



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:04 PM UTC

PDB ID : 6YWE / pdb_00006ywe
EMDB ID : EMD-10965
Title : The structure of the mitoribosome from *Neurospora crassa* in the P/E tRNA bound state
Authors : Amunts, A.; Itoh, Y.; Naschberger, A.
Deposited on : 2020-04-29
Resolution : 2.99 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

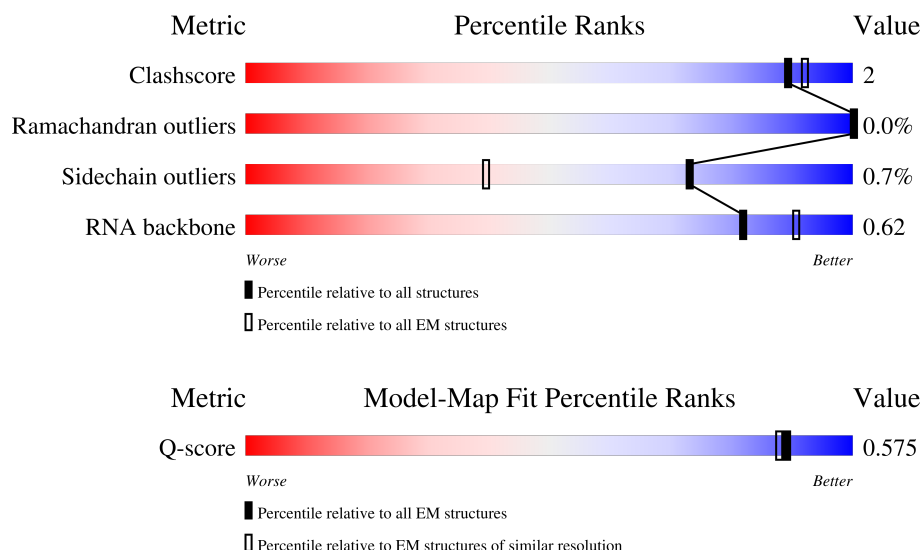
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.99 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	13287 (2.49 - 3.49)

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	A	3464	
2	e	303	
3	B	383	

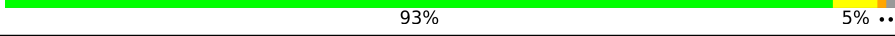
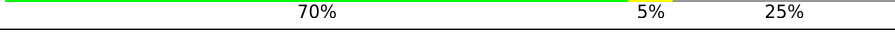
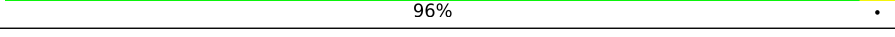
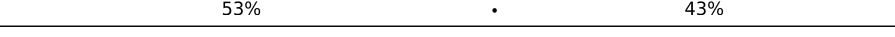
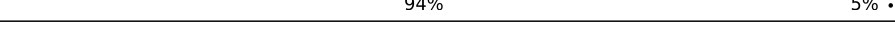
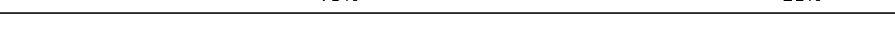
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Mol	Chain	Length	Quality of chain
4	C	384	
5	D	325	
6	E	352	
7	F	255	
8	G	300	
9	f	347	
10	g	158	
11	H	183	
12	I	131	
13	J	312	
14	K	249	
15	L	193	
16	M	258	
17	N	217	
18	O	364	
19	P	228	
20	Q	396	
21	R	447	
22	S	274	
23	T	263	
24	U	161	
25	V	219	
26	W	129	
27	X	59	
28	Y	140	

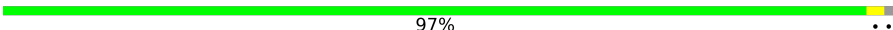
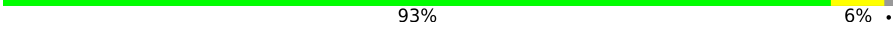
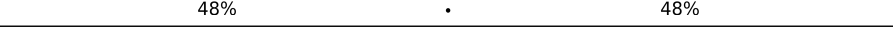
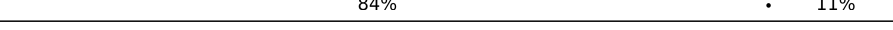
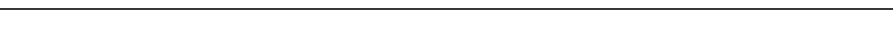
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Mol	Chain	Length	Quality of chain
29	0	124	
30	1	449	
31	2	370	
32	3	103	
33	4	138	
34	5	439	
35	6	368	
36	7	165	
37	8	443	
38	h	98	
39	i	218	
40	9	267	
41	a	225	
42	b	162	
43	c	110	
44	d	292	
45	j	201	
46	bb	74	
47	AA	470	
48	BB	428	
49	CC	508	
50	DD	453	
51	EE	477	
52	FF	117	
53	GG	309	

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Mol	Chain	Length	Quality of chain
54	HH	161	 97% ..
55	II	315	 74% . 22%
56	JJ	268	 65% 5% 30%
57	KK	376	 31% . 67%
58	LL	174	 68% 6% 26%
59	MM	119	 92% 8% .
60	NN	113	 93% 6% .
61	OO	320	 83% . 14%
62	PP	107	 88% . 8%
63	QQ	165	 90% 5% ..
64	RR	256	 48% . 48%
65	SS	91	 80% 9% 11%
66	TT	236	 34% . 63%
67	UU	253	 84% . 11%
68	VV	316	 78% . 17%
69	WW	396	 85% . 11%
70	XX	469	 82% 5% 13%
71	YY	108	 84% 7% 8%
72	ZZ	382	 78% . 18%
73	11	90	 92% 6% .
74	22	344	 10% 90%
75	33	236	 73% 8% 18%
76	44	310	 79% 5% 16%
76	55	310	 71% . 25%
77	66	348	 77% . 19%

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Mol	Chain	Length	Quality of chain
78	77	414	
79	88	508	
80	00	95	
80	99	95	
81	aa	1864	
82	ee	11	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 394184 atoms, of which 175257 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2837	Total	C	H	N	O	P	0	0
			90863	27133	30351	10856	19686	2837		

- Molecule 2 is a protein called 60S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	e	242	Total	C	H	N	O	S	0	0
			3821	1189	1935	332	353	12		

- Molecule 3 is a protein called 60S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	B	326	Total	C	H	N	O	S	0	0
			5136	1578	2592	515	436	15		

- Molecule 4 is a protein called Related to ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	307	Total	C	H	N	O	S	0	0
			4758	1468	2422	447	413	8		

- Molecule 5 is a protein called 60S ribosomal protein L4, variant.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	D	254	Total	C	H	N	O	S	0	0
			4068	1280	2040	372	371	5		

- Molecule 6 is a protein called Related to ribosomal protein L5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	E	309	Total	C	H	N	O	S	0	0
			4910	1558	2461	436	443	12		

- Molecule 7 is a protein called uL6m.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	F	201	Total	C	H	N	O	S	0	0
			3253	1022	1645	290	288	8		

- Molecule 8 is a protein called RIBOSOMAL_L9 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	G	74	Total	C	H	N	O	S	0	0
			1245	390	627	121	104	3		

- Molecule 9 is a protein called Related to ribosomal protein YmL11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	f	245	Total	C	H	N	O	S	0	0
			3801	1202	1925	325	346	3		

- Molecule 10 is a protein called uL11m.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	g	147	Total	C	H	N	O	S	0	0
			2258	700	1154	203	197	4		

- Molecule 11 is a protein called uL13m.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	H	183	Total	C	H	N	O	S	0	0
			2885	899	1459	268	251	8		

- Molecule 12 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	I	119	Total	C	H	N	O	S	0	0
			1898	564	985	182	159	8		

- Molecule 13 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	J	243	Total	C	H	N	O	S	0	0
			3827	1198	1939	346	343	1		

- Molecule 14 is a protein called Related to ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	K	168	Total	C	H	N	O	S	0	0
			2751	850	1401	263	231	6		

- Molecule 15 is a protein called uL17m.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	L	192	Total	C	H	N	O	S	0	0
			3135	960	1590	294	285	6		

- Molecule 16 is a protein called bL19m.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	M	194	Total	C	H	N	O	S	0	0
			3164	981	1628	292	253	10		

- Molecule 17 is a protein called Related to ribosomal protein YmL49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	N	133	Total	C	H	N	O	S	0	0
			2176	673	1120	195	182	6		

- Molecule 18 is a protein called Mitochondrial large ribosomal subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	O	272	Total	C	H	N	O	S	0	0
			4532	1392	2323	424	387	6		

- Molecule 19 is a protein called uL23m.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	P	180	Total	C	H	N	O	S	0	0
			2975	953	1494	270	254	4		

- Molecule 20 is a protein called KOW domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	Q	353	Total	C	H	N	O	S	0	0
			5829	1786	2961	547	524	11		

- Molecule 21 is a protein called Related to 60s ribosomal protein L2 (Mitochondrial).

Mol	Chain	Residues	Atoms						AltConf	Trace
21	R	266	Total	C	H	N	O	S	0	0
			4499	1374	2310	441	370	4		

- Molecule 22 is a protein called bL28m.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	S	179	Total	C	H	N	O	S	0	0
			2979	937	1507	281	252	2		

- Molecule 23 is a protein called 54S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	T	180	Total	C	H	N	O	S	0	0
			2950	937	1453	279	278	3		

- Molecule 24 is a protein called Related to ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	U	138	Total	C	H	N	O	S	0	0
			2263	698	1164	213	185	3		

- Molecule 25 is a protein called Related to ribosomal protein YmL36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	V	100	Total	C	H	N	O	S	0	0
			1577	501	778	143	153	2		

- Molecule 26 is a protein called Related to ribosomal protein YmL32 (Mitochondrial), Mitochondrial ribosomal protein subunit L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	W	59	Total	C	H	N	O	S	0	0
			949	282	489	98	72	8		

- Molecule 27 is a protein called bL33m.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	X	48	Total	C	H	N	O	S	0	0
			836	263	433	71	65	4		

- Molecule 28 is a protein called Related to ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	Y	46	Total	C	H	N	O	S	0	0
			777	224	412	84	56	1		

- Molecule 29 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	0	46	Total	C	H	N	O	S	0	0
			797	240	409	86	58	4		

- Molecule 30 is a protein called PEBP-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	1	367	Total	C	H	N	O	S	0	0
			6014	1899	3029	547	531	8		

- Molecule 31 is a protein called mL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	2	123	Total	C	H	N	O	S	0	0
			2101	660	1055	211	171	4		

- Molecule 32 is a protein called mL41.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	3	95	Total	C	H	N	O	S	0	0
			1536	489	773	135	137	2		

- Molecule 33 is a protein called L51_S25_CI-B8 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	4	137	Total	C	H	N	O	S	0	0
			2139	671	1087	192	183	6		

- Molecule 34 is a protein called Ribonuclease III.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	5	350	Total	C	H	N	O	S	0	0
			5429	1740	2710	477	493	9		

- Molecule 35 is a protein called MRP-L46 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	6	273	Total	C	H	N	O	S	0	0
			4474	1418	2248	399	401	8		

- Molecule 36 is a protein called mL49.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	7	84	Total	C	H	N	O		0	0
			1383	431	709	130	113			

- Molecule 37 is a protein called mL50.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	8	331	Total	C	H	N	O	S	0	0
			5374	1683	2714	480	489	8		

- Molecule 38 is a protein called Probable ribosomal protein YmL44, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	h	98	Total	C	H	N	O	S	0	0
			1577	490	798	139	146	4		

- Molecule 39 is a protein called mL54.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	i	124	Total	C	H	N	O	S	0	0
			1998	613	1022	181	177	5		

- Molecule 40 is a protein called RNase III domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	9	206	Total	C	H	N	O	S	0	0
			3341	1051	1698	295	290	7		

- Molecule 41 is a protein called Related to ribosomal protein YmL20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	a	161	Total	C	H	N	O	S	0	0
			2671	837	1340	253	235	6		

- Molecule 42 is a protein called Mitoc_mL59 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	b	161	Total	C	H	N	O	S	0	0
			2693	840	1379	249	221	4		

- Molecule 43 is a protein called 54S ribosomal protein L31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	c	98	Total	C	H	N	O	S	0	0
			1700	528	873	162	134	3		

- Molecule 44 is a protein called mL67.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	d	235	Total	C	H	N	O	S	0	0
			3797	1180	1909	363	339	6		

- Molecule 45 is a protein called L51_S25_CI-B8 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	j	195	Total	C	H	N	O	S	0	0
			3139	971	1586	290	284	8		

- Molecule 46 is a RNA chain called tRNA P/E state.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	bb	74	Total	C	H	N	O	P	0	0
			2366	702	796	275	519	74		

- Molecule 47 is a protein called bS1m.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	AA	372	Total	C	H	N	O	S	0	0
			5790	1827	2907	507	543	6		

- Molecule 48 is a protein called Mito ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	BB	290	Total	C	H	N	O	S	0	0
			4570	1426	2301	423	414	6		

- Molecule 49 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	CC	438	Total	C	H	N	O	S	0	0
			7538	2388	3897	636	612	5		

- Molecule 50 is a protein called S4 RNA-binding domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	DD	290	Total	C	H	N	O	S	0	0
			4716	1501	2373	430	401	11		

- Molecule 51 is a protein called Related to ribosomal protein S5 (Mitochondrial).

Mol	Chain	Residues	Atoms						AltConf	Trace
51	EE	367	Total	C	H	N	O	S	0	0
			5798	1799	2918	526	543	12		

- Molecule 52 is a protein called Ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	FF	117	Total	C	H	N	O	S	0	0
			1902	591	966	176	166	3		

- Molecule 53 is a protein called Ribosomal_S7 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	GG	223	Total	C	H	N	O	S	0	0
			3523	1098	1799	318	302	6		

- Molecule 54 is a protein called uS8m.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	HH	160	Total	C	H	N	O	S	0	0
			2521	783	1286	226	220	6		

- Molecule 55 is a protein called uS9m.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	II	247	Total	C	H	N	O	S	0	0
			3995	1253	2026	366	345	5		

- Molecule 56 is a protein called 30S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	JJ	188	Total	C	H	N	O	S	0	0
			3105	998	1554	273	272	8		

- Molecule 57 is a protein called Translational machinery component.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	KK	124	Total	C	H	N	O	S	0	0
			2020	625	1025	195	170	5		

- Molecule 58 is a protein called Ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	LL	128	Total	C	H	N	O	S	0	0
			1991	591	1032	198	165	5		

- Molecule 59 is a protein called Probable ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	MM	118	Total	C	H	N	O	S	0	0
			1923	586	986	186	161	4		

- Molecule 60 is a protein called Mitochondrial 37S ribosomal protein MRP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	NN	112	Total	C	H	N	O	S	0	0
			1875	573	961	184	150	7		

- Molecule 61 is a protein called Related to ribosomal protein S15 (Mitochondrial).

Mol	Chain	Residues	Atoms						AltConf	Trace
61	OO	276	Total	C	H	N	O	S	0	0
			4428	1361	2230	431	401	5		

- Molecule 62 is a protein called bS16m.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	PP	98	Total	C	H	N	O		0	0
			1612	510	826	141	135			

- Molecule 63 is a protein called uS17m.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	QQ	158	Total	C	H	N	O	S	0	0
			2561	789	1314	234	219	5		

- Molecule 64 is a protein called Ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	RR	134	Total	C	H	N	O	S	0	0
			2170	679	1090	206	190	5		

- Molecule 65 is a protein called Ribosomal protein S19/S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	SS	81	Total	C	H	N	O	S	0	0
			1325	422	677	118	107	1		

- Molecule 66 is a protein called bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	TT	88	Total	C	H	N	O		0	0
			1518	470	772	157	119			

- Molecule 67 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	UU	224	Total	C	H	N	O	S	0	0
			3686	1165	1842	342	330	7		

- Molecule 68 is a protein called mS26.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	VV	261	Total	C	H	N	O	S	0	0
			4192	1300	2112	390	387	3		

- Molecule 69 is a protein called mS27.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	WW	353	Total	C	H	N	O	S	0	0
			5744	1804	2901	514	515	10		

- Molecule 70 is a protein called Mitochondrial ribosomal protein DAP3.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	XX	408	Total	C	H	N	O	S	0	0
			6446	2010	3271	562	587	16		

- Molecule 71 is a protein called mS33.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	YY	99	Total	C	H	N	O	S	0	0
			1609	491	823	152	142	1		

- Molecule 72 is a protein called 37S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	ZZ	312	Total	C	H	N	O	S	0	0
			5114	1631	2528	450	495	10		

- Molecule 73 is a protein called 37S ribosomal protein mrp10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	11	88	Total	C	H	N	O	S	0	0
			1358	417	686	128	121	6		

- Molecule 74 is a protein called DUF1713 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	22	33	Total	C	H	N	O	S	0	0
			660	187	359	70	43	1		

- Molecule 75 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	33	193	Total	C	H	N	O	S	0	0
			3161	989	1607	295	268	2		

- Molecule 76 is a protein called Manganese and iron superoxide dismutase.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	44	260	Total	C	H	N	O	S	0	0
			4045	1318	1983	355	378	11		
76	55	232	Total	C	H	N	O	S	0	0
			3651	1195	1793	316	337	10		

- Molecule 77 is a protein called mS45.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	66	283	Total	C	H	N	O	S	0	0
			4628	1455	2330	425	414	4		

- Molecule 78 is a protein called mS46.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	77	179	Total	C	H	N	O	S	0	0
			2796	893	1396	227	277	3		

- Molecule 79 is a protein called 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	88	467	Total	C	H	N	O	S	0	0
			7327	2340	3650	634	691	12		

- Molecule 80 is a protein called IF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	00	48	Total	C	H	N	O	0	0
			823	252	417	77	77		
80	99	36	Total	C	H	N	O	0	0
			639	191	333	59	56		

- Molecule 81 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	aa	1435	Total	C	H	N	O	P	0	0
			45981	13712	15373	5486	9975	1435		

- Molecule 82 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	ee	11	Total	C	H	N	O	P	0	0
			347	104	116	37	79	11		

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

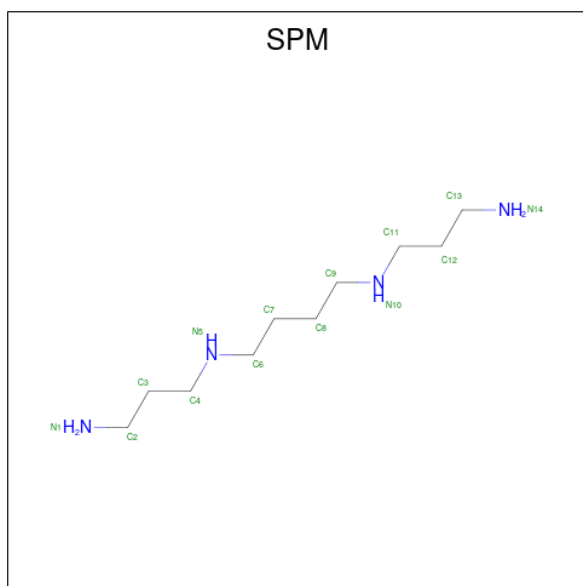
Mol	Chain	Residues	Atoms		AltConf
83	A	135	Total	Mg	0
			135	135	
83	B	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
83	S	1	Total	Mg	0
			1	1	
83	3	1	Total	Mg	0
			1	1	
83	BB	1	Total	Mg	0
			1	1	
83	XX	1	Total	Mg	0
			1	1	
83	YY	1	Total	Mg	0
			1	1	
83	00	1	Total	Mg	0
			1	1	
83	aa	99	Total	Mg	0
			99	99	
83	ee	1	Total	Mg	0
			1	1	

- Molecule 84 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms				AltConf
84	A	1	Total	C	H	N	0
			40	10	26	4	

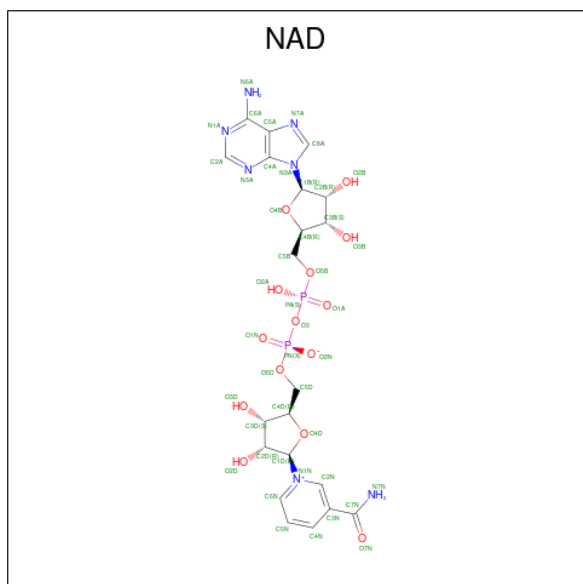
- Molecule 85 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
85	A	38	Total K 38 38	0
85	K	1	Total K 1 1	0
85	2	1	Total K 1 1	0
85	KK	1	Total K 1 1	0
85	77	1	Total K 1 1	0
85	88	1	Total K 1 1	0
85	aa	12	Total K 12 12	0

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

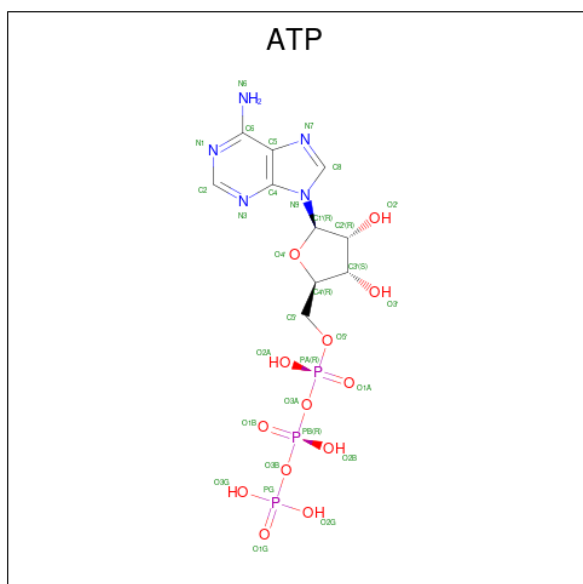
Mol	Chain	Residues	Atoms	AltConf
86	W	1	Total Zn 1 1	0
86	0	1	Total Zn 1 1	0

- Molecule 87 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
87	2	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 88 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).

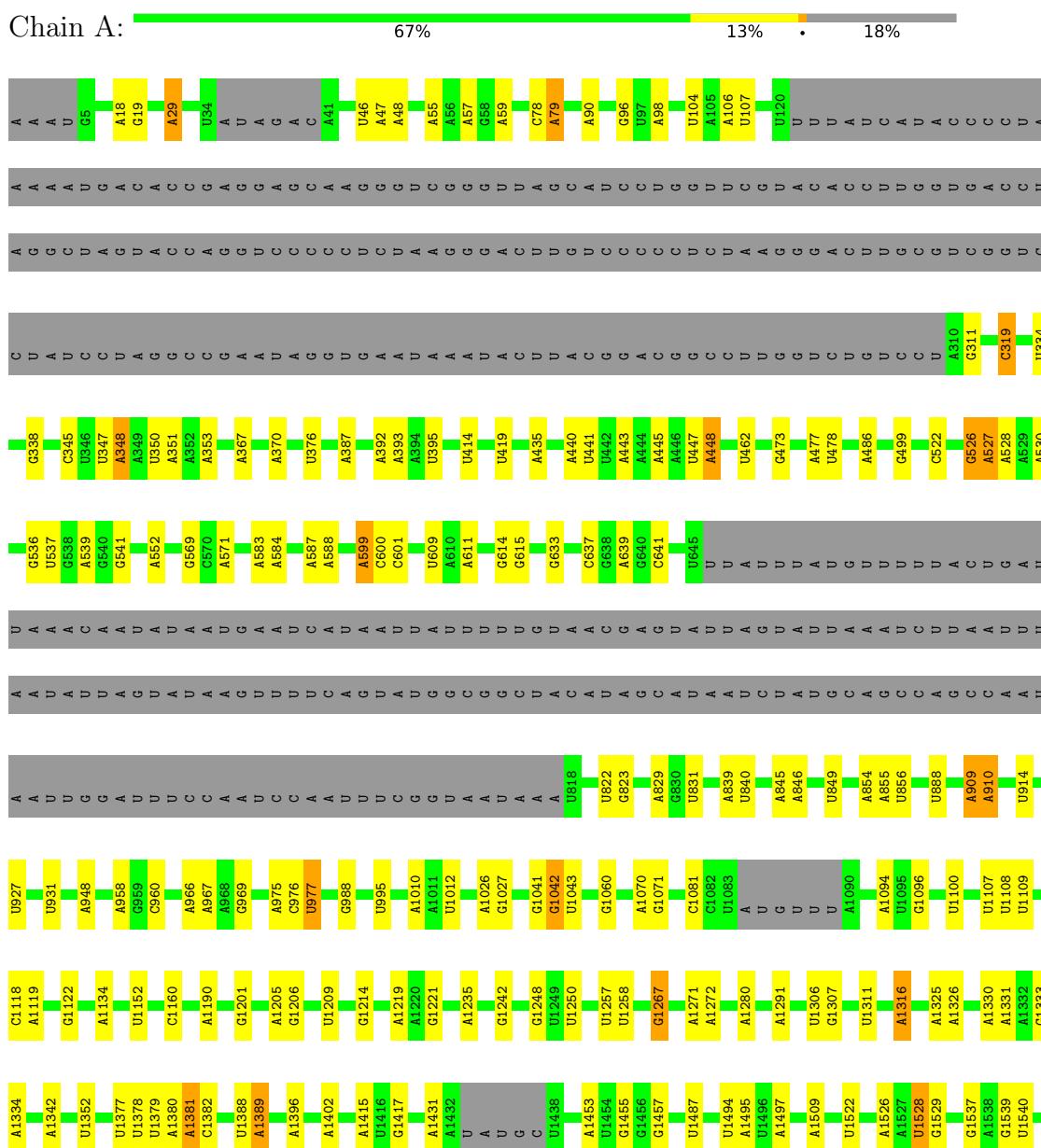


Mol	Chain	Residues	Atoms						AltConf
88	XX	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

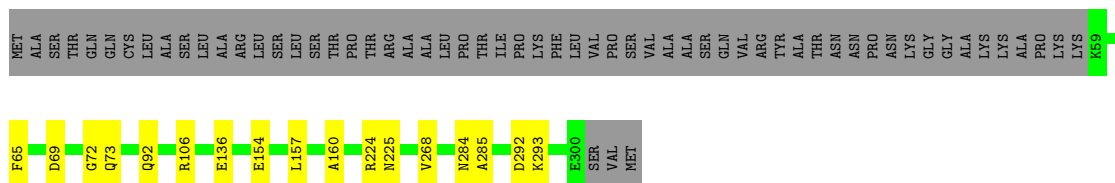
3 Residue-property plots

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

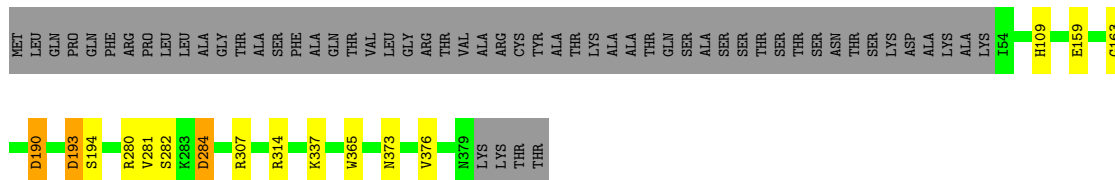
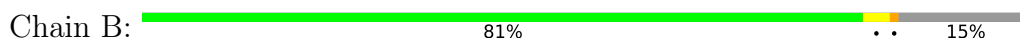
• Molecule 1: 23S rRNA



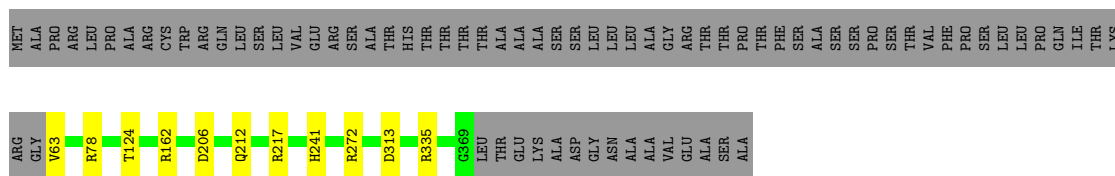
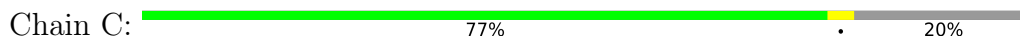




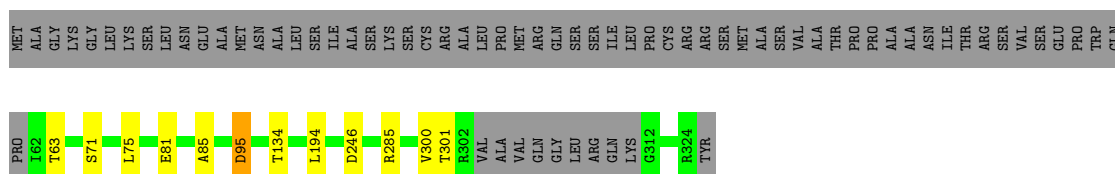
- Molecule 3: 60S ribosomal protein L2, mitochondrial



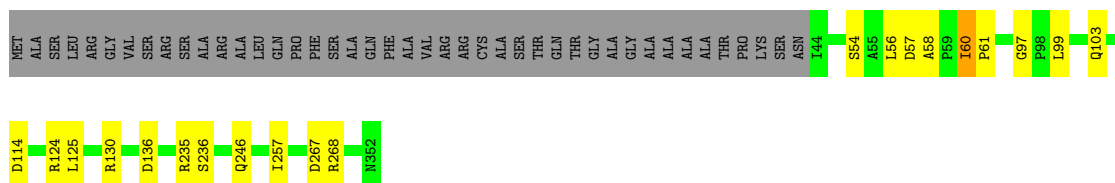
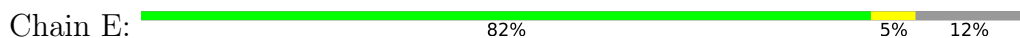
- Molecule 4: Related to ribosomal protein L3, mitochondrial



- Molecule 5: 60S ribosomal protein L4, variant

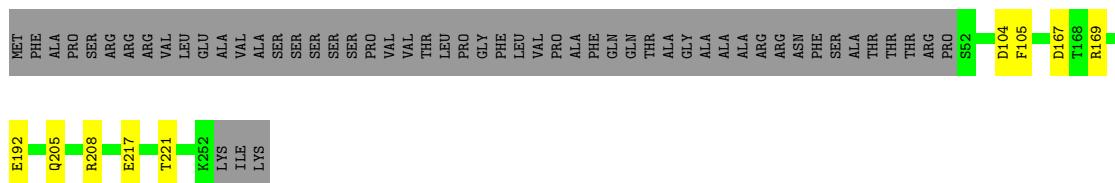


- Molecule 6: Related to ribosomal protein L5, mitochondrial

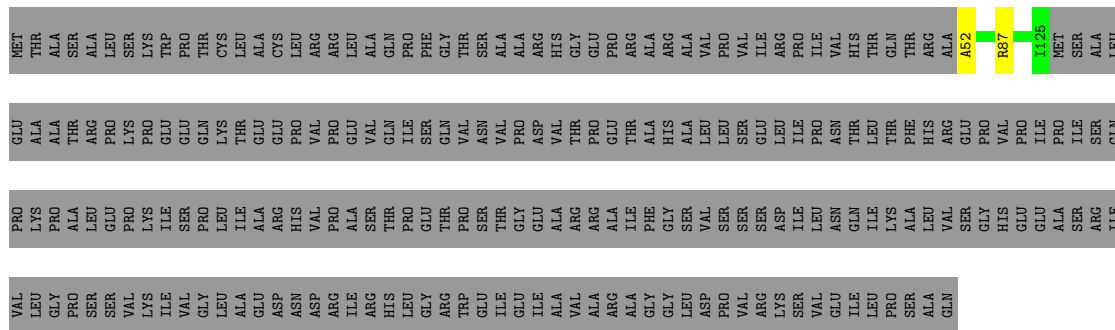


- Molecule 7: uL6m

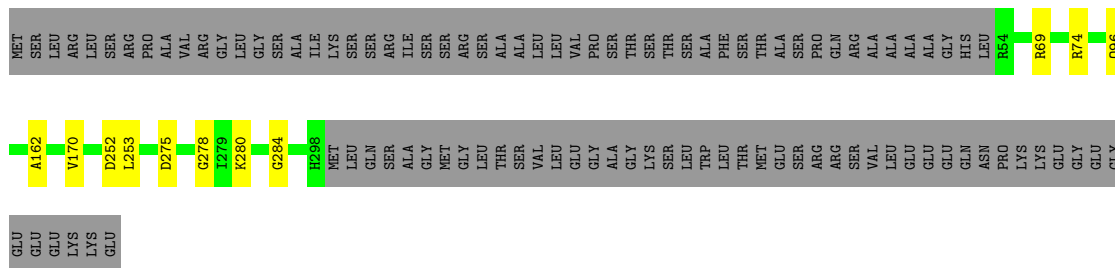




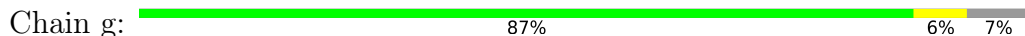
- Molecule 8: RIBOSOMAL L9 domain-containing protein



- Molecule 9: Related to ribosomal protein YmL11, mitochondrial



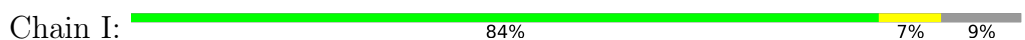
- Molecule 10: uL11m



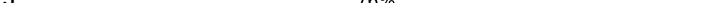
- Molecule 11: uL13m

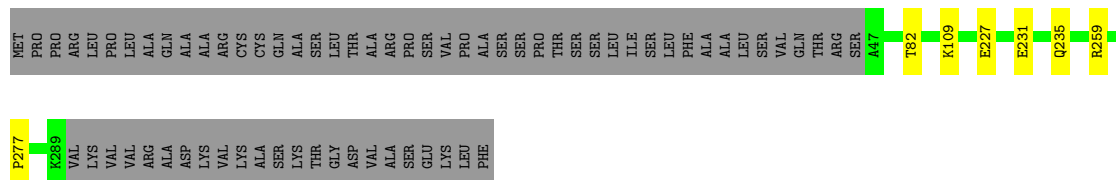


- Molecule 12: Ribosomal protein L14

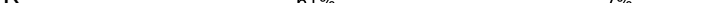


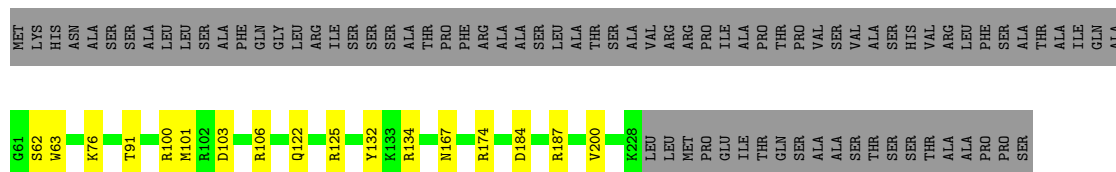
- Molecule 13: Ribosomal protein L15

Chain J:  76% . 22%

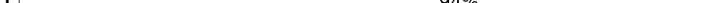


- Molecule 14: Related to ribosomal protein L16, mitochondrial

Chain K:  61% 7% 33%

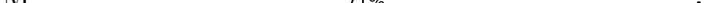


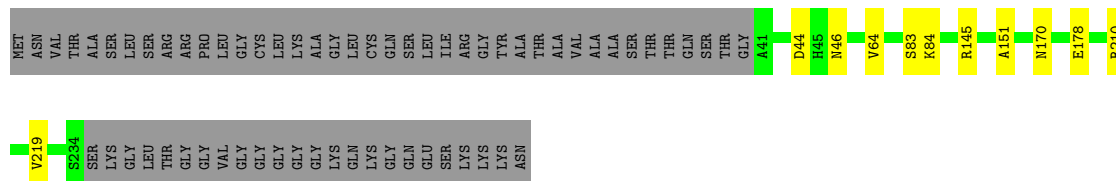
- Molecule 15: uL17m

Chain L:  94% 5%

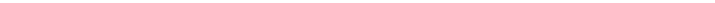


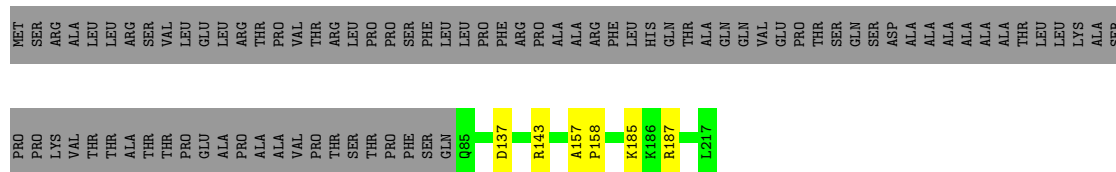
- Molecule 16: bL19m

Chain M:  71% . 25%



- Molecule 17: Related to ribosomal protein YmL49, mitochondrial

Chain N:  59% 1% 39%



- Molecule 18: Mitochondrial large ribosomal subunit

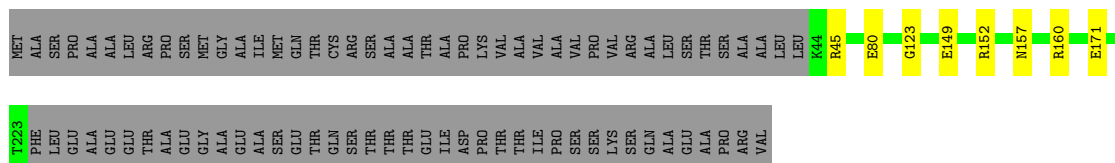
R332	E336	D352	R359	W364																																																																								
GLU	ARG	VAL	GLY	ARG	LEU	GLU	GLY	ASP	SER	ILE	PHE	ALA	ASP	THR	THR	PRO	SER	SER	GLN	LEU	ALA	ALA	GLU	GLN	ASP	LYS	HIS	LYS	LEU	ASN	ARG	SER	THR	THR	THR	THR	ILE	SER	SER	LEU	ASP	GLN	LEU	ALA	PRO	VAL	LEU	ALA	ALA	SER	SER	SER	PRO	ASP	ALA	ALA	ALA	ALA	LYS	ARG	T771	E61	R56	Q51	K43	Gln	Lys	Arg	Thr	Glu	Gln	Thr	Pro	Lys	Arg	Met
A122	K127	E156	R206	K241	T245	A258	T262	F296	T317																																																																			

[illegible]

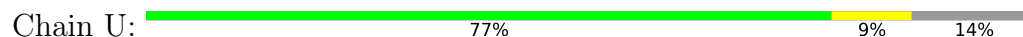
Residue	Position
SER	M1
LEU	P67
GLY	D72
GLY	E73
GLN	R104
GLU	S110
ASP	P111
ALA	N143
ALA	E147
THR	Q164
THR	K169
THR	R177
THR	R208
SER	D213
PRO	T216
GLU	R217
GLN	T218
PRO	R219
VAL	R222
VAL	D248
VAL	R324
SER	G353
HIS	HIS
SER	GLN
PRO	ALA
PRO	PRO
LYS	LYS
LYS	VAL
GLU	LYS
GLU	GLU
THR	THR
VAL	VAL
ALA	ALA
GLN	GLN
THR	THR
LYS	LYS
ALA	ALA
VAL	VAL
GLU	GLU
GLN	GLN
LEU	LEU

[illegible]

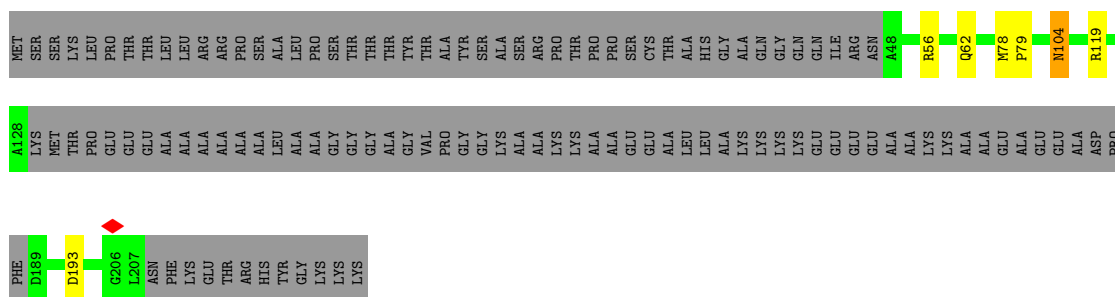
- Molecule 23: 54S ribosomal protein L4, mitochondrial



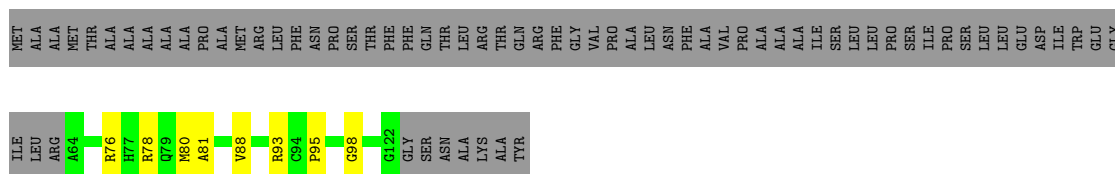
- Molecule 24: Related to ribosomal protein L30



- Molecule 25: Related to ribosomal protein YmL36, mitochondrial



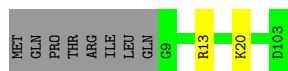
- Molecule 26: Related to ribosomal protein YmL32 (Mitochondrial), Mitochondrial ribosomal protein subunit L32



- Molecule 27: bL33m



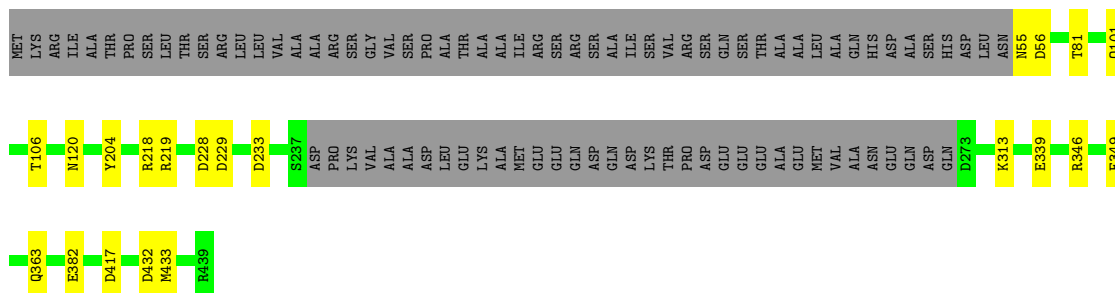
• Molecule 32: mL41

Chain 3:  90% 8%

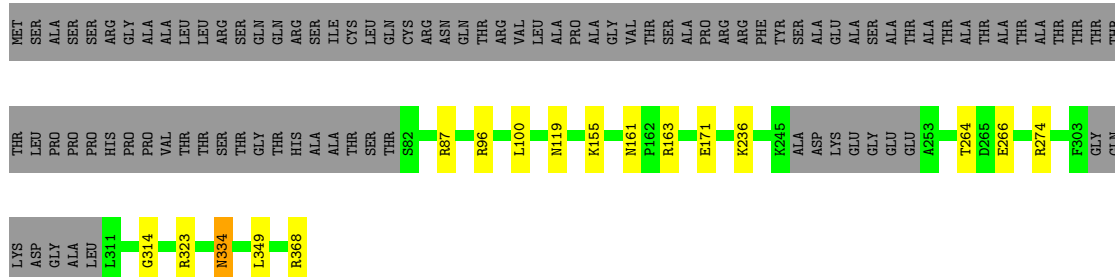
• Molecule 33: L51_S25_CI-B8 domain-containing protein

Chain 4:  93% 5% ..

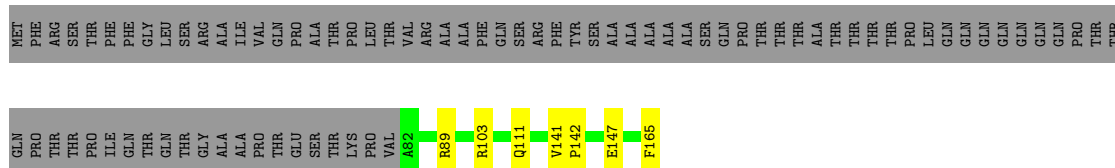
• Molecule 34: Ribonuclease III

Chain 5:  75% 5% 20%

• Molecule 35: MRP-L46 domain-containing protein

Chain 6:  70% 26%

• Molecule 36: mL49

Chain 7:  47% 49%

• Molecule 37: mL50

- Molecule 38: Probable ribosomal protein YmL44, mitochondrial

- Molecule 39: mL54

- Molecule 40: RNase III domain-containing protein

- Molecule 41: Related to ribosomal protein YmL20, mitochondrial

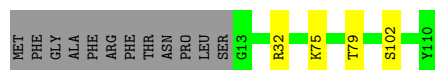
- Molecule 42: Mitoc mL59 domain-containing protein





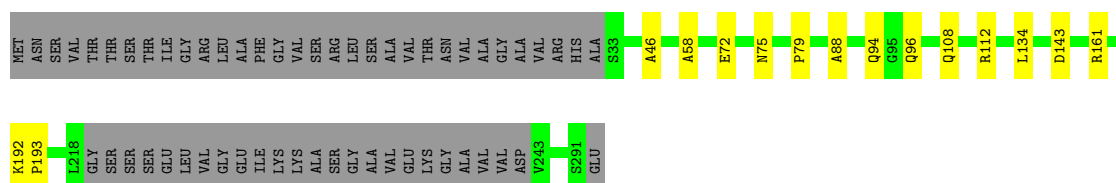
- Molecule 43: 54S ribosomal protein L31, mitochondrial

Chain c: 85% 11%



- Molecule 44: mL67

Chain d: 75% 5% 20%



- Molecule 45: L51_S25_CI-B8 domain-containing protein

Chain j: 84% 12%



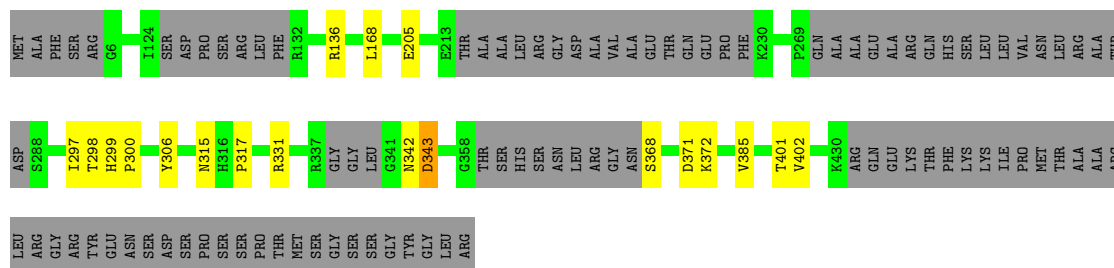
- Molecule 46: tRNA P/E state

Chain bb: 77% 15% 8%



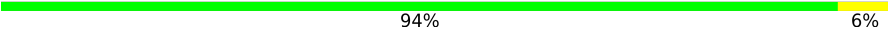
- Molecule 47: bS1m

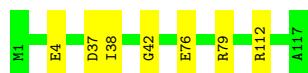
Chain AA: 75% 21%



- Molecule 48: Mito ribosomal protein S2

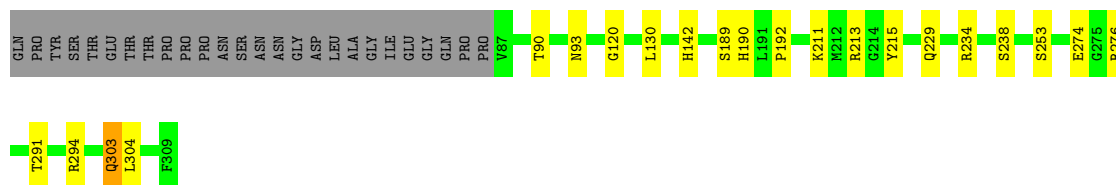
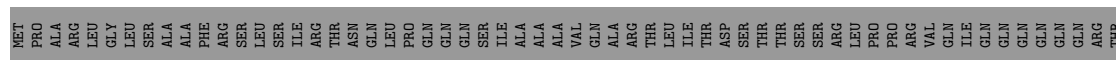
Chain BB: 64% 32%

Chain FF:  94% 6%

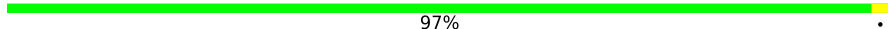


- Molecule 53: Ribosomal_S7 domain-containing protein

Chain GG:  65% 6% 28%



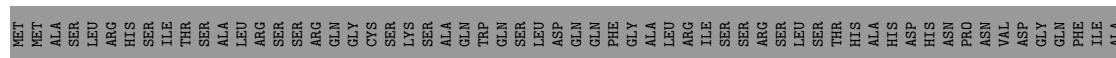
- Molecule 54: uS8m

Chain HH:  97% ..



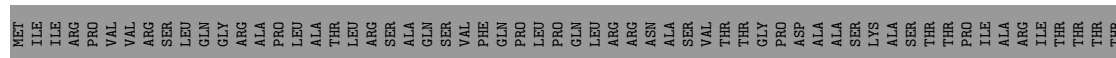
- Molecule 55: uS9m

Chain II:  74% 22% .



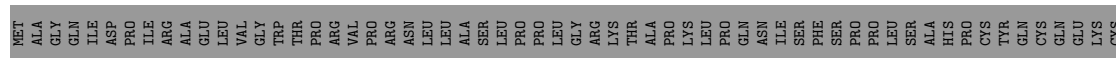
- Molecule 56: 30S ribosomal protein S10, mitochondrial

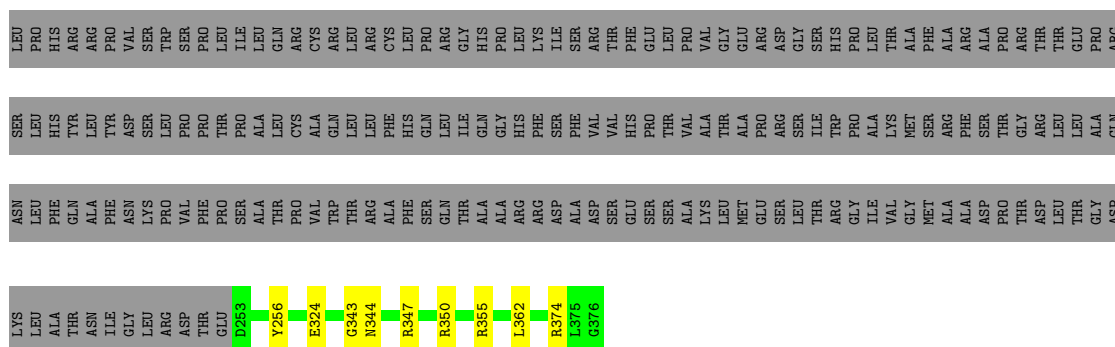
Chain JJ:  65% 5% 30%



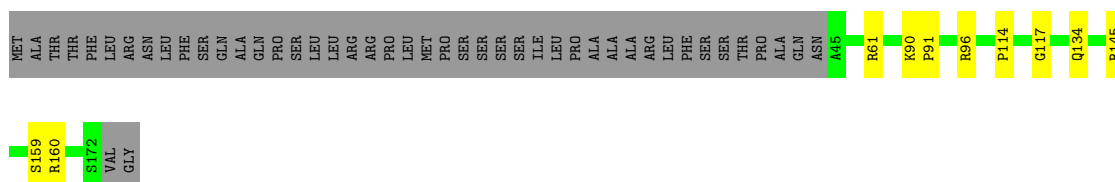
- Molecule 57: Translational machinery component

Chain KK:  31% 67%





- Molecule 58: Ribosomal protein S12



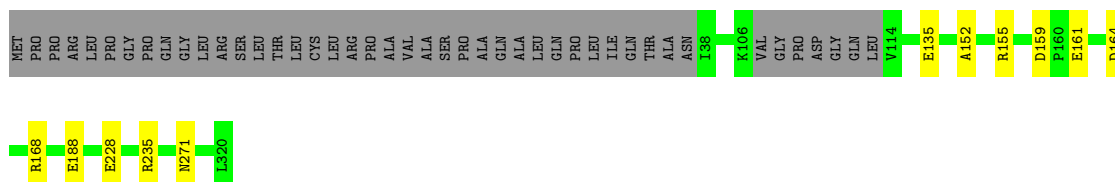
- Molecule 59: Probable ribosomal protein S13



- Molecule 60: Mitochondrial 37S ribosomal protein MRP2

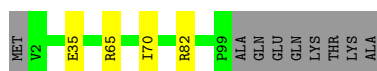


- Molecule 61: Related to ribosomal protein S15 (Mitochondrial)



- Molecule 62: bS16m





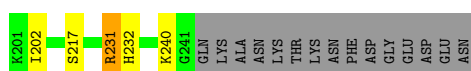
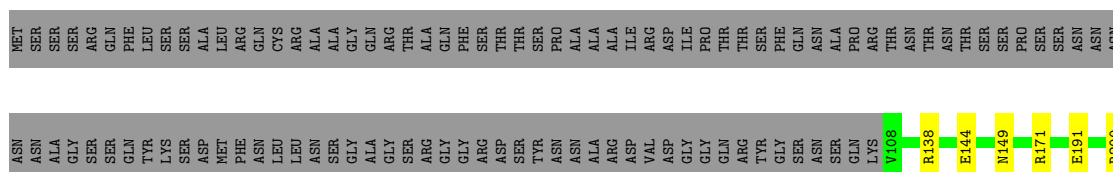
- Molecule 63: uS17m

Chain QQ: 90% 5% . .



- Molecule 64: Ribosomal protein S18

Chain RR: 48% . 48%



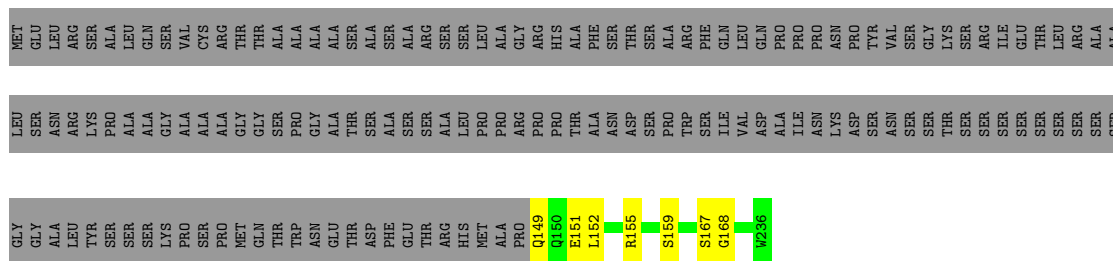
- Molecule 65: Ribosomal protein S19/S15

Chain SS: 80% 9% 11%



- Molecule 66: bS21m

Chain TT: 34% . 63%



- Molecule 67: 37S ribosomal protein S25, mitochondrial

Chain UU: 84% . 11%



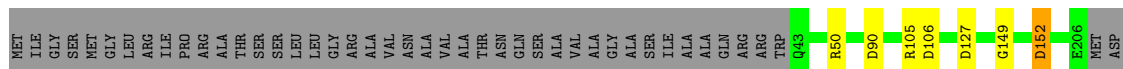
- Molecule 68: mS26

R213	MET
R221	ALA
D238	PRO
E239	THR
A257	LEU
GLY	ALA
S262	ARG
S265	PRO
N272	ARG
E278	SER
N287	SER
ASP	THR
ARG	THR
VAL	CYS
THR	ALA
ALA	ALA
T293	THR
SER	SER
VAL	VAL
R303	VAL
L316	THR
	ARG
	ALA
	ILE
	ALA
	ARG
	SER
	PHE
	SER
	SER
	THR
	THR
	ARG
	ALA
	SER
	ALA
	ARG
	D47
	V61
	P73
	E121
	R125
	R131
	R207

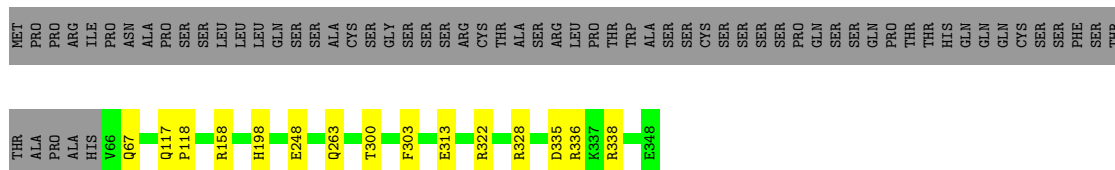
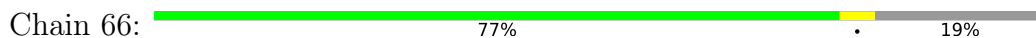
[illegible][illegible]

MET	S2	C16	E17	L18	F19	S20	T21	V73	D74	D75	D76	R77	S100	ALA	ALA	ASP	ALA	LYS	LYS	LYS
-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----	-----	-----	-----

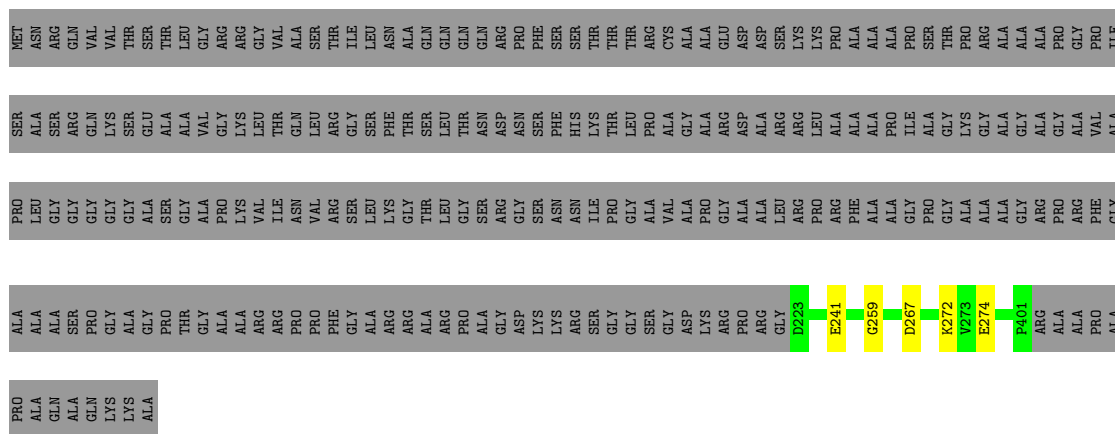
[illegible]



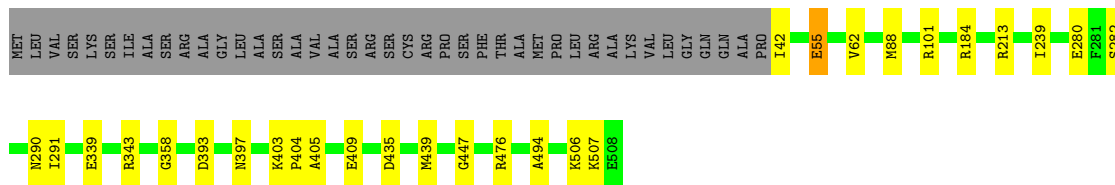
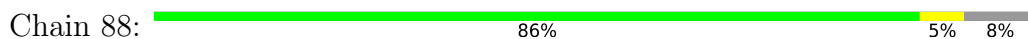
- Molecule 77: mS45



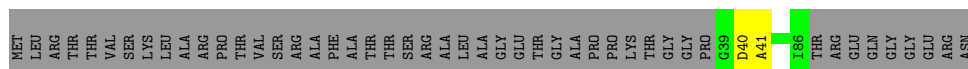
- Molecule 78: mS46



- Molecule 79: 3-hydroxyisobutyryl-CoA hydrolase, mitochondrial



- Molecule 80: IF1

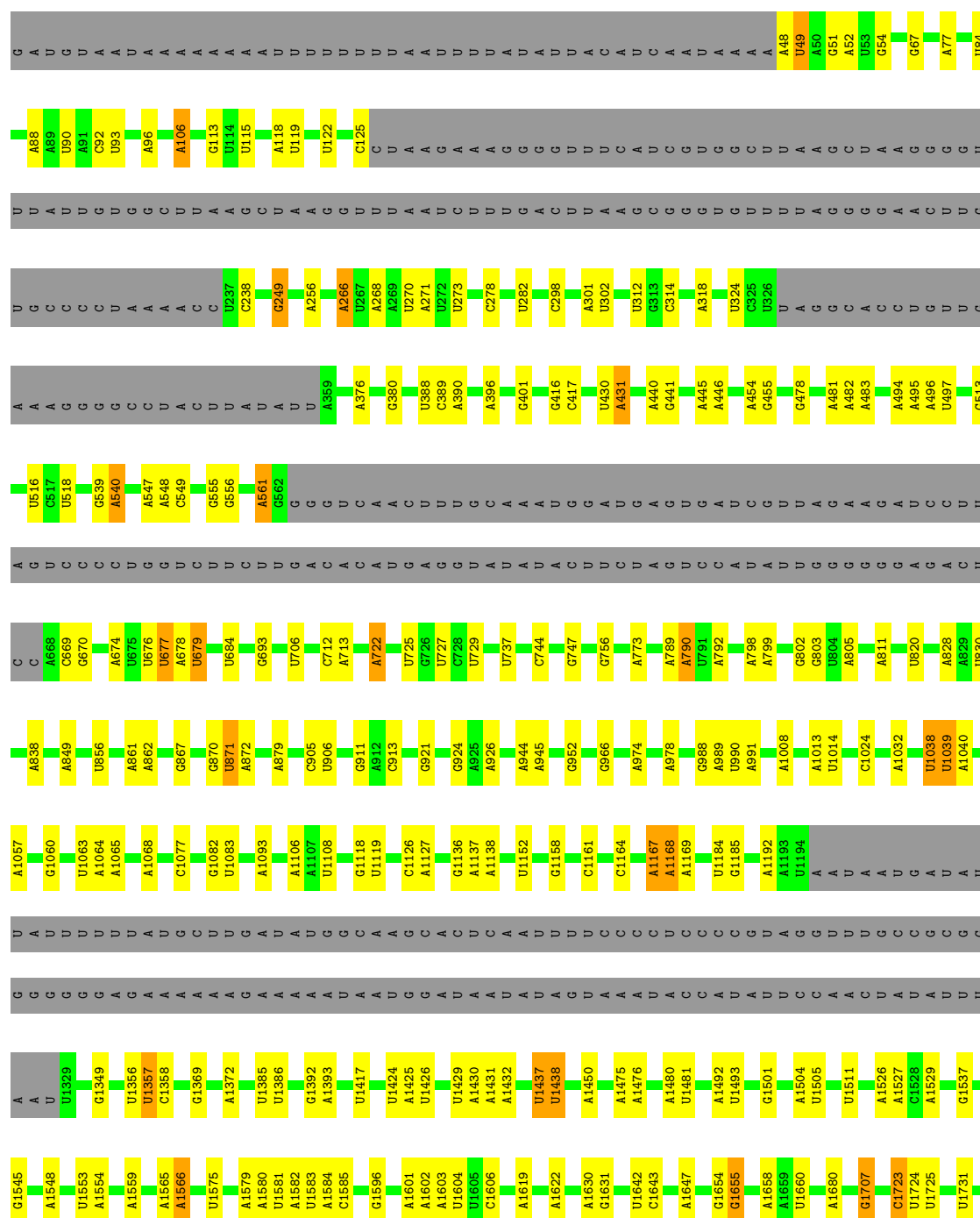


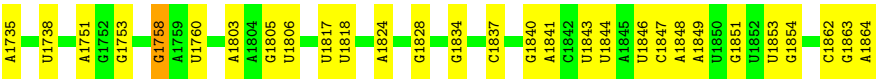
- Molecule 80: IF1



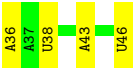


Chain aa: 62% 13% 1% 23%





● Molecule 82: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37908	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	37.644	Depositor
Minimum map value	-21.693	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	1.217	Depositor
Recommended contour level	0.0258	Depositor
Map size ($\text{\AA}$)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.11	0/67768	0.18	0/105530
2	e	0.10	0/1918	0.25	0/2582
3	B	0.15	0/2603	0.30	0/3508
4	C	0.14	0/2380	0.28	0/3209
5	D	0.13	0/2072	0.27	0/2794
6	E	0.17	0/2518	0.31	0/3427
7	F	0.11	0/1644	0.24	0/2218
8	G	0.11	0/630	0.29	0/842
9	f	0.12	0/1923	0.24	0/2631
10	g	0.10	0/1127	0.27	0/1525
11	H	0.15	0/1460	0.29	0/1975
12	I	0.13	0/918	0.28	0/1225
13	J	0.12	0/1931	0.27	0/2597
14	K	0.13	0/1376	0.26	0/1842
15	L	0.14	0/1569	0.29	0/2106
16	M	0.12	0/1572	0.27	0/2117
17	N	0.13	0/1077	0.29	0/1452
18	O	0.13	0/2248	0.27	0/3015
19	P	0.13	0/1523	0.26	0/2058
20	Q	0.12	0/2916	0.27	0/3927
21	R	0.13	0/2227	0.30	0/2978
22	S	0.13	0/1510	0.29	0/2042
23	T	0.12	0/1538	0.27	0/2086
24	U	0.13	0/1117	0.30	0/1496
25	V	0.16	0/816	0.30	0/1104
26	W	0.17	0/467	0.33	0/616
27	X	0.14	0/411	0.30	0/551
28	Y	0.17	0/368	0.38	0/485
29	0	0.16	0/395	0.28	0/523
30	1	0.15	0/3053	0.29	0/4108
31	2	0.19	0/1074	0.34	0/1449
32	3	0.13	0/783	0.26	0/1056

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	4	0.14	0/1077	0.26	0/1453
34	5	0.12	0/2790	0.25	0/3794
35	6	0.17	0/2274	0.30	0/3062
36	7	0.12	0/686	0.28	0/919
37	8	0.10	0/2714	0.28	0/3657
38	h	0.09	0/791	0.25	0/1065
39	i	0.10	0/989	0.26	0/1324
40	9	0.10	0/1678	0.27	0/2267
41	a	0.13	0/1364	0.29	0/1842
42	b	0.11	0/1348	0.25	0/1816
43	c	0.15	0/846	0.29	0/1134
44	d	0.12	0/1930	0.26	0/2597
45	j	0.11	0/1583	0.29	0/2130
46	bb	0.07	0/1751	0.17	0/2720
47	AA	0.11	0/2948	0.27	0/3995
48	BB	0.13	0/2314	0.29	0/3142
49	CC	0.15	0/3712	0.25	0/4978
50	DD	0.14	0/2409	0.29	0/3255
51	EE	0.13	0/2928	0.27	0/3947
52	FF	0.14	0/953	0.27	0/1285
53	GG	0.13	0/1765	0.30	0/2392
54	HH	0.15	0/1259	0.29	0/1707
55	II	0.13	0/2013	0.27	0/2720
56	JJ	0.18	0/1590	0.30	0/2140
57	KK	0.13	0/1015	0.28	0/1357
58	LL	0.13	0/973	0.30	0/1305
59	MM	0.14	0/950	0.32	0/1274
60	NN	0.18	0/929	0.29	0/1243
61	OO	0.13	0/2242	0.27	0/3016
62	PP	0.16	0/806	0.26	0/1096
63	QQ	0.12	0/1268	0.26	0/1701
64	RR	0.14	0/1105	0.31	0/1491
65	SS	0.14	0/667	0.28	0/902
66	TT	0.14	0/761	0.29	0/1015
67	UU	0.13	0/1890	0.28	0/2554
68	VV	0.11	0/2120	0.26	0/2851
69	WW	0.12	0/2897	0.27	0/3911
70	XX	0.14	0/3234	0.26	0/4374
71	YY	0.15	0/797	0.32	0/1070
72	ZZ	0.14	0/2645	0.25	0/3566
73	11	0.12	0/686	0.28	0/929
74	22	0.17	0/301	0.36	0/388
75	33	0.15	0/1589	0.30	0/2140

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	44	0.09	0/2121	0.23	0/2879
76	55	0.09	0/1912	0.25	0/2600
77	66	0.12	0/2348	0.28	0/3163
78	77	0.15	0/1431	0.22	0/1934
79	88	0.11	0/3760	0.25	0/5085
80	00	0.09	0/409	0.20	0/540
80	99	0.08	0/307	0.19	0/405
81	aa	0.11	0/34270	0.17	0/53383
82	ee	0.08	0/257	0.15	0/397
All	All	0.12	0/232334	0.23	0/334984

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60512	30351	30367	129	0
2	e	1886	1935	1935	10	0
3	B	2544	2592	2592	11	0
4	C	2336	2422	2420	10	0
5	D	2028	2040	2040	6	0
6	E	2449	2461	2461	14	0
7	F	1608	1645	1645	6	0
8	G	618	627	627	2	0
9	f	1876	1925	1925	7	0
10	g	1104	1154	1154	7	0
11	H	1426	1459	1459	11	0
12	I	913	985	985	7	0
13	J	1888	1939	1939	4	0
14	K	1350	1401	1401	10	0
15	L	1545	1590	1590	6	0
16	M	1536	1628	1628	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	N	1056	1120	1120	7	0
18	O	2209	2323	2323	12	0
19	P	1481	1494	1494	5	0
20	Q	2868	2961	2961	12	0
21	R	2189	2310	2310	9	0
22	S	1472	1507	1507	5	0
23	T	1497	1453	1453	6	0
24	U	1099	1164	1164	9	0
25	V	799	778	778	8	0
26	W	460	489	488	7	0
27	X	403	433	433	5	0
28	Y	365	412	412	3	0
29	0	388	409	409	2	0
30	1	2985	3029	3029	16	0
31	2	1046	1055	1055	6	0
32	3	763	773	773	2	0
33	4	1052	1087	1087	6	0
34	5	2719	2710	2710	15	0
35	6	2226	2248	2248	12	0
36	7	674	709	709	4	0
37	8	2660	2714	2714	8	0
38	h	779	798	798	4	0
39	i	976	1022	1022	5	0
40	9	1643	1698	1698	10	0
41	a	1331	1340	1340	5	0
42	b	1314	1379	1379	5	0
43	c	827	873	873	2	0
44	d	1888	1909	1909	9	0
45	j	1553	1586	1586	15	0
46	bb	1570	796	798	8	0
47	AA	2883	2907	2907	14	0
48	BB	2269	2301	2301	14	0
49	CC	3641	3897	3897	13	0
50	DD	2343	2373	2373	17	0
51	EE	2880	2918	2918	12	0
52	FF	936	966	966	6	0
53	GG	1724	1799	1799	13	0
54	HH	1235	1286	1286	2	0
55	II	1969	2026	2026	11	0
56	JJ	1551	1554	1554	11	0
57	KK	995	1025	1025	6	0
58	LL	959	1032	1032	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	MM	937	986	986	4	0
60	NN	914	961	961	5	0
61	OO	2198	2230	2230	9	0
62	PP	786	826	826	4	0
63	QQ	1247	1314	1314	5	0
64	RR	1080	1090	1089	7	0
65	SS	648	677	677	9	0
66	TT	746	772	772	4	0
67	UU	1844	1842	1842	7	0
68	VV	2080	2112	2112	12	0
69	WW	2843	2901	2900	8	0
70	XX	3175	3271	3271	14	0
71	YY	786	823	823	5	0
72	ZZ	2586	2528	2528	10	0
73	11	672	686	686	4	0
74	22	301	359	359	0	0
75	33	1554	1607	1607	13	0
76	44	2062	1983	1982	9	0
76	55	1858	1793	1793	9	0
77	66	2298	2330	2330	13	0
78	77	1400	1396	1396	3	0
79	88	3677	3650	3650	17	0
80	00	406	417	417	1	0
80	99	306	333	333	0	0
81	aa	30608	15373	15377	86	0
82	ee	231	116	116	1	0
83	00	1	0	0	0	0
83	3	1	0	0	0	0
83	A	135	0	0	0	0
83	B	1	0	0	0	0
83	BB	1	0	0	0	0
83	S	1	0	0	0	0
83	XX	1	0	0	0	0
83	YY	1	0	0	0	0
83	aa	99	0	0	0	0
83	ee	1	0	0	0	0
84	A	14	26	26	0	0
85	2	1	0	0	0	0
85	77	1	0	0	0	0
85	88	1	0	0	0	0
85	A	38	0	0	0	0
85	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	KK	1	0	0	0	0
85	aa	12	0	0	0	0
86	0	1	0	0	0	0
86	W	1	0	0	0	0
87	2	44	26	26	1	0
88	XX	31	12	12	0	0
All	All	218927	175257	175273	661	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 2.

All (661) 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)
1:A:2276:U:OP1	4:C:63:VAL:N	2.09	0.85
1:A:3094:A:OP1	11:H:94:ARG:NH1	2.11	0.84
1:A:3334:C:OP1	4:C:217:ARG:NH1	2.10	0.84
25:V:119:ARG:NH2	81:aa:1596:G:OP2	2.10	0.84
72:ZZ:212:ARG:NH1	72:ZZ:257:GLU:OE1	2.12	0.83
60:NN:22:ASP:OD2	60:NN:26:ARG:NH1	2.13	0.81
49:CC:295:ASN:ND2	51:EE:292:ASP:O	2.14	0.80
79:88:213:ARG:NH1	79:88:439:MET:O	2.15	0.79
50:DD:80:ASN:O	50:DD:126:ARG:NH1	2.15	0.79
37:8:271:ASN:OD1	37:8:274:ARG:NH2	2.15	0.78
1:A:2757:G:OP2	31:2:285:ARG:NH1	2.17	0.78
9:f:96:GLN:OE1	38:h:24:ARG:NH2	2.16	0.78
47:AA:168:LEU:O	68:VV:303:ARG:NH1	2.16	0.78
18:O:51:GLN:O	18:O:56:ARG:NH1	2.17	0.77
1:A:2034:A:N6	1:A:2046:U:O2	2.18	0.77
31:2:279:ARG:NH2	35:6:171:GLU:OE2	2.18	0.77
57:KK:343:GLY:O	57:KK:350:ARG:NH2	2.18	0.77
60:NN:75:ARG:NH1	60:NN:80:GLY:O	2.17	0.77
79:88:447:GLY:O	79:88:476:ARG:NH1	2.19	0.76
1:A:831:U:OP1	1:A:854:A:O2'	2.03	0.76
12:I:106:ARG:NH1	81:aa:495:A:N7	2.33	0.76
47:AA:331:ARG:NH2	67:UU:194:ASN:OD1	2.19	0.76
1:A:614:G:OP1	1:A:1528:U:O2'	2.04	0.75
1:A:975:A:OP1	28:Y:95:GLY:N	2.19	0.75
1:A:2940:G:N2	1:A:2942:U:O4	2.20	0.75
1:A:2008:U:OP2	1:A:2013:A:N6	2.20	0.74
13:J:231:GLU:O	13:J:235:GLN:NE2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:157:ASN:OD1	23:T:160:ARG:NH1	2.21	0.74
17:N:137:ASP:OD2	24:U:86:ARG:NH2	2.20	0.74
56:JJ:123:ASN:OD1	56:JJ:124:LEU:N	2.21	0.74
75:33:158:VAL:O	75:33:163:ARG:NH2	2.21	0.73
48:BB:274:ASP:OD2	48:BB:362:ARG:NH1	2.21	0.73
45:j:187:ALA:O	45:j:191:SER:OG	2.05	0.73
49:CC:333:LEU:O	51:EE:82:LYS:NZ	2.20	0.73
34:5:204:TYR:OH	40:9:196:MET:O	2.06	0.73
1:A:600:C:OP2	17:N:187:ARG:NH2	2.21	0.73
1:A:2797:C:OP1	27:X:39:LYS:NZ	2.21	0.73
27:X:54:LYS:O	42:b:162:LYS:NZ	2.21	0.72
70:XX:271:LEU:O	70:XX:275:ASN:ND2	2.22	0.72
40:9:66:TRP:O	40:9:135:ARG:NH2	2.22	0.72
48:BB:274:ASP:OD1	55:II:76:ARG:NH1	2.22	0.72
76:55:127:ASP:OD2	76:55:291:LYS:NZ	2.22	0.72
58:LL:117:GLY:O	58:LL:145:ARG:NH2	2.23	0.72
1:A:1330:A:OP2	39:i:198:ARG:NH2	2.22	0.71
7:F:169:ARG:NE	7:F:192:GLU:OE2	2.22	0.71
57:KK:362:LEU:O	81:aa:871:U:O2'	2.07	0.71
47:AA:371:ASP:OD1	47:AA:372:LYS:N	2.24	0.71
52:FF:112:ARG:NH1	68:VV:278:GLU:OE1	2.23	0.71
1:A:966:A:OP1	3:B:314:ARG:NH1	2.24	0.71
48:BB:159:SER:OG	48:BB:162:ASP:OD1	2.08	0.71
62:PP:65:ARG:NH1	77:66:313:GLU:OE2	2.24	0.70
24:U:40:GLU:OE2	24:U:42:GLN:NE2	2.23	0.70
34:5:106:THR:O	34:5:120:ASN:ND2	2.24	0.70
44:d:75:ASN:ND2	44:d:79:PRO:O	2.23	0.70
61:OO:228:GLU:N	61:OO:228:GLU:OE1	2.22	0.70
62:PP:82:ARG:NH1	81:aa:706:U:O5'	2.24	0.70
61:OO:235:ARG:O	68:VV:207:ARG:NH1	2.24	0.70
77:66:336:ARG:NH1	81:aa:549:C:O2	2.25	0.70
35:6:266:GLU:OE1	35:6:274:ARG:NH2	2.25	0.70
51:EE:432:ARG:NH1	81:aa:1057:A:OP1	2.24	0.70
75:33:206:LYS:NZ	81:aa:106:A:OP1	2.25	0.69
31:2:325:ARG:NH1	35:6:264:THR:O	2.24	0.69
25:V:104:ASN:O	25:V:104:ASN:ND2	2.20	0.69
52:FF:76:GLU:OE1	52:FF:79:ARG:NH1	2.25	0.69
70:XX:391:ARG:NH1	70:XX:400:ASP:OD1	2.25	0.69
20:Q:164:GLN:NE2	20:Q:169:LYS:O	2.25	0.69
16:M:151:ALA:O	16:M:170:ASN:ND2	2.26	0.69
5:D:81:GLU:OE2	5:D:285:ARG:NE	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:LL:160:ARG:NH2	81:aa:727:U:OP1	2.26	0.69
1:A:3363:A:O2'	1:A:3365:A:OP2	2.11	0.68
51:EE:288:ASP:OD2	51:EE:308:ARG:NH2	2.26	0.68
63:QQ:94:ALA:O	63:QQ:101:ARG:NH2	2.26	0.68
46:bb:33:U:OP2	55:II:315:ARG:NH2	2.27	0.67
25:V:62:GLN:NE2	25:V:78:MET:SD	2.67	0.67
1:A:2328:G:O2'	8:G:87:ARG:NH2	2.27	0.67
1:A:2558:A:O2'	21:R:370:ARG:NH1	2.27	0.67
1:A:2606:U:OP1	70:XX:262:GLN:NE2	2.27	0.67
7:F:208:ARG:NH2	38:h:97:ASP:O	2.28	0.67
57:KK:324:GLU:OE1	57:KK:355:ARG:NH1	2.28	0.66
1:A:473:G:N7	22:S:147:ARG:NH2	2.44	0.66
1:A:1352:U:OP1	9:f:74:ARG:NH1	2.28	0.66
50:DD:407:ARG:NH1	77:66:198:HIS:O	2.29	0.66
64:RR:138:ARG:NH1	64:RR:144:GLU:OE1	2.29	0.66
1:A:3374:U:O2'	4:C:162:ARG:NH2	2.28	0.66
18:O:258:ALA:O	18:O:262:THR:OG1	2.14	0.66
49:CC:343:ASN:ND2	56:JJ:87:SER:O	2.28	0.66
81:aa:1136:G:N1	81:aa:1622:A:OP2	2.29	0.66
18:O:206:ARG:NH1	26:W:80:MET:SD	2.69	0.65
20:Q:248:ASP:OD1	23:T:123:GLY:N	2.29	0.65
1:A:3033:G:N2	1:A:3033:G:OP2	2.30	0.65
21:R:309:GLY:O	27:X:46:ARG:NH2	2.29	0.65
1:A:1152:U:O2'	14:K:134:ARG:NH2	2.30	0.65
76:44:68:ASN:O	76:44:72:THR:OG1	2.14	0.64
1:A:2689:G:O6	30:1:367:GLU:N	2.31	0.64
1:A:2488:U:OP1	27:X:8:ARG:NH2	2.30	0.64
1:A:3452:A:OP2	34:5:218:ARG:NH1	2.30	0.64
76:44:238:LYS:NZ	76:44:240:GLU:O	2.30	0.64
81:aa:513:G:N2	81:aa:516:U:OP2	2.31	0.64
18:O:364:TRP:O	33:4:125:ARG:NH1	2.30	0.64
65:SS:40:ARG:NH2	81:aa:1604:U:O2	2.30	0.64
79:88:42:ILE:O	79:88:101:ARG:NH2	2.31	0.64
1:A:2154:A:N6	81:aa:1806:U:O2'	2.29	0.64
49:CC:442:ARG:NH2	49:CC:448:ARG:O	2.29	0.64
76:44:208:ASP:OD1	76:44:209:ALA:N	2.31	0.64
81:aa:298:C:N4	81:aa:301:A:OP2	2.31	0.64
6:E:124:ARG:NE	6:E:267:ASP:OD2	2.24	0.64
14:K:103:ASP:OD2	14:K:106:ARG:NH1	2.30	0.64
50:DD:126:ARG:NH2	51:EE:472:TYR:O	2.30	0.64
81:aa:1429:U:O4	81:aa:1430:A:N6	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:OO:161:GLU:N	61:OO:161:GLU:OE1	2.31	0.63
79:88:339:GLU:O	79:88:343:ARG:NH2	2.31	0.63
1:A:2687:G:OP2	30:1:292:ARG:NH1	2.31	0.63
1:A:2481:G:O2'	1:A:2483:G:OP2	2.16	0.63
42:b:157:TRP:NE1	42:b:159:LYS:O	2.32	0.63
55:II:299:LYS:NZ	55:II:303:HIS:O	2.31	0.63
72:ZZ:96:ASP:OD1	72:ZZ:97:ASP:N	2.31	0.63
1:A:599:A:OP2	17:N:187:ARG:NH1	2.31	0.63
18:O:332:ARG:NH1	18:O:336:GLU:OE1	2.32	0.63
42:b:121:GLY:O	42:b:126:ARG:NH2	2.31	0.62
6:E:56:LEU:O	30:1:120:GLN:NE2	2.31	0.62
60:NN:57:GLN:NE2	65:SS:16:PRO:O	2.31	0.62
1:A:1291:A:OP1	9:f:69:ARG:NE	2.32	0.62
6:E:97:GLY:O	6:E:103:GLN:NE2	2.31	0.62
20:Q:104:ARG:NH1	20:Q:143:ASN:O	2.32	0.62
44:d:94:GLN:OE1	44:d:96:GLN:NE2	2.32	0.62
81:aa:1437:U:O2'	81:aa:1438:U:OP2	2.15	0.62
48:BB:135:GLN:NE2	76:44:95:ASP:OD2	2.32	0.62
4:C:212:GLN:NE2	4:C:313:ASP:OD1	2.33	0.62
64:RR:200:ARG:NH2	81:aa:1032:A:OP1	2.33	0.62
19:P:159:THR:OG1	19:P:161:ASP:OD1	2.17	0.61
1:A:1272:A:O2'	1:A:1381:A:N6	2.33	0.61
23:T:80:GLU:O	44:d:161:ARG:NH2	2.33	0.61
10:g:28:SER:O	10:g:32:GLY:N	2.32	0.61
47:AA:306:TYR:OH	67:UU:94:GLU:OE2	2.17	0.61
61:OO:188:GLU:N	61:OO:188:GLU:OE1	2.32	0.61
1:A:29:A:O3'	4:C:78:ARG:NH1	2.33	0.61
1:A:3389:G:O2'	1:A:3409:A:N6	2.33	0.61
6:E:58:ALA:O	30:1:116:ARG:NH2	2.33	0.61
1:A:541:G:N7	28:Y:135:ARG:NH1	2.47	0.61
50:DD:65:ARG:O	77:66:338:ARG:NH1	2.33	0.61
1:A:3366:U:O4	4:C:272:ARG:NH2	2.32	0.61
1:A:615:G:O2'	1:A:2254:G:OP1	2.18	0.61
75:33:211:GLU:N	81:aa:106:A:OP2	2.33	0.61
11:H:153:GLU:OE2	34:5:363:GLN:NE2	2.33	0.61
58:LL:61:ARG:NH1	81:aa:1077:C:OP2	2.34	0.61
45:j:138:ASP:OD1	45:j:139:LYS:N	2.34	0.60
41:a:88:LEU:O	41:a:95:ARG:NH2	2.34	0.60
51:EE:147:ARG:NH2	78:77:241:GLU:O	2.34	0.60
2:e:65:PHE:O	2:e:106:ARG:NH1	2.34	0.60
40:9:165:GLU:OE2	40:9:165:GLU:N	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:8:295:ARG:NH1	37:8:299:GLU:O	2.35	0.60
34:5:313:LYS:NZ	34:5:417:ASP:OD1	2.34	0.60
1:A:96:G:OP2	19:P:93:ARG:NH1	2.31	0.60
67:UU:225:ASN:OD1	67:UU:225:ASN:N	2.34	0.60
1:A:1325:A:N6	10:g:146:ILE:O	2.34	0.60
1:A:445:A:OP2	20:Q:324:ARG:NH2	2.34	0.59
67:UU:150:ASP:OD1	67:UU:153:ARG:NH2	2.36	0.59
9:f:162:ALA:N	9:f:170:VAL:O	2.36	0.59
45:j:42:GLU:N	45:j:42:GLU:OE2	2.36	0.59
15:L:136:ARG:NH2	15:L:137:ASP:OD1	2.35	0.59
79:88:393:ASP:OD2	79:88:397:ASN:ND2	2.36	0.59
18:O:241:LYS:NZ	20:Q:72:ASP:OD1	2.36	0.58
48:BB:209:ARG:NH2	79:88:280:GLU:OE2	2.37	0.58
81:aa:1862:C:N4	81:aa:1863:G:O6	2.36	0.58
40:9:207:ASP:OD1	40:9:208:PHE:N	2.36	0.58
46:bb:43:A:O2'	46:bb:44:U:OP1	2.18	0.58
15:L:139:GLU:OE1	15:L:174:ARG:NE	2.36	0.58
75:33:93:VAL:O	75:33:99:ARG:NH1	2.36	0.58
64:RR:231:ARG:H	64:RR:231:ARG:HD2	1.68	0.58
75:33:165:LYS:NZ	81:aa:324:U:OP2	2.35	0.58
81:aa:478:G:N1	81:aa:481:A:OP2	2.35	0.58
45:j:29:GLU:OE1	45:j:29:GLU:N	2.36	0.58
81:aa:1369:G:N2	81:aa:1372:A:OP2	2.36	0.58
79:88:494:ALA:O	79:88:506:LYS:NZ	2.37	0.58
12:I:73:ARG:NH2	12:I:90:ASP:OD1	2.37	0.58
56:JJ:122:ARG:NH2	81:aa:1432:A:OP1	2.37	0.58
30:1:219:PHE:O	30:1:340:ARG:NH1	2.37	0.57
1:A:977:U:O2	1:A:2307:G:O2'	2.17	0.57
46:bb:6:A:O2'	46:bb:7:G:OP1	2.16	0.57
76:55:259:GLU:N	76:55:259:GLU:OE1	2.37	0.57
19:P:54:ASN:OD1	19:P:56:LEU:N	2.37	0.57
43:c:75:LYS:O	43:c:79:THR:OG1	2.21	0.57
75:33:107:GLN:NE2	75:33:111:GLU:OE2	2.36	0.57
62:PP:70:ILE:O	68:VV:131:ARG:NH1	2.37	0.57
1:A:1719:A:OP1	3:B:307:ARG:NH1	2.37	0.57
1:A:1835:U:OP2	32:3:20:LYS:NZ	2.38	0.57
1:A:3111:G:N2	1:A:3114:A:OP2	2.38	0.57
72:ZZ:50:GLU:O	72:ZZ:51:ASP:OD1	2.23	0.56
42:b:40:HIS:O	42:b:40:HIS:ND1	2.37	0.56
50:DD:134:GLN:NE2	50:DD:442:ASN:OD1	2.38	0.56
68:VV:121:GLU:OE2	68:VV:125:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2925:A:OP2	1:A:2926:C:N4	2.36	0.56
52:FF:112:ARG:NH2	68:VV:272:ASN:O	2.38	0.56
75:33:218:ARG:NH2	81:aa:249:G:OP1	2.37	0.56
30:1:409:GLU:OE1	30:1:409:GLU:N	2.36	0.56
72:ZZ:212:ARG:O	72:ZZ:262:ASN:ND2	2.37	0.56
59:MM:40:HIS:NE2	70:XX:217:GLU:OE1	2.36	0.56
46:bb:25:C:O2'	46:bb:26:A:OP1	2.23	0.56
53:GG:213:ARG:NH1	53:GG:215:TYR:OH	2.39	0.56
81:aa:678:A:O2'	81:aa:679:U:O5'	2.24	0.56
1:A:1455:G:OP1	24:U:30:ARG:NH1	2.39	0.56
35:6:100:LEU:O	35:6:368:ARG:NH1	2.39	0.56
76:55:152:ASP:N	76:55:152:ASP:OD1	2.39	0.56
4:C:206:ASP:OD2	4:C:335:ARG:NH2	2.38	0.55
21:R:336:THR:O	21:R:340:GLY:N	2.34	0.55
29:0:103:GLN:OE1	29:0:124:ARG:NH1	2.38	0.55
61:OO:152:ALA:O	61:OO:155:ARG:NH1	2.39	0.55
31:2:350:TYR:OH	35:6:323:ARG:NH2	2.39	0.55
63:QQ:18:GLU:O	81:aa:820:U:O2'	2.24	0.55
66:TT:149:GLN:N	66:TT:152:LEU:O	2.38	0.55
34:5:349:PHE:O	40:9:72:ARG:NH2	2.37	0.55
9:f:252:ASP:OD1	9:f:253:LEU:N	2.40	0.55
17:N:143:ARG:NE	24:U:75:ASP:OD2	2.35	0.55
20:Q:208:ARG:N	20:Q:222:ARG:O	2.39	0.55
5:D:71:SER:O	5:D:75:LEU:N	2.36	0.55
18:O:156:GLU:OE2	19:P:190:SER:N	2.40	0.55
76:44:128:HIS:NE2	76:44:252:ILE:O	2.40	0.55
47:AA:317:PRO:O	76:55:105:ARG:NH1	2.37	0.54
13:J:259:ARG:NH2	13:J:277:PRO:O	2.41	0.54
37:8:195:GLU:OE1	37:8:339:ARG:NE	2.40	0.54
69:WW:214:LYS:NZ	69:WW:218:GLU:OE2	2.40	0.54
49:CC:135:ARG:NH2	72:ZZ:144:GLU:OE1	2.41	0.54
53:GG:291:THR:O	53:GG:294:ARG:NH2	2.40	0.54
73:11:70:ASN:ND2	81:aa:1851:G:O6	2.39	0.54
76:55:105:ARG:O	76:55:106:ASP:OD1	2.26	0.54
48:BB:173:ASN:OD1	48:BB:174:THR:N	2.41	0.54
50:DD:422:ARG:NH2	50:DD:432:GLU:OE2	2.41	0.54
40:9:96:ASP:OD1	40:9:96:ASP:N	2.40	0.54
45:j:123:ASP:OD1	45:j:124:MET:N	2.40	0.54
1:A:2689:G:OP2	30:1:366:ARG:NH2	2.40	0.54
56:JJ:120:SER:OG	56:JJ:123:ASN:ND2	2.41	0.54
58:LL:159:SER:OG	81:aa:729:U:OP2	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SS:63:ASP:OD1	65:SS:64:LEU:N	2.41	0.54
69:WW:240:GLN:OE1	69:WW:248:TYR:OH	2.25	0.54
7:F:104:ASP:OD1	7:F:105:PHE:N	2.41	0.54
49:CC:334:ASN:O	49:CC:334:ASN:ND2	2.40	0.54
70:XX:378:ARG:NE	70:XX:407:LYS:O	2.41	0.54
11:H:8:THR:N	18:O:352:ASP:OD1	2.40	0.53
45:j:181:ARG:NH2	45:j:185:MET:SD	2.80	0.53
1:A:2537:A:N7	21:R:324:LYS:NZ	2.55	0.53
6:E:268:ARG:NH1	25:V:62:GLN:OE1	2.32	0.53
58:LL:114:PRO:O	58:LL:145:ARG:NE	2.41	0.53
76:55:50:ARG:NH1	76:55:127:ASP:O	2.40	0.53
81:aa:678:A:O2'	81:aa:679:U:O4'	2.16	0.53
1:A:2096:U:OP1	1:A:2862:G:O2'	2.25	0.53
2:e:292:ASP:OD1	2:e:293:LYS:N	2.42	0.53
14:K:122:GLN:OE1	14:K:125:ARG:NH1	2.40	0.53
58:LL:96:ARG:NH1	81:aa:747:G:N7	2.55	0.53
48:BB:115:GLN:OE1	48:BB:115:GLN:N	2.42	0.53
15:L:136:ARG:NH1	26:W:95:PRO:O	2.42	0.53
25:V:79:PRO:O	35:6:155:LYS:NZ	2.41	0.53
13:J:109:LYS:O	30:1:447:ARG:NH1	2.42	0.53
81:aa:789:A:O2'	81:aa:792:A:O2'	2.25	0.53
1:A:2883:A:O2'	1:A:2884:A:OP1	2.25	0.52
30:1:251:ASP:OD1	30:1:252:SER:N	2.41	0.52
1:A:536:G:N2	1:A:539:A:OP2	2.35	0.52
3:B:193:ASP:C	3:B:193:ASP:OD1	2.52	0.52
24:U:98:ASP:OD2	24:U:101:LYS:NZ	2.41	0.52
2:e:284:ASN:OD1	2:e:285:ALA:N	2.42	0.52
12:I:114:GLU:N	12:I:114:GLU:OE2	2.42	0.52
50:DD:61:HIS:NE2	50:DD:145:ASP:OD2	2.40	0.52
53:GG:303:GLN:OE1	82:ee:36:A:O2'	2.28	0.52
14:K:101:MET:O	14:K:167:ASN:N	2.40	0.52
30:1:247:GLY:O	30:1:389:ARG:NH1	2.42	0.52
70:XX:319:SER:OG	70:XX:320:ASP:N	2.43	0.52
3:B:280:ARG:N	3:B:365:TRP:O	2.41	0.52
4:C:124:THR:O	16:M:145:ARG:NH1	2.42	0.52
35:6:87:ARG:N	35:6:314:GLY:O	2.32	0.52
61:OO:159:ASP:OD1	61:OO:159:ASP:N	2.43	0.52
3:B:193:ASP:OD1	3:B:194:SER:N	2.42	0.52
68:VV:213:LYS:NZ	81:aa:944:A:O2'	2.43	0.52
81:aa:1168:A:OP2	81:aa:1642:U:O2'	2.27	0.52
19:P:185:ASN:ND2	20:Q:67:PRO:O	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:d:108:GLN:OE1	44:d:112:ARG:NH2	2.43	0.52
50:DD:186:GLY:O	77:66:158:ARG:NH1	2.40	0.52
53:GG:130:LEU:O	55:II:235:TRP:NE1	2.39	0.52
65:SS:9:LYS:N	81:aa:1603:A:OP1	2.42	0.52
1:A:2846:C:N3	46:bb:76:A:O2'	2.40	0.51
18:O:296:PHE:O	18:O:317:THR:OG1	2.25	0.51
34:5:346:ARG:O	40:9:65:ARG:NH2	2.42	0.51
47:AA:371:ASP:OD1	47:AA:372:LYS:HG2	2.09	0.51
24:U:12:ALA:O	24:U:20:HIS:NE2	2.44	0.51
44:d:143:ASP:OD1	44:d:143:ASP:N	2.42	0.51
53:GG:274:GLU:OE1	53:GG:276:ARG:NE	2.42	0.51
1:A:633:G:OP1	36:7:103:ARG:NH2	2.44	0.51
21:R:136:HIS:ND1	21:R:138:ASP:OD1	2.43	0.51
35:6:96:ARG:NH2	35:6:236:LYS:O	2.43	0.51
50:DD:430:GLU:OE1	77:66:117:GLN:NE2	2.43	0.51
40:9:80:LEU:O	41:a:151:ARG:NH2	2.43	0.51
48:BB:161:GLU:OE1	48:BB:161:GLU:N	2.43	0.51
65:SS:40:ARG:NH1	65:SS:79:SER:O	2.44	0.51
1:A:59:A:OP1	26:W:76:ARG:NE	2.39	0.51
51:EE:379:TYR:N	51:EE:383:THR:O	2.42	0.51
1:A:2616:C:OP1	21:R:352:ARG:NH1	2.44	0.51
1:A:2883:A:O2'	1:A:2884:A:P	2.68	0.51
52:FF:4:GLU:OE2	64:RR:171:ARG:NE	2.42	0.51
5:D:95:ASP:OD1	5:D:95:ASP:N	2.36	0.51
5:D:300:VAL:O	5:D:300:VAL:HG13	2.11	0.51
73:11:13:GLN:O	81:aa:1846:U:N3	2.39	0.51
40:9:169:ASP:OD1	40:9:171:TYR:N	2.45	0.50
6:E:60:ILE:HG23	6:E:61:PRO:HD2	1.93	0.50
18:O:359:ARG:NH1	41:a:51:LEU:O	2.43	0.50
81:aa:1758:G:OP2	81:aa:1758:G:N2	2.40	0.50
46:bb:25:C:HO2'	46:bb:26:A:P	2.34	0.50
59:MM:70:ARG:NH1	59:MM:118:HIS:O	2.44	0.50
69:WW:206:ASP:O	69:WW:268:ARG:NH1	2.44	0.50
20:Q:213:ASP:N	20:Q:218:THR:O	2.44	0.50
1:A:601:C:OP1	17:N:185:LYS:NZ	2.44	0.50
28:Y:137:ARG:NH1	28:Y:140:ALA:O	2.44	0.50
81:aa:1545:G:N2	81:aa:1548:A:OP2	2.37	0.50
1:A:527:A:N3	1:A:530:A:O2'	2.44	0.50
50:DD:407:ARG:NH2	77:66:118:PRO:O	2.45	0.50
63:QQ:157:LYS:O	63:QQ:160:SER:OG	2.29	0.50
77:66:335:ASP:OD2	81:aa:88:A:O2'	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:A:O2'	1:A:499:G:OP1	2.29	0.50
37:8:242:ASN:N	37:8:242:ASN:OD1	2.45	0.50
81:aa:1501:G:OP2	81:aa:1606:C:N4	2.38	0.50
38:h:8:ASP:OD1	38:h:8:ASP:N	2.44	0.50
68:VV:73:PRO:O	77:66:322:ARG:NH1	2.45	0.50
14:K:91:THR:O	14:K:134:ARG:NH1	2.45	0.50
23:T:171:GLU:OE1	23:T:171:GLU:N	2.45	0.50
81:aa:1082:G:O2'	81:aa:1083:U:OP2	2.30	0.50
64:RR:217:SER:OG	81:aa:871:U:OP1	2.30	0.49
76:44:68:ASN:OD1	76:44:72:THR:OG1	2.26	0.49
2:e:136:GLU:OE2	2:e:154:GLU:N	2.43	0.49
17:N:157:ALA:HB3	17:N:158:PRO:CD	2.42	0.49
6:E:114:ASP:OD1	6:E:114:ASP:N	2.38	0.49
1:A:57:A:O2'	26:W:81:ALA:O	2.27	0.49
1:A:1396:A:OP2	43:c:32:ARG:NH2	2.45	0.49
37:8:220:ASP:OD2	37:8:224:ARG:NE	2.41	0.49
44:d:46:ALA:O	44:d:58:ALA:N	2.41	0.49
1:A:1689:G:OP2	1:A:1689:G:N2	2.35	0.49
1:A:2369:A:OP2	45:j:43:GLU:N	2.40	0.49
59:MM:2:VAL:N	59:MM:9:PHE:O	2.46	0.49
75:33:104:ARG:NH1	75:33:201:ASP:OD2	2.46	0.49
77:66:67:GLN:NE2	81:aa:561:A:O4'	2.45	0.49
81:aa:693:G:N1	81:aa:722:A:OP2	2.35	0.49
1:A:2040:U:O2'	1:A:2041:A:OP2	2.23	0.49
16:M:178:GLU:OE2	16:M:210:ARG:NE	2.46	0.49
25:V:56:ARG:NH2	35:6:119:ASN:OD1	2.42	0.49
48:BB:112:LYS:O	48:BB:115:GLN:NE2	2.45	0.49
70:XX:423:ARG:NH1	72:ZZ:327:ASP:OD1	2.43	0.49
70:XX:440:ASP:OD1	70:XX:440:ASP:N	2.46	0.49
54:HH:103:ARG:NH1	81:aa:790:A:O2'	2.45	0.49
20:Q:72:ASP:OD1	20:Q:73:GLU:N	2.40	0.49
33:4:132:HIS:NE2	34:5:382:GLU:OE2	2.43	0.49
56:JJ:150:ARG:NH2	81:aa:1431:A:OP2	2.46	0.49
79:88:184:ARG:NE	79:88:239:ILE:O	2.35	0.49
11:H:118:GLU:OE2	11:H:122:LYS:NZ	2.44	0.49
14:K:132:TYR:OH	14:K:174:ARG:NH1	2.46	0.49
1:A:1865:G:N1	1:A:1868:A:OP2	2.41	0.48
1:A:2883:A:HO2'	1:A:2884:A:P	2.36	0.48
73:11:17:ARG:NH1	81:aa:1846:U:OP2	2.46	0.48
73:11:29:ALA:O	73:11:32:SER:OG	2.31	0.48
75:33:184:PRO:O	81:aa:119:U:O2'	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3107:G:O2'	1:A:3108:U:OP2	2.31	0.48
26:W:93:ARG:NH2	26:W:98:GLY:O	2.45	0.48
79:88:55:GLU:OE2	79:88:55:GLU:HA	2.13	0.48
1:A:2634:A:OP1	6:E:235:ARG:NH1	2.44	0.48
6:E:57:ASP:OD2	30:1:123:ARG:NH2	2.47	0.48
55:II:187:GLN:NE2	81:aa:1424:U:O4	2.46	0.48
1:A:3455:U:O2'	40:9:219:ARG:NH1	2.47	0.48
12:I:116:ARG:NH1	12:I:130:GLN:OE1	2.46	0.48
22:S:93:THR:OG1	22:S:140:ARG:NH1	2.44	0.48
37:8:259:LYS:HD3	37:8:259:LYS:C	2.39	0.48
79:88:405:ALA:N	79:88:409:GLU:OE2	2.47	0.48
15:L:59:ASP:OD1	15:L:86:ARG:NH1	2.44	0.48
25:V:104:ASN:HD22	25:V:104:ASN:C	2.16	0.48
53:GG:90:THR:N	53:GG:93:ASN:OD1	2.40	0.48
1:A:1971:A:OP2	23:T:45:ARG:NH2	2.47	0.48
1:A:2286:U:O2'	1:A:3066:A:N6	2.45	0.48
49:CC:103:LYS:N	81:aa:677:U:OP1	2.43	0.48
1:A:2828:G:N2	1:A:2831:A:OP2	2.44	0.48
56:JJ:243:HIS:ND1	56:JJ:244:VAL:O	2.46	0.48
68:VV:61:VAL:HG23	68:VV:61:VAL:O	2.13	0.48
77:66:248:GLU:N	77:66:248:GLU:OE1	2.47	0.48
49:CC:478:ARG:NH1	60:NN:101:LEU:O	2.46	0.48
16:M:46:ASN:O	16:M:64:VAL:N	2.47	0.48
35:6:334:ASN:C	35:6:334:ASN:HD22	2.22	0.48
77:66:300:THR:OG1	77:66:303:PHE:O	2.30	0.48
1:A:1976:G:O2'	81:aa:1723:C:N4	2.45	0.47
1:A:2058:G:O2'	1:A:2206:U:OP2	2.32	0.47
1:A:2295:A:H2'	1:A:2295:A:N3	2.29	0.47
65:SS:40:ARG:NH1	65:SS:79:SER:OG	2.46	0.47
81:aa:1356:U:H4'	81:aa:1357:U:H5'	1.96	0.47
1:A:2453:G:O4'	1:A:2899:U:O2'	2.32	0.47
1:A:2512:A:OP2	30:1:182:ARG:NH2	2.47	0.47
2:e:157:LEU:O	2:e:160:ALA:N	2.48	0.47
20:Q:147:GLU:OE1	20:Q:177:ARG:NH1	2.47	0.47
45:j:42:GLU:O	45:j:76:GLN:NE2	2.48	0.47
1:A:2174:U:O4'	1:A:3043:C:O2'	2.32	0.47
1:A:3372:G:OP1	4:C:162:ARG:NH1	2.42	0.47
11:H:29:SER:O	11:H:32:LYS:NZ	2.47	0.47
47:AA:299:HIS:CD2	47:AA:300:PRO:HD2	2.49	0.47
70:XX:259:ASP:OD1	70:XX:259:ASP:N	2.43	0.47
1:A:537:U:O2'	32:3:13:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:U:O2'	1:A:1895:U:OP1	2.31	0.47
5:D:246:ASP:OD1	5:D:246:ASP:N	2.48	0.47
64:RR:231:ARG:HD2	64:RR:231:ARG:N	2.29	0.47
69:WW:129:ASN:OD1	69:WW:130:GLY:N	2.47	0.47
1:A:1311:U:OP2	10:g:102:LYS:NZ	2.40	0.47
3:B:373:ASN:ND2	3:B:376:VAL:O	2.42	0.47
68:VV:238:ASP:OD1	68:VV:239:GLU:N	2.47	0.47
34:5:229:ASP:OD1	34:5:233:ASP:N	2.48	0.47
36:7:89:ARG:NE	36:7:165:PHE:O	2.47	0.47
37:8:243:GLU:OE1	37:8:243:GLU:N	2.42	0.47
51:EE:135:ASP:OD1	51:EE:136:ASP:N	2.47	0.47
55:II:160:GLN:NE2	55:II:164:ASP:OD1	2.48	0.47
70:XX:150:LEU:O	70:XX:190:GLN:NE2	2.43	0.47
51:EE:240:ASP:OD1	51:EE:240:ASP:N	2.45	0.47
1:A:2408:U:O2'	1:A:2410:A:O2'	2.33	0.47
48:BB:153:ASN:OD1	48:BB:353:ARG:NH1	2.48	0.47
57:KK:374:ARG:NH1	81:aa:1834:G:OP1	2.48	0.47
70:XX:60:ARG:NH2	81:aa:1137:A:OP1	2.46	0.47
1:A:2085:A:OP2	1:A:2124:G:N1	2.37	0.46
10:g:118:LYS:NZ	39:i:102:LEU:O	2.40	0.46
34:5:432:ASP:OD1	34:5:433:MET:N	2.48	0.46
53:GG:142:HIS:NE2	53:GG:238:SER:OG	2.47	0.46
6:E:236:SER:OG	6:E:246:GLN:O	2.30	0.46
72:ZZ:241:ARG:NH1	81:aa:1554:A:O5'	2.48	0.46
79:88:403:LYS:HB3	79:88:404:PRO:HD3	1.96	0.46
23:T:149:GLU:OE1	23:T:152:ARG:NH2	2.48	0.46
50:DD:161:ARG:NH2	81:aa:555:G:OP2	2.38	0.46
1:A:1201:G:O6	14:K:76:LYS:NZ	2.47	0.46
1:A:3047:G:N2	1:A:3050:A:OP2	2.35	0.46
11:H:63:ASP:OD2	11:H:65:SER:OG	2.28	0.46
37:8:420:ARG:O	37:8:421:GLU:HB2	2.16	0.46
50:DD:199:ALA:O	50:DD:396:ARG:NH1	2.39	0.46
1:A:1042:G:O2'	1:A:1043:U:OP2	2.28	0.46
3:B:282:SER:OG	3:B:284:ASP:OD1	2.33	0.46
69:WW:100:GLN:NE2	69:WW:101:PRO:O	2.49	0.46
1:A:637:C:O2'	1:A:641:C:OP1	2.32	0.46
1:A:2090:A:N7	8:G:52:ALA:N	2.64	0.46
11:H:108:ASP:OD2	29:0:102:ARG:NH1	2.43	0.46
33:4:2:THR:N	34:5:339:GLU:OE2	2.49	0.46
64:RR:240:LYS:NZ	81:aa:905:C:O2	2.49	0.46
34:5:55:ASN:OD1	34:5:56:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:YY:16:CYS:SG	71:YY:21:THR:OG1	2.74	0.46
81:aa:870:G:H2'	81:aa:871:U:C6	2.51	0.46
18:O:241:LYS:O	18:O:245:THR:OG1	2.27	0.46
1:A:2584:U:O4	1:A:2585:A:N6	2.50	0.46
50:DD:8:LYS:HB3	50:DD:11:SER:HB2	1.97	0.46
79:88:435:ASP:N	79:88:435:ASP:OD1	2.48	0.45
81:aa:966:G:H4'	81:aa:1824:A:H4'	1.98	0.45
1:A:1906:C:O2	4:C:241:HIS:NE2	2.44	0.45
16:M:44:ASP:N	16:M:44:ASP:OD1	2.48	0.45
16:M:219:VAL:HG12	16:M:219:VAL:O	2.16	0.45
66:TT:167:SER:OG	66:TT:168:GLY:N	2.49	0.45
81:aa:1008:A:O2'	81:aa:1093:A:N1	2.48	0.45
12:I:10:CYS:O	12:I:45:ARG:NH1	2.50	0.45
39:i:143:ALA:O	39:i:147:ALA:N	2.49	0.45
46:bb:25:C:O2'	46:bb:26:A:P	2.73	0.45
57:KK:344:ASN:O	57:KK:347:ARG:NH2	2.42	0.45
71:YY:18:LEU:HD21	72:ZZ:273:MET:HG2	1.99	0.45
49:CC:63:PHE:N	72:ZZ:206:GLU:OE1	2.50	0.45
69:WW:91:ASP:OD1	69:WW:91:ASP:N	2.49	0.45
1:A:1041:G:O2'	1:A:1042:G:O5'	2.30	0.45
17:N:157:ALA:HB3	17:N:158:PRO:HD3	1.98	0.45
25:V:193:ASP:N	25:V:193:ASP:OD1	2.48	0.45
65:SS:9:LYS:NZ	81:aa:1602:A:OP1	2.35	0.45
81:aa:48:A:O2'	81:aa:49:U:O5'	2.32	0.45
1:A:2138:U:OP1	3:B:337:LYS:NZ	2.50	0.45
22:S:106:ASN:N	22:S:115:THR:O	2.40	0.45
79:88:507:LYS:O	79:88:507:LYS:HG2	2.17	0.45
3:B:284:ASP:OD1	3:B:284:ASP:N	2.40	0.45
1:A:3406:U:H3'	1:A:3407:U:H5''	1.99	0.45
2:e:92:GLN:OE1	2:e:92:GLN:N	2.50	0.45
69:WW:330:HIS:NE2	69:WW:370:GLU:OE2	2.49	0.45
76:55:90:ASP:OD1	76:55:90:ASP:N	2.48	0.45
71:YY:76:ASP:OD1	71:YY:77:ARG:N	2.49	0.45
81:aa:266:A:OP2	81:aa:440:A:N6	2.45	0.45
3:B:190:ASP:OD1	3:B:190:ASP:N	2.48	0.45
15:L:37:THR:OG1	15:L:38:THR:N	2.50	0.45
34:5:101:GLN:OE1	34:5:101:GLN:N	2.50	0.45
81:aa:1707:G:N3	81:aa:1707:G:H2'	2.32	0.45
1:A:526:G:O2'	1:A:527:A:P	2.75	0.44
1:A:2897:G:H2'	1:A:2951:U:H5''	1.99	0.44
9:f:275:ASP:OD1	9:f:278:GLY:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1267:G:N7	11:H:86:LYS:NZ	2.53	0.44
1:A:1539:G:O2'	1:A:1540:U:OP2	2.33	0.44
1:A:1316:A:N7	1:A:1342:A:O2'	2.48	0.44
34:5:219:ARG:NH2	34:5:228:ASP:OD2	2.50	0.44
36:7:111:GLN:NE2	36:7:147:GLU:OE2	2.50	0.44
47:AA:368:SER:N	47:AA:371:ASP:OD2	2.50	0.44
71:YY:16:CYS:O	71:YY:20:SER:N	2.50	0.44
81:aa:870:G:O2'	81:aa:871:U:P	2.75	0.44
1:A:1209:U:O2'	1:A:2475:A:N3	2.46	0.44
41:a:173:THR:HG22	41:a:175:VAL:H	1.82	0.44
65:SS:27:GLU:OE1	65:SS:28:PRO:HD2	2.18	0.44
81:aa:1565:A:H2'	81:aa:1566:A:H4'	2.00	0.44
48:BB:281:GLU:OE1	48:BB:281:GLU:N	2.47	0.44
51:EE:377:PRO:O	51:EE:450:GLN:NE2	2.50	0.44
53:GG:234:ARG:NH2	81:aa:1660:U:OP2	2.51	0.44
35:6:161:ASN:ND2	35:6:163:ARG:O	2.50	0.44
52:FF:42:GLY:HA3	68:VV:265:SER:HA	2.00	0.44
61:OO:164:ASP:OD1	61:OO:168:ARG:NH2	2.46	0.44
71:YY:20:SER:O	71:YY:20:SER:OG	2.34	0.44
1:A:345:C:O2'	1:A:348:A:N6	2.50	0.44
1:A:2851:G:O2'	27:X:21:GLY:O	2.36	0.44
11:H:97:THR:HG22	11:H:97:THR:O	2.17	0.44
21:R:182:SER:OG	21:R:183:ALA:N	2.51	0.44
47:AA:297:ILE:HG13	47:AA:298:THR:HG23	2.00	0.44
58:LL:134:GLN:OE1	58:LL:134:GLN:N	2.43	0.44
1:A:2040:U:OP1	22:S:118:LYS:NZ	2.50	0.43
45:j:103:SER:OG	45:j:104:ALA:N	2.51	0.43
61:OO:135:GLU:OE1	68:VV:221:ARG:NH1	2.51	0.43
78:77:267:ASP:O	78:77:272:LYS:NZ	2.51	0.43
1:A:2491:A:N6	1:A:2637:U:OP2	2.51	0.43
1:A:1634:G:OP1	22:S:120:ARG:NH2	2.51	0.43
7:F:217:GLU:O	7:F:221:THR:OG1	2.34	0.43
1:A:447:U:O2'	42:b:63:TRP:O	2.32	0.43
1:A:1991:A:N3	1:A:1991:A:H2'	2.32	0.43
10:g:148:GLN:O	10:g:151:SER:OG	2.29	0.43
41:a:67:ASP:N	41:a:67:ASP:OD1	2.50	0.43
5:D:63:THR:O	5:D:85:ALA:N	2.45	0.43
14:K:184:ASP:OD1	14:K:187:ARG:NH2	2.44	0.43
36:7:141:VAL:N	36:7:142:PRO:CD	2.81	0.43
21:R:353:GLU:OE1	21:R:353:GLU:HA	2.18	0.43
45:j:93:LYS:N	45:j:94:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1378:U:O4	1:A:2259:A:O2'	2.33	0.43
3:B:159:GLU:O	3:B:163:GLY:N	2.47	0.43
56:JJ:102:ARG:NH1	56:JJ:144:GLY:O	2.52	0.43
72:ZZ:78:ASP:N	72:ZZ:78:ASP:OD1	2.51	0.43
78:77:259:GLY:N	78:77:274:GLU:OE2	2.48	0.43
81:aa:871:U:H2'	81:aa:872:A:O4'	2.18	0.43
81:aa:1013:A:OP1	81:aa:1837:C:O2'	2.36	0.43
1:A:319:C:O2	20:Q:219:ARG:NH2	2.52	0.43
1:A:1214:G:H4'	24:U:14:GLY:O	2.18	0.43
31:2:315:GLU:O	31:2:319:THR:HG23	2.18	0.43
56:JJ:102:ARG:NH2	56:JJ:144:GLY:O	2.52	0.43
56:JJ:169:GLU:OE1	60:NN:97:ARG:NH2	2.49	0.43
81:aa:798:A:O2'	81:aa:1108:U:O2'	2.29	0.43
20:Q:110:SER:HB2	20:Q:111:PRO:HD2	2.01	0.43
33:4:81:ARG:NH1	33:4:107:GLY:O	2.49	0.43
47:AA:315:ASN:N	67:UU:172:GLU:OE2	2.52	0.43
50:DD:55:ARG:NH2	50:DD:62:ILE:O	2.48	0.43
79:88:290:ASN:OD1	79:88:291:ILE:N	2.48	0.43
1:A:909:A:O2'	1:A:910:A:P	2.77	0.42
1:A:1388:U:H4'	1:A:1389:A:O4'	2.19	0.42
31:2:254:ILE:N	31:2:254:ILE:HD13	2.34	0.42
53:GG:211:LYS:N	53:GG:229:GLN:O	2.48	0.42
61:OO:271:ASN:OD1	81:aa:926:A:N6	2.52	0.42
1:A:3095:G:OP1	11:H:101:SER:OG	2.35	0.42
24:U:130:ASP:OD1	24:U:131:GLY:N	2.52	0.42
70:XX:72:SER:OG	70:XX:73:GLY:N	2.50	0.42
11:H:155:LEU:O	11:H:157:ARG:NH2	2.52	0.42
33:4:49:LEU:N	33:4:50:PRO:CD	2.82	0.42
39:i:176:LEU:O	39:i:178:GLY:N	2.51	0.42
57:KK:256:TYR:O	57:KK:324:GLU:N	2.49	0.42
70:XX:85:ARG:NH2	81:aa:1575:U:OP2	2.47	0.42
1:A:1306:U:OP2	10:g:127:LYS:NZ	2.43	0.42
24:U:81:GLU:O	24:U:99:PHE:N	2.49	0.42
2:e:224:ARG:O	2:e:225:ASN:C	2.62	0.42
14:K:62:SER:OG	14:K:63:TRP:N	2.52	0.42
14:K:100:ARG:HB2	14:K:200:VAL:HG21	2.01	0.42
15:L:109:SER:O	15:L:110:GLN:HB2	2.18	0.42
45:j:54:GLU:O	45:j:58:LYS:NZ	2.49	0.42
45:j:86:PHE:O	45:j:86:PHE:CG	2.72	0.42
45:j:97:THR:OG1	45:j:98:PRO:HD3	2.19	0.42
50:DD:138:ALA:N	50:DD:139:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:FF:37:ASP:OD1	52:FF:38:ILE:N	2.52	0.42
53:GG:303:GLN:H	53:GG:303:GLN:HG2	1.71	0.42
81:aa:539:G:C4'	81:aa:540:A:OP2	2.68	0.42
2:e:72:GLY:O	2:e:73:GLN:C	2.63	0.42
39:i:140:ARG:O	39:i:144:MET:N	2.48	0.42
47:AA:342:ASN:O	47:AA:343:ASP:CB	2.67	0.42
55:II:298:ARG:NH1	55:II:299:LYS:O	2.52	0.42
62:PP:35:GLU:OE2	62:PP:65:ARG:NH2	2.42	0.42
44:d:192:LYS:N	44:d:193:PRO:HD2	2.35	0.42
49:CC:441:GLY:HA2	81:aa:1349:G:H5'	2.01	0.42
69:WW:205:SER:O	69:WW:205:SER:OG	2.35	0.42
70:XX:323:ASN:OD1	70:XX:327:GLU:N	2.43	0.42
76:44:53:PHE:O	76:44:57:GLY:N	2.53	0.42
1:A:571:A:N6	1:A:2255:A:H4'	2.35	0.42
51:EE:346:GLY:N	51:EE:421:ALA:O	2.47	0.42
63:QQ:63:ASN:OD1	63:QQ:63:ASN:N	2.53	0.42
75:33:83:LEU:O	75:33:106:ARG:NH2	2.49	0.42
76:44:191:TYR:O	76:44:192:LEU:C	2.63	0.42
1:A:1537:G:OP1	26:W:78:ARG:NH1	2.46	0.42
9:f:280:LYS:O	9:f:284:GLY:N	2.51	0.42
34:5:81:THR:O	34:5:81:THR:OG1	2.35	0.42
81:aa:870:G:O2'	81:aa:871:U:OP1	2.34	0.42
16:M:83:SER:O	16:M:84:LYS:HB3	2.18	0.41
30:1:367:GLU:O	30:1:367:GLU:HG3	2.20	0.41
1:A:2545:U:O4	1:A:2597:U:O2'	2.30	0.41
50:DD:126:ARG:O	50:DD:127:LYS:HG2	2.20	0.41
65:SS:27:GLU:O	65:SS:28:PRO:C	2.62	0.41
1:A:822:U:N3	1:A:823:G:O6	2.54	0.41
1:A:2105:A:N3	1:A:2105:A:H2'	2.35	0.41
1:A:2174:U:OP1	1:A:3056:U:O2'	2.35	0.41
44:d:72:GLU:O	44:d:72:GLU:HG3	2.19	0.41
46:bb:1:G:N2	46:bb:73:A:O4'	2.53	0.41
10:g:29:PRO:N	10:g:30:PRO:HD2	2.36	0.41
33:4:104:ASP:OD1	33:4:104:ASP:N	2.52	0.41
54:HH:114:ARG:NH2	81:aa:49:U:OP1	2.49	0.41
79:88:213:ARG:NH2	79:88:358:GLY:O	2.51	0.41
81:aa:712:C:H2'	81:aa:713:A:O4'	2.21	0.41
81:aa:988:G:O6	81:aa:989:A:N6	2.50	0.41
48:BB:299:ASN:OD1	48:BB:299:ASN:N	2.53	0.41
49:CC:163:GLU:O	49:CC:168:SER:OG	2.34	0.41
50:DD:406:PRO:HB2	50:DD:408:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:UU:126:SER:OG	67:UU:127:GLY:N	2.53	0.41
59:MM:66:GLU:OE2	59:MM:66:GLU:HA	2.19	0.41
75:33:81:PHE:HA	75:33:106:ARG:HD2	2.02	0.41
75:33:231:GLU:OE2	75:33:232:LYS:N	2.53	0.41
7:F:167:ASP:OD1	7:F:169:ARG:NH1	2.54	0.41
45:j:148:THR:OG1	45:j:149:ALA:N	2.54	0.41
47:AA:385:VAL:HG21	47:AA:402:VAL:CG1	2.51	0.41
53:GG:120:GLY:O	55:II:242:ARG:NH1	2.49	0.41
66:TT:151:GLU:N	66:TT:151:GLU:OE1	2.54	0.41
6:E:136:ASP:OD2	35:6:323:ARG:NH2	2.54	0.41
81:aa:1038:U:H4'	81:aa:1039:U:OP2	2.20	0.41
81:aa:1167:A:H4'	81:aa:1168:A:H5''	2.02	0.41
1:A:55:A:H2	1:A:3079:A:H2'	1.86	0.41
1:A:79:A:N6	1:A:528:A:N3	2.69	0.41
1:A:3168:U:H4'	12:I:85:VAL:HG21	2.02	0.41
2:e:268:VAL:HG23	2:e:268:VAL:O	2.21	0.41
6:E:130:ARG:NH1	87:2:4301:NAD:O1A	2.48	0.41
13:J:227:GLU:H	13:J:227:GLU:CD	2.28	0.41
51:EE:261:ASN:OD1	51:EE:261:ASN:N	2.52	0.41
55:II:197:ARG:NH1	81:aa:1631:G:O6	2.54	0.41
55:II:232:SER:O	55:II:265:THR:OG1	2.35	0.41
56:JJ:226:SER:O	56:JJ:227:LYS:C	2.64	0.41
63:QQ:143:ARG:O	63:QQ:147:HIS:ND1	2.54	0.41
1:A:2282:U:O2'	1:A:3364:A:N1	2.53	0.41
6:E:99:LEU:HA	30:1:207:MET:HE1	2.03	0.41
18:O:127:LYS:O	18:O:127:LYS:HG2	2.21	0.41
45:j:11:VAL:HG23	45:j:12:ARG:N	2.36	0.41
47:AA:136:ARG:NH2	76:55:149:GLY:O	2.54	0.41
49:CC:74:PHE:O	49:CC:77:ASN:N	2.54	0.41
49:CC:368:SER:OG	56:JJ:82:GLN:N	2.51	0.41
58:LL:90:LYS:HB3	58:LL:91:PRO:HD3	2.03	0.41
67:UU:89:ARG:NH1	81:aa:1039:U:O4	2.52	0.41
75:33:138:SER:HB3	75:33:139:PRO:HD2	2.03	0.41
77:66:328:ARG:HH21	77:66:328:ARG:HG2	1.85	0.41
1:A:338:G:OP1	1:A:1645:C:O2'	2.38	0.40
1:A:2337:U:O2'	1:A:2339:U:OP1	2.36	0.40
30:1:267:ASP:OD1	30:1:271:ARG:NH1	2.52	0.40
44:d:88:ALA:O	44:d:134:LEU:N	2.46	0.40
55:II:199:ALA:HB2	81:aa:1655:G:OP1	2.21	0.40
7:F:205:GLN:NE2	38:h:98:GLY:O	2.55	0.40
47:AA:401:THR:O	47:AA:401:THR:OG1	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:GG:303:GLN:O	53:GG:304:LEU:HD23	2.20	0.40
76:55:299:GLU:N	76:55:299:GLU:OE2	2.55	0.40
80:00:40:ASP:OD1	80:00:41:ALA:N	2.54	0.40
1:A:2148:A:N3	1:A:2148:A:H2'	2.37	0.40
1:A:2536:A:OP1	21:R:262:ARG:NH2	2.55	0.40
2:e:69:ASP:OD1	2:e:69:ASP:C	2.64	0.40
6:E:267:ASP:C	6:E:267:ASP:OD1	2.63	0.40
12:I:106:ARG:NH2	81:aa:494:A:OP2	2.54	0.40
26:W:88:VAL:HG23	26:W:88:VAL:O	2.20	0.40
79:88:62:VAL:CG2	79:88:88:MET:HG3	2.52	0.40
81:aa:396:A:N6	81:aa:431:A:O4'	2.54	0.40
81:aa:1060:G:O2'	81:aa:1065:A:N1	2.48	0.40
1:A:1221:G:O2'	1:A:1402:A:O2'	2.35	0.40
30:1:271:ARG:HG2	30:1:273:LEU:HD13	2.02	0.40
48:BB:173:ASN:OD1	48:BB:175:SER:N	2.39	0.40
48:BB:205:ARG:NH2	79:88:282:SER:O	2.54	0.40
53:GG:189:SER:O	53:GG:192:PRO:HD2	2.21	0.40
66:TT:155:ARG:NH1	81:aa:906:U:OP1	2.52	0.40
76:44:95:ASP:OD1	76:44:95:ASP:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	e	240/303 (79%)	231 (96%)	9 (4%)	0	100	100
3	B	324/383 (85%)	318 (98%)	6 (2%)	0	100	100
4	C	305/384 (79%)	299 (98%)	6 (2%)	0	100	100
5	D	250/325 (77%)	244 (98%)	6 (2%)	0	100	100
6	E	307/352 (87%)	301 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	F	199/255 (78%)	199 (100%)	0	0	100	100
8	G	72/300 (24%)	72 (100%)	0	0	100	100
9	f	243/347 (70%)	240 (99%)	3 (1%)	0	100	100
10	g	145/158 (92%)	142 (98%)	3 (2%)	0	100	100
11	H	181/183 (99%)	179 (99%)	2 (1%)	0	100	100
12	I	115/131 (88%)	113 (98%)	2 (2%)	0	100	100
13	J	241/312 (77%)	235 (98%)	6 (2%)	0	100	100
14	K	166/249 (67%)	165 (99%)	1 (1%)	0	100	100
15	L	190/193 (98%)	189 (100%)	1 (0%)	0	100	100
16	M	192/258 (74%)	190 (99%)	2 (1%)	0	100	100
17	N	131/217 (60%)	125 (95%)	6 (5%)	0	100	100
18	O	268/364 (74%)	265 (99%)	3 (1%)	0	100	100
19	P	178/228 (78%)	177 (99%)	1 (1%)	0	100	100
20	Q	351/396 (89%)	348 (99%)	3 (1%)	0	100	100
21	R	262/447 (59%)	260 (99%)	2 (1%)	0	100	100
22	S	175/274 (64%)	173 (99%)	2 (1%)	0	100	100
23	T	178/263 (68%)	177 (99%)	1 (1%)	0	100	100
24	U	134/161 (83%)	132 (98%)	2 (2%)	0	100	100
25	V	96/219 (44%)	95 (99%)	1 (1%)	0	100	100
26	W	57/129 (44%)	55 (96%)	2 (4%)	0	100	100
27	X	46/59 (78%)	45 (98%)	1 (2%)	0	100	100
28	Y	44/140 (31%)	44 (100%)	0	0	100	100
29	0	44/124 (36%)	43 (98%)	1 (2%)	0	100	100
30	1	365/449 (81%)	359 (98%)	6 (2%)	0	100	100
31	2	121/370 (33%)	121 (100%)	0	0	100	100
32	3	93/103 (90%)	91 (98%)	2 (2%)	0	100	100
33	4	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
34	5	346/439 (79%)	342 (99%)	4 (1%)	0	100	100
35	6	267/368 (73%)	262 (98%)	5 (2%)	0	100	100
36	7	82/165 (50%)	81 (99%)	1 (1%)	0	100	100
37	8	329/443 (74%)	318 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	h	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
39	i	120/218 (55%)	114 (95%)	6 (5%)	0	100	100
40	9	204/267 (76%)	202 (99%)	2 (1%)	0	100	100
41	a	157/225 (70%)	157 (100%)	0	0	100	100
42	b	159/162 (98%)	158 (99%)	1 (1%)	0	100	100
43	c	96/110 (87%)	95 (99%)	1 (1%)	0	100	100
44	d	231/292 (79%)	229 (99%)	2 (1%)	0	100	100
45	j	193/201 (96%)	176 (91%)	17 (9%)	0	100	100
47	AA	360/470 (77%)	351 (98%)	8 (2%)	1 (0%)	36	70
48	BB	288/428 (67%)	279 (97%)	9 (3%)	0	100	100
49	CC	432/508 (85%)	425 (98%)	7 (2%)	0	100	100
50	DD	286/453 (63%)	277 (97%)	9 (3%)	0	100	100
51	EE	363/477 (76%)	356 (98%)	7 (2%)	0	100	100
52	FF	115/117 (98%)	115 (100%)	0	0	100	100
53	GG	221/309 (72%)	221 (100%)	0	0	100	100
54	HH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
55	II	245/315 (78%)	242 (99%)	3 (1%)	0	100	100
56	JJ	186/268 (69%)	180 (97%)	6 (3%)	0	100	100
57	KK	122/376 (32%)	119 (98%)	3 (2%)	0	100	100
58	LL	126/174 (72%)	118 (94%)	8 (6%)	0	100	100
59	MM	116/119 (98%)	113 (97%)	3 (3%)	0	100	100
60	NN	110/113 (97%)	110 (100%)	0	0	100	100
61	OO	272/320 (85%)	270 (99%)	2 (1%)	0	100	100
62	PP	96/107 (90%)	95 (99%)	1 (1%)	0	100	100
63	QQ	156/165 (94%)	156 (100%)	0	0	100	100
64	RR	132/256 (52%)	129 (98%)	3 (2%)	0	100	100
65	SS	79/91 (87%)	75 (95%)	4 (5%)	0	100	100
66	TT	86/236 (36%)	85 (99%)	1 (1%)	0	100	100
67	UU	222/253 (88%)	218 (98%)	4 (2%)	0	100	100
68	VV	255/316 (81%)	252 (99%)	3 (1%)	0	100	100
69	WW	349/396 (88%)	345 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	XX	404/469 (86%)	395 (98%)	9 (2%)	0	100	100
71	YY	97/108 (90%)	96 (99%)	1 (1%)	0	100	100
72	ZZ	310/382 (81%)	307 (99%)	3 (1%)	0	100	100
73	11	86/90 (96%)	83 (96%)	3 (4%)	0	100	100
74	22	31/344 (9%)	31 (100%)	0	0	100	100
75	33	191/236 (81%)	182 (95%)	9 (5%)	0	100	100
76	44	258/310 (83%)	252 (98%)	6 (2%)	0	100	100
76	55	228/310 (74%)	223 (98%)	5 (2%)	0	100	100
77	66	281/348 (81%)	278 (99%)	3 (1%)	0	100	100
78	77	177/414 (43%)	174 (98%)	3 (2%)	0	100	100
79	88	465/508 (92%)	454 (98%)	11 (2%)	0	100	100
80	00	46/95 (48%)	46 (100%)	0	0	100	100
80	99	34/95 (36%)	34 (100%)	0	0	100	100
All	All	15511/21339 (73%)	15228 (98%)	282 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
47	AA	343	ASP

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	
2	e	207/256 (81%)	207 (100%)	0	100	100
3	B	267/312 (86%)	262 (98%)	5 (2%)	50	76
4	C	242/303 (80%)	242 (100%)	0	100	100
5	D	216/274 (79%)	212 (98%)	4 (2%)	50	76
6	E	267/296 (90%)	263 (98%)	4 (2%)	57	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	F	173/216 (80%)	173 (100%)	0	100	100
8	G	64/254 (25%)	64 (100%)	0	100	100
9	f	206/287 (72%)	206 (100%)	0	100	100
10	g	120/124 (97%)	120 (100%)	0	100	100
11	H	149/149 (100%)	149 (100%)	0	100	100
12	I	100/105 (95%)	100 (100%)	0	100	100
13	J	198/255 (78%)	197 (100%)	1 (0%)	81	89
14	K	142/205 (69%)	142 (100%)	0	100	100
15	L	164/165 (99%)	164 (100%)	0	100	100
16	M	164/209 (78%)	164 (100%)	0	100	100
17	N	119/188 (63%)	119 (100%)	0	100	100
18	O	235/315 (75%)	234 (100%)	1 (0%)	84	90
19	P	158/196 (81%)	156 (99%)	2 (1%)	61	81
20	Q	312/347 (90%)	311 (100%)	1 (0%)	86	91
21	R	226/359 (63%)	224 (99%)	2 (1%)	70	85
22	S	159/242 (66%)	158 (99%)	1 (1%)	78	88
23	T	161/224 (72%)	161 (100%)	0	100	100
24	U	118/138 (86%)	118 (100%)	0	100	100
25	V	86/170 (51%)	85 (99%)	1 (1%)	63	82
26	W	50/102 (49%)	50 (100%)	0	100	100
27	X	46/54 (85%)	46 (100%)	0	100	100
28	Y	38/116 (33%)	37 (97%)	1 (3%)	40	72
29	0	41/108 (38%)	41 (100%)	0	100	100
30	1	316/384 (82%)	312 (99%)	4 (1%)	61	81
31	2	109/317 (34%)	108 (99%)	1 (1%)	70	85
32	3	83/91 (91%)	83 (100%)	0	100	100
33	4	113/114 (99%)	112 (99%)	1 (1%)	70	85
34	5	279/351 (80%)	279 (100%)	0	100	100
35	6	238/310 (77%)	236 (99%)	2 (1%)	73	86
36	7	69/136 (51%)	69 (100%)	0	100	100
37	8	285/378 (75%)	278 (98%)	7 (2%)	42	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	h	88/88 (100%)	88 (100%)	0	100	100
39	i	101/162 (62%)	100 (99%)	1 (1%)	68	84
40	9	176/225 (78%)	173 (98%)	3 (2%)	53	78
41	a	146/196 (74%)	144 (99%)	2 (1%)	59	80
42	b	141/141 (100%)	140 (99%)	1 (1%)	76	86
43	c	86/96 (90%)	85 (99%)	1 (1%)	63	82
44	d	201/243 (83%)	201 (100%)	0	100	100
45	j	168/171 (98%)	166 (99%)	2 (1%)	63	82
47	AA	314/393 (80%)	313 (100%)	1 (0%)	86	91
48	BB	237/347 (68%)	236 (100%)	1 (0%)	84	90
49	CC	405/461 (88%)	403 (100%)	2 (0%)	81	89
50	DD	242/377 (64%)	239 (99%)	3 (1%)	63	82
51	EE	308/392 (79%)	306 (99%)	2 (1%)	78	88
52	FF	99/99 (100%)	99 (100%)	0	100	100
53	GG	186/260 (72%)	183 (98%)	3 (2%)	55	79
54	HH	134/135 (99%)	132 (98%)	2 (2%)	57	80
55	II	206/263 (78%)	206 (100%)	0	100	100
56	JJ	166/227 (73%)	166 (100%)	0	100	100
57	KK	108/324 (33%)	108 (100%)	0	100	100
58	LL	103/142 (72%)	103 (100%)	0	100	100
59	MM	98/99 (99%)	95 (97%)	3 (3%)	35	68
60	NN	96/97 (99%)	96 (100%)	0	100	100
61	OO	230/265 (87%)	230 (100%)	0	100	100
62	PP	85/92 (92%)	85 (100%)	0	100	100
63	QQ	132/138 (96%)	130 (98%)	2 (2%)	57	80
64	RR	118/218 (54%)	113 (96%)	5 (4%)	26	61
65	SS	70/80 (88%)	70 (100%)	0	100	100
66	TT	75/191 (39%)	74 (99%)	1 (1%)	61	81
67	UU	193/218 (88%)	190 (98%)	3 (2%)	55	79
68	VV	224/268 (84%)	224 (100%)	0	100	100
69	WW	300/333 (90%)	296 (99%)	4 (1%)	61	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	XX	345/391 (88%)	343 (99%)	2 (1%)	78	88
71	YY	83/89 (93%)	81 (98%)	2 (2%)	43	73
72	ZZ	278/328 (85%)	277 (100%)	1 (0%)	84	90
73	11	73/75 (97%)	73 (100%)	0	100	100
74	22	33/293 (11%)	33 (100%)	0	100	100
75	33	163/195 (84%)	163 (100%)	0	100	100
76	44	215/250 (86%)	214 (100%)	1 (0%)	81	89
76	55	195/250 (78%)	192 (98%)	3 (2%)	57	80
77	66	245/303 (81%)	244 (100%)	1 (0%)	84	90
78	77	153/304 (50%)	153 (100%)	0	100	100
79	88	388/419 (93%)	387 (100%)	1 (0%)	86	91
80	00	43/78 (55%)	43 (100%)	0	100	100
80	99	34/78 (44%)	33 (97%)	1 (3%)	37	70
All	All	13404/17844 (75%)	13312 (99%)	92 (1%)	73	86

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	109	HIS
3	B	190	ASP
3	B	193	ASP
3	B	281	VAL
3	B	284	ASP
5	D	95	ASP
5	D	134	THR
5	D	194	LEU
5	D	301	THR
6	E	54	SER
6	E	60	ILE
6	E	125	LEU
6	E	257	ILE
13	J	82	THR
18	O	61	GLU
19	P	52	GLU
19	P	53	PHE
20	Q	216	THR
21	R	334	ARG

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Mol	Chain	Res	Type
21	R	353	GLU
22	S	211	SER
25	V	104	ASN
28	Y	111	ARG
30	1	273	LEU
30	1	341	LEU
30	1	366	ARG
30	1	409	GLU
31	2	251	ILE
33	4	104	ASP
35	6	334	ASN
35	6	349	LEU
37	8	180	THR
37	8	235	ASN
37	8	261	TYR
37	8	263	GLN
37	8	319	ASN
37	8	350	ASP
37	8	362	PHE
39	i	181	ASN
40	9	69	THR
40	9	92	MET
40	9	96	ASP
41	a	67	ASP
41	a	180	CYS
42	b	92	THR
43	c	102	SER
45	j	161	LEU
45	j	191	SER
47	AA	205	GLU
48	BB	385	LEU
49	CC	101	LEU
49	CC	419	ILE
50	DD	86	MET
50	DD	407	ARG
50	DD	447	ASN
51	EE	261	ASN
51	EE	343	ASN
53	GG	190	HIS
53	GG	253	SER
53	GG	303	GLN
54	HH	29	THR

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Mol	Chain	Res	Type
54	HH	143	GLU
59	MM	60	LEU
59	MM	63	MET
59	MM	68	ASP
63	QQ	29	ILE
63	QQ	63	ASN
64	RR	149	ASN
64	RR	191	GLU
64	RR	202	ILE
64	RR	231	ARG
64	RR	232	HIS
66	TT	159	SER
67	UU	218	MET
67	UU	221	ASN
67	UU	225	ASN
69	WW	74	GLU
69	WW	91	ASP
69	WW	95	ILE
69	WW	308	ASP
70	XX	182	THR
70	XX	186	LEU
71	YY	73	VAL
71	YY	74	ASP
72	ZZ	85	GLU
76	44	302	ILE
76	55	152	ASP
76	55	247	THR
76	55	254	CYS
77	66	263	GLN
79	88	55	GLU
80	99	58	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	281	GLN
11	H	18	HIS
12	I	3	GLN
13	J	90	HIS
13	J	228	HIS
13	J	263	HIS
16	M	45	HIS

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Mol	Chain	Res	Type
16	M	214	HIS
21	R	117	HIS
21	R	149	ASN
22	S	89	HIS
23	T	46	HIS
23	T	122	HIS
23	T	178	ASN
27	X	53	GLN
30	1	218	GLN
30	1	362	HIS
30	1	365	ASN
35	6	150	HIS
35	6	334	ASN
37	8	263	GLN
41	a	201	ASN
45	j	128	ASN
47	AA	32	ASN
47	AA	250	ASN
49	CC	66	ASN
50	DD	162	GLN
50	DD	381	ASN
51	EE	102	HIS
51	EE	343	ASN
52	FF	54	GLN
52	FF	57	HIS
52	FF	74	HIS
54	HH	5	GLN
56	JJ	161	HIS
57	KK	318	ASN
59	MM	108	ASN
60	NN	23	HIS
61	OO	145	HIS
61	OO	301	HIS
63	QQ	20	HIS
67	UU	8	GLN
67	UU	32	ASN
68	VV	66	GLN
69	WW	47	ASN
69	WW	279	GLN
69	WW	295	GLN
70	XX	107	ASN
70	XX	314	HIS

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Mol	Chain	Res	Type
74	22	336	ASN
75	33	122	HIS
76	44	93	GLN
76	44	120	HIS
76	55	147	ASN
76	55	181	GLN
76	55	237	ASN
77	66	311	ASN
79	88	69	ASN
79	88	180	HIS
80	99	73	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2819/3464 (81%)	360 (12%)	7 (0%)
46	bb	73/74 (98%)	13 (17%)	0
81	aa	1430/1864 (76%)	189 (13%)	0
82	ee	10/11 (90%)	3 (30%)	0
All	All	4332/5413 (80%)	565 (13%)	7 (0%)

All (565) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	18	A
1	A	19	G
1	A	29	A
1	A	46	U
1	A	47	A
1	A	48	A
1	A	78	C
1	A	79	A
1	A	90	A
1	A	98	A
1	A	104	U
1	A	106	A
1	A	107	U
1	A	311	G
1	A	319	C
1	A	334	U
1	A	347	U

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Mol	Chain	Res	Type
1	A	348	A
1	A	350	U
1	A	351	A
1	A	353	A
1	A	367	A
1	A	370	A
1	A	376	U
1	A	387	A
1	A	392	A
1	A	393	A
1	A	395	U
1	A	414	U
1	A	419	U
1	A	435	A
1	A	440	A
1	A	441	U
1	A	443	A
1	A	448	A
1	A	462	U
1	A	477	A
1	A	478	U
1	A	486	A
1	A	522	C
1	A	526	G
1	A	527	A
1	A	552	A
1	A	569	G
1	A	583	A
1	A	584	A
1	A	587	A
1	A	588	A
1	A	599	A
1	A	609	U
1	A	611	A
1	A	639	A
1	A	829	A
1	A	839	A
1	A	840	U
1	A	845	A
1	A	846	A
1	A	849	U
1	A	855	A

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Mol	Chain	Res	Type
1	A	856	U
1	A	888	U
1	A	910	A
1	A	914	U
1	A	931	U
1	A	948	A
1	A	958	A
1	A	960	C
1	A	967	A
1	A	969	G
1	A	976	C
1	A	977	U
1	A	988	G
1	A	995	U
1	A	1010	A
1	A	1012	U
1	A	1026	A
1	A	1027	G
1	A	1042	G
1	A	1060	G
1	A	1070	A
1	A	1071	G
1	A	1081	C
1	A	1094	A
1	A	1096	G
1	A	1100	U
1	A	1107	U
1	A	1108	U
1	A	1109	U
1	A	1118	C
1	A	1119	A
1	A	1122	G
1	A	1134	A
1	A	1160	C
1	A	1190	A
1	A	1206	G
1	A	1219	A
1	A	1235	A
1	A	1242	G
1	A	1248	G
1	A	1250	U
1	A	1257	U

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Mol	Chain	Res	Type
1	A	1258	U
1	A	1267	G
1	A	1271	A
1	A	1280	A
1	A	1307	G
1	A	1316	A
1	A	1326	A
1	A	1331	A
1	A	1333	G
1	A	1334	A
1	A	1377	U
1	A	1379	U
1	A	1380	A
1	A	1381	A
1	A	1382	C
1	A	1389	A
1	A	1415	A
1	A	1417	G
1	A	1431	A
1	A	1453	A
1	A	1457	G
1	A	1487	U
1	A	1494	U
1	A	1495	A
1	A	1497	A
1	A	1509	A
1	A	1522	U
1	A	1526	A
1	A	1528	U
1	A	1529	G
1	A	1565	A
1	A	1566	A
1	A	1567	A
1	A	1568	A
1	A	1578	G
1	A	1589	A
1	A	1590	A
1	A	1591	A
1	A	1595	U
1	A	1604	G
1	A	1605	U
1	A	1613	C

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Mol	Chain	Res	Type
1	A	1620	U
1	A	1626	U
1	A	1627	A
1	A	1634	G
1	A	1648	U
1	A	1703	A
1	A	1719	A
1	A	1722	A
1	A	1726	A
1	A	1842	A
1	A	1843	A
1	A	1844	U
1	A	1852	A
1	A	1866	A
1	A	1880	U
1	A	1881	G
1	A	1882	A
1	A	1884	U
1	A	1910	G
1	A	1921	A
1	A	1922	C
1	A	1951	A
1	A	1970	A
1	A	1971	A
1	A	1977	A
1	A	1985	U
1	A	1988	A
1	A	1991	A
1	A	1993	U
1	A	2002	A
1	A	2011	U
1	A	2029	C
1	A	2030	A
1	A	2032	A
1	A	2039	A
1	A	2041	A
1	A	2048	A
1	A	2051	A
1	A	2052	U
1	A	2080	U
1	A	2105	A
1	A	2106	A

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Mol	Chain	Res	Type
1	A	2108	A
1	A	2136	A
1	A	2142	G
1	A	2143	G
1	A	2149	G
1	A	2150	C
1	A	2154	A
1	A	2164	G
1	A	2165	G
1	A	2172	A
1	A	2173	A
1	A	2190	U
1	A	2198	U
1	A	2199	G
1	A	2202	U
1	A	2205	A
1	A	2206	U
1	A	2207	G
1	A	2226	U
1	A	2228	U
1	A	2258	A
1	A	2265	C
1	A	2266	A
1	A	2268	A
1	A	2278	C
1	A	2287	A
1	A	2290	C
1	A	2291	G
1	A	2295	A
1	A	2304	G
1	A	2328	G
1	A	2337	U
1	A	2346	U
1	A	2347	U
1	A	2348	C
1	A	2367	A
1	A	2369	A
1	A	2371	G
1	A	2372	A
1	A	2384	C
1	A	2409	U
1	A	2411	A

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Mol	Chain	Res	Type
1	A	2418	A
1	A	2419	A
1	A	2420	U
1	A	2421	U
1	A	2427	A
1	A	2439	A
1	A	2440	G
1	A	2441	A
1	A	2477	A
1	A	2486	U
1	A	2506	G
1	A	2509	U
1	A	2511	C
1	A	2541	A
1	A	2543	C
1	A	2547	A
1	A	2548	U
1	A	2549	G
1	A	2555	C
1	A	2556	A
1	A	2558	A
1	A	2559	G
1	A	2582	G
1	A	2583	G
1	A	2592	A
1	A	2595	A
1	A	2596	A
1	A	2598	U
1	A	2602	U
1	A	2603	A
1	A	2605	G
1	A	2609	U
1	A	2612	U
1	A	2613	U
1	A	2619	A
1	A	2621	A
1	A	2622	U
1	A	2623	U
1	A	2626	U
1	A	2627	U
1	A	2628	C
1	A	2629	U

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Mol	Chain	Res	Type
1	A	2631	A
1	A	2638	A
1	A	2648	U
1	A	2649	U
1	A	2658	A
1	A	2659	G
1	A	2666	G
1	A	2685	A
1	A	2686	U
1	A	2690	G
1	A	2694	G
1	A	2705	U
1	A	2706	C
1	A	2710	U
1	A	2711	U
1	A	2719	U
1	A	2720	U
1	A	2721	U
1	A	2722	U
1	A	2723	U
1	A	2756	U
1	A	2758	U
1	A	2775	U
1	A	2784	U
1	A	2795	U
1	A	2797	C
1	A	2806	U
1	A	2808	A
1	A	2810	A
1	A	2811	A
1	A	2836	G
1	A	2838	C
1	A	2843	G
1	A	2852	A
1	A	2858	A
1	A	2875	U
1	A	2881	G
1	A	2882	A
1	A	2883	A
1	A	2884	A
1	A	2891	G
1	A	2897	G

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Mol	Chain	Res	Type
1	A	2898	A
1	A	2899	U
1	A	2900	A
1	A	2909	A
1	A	2912	U
1	A	2927	A
1	A	2942	U
1	A	2949	C
1	A	2969	A
1	A	2971	C
1	A	2980	U
1	A	2981	G
1	A	3018	A
1	A	3019	A
1	A	3025	C
1	A	3030	G
1	A	3034	G
1	A	3053	C
1	A	3054	A
1	A	3055	G
1	A	3061	U
1	A	3062	U
1	A	3065	U
1	A	3081	U
1	A	3082	U
1	A	3124	G
1	A	3125	G
1	A	3156	U
1	A	3259	A
1	A	3260	C
1	A	3262	A
1	A	3263	U
1	A	3276	G
1	A	3288	A
1	A	3296	A
1	A	3310	A
1	A	3349	A
1	A	3359	A
1	A	3391	A
1	A	3399	A
1	A	3407	U
1	A	3408	A

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Mol	Chain	Res	Type
1	A	3413	A
1	A	3420	A
1	A	3424	A
1	A	3425	U
1	A	3429	A
1	A	3447	A
1	A	3449	U
46	bb	7	G
46	bb	14	A
46	bb	18	G
46	bb	19	G
46	bb	21	A
46	bb	26	A
46	bb	43	A
46	bb	44	U
46	bb	48	U
46	bb	56	C
46	bb	71	C
46	bb	73	A
46	bb	76	A
81	aa	49	U
81	aa	51	G
81	aa	52	A
81	aa	54	G
81	aa	67	G
81	aa	77	A
81	aa	84	U
81	aa	90	U
81	aa	92	C
81	aa	93	U
81	aa	96	A
81	aa	106	A
81	aa	113	G
81	aa	115	U
81	aa	118	A
81	aa	122	U
81	aa	125	C
81	aa	238	C
81	aa	249	G
81	aa	256	A
81	aa	266	A
81	aa	268	A

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Mol	Chain	Res	Type
81	aa	270	U
81	aa	271	A
81	aa	273	U
81	aa	278	C
81	aa	282	U
81	aa	302	U
81	aa	312	U
81	aa	314	C
81	aa	318	A
81	aa	376	A
81	aa	380	G
81	aa	388	U
81	aa	389	C
81	aa	390	A
81	aa	401	G
81	aa	416	G
81	aa	417	C
81	aa	430	U
81	aa	431	A
81	aa	441	G
81	aa	445	A
81	aa	446	A
81	aa	454	A
81	aa	455	G
81	aa	482	A
81	aa	483	A
81	aa	496	A
81	aa	497	U
81	aa	518	U
81	aa	540	A
81	aa	547	A
81	aa	548	A
81	aa	556	G
81	aa	561	A
81	aa	669	C
81	aa	670	G
81	aa	674	A
81	aa	676	U
81	aa	677	U
81	aa	679	U
81	aa	684	U
81	aa	722	A

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Mol	Chain	Res	Type
81	aa	725	U
81	aa	737	U
81	aa	744	C
81	aa	756	G
81	aa	773	A
81	aa	790	A
81	aa	799	A
81	aa	802	G
81	aa	803	G
81	aa	805	A
81	aa	811	A
81	aa	828	A
81	aa	830	U
81	aa	838	A
81	aa	849	A
81	aa	856	U
81	aa	861	A
81	aa	862	A
81	aa	867	G
81	aa	871	U
81	aa	879	A
81	aa	911	G
81	aa	913	C
81	aa	921	G
81	aa	924	G
81	aa	945	A
81	aa	952	G
81	aa	974	A
81	aa	978	A
81	aa	990	U
81	aa	991	A
81	aa	1014	U
81	aa	1024	C
81	aa	1038	U
81	aa	1039	U
81	aa	1040	A
81	aa	1063	U
81	aa	1064	A
81	aa	1068	A
81	aa	1106	A
81	aa	1118	G
81	aa	1119	U

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Mol	Chain	Res	Type
81	aa	1126	C
81	aa	1127	A
81	aa	1138	A
81	aa	1152	U
81	aa	1158	G
81	aa	1161	C
81	aa	1164	C
81	aa	1167	A
81	aa	1168	A
81	aa	1169	A
81	aa	1184	U
81	aa	1185	G
81	aa	1192	A
81	aa	1357	U
81	aa	1358	C
81	aa	1385	U
81	aa	1386	U
81	aa	1392	G
81	aa	1393	A
81	aa	1417	U
81	aa	1425	A
81	aa	1426	U
81	aa	1437	U
81	aa	1438	U
81	aa	1450	A
81	aa	1475	A
81	aa	1476	A
81	aa	1480	A
81	aa	1481	U
81	aa	1492	A
81	aa	1493	U
81	aa	1504	A
81	aa	1505	U
81	aa	1511	U
81	aa	1526	A
81	aa	1527	A
81	aa	1529	A
81	aa	1537	G
81	aa	1553	U
81	aa	1559	A
81	aa	1566	A
81	aa	1579	A

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Mol	Chain	Res	Type
81	aa	1580	A
81	aa	1581	U
81	aa	1582	A
81	aa	1583	U
81	aa	1584	A
81	aa	1585	C
81	aa	1601	A
81	aa	1619	A
81	aa	1630	A
81	aa	1643	C
81	aa	1647	A
81	aa	1654	G
81	aa	1655	G
81	aa	1658	A
81	aa	1680	A
81	aa	1707	G
81	aa	1723	C
81	aa	1724	U
81	aa	1725	U
81	aa	1731	U
81	aa	1735	A
81	aa	1738	U
81	aa	1751	A
81	aa	1753	G
81	aa	1758	G
81	aa	1760	U
81	aa	1803	A
81	aa	1805	G
81	aa	1817	U
81	aa	1818	U
81	aa	1828	G
81	aa	1840	G
81	aa	1841	A
81	aa	1843	U
81	aa	1844	U
81	aa	1847	C
81	aa	1848	A
81	aa	1849	A
81	aa	1853	U
81	aa	1854	G
81	aa	1864	A
82	ee	38	U

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Mol	Chain	Res	Type
82	ee	43	A
82	ee	46	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	526	G
1	A	909	A
1	A	1205	A
1	A	2051	A
1	A	2648	U
1	A	2720	U
1	A	2883	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 302 ligands modelled in this entry, 299 are monoatomic - leaving 3 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
88	ATP	XX	501	83	32,33,33	2.46	6 (18%)	48,52,52	1.79	8 (16%)
87	NAD	2	4301	85	46,48,48	0.87	1 (2%)	64,73,73	1.32	7 (10%)
84	SPM	A	3636	-	13,13,13	0.33	0	12,12,12	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	ATP	XX	501	83	-	1/22/38/38	0/3/3/3
87	NAD	2	4301	85	-	3/30/62/62	0/5/5/5
84	SPM	A	3636	-	-	4/11/11/11	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	XX	501	ATP	C2'-C1'	-8.11	1.28	1.53
88	XX	501	ATP	PB-O3A	5.78	1.65	1.59
88	XX	501	ATP	PA-O3A	5.74	1.65	1.59
88	XX	501	ATP	PB-O3B	5.14	1.65	1.59
88	XX	501	ATP	C8-N9	-2.47	1.33	1.37
87	2	4301	NAD	C2N-N1N	-2.31	1.32	1.35
88	XX	501	ATP	C5-N7	-2.06	1.35	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	XX	501	ATP	C4-N9-C8	6.04	112.08	105.74
87	2	4301	NAD	C5A-C4A-N3A	-5.64	118.95	126.72
88	XX	501	ATP	N9-C8-N7	-4.96	106.91	113.94
88	XX	501	ATP	N3-C4-N9	4.39	134.64	127.17
88	XX	501	ATP	C5-C4-N3	-4.29	120.81	126.72
87	2	4301	NAD	N3A-C4A-N9A	4.18	134.28	127.17
88	XX	501	ATP	C5-N7-C8	3.19	108.47	103.45
87	2	4301	NAD	C5A-N7A-C8A	3.02	108.20	103.45
87	2	4301	NAD	C2A-N3A-C4A	2.97	119.09	111.83
87	2	4301	NAD	N9A-C8A-N7A	-2.78	109.99	113.94
88	XX	501	ATP	C1'-N9-C8	-2.74	121.02	127.09
87	2	4301	NAD	N3A-C2A-N1A	-2.63	124.60	128.58
87	2	4301	NAD	C4A-C5A-N7A	-2.60	107.61	110.58
88	XX	501	ATP	C3'-C2'-C1'	2.32	105.86	101.46
88	XX	501	ATP	C4-C5-N7	-2.26	108.00	110.58

There are no chirality outliers.

All (8) torsion outliers are listed below:

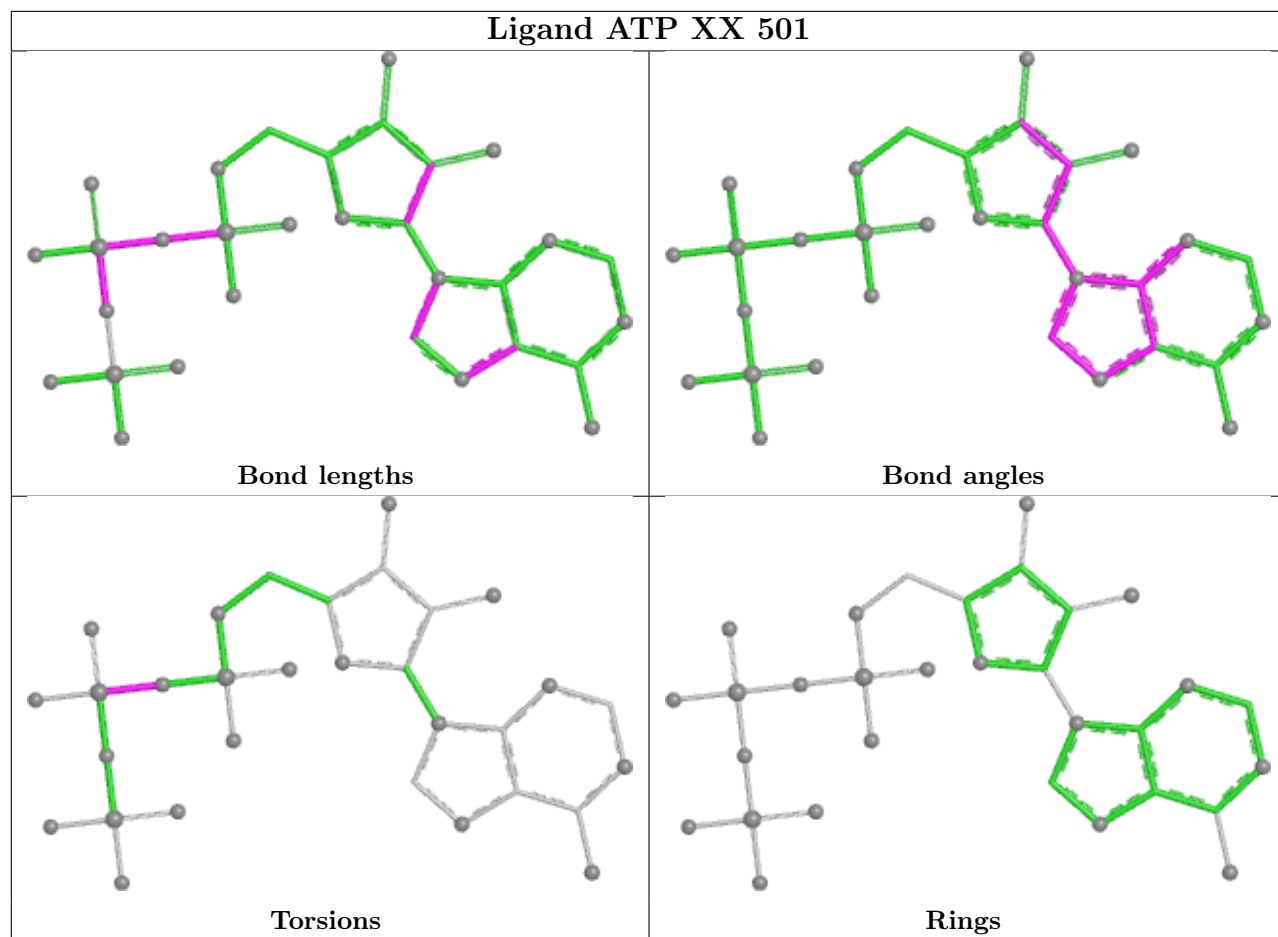
Mol	Chain	Res	Type	Atoms
87	2	4301	NAD	O4D-C1D-N1N-C6N
84	A	3636	SPM	N5-C6-C7-C8
84	A	3636	SPM	C8-C9-N10-C11
87	2	4301	NAD	C3B-C4B-C5B-O5B
88	XX	501	ATP	PA-O3A-PB-O2B
87	2	4301	NAD	O4B-C4B-C5B-O5B
84	A	3636	SPM	C12-C11-N10-C9
84	A	3636	SPM	C7-C6-N5-C4

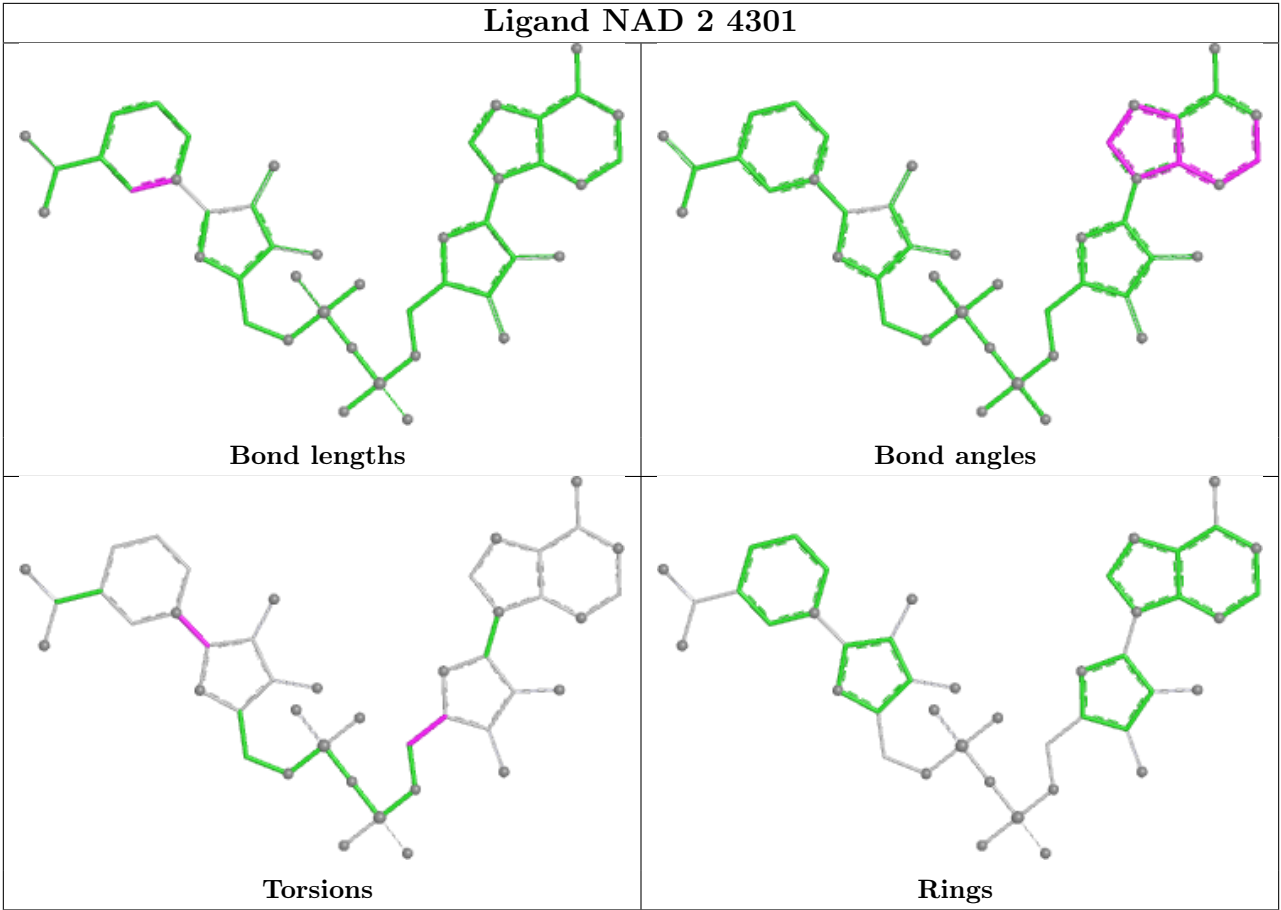
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	2	4301	NAD	1	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
46	bb	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	bb	16:U	O3'	18:G	P	3.28
1	bb	46:G	O3'	48:U	P	3.20

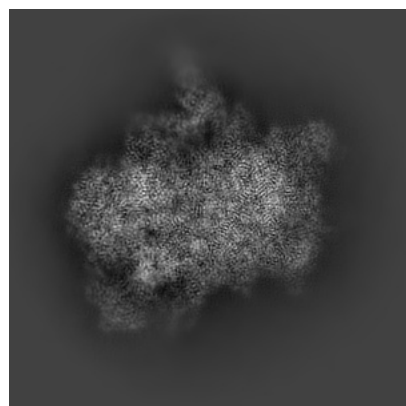
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10965. These allow visual inspection of the internal detail of the map and identification of artifacts.

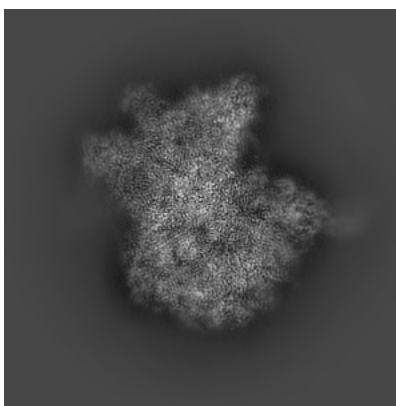
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

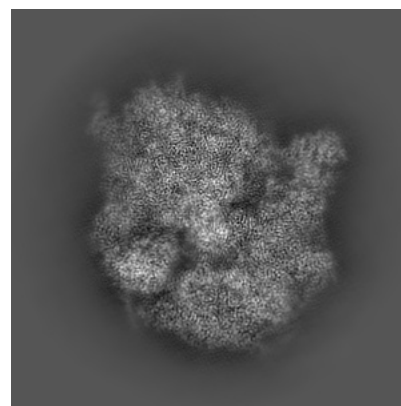
6.1.1 Primary map



X

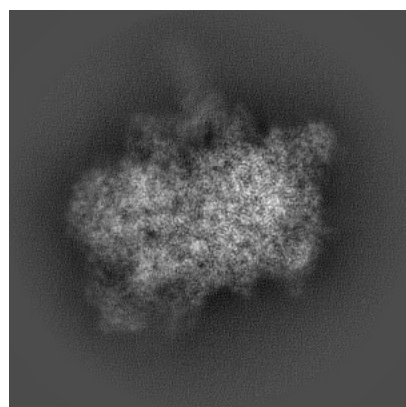


Y

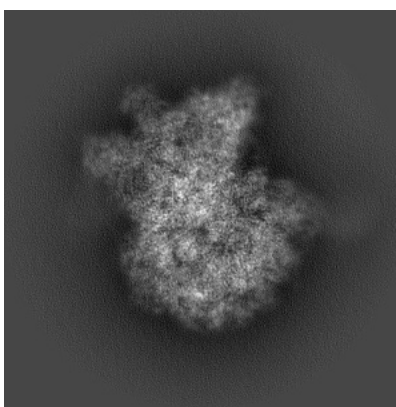


Z

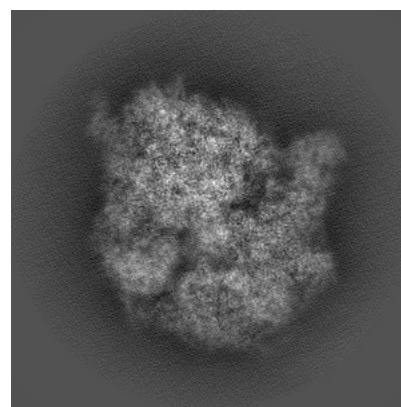
6.1.2 Raw map



X



Y

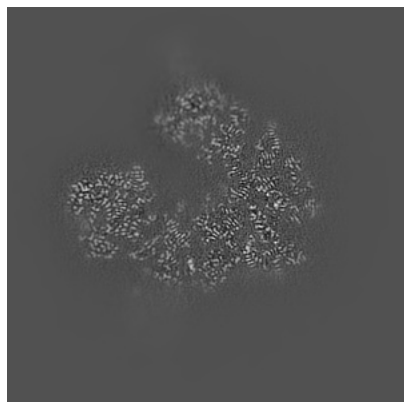


Z

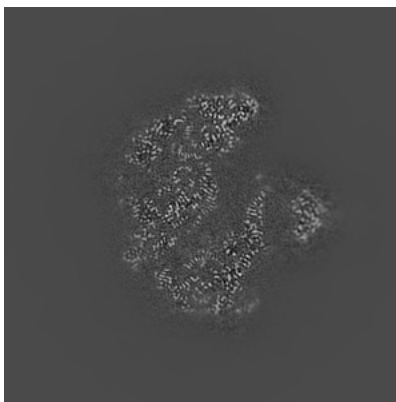
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

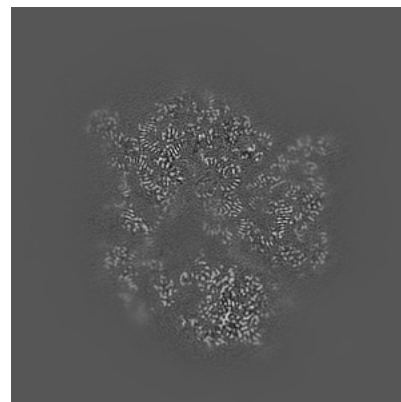
6.2.1 Primary map



X Index: 200

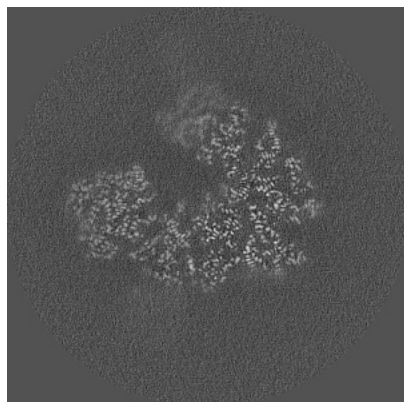


Y Index: 200

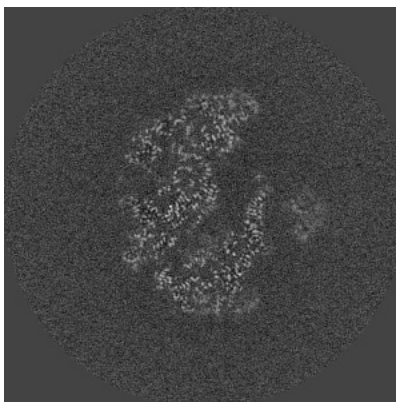


Z Index: 200

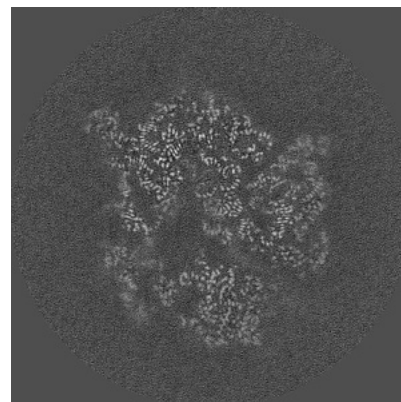
6.2.2 Raw map



X Index: 200



Y Index: 200

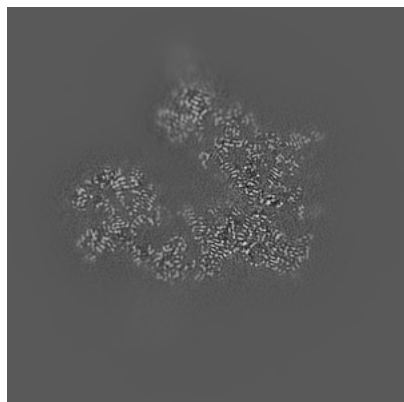


Z Index: 200

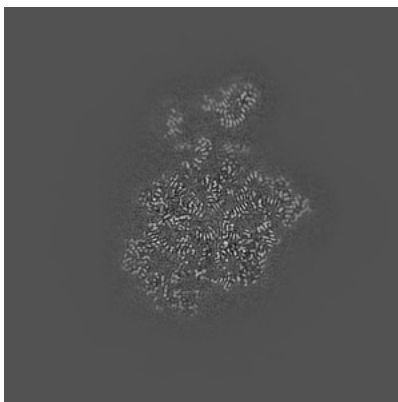
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

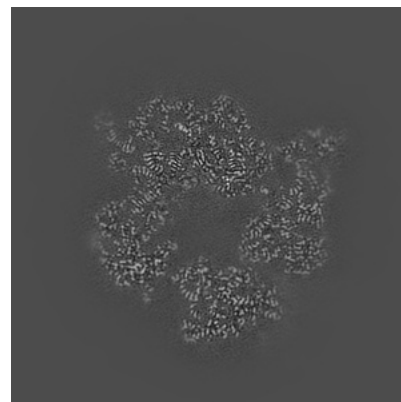
6.3.1 Primary map



X Index: 192

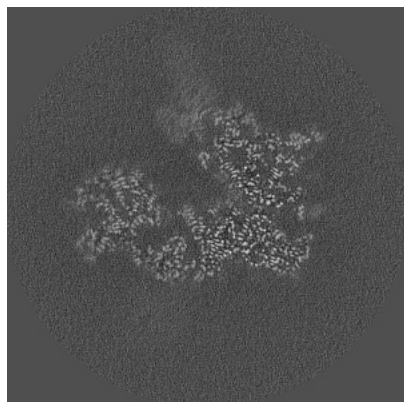


Y Index: 228

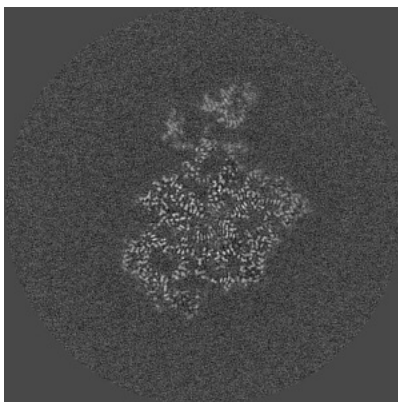


Z Index: 215

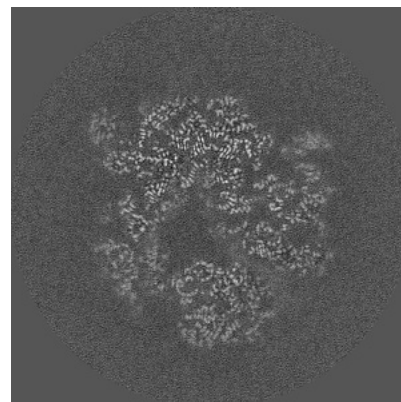
6.3.2 Raw map



X Index: 192



Y Index: 227

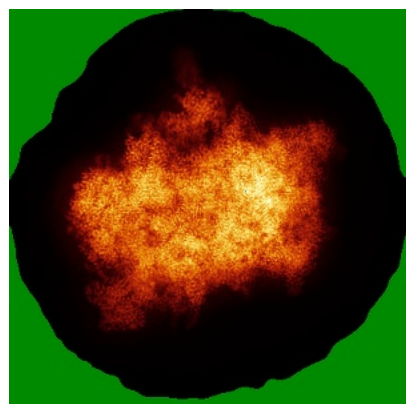


Z Index: 206

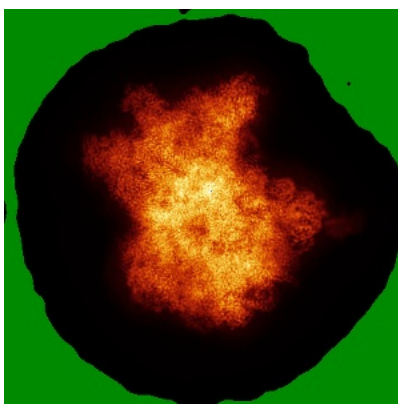
The images above show the largest variance slices of the map in three orthogonal directions.

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

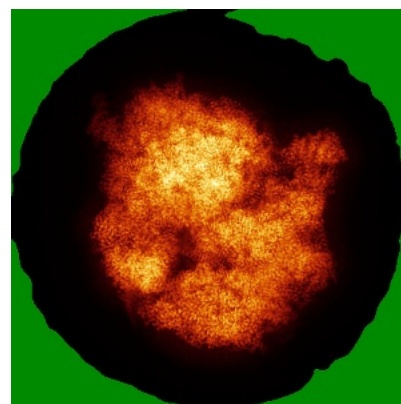
6.4.1 Primary map



X

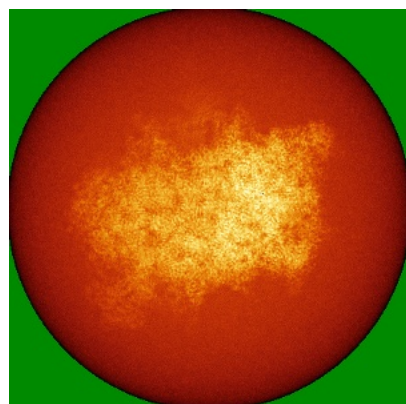


Y

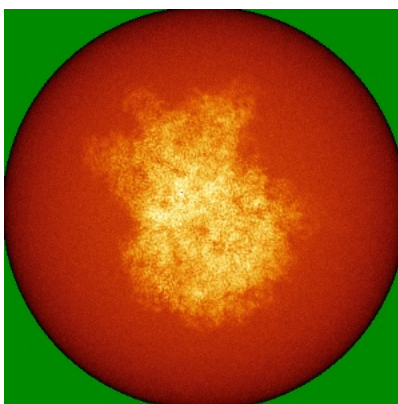


Z

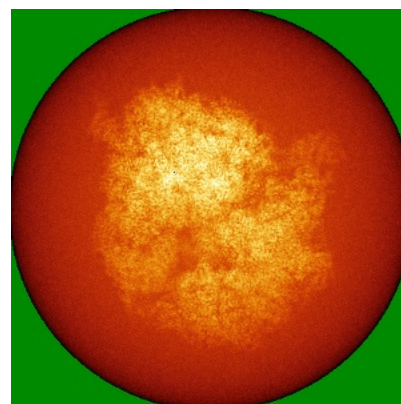
6.4.2 Raw map



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.

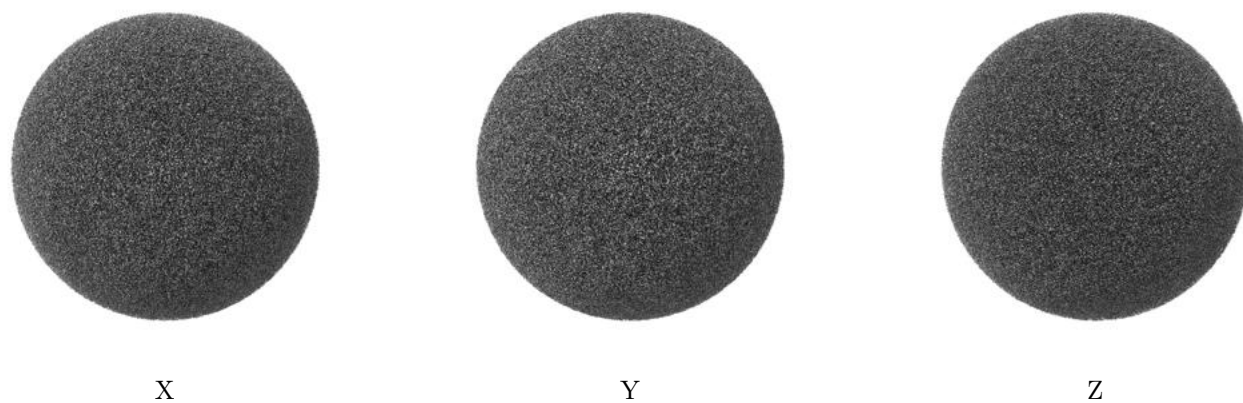
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0258. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

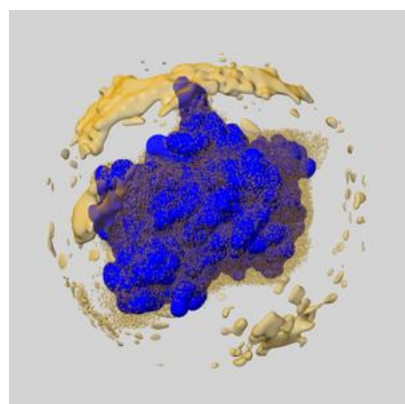
6.6 Mask visualisation [i](#)

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

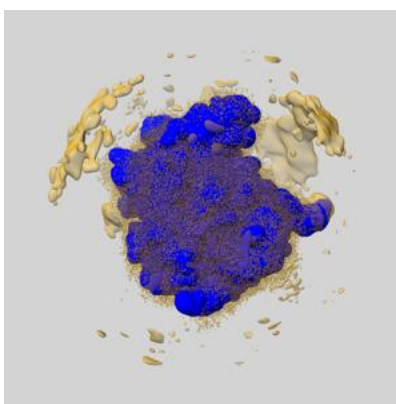
A mask typically either:

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

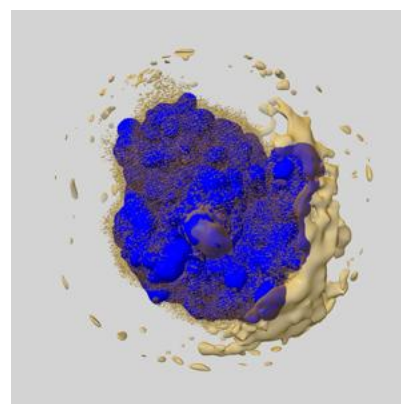
6.6.1 emd_10965_msk_1.map [i](#)



X



Y

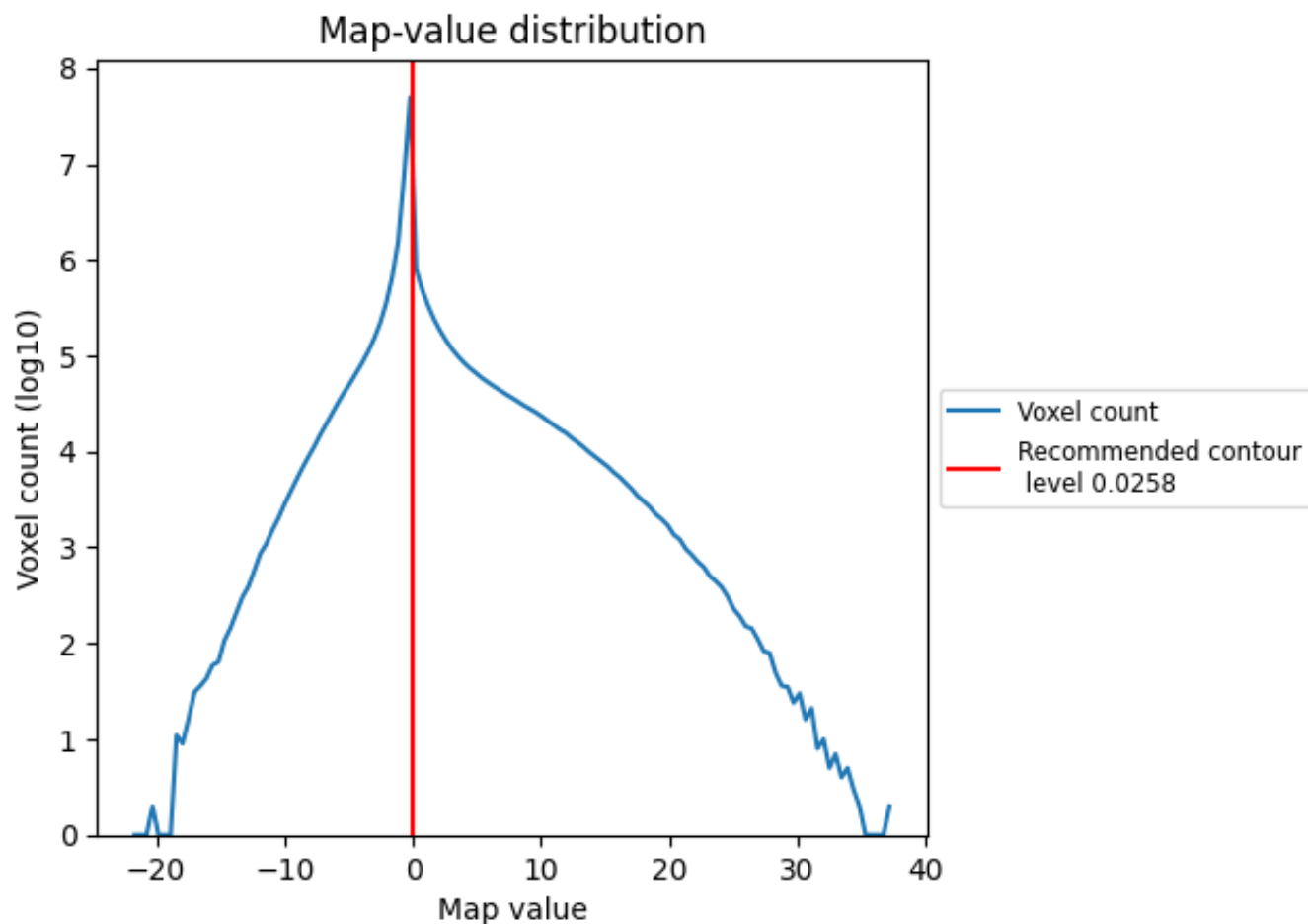


Z

7 Map analysis [i](#)

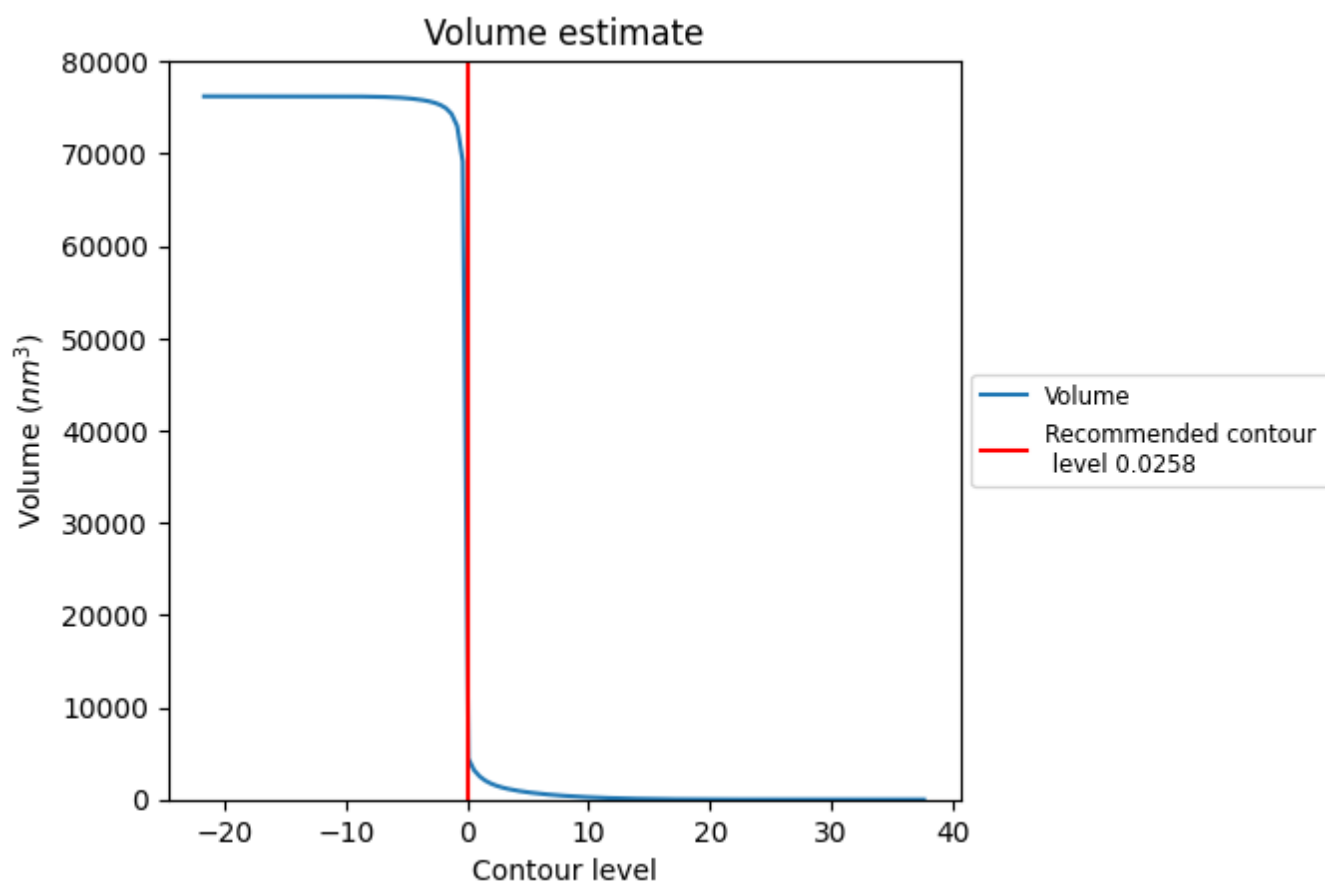
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

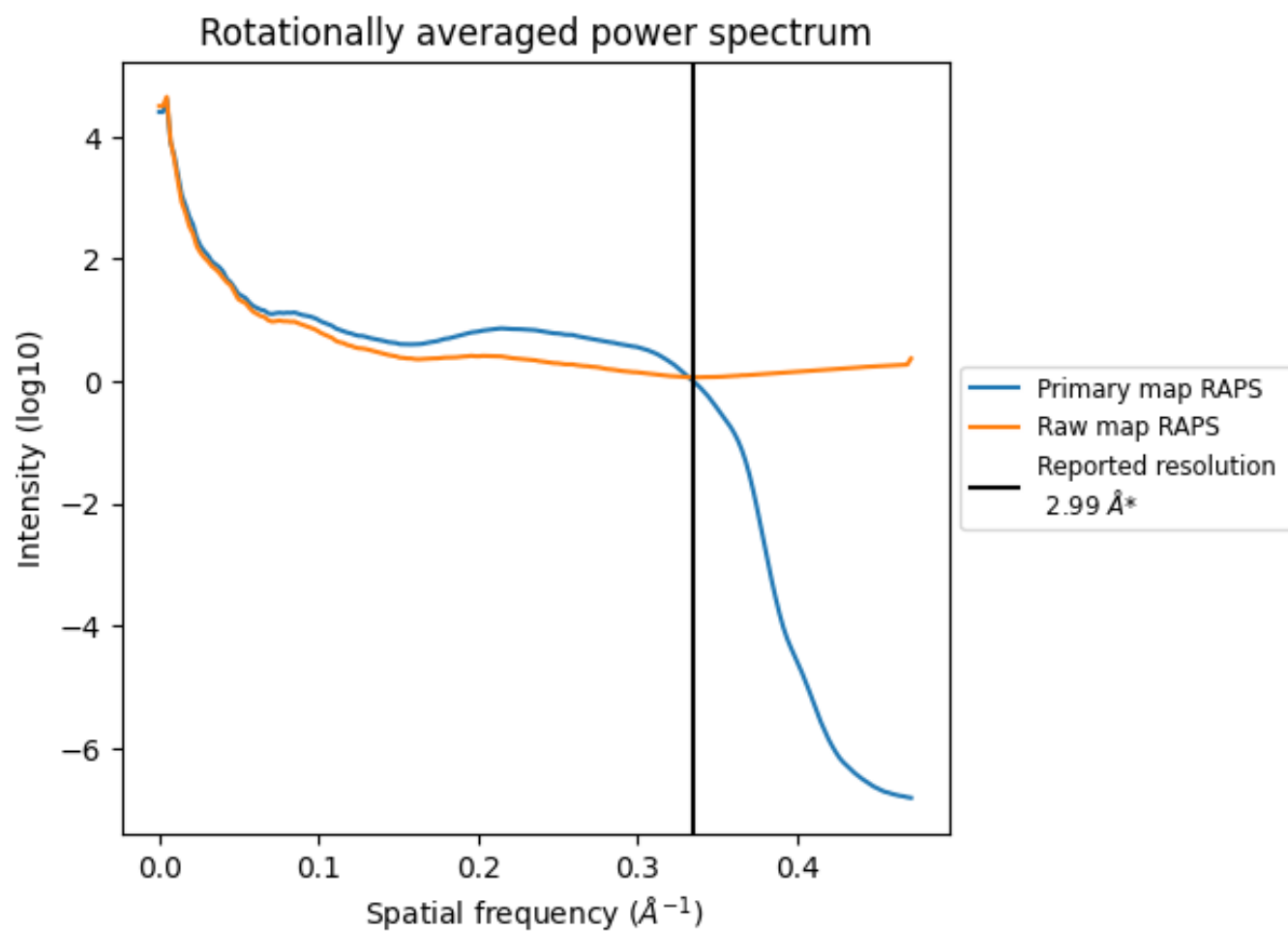
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 14015 nm³; this corresponds to an approximate mass of 12660 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 ⓘ

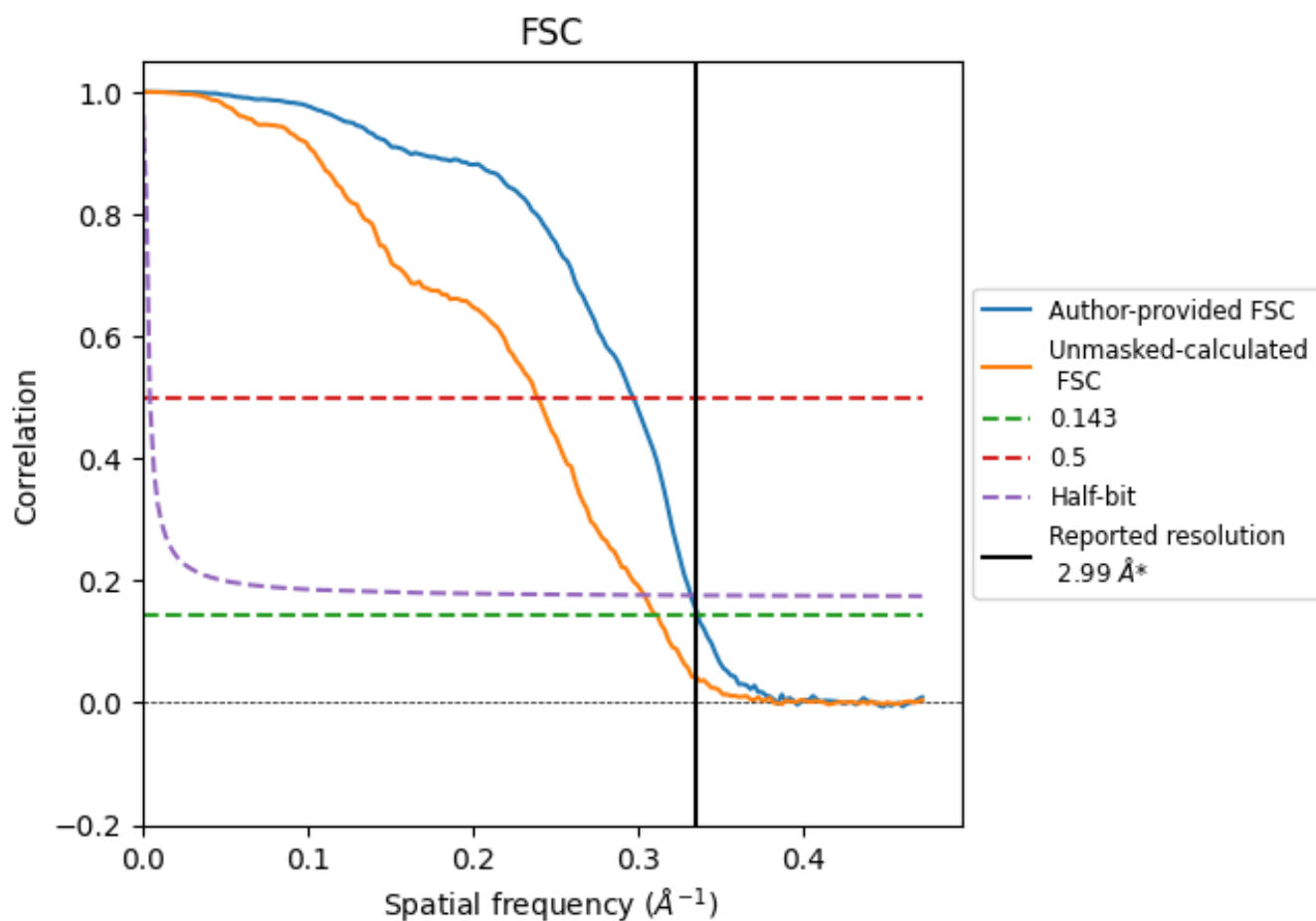


*Reported resolution corresponds to spatial frequency of $0.334 \text{ \AA}^{-1}$

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 $0.334 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

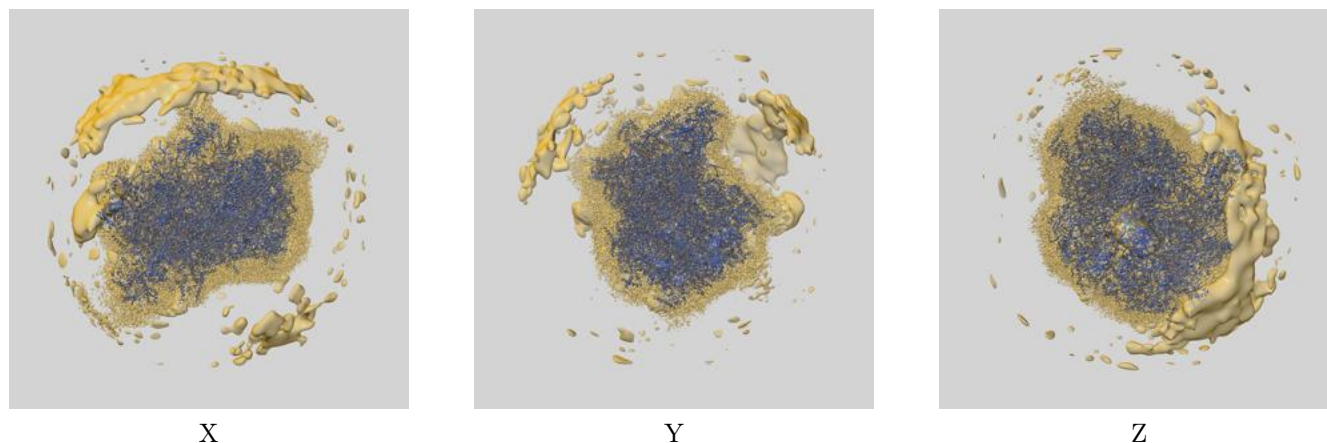
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.99	-	-
Author-provided FSC curve	2.98	3.37	3.01
Unmasked-calculated*	3.21	4.19	3.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

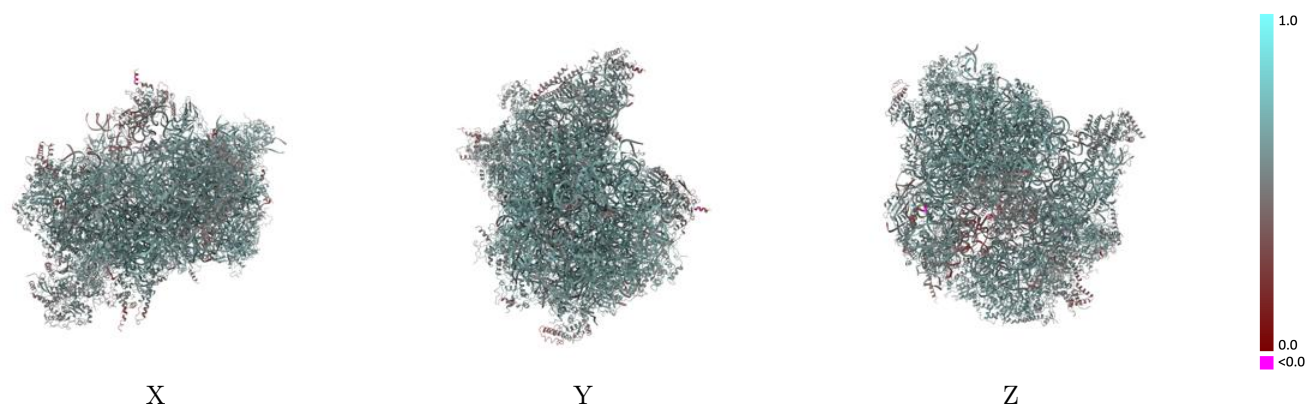
This section contains information regarding the fit between EMDB map EMD-10965 and PDB model 6YWE. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



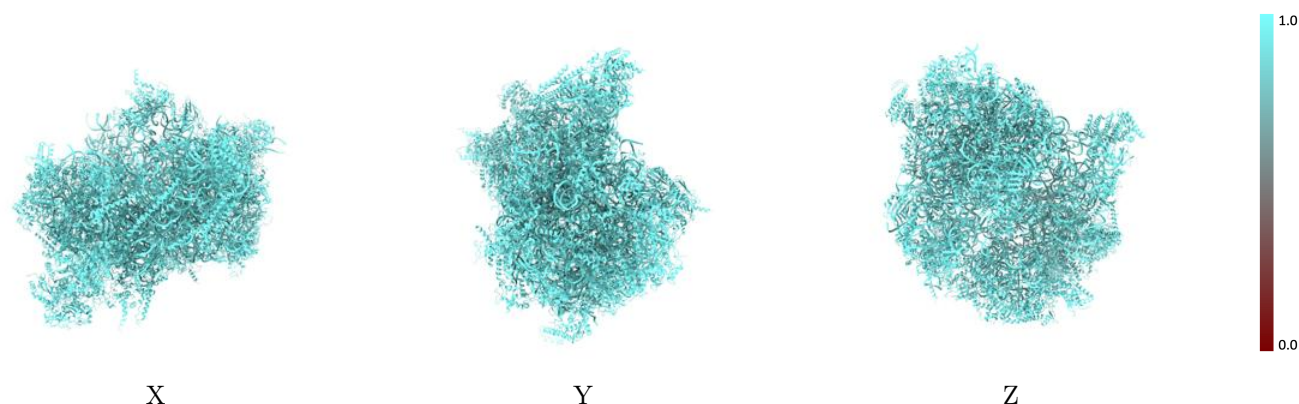
The images above show the 3D surface view of the map at the recommended contour level 0.0258 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



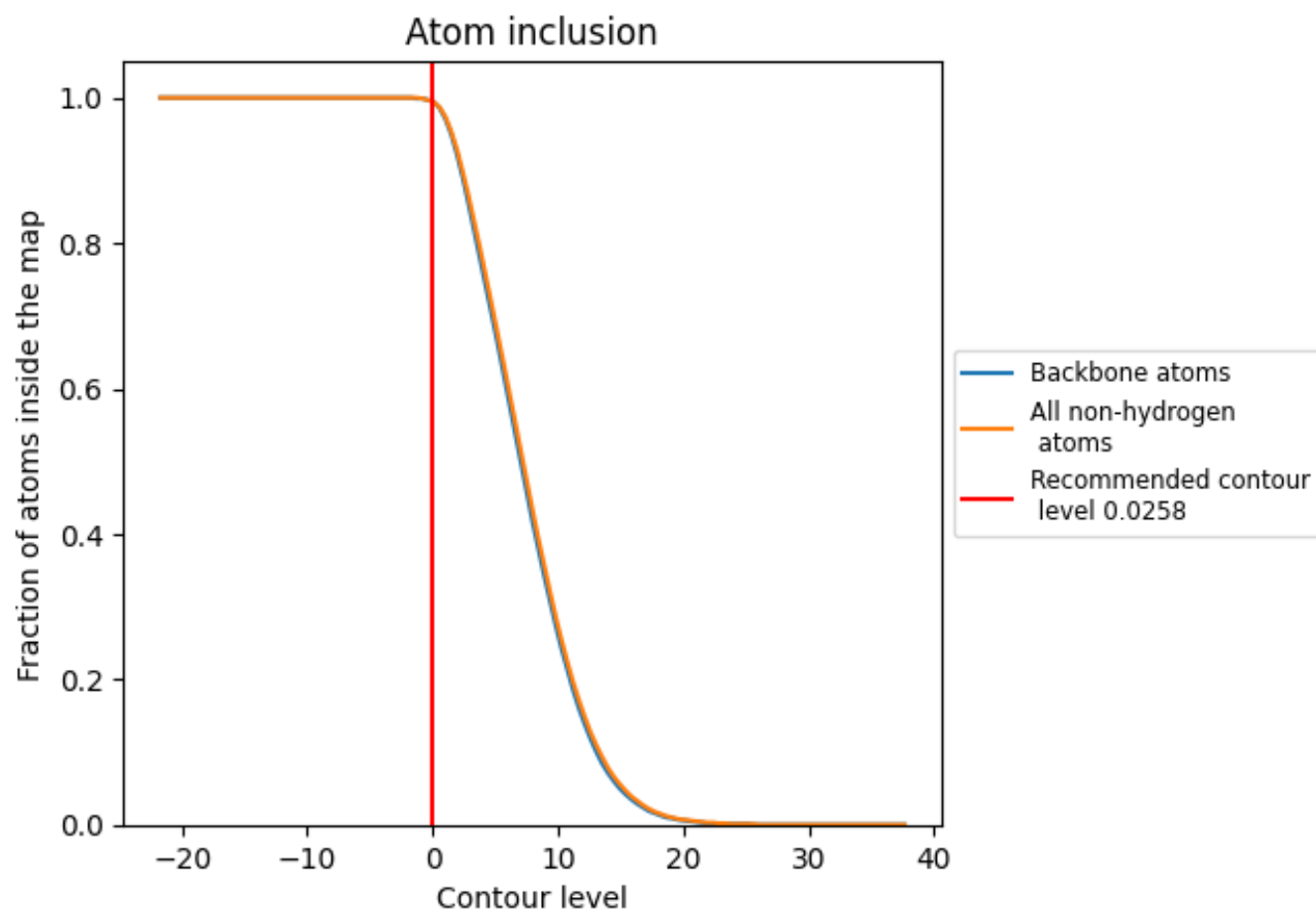
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0258).

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0258) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9950	 0.5750
0	 1.0000	 0.6380
00	 0.9900	 0.4530
1	 0.9960	 0.5800
11	 0.9910	 0.5630
2	 0.9900	 0.5980
22	 0.9930	 0.6020
3	 0.9930	 0.5980
33	 0.9930	 0.5540
4	 0.9930	 0.6220
44	 0.9950	 0.5050
5	 0.9950	 0.5880
55	 0.9960	 0.5010
6	 0.9930	 0.5770
66	 0.9930	 0.5580
7	 0.9940	 0.5870
77	 0.9880	 0.5660
8	 0.9940	 0.4970
88	 0.9920	 0.5390
9	 0.9980	 0.5520
99	 0.9800	 0.3730
A	 0.9980	 0.5980
AA	 0.9930	 0.5050
B	 0.9980	 0.6220
BB	 0.9930	 0.5640
C	 0.9960	 0.6290
CC	 0.9920	 0.5550
D	 0.9940	 0.5910
DD	 0.9970	 0.5760
E	 0.9920	 0.5870
EE	 0.9940	 0.5690
F	 0.9940	 0.5530
FF	 0.9930	 0.5930
G	 0.9970	 0.5650
GG	 0.9870	 0.5630



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Chain	Atom inclusion	Q-score
H	 0.9970	 0.6320
HH	 0.9870	 0.6050
I	 0.9970	 0.6120
II	 0.9940	 0.5680
J	 0.9920	 0.6030
JJ	 0.9930	 0.5950
K	 0.9920	 0.6030
KK	 0.9940	 0.5930
L	 0.9970	 0.6150
LL	 0.9950	 0.5910
M	 0.9970	 0.5900
MM	 0.9950	 0.5790
N	 0.9990	 0.6050
NN	 0.9950	 0.6220
O	 0.9910	 0.5940
OO	 0.9940	 0.5550
P	 0.9930	 0.6050
PP	 0.9940	 0.5940
Q	 0.9910	 0.5720
QQ	 0.9900	 0.5530
R	 0.9960	 0.5310
RR	 0.9900	 0.5350
S	 0.9970	 0.5860
SS	 0.9910	 0.5690
T	 0.9960	 0.5970
TT	 0.9930	 0.5970
U	 0.9920	 0.5910
UU	 0.9910	 0.5600
V	 0.9820	 0.5570
VV	 0.9920	 0.5410
W	 0.9910	 0.6220
WW	 0.9920	 0.5090
X	 0.9970	 0.6010
XX	 0.9910	 0.5690
Y	 0.9910	 0.6430
YY	 0.9860	 0.5850
ZZ	 0.9940	 0.5300
a	 0.9950	 0.5710
aa	 0.9980	 0.5990
b	 0.9950	 0.5670
bb	 0.9960	 0.3960
c	 0.9960	 0.6320

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Chain	Atom inclusion	Q-score
d	 0.9940	 0.6000
e	 0.9880	 0.4320
ee	 0.9870	 0.5170
f	 0.9910	 0.4420
g	 0.9980	 0.4430
h	 0.9840	 0.4350
i	 0.9800	 0.4070
j	 0.9850	 0.4180