:Br:40:PRO:HG2	47:Br:43:TYR:HE1	1.75	0.50
57:AB:268:LEU:HD13	57:AB:285:LEU:HD12	1.93	0.50
87:Ag:321:LEU:HD11	87:Ag:365:MET:HE1	1.93	0.50
29:BY:57:ARG:NH2	30:BZ:174:ILE:O	2.45	0.50
44:Bo:210:ASP:OD2	44:Bo:268:ARG:NH1	2.45	0.50
68:AM:42:PRO:HG2	68:AM:45:GLY:HA3	1.93	0.50
79:AX:178:ASP:HB3	79:AX:236:THR:HG21	1.93	0.50
3:B8:644:G:P	12:BH:93:ARG:HH12	2.34	0.50
26:BV:16:ARG:NH2	26:BV:50:ASP:OD2	2.44	0.50
39:Bi:49:ALA:O	39:Bi:61:ARG:NH1	2.40	0.50
42:Bm:113:LEU:HD12	42:Bm:311:ALA:HB1	1.92	0.50
43:Bn:175:VAL:HG22	43:Bn:204:VAL:HG22	1.92	0.50
58:AC:72:HIS:HD2	58:AC:74:GLY:H	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AY:272:ILE:HG22	80:AY:276:LYS:HE3	1.93	0.50
3:B8:84:G:OP2	15:BK:113:ARG:NH2	2.44	0.50
3:B8:617:A:HO2'	49:Bt:39:TYR:HH	1.55	0.50
3:B8:1331:G:HO2'	3:B8:1377:U:HO2'	1.60	0.50
11:BG:75:THR:HB	11:BG:83:LYS:HG2	1.91	0.50
23:BS:145:VAL:HG11	28:BX:160:VAL:HG11	1.94	0.50
56:AA:393:A:H5'	67:AL:133:LEU:HD21	1.93	0.50
56:AA:579:A:OP2	66:AK:108:ARG:NH1	2.44	0.50
69:AN:62:ASP:OD1	69:AN:88:VAL:N	2.44	0.50
78:AW:144:ARG:HB2	78:AW:171:LEU:HD11	1.93	0.50
79:AX:264:VAL:HG12	79:AX:268:TRP:HZ3	1.76	0.50
79:AX:294:LYS:NZ	99:AX:503:GDP:O1B	2.44	0.50
88:Ai:76:ARG:HH21	88:Ai:81:LYS:HE2	1.76	0.50
4:B9:17:U:OP2	4:B9:58:A:N6	2.45	0.50
18:BN:102:TRP:O	18:BN:106:PHE:HB3	2.12	0.50
19:BO:201:VAL:HG22	40:Bj:86:VAL:HG13	1.94	0.50
27:BW:151:TRP:HH2	43:Bn:54:PHE:HB3	1.76	0.50
42:Bm:181:VAL:HG21	42:Bm:294:LEU:HD22	1.94	0.50
49:Bt:237:PRO:HG3	49:Bt:298:ARG:HE	1.76	0.50
52:Bw:97:ALA:HB3	52:Bw:103:ALA:HB2	1.93	0.50
73:AR:229:PRO:HB2	73:AR:231:ILE:HG22	1.94	0.50
74:AS:34:ILE:HD11	83:Ab:137:ARG:HD3	1.93	0.50
33:Bc:92:TYR:HB3	33:Bc:96:LEU:HD21	1.93	0.50
43:Bn:197:GLU:OE1	43:Bn:197:GLU:N	2.44	0.50
48:Bs:133:PHE:HB3	49:Bt:259:ARG:HD3	1.94	0.50
56:AA:735:G:N3	79:AX:163:ASN:ND2	2.58	0.50
57:AB:190:LYS:NZ	57:AB:251:GLU:OE1	2.42	0.50
75:AT:2:PRO:HB2	75:AT:8:PRO:HB3	1.94	0.50
80:AY:339:ILE:HG12	80:AY:386:LEU:HD13	1.94	0.50
3:B8:789:A:O2'	17:BM:215:PHE:O	2.23	0.50
3:B8:1355:A:O2'	3:B8:1460:A:N1	2.44	0.50
21:BQ:43:GLY:HA3	21:BQ:76:ARG:HH11	1.77	0.50
42:Bm:125:LYS:HG2	42:Bm:371:LYS:HG3	1.93	0.50
49:Bt:245:LEU:HD22	49:Bt:250:ILE:HD12	1.94	0.50
60:AE:37:ARG:HG2	60:AE:38:ASN:HD22	1.76	0.50
76:AU:141:LEU:HD23	76:AU:144:ARG:HH12	1.77	0.50
1:B6:76:LEU:HA	1:B6:79:ILE:HG12	1.93	0.49
3:B8:154:A:OP1	12:BH:95:ARG:NH2	2.45	0.49
56:AA:127:A:H2'	56:AA:128:C:O4'	2.12	0.49
56:AA:896:A:O2'	59:AD:183:LYS:NZ	2.45	0.49
61:AF:78:PRO:HG2	61:AF:81:LYS:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
89:Aj:143:PRO:HD2	89:Aj:146:GLU:HB2	1.94	0.49
4:B9:72:C:O4'	51:Bv:267:LYS:NZ	2.36	0.49
19:BO:102:VAL:HB	19:BO:105:LEU:HB2	1.94	0.49
31:Ba:100:GLN:NE2	31:Ba:103:GLU:OE2	2.45	0.49
61:AF:155:VAL:H	61:AF:227:HIS:CE1	2.31	0.49
72:AQ:58:GLU:HG2	72:AQ:62:ARG:HH12	1.77	0.49
83:Ab:157:THR:HG23	83:Ab:253:GLN:HE21	1.77	0.49
89:Aj:91:GLU:HG3	89:Aj:121:LYS:HA	1.94	0.49
3:B8:1231:U:H5''	15:BK:135:LYS:HD3	1.94	0.49
5:BA:202:ARG:NH1	49:Bt:287:GLU:OE2	2.45	0.49
17:BM:334:ASP:HB3	17:BM:337:VAL:HG23	1.94	0.49
28:BX:77:SER:HB2	28:BX:80:PHE:HD2	1.76	0.49
54:By:143:GLU:O	54:By:147:SER:OG	2.29	0.49
57:AB:109:LYS:HE2	58:AC:69:LEU:HD23	1.94	0.49
69:AN:53:ASP:OD2	69:AN:57:GLN:N	2.39	0.49
3:B8:1187:U:O2'	3:B8:1189:U:OP2	2.30	0.49
3:B8:1425:A:O2'	62:AG:69:C:OP2	2.28	0.49
19:BO:201:VAL:HG13	40:Bj:86:VAL:HG22	1.94	0.49
51:Bv:58:LEU:N	51:Bv:153:LEU:O	2.42	0.49
52:Bw:173:ILE:O	52:Bw:177:ASN:ND2	2.35	0.49
86:Ae:192:LEU:HD21	86:Ae:250:ILE:HB	1.93	0.49
89:Aj:119:THR:HG22	89:Aj:124:THR:HG22	1.93	0.49
5:BA:66:ARG:HH21	50:Bu:230:ARG:HD2	1.77	0.49
7:BC:189:PRO:O	46:Bq:93:THR:OG1	2.26	0.49
77:AV:252:GLY:O	77:AV:264:GLN:NE2	2.38	0.49
79:AX:244:LYS:HD2	99:AX:503:GDP:H5'	1.94	0.49
79:AX:275:ARG:HH21	79:AX:281:ILE:HG22	1.76	0.49
3:B8:532:A:OP1	33:Bc:123:LYS:NZ	2.37	0.49
5:BA:77:GLN:H	5:BA:171:HIS:CD2	2.30	0.49
43:Bn:139:TRP:CD1	43:Bn:143:CYS:HG	2.30	0.49
51:Bv:147:THR:HG21	51:Bv:248:LYS:HB3	1.93	0.49
79:AX:367:HIS:HB3	79:AX:370:ALA:HB2	1.94	0.49
82:Aa:162:LYS:HE2	82:Aa:166:LEU:HD11	1.95	0.49
83:Ab:68:HIS:HB2	83:Ab:71:PHE:HB2	1.95	0.49
3:B8:1124:C:H2'	3:B8:1125:U:C6	2.48	0.49
5:BA:101:LEU:HD22	5:BA:116:LYS:HG3	1.94	0.49
79:AX:161:VAL:HG21	79:AX:266:ALA:HB1	1.95	0.49
53:Bx:77:ASP:HB2	53:Bx:78:PRO:HD3	1.95	0.49
63:AH:76:LEU:HB3	63:AH:145:LEU:HB2	1.95	0.49
63:AH:96:VAL:HG22	63:AH:106:ILE:HD11	1.94	0.49
68:AM:20:ARG:NH2	68:AM:41:CYS:SG	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:480:G:OP2	30:BZ:108:HIS:ND1	2.44	0.49
3:B8:515:A:H2'	3:B8:541:A:H5'	1.95	0.49
3:B8:1014:A:OP1	29:BY:34:ARG:NH2	2.45	0.49
23:BS:94:PRO:O	23:BS:97:THR:OG1	2.27	0.49
39:Bi:195:ASP:HB2	39:Bi:234:GLN:HB2	1.94	0.49
40:Bj:117:PRO:HB2	40:Bj:261:ASN:HD21	1.78	0.49
43:Bn:87:ARG:NH2	43:Bn:153:GLU:OE2	2.46	0.49
49:Bt:148:LEU:HD13	49:Bt:149:PRO:HD2	1.95	0.49
56:AA:28:U:H2'	56:AA:29:A:H8	1.77	0.49
58:AC:115:ASN:HB3	80:AY:303:TRP:CE2	2.47	0.49
64:Al:-4:A:O2'	64:Al:-3:A:N7	2.45	0.49
87:Ag:317:PRO:HG2	87:Ag:349:MET:HE3	1.95	0.49
3:B8:71:U:H3	3:B8:94:U:H3	1.61	0.49
3:B8:1360:U:H2'	3:B8:1361:A:H8	1.77	0.49
6:BB:88:LYS:NZ	6:BB:91:ASP:OD1	2.46	0.49
19:BO:178:ASN:HD22	19:BO:216:ARG:HH22	1.61	0.49
24:BT:44:ARG:HG3	24:BT:45:ARG:HG3	1.95	0.49
25:BU:65:GLU:OE1	25:BU:65:GLU:N	2.46	0.49
26:BV:32:LEU:HB3	26:BV:52:LEU:HD22	1.95	0.49
42:Bm:310:ARG:HA	42:Bm:313:MET:HE2	1.95	0.49
56:AA:357:G:H21	88:Ai:100:GLN:HE22	1.60	0.49
57:AB:254:ILE:O	57:AB:258:SER:OG	2.29	0.49
62:AG:47:U:H3	62:AG:58:U:H3	1.61	0.49
36:Bf:138:CYS:SG	36:Bf:139:SER:N	2.86	0.48
37:Bg:40:PRO:HG3	37:Bg:51:GLN:HB3	1.93	0.48
55:Bz:69:HIS:CD2	55:Bz:71:LYS:H	2.30	0.48
56:AA:308:A:N1	75:AT:68:LYS:NZ	2.49	0.48
66:AK:53:ARG:O	66:AK:56:SER:OG	2.30	0.48
77:AV:112:ILE:HD11	77:AV:132:LEU:HD23	1.95	0.48
3:B8:575:C:H5	38:Bh:186:SER:HA	1.77	0.48
12:BH:152:PRO:HG3	12:BH:173:ARG:HH11	1.77	0.48
20:BP:97:ALA:HB3	20:BP:154:LEU:HB2	1.95	0.48
30:BZ:105:PHE:HE1	31:Ba:49:TRP:HB3	1.77	0.48
43:Bn:307:HIS:HB2	43:Bn:311:MET:HE2	1.95	0.48
44:Bo:113:TYR:OH	44:Bo:268:ARG:NH2	2.39	0.48
45:Bp:174:GLN:HG2	52:Bw:183:LYS:HG2	1.95	0.48
56:AA:312:A:H2'	56:AA:313:A:C8	2.48	0.48
56:AA:562:A:H8	56:AA:708:A:H61	1.61	0.48
87:Ag:198:SER:HB2	87:Ag:246:ARG:HD2	1.95	0.48
3:B8:132:G:O2'	7:BC:40:ARG:O	2.31	0.48
17:BM:97:VAL:O	17:BM:197:HIS:NE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Bj:128:ASP:HB2	40:Bj:291:VAL:HG23	1.94	0.48
50:Bu:251:HIS:HE1	50:Bu:253:VAL:HB	1.78	0.48
56:AA:262:C:N4	56:AA:263:G:O6	2.47	0.48
73:AR:181:THR:HG22	73:AR:194:ILE:HG23	1.96	0.48
75:AT:90:VAL:HG21	75:AT:98:ILE:HD11	1.95	0.48
86:Ae:491:PRO:O	86:Ae:524:HIS:NE2	2.38	0.48
3:B8:143:A:H2'	3:B8:144:A:C8	2.48	0.48
3:B8:1292:A:N6	3:B8:1304:G:O2'	2.45	0.48
21:BQ:117:VAL:HG12	21:BQ:141:VAL:HG23	1.95	0.48
42:Bm:288:PRO:HD2	42:Bm:324:GLN:CD	2.38	0.48
50:Bu:88:TYR:OH	50:Bu:108:ARG:NH1	2.45	0.48
50:Bu:138:PRO:HB2	50:Bu:192:PRO:HG2	1.95	0.48
56:AA:801:A:N6	56:AA:802:A:N1	2.61	0.48
63:AH:55:PRO:HA	86:Ae:443:ASN:HB3	1.94	0.48
70:AO:110:ASP:OD1	70:AO:110:ASP:N	2.45	0.48
79:AX:168:LEU:O	79:AX:178:ASP:N	2.42	0.48
3:B8:623:G:O2'	18:BN:105:ASN:ND2	2.46	0.48
3:B8:1266:U:H2'	3:B8:1267:A:H8	1.77	0.48
3:B8:1323:U:O2'	3:B8:1327:U:OP1	2.30	0.48
17:BM:206:VAL:HG13	17:BM:297:VAL:HG13	1.95	0.48
21:BQ:85:PRO:O	21:BQ:124:LYS:NZ	2.44	0.48
38:Bh:144:LYS:H	38:Bh:144:LYS:HD2	1.77	0.48
42:Bm:207:ASN:HD21	42:Bm:229:ARG:HD2	1.77	0.48
45:Bp:67:ARG:NE	62:AG:43:A:H4'	2.28	0.48
63:AH:82:GLY:HA3	63:AH:168:VAL:HG12	1.94	0.48
66:AK:41:ARG:NH1	81:AZ:48:THR:O	2.45	0.48
12:BH:138:ARG:HA	12:BH:141:MET:HE2	1.96	0.48
35:Be:101:TRP:NE1	48:Bs:48:GLU:OE2	2.33	0.48
38:Bh:155:SER:OG	38:Bh:158:SER:OG	2.32	0.48
39:Bi:145:LEU:HD22	39:Bi:402:ASN:HA	1.96	0.48
42:Bm:174:GLU:HA	42:Bm:296:SER:HB2	1.95	0.48
42:Bm:322:LEU:HG	42:Bm:326:ARG:HH12	1.79	0.48
48:Bs:75:VAL:HG13	48:Bs:87:GLU:HB2	1.95	0.48
56:AA:104:A:OP2	69:AN:49:TYR:OH	2.18	0.48
61:AF:61:GLU:HA	61:AF:64:TYR:CE2	2.49	0.48
71:AP:81:LEU:HB3	71:AP:112:ILE:HG12	1.94	0.48
77:AV:325:ARG:NH2	77:AV:376:GLU:OE2	2.47	0.48
11:BG:148:ARG:HD2	11:BG:151:LEU:HD11	1.96	0.48
17:BM:78:CYS:HB3	17:BM:81:LYS:HB2	1.96	0.48
18:BN:220:ASP:OD1	18:BN:221:LEU:N	2.46	0.48
39:Bi:156:ARG:HH11	39:Bi:161:GLN:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:AC:92:LEU:HD11	58:AC:117:LEU:HD21	1.96	0.48
59:AD:172:ASP:OD1	59:AD:175:ARG:NH2	2.43	0.48
86:Ae:382:PHE:O	86:Ae:392:SER:OG	2.31	0.48
86:Ae:559:LYS:NZ	86:Ae:563:GLU:OE2	2.46	0.48
3:B8:1458:G:O2'	3:B8:1467:G:O6	2.30	0.48
7:BC:23:MET:SD	7:BC:114:PRO:HG3	2.54	0.48
19:BO:156:GLN:HE22	19:BO:226:ASN:HB2	1.77	0.48
44:Bo:253:ARG:HG3	44:Bo:258:ILE:HG12	1.96	0.48
56:AA:237:U:O2'	56:AA:238:C:O4'	2.25	0.48
73:AR:104:MET:HG3	73:AR:290:PHE:HE2	1.78	0.48
85:Ad:288:HIS:CE1	85:Ad:310:ARG:HG2	2.49	0.48
3:B8:776:C:O2'	3:B8:777:A:H2'	2.14	0.48
3:B8:1336:A:H2'	3:B8:1337:G:H8	1.79	0.48
3:B8:1396:C:H41	82:Aa:317:LYS:HA	1.79	0.48
44:Bo:305:HIS:CD2	44:Bo:307:THR:H	2.32	0.48
70:AO:225:ARG:HB2	76:AU:47:ALA:HB1	1.96	0.48
3:B8:250:A:N6	3:B8:341:G:O6	2.45	0.48
4:B9:23:A:OP1	27:BW:113:LYS:NZ	2.44	0.48
26:BV:38:ARG:NH2	26:BV:82:GLU:OE1	2.47	0.48
40:Bj:115:THR:OG1	40:Bj:116:ASN:N	2.47	0.48
73:AR:101:LEU:HB3	73:AR:150:MET:HE1	1.96	0.48
77:AV:144:LEU:HD13	77:AV:149:ILE:HD11	1.96	0.48
3:B8:1140:A:H2'	3:B8:1141:A:H8	1.79	0.47
20:BP:94:ARG:HH21	20:BP:158:GLU:H	1.60	0.47
25:BU:72:ILE:HD11	25:BU:96:TYR:CZ	2.49	0.47
44:Bo:273:PHE:HB2	44:Bo:300:VAL:HG22	1.96	0.47
68:AM:111:ARG:NH2	70:AO:233:GLU:O	2.45	0.47
3:B8:8:C:H5	49:Bt:31:ALA:HB2	1.78	0.47
3:B8:197:U:O2'	29:BY:38:CYS:SG	2.60	0.47
3:B8:247:C:H2'	3:B8:248:A:C8	2.50	0.47
3:B8:465:A:N6	35:Be:16:GLN:OE1	2.47	0.47
3:B8:1295:G:H2'	3:B8:1298:C:H42	1.79	0.47
39:Bi:197:LYS:HB3	39:Bi:230:LYS:HE3	1.96	0.47
39:Bi:243:GLU:HA	39:Bi:350:VAL:HG21	1.96	0.47
51:Bv:42:SER:OG	51:Bv:43:SER:N	2.46	0.47
67:AL:165:LYS:NZ	67:AL:191:THR:H	2.12	0.47
75:AT:132:ARG:NH1	75:AT:136:LEU:O	2.47	0.47
87:Ag:269:ALA:HB1	87:Ag:356:PHE:HE2	1.79	0.47
6:BB:71:ARG:NH1	6:BB:73:GLN:OE1	2.40	0.47
7:BC:121:LYS:HE3	7:BC:130:PRO:HB2	1.96	0.47
56:AA:245:C:OP1	82:Aa:259:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:AF:140:ASN:OD1	61:AF:143:THR:N	2.41	0.47
78:AW:115:ILE:HD13	78:AW:141:VAL:HG21	1.96	0.47
79:AX:46:ALA:HB3	79:AX:357:GLN:HG3	1.96	0.47
88:Ai:155:GLY:HA2	88:Ai:181:THR:HG23	1.96	0.47
88:Ai:156:LEU:HA	88:Ai:160:ARG:HD2	1.95	0.47
3:B8:844:A:O2'	3:B8:873:U:OP1	2.28	0.47
3:B8:1360:U:H2'	3:B8:1361:A:C8	2.49	0.47
62:AG:22:U:H2'	62:AG:23:A:H8	1.80	0.47
69:AN:74:THR:HG23	69:AN:77:VAL:H	1.79	0.47
77:AV:185:ASN:HD22	77:AV:220:LEU:HD23	1.80	0.47
80:AY:353:ASN:ND2	81:AZ:37:PHE:O	2.42	0.47
89:Aj:132:GLU:HG2	89:Aj:133:GLN:HG3	1.96	0.47
3:B8:226:U:OP1	15:BK:168:ARG:NE	2.40	0.47
3:B8:721:A:H5''	42:Bm:301:PRO:HB3	1.96	0.47
7:BC:112:GLU:OE2	50:Bu:74:ARG:NH1	2.48	0.47
22:BR:112:LEU:HD13	22:BR:121:MET:HG3	1.96	0.47
26:BV:55:TYR:HE1	28:BX:270:MET:HB2	1.78	0.47
40:Bj:133:LYS:HG2	40:Bj:134:LYS:H	1.80	0.47
40:Bj:291:VAL:HG12	40:Bj:292:ARG:HG3	1.96	0.47
46:Bq:21:TRP:HE3	46:Bq:25:ARG:HH21	1.62	0.47
56:AA:901:A:O2'	59:AD:171:ARG:NH1	2.47	0.47
57:AB:63:ALA:HB3	57:AB:66:GLN:HB3	1.97	0.47
57:AB:215:PRO:HB2	57:AB:216:LEU:HD12	1.95	0.47
58:AC:134:PHE:CD2	85:Ad:144:LEU:HG	2.49	0.47
68:AM:54:TYR:HD1	68:AM:66:VAL:HG22	1.78	0.47
82:Aa:284:VAL:HG13	82:Aa:375:GLN:HE22	1.78	0.47
9:BE:40:PRO:HB3	9:BE:43:TYR:CZ	2.50	0.47
49:Bt:101:GLU:O	49:Bt:105:ARG:HG2	2.14	0.47
56:AA:888:A:H1'	77:AV:106:PRO:HD3	1.97	0.47
73:AR:347:LEU:HD22	73:AR:368:LEU:HD11	1.96	0.47
81:AZ:74:GLU:HB3	85:Ad:95:ALA:HB2	1.96	0.47
83:Ab:219:VAL:HG22	83:Ab:233:TYR:HB2	1.97	0.47
86:Ae:364:LYS:NZ	86:Ae:369:GLU:OE1	2.47	0.47
3:B8:249:G:N2	3:B8:344:U:O2	2.48	0.47
3:B8:295:G:N3	3:B8:297:A:N6	2.62	0.47
3:B8:560:A:H3'	3:B8:561:C:O2	2.14	0.47
7:BC:49:ILE:O	7:BC:81:ARG:NH2	2.46	0.47
9:BE:6:VAL:HG13	9:BE:11:TRP:HE1	1.78	0.47
16:BL:290:LEU:HD12	16:BL:291:PRO:HD2	1.97	0.47
27:BW:118:SER:HB3	27:BW:121:ASN:OD1	2.15	0.47
30:BZ:133:ARG:HH22	30:BZ:155:LYS:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Bm:249:LYS:HG2	42:Bm:370:VAL:HG22	1.97	0.47
48:Bs:126:ILE:O	48:Bs:127:GLN:HG2	2.14	0.47
56:AA:201:A:H2'	56:AA:202:A:C8	2.50	0.47
56:AA:630:A:H2'	56:AA:631:A:C8	2.50	0.47
57:AB:116:LEU:HD11	63:AH:163:ASN:HB3	1.95	0.47
74:AS:71:ARG:HH12	78:AW:91:THR:HG22	1.80	0.47
79:AX:119:PRO:HB3	79:AX:301:GLN:HE22	1.79	0.47
1:B2:77:LEU:HD23	20:BP:197:LEU:HD22	1.97	0.47
18:BN:123:GLY:HA3	18:BN:142:ARG:HG2	1.97	0.47
21:BQ:119:GLU:HG2	33:Bc:75:VAL:HG11	1.95	0.47
40:Bj:96:ILE:HG21	40:Bj:303:LEU:HD13	1.96	0.47
3:B8:528:U:O2'	33:Bc:115:ARG:NH2	2.48	0.47
3:B8:723:A:H3'	3:B8:724:A:H5''	1.97	0.47
20:BP:61:ASN:HD22	20:BP:63:ARG:H	1.61	0.47
29:BY:57:ARG:HH12	30:BZ:173:LYS:HB3	1.80	0.47
40:Bj:143:VAL:HG22	40:Bj:242:GLU:HA	1.96	0.47
43:Bn:214:TRP:HB3	43:Bn:272:LEU:HD11	1.96	0.47
51:Bv:205:LEU:HB3	52:Bw:168:GLU:HG3	1.96	0.47
56:AA:512:A:H2'	56:AA:513:A:H8	1.79	0.47
57:AB:171:ARG:O	57:AB:220:ASN:ND2	2.48	0.47
79:AX:384:ASN:HB3	87:Ag:302:LEU:HD22	1.97	0.47
11:BG:59:ASP:O	35:Be:51:ARG:NH2	2.47	0.47
23:BS:75:LEU:HD21	23:BS:105:VAL:HG21	1.97	0.47
27:BW:52:ASN:OD1	27:BW:55:ASN:N	2.48	0.47
28:BX:221:LYS:NZ	28:BX:241:LYS:O	2.42	0.47
36:Bf:114:VAL:HG22	36:Bf:161:SER:HA	1.97	0.47
45:Bp:77:LYS:HZ3	62:AG:48:G:P	2.37	0.47
87:Ag:365:MET:HG3	87:Ag:370:LEU:HB2	1.96	0.47
3:B8:188:C:H3'	30:BZ:181:ARG:NH2	2.30	0.46
17:BM:76:LYS:HG3	17:BM:170:LEU:HD21	1.96	0.46
56:AA:35:U:H2'	56:AA:36:A:H8	1.81	0.46
56:AA:895:U:H2'	56:AA:896:A:C8	2.50	0.46
69:AN:69:LEU:HD12	69:AN:70:PRO:HD2	1.97	0.46
79:AX:205:GLU:HG2	79:AX:248:ARG:HH22	1.79	0.46
89:Aj:78:ARG:NH2	89:Aj:142:VAL:O	2.48	0.46
1:B3:76:LEU:HD11	1:B6:79:ILE:HG21	1.97	0.46
11:BG:48:PRO:HD3	35:Be:50:SER:OG	2.15	0.46
29:BY:111:LYS:NZ	47:Br:64:SER:OG	2.26	0.46
56:AA:388:U:H5''	60:AE:72:ALA:HB1	1.97	0.46
67:AL:93:LEU:HD11	76:AU:167:PHE:HE2	1.80	0.46
73:AR:240:MET:HB3	73:AR:245:GLN:HB2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:AS:5:ARG:O	83:Ab:213:LYS:NZ	2.38	0.46
86:Ae:631:ILE:HG22	86:Ae:635:LYS:HE3	1.97	0.46
88:Ai:100:GLN:HE21	88:Ai:108:PRO:HB3	1.80	0.46
3:B8:114:A:N3	3:B8:116:A:O2'	2.42	0.46
18:BN:49:ARG:HB3	18:BN:80:THR:OG1	2.15	0.46
20:BP:99:CYS:N	20:BP:152:LEU:O	2.47	0.46
20:BP:225:GLN:HB2	20:BP:226:PRO:HD3	1.96	0.46
56:AA:191:C:H42	56:AA:208:A:H62	1.63	0.46
60:AE:24:ARG:NH2	60:AE:87:ASP:OD2	2.48	0.46
3:B8:792:G:H2'	3:B8:793:A:H8	1.79	0.46
17:BM:96:ARG:NH2	17:BM:197:HIS:O	2.47	0.46
43:Bn:198:ALA:O	43:Bn:254:TYR:OH	2.32	0.46
58:AC:75:ASN:OD1	66:AK:104:TRP:NE1	2.44	0.46
72:AQ:83:PRO:HG2	72:AQ:84:TRP:CD1	2.51	0.46
85:Ad:243:VAL:HG11	85:Ad:268:PHE:HE1	1.81	0.46
86:Ae:627:PRO:HB3	86:Ae:657:THR:HA	1.98	0.46
26:BV:150:LEU:HD23	44:Bo:312:LEU:HD21	1.97	0.46
50:Bu:226:ASP:OD1	50:Bu:227:ARG:N	2.48	0.46
51:Bv:214:LYS:HG2	51:Bv:230:LYS:HG2	1.97	0.46
56:AA:210:U:O4	56:AA:211:A:N6	2.48	0.46
61:AF:114:THR:HG21	61:AF:205:LEU:HD22	1.98	0.46
74:AS:77:ALA:O	74:AS:134:ARG:NH1	2.49	0.46
89:Aj:82:ARG:HB3	89:Aj:85:TRP:CE3	2.50	0.46
4:B9:50:A:H2'	4:B9:51:G:C8	2.51	0.46
40:Bj:130:THR:HG22	40:Bj:131:LEU:H	1.81	0.46
56:AA:68:G:H4'	56:AA:208:A:H4'	1.98	0.46
56:AA:124:A:H2'	56:AA:125:U:O4'	2.15	0.46
58:AC:132:PHE:HD2	86:Ae:95:LEU:HD21	1.81	0.46
3:B8:220:G:N3	3:B8:231:C:O2'	2.49	0.46
3:B8:725:C:H5	42:Bm:389:LEU:H	1.64	0.46
4:B9:51:G:N2	4:B9:61:U:O2	2.48	0.46
6:BB:8:PRO:HG3	46:Bq:132:ASN:O	2.16	0.46
21:BQ:25:ARG:HB2	21:BQ:28:GLN:HB3	1.97	0.46
36:Bf:190:LYS:HE2	43:Bn:184:LEU:HD23	1.96	0.46
58:AC:76:LEU:O	66:AK:103:ARG:NH2	2.43	0.46
73:AR:226:ILE:HD12	75:AT:144:GLU:HB3	1.98	0.46
85:Ad:149:MET:HG2	85:Ad:154:VAL:HG22	1.98	0.46
1:B3:72:ALA:HB1	1:B6:77:LEU:HG	1.98	0.46
3:B8:1513:U:H2'	3:B8:1514:A:H8	1.81	0.46
21:BQ:151:LEU:HG	21:BQ:153:ILE:HD13	1.98	0.46
27:BW:91:GLU:HG3	27:BW:106:SER:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:AC:106:ASP:OD1	58:AC:106:ASP:N	2.48	0.46
60:AE:80:GLU:O	60:AE:83:SER:OG	2.32	0.46
86:Ae:453:SER:H	86:Ae:456:ARG:HD2	1.81	0.46
88:Ai:121:ASN:O	88:Ai:124:LYS:HG2	2.16	0.46
3:B8:348:G:C8	18:BN:118:ALA:HB2	2.51	0.46
3:B8:1326:A:O2'	3:B8:1328:G:OP2	2.34	0.46
18:BN:220:ASP:O	18:BN:245:ALA:N	2.47	0.46
35:Be:82:PHE:CG	35:Be:83:PRO:HD2	2.51	0.46
56:AA:166:G:H2'	56:AA:167:G:H8	1.81	0.46
56:AA:248:C:H41	65:AJ:78:ARG:NH2	2.14	0.46
56:AA:826:C:H2'	56:AA:827:A:H8	1.81	0.46
68:AM:50:GLN:HB3	75:AT:128:HIS:CD2	2.51	0.46
82:Aa:205:ARG:HB2	82:Aa:235:LEU:HD13	1.98	0.46
86:Ae:568:ARG:HG2	86:Ae:572:PRO:HB3	1.97	0.46
4:B9:7:G:O6	4:B9:62:C:N4	2.49	0.46
18:BN:92:ARG:HB2	18:BN:176:VAL:HG11	1.96	0.46
44:Bo:175:ALA:HB1	44:Bo:295:GLY:O	2.17	0.46
49:Bt:166:VAL:HG11	49:Bt:192:ARG:HG3	1.98	0.46
62:AG:38:C:H2'	62:AG:39:G:H8	1.80	0.46
65:AJ:32:THR:OG1	65:AJ:33:LEU:N	2.49	0.46
86:Ae:584:VAL:HG22	86:Ae:613:LEU:HD13	1.98	0.46
18:BN:171:VAL:HG12	18:BN:175:LYS:HE3	1.98	0.45
19:BO:160:GLY:O	19:BO:163:THR:OG1	2.26	0.45
19:BO:223:VAL:HG13	40:Bj:86:VAL:HG21	1.98	0.45
44:Bo:206:LEU:HD21	44:Bo:254:PHE:HE2	1.80	0.45
56:AA:257:U:H3'	82:Aa:392:GLN:HE22	1.80	0.45
56:AA:576:C:O2'	56:AA:809:G:O2'	2.23	0.45
56:AA:895:U:H2'	56:AA:896:A:H8	1.81	0.45
3:B8:1196:G:OP2	43:Bn:368:ARG:NH1	2.49	0.45
39:Bi:233:ASN:HB2	39:Bi:293:PHE:HB2	1.98	0.45
57:AB:168:PRO:O	57:AB:171:ARG:NH1	2.50	0.45
68:AM:63:GLU:HG2	73:AR:177:LYS:HE3	1.97	0.45
79:AX:59:ARG:HE	79:AX:61:GLN:HE22	1.64	0.45
79:AX:321:ALA:HB1	79:AX:326:GLU:HG3	1.97	0.45
1:B2:76:LEU:HB3	20:BP:197:LEU:HD23	1.98	0.45
3:B8:1266:U:H2'	3:B8:1267:A:C8	2.51	0.45
3:B8:1377:U:H2'	3:B8:1378:U:C6	2.52	0.45
4:B9:73:A:H61	51:Bv:231:VAL:HG21	1.81	0.45
24:BT:119:THR:HG22	24:BT:123:ASN:HD21	1.81	0.45
24:BT:153:ASN:HB2	24:BT:256:LEU:HD23	1.99	0.45
42:Bm:289:HIS:ND1	42:Bm:290:THR:OG1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Ad:159:GLN:HG2	85:Ad:160:ARG:H	1.81	0.45
3:B8:198:U:H2'	3:B8:199:A:C8	2.51	0.45
3:B8:925:G:N2	3:B8:964:A:OP2	2.34	0.45
6:BB:8:PRO:HD2	6:BB:17:LEU:HD11	1.98	0.45
11:BG:72:ILE:HD11	11:BG:118:ARG:HB2	1.98	0.45
24:BT:111:ASP:OD1	24:BT:111:ASP:N	2.49	0.45
28:BX:117:LEU:HG	28:BX:176:VAL:HG22	1.99	0.45
38:Bh:35:PHE:N	38:Bh:56:THR:HG1	2.13	0.45
47:Br:62:HIS:O	47:Br:62:HIS:ND1	2.45	0.45
51:Bv:251:HIS:HD2	51:Bv:252:HIS:HD2	1.65	0.45
56:AA:220:U:H2'	56:AA:221:A:C8	2.52	0.45
56:AA:712:A:H2'	56:AA:713:A:H8	1.81	0.45
56:AA:897:C:H2'	56:AA:898:A:H8	1.81	0.45
61:AF:57:GLU:OE1	61:AF:60:GLU:N	2.36	0.45
77:AV:223:LEU:HD22	77:AV:397:SER:HB2	1.98	0.45
3:B8:165:A:H5''	29:BY:31:PHE:CE1	2.51	0.45
24:BT:112:PRO:HB3	24:BT:152:VAL:HG12	1.98	0.45
38:Bh:176:VAL:HG21	38:Bh:196:HIS:CE1	2.51	0.45
56:AA:58:U:OP1	89:Aj:53:ARG:NH1	2.49	0.45
56:AA:166:G:H2'	56:AA:167:G:C8	2.52	0.45
60:AE:114:GLU:HG3	84:Ac:7:ARG:HA	1.98	0.45
80:AY:321:HIS:CE1	80:AY:322:GLU:HG3	2.52	0.45
85:Ad:242:ARG:HD2	85:Ad:258:ILE:HD11	1.99	0.45
32:Bb:33:PHE:HD1	32:Bb:87:LEU:HD12	1.81	0.45
34:Bd:62:GLY:HA3	45:Bp:182:ILE:H	1.82	0.45
38:Bh:60:SER:HB2	38:Bh:75:TRP:CH2	2.51	0.45
43:Bn:204:VAL:HB	43:Bn:245:VAL:HG21	1.99	0.45
44:Bo:177:CYS:HB3	44:Bo:294:GLN:HG2	1.98	0.45
49:Bt:105:ARG:HA	49:Bt:105:ARG:HH11	1.81	0.45
51:Bv:162:ARG:HD2	51:Bv:169:ASP:HB3	1.99	0.45
56:AA:826:C:H2'	56:AA:827:A:C8	2.52	0.45
62:AG:16:A:H5'	62:AG:55:C:N3	2.32	0.45
74:AS:42:ARG:HH21	74:AS:47:ARG:HE	1.64	0.45
75:AT:89:ASP:OD2	76:AU:120:ARG:NH2	2.49	0.45
85:Ad:341:ASN:HD22	85:Ad:344:ASN:HD22	1.65	0.45
3:B8:78:A:OP2	15:BK:108:LYS:NZ	2.43	0.45
24:BT:127:VAL:HG21	24:BT:138:VAL:HG21	1.99	0.45
24:BT:208:GLU:HB3	37:Bg:103:LEU:HD11	1.98	0.45
65:AJ:37:HIS:ND1	69:AN:36:ASP:OD2	2.48	0.45
73:AR:323:VAL:HG21	73:AR:350:ILE:HG12	1.99	0.45
80:AY:319:GLU:HG3	80:AY:320:PHE:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:1458:G:N2	3:B8:1468:A:OP2	2.44	0.45
18:BN:231:VAL:HG13	37:Bg:26:ARG:HD2	1.99	0.45
45:Bp:110:GLU:OE2	45:Bp:113:ARG:NH1	2.50	0.45
79:AX:347:TYR:CZ	79:AX:387:PRO:HB3	2.51	0.45
3:B8:87:A:OP1	55:Bz:118:TYR:OH	2.30	0.45
7:BC:181:ASP:O	10:BF:95:LYS:NZ	2.50	0.45
40:Bj:105:LEU:HD12	40:Bj:108:LYS:HD3	1.97	0.45
42:Bm:272:ASP:OD1	42:Bm:272:ASP:N	2.49	0.45
51:Bv:45:TRP:CG	51:Bv:230:LYS:HE3	2.52	0.45
51:Bv:152:LYS:HB3	51:Bv:155:ARG:HB2	1.99	0.45
56:AA:887:U:H2'	56:AA:888:A:H8	1.82	0.45
71:AP:112:ILE:O	71:AP:116:GLN:HG2	2.17	0.45
89:Aj:145:HIS:CD2	89:Aj:146:GLU:HG2	2.52	0.45
18:BN:262:THR:O	18:BN:265:THR:OG1	2.32	0.45
42:Bm:173:ARG:HA	42:Bm:176:TYR:CE2	2.52	0.45
43:Bn:261:ARG:HH21	43:Bn:341:VAL:HG11	1.82	0.45
56:AA:546:U:H2'	56:AA:547:A:C8	2.51	0.45
56:AA:923:G:H1'	56:AA:944:MA6:H2	1.97	0.45
67:AL:113:MET:HB2	67:AL:117:LEU:HD12	1.99	0.45
73:AR:170:LEU:HD12	73:AR:197:ARG:NH2	2.32	0.45
79:AX:59:ARG:HE	79:AX:61:GLN:NE2	2.15	0.45
4:B9:18:U:H2'	4:B9:19:A:C8	2.53	0.44
25:BU:54:GLU:H	25:BU:54:GLU:CD	2.25	0.44
34:Bd:82:LEU:HD12	34:Bd:85:LEU:HD12	1.98	0.44
43:Bn:173:LEU:HD12	43:Bn:272:LEU:HD22	1.98	0.44
43:Bn:257:PRO:HB3	43:Bn:268:PHE:CZ	2.52	0.44
56:AA:374:C:OP2	84:Ac:9:ARG:NH2	2.33	0.44
77:AV:211:GLU:OE2	89:Aj:78:ARG:NH1	2.50	0.44
82:Aa:393:ASP:OD1	82:Aa:407:ILE:HG13	2.17	0.44
85:Ad:140:LEU:HD23	85:Ad:146:ILE:HG21	1.98	0.44
89:Aj:94:TYR:O	89:Aj:119:THR:OG1	2.27	0.44
18:BN:241:ASN:OD1	37:Bg:25:TYR:N	2.50	0.44
43:Bn:194:THR:HB	43:Bn:197:GLU:OE1	2.18	0.44
48:Bs:93:SER:O	48:Bs:97:ILE:HG12	2.17	0.44
60:AE:42:LEU:HB2	60:AE:63:TYR:HB2	1.99	0.44
80:AY:254:GLN:NE2	86:Ae:332:LYS:HB3	2.32	0.44
86:Ae:473:GLN:NE2	86:Ae:475:ASP:OD2	2.49	0.44
3:B8:118:U:H5''	14:BJ:91:LYS:HB2	1.99	0.44
3:B8:247:C:H2'	3:B8:248:A:H8	1.82	0.44
3:B8:644:G:O6	5:BA:81:SER:OG	2.25	0.44
3:B8:927:A:H2'	3:B8:928:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:1016:C:OP1	12:BH:86:SER:OG	2.27	0.44
4:B9:59:G:H2'	4:B9:60:C:C6	2.52	0.44
8:BD:62:HIS:H	8:BD:65:ASN:ND2	2.15	0.44
16:BL:178:ARG:NH1	16:BL:181:ASP:OD1	2.50	0.44
40:Bj:95:GLN:HG3	40:Bj:96:ILE:HG13	1.99	0.44
61:AF:88:ASP:OD2	61:AF:146:HIS:NE2	2.45	0.44
77:AV:303:MET:HE1	77:AV:375:PHE:HD1	1.81	0.44
85:Ad:108:ALA:O	85:Ad:114:ARG:NH1	2.51	0.44
3:B8:33:A:C6	46:Bq:30:PHE:HB2	2.52	0.44
3:B8:813:A:N6	3:B8:815:A:N1	2.66	0.44
3:B8:1122:A:H2'	3:B8:1123:A:C8	2.52	0.44
3:B8:1309:U:H2'	3:B8:1310:A:C8	2.52	0.44
17:BM:45:SER:O	44:Bo:303:ARG:NH2	2.50	0.44
17:BM:347:PHE:CG	28:BX:124:PRO:HG3	2.52	0.44
18:BN:61:PRO:HA	18:BN:84:PRO:HD3	2.00	0.44
19:BO:174:VAL:HG13	19:BO:192:HIS:CD2	2.52	0.44
22:BR:132:ASP:OD1	22:BR:132:ASP:N	2.51	0.44
34:Bd:64:THR:O	45:Bp:178:TYR:N	2.49	0.44
40:Bj:123:LEU:HD21	40:Bj:125:LEU:HD21	1.99	0.44
56:AA:424:G:H2'	56:AA:425:G:H8	1.82	0.44
56:AA:552:A:H2'	56:AA:553:G:C8	2.53	0.44
61:AF:196:HIS:HB3	61:AF:199:VAL:HG12	1.99	0.44
69:AN:74:THR:OG1	69:AN:75:LYS:N	2.51	0.44
78:AW:153:ARG:NH1	78:AW:158:THR:O	2.50	0.44
85:Ad:103:LEU:HD11	85:Ad:123:ARG:HB2	1.99	0.44
85:Ad:296:LEU:HD22	85:Ad:352:GLY:HA3	1.98	0.44
86:Ae:301:ILE:HG21	86:Ae:341:ILE:HG12	2.00	0.44
5:BA:78:ILE:HG22	5:BA:80:TYR:H	1.83	0.44
20:BP:224:HIS:CD2	20:BP:228:GLN:HE21	2.36	0.44
22:BR:155:LEU:HB2	38:Bh:86:VAL:HG11	2.00	0.44
29:BY:11:ARG:NH1	29:BY:13:ARG:HD2	2.32	0.44
29:BY:141:ILE:HG21	30:BZ:76:GLU:HG2	2.00	0.44
34:Bd:97:ARG:HH21	45:Bp:189:GLU:CD	2.26	0.44
43:Bn:86:ASP:OD1	43:Bn:86:ASP:N	2.48	0.44
49:Bt:228:LEU:HB2	49:Bt:307:PHE:CD1	2.53	0.44
56:AA:11:G:H21	85:Ad:230:ASN:HA	1.82	0.44
65:AJ:104:GLU:HG2	65:AJ:105:HIS:ND1	2.33	0.44
87:Ag:161:LEU:HD11	87:Ag:245:PHE:HZ	1.82	0.44
3:B8:311:A:H5'	16:BL:262:GLY:HA2	2.00	0.44
4:B9:17:U:H1'	43:Bn:98:SER:HA	2.00	0.44
5:BA:151:LEU:HB2	5:BA:167:LYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BH:182:PRO:HG2	12:BH:185:PHE:HB2	2.00	0.44
24:BT:30:ASN:OD1	35:Be:86:ARG:NH2	2.50	0.44
26:BV:30:GLN:NE2	26:BV:78:PHE:O	2.50	0.44
37:Bg:149:ASP:HA	37:Bg:152:ARG:HE	1.82	0.44
56:AA:430:A:OP1	62:AG:35:C:O2'	2.35	0.44
63:AH:121:LEU:HB2	66:AK:108:ARG:NE	2.32	0.44
2:B7:76:A:OP2	3:B8:1255:A:O2'	2.36	0.44
3:B8:299:A:OP2	3:B8:833:C:N4	2.51	0.44
3:B8:699:G:H2'	3:B8:700:A:C8	2.53	0.44
5:BA:154:ILE:HG13	50:Bu:52:SER:HB3	2.00	0.44
42:Bm:300:ARG:HE	42:Bm:303:ARG:HH22	1.65	0.44
49:Bt:126:SER:OG	49:Bt:193:GLN:NE2	2.50	0.44
95:AA:1120:SPM:H91	95:AA:1120:SPM:H62	1.83	0.44
75:AT:29:VAL:HB	75:AT:79:TYR:HB2	1.99	0.44
75:AT:35:ASN:HD21	75:AT:72:PRO:HA	1.82	0.44
77:AV:291:TRP:HH2	89:Aj:142:VAL:HG12	1.82	0.44
3:B8:294:G:H5'	5:BA:159:ARG:HD2	1.98	0.44
18:BN:279:ARG:HH12	18:BN:282:PRO:HD3	1.83	0.44
42:Bm:107:PHE:HB2	42:Bm:265:LEU:HD22	1.99	0.44
42:Bm:118:LYS:HB3	42:Bm:256:PHE:HE2	1.82	0.44
56:AA:901:A:O3'	59:AD:171:ARG:NH1	2.50	0.44
3:B8:1531:C:H1'	38:Bh:135:LEU:HD12	2.00	0.44
18:BN:219:VAL:HG21	18:BN:261:LEU:HD23	1.98	0.44
62:AG:26:G:H2'	62:AG:27:G:H8	1.83	0.44
66:AK:37:ASP:HB3	81:AZ:52:TYR:HE2	1.81	0.44
83:Ab:242:PRO:N	83:Ab:243:PRO:HD2	2.33	0.44
86:Ae:156:ALA:HB3	86:Ae:172:MET:HE1	2.00	0.44
89:Aj:78:ARG:HH21	89:Aj:141:LEU:HG	1.83	0.44
9:BE:215:GLN:NE2	9:BE:219:GLU:OE2	2.44	0.43
16:BL:177:ALA:HB1	16:BL:245:VAL:HG11	1.99	0.43
18:BN:174:LEU:HD21	18:BN:249:ASN:HA	1.99	0.43
20:BP:71:PRO:HA	20:BP:72:PRO:HD3	1.89	0.43
30:BZ:98:ARG:HB3	48:Bs:126:ILE:HD13	1.99	0.43
39:Bi:206:ARG:HD3	39:Bi:373:LEU:HD23	2.00	0.43
69:AN:11:LYS:HA	69:AN:68:ALA:HB2	2.00	0.43
3:B8:232:U:H2'	3:B8:233:A:H8	1.82	0.43
3:B8:299:A:H61	3:B8:1432:U:H3	1.66	0.43
3:B8:1118:A:H5''	3:B8:1119:C:H2'	2.00	0.43
30:BZ:147:LEU:HD22	47:Br:59:VAL:HG12	2.00	0.43
56:AA:220:U:OP1	70:AO:89:ARG:NH2	2.47	0.43
74:AS:63:ILE:HD11	83:Ab:107:GLY:HA3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:AY:285:PRO:O	80:AY:287:GLN:NE2	2.51	0.43
3:B8:364:A:O2'	3:B8:385:U:H5''	2.18	0.43
3:B8:1336:A:H2'	3:B8:1337:G:C8	2.53	0.43
6:BB:21:ARG:NH1	10:BF:145:ASP:OD1	2.49	0.43
7:BC:60:ASP:HB3	7:BC:157:PRO:HB3	2.00	0.43
13:BI:54:VAL:HB	37:Bg:128:MET:HE3	2.00	0.43
39:Bi:91:TYR:HE2	39:Bi:223:LEU:HD22	1.83	0.43
42:Bm:332:ASP:N	42:Bm:332:ASP:OD1	2.51	0.43
47:Br:105:GLN:O	47:Br:109:ILE:HG12	2.18	0.43
51:Bv:151:ARG:NH1	51:Bv:254:TRP:O	2.51	0.43
53:Bx:73:GLN:HB3	53:Bx:162:LEU:HD11	2.00	0.43
56:AA:29:A:H2'	56:AA:30:A:C8	2.53	0.43
67:AL:144:MET:HE2	67:AL:144:MET:HA	1.99	0.43
3:B8:1116:A:H2'	3:B8:1117:A:O4'	2.19	0.43
3:B8:1296:U:O4	82:Aa:104:ARG:HD2	2.18	0.43
39:Bi:226:GLN:HE21	39:Bi:228:ASN:HD21	1.66	0.43
45:Bp:67:ARG:HH22	62:AG:10:A:P	2.40	0.43
45:Bp:72:ILE:HD11	52:Bw:211:LEU:HD11	1.99	0.43
57:AB:108:LEU:HD21	58:AC:120:CYS:HB3	2.00	0.43
77:AV:268:TYR:HB3	77:AV:299:ALA:HB2	1.99	0.43
3:B8:170:U:H3	5:BA:205:THR:H	1.67	0.43
3:B8:467:A:H62	3:B8:468:A:H62	1.65	0.43
3:B8:562:A:H61	3:B8:1311:G:H1'	1.83	0.43
3:B8:687:U:OP1	5:BA:153:ARG:NE	2.43	0.43
3:B8:1050:C:H2'	3:B8:1327:U:H4'	1.99	0.43
4:B9:49:G:N2	4:B9:63:C:O2	2.52	0.43
5:BA:189:THR:HG23	5:BA:192:ALA:H	1.84	0.43
12:BH:156:THR:HG23	12:BH:173:ARG:HG3	2.01	0.43
58:AC:72:HIS:CD2	58:AC:74:GLY:H	2.34	0.43
69:AN:41:LYS:HB2	75:AT:11:ARG:HD2	1.99	0.43
77:AV:311:GLU:HA	77:AV:388:VAL:HG11	2.00	0.43
4:B9:51:G:H1	4:B9:60:C:H42	1.67	0.43
6:BB:27:GLN:HG2	10:BF:115:LEU:HB3	2.01	0.43
22:BR:156:ASP:OD1	22:BR:156:ASP:N	2.52	0.43
32:Bb:46:ASN:OD1	32:Bb:46:ASN:N	2.52	0.43
34:Bd:72:PRO:HG2	51:Bv:87:HIS:CD2	2.53	0.43
47:Br:49:LEU:HD23	47:Br:60:CYS:HB3	2.01	0.43
49:Bt:73:GLN:O	49:Bt:77:HIS:ND1	2.41	0.43
56:AA:520:G:H4'	59:AD:132:LYS:HE3	2.01	0.43
58:AC:115:ASN:HB3	80:AY:303:TRP:CZ2	2.54	0.43
75:AT:51:ASN:OD1	75:AT:95:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:AV:196:ASN:HB3	77:AV:199:ASP:OD1	2.19	0.43
3:B8:8:C:N4	3:B8:108:A:OP2	2.52	0.43
3:B8:514:A:H4'	3:B8:515:A:H2	1.83	0.43
3:B8:842:U:O2'	16:BL:261:ALA:HB2	2.19	0.43
12:BH:108:ASP:OD1	12:BH:109:VAL:N	2.52	0.43
17:BM:274:TRP:HE1	17:BM:286:ASN:HB2	1.84	0.43
53:Bx:138:THR:HG22	53:Bx:149:VAL:HG22	2.00	0.43
56:AA:477:A:H2'	56:AA:478:A:H8	1.82	0.43
3:B8:17:C:H2'	3:B8:18:A:O4'	2.19	0.43
3:B8:680:C:H2'	3:B8:681:A:H8	1.84	0.43
3:B8:737:G:H2'	3:B8:738:U:C6	2.54	0.43
3:B8:1111:G:H5'	40:Bj:116:ASN:HB2	2.01	0.43
18:BN:234:THR:HG21	18:BN:242:LEU:HB2	2.01	0.43
42:Bm:297:ALA:HB3	42:Bm:303:ARG:HG3	2.00	0.43
43:Bn:238:THR:HG21	43:Bn:281:PHE:HB2	2.01	0.43
45:Bp:195:ILE:H	45:Bp:195:ILE:HG12	1.57	0.43
56:AA:631:A:H4'	58:AC:46:LYS:HE3	2.00	0.43
67:AL:86:VAL:HG13	76:AU:161:GLN:HE22	1.83	0.43
74:AS:104:ILE:O	74:AS:107:GLN:HG3	2.18	0.43
87:Ag:177:ASN:HA	87:Ag:180:ARG:HE	1.83	0.43
3:B8:2:C:O2'	5:BA:147:ARG:O	2.35	0.43
20:BP:188:ARG:HD2	32:Bb:55:VAL:HB	2.00	0.43
34:Bd:46:ARG:HG3	34:Bd:47:GLN:H	1.84	0.43
56:AA:356:A:H2'	56:AA:357:G:H8	1.83	0.43
56:AA:540:U:H1'	56:AA:541:C:H5	1.84	0.43
1:B3:71:ILE:HG12	1:B4:67:LEU:HD13	2.00	0.43
1:B3:76:LEU:HD21	1:B6:79:ILE:HD13	2.01	0.43
3:B8:447:A:HO2'	3:B8:1279:G:HO2'	1.67	0.43
3:B8:1177:U:H4'	25:BU:144:LYS:HD3	2.01	0.43
3:B8:1531:C:OP2	38:Bh:146:ARG:NH2	2.52	0.43
12:BH:132:LYS:NZ	12:BH:136:GLU:OE2	2.51	0.43
17:BM:97:VAL:HG22	17:BM:181:VAL:HG21	2.00	0.43
17:BM:222:TRP:CD1	17:BM:256:LYS:HB3	2.54	0.43
19:BO:178:ASN:HD22	19:BO:178:ASN:H	1.67	0.43
32:Bb:93:HIS:HE1	38:Bh:47:THR:HG21	1.84	0.43
39:Bi:132:ASP:OD1	39:Bi:132:ASP:N	2.44	0.43
42:Bm:192:ILE:HD11	42:Bm:199:ALA:HB2	2.01	0.43
44:Bo:140:TRP:HZ2	44:Bo:175:ALA:HA	1.84	0.43
46:Bq:129:TYR:HB3	46:Bq:130:PRO:HD3	2.00	0.43
49:Bt:60:ARG:HD2	49:Bt:63:LYS:HD2	2.01	0.43
69:AN:69:LEU:HD13	69:AN:80:GLU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:AS:67:GLU:OE2	78:AW:86:ARG:NH2	2.43	0.43
75:AT:2:PRO:HB3	75:AT:11:ARG:NH2	2.34	0.43
86:Ae:312:PHE:HZ	86:Ae:355:PRO:HG2	1.83	0.43
89:Aj:3:ARG:HG3	89:Aj:5:LYS:H	1.84	0.43
3:B8:660:C:O3'	26:BV:81:THR:OG1	2.32	0.42
3:B8:670:A:H5''	46:Bq:28:ARG:HD3	2.01	0.42
17:BM:79:PRO:HB3	17:BM:191:THR:HG23	2.01	0.42
17:BM:149:GLY:O	17:BM:173:LYS:HD2	2.19	0.42
18:BN:276:HIS:O	53:Bx:90:ARG:NH2	2.52	0.42
26:BV:117:ASP:OD1	26:BV:117:ASP:N	2.51	0.42
27:BW:125:CYS:HB3	27:BW:161:LEU:HD12	2.00	0.42
47:Br:109:ILE:HG23	47:Br:123:TRP:HB2	2.00	0.42
50:Bu:288:LYS:NZ	50:Bu:291:GLU:HB2	2.34	0.42
56:AA:866:U:H2'	56:AA:867:G:C8	2.54	0.42
60:AE:3:ARG:NH2	60:AE:70:ALA:O	2.38	0.42
69:AN:35:LEU:HB2	69:AN:42:TYR:CE1	2.54	0.42
71:AP:96:HIS:CD2	71:AP:97:ILE:HG13	2.54	0.42
77:AV:157:LEU:HD13	77:AV:190:TYR:CE2	2.54	0.42
1:B1:40:LEU:HA	1:B1:43:ILE:HD12	2.01	0.42
1:B1:40:LEU:HD21	1:B3:90:LEU:HD11	2.00	0.42
3:B8:1041:A:H5''	12:BH:93:ARG:HG3	2.01	0.42
3:B8:1089:G:H2'	3:B8:1090:U:C6	2.53	0.42
4:B9:58:A:H2'	4:B9:59:G:C8	2.53	0.42
18:BN:132:GLY:HA3	50:Bu:42:THR:HG21	2.01	0.42
19:BO:110:ASP:OD1	19:BO:111:LEU:N	2.52	0.42
27:BW:178:ILE:HG22	27:BW:179:TYR:HD2	1.84	0.42
32:Bb:17:ARG:HG2	32:Bb:65:ASP:HB3	2.01	0.42
43:Bn:286:ARG:NH1	43:Bn:295:GLN:O	2.53	0.42
44:Bo:78:MET:HE1	44:Bo:91:HIS:CE1	2.54	0.42
49:Bt:112:LYS:HE3	49:Bt:116:LEU:HB2	2.00	0.42
56:AA:36:A:H2'	56:AA:37:A:C8	2.55	0.42
56:AA:129:G:H2'	56:AA:130:G:H8	1.84	0.42
95:AA:1120:SPM:H42	95:AA:1120:SPM:H71	1.87	0.42
57:AB:117:THR:HG22	57:AB:118:PRO:HD2	2.01	0.42
73:AR:105:THR:OG1	73:AR:285:ARG:O	2.27	0.42
85:Ad:150:ARG:HB2	85:Ad:155:GLN:HE21	1.84	0.42
1:B2:76:LEU:HD12	20:BP:194:TYR:CZ	2.53	0.42
3:B8:443:G:H5''	25:BU:134:LYS:HD3	2.01	0.42
20:BP:123:MET:HB3	20:BP:154:LEU:HD23	2.01	0.42
22:BR:73:GLU:OE2	38:Bh:149:ARG:NH2	2.52	0.42
27:BW:123:VAL:HG11	43:Bn:128:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Bi:291:THR:HG22	39:Bi:352:GLN:HB2	2.00	0.42
43:Bn:224:HIS:CE1	43:Bn:227:GLU:H	2.38	0.42
46:Bq:68:LEU:HD12	46:Bq:68:LEU:HA	1.88	0.42
56:AA:762:G:N2	56:AA:764:A:H3'	2.35	0.42
62:AG:38:C:H2'	62:AG:39:G:C8	2.54	0.42
83:Ab:92:HIS:HD2	83:Ab:224:THR:HG22	1.85	0.42
83:Ab:218:THR:H	83:Ab:232:THR:HG22	1.84	0.42
86:Ae:152:VAL:HA	86:Ae:172:MET:HE3	2.00	0.42
3:B8:409:A:H61	52:Bw:48:TYR:HE2	1.67	0.42
8:BD:74:ARG:HD3	8:BD:75:TRP:CZ2	2.54	0.42
9:BE:163:ARG:NH1	42:Bm:55:LEU:HD11	2.34	0.42
16:BL:127:VAL:HG22	16:BL:143:VAL:HG22	2.02	0.42
21:BQ:73:LYS:HE2	21:BQ:79:GLU:HG3	2.01	0.42
21:BQ:141:VAL:HG11	33:Bc:95:TRP:HZ3	1.83	0.42
23:BS:104:ASN:ND2	28:BX:158:GLN:OE1	2.44	0.42
24:BT:247:ILE:HD12	24:BT:247:ILE:HA	1.90	0.42
35:Be:23:ARG:HA	35:Be:24:PRO:HD3	1.87	0.42
56:AA:48:C:H2'	56:AA:171:C:H41	1.84	0.42
75:AT:7:PHE:HB2	75:AT:10:ARG:HH11	1.83	0.42
82:Aa:325:VAL:HG22	82:Aa:332:VAL:HG22	2.02	0.42
15:BK:113:ARG:HH21	24:BT:80:LYS:HE3	1.83	0.42
17:BM:151:THR:HG23	17:BM:171:PRO:HB2	2.01	0.42
19:BO:115:LYS:HE3	19:BO:118:VAL:HG21	2.01	0.42
23:BS:58:ILE:HD11	23:BS:76:ALA:HB2	2.01	0.42
28:BX:57:PRO:HA	28:BX:58:PRO:HD3	1.97	0.42
31:Ba:111:LYS:N	43:Bn:308:GLN:OE1	2.52	0.42
43:Bn:195:PRO:HG3	43:Bn:321:CYS:SG	2.60	0.42
56:AA:458:C:H1'	56:AA:476:A:H61	1.85	0.42
56:AA:550:G:N1	56:AA:782:G:OP2	2.53	0.42
74:AS:111:GLU:HB2	74:AS:117:LEU:HD21	2.01	0.42
77:AV:280:LEU:HD22	77:AV:293:PRO:HB3	2.01	0.42
83:Ab:94:ALA:N	83:Ab:111:GLY:O	2.52	0.42
6:BB:25:PHE:CE1	10:BF:111:ARG:HD3	2.54	0.42
19:BO:116:LYS:HE2	19:BO:120:ARG:NH2	2.33	0.42
19:BO:159:ALA:O	19:BO:163:THR:HG23	2.20	0.42
21:BQ:43:GLY:HA3	21:BQ:76:ARG:NH1	2.35	0.42
32:Bb:57:HIS:ND1	32:Bb:58:ASP:OD1	2.43	0.42
39:Bi:397:GLU:HB3	39:Bi:406:GLY:HA3	2.00	0.42
42:Bm:277:THR:OG1	42:Bm:278:GLY:N	2.53	0.42
70:AO:202:TRP:CD1	70:AO:202:TRP:H	2.38	0.42
85:Ad:374:ARG:HB2	85:Ad:377:CYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:Ai:112:ALA:HB3	88:Ai:137:ALA:HB2	2.00	0.42
3:B8:435:C:H2'	3:B8:436:U:C6	2.54	0.42
3:B8:680:C:H2'	3:B8:681:A:C8	2.55	0.42
17:BM:196:ALA:HB1	17:BM:199:ARG:HH12	1.82	0.42
20:BP:52:GLU:HG2	25:BU:250:ARG:HH12	1.84	0.42
20:BP:123:MET:HE3	20:BP:152:LEU:HD11	2.02	0.42
21:BQ:115:LYS:HE3	21:BQ:115:LYS:HB2	1.88	0.42
24:BT:142:GLU:N	24:BT:142:GLU:OE1	2.53	0.42
37:Bg:41:ASP:OD1	37:Bg:41:ASP:N	2.53	0.42
57:AB:158:TYR:HE2	57:AB:169:LYS:HB2	1.84	0.42
57:AB:213:ARG:NH2	80:AY:351:SER:OG	2.52	0.42
57:AB:233:HIS:HE1	63:AH:188:ILE:HB	1.85	0.42
77:AV:74:TYR:CD2	77:AV:409:GLU:HG2	2.53	0.42
79:AX:54:ASP:HB3	79:AX:57:LYS:HG2	2.02	0.42
79:AX:271:THR:HG22	79:AX:273:LEU:H	1.83	0.42
82:Aa:93:LEU:HD21	82:Aa:106:LEU:HB2	2.02	0.42
83:Ab:182:LEU:HB2	83:Ab:186:VAL:HG21	2.01	0.42
89:Aj:42:MET:HE3	89:Aj:42:MET:HB3	1.98	0.42
7:BC:62:VAL:HB	7:BC:120:VAL:HG13	2.02	0.42
7:BC:137:PHE:CZ	7:BC:141:GLY:HA2	2.54	0.42
16:BL:141:ALA:HB2	16:BL:154:ALA:HB2	2.00	0.42
21:BQ:23:ILE:HG13	21:BQ:67:PRO:HA	2.00	0.42
51:Bv:215:PHE:CE1	51:Bv:229:ALA:HB3	2.55	0.42
56:AA:432:A:O2'	56:AA:434:A:N7	2.45	0.42
77:AV:378:LEU:O	77:AV:382:LEU:HG	2.20	0.42
85:Ad:142:PRO:HA	85:Ad:146:ILE:HG13	2.01	0.42
3:B8:1003:C:H2'	3:B8:1004:A:H8	1.85	0.42
6:BB:3:ARG:HG2	6:BB:23:ASN:HB3	2.01	0.42
7:BC:191:LEU:HD12	46:Bq:116:GLY:HA3	2.01	0.42
9:BE:100:ARG:NH1	19:BO:75:ARG:HE	2.18	0.42
10:BF:105:TYR:CE1	46:Bq:60:VAL:HG12	2.55	0.42
24:BT:30:ASN:CG	35:Be:86:ARG:HH22	2.27	0.42
27:BW:117:TYR:CZ	43:Bn:120:GLU:HG2	2.55	0.42
28:BX:123:ASP:OD1	28:BX:123:ASP:N	2.46	0.42
30:BZ:168:THR:OG1	30:BZ:169:GLU:N	2.51	0.42
49:Bt:188:PRO:N	49:Bt:189:PRO:HD2	2.35	0.42
49:Bt:220:ILE:O	49:Bt:223:MET:HG2	2.20	0.42
70:AO:67:ARG:HD2	70:AO:68:TYR:CE2	2.55	0.42
71:AP:98:THR:HG22	71:AP:100:LEU:HG	2.02	0.42
86:Ae:160:ARG:NH1	86:Ae:172:MET:SD	2.93	0.42
86:Ae:412:ASP:N	86:Ae:415:ASP:OD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:1530:C:H4'	38:Bh:132:ARG:HD3	2.02	0.42
18:BN:191:ASP:O	18:BN:192:SER:OG	2.38	0.42
21:BQ:140:VAL:O	21:BQ:144:ILE:HG12	2.20	0.42
24:BT:72:THR:OG1	24:BT:77:ARG:NH2	2.53	0.42
26:BV:83:LYS:HB2	39:Bi:47:ILE:HA	2.02	0.42
26:BV:110:ILE:HD13	26:BV:110:ILE:HA	1.87	0.42
35:Be:15:ARG:HB3	35:Be:18:ILE:HG12	2.01	0.42
52:Bw:94:HIS:HB2	52:Bw:185:SER:HB3	2.02	0.42
61:AF:180:ARG:HG2	61:AF:184:MET:HE3	2.01	0.42
62:AG:1:A:H61	62:AG:67:U:H3	1.67	0.42
79:AX:141:LEU:HD11	79:AX:151:ILE:HG23	2.01	0.42
88:Ai:87:ILE:HD11	88:Ai:150:ARG:NH2	2.35	0.42
89:Aj:85:TRP:HD1	89:Aj:89:HIS:CD2	2.37	0.42
3:B8:641:U:H1'	12:BH:84:ARG:HG3	2.01	0.41
3:B8:675:U:H5''	6:BB:78:ARG:HB2	2.02	0.41
10:BF:153:ASP:OD1	10:BF:154:ALA:N	2.52	0.41
12:BH:144:GLN:NE2	12:BH:173:ARG:HH21	2.09	0.41
18:BN:48:LEU:HD22	54:By:95:VAL:HG12	2.02	0.41
32:Bb:67:LEU:HD12	32:Bb:72:HIS:O	2.19	0.41
34:Bd:86:SER:O	34:Bd:90:ARG:N	2.37	0.41
43:Bn:262:GLY:HA3	43:Bn:342:PHE:HB2	2.01	0.41
56:AA:177:U:H2'	56:AA:178:G:H8	1.85	0.41
58:AC:37:ASN:O	58:AC:43:ARG:NH2	2.52	0.41
58:AC:89:ASP:O	58:AC:93:ARG:HG2	2.20	0.41
70:AO:73:VAL:HG12	70:AO:106:PRO:HB3	2.02	0.41
82:Aa:253:TYR:O	82:Aa:399:ARG:NH2	2.53	0.41
87:Ag:127:HIS:CD2	87:Ag:129:GLU:H	2.37	0.41
3:B8:330:A:H8	3:B8:830:U:O2'	2.03	0.41
3:B8:722:A:H5'	42:Bm:300:ARG:HB3	2.02	0.41
3:B8:801:G:O2'	23:BS:36:THR:HG22	2.20	0.41
3:B8:1376:OMG:H1'	3:B8:1405:A:N3	2.36	0.41
21:BQ:115:LYS:NZ	33:Bc:86:LEU:HB2	2.35	0.41
39:Bi:244:PHE:HE2	39:Bi:365:CYS:HB3	1.84	0.41
39:Bi:265:LEU:N	39:Bi:266:PRO:HA	2.35	0.41
45:Bp:200:THR:HG22	52:Bw:200:ALA:HB3	2.01	0.41
56:AA:220:U:H2'	56:AA:221:A:H8	1.85	0.41
56:AA:728:U:H2'	56:AA:729:A:H8	1.85	0.41
67:AL:117:LEU:HD11	67:AL:128:ALA:HA	2.02	0.41
80:AY:319:GLU:HB3	80:AY:321:HIS:CD2	2.54	0.41
80:AY:338:PRO:HD2	80:AY:386:LEU:HD21	2.02	0.41
82:Aa:162:LYS:HA	82:Aa:165:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Ae:377:TYR:OH	86:Ae:414:ASP:OD2	2.39	0.41
86:Ae:382:PHE:CG	86:Ae:395:ILE:HG13	2.55	0.41
5:BA:59:PRO:HA	50:Bu:229:GLY:HA2	2.03	0.41
25:BU:76:SER:HB2	25:BU:155:LYS:HB2	2.01	0.41
28:BX:123:ASP:HA	28:BX:124:PRO:HD3	1.92	0.41
30:BZ:67:ASP:OD1	30:BZ:68:ILE:N	2.52	0.41
34:Bd:120:LYS:HE2	34:Bd:123:TRP:CZ3	2.54	0.41
56:AA:443:U:H2'	56:AA:444:G:C8	2.54	0.41
56:AA:750:G:N2	56:AA:776:A:N7	2.69	0.41
56:AA:854:C:H2'	56:AA:855:C:C6	2.55	0.41
57:AB:67:ASP:OD1	57:AB:67:ASP:N	2.52	0.41
61:AF:157:GLY:HA2	61:AF:226:MET:HE2	2.02	0.41
62:AG:18:A:H61	62:AG:44:U:H5''	1.84	0.41
67:AL:109:LYS:HG2	67:AL:113:MET:HE3	2.02	0.41
88:Ai:71:GLN:HG3	88:Ai:72:GLU:H	1.85	0.41
3:B8:913:G:H21	3:B8:914:A:H62	1.67	0.41
4:B9:8:U:H3	4:B9:13:U:H3	1.67	0.41
5:BA:55:ILE:O	50:Bu:227:ARG:NH2	2.53	0.41
5:BA:60:GLN:HE22	5:BA:67:ARG:HB2	1.85	0.41
20:BP:101:HIS:HB3	20:BP:150:HIS:ND1	2.35	0.41
34:Bd:53:TYR:CE1	34:Bd:72:PRO:HG3	2.56	0.41
40:Bj:119:GLN:HB2	40:Bj:260:LEU:HB2	2.01	0.41
47:Br:77:ARG:HB2	47:Br:78:PRO:HD3	2.01	0.41
50:Bu:185:PHE:HZ	50:Bu:188:SER:HB2	1.85	0.41
56:AA:303:U:OP2	56:AA:398:G:N1	2.52	0.41
56:AA:527:G:N2	56:AA:839:C:O2	2.53	0.41
57:AB:140:ASP:OD1	57:AB:140:ASP:N	2.46	0.41
61:AF:91:ILE:HG23	61:AF:111:MET:HE2	2.02	0.41
61:AF:200:LEU:HB3	61:AF:202:PRO:HD2	2.02	0.41
68:AM:29:ARG:NH1	68:AM:57:LEU:HB2	2.35	0.41
70:AO:173:ARG:HA	73:AR:221:ARG:NH1	2.36	0.41
77:AV:401:ALA:O	77:AV:405:LEU:HB3	2.20	0.41
79:AX:377:LYS:HB3	87:Ag:324:LEU:HD12	2.02	0.41
3:B8:655:C:OP1	12:BH:131:ARG:NH1	2.52	0.41
3:B8:1224:C:H2'	3:B8:1225:A:C8	2.55	0.41
19:BO:85:ASP:HB3	19:BO:88:HIS:HD2	1.86	0.41
36:Bf:71:ILE:HD11	36:Bf:154:ARG:HG3	2.02	0.41
44:Bo:84:THR:O	44:Bo:87:SER:OG	2.37	0.41
49:Bt:312:ARG:HD3	49:Bt:313:PRO:HD2	2.02	0.41
51:Bv:200:MET:HG2	51:Bv:241:GLY:C	2.46	0.41
52:Bw:88:TYR:HE1	52:Bw:164:ALA:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AA:404:C:H5''	67:AL:151:LYS:HD2	2.03	0.41
56:AA:620:C:H5'	63:AH:122:LYS:HE2	2.02	0.41
68:AM:35:VAL:HG23	68:AM:50:GLN:HA	2.02	0.41
3:B8:36:A:C4	46:Bq:32:LYS:HG3	2.55	0.41
3:B8:83:A:OP2	3:B8:1235:C:O2'	2.27	0.41
3:B8:624:A:O2'	18:BN:108:ARG:NH1	2.54	0.41
3:B8:1109:A:H8	19:BO:179:ASN:HD21	1.69	0.41
9:BE:20:ILE:HD12	9:BE:20:ILE:H	1.86	0.41
18:BN:64:ALA:HA	54:By:118:LEU:HD12	2.03	0.41
32:Bb:81:LEU:HD21	38:Bh:49:ILE:HG22	2.02	0.41
43:Bn:118:GLU:CD	43:Bn:118:GLU:H	2.29	0.41
52:Bw:127:MET:HB3	52:Bw:154:GLU:HB3	2.03	0.41
56:AA:285:C:H41	65:AJ:44:HIS:HA	1.86	0.41
56:AA:409:G:H4'	56:AA:939:A:H4'	2.02	0.41
56:AA:663:A:H61	56:AA:670:A:H61	1.68	0.41
56:AA:704:U:H2'	56:AA:705:G:H8	1.84	0.41
57:AB:211:THR:OG1	57:AB:220:ASN:OD1	2.25	0.41
63:AH:128:LYS:HG2	63:AH:131:ARG:HH21	1.86	0.41
72:AQ:82:ASP:OD1	72:AQ:82:ASP:N	2.50	0.41
88:Ai:186:5F0:O	88:Ai:186:5F0:N	2.52	0.41
6:BB:2:AYA:HM1	46:Bq:58:LEU:HD21	2.02	0.41
16:BL:67:LYS:HB2	42:Bm:35:VAL:HG21	2.02	0.41
16:BL:156:GLU:N	16:BL:247:ARG:O	2.54	0.41
18:BN:58:HIS:CD2	18:BN:59:ARG:HG3	2.55	0.41
24:BT:46:GLY:C	24:BT:48:LYS:H	2.29	0.41
27:BW:82:ARG:HB3	27:BW:93:LEU:HB2	2.03	0.41
30:BZ:112:VAL:HG11	30:BZ:199:ILE:HG12	2.02	0.41
34:Bd:82:LEU:HD21	34:Bd:94:PHE:HE1	1.85	0.41
42:Bm:94:HIS:HA	42:Bm:99:TYR:CG	2.55	0.41
43:Bn:362:PRO:HB2	43:Bn:364:ARG:HG2	2.02	0.41
49:Bt:148:LEU:HD22	49:Bt:305:PHE:HB3	2.02	0.41
50:Bu:113:LYS:HA	50:Bu:113:LYS:HD3	1.95	0.41
61:AF:116:GLU:O	61:AF:120:ARG:HG2	2.20	0.41
66:AK:51:ARG:NH1	66:AK:82:SER:O	2.54	0.41
71:AP:95:ARG:NH1	71:AP:102:GLY:HA2	2.34	0.41
71:AP:124:THR:HG23	71:AP:125:TYR:HD1	1.85	0.41
77:AV:163:ASP:OD1	77:AV:163:ASP:N	2.53	0.41
77:AV:270:LEU:HG	77:AV:320:LEU:HD21	2.03	0.41
78:AW:118:GLY:HA2	83:Ab:87:ARG:NH2	2.36	0.41
82:Aa:103:ARG:HG2	82:Aa:107:ASN:HD21	1.86	0.41
3:B8:218:A:C5	43:Bn:379:ILE:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BC:15:LEU:HD21	7:BC:26:PRO:HB3	2.03	0.41
9:BE:227:PHE:HD1	10:BF:158:LEU:HD12	1.85	0.41
12:BH:156:THR:HB	26:BV:130:CYS:SG	2.60	0.41
18:BN:62:VAL:HG13	18:BN:82:LEU:HB2	2.03	0.41
24:BT:218:LYS:HE2	24:BT:218:LYS:HB2	1.92	0.41
40:Bj:128:ASP:O	40:Bj:282:ARG:NH2	2.54	0.41
43:Bn:215:THR:HB	43:Bn:273:PHE:HB2	2.02	0.41
45:Bp:182:ILE:HD11	45:Bp:185:TYR:CD1	2.56	0.41
57:AB:69:PRO:HB3	57:AB:120:ALA:HB2	2.02	0.41
57:AB:189:LYS:HE3	57:AB:189:LYS:HB3	1.92	0.41
67:AL:82:GLY:HA3	67:AL:85:LYS:HE3	2.02	0.41
70:AO:91:ARG:HE	70:AO:94:CYS:HB3	1.86	0.41
77:AV:99:LYS:HB3	77:AV:99:LYS:HE3	1.81	0.41
84:Ac:113:ASN:OD1	84:Ac:114:LYS:N	2.53	0.41
85:Ad:289:THR:HG23	85:Ad:331:ASP:O	2.20	0.41
1:B2:70:ASP:O	1:B2:74:LEU:HG	2.21	0.41
3:B8:273:A:O2'	3:B8:274:A:H5''	2.21	0.41
3:B8:348:G:O6	55:Bz:113:ARG:NH1	2.47	0.41
3:B8:402:A:C4	8:BD:74:ARG:HG3	2.55	0.41
3:B8:619:C:H2'	3:B8:620:A:H8	1.86	0.41
3:B8:860:G:O5'	16:BL:136:ARG:NH2	2.53	0.41
3:B8:914:A:O2'	56:AA:943:G:N3	2.53	0.41
3:B8:1396:C:H5	82:Aa:317:LYS:HD2	1.86	0.41
3:B8:1426:G:H2'	3:B8:1427:G:H8	1.86	0.41
3:B8:1519:U:H5'	38:Bh:99:MET:O	2.21	0.41
14:BJ:85:ARG:HH21	14:BJ:90:ARG:NE	2.18	0.41
17:BM:121:LEU:HD12	28:BX:91:LYS:HG3	2.03	0.41
18:BN:59:ARG:HE	18:BN:84:PRO:HB2	1.86	0.41
20:BP:94:ARG:HH21	20:BP:158:GLU:N	2.19	0.41
24:BT:97:SER:OG	24:BT:143:GLU:HB3	2.20	0.41
30:BZ:88:ASN:HA	30:BZ:91:ILE:HG22	2.03	0.41
34:Bd:41:LEU:HD11	51:Bv:67:GLN:HB3	2.03	0.41
34:Bd:111:SER:OG	81:AZ:10:ARG:NH2	2.54	0.41
38:Bh:108:CYS:SG	38:Bh:111:GLU:HB2	2.61	0.41
39:Bi:410:ASP:OD1	39:Bi:410:ASP:N	2.54	0.41
43:Bn:238:THR:HG23	43:Bn:281:PHE:HD2	1.86	0.41
46:Bq:73:ASN:OD1	46:Bq:74:TYR:N	2.54	0.41
49:Bt:245:LEU:HD12	49:Bt:253:PRO:HD3	2.02	0.41
53:Bx:76:ARG:HD3	53:Bx:165:GLY:HA3	2.02	0.41
56:AA:704:U:H2'	56:AA:705:G:C8	2.56	0.41
56:AA:855:C:H2'	56:AA:856:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:AB:68:TRP:N	57:AB:69:PRO:HD2	2.36	0.41
57:AB:214:CYS:HB3	57:AB:219:GLN:HB2	2.03	0.41
58:AC:100:PHE:HB3	58:AC:103:CYS:SG	2.61	0.41
71:AP:63:LEU:HD12	71:AP:63:LEU:H	1.86	0.41
73:AR:282:ASP:HA	73:AR:285:ARG:HG2	2.03	0.41
80:AY:242:ILE:HB	86:Ae:357:LEU:HD22	2.02	0.41
80:AY:321:HIS:ND1	80:AY:322:GLU:HG3	2.36	0.41
82:Aa:180:TYR:HB3	82:Aa:181:ASP:H	1.58	0.41
86:Ae:644:VAL:HG12	86:Ae:648:LEU:HG	2.03	0.41
3:B8:354:U:H2'	3:B8:355:G:H8	1.85	0.41
3:B8:717:A:O2'	42:Bm:266:GLN:HG3	2.21	0.41
3:B8:1230:U:H5'	3:B8:1231:U:C5'	2.51	0.41
7:BC:88:VAL:HG21	7:BC:91:LEU:HB2	2.03	0.41
9:BE:196:ILE:HG23	9:BE:200:GLU:HB2	2.03	0.41
16:BL:155:THR:O	16:BL:249:SER:HB3	2.21	0.41
30:BZ:60:LEU:O	38:Bh:187:TYR:OH	2.36	0.41
38:Bh:72:ILE:HG12	38:Bh:107:LEU:HD22	2.03	0.41
45:Bp:91:PRO:HD2	45:Bp:94:PHE:HE2	1.86	0.41
56:AA:335:A:H2'	56:AA:336:A:C8	2.56	0.41
56:AA:647:A:N6	72:AQ:80:ARG:O	2.53	0.41
57:AB:89:MET:HG2	57:AB:107:LEU:HG	2.02	0.41
61:AF:66:ARG:HA	61:AF:69:LYS:HB3	2.02	0.41
63:AH:128:LYS:HE2	63:AH:131:ARG:NH2	2.35	0.41
70:AO:235:MET:HE1	73:AR:171:GLU:HB3	2.03	0.41
72:AQ:85:GLN:HB3	87:Ag:228:ARG:HH11	1.85	0.41
82:Aa:126:THR:HG22	82:Aa:159:ILE:HG23	2.02	0.41
82:Aa:258:HIS:HB3	82:Aa:388:TYR:HE1	1.86	0.41
82:Aa:389:ASN:HB3	82:Aa:394[A]:ARG:HG3	2.01	0.41
3:B8:1094:A:H2'	3:B8:1118:A:N1	2.35	0.40
4:B9:12:U:H3	4:B9:24:A:H61	1.69	0.40
10:BF:212:ARG:HD3	55:Bz:104:ILE:HD11	2.04	0.40
24:BT:26:ASN:OD1	24:BT:26:ASN:N	2.54	0.40
26:BV:34:THR:OG1	26:BV:81:THR:HG22	2.21	0.40
42:Bm:125:LYS:HG3	42:Bm:253:LEU:HD11	2.03	0.40
42:Bm:347:THR:HG22	42:Bm:349:GLY:H	1.86	0.40
45:Bp:139:LEU:HD23	52:Bw:169:ILE:HG23	2.03	0.40
48:Bs:72:VAL:HG13	48:Bs:90:HIS:HB2	2.03	0.40
56:AA:512:A:H2'	56:AA:513:A:C8	2.55	0.40
56:AA:814:A:OP2	87:Ag:378:ARG:NH1	2.52	0.40
57:AB:80:PRO:HG2	58:AC:156:GLN:NE2	2.35	0.40
63:AH:76:LEU:HG	63:AH:174:LYS:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AL:233:VAL:HG12	67:AL:237:LYS:HE3	2.02	0.40
76:AU:194:GLU:HG3	76:AU:196:LEU:HD13	2.04	0.40
79:AX:152:LEU:HD12	79:AX:259:VAL:HG22	2.03	0.40
80:AY:376:ARG:NH2	80:AY:386:LEU:O	2.53	0.40
82:Aa:296:ASP:N	82:Aa:296:ASP:OD1	2.55	0.40
85:Ad:220:THR:HB	85:Ad:247:VAL:HG12	2.01	0.40
5:BA:210:LEU:HD12	29:BY:104:ASP:HB3	2.03	0.40
18:BN:120:VAL:HG11	18:BN:142:ARG:HD2	2.03	0.40
19:BO:193:PHE:O	19:BO:198:GLY:N	2.54	0.40
44:Bo:313:LEU:O	44:Bo:316:SER:OG	2.32	0.40
45:Bp:82:LEU:HA	52:Bw:198:PHE:HA	2.03	0.40
56:AA:369:U:O2	71:AP:92:ILE:N	2.54	0.40
56:AA:633:C:H2'	56:AA:634:C:C6	2.57	0.40
57:AB:166:ARG:HD3	86:Ae:134:GLU:HB3	2.03	0.40
61:AF:52:ARG:NH2	87:Ag:320:PHE:O	2.54	0.40
62:AG:7:G:N2	62:AG:62:C:O2	2.54	0.40
75:AT:48:VAL:HG13	75:AT:52:ILE:HD12	2.03	0.40
77:AV:147:TRP:HB3	77:AV:423:TRP:CG	2.56	0.40
79:AX:101:ARG:NH2	79:AX:345:SER:O	2.52	0.40
79:AX:210:ASN:ND2	79:AX:213:GLU:OE2	2.55	0.40
80:AY:242:ILE:HG21	86:Ae:395:ILE:HD13	2.02	0.40
86:Ae:627:PRO:O	86:Ae:631:ILE:HG12	2.22	0.40
3:B8:449:C:H4'	3:B8:1319:G:O2'	2.21	0.40
9:BE:227:PHE:HE2	46:Bq:112:LEU:HD23	1.85	0.40
17:BM:142:MET:HE3	17:BM:180:ASN:HB3	2.04	0.40
18:BN:284:TYR:HB2	18:BN:285:PRO:HD2	2.03	0.40
28:BX:82:PRO:HA	28:BX:83:PRO:HD3	1.95	0.40
31:Ba:112:SER:HB3	43:Bn:88:VAL:HG13	2.03	0.40
31:Ba:113:LYS:NZ	43:Bn:312:THR:OG1	2.40	0.40
50:Bu:85:PHE:HB2	50:Bu:198:ARG:HH21	1.85	0.40
58:AC:47:GLY:HA2	58:AC:166:TYR:HD2	1.86	0.40
60:AE:28:ALA:O	60:AE:32:ARG:HG2	2.21	0.40
62:AG:47:U:H2'	62:AG:48:G:C8	2.56	0.40
63:AH:63:ILE:HG22	86:Ae:63:LYS:HB3	2.02	0.40
3:B8:144:A:H2'	3:B8:145:A:C8	2.57	0.40
3:B8:178:C:HO2'	29:BY:55:ARG:HH22	1.61	0.40
3:B8:391:A:N6	35:Be:78:GLN:OE1	2.55	0.40
3:B8:1212:U:H2'	3:B8:1213:A:C8	2.57	0.40
3:B8:1513:U:OP2	3:B8:1525:C:N4	2.55	0.40
4:B9:14:A:H2'	4:B9:15:A:O4'	2.21	0.40
8:BD:102:GLU:OE2	43:Bn:74:TYR:N	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BD:139:GLU:HG3	27:BW:63:ARG:HG3	2.04	0.40
9:BE:226:LEU:HD12	10:BF:157:LEU:HB3	2.03	0.40
22:BR:17:VAL:HG11	48:Bs:136:LYS:NZ	2.37	0.40
25:BU:104:MET:HE3	25:BU:104:MET:HB3	1.99	0.40
25:BU:202:GLN:NE2	25:BU:240:ARG:HH12	2.19	0.40
27:BW:114:LYS:HG3	27:BW:115:HIS:CD2	2.57	0.40
45:Bp:168:LEU:HD21	52:Bw:171:LEU:HD12	2.04	0.40
51:Bv:278:ASP:OD1	51:Bv:278:ASP:N	2.53	0.40
56:AA:28:U:H2'	56:AA:29:A:C8	2.55	0.40
58:AC:73:THR:HG23	58:AC:76:LEU:HD12	2.02	0.40
80:AY:289:GLY:O	80:AY:293:MET:HG2	2.22	0.40
85:Ad:111:ARG:HB2	85:Ad:114:ARG:HH12	1.86	0.40
3:B8:617:A:H4'	3:B8:618:A:C2	2.56	0.40
3:B8:1414:C:H2'	3:B8:1415:G:C8	2.57	0.40
5:BA:60:GLN:NE2	5:BA:67:ARG:HB2	2.36	0.40
18:BN:249:ASN:O	18:BN:253:MET:HG3	2.21	0.40
23:BS:62:ASN:OD1	23:BS:63:LYS:N	2.54	0.40
30:BZ:99:LEU:HD23	30:BZ:142:ALA:HB2	2.04	0.40
33:Bc:106:LYS:HB2	33:Bc:109:GLU:OE1	2.21	0.40
34:Bd:79:PRO:O	45:Bp:192:TYR:OH	2.35	0.40
42:Bm:361:THR:OG1	42:Bm:370:VAL:O	2.28	0.40
45:Bp:70:LYS:HE3	45:Bp:74:ARG:NE	2.37	0.40
51:Bv:242:ASP:OD1	51:Bv:242:ASP:N	2.55	0.40
52:Bw:84:THR:HG22	52:Bw:85:ASP:H	1.86	0.40
52:Bw:131:THR:HG23	52:Bw:151:THR:HG22	2.03	0.40
56:AA:38:U:H2'	56:AA:39:A:H8	1.86	0.40
56:AA:663:A:H5'	87:Ag:117:PHE:HB3	2.04	0.40
57:AB:58:ARG:NH2	86:Ae:91:ASP:OD1	2.48	0.40
57:AB:214:CYS:HB2	57:AB:220:ASN:CG	2.46	0.40
58:AC:43:ARG:HD3	58:AC:43:ARG:HA	1.90	0.40
63:AH:78:VAL:HG22	63:AH:172:VAL:HG12	2.04	0.40
77:AV:262:SER:HB3	77:AV:313:GLY:HA3	2.02	0.40
79:AX:83:PRO:HG2	79:AX:86:PHE:HB3	2.04	0.40
79:AX:83:PRO:HA	79:AX:84:PRO:HD3	1.95	0.40
79:AX:150:LEU:HD23	79:AX:257:LEU:HD13	2.03	0.40
88:Ai:65:TYR:HA	88:Ai:66:PRO:HD3	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B1	43/198 (22%)	41 (95%)	2 (5%)	0	100	100
1	B2	25/198 (13%)	25 (100%)	0	0	100	100
1	B3	26/198 (13%)	26 (100%)	0	0	100	100
1	B4	25/198 (13%)	25 (100%)	0	0	100	100
1	B5	25/198 (13%)	25 (100%)	0	0	100	100
1	B6	24/198 (12%)	24 (100%)	0	0	100	100
5	BA	164/210 (78%)	159 (97%)	5 (3%)	0	100	100
6	BB	147/150 (98%)	144 (98%)	3 (2%)	0	100	100
7	BC	204/216 (94%)	199 (98%)	5 (2%)	0	100	100
8	BD	110/148 (74%)	109 (99%)	1 (1%)	0	100	100
9	BE	242/256 (94%)	238 (98%)	4 (2%)	0	100	100
10	BF	177/250 (71%)	175 (99%)	2 (1%)	0	100	100
11	BG	105/161 (65%)	105 (100%)	0	0	100	100
12	BH	108/207 (52%)	108 (100%)	0	0	100	100
13	BI	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
14	BJ	44/95 (46%)	43 (98%)	1 (2%)	0	100	100
15	BK	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
16	BL	238/306 (78%)	229 (96%)	8 (3%)	1 (0%)	30	61
17	BM	305/399 (76%)	296 (97%)	9 (3%)	0	100	100
18	BN	249/294 (85%)	247 (99%)	2 (1%)	0	100	100
19	BO	200/268 (75%)	188 (94%)	12 (6%)	0	100	100
20	BP	210/257 (82%)	207 (99%)	3 (1%)	0	100	100
21	BQ	174/192 (91%)	171 (98%)	3 (2%)	0	100	100
22	BR	175/197 (89%)	171 (98%)	4 (2%)	0	100	100
23	BS	113/325 (35%)	112 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	BT	286/296 (97%)	274 (96%)	12 (4%)	0	100	100
25	BU	220/251 (88%)	215 (98%)	5 (2%)	0	100	100
26	BV	151/169 (89%)	147 (97%)	4 (3%)	0	100	100
27	BW	141/188 (75%)	135 (96%)	6 (4%)	0	100	100
28	BX	238/303 (78%)	234 (98%)	4 (2%)	0	100	100
29	BY	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
30	BZ	153/209 (73%)	151 (99%)	2 (1%)	0	100	100
31	Ba	95/160 (59%)	94 (99%)	1 (1%)	0	100	100
32	Bb	95/112 (85%)	91 (96%)	4 (4%)	0	100	100
33	Bc	82/138 (59%)	82 (100%)	0	0	100	100
34	Bd	90/126 (71%)	88 (98%)	2 (2%)	0	100	100
35	Be	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
36	Bf	147/205 (72%)	144 (98%)	3 (2%)	0	100	100
37	Bg	133/222 (60%)	132 (99%)	1 (1%)	0	100	100
38	Bh	160/196 (82%)	152 (95%)	8 (5%)	0	100	100
39	Bi	385/433 (89%)	371 (96%)	13 (3%)	1 (0%)	36	65
40	Bj	160/304 (53%)	156 (98%)	4 (2%)	0	100	100
41	Bl	36/100 (36%)	36 (100%)	0	0	100	100
42	Bm	391/423 (92%)	384 (98%)	7 (2%)	0	100	100
43	Bn	352/380 (93%)	334 (95%)	18 (5%)	0	100	100
44	Bo	293/334 (88%)	284 (97%)	9 (3%)	0	100	100
45	Bp	141/162 (87%)	135 (96%)	6 (4%)	0	100	100
46	Bq	120/135 (89%)	115 (96%)	5 (4%)	0	100	100
47	Br	106/142 (75%)	102 (96%)	4 (4%)	0	100	100
48	Bs	149/159 (94%)	146 (98%)	3 (2%)	0	100	100
49	Bt	287/332 (86%)	283 (99%)	4 (1%)	0	100	100
50	Bu	258/306 (84%)	253 (98%)	5 (2%)	0	100	100
51	Bv	236/279 (85%)	229 (97%)	7 (3%)	0	100	100
52	Bw	163/269 (61%)	156 (96%)	7 (4%)	0	100	100
53	Bx	131/166 (79%)	128 (98%)	3 (2%)	0	100	100
54	By	107/198 (54%)	104 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	Bz	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
57	AB	273/366 (75%)	270 (99%)	3 (1%)	0	100	100
58	AC	130/167 (78%)	126 (97%)	4 (3%)	0	100	100
59	AD	70/199 (35%)	70 (100%)	0	0	100	100
60	AE	120/124 (97%)	118 (98%)	2 (2%)	0	100	100
61	AF	206/242 (85%)	202 (98%)	4 (2%)	0	100	100
63	AH	138/200 (69%)	134 (97%)	3 (2%)	1 (1%)	18	51
65	AJ	107/139 (77%)	106 (99%)	1 (1%)	0	100	100
66	AK	99/128 (77%)	99 (100%)	0	0	100	100
67	AL	173/259 (67%)	170 (98%)	3 (2%)	0	100	100
68	AM	115/135 (85%)	111 (96%)	4 (4%)	0	100	100
69	AN	110/130 (85%)	106 (96%)	4 (4%)	0	100	100
70	AO	188/258 (73%)	187 (100%)	1 (0%)	0	100	100
71	AP	95/143 (66%)	95 (100%)	0	0	100	100
72	AQ	84/87 (97%)	84 (100%)	0	0	100	100
73	AR	290/382 (76%)	287 (99%)	3 (1%)	0	100	100
74	AS	133/190 (70%)	131 (98%)	2 (2%)	0	100	100
75	AT	167/173 (96%)	165 (99%)	2 (1%)	0	100	100
76	AU	175/205 (85%)	175 (100%)	0	0	100	100
77	AV	386/395 (98%)	373 (97%)	13 (3%)	0	100	100
78	AW	97/188 (52%)	96 (99%)	1 (1%)	0	100	100
79	AX	351/410 (86%)	344 (98%)	7 (2%)	0	100	100
80	AY	147/381 (39%)	145 (99%)	2 (1%)	0	100	100
81	AZ	97/148 (66%)	96 (99%)	1 (1%)	0	100	100
82	Aa	380/474 (80%)	373 (98%)	7 (2%)	0	100	100
83	Ab	218/289 (75%)	211 (97%)	7 (3%)	0	100	100
84	Ac	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
85	Ad	341/430 (79%)	332 (97%)	9 (3%)	0	100	100
86	Ae	584/692 (84%)	576 (99%)	8 (1%)	0	100	100
87	Ag	326/397 (82%)	322 (99%)	4 (1%)	0	100	100
88	Ai	134/196 (68%)	131 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
89	Aj	211/505 (42%)	209 (99%)	2 (1%)	0	100	100
All	All	14966/20598 (73%)	14638 (98%)	325 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
63	AH	126	ILE
39	Bi	159	VAL
16	BL	208	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	30/157 (19%)	30 (100%)	0	100	100
1	B2	26/157 (17%)	25 (96%)	1 (4%)	29	55
1	B3	27/157 (17%)	27 (100%)	0	100	100
1	B4	26/157 (17%)	26 (100%)	0	100	100
1	B5	26/157 (17%)	26 (100%)	0	100	100
1	B6	25/157 (16%)	25 (100%)	0	100	100
5	BA	144/180 (80%)	144 (100%)	0	100	100
6	BB	116/134 (87%)	116 (100%)	0	100	100
7	BC	185/192 (96%)	185 (100%)	0	100	100
8	BD	91/115 (79%)	90 (99%)	1 (1%)	65	74
9	BE	219/229 (96%)	216 (99%)	3 (1%)	59	71
10	BF	164/226 (73%)	163 (99%)	1 (1%)	78	79
11	BG	99/150 (66%)	99 (100%)	0	100	100
12	BH	99/177 (56%)	99 (100%)	0	100	100
13	BI	49/60 (82%)	48 (98%)	1 (2%)	48	66
14	BJ	41/78 (53%)	41 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	BK	87/162 (54%)	87 (100%)	0	100	100
16	BL	193/248 (78%)	191 (99%)	2 (1%)	68	75
17	BM	263/320 (82%)	263 (100%)	0	100	100
18	BN	218/251 (87%)	217 (100%)	1 (0%)	81	80
19	BO	181/228 (79%)	179 (99%)	2 (1%)	65	74
20	BP	192/231 (83%)	189 (98%)	3 (2%)	55	69
21	BQ	138/151 (91%)	136 (99%)	2 (1%)	59	71
22	BR	155/173 (90%)	154 (99%)	1 (1%)	78	79
23	BS	99/243 (41%)	98 (99%)	1 (1%)	68	75
24	BT	245/249 (98%)	245 (100%)	0	100	100
25	BU	190/210 (90%)	189 (100%)	1 (0%)	81	80
26	BV	132/143 (92%)	132 (100%)	0	100	100
27	BW	123/161 (76%)	121 (98%)	2 (2%)	55	69
28	BX	212/266 (80%)	211 (100%)	1 (0%)	81	80
29	BY	118/127 (93%)	118 (100%)	0	100	100
30	BZ	136/178 (76%)	136 (100%)	0	100	100
31	Ba	77/129 (60%)	76 (99%)	1 (1%)	61	72
32	Bb	79/88 (90%)	76 (96%)	3 (4%)	29	55
33	Bc	79/114 (69%)	78 (99%)	1 (1%)	61	72
34	Bd	79/114 (69%)	77 (98%)	2 (2%)	42	63
35	Be	75/82 (92%)	74 (99%)	1 (1%)	61	72
36	Bf	126/177 (71%)	126 (100%)	0	100	100
37	Bg	115/183 (63%)	114 (99%)	1 (1%)	70	76
38	Bh	149/173 (86%)	148 (99%)	1 (1%)	76	78
39	Bi	340/373 (91%)	337 (99%)	3 (1%)	70	76
40	Bj	150/267 (56%)	149 (99%)	1 (1%)	76	78
41	Bl	36/77 (47%)	36 (100%)	0	100	100
42	Bm	348/365 (95%)	343 (99%)	5 (1%)	59	71
43	Bn	310/328 (94%)	309 (100%)	1 (0%)	86	83
44	Bo	271/299 (91%)	269 (99%)	2 (1%)	76	78
45	Bp	132/150 (88%)	131 (99%)	1 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	Bq	100/108 (93%)	100 (100%)	0	100	100
47	Br	103/133 (77%)	102 (99%)	1 (1%)	68	75
48	Bs	130/135 (96%)	128 (98%)	2 (2%)	57	70
49	Bt	251/284 (88%)	250 (100%)	1 (0%)	84	81
50	Bu	236/275 (86%)	233 (99%)	3 (1%)	61	72
51	Bv	210/242 (87%)	209 (100%)	1 (0%)	81	80
52	Bw	135/226 (60%)	133 (98%)	2 (2%)	57	70
53	Bx	122/147 (83%)	122 (100%)	0	100	100
54	By	103/178 (58%)	103 (100%)	0	100	100
55	Bz	88/113 (78%)	88 (100%)	0	100	100
57	AB	249/322 (77%)	244 (98%)	5 (2%)	48	66
58	AC	115/142 (81%)	114 (99%)	1 (1%)	70	76
59	AD	66/174 (38%)	66 (100%)	0	100	100
60	AE	107/109 (98%)	105 (98%)	2 (2%)	50	67
61	AF	181/205 (88%)	181 (100%)	0	100	100
63	AH	130/180 (72%)	130 (100%)	0	100	100
65	AJ	92/116 (79%)	91 (99%)	1 (1%)	65	74
66	AK	92/114 (81%)	92 (100%)	0	100	100
67	AL	159/222 (72%)	159 (100%)	0	100	100
68	AM	97/113 (86%)	95 (98%)	2 (2%)	47	65
69	AN	97/114 (85%)	97 (100%)	0	100	100
70	AO	170/225 (76%)	169 (99%)	1 (1%)	78	79
71	AP	89/127 (70%)	89 (100%)	0	100	100
72	AQ	77/78 (99%)	76 (99%)	1 (1%)	61	72
73	AR	258/330 (78%)	257 (100%)	1 (0%)	84	81
74	AS	113/162 (70%)	111 (98%)	2 (2%)	51	68
75	AT	152/155 (98%)	151 (99%)	1 (1%)	76	78
76	AU	149/168 (89%)	148 (99%)	1 (1%)	76	78
77	AV	325/347 (94%)	323 (99%)	2 (1%)	78	79
78	AW	86/160 (54%)	84 (98%)	2 (2%)	44	64
79	AX	312/361 (86%)	311 (100%)	1 (0%)	86	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
80	AY	134/342 (39%)	133 (99%)	1 (1%)	76	78
81	AZ	86/125 (69%)	86 (100%)	0	100	100
82	Aa	339/424 (80%)	336 (99%)	3 (1%)	70	76
83	Ab	187/233 (80%)	187 (100%)	0	100	100
84	Ac	100/102 (98%)	97 (97%)	3 (3%)	36	59
85	Ad	282/351 (80%)	275 (98%)	7 (2%)	42	63
86	Ae	521/604 (86%)	521 (100%)	0	100	100
87	Ag	273/333 (82%)	272 (100%)	1 (0%)	84	81
88	Ai	102/150 (68%)	102 (100%)	0	100	100
89	Aj	188/404 (46%)	185 (98%)	3 (2%)	55	69
All	All	13221/17576 (75%)	13124 (99%)	97 (1%)	73	78

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B2	86	LEU
8	BD	40	LYS
9	BE	6	VAL
9	BE	46	HIS
9	BE	196	ILE
10	BF	155	LEU
13	BI	50	VAL
16	BL	173	MET
16	BL	216	VAL
18	BN	106	PHE
19	BO	118	VAL
19	BO	238	VAL
20	BP	150	HIS
20	BP	171	ILE
20	BP	174	LEU
21	BQ	56	LYS
21	BQ	58	LYS
22	BR	67	PHE
23	BS	89	HIS
25	BU	59	VAL
27	BW	101	VAL
27	BW	149	THR
28	BX	265	LEU

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Mol	Chain	Res	Type
31	Ba	45	GLU
32	Bb	10	LEU
32	Bb	47	LEU
32	Bb	75	ILE
33	Bc	113	GLU
34	Bd	66	HIS
34	Bd	122	PHE
35	Be	101	TRP
37	Bg	41	ASP
38	Bh	70	CYS
39	Bi	124	LYS
39	Bi	210	ILE
39	Bi	399	ILE
40	Bj	130	THR
42	Bm	121	LEU
42	Bm	152	GLU
42	Bm	256	PHE
42	Bm	270	VAL
42	Bm	398	VAL
43	Bn	376	THR
44	Bo	104	LEU
44	Bo	260	VAL
45	Bp	195	ILE
47	Br	41	ASP
48	Bs	75	VAL
48	Bs	84	VAL
49	Bt	148	LEU
50	Bu	57	VAL
50	Bu	186	VAL
50	Bu	238	VAL
51	Bv	278	ASP
52	Bw	84	THR
52	Bw	146	LEU
57	AB	87	VAL
57	AB	93	VAL
57	AB	117	THR
57	AB	159	VAL
57	AB	211	THR
58	AC	167	ILE
60	AE	88	VAL
60	AE	111	VAL
65	AJ	126	VAL

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Mol	Chain	Res	Type
68	AM	35	VAL
68	AM	93	LEU
70	AO	179	THR
72	AQ	27	ASN
73	AR	337	GLN
74	AS	51	LEU
74	AS	83	LYS
75	AT	90	VAL
76	AU	42	VAL
77	AV	156	CYS
77	AV	388	VAL
78	AW	109	VAL
78	AW	148	LEU
79	AX	108	LEU
80	AY	358	VAL
82	Aa	147	GLN
82	Aa	275	ILE
82	Aa	284	VAL
84	Ac	29	LEU
84	Ac	95	GLU
84	Ac	117	VAL
85	Ad	91	THR
85	Ad	118	THR
85	Ad	172	MET
85	Ad	296	LEU
85	Ad	340	VAL
85	Ad	370	VAL
85	Ad	421	VAL
87	Ag	286	VAL
89	Aj	40	THR
89	Aj	100	VAL
89	Aj	211	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (206) such sidechains are listed below:

Mol	Chain	Res	Type
5	BA	60	GLN
5	BA	77	GLN
5	BA	99	GLN
5	BA	113	GLN
5	BA	171	HIS
5	BA	193	HIS

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Mol	Chain	Res	Type
5	BA	199	GLN
5	BA	208	HIS
6	BB	82	HIS
8	BD	107	ASN
9	BE	42	HIS
10	BF	197	ASN
12	BH	96	ASN
12	BH	144	GLN
14	BJ	57	GLN
15	BK	118	HIS
15	BK	154	GLN
16	BL	228	GLN
17	BM	117	HIS
17	BM	139	ASN
17	BM	156	HIS
18	BN	97	HIS
18	BN	201	GLN
18	BN	241	ASN
18	BN	251	HIS
18	BN	277	ASN
19	BO	88	HIS
19	BO	178	ASN
19	BO	239	ASN
20	BP	61	ASN
20	BP	73	GLN
20	BP	101	HIS
20	BP	142	ASN
20	BP	224	HIS
21	BQ	84	GLN
21	BQ	103	HIS
21	BQ	133	GLN
22	BR	40	GLN
22	BR	89	GLN
22	BR	160	GLN
23	BS	33	GLN
23	BS	52	HIS
23	BS	59	HIS
23	BS	142	GLN
24	BT	87	HIS
24	BT	94	GLN
24	BT	153	ASN
24	BT	170	ASN

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Mol	Chain	Res	Type
25	BU	101	HIS
25	BU	138	GLN
25	BU	202	GLN
26	BV	98	GLN
26	BV	148	GLN
27	BW	52	ASN
27	BW	55	ASN
27	BW	96	HIS
28	BX	175	GLN
28	BX	253	GLN
29	BY	70	ASN
29	BY	147	GLN
30	BZ	183	ASN
31	Ba	100	GLN
32	Bb	84	GLN
33	Bc	82	GLN
33	Bc	124	HIS
34	Bd	60	GLN
35	Be	30	GLN
35	Be	85	HIS
36	Bf	103	HIS
36	Bf	162	GLN
37	Bg	106	GLN
37	Bg	119	GLN
37	Bg	130	GLN
37	Bg	140	GLN
38	Bh	112	HIS
39	Bi	104	ASN
39	Bi	148	HIS
39	Bi	173	GLN
39	Bi	228	ASN
39	Bi	240	GLN
39	Bi	379	GLN
39	Bi	414	GLN
42	Bm	119	GLN
42	Bm	146	HIS
42	Bm	160	HIS
42	Bm	186	GLN
42	Bm	214	ASN
42	Bm	266	GLN
42	Bm	280	GLN
42	Bm	343	GLN

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Mol	Chain	Res	Type
42	Bm	358	GLN
42	Bm	380	GLN
44	Bo	197	HIS
44	Bo	305	HIS
45	Bp	158	HIS
45	Bp	186	GLN
46	Bq	50	GLN
46	Bq	132	ASN
47	Br	71	HIS
48	Bs	24	GLN
48	Bs	58	ASN
48	Bs	81	ASN
48	Bs	127	GLN
49	Bt	42	GLN
49	Bt	69	HIS
49	Bt	123	GLN
49	Bt	193	GLN
50	Bu	69	HIS
50	Bu	107	GLN
50	Bu	196	GLN
50	Bu	217	HIS
51	Bv	251	HIS
52	Bw	54	HIS
52	Bw	66	GLN
52	Bw	92	ASN
52	Bw	111	HIS
52	Bw	136	GLN
53	Bx	93	ASN
53	Bx	155	GLN
54	By	88	GLN
54	By	96	HIS
55	Bz	69	HIS
55	Bz	122	ASN
57	AB	115	HIS
58	AC	81	HIS
58	AC	156	GLN
60	AE	38	ASN
61	AF	227	HIS
65	AJ	57	GLN
66	AK	68	GLN
67	AL	139	ASN
67	AL	143	HIS

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Mol	Chain	Res	Type
67	AL	153	HIS
67	AL	213	GLN
68	AM	75	HIS
68	AM	100	HIS
69	AN	23	GLN
69	AN	90	GLN
70	AO	147	HIS
71	AP	72	HIS
71	AP	83	GLN
73	AR	132	GLN
73	AR	289	HIS
73	AR	324	HIS
75	AT	95	ASN
75	AT	146	GLN
76	AU	135	GLN
76	AU	155	GLN
76	AU	161	GLN
77	AV	89	HIS
77	AV	118	ASN
77	AV	137	HIS
77	AV	185	ASN
77	AV	196	ASN
77	AV	219	GLN
77	AV	228	HIS
77	AV	301	GLN
77	AV	399	GLN
77	AV	404	GLN
78	AW	104	GLN
78	AW	174	GLN
79	AX	153	HIS
79	AX	169	GLN
79	AX	175	GLN
79	AX	301	GLN
80	AY	287	GLN
81	AZ	75	HIS
82	Aa	107	ASN
82	Aa	124	GLN
82	Aa	164	ASN
82	Aa	183	ASN
82	Aa	202	GLN
82	Aa	336	GLN
82	Aa	381	GLN

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Mol	Chain	Res	Type
82	Aa	392	GLN
82	Aa	440	HIS
83	Ab	133	HIS
83	Ab	166	HIS
83	Ab	177	ASN
83	Ab	265	GLN
85	Ad	130	GLN
85	Ad	155	GLN
85	Ad	196	ASN
85	Ad	344	ASN
85	Ad	360	GLN
85	Ad	415	GLN
86	Ae	136	HIS
86	Ae	260	HIS
86	Ae	380	GLN
86	Ae	443	ASN
86	Ae	466	ASN
86	Ae	473	GLN
86	Ae	494	GLN
86	Ae	543	HIS
87	Ag	127	HIS
87	Ag	163	HIS
87	Ag	256	GLN
88	Ai	71	GLN
88	Ai	73	ASN
88	Ai	89	HIS
88	Ai	98	GLN
88	Ai	100	GLN
88	Ai	106	HIS
88	Ai	107	GLN
89	Aj	32	GLN
89	Aj	111	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B7	2/3 (66%)	1 (50%)	0
3	B8	1570/1571 (99%)	259 (16%)	0
4	B9	72/73 (98%)	13 (18%)	0
56	AA	959/960 (99%)	140 (14%)	0
62	AG	70/71 (98%)	9 (12%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
64	AI	8/9 (88%)	2 (25%)	0
All	All	2681/2687 (99%)	424 (15%)	0

All (424) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B7	76	A
3	B8	15	A
3	B8	19	U
3	B8	20	A
3	B8	21	C
3	B8	27	A
3	B8	31	A
3	B8	32	C
3	B8	36	A
3	B8	40	C
3	B8	42	C
3	B8	45	A
3	B8	46	A
3	B8	56	A
3	B8	57	A
3	B8	59	A
3	B8	60	U
3	B8	68	A
3	B8	69	C
3	B8	82	G
3	B8	83	A
3	B8	104	C
3	B8	105	G
3	B8	109	U
3	B8	112	A
3	B8	115	U
3	B8	129	A
3	B8	139	G
3	B8	140	A
3	B8	141	A
3	B8	142	U
3	B8	143	A
3	B8	163	C
3	B8	164	A
3	B8	168	A
3	B8	172	C

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Mol	Chain	Res	Type
3	B8	179	U
3	B8	180	A
3	B8	189	A
3	B8	190	U
3	B8	192	A
3	B8	205	A
3	B8	218	A
3	B8	219	A
3	B8	225	C
3	B8	228	U
3	B8	229	A
3	B8	239	C
3	B8	254	G
3	B8	263	G
3	B8	272	A
3	B8	273	A
3	B8	275	A
3	B8	277	A
3	B8	311	A
3	B8	322	G
3	B8	324	G
3	B8	329	A
3	B8	330	A
3	B8	331	A
3	B8	336	A
3	B8	340	A
3	B8	352	G
3	B8	359	G
3	B8	369	G
3	B8	373	U
3	B8	374	U
3	B8	376	A
3	B8	392	U
3	B8	409	A
3	B8	427	G
3	B8	428	A
3	B8	433	G
3	B8	434	U
3	B8	445	A
3	B8	446	C
3	B8	448	G
3	B8	459	A

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Mol	Chain	Res	Type
3	B8	460	C
3	B8	475	C
3	B8	479	A
3	B8	480	G
3	B8	488	U
3	B8	490	U
3	B8	491	U
3	B8	492	A
3	B8	497	U
3	B8	498	A
3	B8	501	A
3	B8	502	U
3	B8	503	A
3	B8	506	A
3	B8	515	A
3	B8	518	A
3	B8	532	A
3	B8	534	A
3	B8	549	C
3	B8	560	A
3	B8	570	A
3	B8	574	A
3	B8	575	C
3	B8	576	U
3	B8	578	A
3	B8	579	U
3	B8	580	A
3	B8	584	A
3	B8	586	C
3	B8	592	G
3	B8	595	C
3	B8	596	A
3	B8	617	A
3	B8	618	A
3	B8	625	A
3	B8	631	A
3	B8	633	U
3	B8	634	G
3	B8	640	A
3	B8	684	A
3	B8	689	A
3	B8	693	U

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Mol	Chain	Res	Type
3	B8	695	U
3	B8	704	U
3	B8	707	A
3	B8	713	A
3	B8	720	C
3	B8	722	A
3	B8	724	A
3	B8	725	C
3	B8	727	A
3	B8	728	C
3	B8	737	G
3	B8	746	U
3	B8	747	U
3	B8	748	A
3	B8	753	G
3	B8	777	A
3	B8	783	A
3	B8	809	G
3	B8	817	A
3	B8	825	C
3	B8	852	C
3	B8	854	U
3	B8	855	U
3	B8	859	A
3	B8	864	U
3	B8	872	A
3	B8	889	C
3	B8	890	C
3	B8	897	A
3	B8	902	C
3	B8	922	A
3	B8	923	A
3	B8	924	G
3	B8	925	G
3	B8	933	A
3	B8	950	U
3	B8	958	U
3	B8	959	G
3	B8	960	U
3	B8	964	A
3	B8	965	A
3	B8	967	G

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Mol	Chain	Res	Type
3	B8	977	G
3	B8	1015	C
3	B8	1016	C
3	B8	1018	U
3	B8	1026	A
3	B8	1027	G
3	B8	1028	A
3	B8	1038	A
3	B8	1050	C
3	B8	1051	G
3	B8	1055	A
3	B8	1056	G
3	B8	1057	A
3	B8	1063	U
3	B8	1064	G
3	B8	1093	A
3	B8	1094	A
3	B8	1095	C
3	B8	1096	A
3	B8	1097	A
3	B8	1099	U
3	B8	1100	C
3	B8	1105	A
3	B8	1107	A
3	B8	1113	A
3	B8	1114	U
3	B8	1115	A
3	B8	1119	C
3	B8	1120	A
3	B8	1121	U
3	B8	1146	G
3	B8	1167	C
3	B8	1168	A
3	B8	1169	A
3	B8	1180	G
3	B8	1183	U
3	B8	1188	U
3	B8	1195	A
3	B8	1204	A
3	B8	1206	U
3	B8	1207	C
3	B8	1215	C

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Mol	Chain	Res	Type
3	B8	1217	A
3	B8	1218	U
3	B8	1220	A
3	B8	1221	C
3	B8	1222	A
3	B8	1226	C
3	B8	1231	U
3	B8	1233	A
3	B8	1240	A
3	B8	1241	U
3	B8	1243	U
3	B8	1246	A
3	B8	1247	U
3	B8	1249	A
3	B8	1253	G
3	B8	1254	A
3	B8	1264	C
3	B8	1271	A
3	B8	1291	U
3	B8	1299	C
3	B8	1314	U
3	B8	1325	G
3	B8	1326	A
3	B8	1327	U
3	B8	1328	G
3	B8	1332	G
3	B8	1341	A
3	B8	1342	C
3	B8	1389	A
3	B8	1390	G
3	B8	1396	C
3	B8	1425	A
3	B8	1426	G
3	B8	1432	U
3	B8	1433	U
3	B8	1436	U
3	B8	1445	U
3	B8	1448	A
3	B8	1468	A
3	B8	1485	A
3	B8	1493	A
3	B8	1494	A

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Mol	Chain	Res	Type
3	B8	1498	C
3	B8	1504	A
3	B8	1505	G
3	B8	1509	U
3	B8	1525	C
3	B8	1526	U
3	B8	1527	U
3	B8	1528	A
3	B8	1536	U
3	B8	1551	C
3	B8	1553	A
3	B8	1558	U
3	B8	1561	A
3	B8	1571	A
4	B9	8	U
4	B9	17	U
4	B9	18	U
4	B9	23	A
4	B9	34	U
4	B9	35	G
4	B9	48	U
4	B9	49	G
4	B9	55	C
4	B9	56	A
4	B9	57	C
4	B9	58	A
4	B9	71	C
56	AA	5	A
56	AA	18	G
56	AA	34	U
56	AA	42	A
56	AA	43	U
56	AA	58	U
56	AA	65	C
56	AA	66	C
56	AA	75	A
56	AA	77	G
56	AA	92	A
56	AA	93	A
56	AA	98	A
56	AA	108	G
56	AA	115	A

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Mol	Chain	Res	Type
56	AA	120	A
56	AA	125	U
56	AA	126	A
56	AA	127	A
56	AA	139	A
56	AA	147	G
56	AA	152	A
56	AA	161	C
56	AA	170	A
56	AA	186	U
56	AA	191	C
56	AA	192	C
56	AA	203	G
56	AA	208	A
56	AA	216	A
56	AA	217	U
56	AA	223	U
56	AA	244	C
56	AA	250	A
56	AA	257	U
56	AA	258	C
56	AA	261	A
56	AA	273	A
56	AA	287	C
56	AA	288	G
56	AA	293	A
56	AA	296	G
56	AA	297	A
56	AA	309	A
56	AA	310	A
56	AA	314	A
56	AA	317	A
56	AA	319	A
56	AA	320	A
56	AA	328	A
56	AA	354	C
56	AA	355	U
56	AA	367	A
56	AA	368	A
56	AA	372	C
56	AA	381	G
56	AA	395	C

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Mol	Chain	Res	Type
56	AA	396	C
56	AA	399	A
56	AA	417	C
56	AA	421	A
56	AA	455	A
56	AA	456	A
56	AA	457	C
56	AA	461	A
56	AA	465	G
56	AA	471	U
56	AA	472	A
56	AA	477	A
56	AA	495	U
56	AA	502	A
56	AA	530	G
56	AA	538	C
56	AA	539	A
56	AA	540	U
56	AA	541	C
56	AA	566	U
56	AA	571	A
56	AA	574	C
56	AA	576	C
56	AA	596	U
56	AA	597	U
56	AA	604	U
56	AA	613	A
56	AA	625	U
56	AA	626	C
56	AA	639	A
56	AA	641	A
56	AA	644	A
56	AA	645	A
56	AA	646	C
56	AA	665	A
56	AA	681	A
56	AA	682	G
56	AA	685	C
56	AA	698	A
56	AA	699	U
56	AA	708	A
56	AA	711	A

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Mol	Chain	Res	Type
56	AA	720	A
56	AA	722	A
56	AA	724	U
56	AA	731	A
56	AA	733	A
56	AA	739	A
56	AA	740	U
56	AA	743	A
56	AA	745	C
56	AA	748	A
56	AA	751	A
56	AA	752	A
56	AA	753	A
56	AA	766	C
56	AA	780	A
56	AA	790	A
56	AA	808	U
56	AA	823	G
56	AA	825	C
56	AA	826	C
56	AA	838	A
56	AA	869	A
56	AA	884	C
56	AA	885	U
56	AA	893	A
56	AA	896	A
56	AA	899	C
56	AA	919	A
56	AA	920	G
56	AA	925	A
56	AA	928	A
56	AA	929	A
56	AA	930	G
56	AA	932	U
56	AA	933	A
56	AA	943	G
56	AA	945	MA6
56	AA	955	G
56	AA	956	G
56	AA	959	U
56	AA	960	A
62	AG	8	U

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Mol	Chain	Res	Type
62	AG	11	G
62	AG	16	A
62	AG	17	U
62	AG	45	G
62	AG	52	A
62	AG	53	U
62	AG	55	C
62	AG	71	A
64	AI	2	G
64	AI	4	C

There are no RNA pucker outliers to report.

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

17 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
88	5F0	Ai	186	88	8,8,9	1.45	2 (25%)	8,9,11	1.61	1 (12%)
6	AYA	BB	2	6	6,7,8	0.77	0	6,8,10	0.56	0
32	AYA	Bb	2	32	6,7,8	0.73	0	6,8,10	0.68	0
3	OMG	B8	1151	62,91,3	23,26,27	1.19	3 (13%)	32,38,41	1.93	6 (18%)
72	AYA	AQ	2	72	6,7,8	0.77	0	6,8,10	0.60	0
3	OMG	B8	1376	3	23,26,27	1.19	3 (13%)	32,38,41	1.92	6 (18%)
56	5MC	AA	848	56	19,22,23	1.56	3 (15%)	26,32,35	1.08	2 (7%)
22	SAC	BR	2	22	7,8,9	0.57	0	7,9,11	1.02	1 (14%)
84	AYA	Ac	2	84	6,7,8	0.79	0	6,8,10	0.59	0
3	1MA	B8	949	3	21,25,26	0.42	0	30,37,40	0.76	1 (3%)
56	MA6	AA	944	56	23,26,27	2.37	5 (21%)	33,38,41	3.78	13 (39%)
3	OMU	B8	1375	91,3	19,22,23	1.20	3 (15%)	25,31,34	1.78	5 (20%)
3	PSU	B8	1403	3	18,21,22	1.39	2 (11%)	21,30,33	2.00	3 (14%)
56	B8T	AA	846	56	19,22,23	0.39	0	25,31,34	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	MA6	AA	945	56	23,26,27	2.34	5 (21%)	33,38,41	3.78	13 (39%)
4	MIA	B9	38	4	28,31,32	0.60	1 (3%)	38,44,47	3.89	1 (2%)
56	5MU	AA	428	56	19,22,23	1.39	6 (31%)	27,32,35	2.08	6 (22%)

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
88	5F0	Ai	186	88	-	3/9/9/10	-
6	AYA	BB	2	6	-	2/5/6/8	-
32	AYA	Bb	2	32	-	3/5/6/8	-
3	OMG	B8	1151	62,91,3	-	0/9/27/28	0/3/3/3
72	AYA	AQ	2	72	-	2/5/6/8	-
3	OMG	B8	1376	3	-	0/9/27/28	0/3/3/3
56	5MC	AA	848	56	-	0/7/25/26	0/2/2/2
22	SAC	BR	2	22	-	4/7/8/10	-
84	AYA	Ac	2	84	-	4/5/6/8	-
3	1MA	B8	949	3	-	0/7/25/26	0/3/3/3
56	MA6	AA	944	56	-	0/11/29/30	0/3/3/3
3	OMU	B8	1375	91,3	-	0/9/27/28	0/2/2/2
3	PSU	B8	1403	3	-	0/7/25/26	0/2/2/2
56	B8T	AA	846	56	-	0/7/27/28	0/2/2/2
56	MA6	AA	945	56	-	4/11/29/30	0/3/3/3
4	MIA	B9	38	4	-	0/15/33/34	0/3/3/3
56	5MU	AA	428	56	-	0/7/25/26	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	AA	944	MA6	C5-N7	7.04	1.51	1.39
56	AA	945	MA6	C5-N7	6.94	1.51	1.39
56	AA	944	MA6	C8-N9	-5.76	1.27	1.37
56	AA	945	MA6	C8-N9	-5.67	1.27	1.37
56	AA	848	5MC	C5-C4	5.56	1.48	1.44
56	AA	944	MA6	C4-N9	-3.92	1.29	1.37
56	AA	945	MA6	C4-N9	-3.91	1.29	1.37
56	AA	944	MA6	C5-C4	3.43	1.45	1.39
56	AA	945	MA6	C5-C4	3.32	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	AA	944	MA6	C6-N6	3.23	1.45	1.36
3	B8	1403	PSU	C6-C5	3.21	1.38	1.35
56	AA	945	MA6	C6-N6	3.18	1.45	1.36
3	B8	1376	OMG	C5-C4	3.07	1.47	1.38
3	B8	1151	OMG	C5-C4	3.05	1.47	1.38
88	Ai	186	5F0	OD1-C1	2.88	1.40	1.33
3	B8	1403	PSU	C4-N3	-2.74	1.33	1.38
56	AA	848	5MC	C6-C5	2.71	1.39	1.34
56	AA	428	5MU	C6-C5	2.70	1.39	1.34
56	AA	428	5MU	C4-N3	-2.61	1.34	1.38
3	B8	1376	OMG	C6-N1	-2.59	1.34	1.38
3	B8	1375	OMU	C4-N3	-2.59	1.34	1.38
3	B8	1151	OMG	C6-N1	-2.54	1.34	1.38
4	B9	38	MIA	C2-S10	2.29	1.77	1.75
56	AA	428	5MU	C6-N1	-2.27	1.34	1.38
56	AA	428	5MU	C4-C5	2.26	1.48	1.44
56	AA	848	5MC	C6-N1	-2.22	1.34	1.38
88	Ai	186	5F0	OD1-CXT	-2.21	1.40	1.45
3	B8	1375	OMU	C2-N3	-2.16	1.34	1.38
3	B8	1151	OMG	C5-N7	-2.14	1.34	1.39
3	B8	1376	OMG	C5-N7	-2.12	1.34	1.39
56	AA	428	5MU	C2-N3	-2.11	1.34	1.38
3	B8	1375	OMU	C5-C4	-2.02	1.39	1.43
56	AA	428	5MU	C2-N1	2.02	1.41	1.38

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B9	38	MIA	C11-S10-C2	23.75	120.07	102.25
56	AA	945	MA6	C4-N9-C8	15.08	121.57	105.74
56	AA	944	MA6	C4-N9-C8	15.07	121.56	105.74
56	AA	945	MA6	N3-C4-N9	6.73	138.60	127.17
56	AA	944	MA6	N3-C4-N9	6.38	138.02	127.17
56	AA	944	MA6	C4-C5-N7	-6.35	103.32	110.58
3	B8	1403	PSU	N1-C2-N3	6.28	121.79	115.17
3	B8	1151	OMG	C5-C4-N3	-5.99	118.86	128.39
3	B8	1376	OMG	C5-C4-N3	-5.94	118.93	128.39
56	AA	944	MA6	N9-C8-N7	-5.74	105.80	113.94
56	AA	945	MA6	C4-C5-N7	-5.71	104.06	110.58
56	AA	945	MA6	N9-C8-N7	-5.47	106.17	113.94
56	AA	945	MA6	C5-C4-N3	-5.39	119.29	126.72
56	AA	944	MA6	C5-C4-N3	-5.38	119.31	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	AA	428	5MU	C4-N3-C2	-5.03	120.75	127.34
56	AA	428	5MU	N3-C2-N1	4.85	121.20	114.89
3	B8	1151	OMG	C2-N3-C4	4.82	120.60	112.30
3	B8	1376	OMG	C2-N3-C4	4.79	120.56	112.30
3	B8	1375	OMU	C4-N3-C2	-4.79	120.66	126.61
3	B8	1151	OMG	N9-C4-N3	4.56	135.07	125.95
3	B8	1376	OMG	N9-C4-N3	4.47	134.90	125.95
56	AA	428	5MU	C5-C4-N3	4.40	119.15	115.32
56	AA	944	MA6	N1-C2-N3	-4.27	122.11	128.58
56	AA	945	MA6	N1-C2-N3	-4.20	122.23	128.58
3	B8	1375	OMU	N3-C2-N1	4.16	120.30	114.89
56	AA	428	5MU	O4-C4-C5	-4.09	120.23	124.92
3	B8	1403	PSU	C4-N3-C2	-3.99	120.88	126.37
56	AA	944	MA6	C2-N1-C6	3.94	121.44	111.83
56	AA	945	MA6	C2-N1-C6	3.83	121.18	111.83
3	B8	1375	OMU	C5-C4-N3	3.79	120.11	114.80
56	AA	944	MA6	C6-C5-N7	3.63	139.22	133.43
56	AA	428	5MU	C5-C6-N1	-3.54	119.47	123.31
56	AA	944	MA6	C4-N9-C1'	-3.51	118.42	126.63
3	B8	1403	PSU	O2-C2-N1	-3.49	119.19	122.79
56	AA	945	MA6	C1'-N9-C8	-3.45	119.44	127.09
56	AA	945	MA6	C5-C4-N9	-3.40	102.10	105.81
88	Ai	186	5F0	OD1-C1-CA	3.38	120.09	111.50
56	AA	944	MA6	C2-N3-C4	3.28	119.83	111.83
56	AA	945	MA6	C4-N9-C1'	-3.27	118.99	126.63
56	AA	848	5MC	C5-C6-N1	-3.24	119.80	123.31
56	AA	945	MA6	C2-N3-C4	3.21	119.66	111.83
56	AA	944	MA6	C1'-N9-C8	-3.19	120.02	127.09
3	B8	1376	OMG	C6-C5-N7	3.14	136.01	130.29
3	B8	1375	OMU	O4-C4-C5	-3.07	119.87	125.16
56	AA	945	MA6	C6-C5-N7	3.06	138.32	133.43
3	B8	1151	OMG	C6-C5-N7	3.02	135.78	130.29
56	AA	944	MA6	C5-C4-N9	-2.88	102.67	105.81
56	AA	945	MA6	C5-C6-N6	-2.68	121.09	125.33
56	AA	848	5MC	C5-C4-N3	-2.61	119.08	121.75
22	BR	2	SAC	O-C-CA	-2.58	118.13	124.77
56	AA	428	5MU	O2-C2-N1	-2.58	119.44	122.80
3	B8	1375	OMU	O2-C2-N1	-2.41	119.67	122.80
3	B8	1376	OMG	C4-C5-N7	-2.40	106.86	110.67
3	B8	1151	OMG	C4-C5-N7	-2.35	106.95	110.67
3	B8	1151	OMG	O6-C6-C5	-2.17	120.79	126.53
3	B8	949	1MA	N1-C6-N6	2.17	125.16	119.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B8	1376	OMG	O6-C6-C5	-2.10	120.98	126.53
56	AA	944	MA6	C5-N7-C8	2.04	106.65	103.45

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	BB	2	AYA	O-C-CA-CB
22	BR	2	SAC	C2A-C1A-N-CA
22	BR	2	SAC	OAC-C1A-N-CA
22	BR	2	SAC	C-CA-CB-OG
72	AQ	2	AYA	OT-CT-N-CA
84	Ac	2	AYA	O-C-CA-CB
56	AA	945	MA6	C5-C6-N6-C9
88	Ai	186	5F0	OD1-C1-CA-CB
72	AQ	2	AYA	CM-CT-N-CA
84	Ac	2	AYA	CM-CT-N-CA
32	Bb	2	AYA	CM-CT-N-CA
84	Ac	2	AYA	OT-CT-N-CA
56	AA	945	MA6	N1-C6-N6-C9
32	Bb	2	AYA	OT-CT-N-CA
22	BR	2	SAC	N-CA-CB-OG
88	Ai	186	5F0	O1-C1-CA-CB
6	BB	2	AYA	C-CA-N-CT
32	Bb	2	AYA	C-CA-N-CT
56	AA	945	MA6	C5-C6-N6-C10
84	Ac	2	AYA	C-CA-N-CT
56	AA	945	MA6	C4'-C5'-O5'-P
88	Ai	186	5F0	O1-C1-OD1-CXT

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	Ai	186	5F0	1	0
6	BB	2	AYA	1	0
3	B8	1376	OMG	1	0
22	BR	2	SAC	1	0
56	AA	944	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 385 ligands modelled in this entry, 376 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
92	PHE	B9	101	4	10,11,12	0.39	0	8,13,15	0.19	0
95	SPM	AA	1120	-	13,13,13	0.35	0	12,12,12	0.94	0
96	SPD	AA	1121	-	9,9,9	0.32	0	8,8,8	0.86	0
94	FES	AT	201	75,68	0,4,4	-	-	-		
94	FES	Bh	201	38,20	0,4,4	-	-	-		
94	FES	AP	201	60,71	0,4,4	-	-	-		
98	ATP	AX	501	90	32,33,33	0.28	0	48,52,52	0.28	0
97	FME	AG	101	62	8,9,10	0.58	0	8,9,11	0.93	1 (12%)
99	GDP	AX	503	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	PHE	B9	101	4	-	1/5/6/8	0/1/1/1
95	SPM	AA	1120	-	-	2/11/11/11	-
96	SPD	AA	1121	-	-	0/7/7/7	-
94	FES	AT	201	75,68	-	-	0/1/1/1
94	FES	Bh	201	38,20	-	-	0/1/1/1
94	FES	AP	201	60,71	-	-	0/1/1/1
98	ATP	AX	501	90	-	3/22/38/38	0/3/3/3
97	FME	AG	101	62	-	2/7/9/11	-
99	GDP	AX	503	-	-	2/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
99	AX	503	GDP	C5-C4	3.20	1.47	1.38
99	AX	503	GDP	C6-N1	-2.36	1.34	1.38
99	AX	503	GDP	C5-N7	-2.04	1.35	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
99	AX	503	GDP	C5-C4-N3	-6.19	118.54	128.39
99	AX	503	GDP	C2-N3-C4	5.04	120.98	112.30
99	AX	503	GDP	N9-C4-N3	4.63	135.21	125.95
99	AX	503	GDP	C6-C5-N7	3.15	136.02	130.29
97	AG	101	FME	O-C-CA	-2.58	118.14	124.77
99	AX	503	GDP	C4-C5-N7	-2.53	106.65	110.67
99	AX	503	GDP	C3'-C2'-C1'	2.20	105.63	101.46
99	AX	503	GDP	O6-C6-C5	-2.11	120.96	126.53

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	B9	101	PHE	O-C-CA-CB
97	AG	101	FME	O1-CN-N-CA
97	AG	101	FME	CB-CA-N-CN
98	AX	501	ATP	O4'-C4'-C5'-O5'
99	AX	503	GDP	O4'-C4'-C5'-O5'
98	AX	501	ATP	C3'-C4'-C5'-O5'
99	AX	503	GDP	C3'-C4'-C5'-O5'
95	AA	1120	SPM	N5-C6-C7-C8
95	AA	1120	SPM	C6-C7-C8-C9
98	AX	501	ATP	PB-O3B-PG-O3G

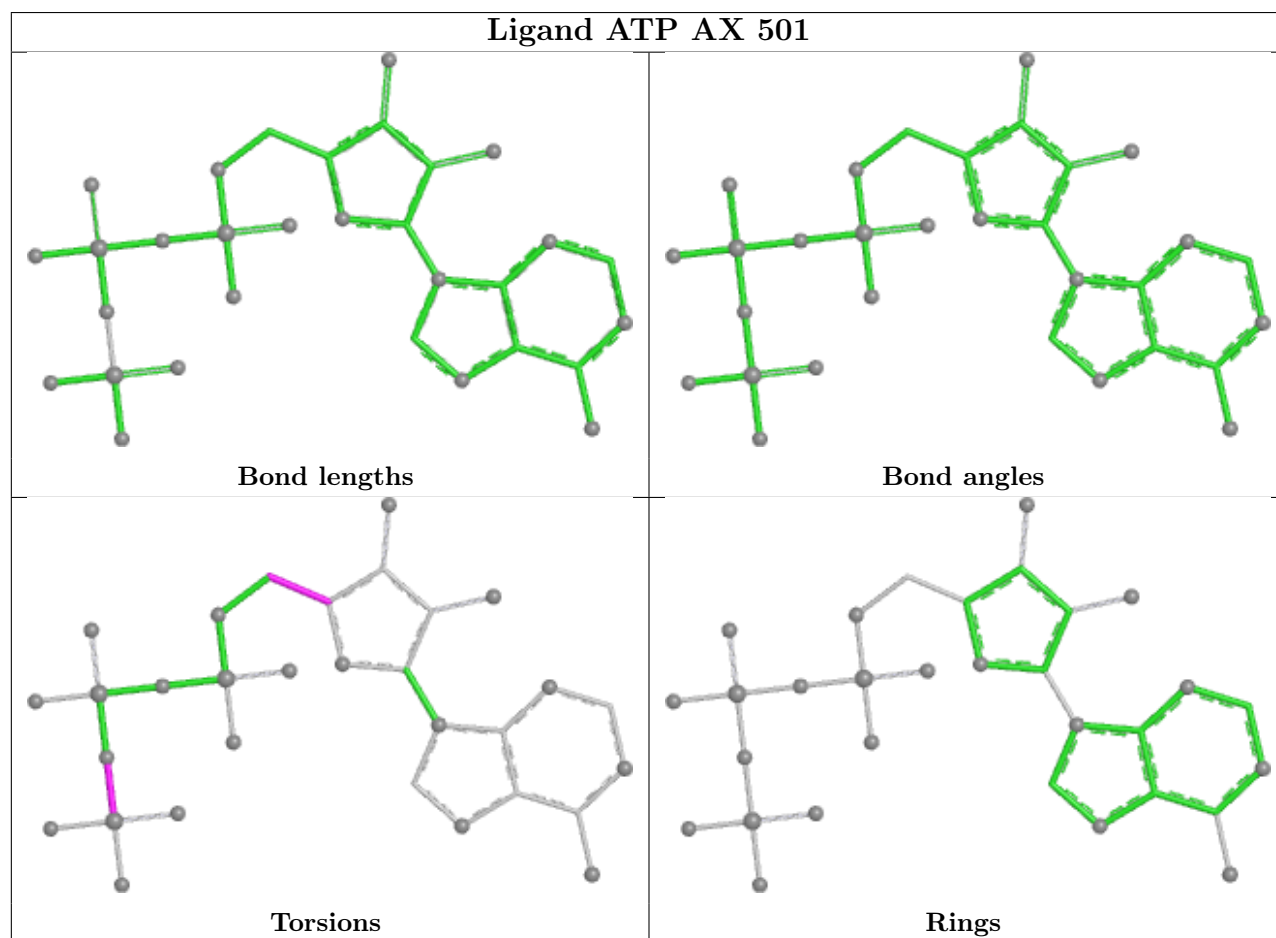
There are no ring outliers.

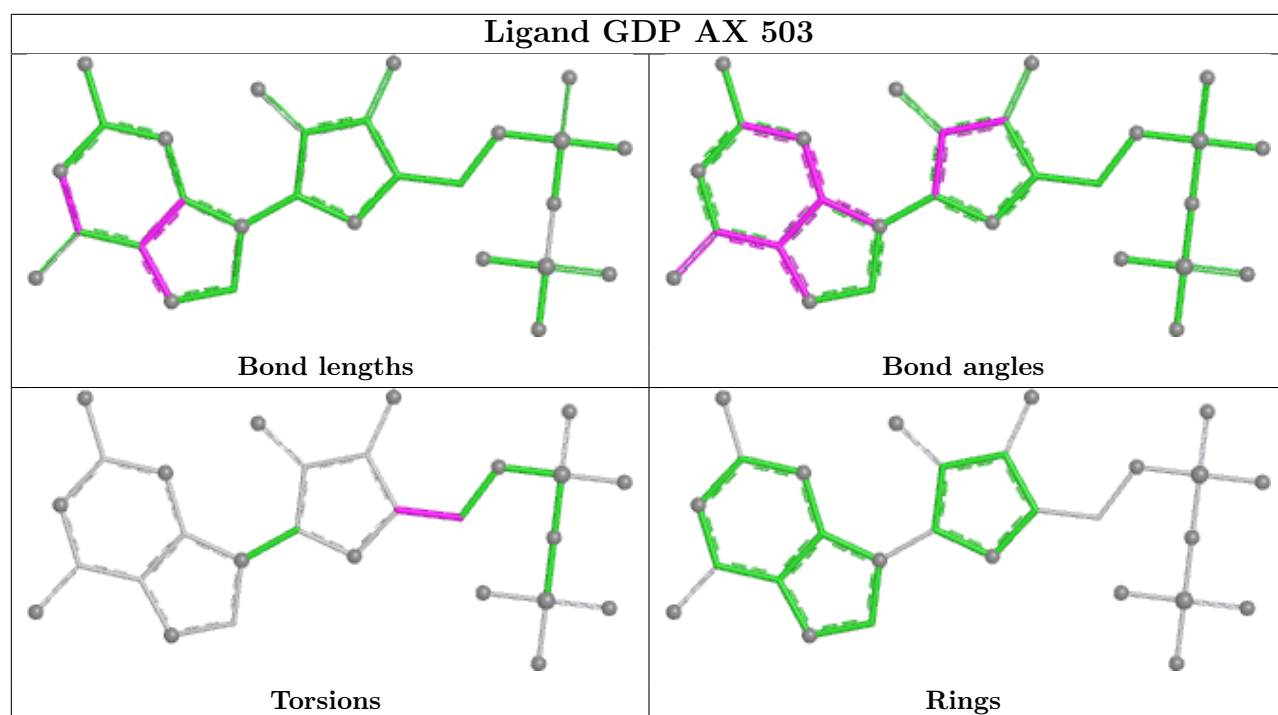
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
92	B9	101	PHE	1	0
95	AA	1120	SPM	3	0
99	AX	503	GDP	3	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.

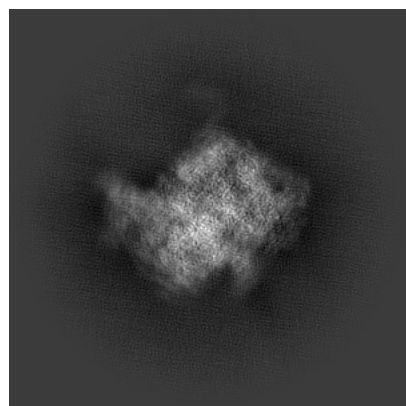
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16894. These allow visual inspection of the internal detail of the map and identification of artifacts.

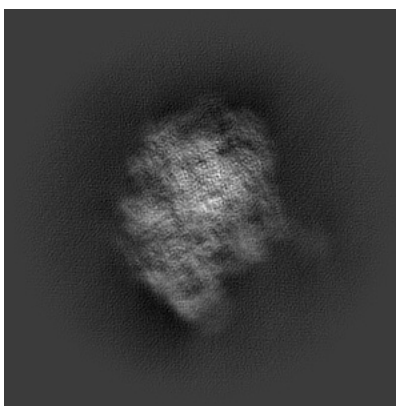
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

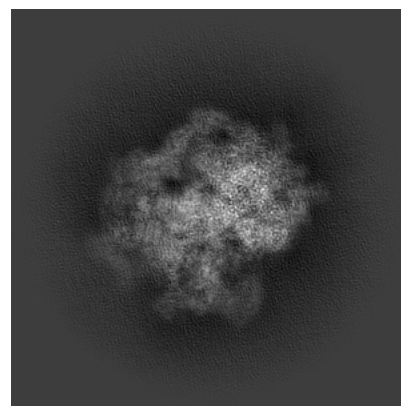
6.1.1 Primary map



X

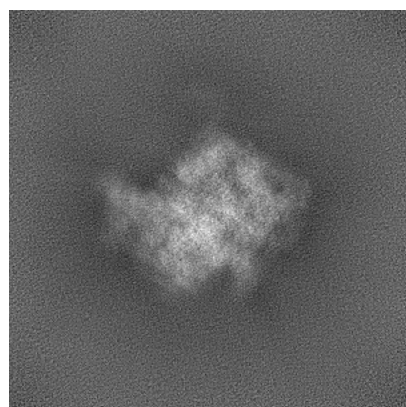


Y

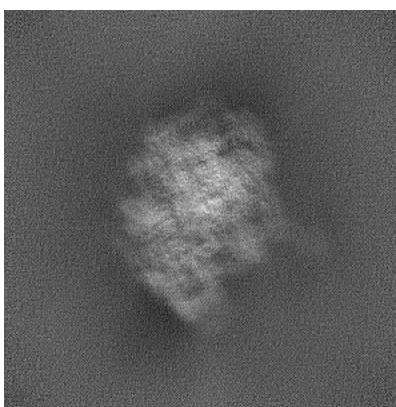


Z

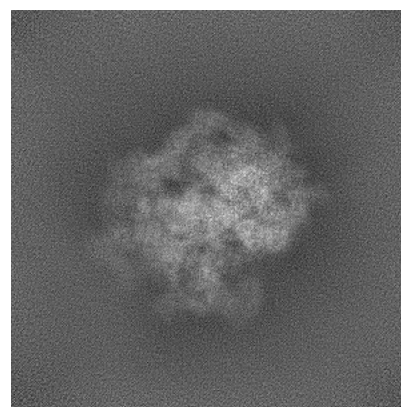
6.1.2 Raw map



X



Y

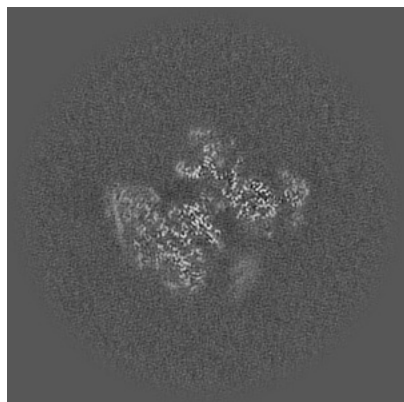


Z

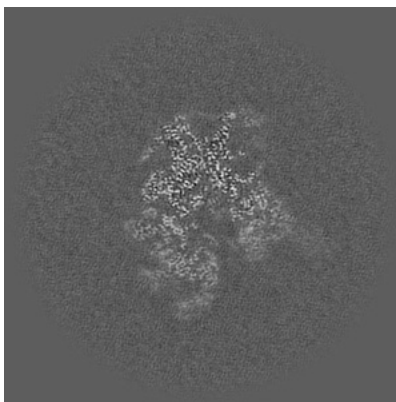
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

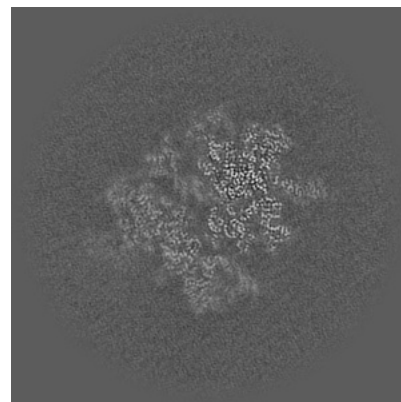
6.2.1 Primary map



X Index: 250

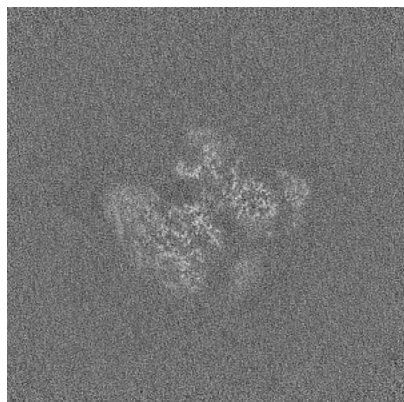


Y Index: 250

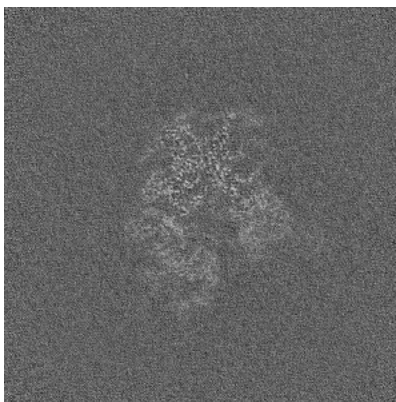


Z Index: 250

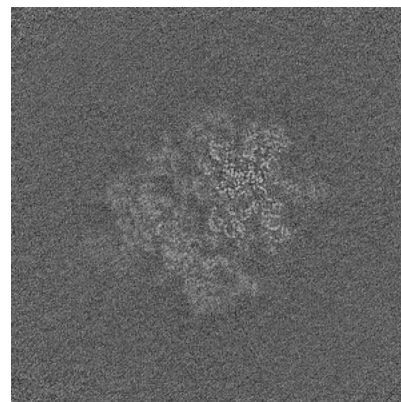
6.2.2 Raw map



X Index: 250



Y Index: 250

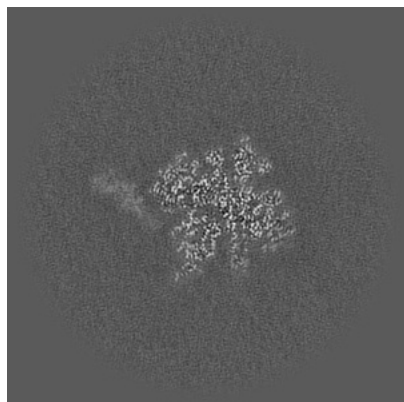


Z Index: 250

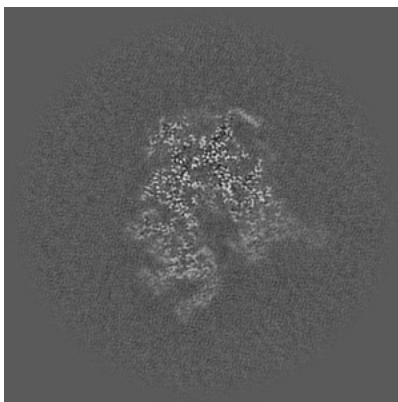
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

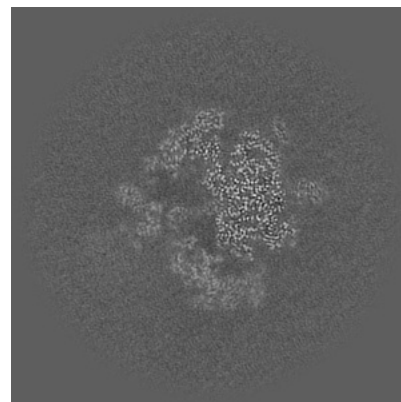
6.3.1 Primary map



X Index: 291

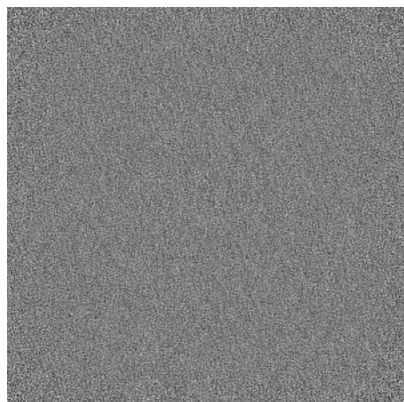


Y Index: 253

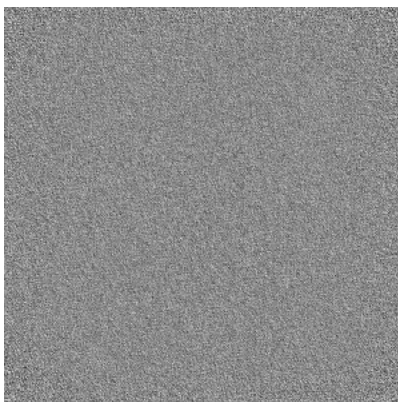


Z Index: 263

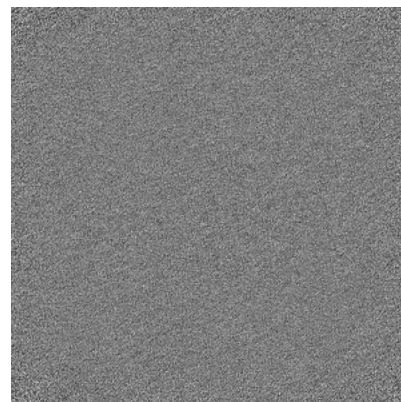
6.3.2 Raw map



X Index: 0



Y Index: 0

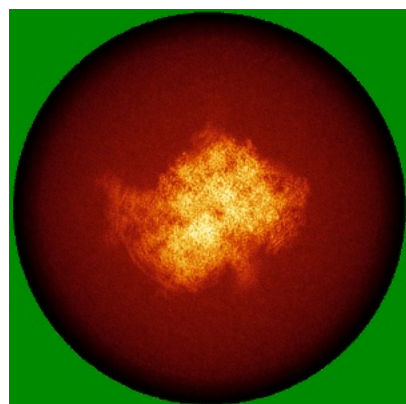


Z Index: 0

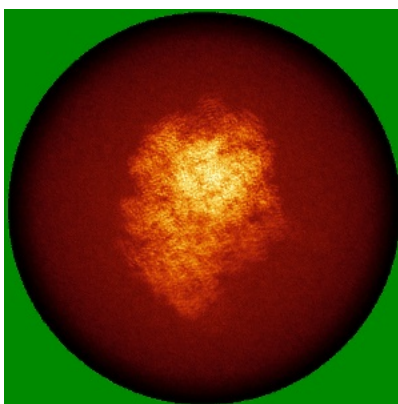
The images above show the largest variance slices of the map in three orthogonal directions.

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

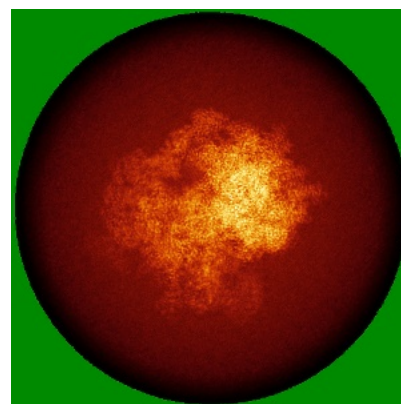
6.4.1 Primary map



X

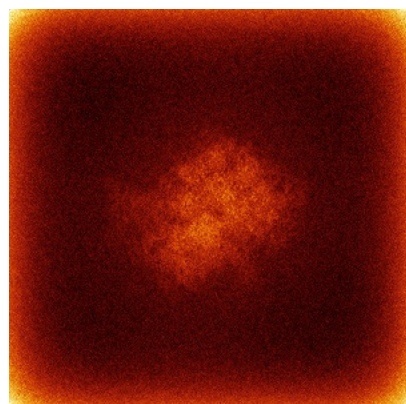


Y

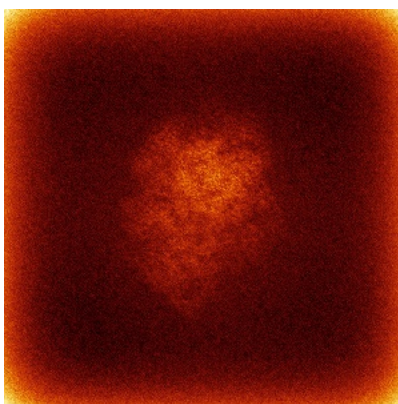


Z

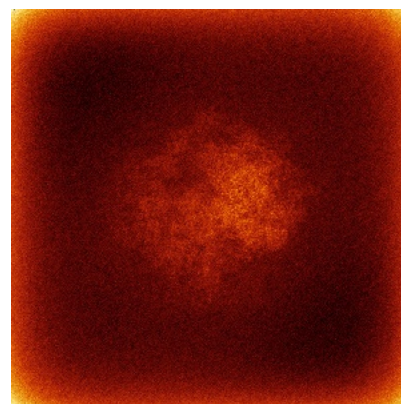
6.4.2 Raw map



X



Y

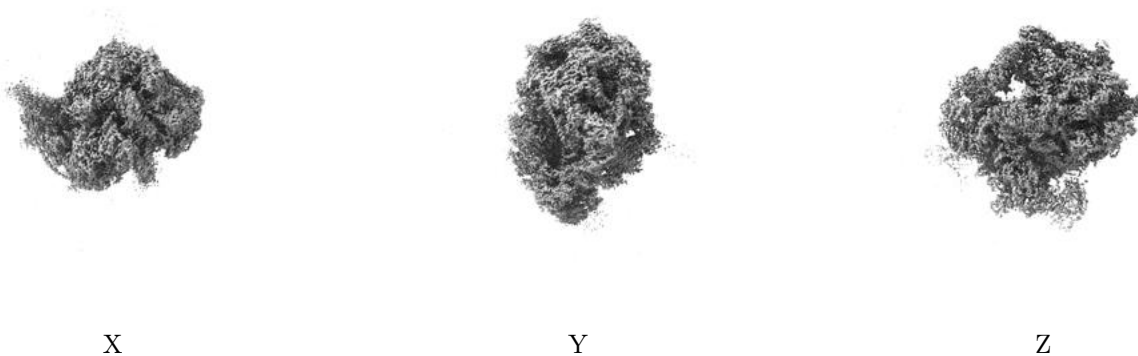


Z

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.

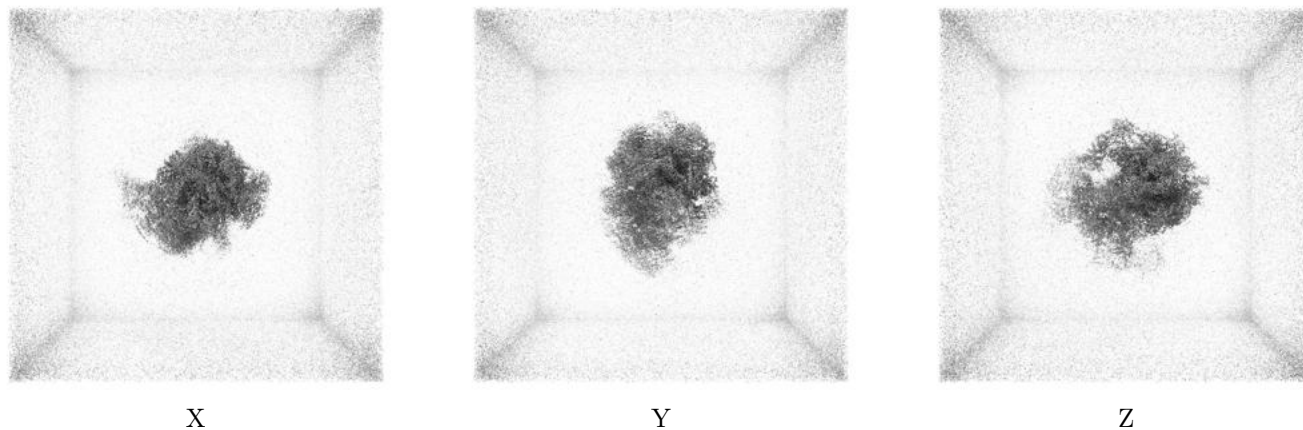
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

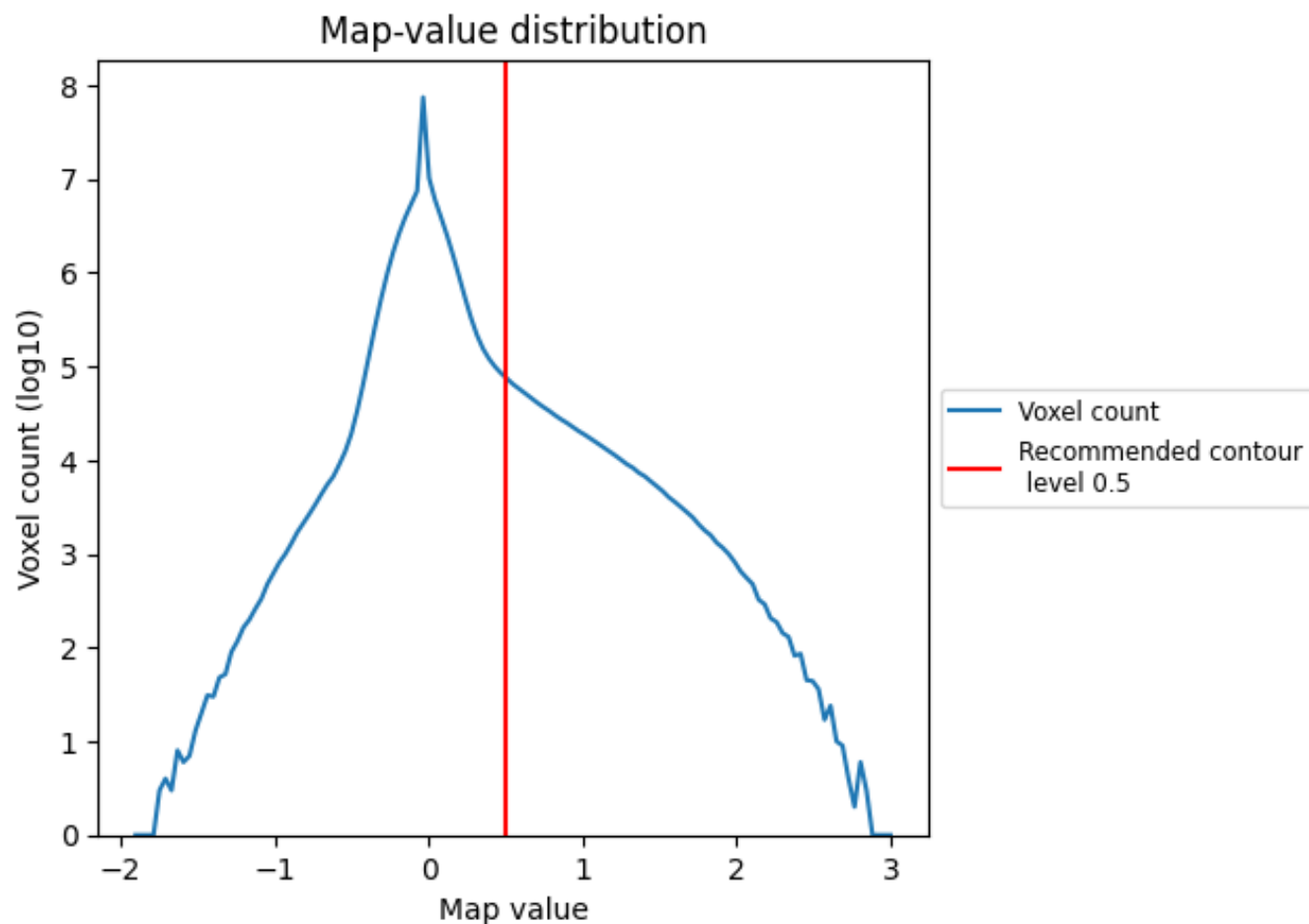
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

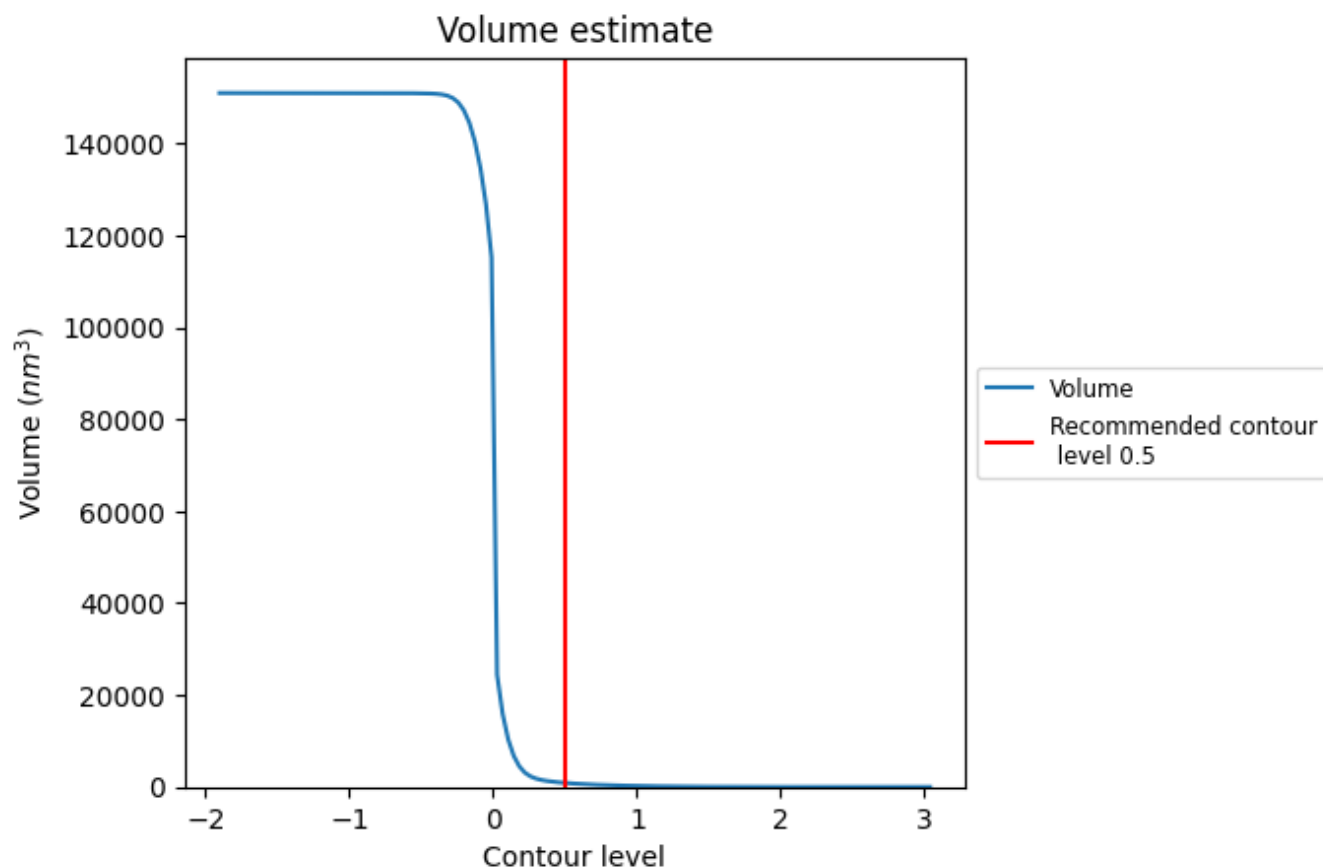
This section contains the results of statistical analysis of the map.

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.

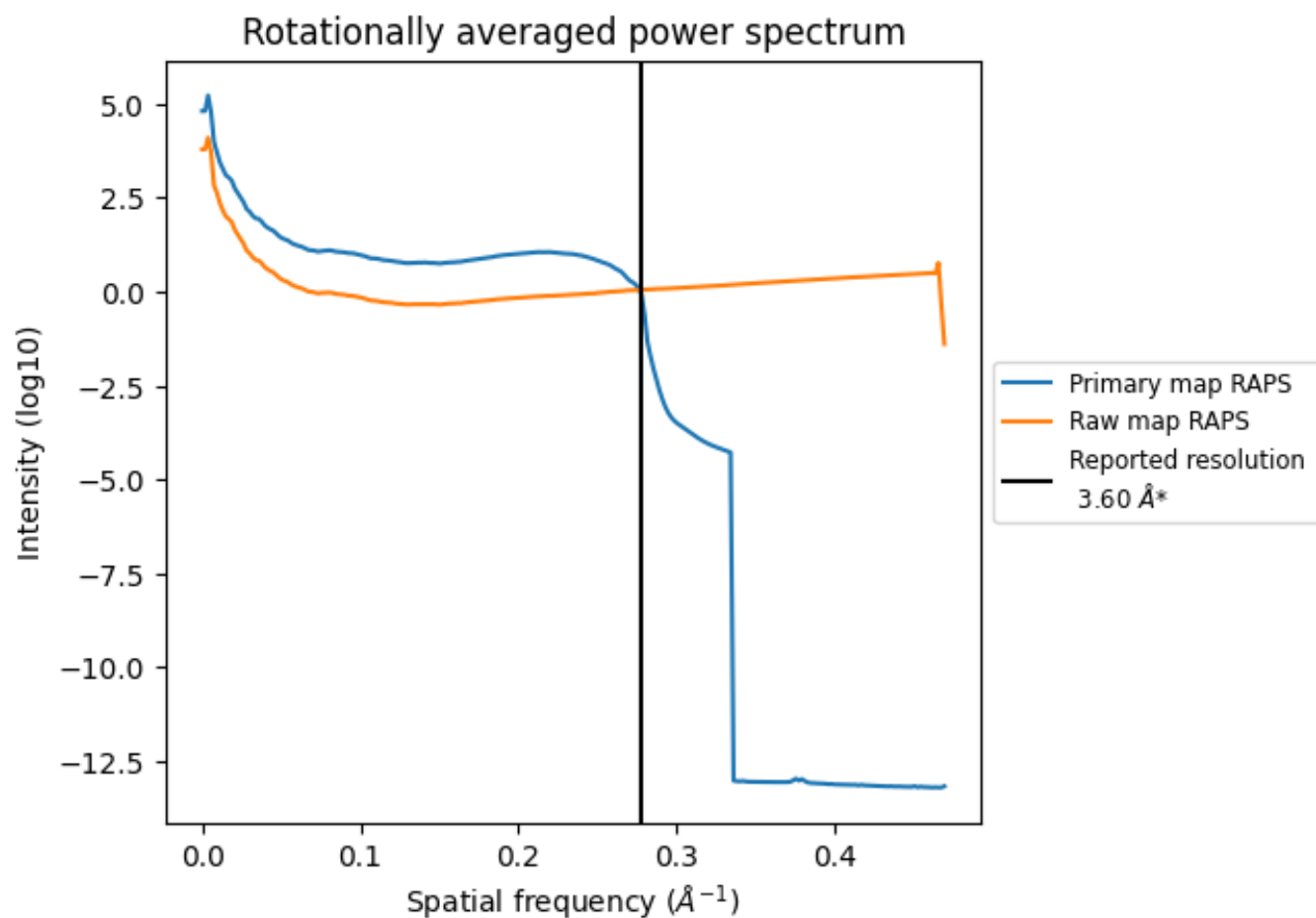
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 880 nm^3 ; this corresponds to an approximate mass of 795 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 ⓘ

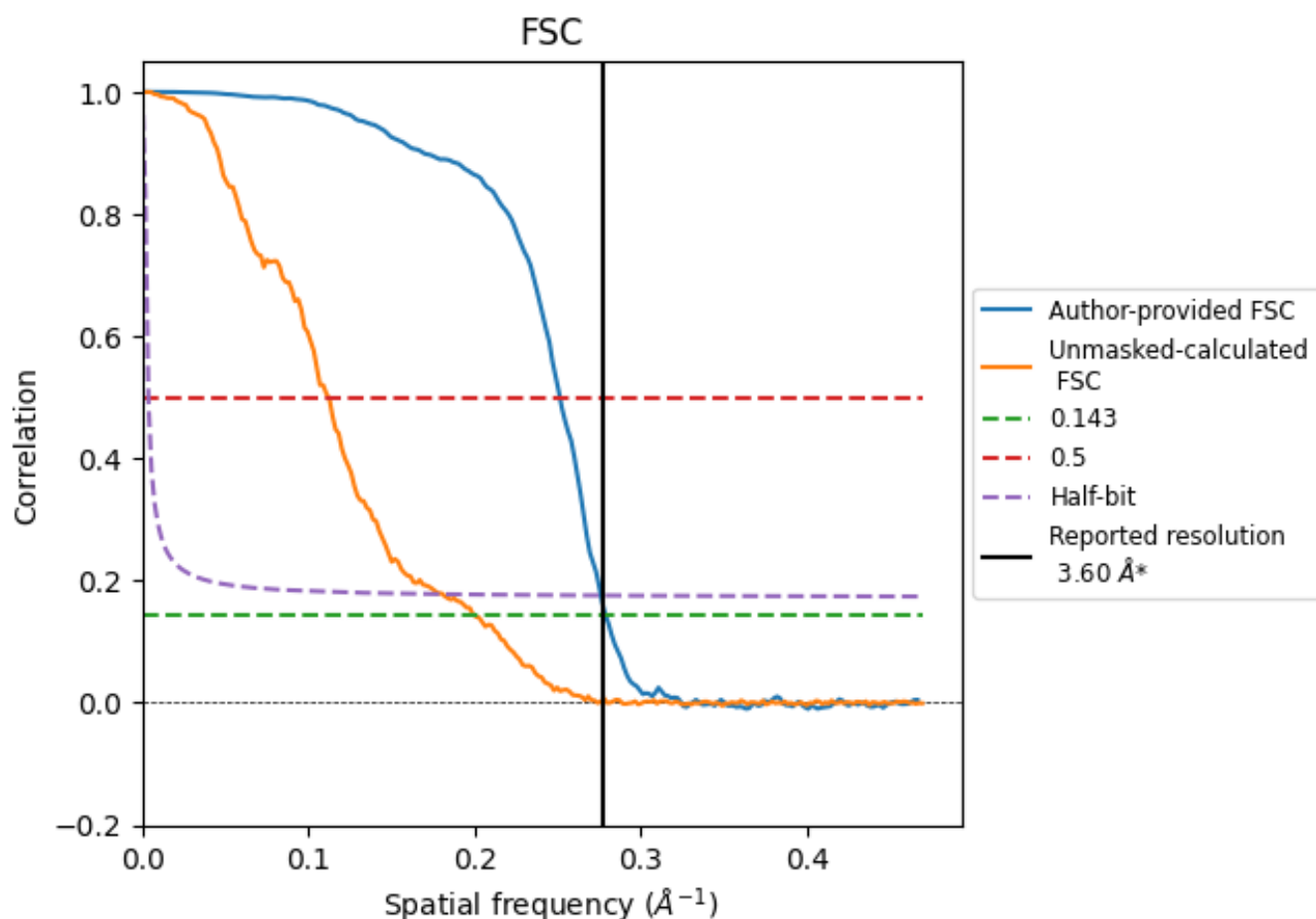


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

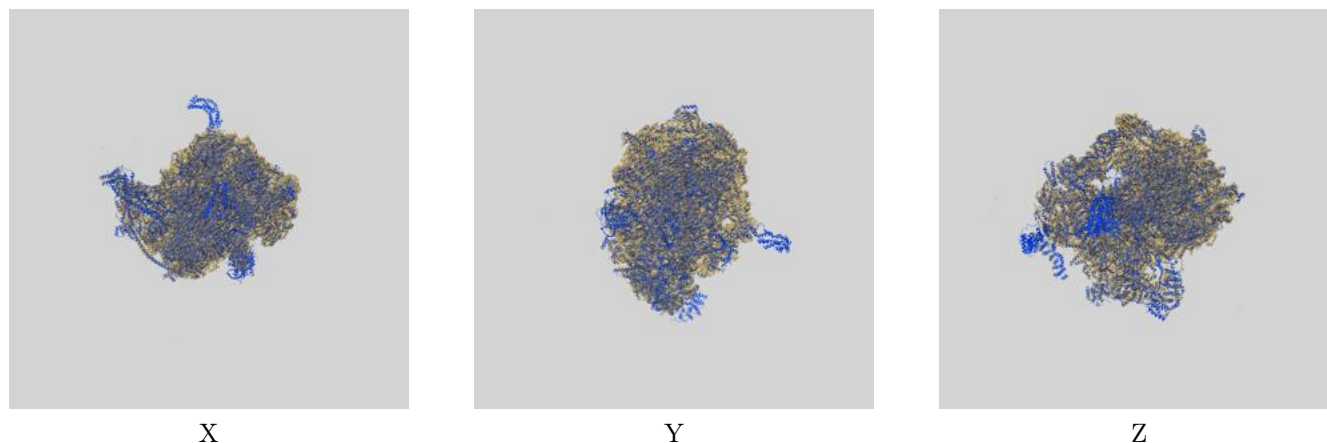
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	3.98	3.62
Unmasked-calculated*	5.00	8.92	5.53

*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 5.00 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

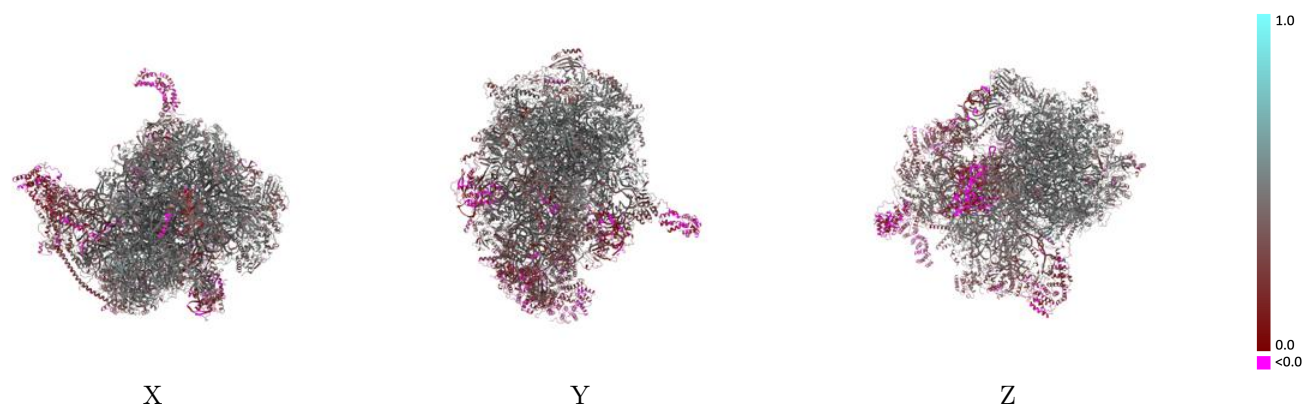
This section contains information regarding the fit between EMDB map EMD-16894 and PDB model 8OIN. Per-residue inclusion information can be found in section [3](#) on page [28](#).

9.1 Map-model overlay [i](#)



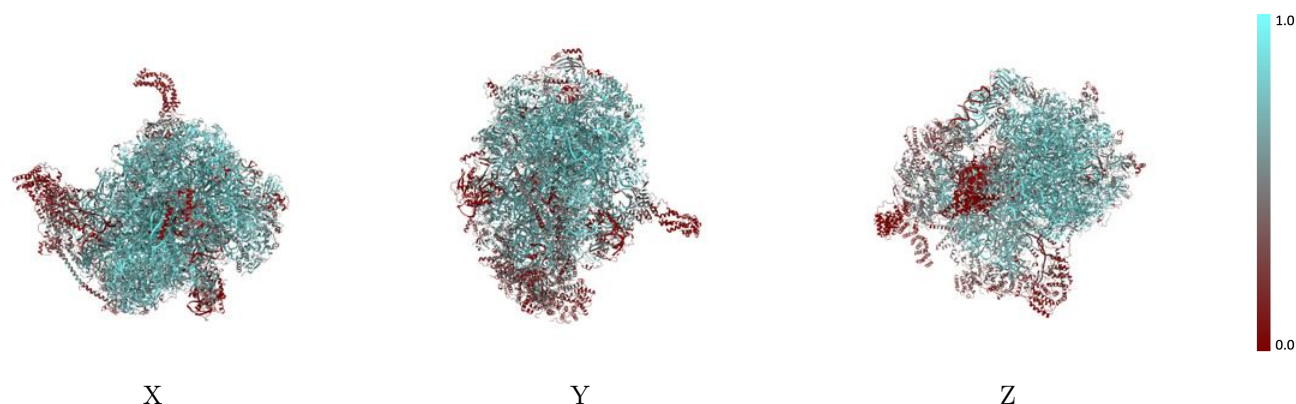
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



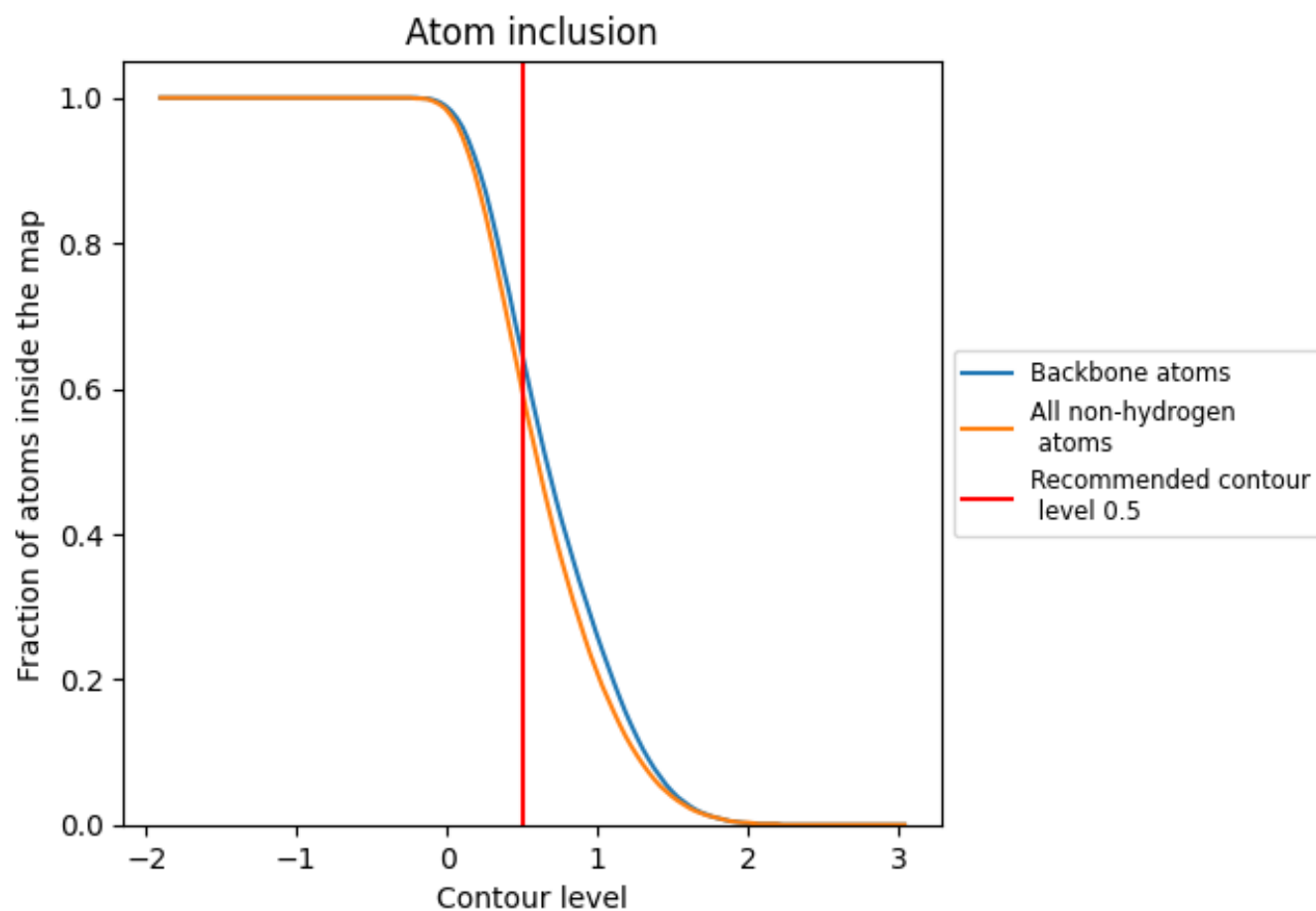
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 60% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5970	 0.3840
AA	 0.7520	 0.4070
AB	 0.3430	 0.2840
AC	 0.5180	 0.4150
AD	 0.6490	 0.4510
AE	 0.6030	 0.4180
AF	 0.4550	 0.3200
AG	 0.4840	 0.3230
AH	 0.4450	 0.3420
AI	 0.7470	 0.4470
AJ	 0.5680	 0.4440
AK	 0.5500	 0.4110
AL	 0.5390	 0.3830
AM	 0.4060	 0.3320
AN	 0.5920	 0.4030
AO	 0.3760	 0.3220
AP	 0.5740	 0.4030
AQ	 0.6480	 0.4300
AR	 0.2430	 0.2670
AS	 0.3750	 0.2950
AT	 0.5360	 0.3740
AU	 0.4150	 0.2690
AV	 0.1150	 0.1370
AW	 0.4350	 0.3570
AX	 0.2690	 0.2030
AY	 0.2530	 0.2350
AZ	 0.3890	 0.3370
Aa	 0.2460	 0.2700
Ab	 0.5880	 0.3910
Ac	 0.4780	 0.3630
Ad	 0.4920	 0.3900
Ae	 0.0600	 0.1060
Ag	 0.4520	 0.3230
Ai	 0.6200	 0.4200
Aj	 0.2400	 0.2550



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Chain	Atom inclusion	Q-score
B1	0.0190	0.0620
B2	0.0000	0.0960
B3	0.0000	0.0660
B4	0.0050	0.0570
B5	0.0000	0.0690
B6	0.0000	0.0150
B7	0.0320	0.1360
B8	0.8300	0.4530
B9	0.4850	0.2420
BA	0.7320	0.4940
BB	0.6760	0.4460
BC	0.4610	0.3960
BD	0.7840	0.5030
BE	0.5830	0.4210
BF	0.7220	0.4600
BG	0.7950	0.4910
BH	0.7190	0.4780
BI	0.4520	0.3930
BJ	0.8210	0.5180
BK	0.8020	0.5130
BL	0.7650	0.4890
BM	0.7590	0.4750
BN	0.7470	0.4830
BO	0.2260	0.2160
BP	0.3440	0.2660
BQ	0.2190	0.2150
BR	0.7910	0.4950
BS	0.7030	0.4750
BT	0.7190	0.4690
BU	0.7610	0.4780
BV	0.7480	0.4920
BW	0.6930	0.4530
BX	0.6500	0.4540
BY	0.7710	0.4940
BZ	0.7550	0.4880
Ba	0.7000	0.4560
Bb	0.4840	0.3510
Bc	0.3490	0.2680
Bd	0.3510	0.2650
Be	0.8110	0.5000
Bf	0.3990	0.3500
Bg	0.4530	0.3670

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Chain	Atom inclusion	Q-score
Bh	 0.7200	 0.4550
Bi	 0.7340	 0.4590
Bj	 0.0300	 0.0700
Bl	 0.8010	 0.4990
Bm	 0.7200	 0.4490
Bn	 0.6980	 0.4250
Bo	 0.6460	 0.4280
Bp	 0.4420	 0.3250
Bq	 0.5770	 0.4220
Br	 0.6210	 0.4300
Bs	 0.7700	 0.4910
Bt	 0.7120	 0.4540
Bu	 0.4000	 0.3590
Bv	 0.3970	 0.2620
Bw	 0.4900	 0.3630
Bx	 0.7250	 0.4680
By	 0.2870	 0.3620
Bz	 0.7870	 0.4960