



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 02:54 AM UTC

PDB ID : 7A5J / pdb_00007a5j
EMDB ID : EMD-11645
Title : Structure of the split human mitoribosomal large subunit with P-and E-site mt-tRNAs
Authors : Desai, N.; Yang, H.; Chandrasekaran, V.; Kazi, R.; Minczuk, M.; Ramakrishnan, V.
Deposited on : 2020-08-21
Resolution : 3.10 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:

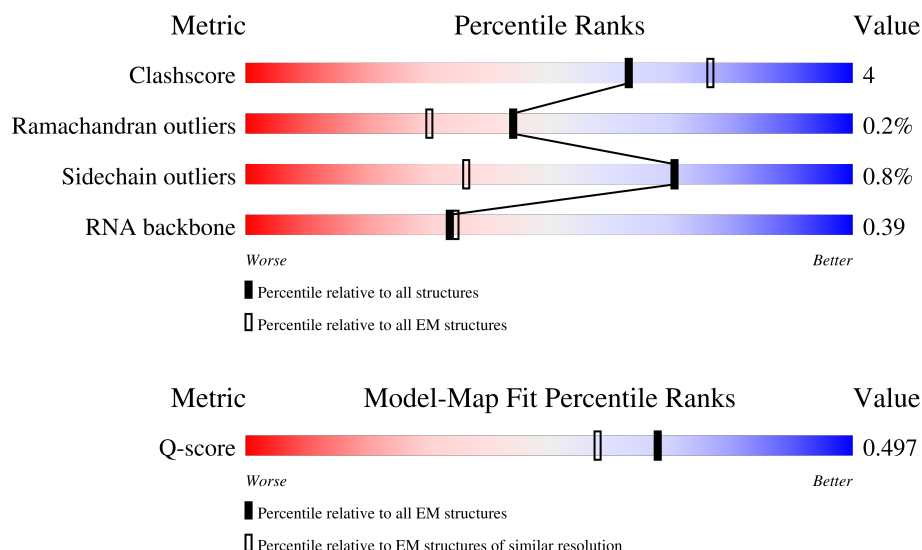
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	305	
2	E	348	
3	F	311	

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Mol	Chain	Length	Quality of chain
4	C	267	
4	H	267	
5	I	261	
6	J	192	
7	K	178	
8	L	145	
9	M	296	
10	N	251	
11	O	175	
12	P	179	
13	Q	292	
14	R	149	
15	S	205	
16	T	212	
17	U	153	
18	V	216	
19	W	148	
20	X	256	
21	Y	250	
22	Z	161	
23	0	188	
24	1	65	
25	2	92	
26	3	188	
27	4	103	

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Mol	Chain	Length	Quality of chain
28	5	423	
29	6	380	
30	7	338	
31	8	206	
32	9	137	
33	a	142	
34	b	155	
35	c	332	
36	d	306	
37	e	279	
38	f	194	
39	g	166	
40	h	158	
41	i	128	
42	j	123	
43	k	112	
44	l	138	
45	m	128	
46	o	102	
47	p	206	
48	q	222	
49	r	196	
50	s	439	
51	t	28	
52	u	234	

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Mol	Chain	Length	Quality of chain
53	v	70	
54	w	156	
55	n	229	
56	A	1559	
57	B	69	
58	Y2	29	
59	G	73	
59	x	73	
60	y	32	
61	z	14	

2 Entry composition [i](#)

There are 65 unique types of molecules in this entry. The entry contains 106132 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	236	Total	C	N	O	S	0	0
			1842	1145	373	315	9		

- Molecule 2 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	304	Total	C	N	O	S	0	0
			2396	1539	416	430	11		

- Molecule 3 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	250	Total	C	N	O	S	0	0
			2013	1294	365	348	6		

- Molecule 4 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	95	Total	C	N	O		0	0
			784	498	152	134			
4	C	80	Total	C	N	O	S	0	0
			648	421	111	112	4		

- Molecule 5 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 6 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	140	Total	C	N	O	S	0	0
			1061	680	192	187	2		

- Molecule 7 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 8 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 9 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 10 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	205	Total	C	N	O	S	0	0
			1654	1056	308	280	10		

- Molecule 11 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 12 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	141	Total	C	N	O	S	0	0
			1148	719	221	203	5		

- Molecule 13 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	217	Total	C	N	O	S	0	0
			1805	1159	317	320	9		

- Molecule 14 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 15 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	156	Total	C	N	O	S	0	0
			1251	806	222	219	4		

- Molecule 16 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 17 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	152	Total	C	N	O	S	0	0
			1218	772	233	210	3		

- Molecule 18 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	202	Total	C	N	O	S	0	0
			1624	1032	291	293	8		

- Molecule 19 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	109	Total	C	N	O	S	0	0
			859	552	162	142	3		

- Molecule 20 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	243	Total	C	N	O	S	0	0
			2035	1317	351	362	5		

- Molecule 21 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 22 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 23 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 24 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 25 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	45	Total	C	N	O	S	0	0
			367	227	81	58	1		

- Molecule 26 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 27 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	37	Total	C	N	O	S	0	0
			333	212	71	47	3		

- Molecule 28 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	387	Total	C	N	O	S	0	0
			3156	2039	548	558	11		

- Molecule 29 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	324	Total	C	N	O	S	0	0
			2640	1694	470	468	8		

- Molecule 30 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	7	287	Total	C	N	O	S	0	0
			2334	1495	397	425	17		

- Molecule 31 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	8	110	Total	C	N	O	S	0	0
			890	567	155	166	2		

- Molecule 32 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	9	117	Total	C	N	O	S	0	0
			947	614	163	168	2		

- Molecule 33 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	82	Total	C	N	O	S	0	0
			686	434	124	123	5		

- Molecule 34 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 35 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 36 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	211	Total	C	N	O	S	0	0
			1741	1123	299	309	10		

- Molecule 37 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	217	Total	C	N	O	S	0	0
			1762	1124	310	323	5		

- Molecule 38 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	116	Total	C	N	O	S	0	0
			915	585	152	175	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	129	Total	C	N	O	S	0	0
			1067	690	185	190	2		

- Molecule 40 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	100	Total	C	N	O	S	0	0
			827	524	146	155	2		

- Molecule 41 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	97	Total	C	N	O	S	0	0
			827	532	165	126	4		

- Molecule 42 is a protein called cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	85	Total	C	N	O	S	0	0
			684	423	133	126	2		

- Molecule 43 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	80	Total	C	N	O	S	0	0
			627	392	116	114	5		

- Molecule 44 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	l	23	Total	C	N	O	0	0
			221	137	52	32		

- Molecule 45 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	45	Total	C	N	O	S	0	0
			372	232	76	62	2		

- Molecule 46 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	91	Total	C	N	O	S	0	0
			771	487	156	125	3		

- Molecule 47 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	127	Total	C	N	O	S	0	0
			1058	661	201	192	4		

- Molecule 48 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 49 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

- Molecule 50 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 51 is a protein called Unknown protein/protein extension.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	t	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 52 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	111	Total	C	N	O	S	0	0
			927	595	155	167	10		

- Molecule 53 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	v	69	Total	C	N	O	0	0
			588	372	116	100		

- Molecule 54 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	w	79	Total	C	N	O	P	S	0	0
			659	421	97	134	1	6		

- Molecule 55 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	n	228	Total	C	N	O	S	4	0
			1767	1121	321	322	3		

- Molecule 56 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	A	1492	Total	C	N	O	P	0	0
			31684	14216	5726	10250	1492		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3107	U	UNK	conflict	GB 1025814679

- Molecule 57 is a RNA chain called mt-tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B	56	Total	C	N	O	P	0	0
			1191	534	214	387	56		

- Molecule 58 is a protein called nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	Y2	29	Total	C	N	O	0	0
			145	87	29	29		

- Molecule 59 is a RNA chain called mt-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	G	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		
59	x	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		

- Molecule 60 is a protein called Unknown protein/protein extension.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	y	32	Total	C	N	O	0	0
			160	96	32	32		

- Molecule 61 is a protein called unknown protein/protein extension.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	z	14	Total	C	N	O	0	0
			70	42	14	14		

- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	D	1	Total	Mg	0
			1	1	
62	g	1	Total	Mg	0
			1	1	
62	A	90	Total	Mg	0
			90	90	

- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
63	0	1	Total	Zn	0
			1	1	
63	4	1	Total	Zn	0
			1	1	
63	r	1	Total	Zn	0
			1	1	

- Molecule 64 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
64	n	2	Total	Cl	0
			2	2	

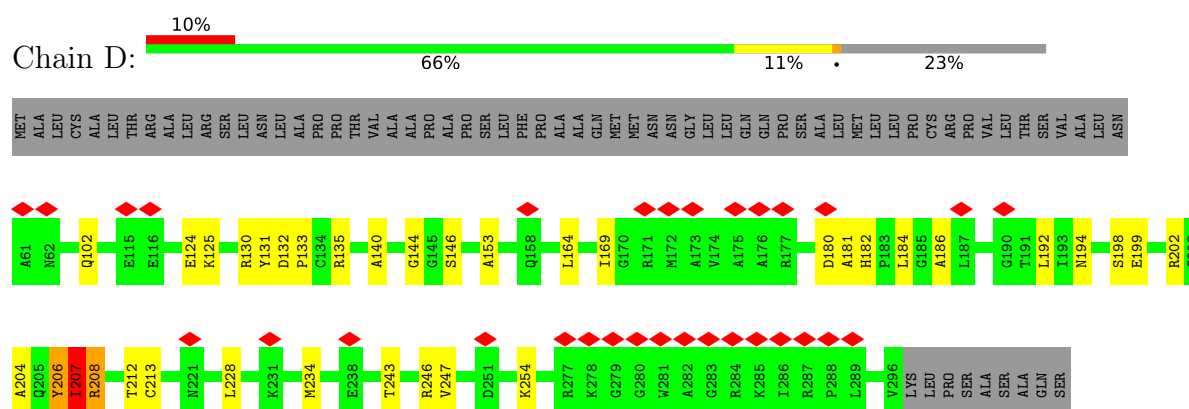
- Molecule 65 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
65	n	3	Total	Na	0
			3	3	
65	A	1	Total	Na	0
			1	1	

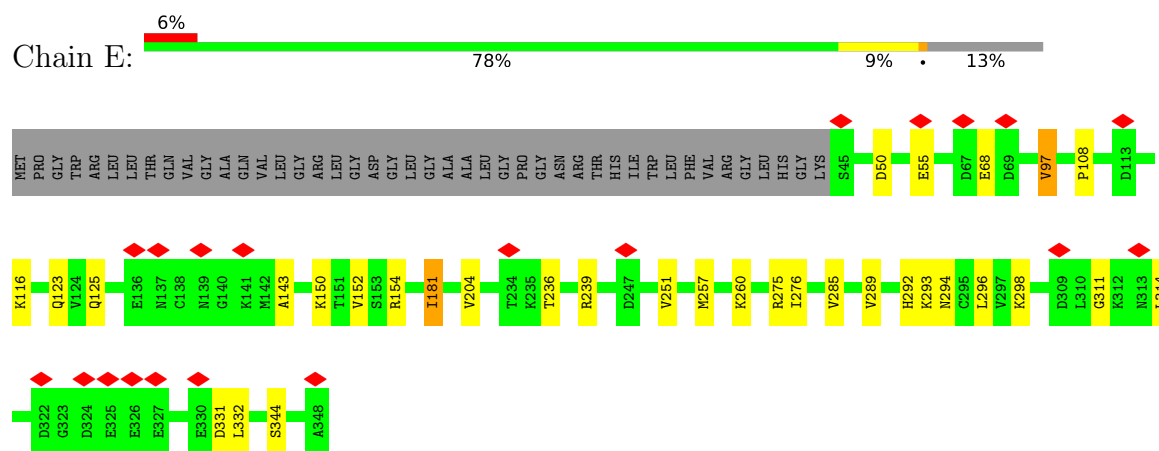
3 Residue-property plots

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.

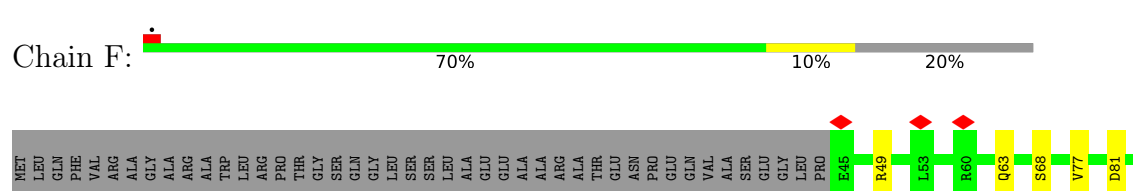
- Molecule 1: 39S ribosomal protein L2, mitochondrial

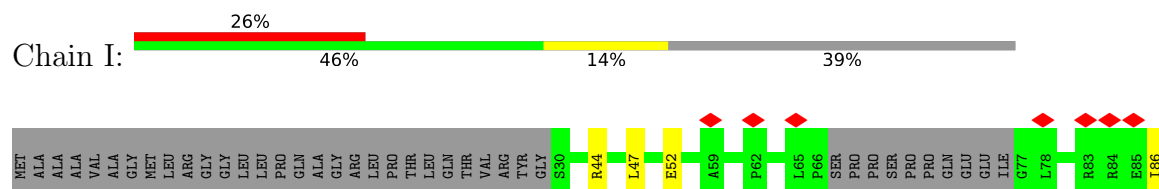


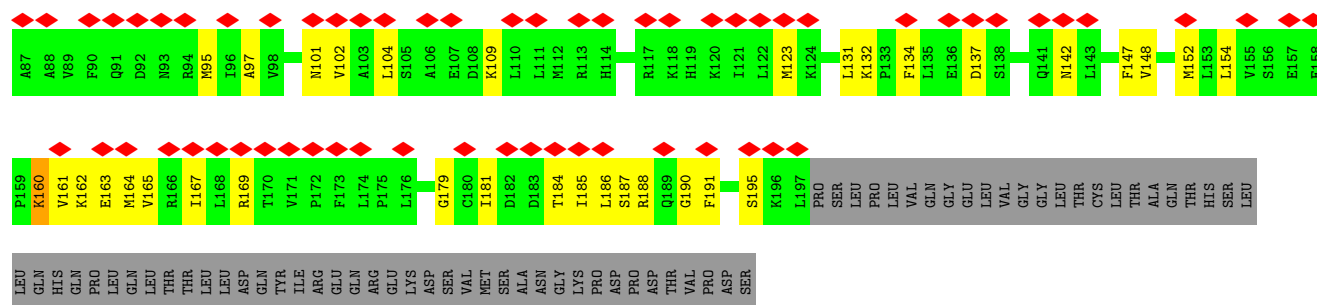
- Molecule 2: 39S ribosomal protein L3, mitochondrial



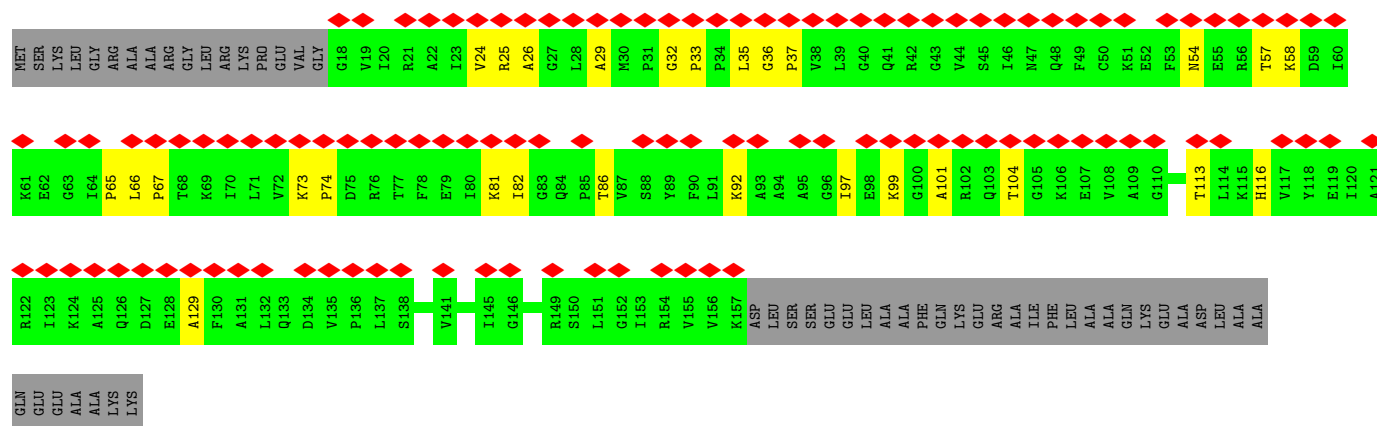
- Molecule 3: 39S ribosomal protein L4, mitochondrial



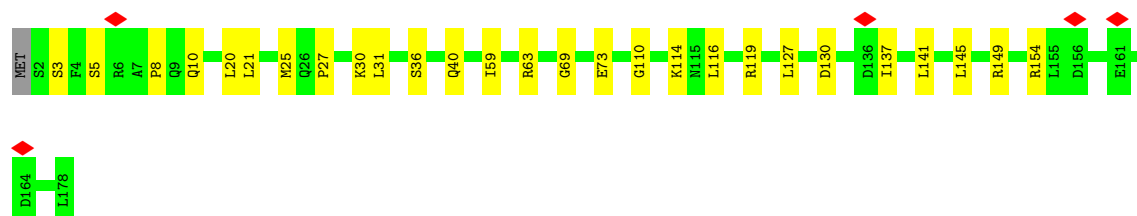
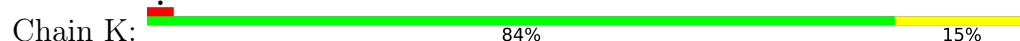




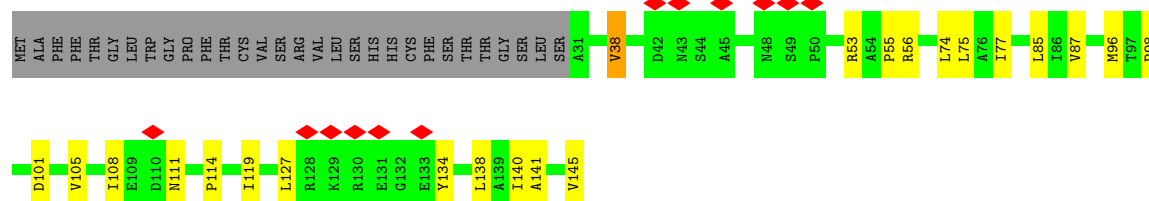
- Molecule 6: 39S ribosomal protein L11, mitochondrial



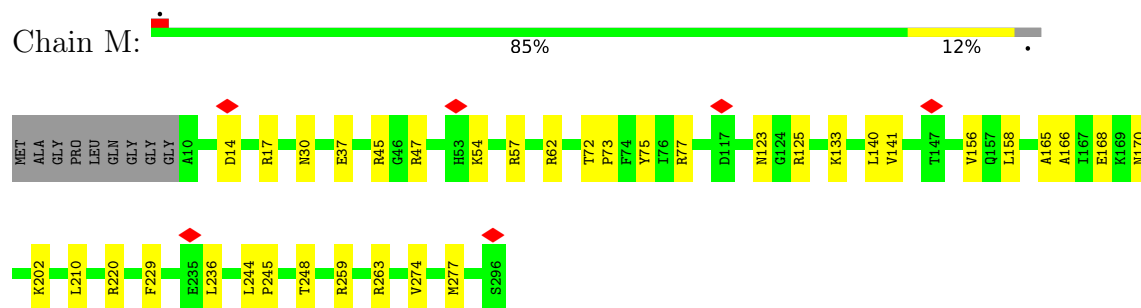
- Molecule 7: 39S ribosomal protein L13, mitochondrial



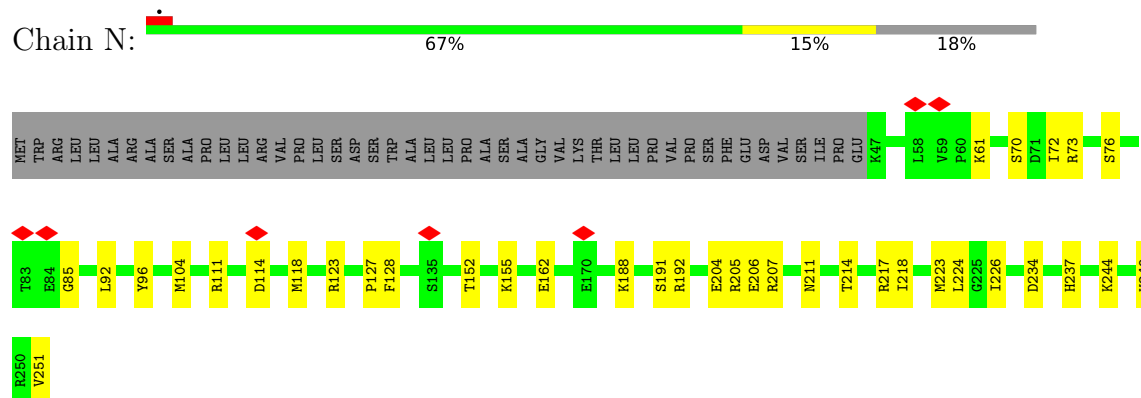
- Molecule 8: 39S ribosomal protein L14, mitochondrial



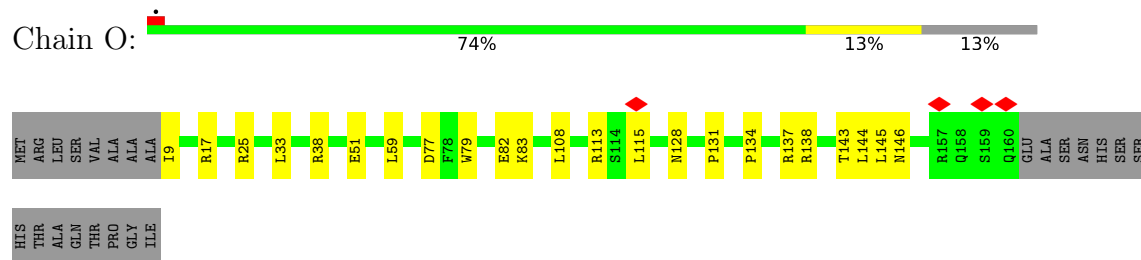
- Molecule 9: 39S ribosomal protein L15, mitochondrial



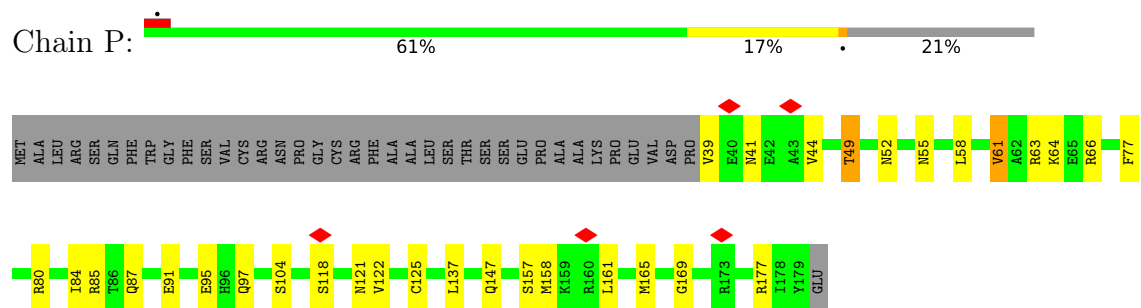
- Molecule 10: 39S ribosomal protein L16, mitochondrial



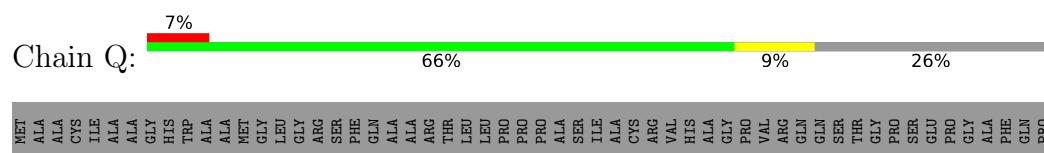
- Molecule 11: 39S ribosomal protein L17, mitochondrial

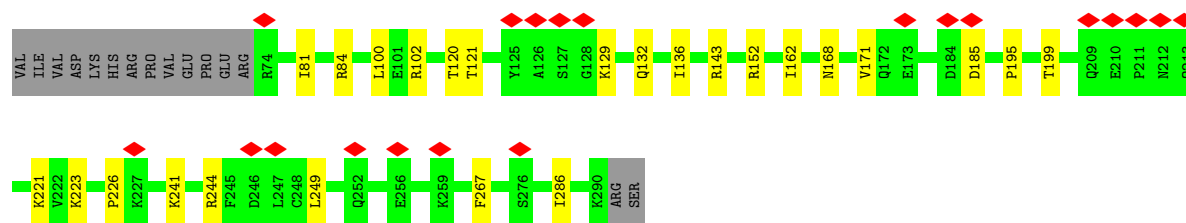


- Molecule 12: Mitochondrial ribosomal protein L18, isoform CRA_b

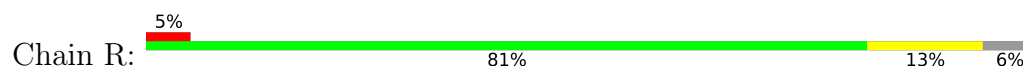


- Molecule 13: 39S ribosomal protein L19, mitochondrial

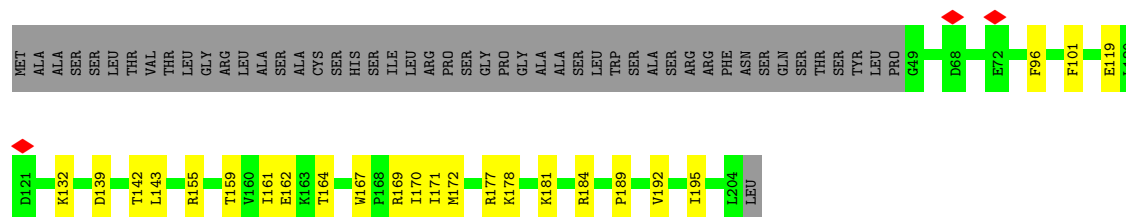




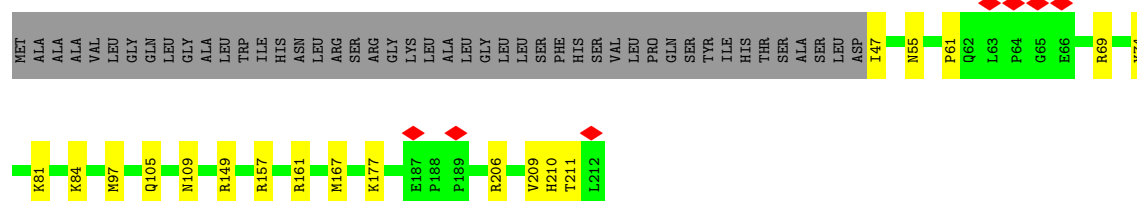
- Molecule 14: 39S ribosomal protein L20, mitochondrial



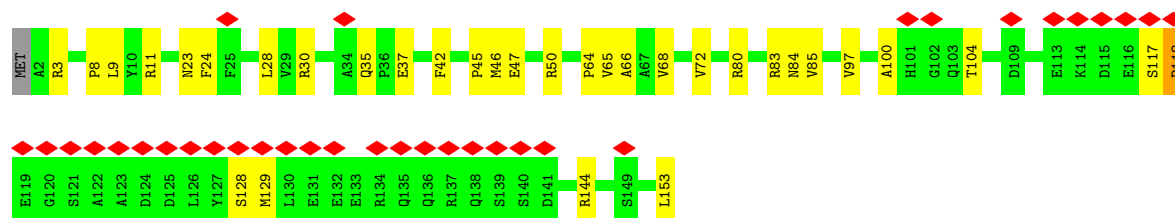
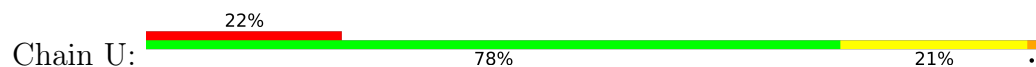
- Molecule 15: 39S ribosomal protein L21, mitochondrial



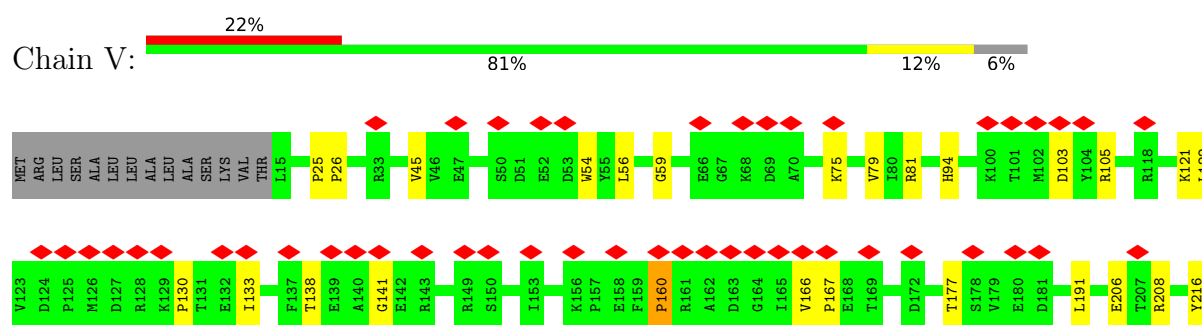
- Molecule 16: 39S ribosomal protein L22, mitochondrial



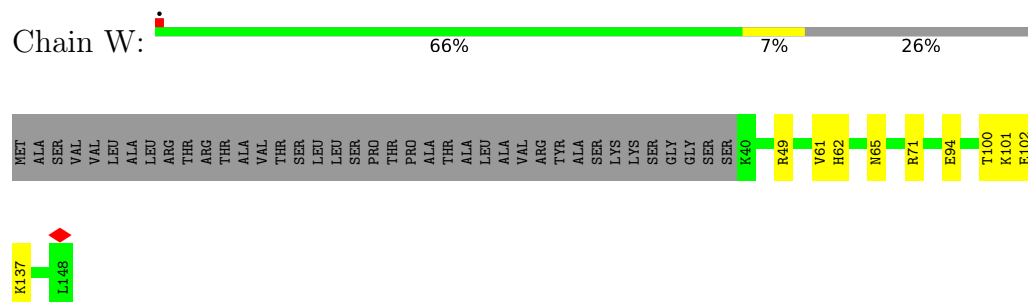
- Molecule 17: 39S ribosomal protein L23, mitochondrial



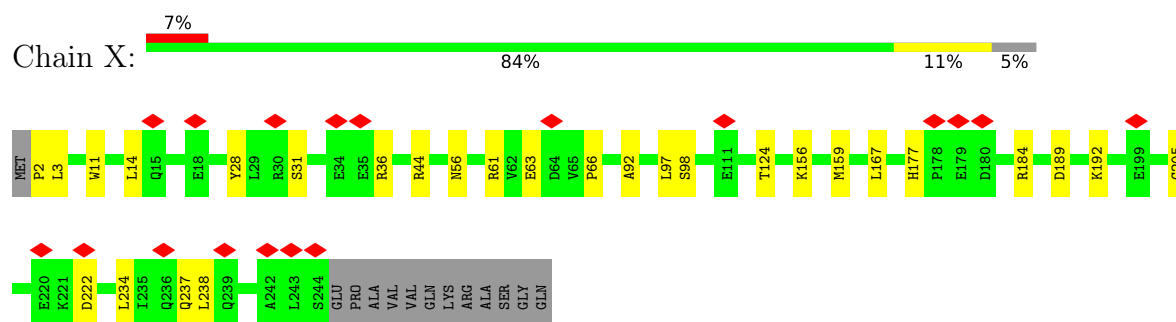
- Molecule 18: 39S ribosomal protein L24, mitochondrial



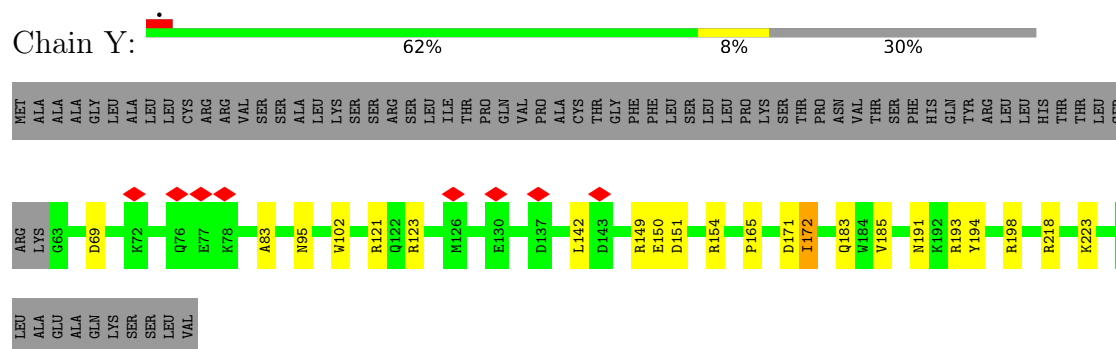
- Molecule 19: 39S ribosomal protein L27, mitochondrial



- Molecule 20: 39S ribosomal protein L28, mitochondrial

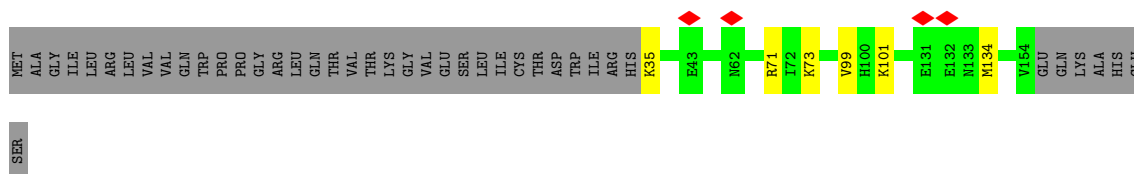


- Molecule 21: 39S ribosomal protein L47, mitochondrial

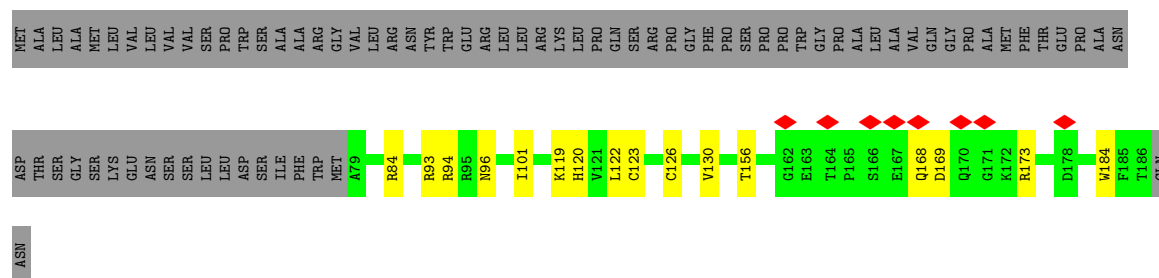


- Molecule 22: 39S ribosomal protein L30, mitochondrial





- Molecule 23: 39S ribosomal protein L32, mitochondrial



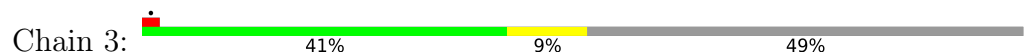
- Molecule 24: 39S ribosomal protein L33, mitochondrial



- Molecule 25: 39S ribosomal protein L34, mitochondrial

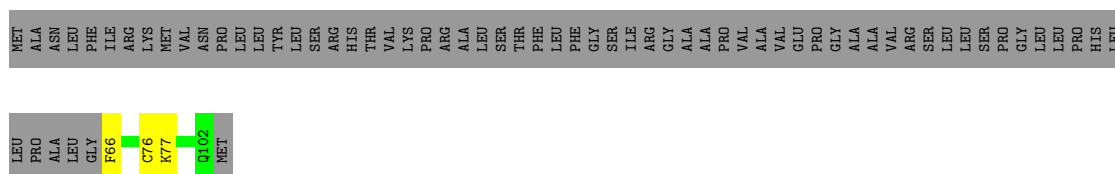


- Molecule 26: 39S ribosomal protein L35, mitochondrial

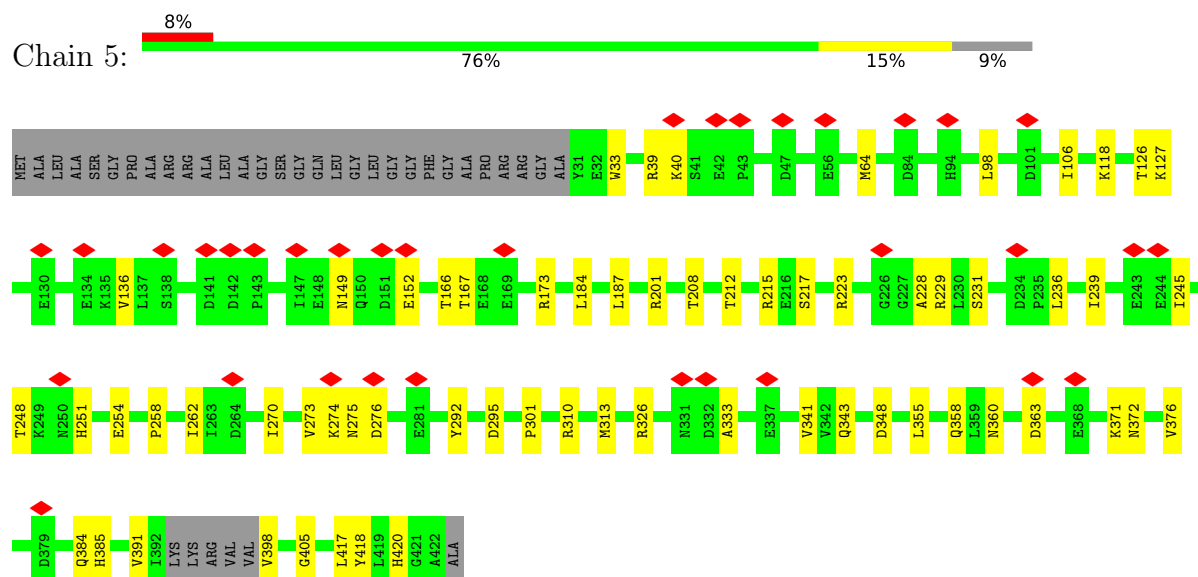


- Molecule 27: 39S ribosomal protein L36, mitochondrial

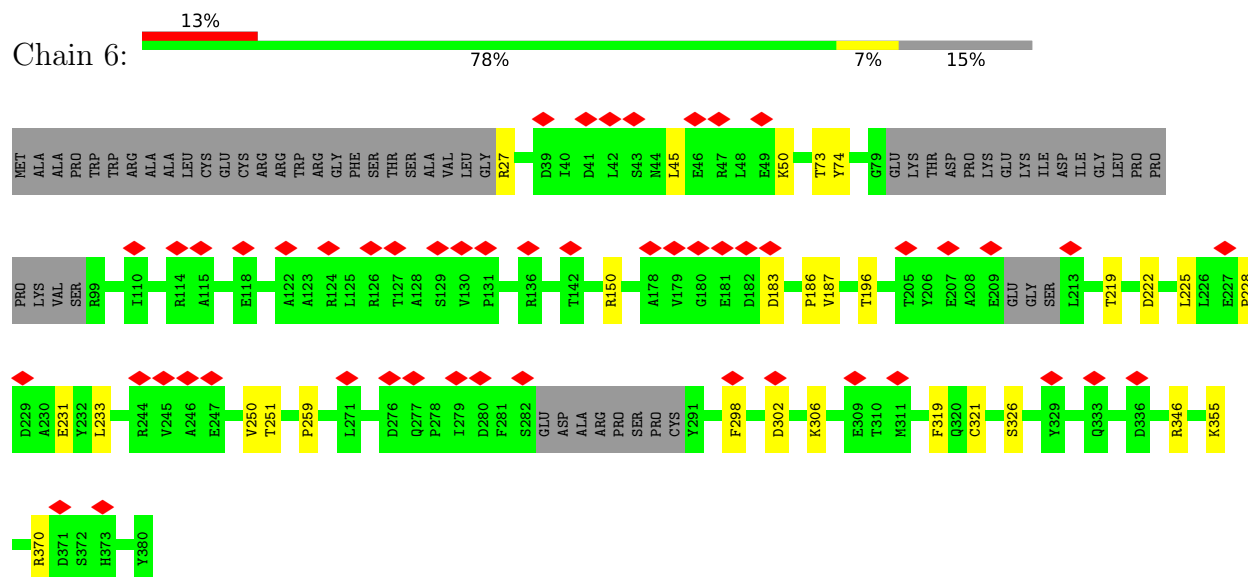




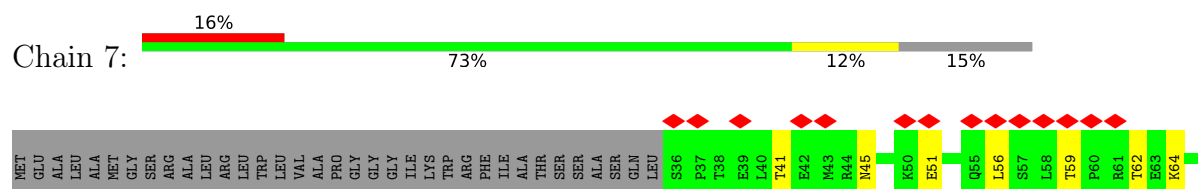
- Molecule 28: 39S ribosomal protein L37, mitochondrial

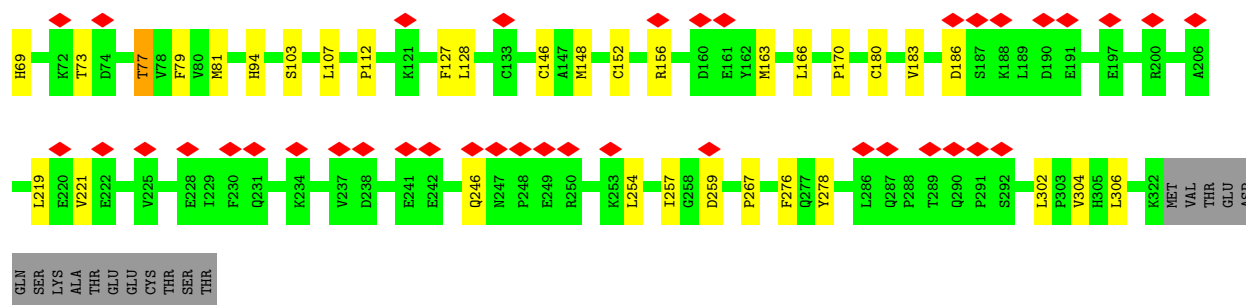


- Molecule 29: 39S ribosomal protein L38, mitochondrial

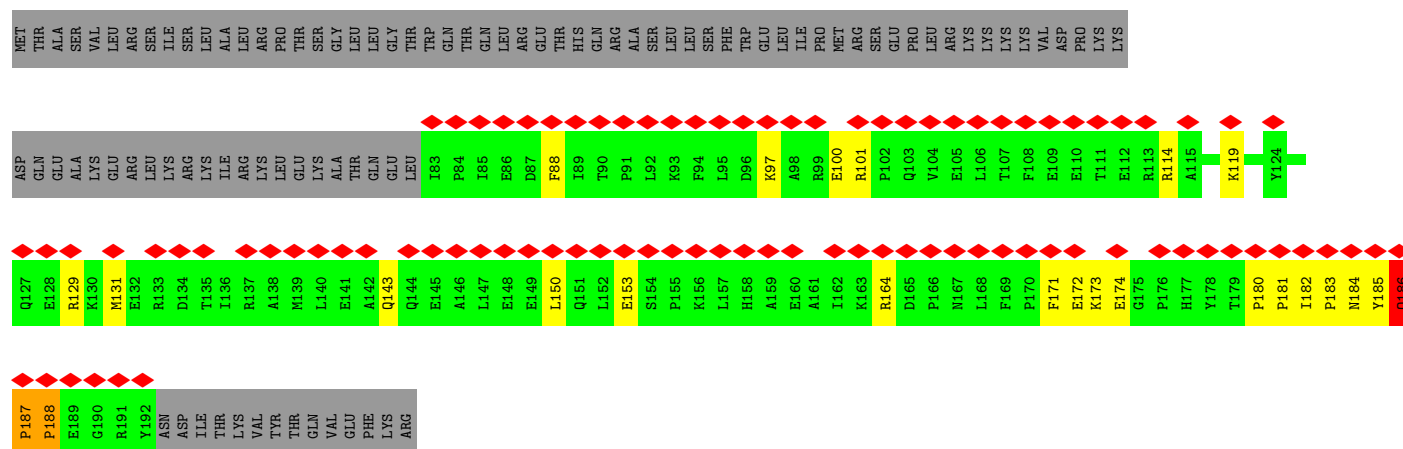
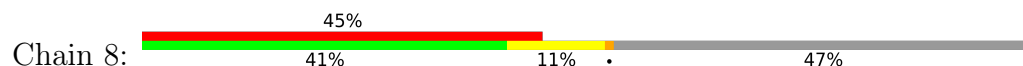


- Molecule 30: 39S ribosomal protein L39, mitochondrial

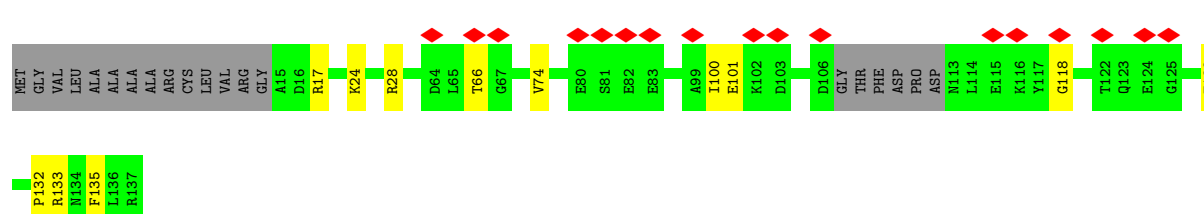




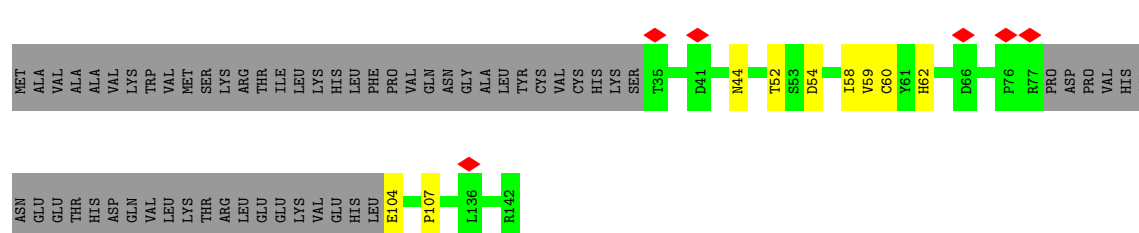
- Molecule 31: 39S ribosomal protein L40, mitochondrial



- Molecule 32: 39S ribosomal protein L41, mitochondrial



- Molecule 33: 39S ribosomal protein L42, mitochondrial



- Molecule 34: 39S ribosomal protein L43, mitochondrial

Frequency	Percentage
Daily	84%
Weekly	11%
Monthly	5%



Frequency	Percentage
5%	5%
79%	79%
17%	17%

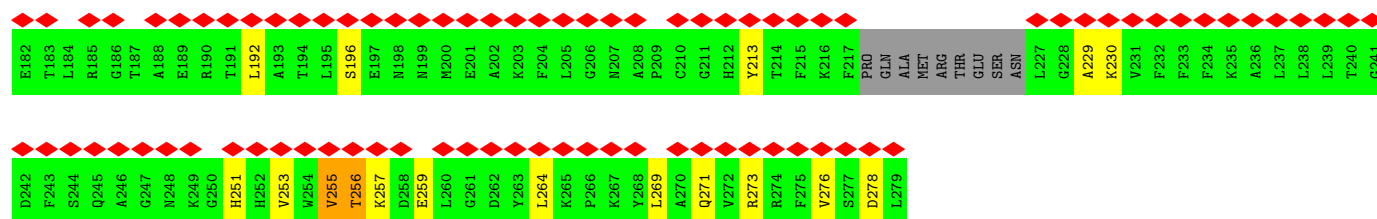


Category	Percentage
Very bad	20%
Bad	57%
Okay	11%
Good	31%

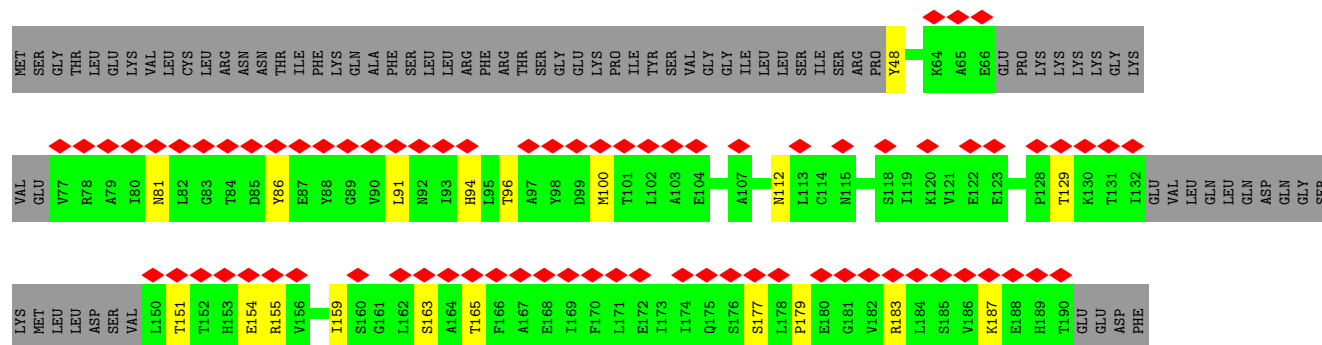
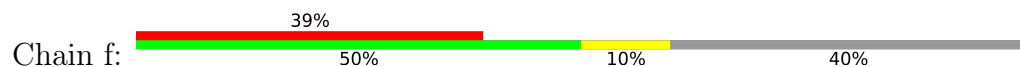


Category	Percentage
Good country	73%
Bad country	22%

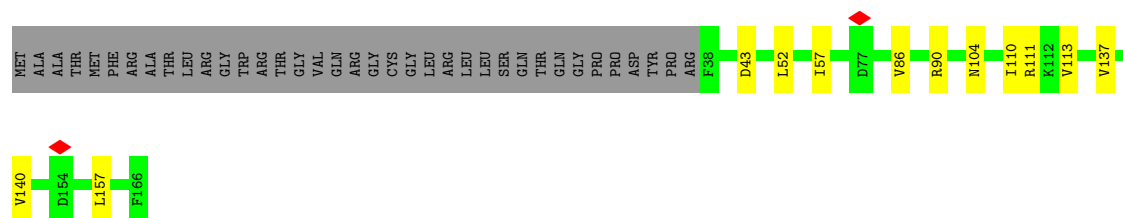




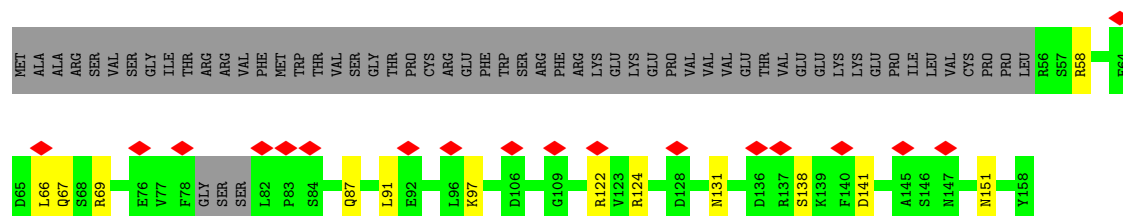
• Molecule 38: 39S ribosomal protein L48, mitochondrial



• Molecule 39: 39S ribosomal protein L49, mitochondrial

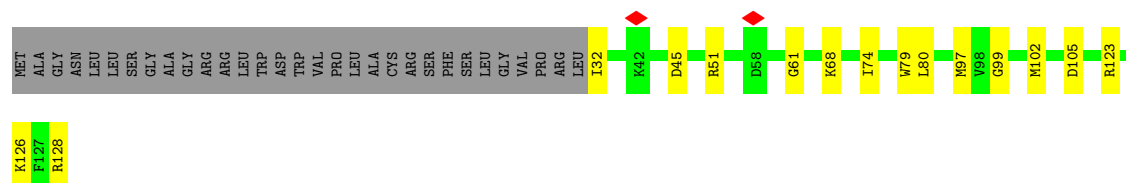


• Molecule 40: 39S ribosomal protein L50, mitochondrial

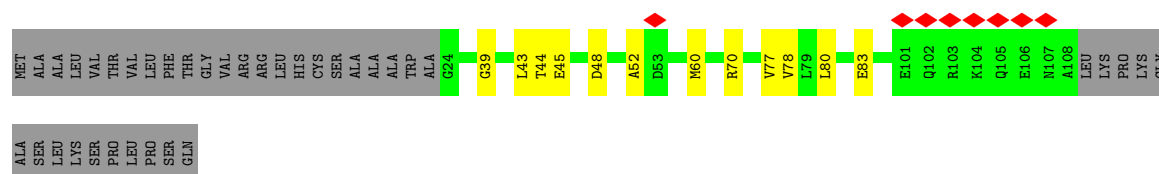


• Molecule 41: 39S ribosomal protein L51, mitochondrial

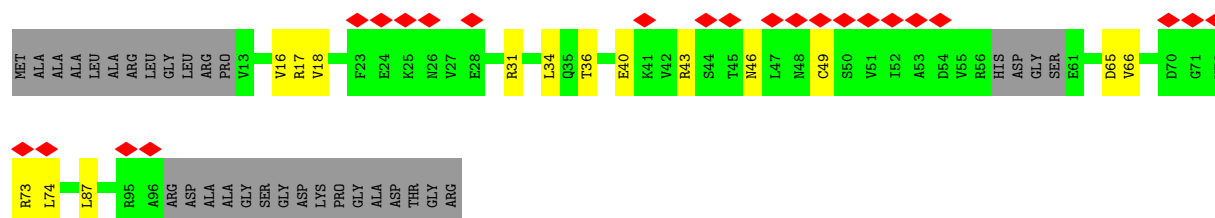




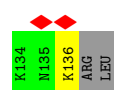
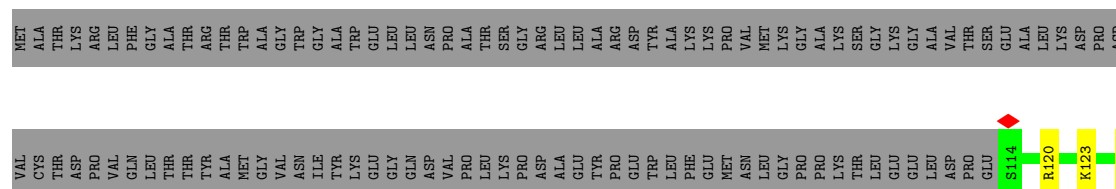
- Molecule 42: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA



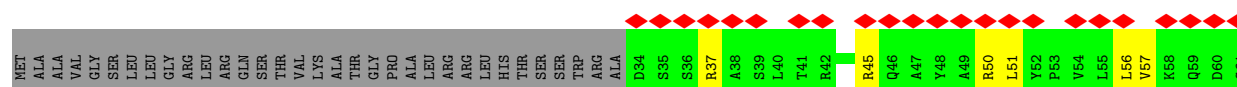
- Molecule 43: 39S ribosomal protein L53, mitochondrial

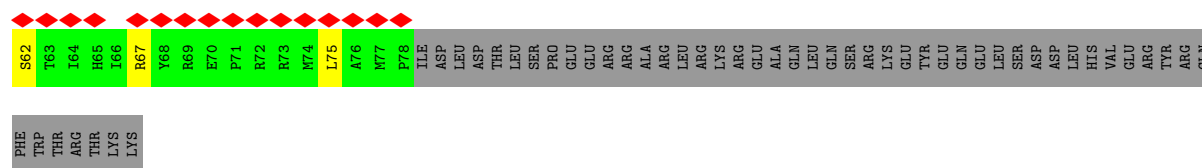


- Molecule 44: 39S ribosomal protein L54, mitochondrial

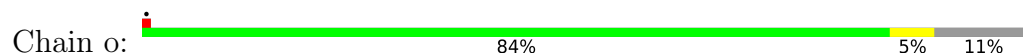


- Molecule 45: 39S ribosomal protein L55, mitochondrial

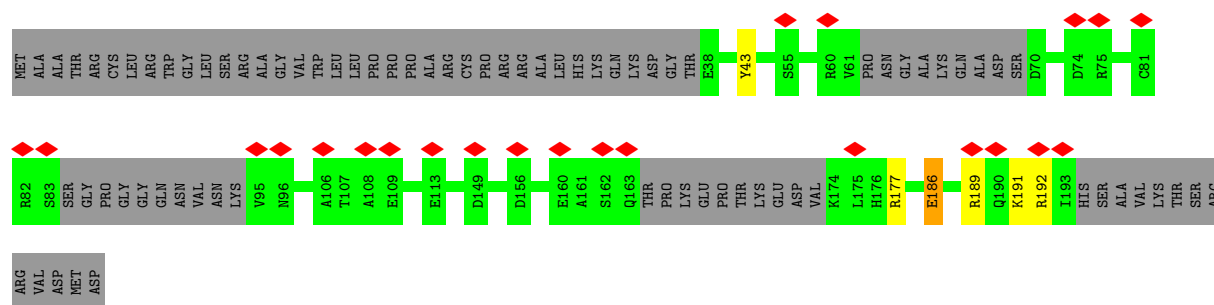




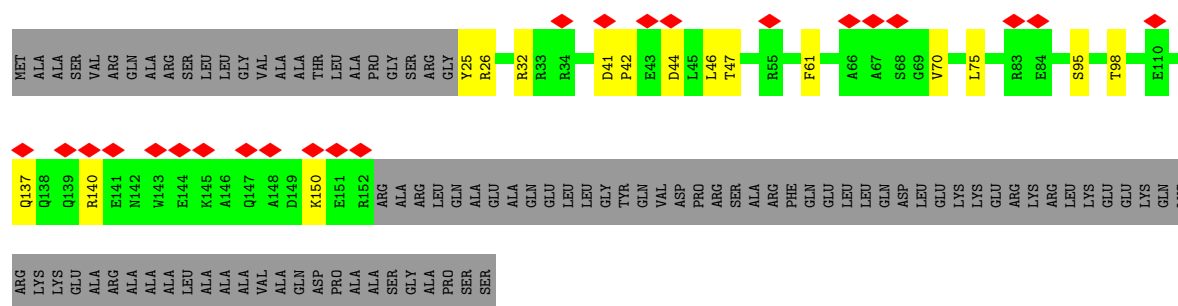
- Molecule 46: Ribosomal protein 63, mitochondrial



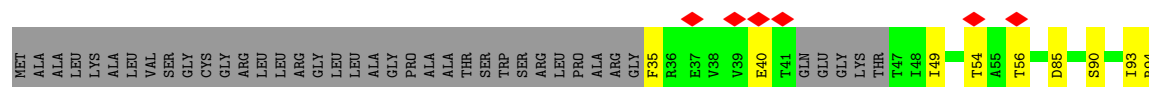
- Molecule 47: Peptidyl-tRNA hydrolase ICT1, mitochondrial

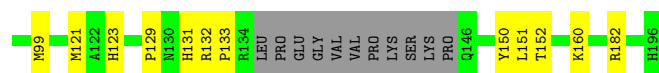


- Molecule 48: Growth arrest and DNA damage-inducible proteins-interacting protein 1



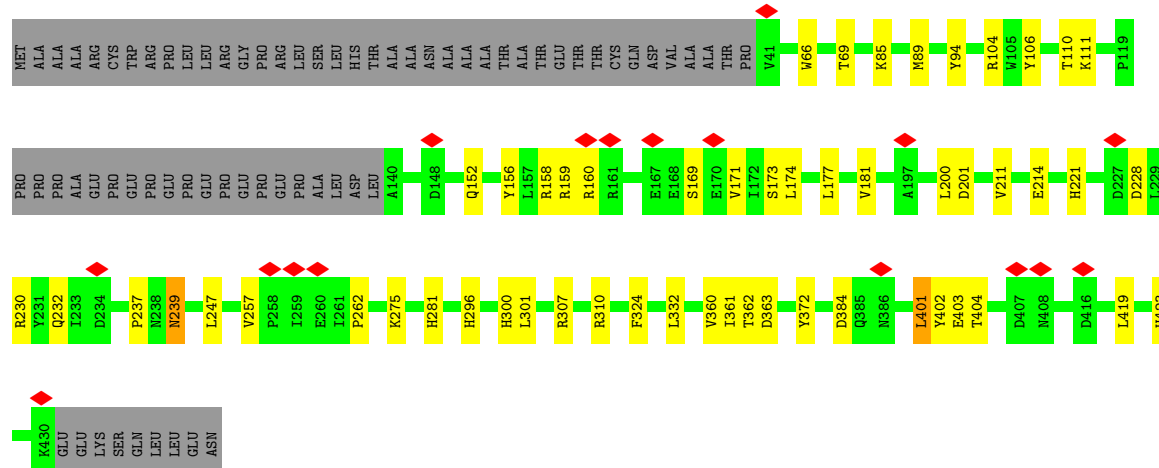
- Molecule 49: 39S ribosomal protein S18a, mitochondrial





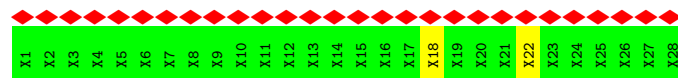
- Molecule 50: 39S ribosomal protein S30, mitochondrial

Chain s: 72% 12% 16%



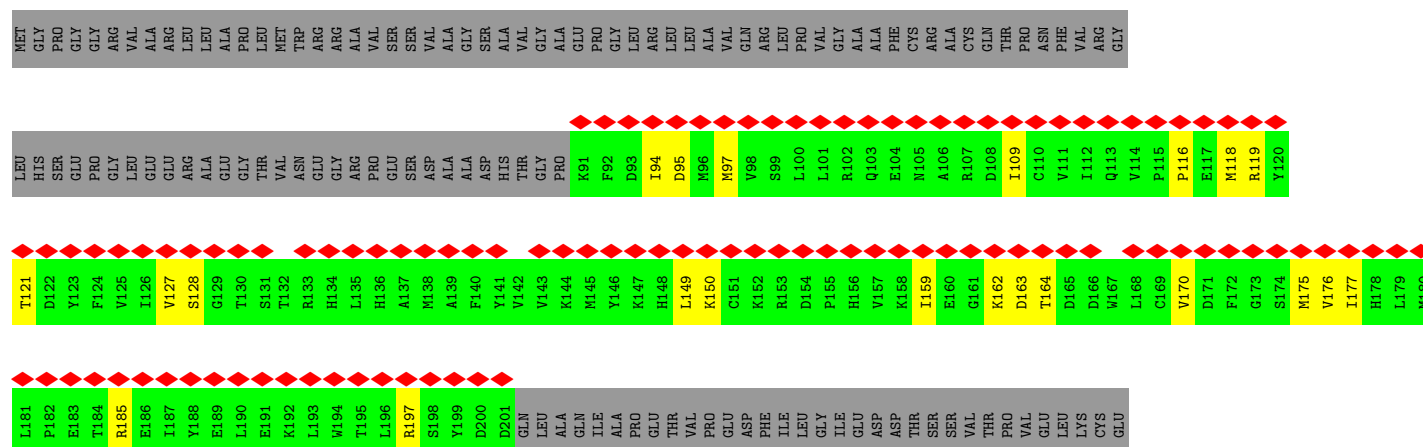
- Molecule 51: Unknown protein/protein extension

Chain t: 100% 93% 7%



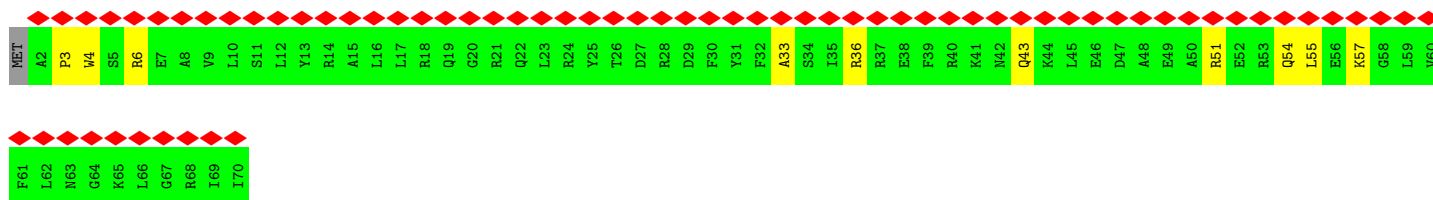
- Molecule 52: Mitochondrial assembly of ribosomal large subunit protein 1

Chain u: 46% 38% 9% 53%

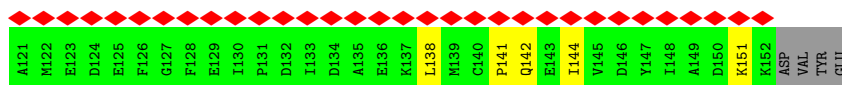
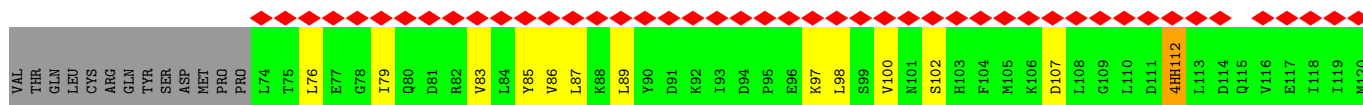
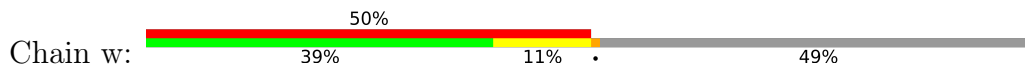


- Molecule 53: MIEF1 upstream open reading frame protein

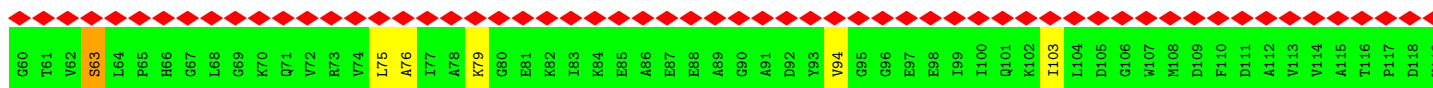
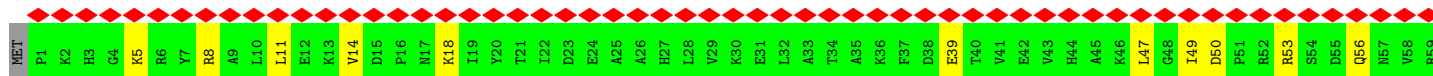
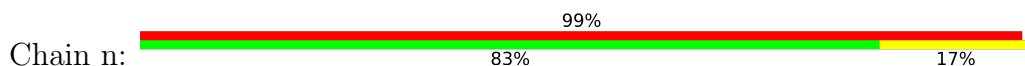
Chain v: 99% 84% 14%



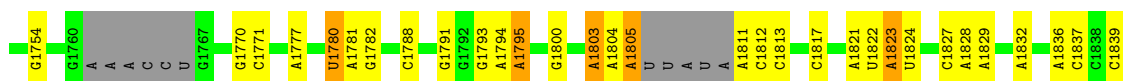
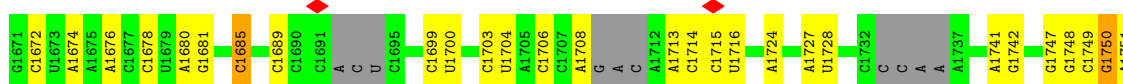
• Molecule 54: Acyl carrier protein, mitochondrial

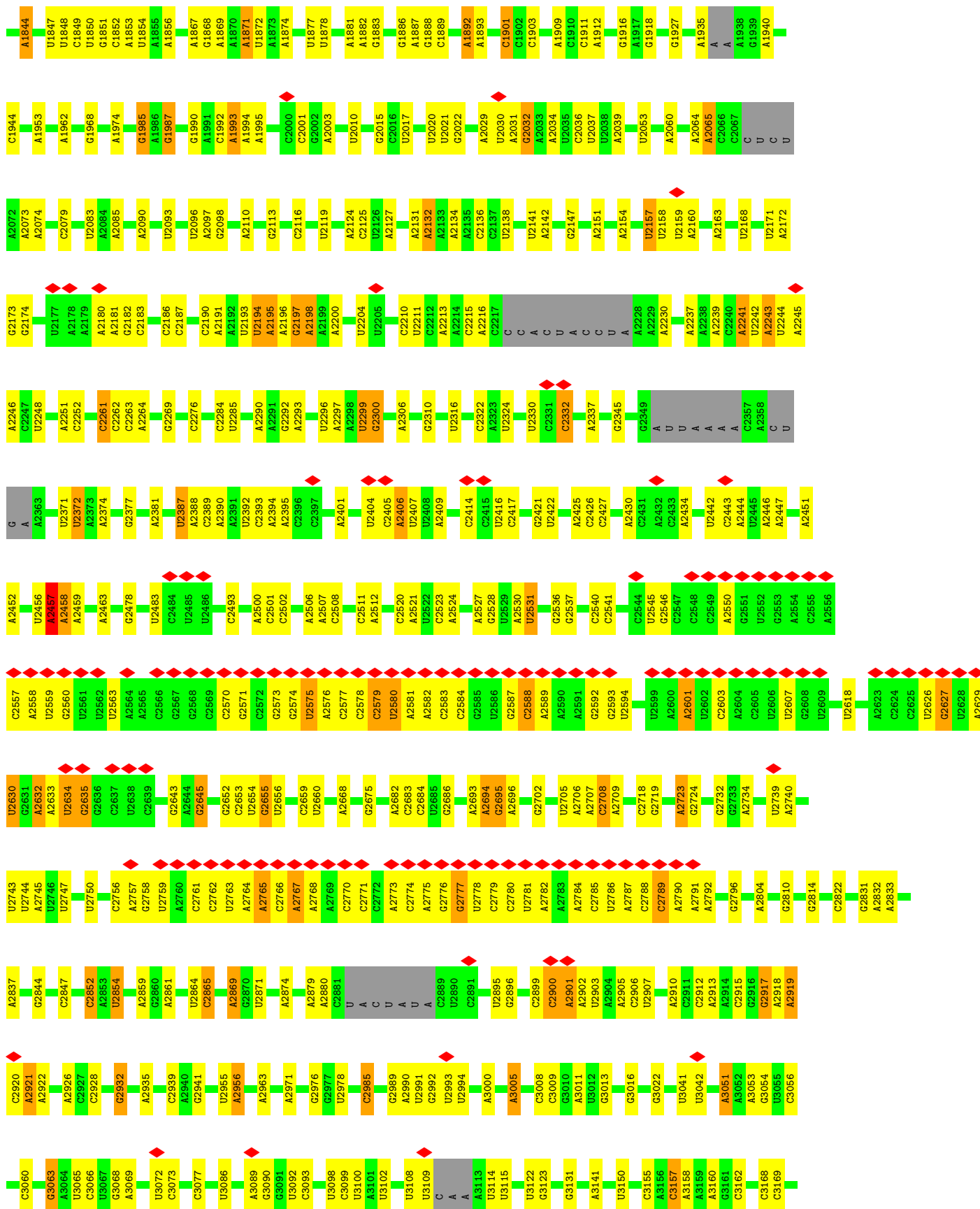


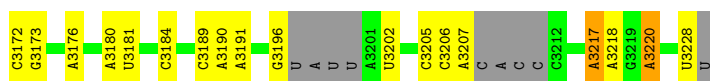
• Molecule 55: 50S ribosomal protein L1



• Molecule 56: 16S rRNA



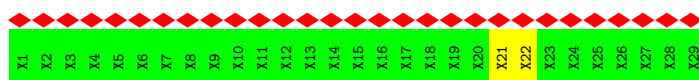




• Molecule 57: mt-tRNA^{Val}



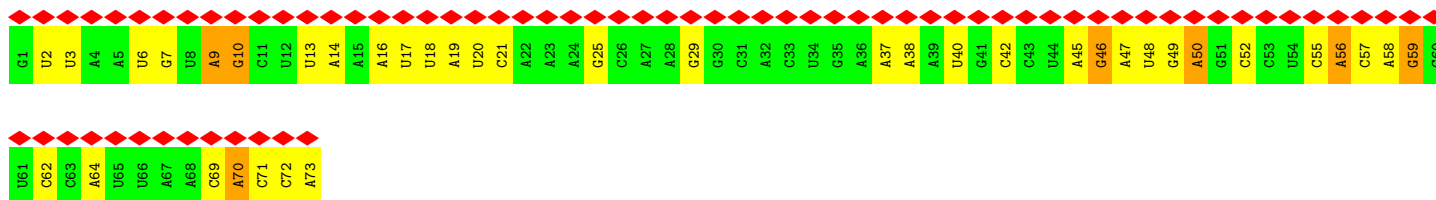
• Molecule 58: nascent chain



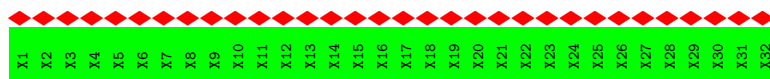
• Molecule 59: mt-tRNA



• Molecule 59: mt-tRNA



• Molecule 60: Unknown protein/protein extension



• Molecule 61: unknown protein/protein extension



X7	X8	X9	X10	X11	X12	X13	X14	X15	X16	X17	X18	X19	X20
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54398	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.926	Depositor
Minimum map value	-0.488	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	644.80255, 644.80255, 644.80255	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25938, 1.25938, 1.25938	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ZN, CL, MG, 4HH

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	D	0.38	0/1879	0.64	1/2527 (0.0%)
2	E	0.45	0/2465	0.60	0/3344
3	F	0.47	0/2071	0.60	1/2817 (0.0%)
4	C	0.34	1/665 (0.2%)	0.74	0/905
4	H	0.43	0/798	0.63	0/1073
5	I	0.30	0/1308	0.69	1/1761 (0.1%)
6	J	0.28	0/1077	0.70	0/1452
7	K	0.47	0/1495	0.58	1/2029 (0.0%)
8	L	0.39	0/904	0.64	1/1218 (0.1%)
9	M	0.47	0/2359	0.60	0/3185
10	N	0.42	0/1697	0.59	0/2281
11	O	0.46	0/1269	0.59	0/1708
12	P	0.41	0/1173	0.60	1/1588 (0.1%)
13	Q	0.38	0/1846	0.60	0/2487
14	R	0.50	0/1174	0.60	0/1572
15	S	0.49	0/1276	0.62	0/1729
16	T	0.47	0/1402	0.56	0/1886
17	U	0.44	0/1247	0.74	1/1689 (0.1%)
18	V	0.33	0/1666	0.62	4/2260 (0.2%)
19	W	0.50	0/881	0.54	0/1188
20	X	0.40	0/2090	0.58	2/2825 (0.1%)
21	Y	0.42	0/1552	0.53	0/2079
22	Z	0.44	0/1003	0.57	0/1354
23	0	0.40	0/895	0.57	0/1201
24	1	0.43	0/438	0.60	0/583
25	2	0.51	0/373	0.61	0/496
26	3	0.52	0/852	0.56	0/1136
27	4	0.47	0/341	0.55	0/451
28	5	0.39	0/3250	0.59	2/4429 (0.0%)
29	6	0.35	0/2726	0.56	0/3715
30	7	0.35	0/2391	0.62	2/3234 (0.1%)
31	8	0.28	0/909	0.82	7/1227 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.40	0/972	0.60	0/1306
33	a	0.37	0/709	0.51	0/963
34	b	0.44	0/1202	0.63	0/1626
35	c	0.36	0/2264	0.53	0/3059
36	d	0.30	0/1790	0.52	0/2423
37	e	0.26	0/1797	0.64	2/2422 (0.1%)
38	f	0.29	0/931	0.57	0/1259
39	g	0.42	0/1102	0.58	0/1503
40	h	0.32	0/847	0.50	0/1150
41	i	0.54	1/849 (0.1%)	0.62	0/1135
42	j	0.38	0/698	0.53	0/940
43	k	0.32	0/635	0.60	0/855
44	l	0.26	0/226	0.45	0/299
45	m	0.27	0/379	0.73	0/510
46	o	0.45	0/792	0.61	0/1064
47	p	0.30	0/1071	0.51	0/1433
48	q	0.31	0/1107	0.50	0/1498
49	r	0.42	0/1238	0.60	2/1676 (0.1%)
50	s	0.42	0/3114	0.58	0/4225
52	u	0.24	0/949	0.55	0/1281
53	v	0.21	0/597	0.57	0/796
54	w	0.24	0/640	0.58	0/860
55	n	0.27	0/1813	0.70	0/2443
56	A	0.44	0/35440	0.46	9/55140 (0.0%)
57	B	0.23	0/1328	0.34	0/2056
59	G	0.17	0/1731	0.36	0/2693
59	x	0.17	0/1731	0.36	0/2693
All	All	0.40	2/111424 (0.0%)	0.54	37/158737 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
5	I	0	1
15	S	0	1
28	5	0	1
31	8	0	2
58	Y2	0	2
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	i	68	LYS	C-N	-5.88	1.24	1.33
4	C	184	LEU	C-N	-5.29	1.25	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	A	2920	C	OP1-P-OP2	-13.31	79.67	119.60
56	A	2920	C	O5'-P-OP2	-11.36	73.93	108.00
56	A	2919	A	OP1-P-O3'	-10.52	76.44	108.00
56	A	2919	A	OP2-P-O3'	9.42	136.26	108.00
30	7	246	GLN	CA-C-N	9.40	138.79	120.94
30	7	246	GLN	C-N-CA	9.40	138.79	120.94
5	I	102	VAL	N-CA-C	-9.30	104.27	113.20
56	A	2920	C	O5'-P-OP1	7.68	131.05	108.00
31	8	188	PRO	N-CA-CB	7.12	110.72	103.25
31	8	187	PRO	N-CA-CB	7.08	109.95	103.08
31	8	183	PRO	N-CA-CB	6.91	110.50	103.25
8	L	140	ILE	N-CA-C	-6.35	107.68	113.71
18	V	160	PRO	N-CA-CB	6.33	109.90	103.25
18	V	166	VAL	CA-C-N	6.14	127.51	119.84
18	V	166	VAL	C-N-CA	6.14	127.51	119.84
31	8	185	TYR	N-CA-C	6.05	116.00	108.19
17	U	118	PRO	N-CA-CB	6.03	109.58	103.25
7	K	137	ILE	N-CA-C	-5.96	107.00	112.96
37	e	178	TRP	CA-C-N	5.90	136.64	122.36
37	e	178	TRP	C-N-CA	5.90	136.64	122.36
18	V	167	PRO	N-CA-CB	5.79	109.33	103.25
56	A	2919	A	O3'-P-O5'	-5.79	95.31	104.00
49	r	131	HIS	CA-C-N	5.46	128.95	120.60
49	r	131	HIS	C-N-CA	5.46	128.95	120.60
31	8	186	GLN	CA-C-N	5.44	125.98	120.38
31	8	186	GLN	C-N-CA	5.44	125.98	120.38
1	D	207	ILE	N-CA-C	5.25	120.25	109.34
12	P	61	VAL	N-CA-C	-5.16	108.26	113.47
28	5	215	ARG	CA-C-N	5.15	131.38	121.54
28	5	215	ARG	C-N-CA	5.15	131.38	121.54
20	X	36	ARG	CA-C-N	5.13	127.55	120.67
20	X	36	ARG	C-N-CA	5.13	127.55	120.67
3	F	86	VAL	N-CA-C	-5.12	107.82	112.12
56	A	1823	A	P-O3'-C3'	5.11	127.86	120.20
56	A	2243	A	P-O3'-C3'	5.10	127.86	120.20
56	A	2457	A	P-O3'-C3'	5.10	127.85	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	8	184	ASN	N-CA-C	5.07	116.50	111.07

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	5	217	SER	Peptide
31	8	180	PRO	Peptide
31	8	186	GLN	Peptide
1	D	206	TYR	Peptide
5	I	160	LYS	Peptide
15	S	101	PHE	Peptide
58	Y2	21	UNK	Peptide
58	Y2	22	UNK	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1842	0	1896	24	0
2	E	2396	0	2402	18	0
3	F	2013	0	2044	21	0
4	C	648	0	657	13	0
4	H	784	0	832	5	0
5	I	1283	0	1369	22	0
6	J	1061	0	1141	15	0
7	K	1451	0	1448	19	0
8	L	889	0	941	15	0
9	M	2305	0	2378	24	0
10	N	1654	0	1681	23	0
11	O	1245	0	1283	18	0
12	P	1148	0	1148	24	0
13	Q	1805	0	1841	17	0
14	R	1153	0	1214	17	0
15	S	1251	0	1322	18	0
16	T	1368	0	1410	15	0
17	U	1218	0	1186	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	V	1624	0	1606	14	0
19	W	859	0	888	7	0
20	X	2035	0	2054	18	0
21	Y	1517	0	1561	19	0
22	Z	978	0	1030	7	0
23	0	880	0	902	13	0
24	1	433	0	475	4	0
25	2	367	0	393	2	0
26	3	831	0	883	14	0
27	4	333	0	353	2	0
28	5	3156	0	3138	42	0
29	6	2640	0	2464	20	0
30	7	2334	0	2343	24	0
31	8	890	0	864	15	0
32	9	947	0	949	13	0
33	a	686	0	658	7	0
34	b	1178	0	1180	14	0
35	c	2217	0	2220	9	0
36	d	1741	0	1727	24	0
37	e	1762	0	1767	31	0
38	f	915	0	917	14	0
39	g	1067	0	1056	8	0
40	h	827	0	806	9	0
41	i	827	0	857	12	0
42	j	684	0	673	10	0
43	k	627	0	636	9	0
44	l	221	0	227	3	0
45	m	372	0	387	6	0
46	o	771	0	775	3	0
47	p	1058	0	1083	5	0
48	q	1076	0	1049	11	0
49	r	1203	0	1220	16	0
50	s	3036	0	3022	35	0
51	t	140	0	30	1	0
52	u	927	0	921	16	0
53	v	588	0	604	8	0
54	w	659	0	655	14	0
55	n	1767	0	1829	21	0
56	A	31684	0	16102	146	0
57	B	1191	0	607	9	0
58	Y2	145	0	39	0	0
59	G	1547	0	787	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	x	1547	0	788	8	0
60	y	160	0	34	0	0
61	z	70	0	16	0	0
62	A	90	0	0	0	0
62	D	1	0	0	0	0
62	g	1	0	0	0	0
63	0	1	0	0	0	0
63	4	1	0	0	0	0
63	r	1	0	0	0	0
64	n	2	0	0	0	0
65	A	1	0	0	0	0
65	n	3	0	0	0	0
All	All	106132	0	88768	793	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (793) 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)
49:r:35:PHE:N	49:r:56:THR:HG1	1.73	0.87
28:5:126:THR:HG22	28:5:372:ASN:HB2	1.73	0.70
30:7:163:MET:HB3	30:7:186:ASP:HB3	1.74	0.69
12:P:87:GLN:HE22	57:B:1625:A:H62	1.41	0.69
12:P:58:LEU:HD23	47:p:177:ARG:HH21	1.59	0.68
56:A:2545:U:H5''	56:A:2546:G:H5'	1.77	0.67
5:I:104:LEU:HB2	5:I:109:LYS:HG3	1.75	0.67
55:n:50:ASP:H	55:n:56:GLN:HG2	1.61	0.66
17:U:64:PRO:HB2	17:U:100:ALA:HB3	1.78	0.65
26:3:188:VAL:HG11	39:g:104:ASN:HB3	1.78	0.65
41:i:32:ILE:HD13	56:A:1813:C:H2'	1.80	0.64
21:Y:193:ARG:NH2	56:A:1706:C:OP1	2.31	0.64
53:v:33:ALA:HA	53:v:36:ARG:HD3	1.79	0.63
1:D:124:GLU:HG2	1:D:144:GLY:HA3	1.81	0.63
5:I:97:ALA:HB3	5:I:154:LEU:HB2	1.80	0.63
57:B:1607:U:H3	57:B:1664:G:H1	1.47	0.63
12:P:44:VAL:HG13	29:6:225:LEU:HB3	1.81	0.63
28:5:229:ARG:NH1	28:5:231:SER:OG	2.31	0.63
27:4:66:PHE:N	56:A:3013:G:HO2'	1.97	0.62
56:A:1747:G:N2	56:A:1750:G:O2'	2.32	0.62
55:n:47:LEU:HB2	55:n:49:ILE:HG12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:n:120:MET:HA	55:n:123:VAL:HG12	1.81	0.62
14:R:99:ARG:NH2	56:A:2248:U:OP1	2.29	0.62
43:k:17:ARG:HB3	43:k:65:ASP:HB3	1.81	0.62
56:A:1871:A:N7	56:A:1901:C:N4	2.48	0.61
50:s:211:VAL:HG22	50:s:230:ARG:HG3	1.82	0.61
4:C:167:LEU:HD21	4:C:233:VAL:HB	1.83	0.61
5:I:164:MET:HA	5:I:167:ILE:HD12	1.82	0.61
7:K:110:GLY:O	7:K:114:LYS:NZ	2.33	0.61
16:T:55:ASN:ND2	16:T:74:TYR:O	2.33	0.61
55:n:103:ILE:HD11	55:n:127:LEU:HD21	1.82	0.61
8:L:96:MET:SD	13:Q:168:ASN:ND2	2.73	0.61
21:Y:151:ASP:OD1	21:Y:154:ARG:NH1	2.34	0.60
17:U:46:MET:HE1	17:U:72:VAL:HG13	1.83	0.60
23:0:119:LYS:O	23:0:120:HIS:ND1	2.33	0.60
34:b:62:VAL:HA	40:h:151:ASN:HB2	1.83	0.60
35:c:94:ASN:HA	35:c:122:ASN:HB2	1.84	0.60
50:s:152:GLN:HA	50:s:156:TYR:HB2	1.83	0.60
15:S:177:ARG:NH2	56:A:1853:A:OP2	2.34	0.60
31:8:100:GLU:HG2	31:8:101:ARG:HE	1.66	0.60
39:g:111:ARG:NH2	56:A:1881:A:OP2	2.35	0.60
11:O:33:LEU:HD21	11:O:59:LEU:HD22	1.83	0.60
41:i:99:GLY:HA2	41:i:102:MET:HE3	1.83	0.59
1:D:130:ARG:NH1	1:D:131:TYR:O	2.35	0.59
28:5:173:ARG:NH2	56:A:2395:A:OP1	2.36	0.59
12:P:52:ASN:HB3	12:P:55:ASN:HB2	1.84	0.59
12:P:77:PHE:O	12:P:97:GLN:NE2	2.35	0.59
9:M:202:LYS:HD2	9:M:263:ARG:HE	1.68	0.59
52:u:149:LEU:HD23	52:u:150:LYS:HB2	1.83	0.59
6:J:92:LYS:HB2	6:J:97:ILE:HB	1.82	0.59
20:X:61:ARG:NH2	20:X:63:GLU:OE1	2.35	0.59
7:K:27:PRO:HG2	7:K:30:LYS:HB2	1.85	0.59
17:U:66:ALA:HB2	17:U:100:ALA:HB2	1.84	0.59
1:D:246:ARG:NH2	56:A:2531:U:O4	2.36	0.59
7:K:154:ARG:HD3	49:r:129:PRO:HG3	1.84	0.59
31:8:172:GLU:OE2	38:f:183:ARG:NH1	2.35	0.59
37:e:146:ARG:HB3	37:e:253:VAL:HG13	1.85	0.59
47:p:186:GLU:HG3	47:p:189:ARG:HE	1.68	0.59
54:w:76:LEU:HA	54:w:79:ILE:HD12	1.84	0.59
27:4:76:CYS:SG	27:4:77:LYS:N	2.76	0.59
28:5:341:VAL:HG22	28:5:358:GLN:HG2	1.85	0.59
29:6:259:PRO:HG3	29:6:321:CYS:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:b:27:GLN:HE21	34:b:80:LEU:HA	1.67	0.59
11:O:25:ARG:NH2	11:O:51:GLU:OE2	2.36	0.58
12:P:87:GLN:HE21	57:B:1643:A:H61	1.49	0.58
37:e:43:SER:OG	37:e:45:TRP:NE1	2.36	0.58
56:A:2902:A:H61	56:A:2907:U:H3	1.50	0.58
5:I:148:VAL:O	43:k:31:ARG:NH2	2.37	0.58
9:M:54:LYS:NZ	56:A:1848:U:OP1	2.33	0.58
56:A:1800:G:H22	56:A:1803:A:H5'	1.67	0.58
9:M:140:LEU:HB2	9:M:156:VAL:HG21	1.84	0.58
1:D:228:LEU:HD11	1:D:234:MET:HE3	1.85	0.58
9:M:77:ARG:NH1	56:A:2917:G:O6	2.36	0.58
5:I:187:SER:OG	5:I:188:ARG:N	2.37	0.58
14:R:11:ARG:HH22	56:A:2276:C:H1'	1.69	0.58
50:s:201:ASP:OD1	50:s:201:ASP:N	2.36	0.58
28:5:301:PRO:HB3	56:A:2389:C:H5''	1.86	0.58
52:u:94:ILE:HA	52:u:97:MET:HB2	1.86	0.58
9:M:166:ALA:O	9:M:170:ASN:ND2	2.36	0.57
59:x:25:G:N2	59:x:42:C:O2	2.37	0.57
13:Q:121:THR:HG22	13:Q:171:VAL:HG12	1.86	0.57
16:T:161:ARG:O	56:A:2430:A:N6	2.38	0.57
30:7:51:GLU:HG3	30:7:219:LEU:HD21	1.84	0.57
56:A:1777:A:N6	56:A:1780:U:OP2	2.32	0.57
2:E:50:ASP:O	11:O:138:ARG:NH2	2.36	0.57
2:E:68:GLU:OE1	2:E:154:ARG:NH1	2.38	0.57
12:P:84:ILE:HB	12:P:91:GLU:HB3	1.85	0.57
15:S:155:ARG:NH1	42:j:52:ALA:O	2.36	0.57
2:E:275:ARG:NH2	2:E:331:ASP:OD1	2.37	0.57
56:A:2196:A:O2'	56:A:2213:A:N1	2.34	0.57
3:F:114:THR:O	3:F:156:ARG:NH2	2.38	0.57
12:P:85:ARG:NH1	12:P:125:CYS:SG	2.78	0.57
5:I:181:ILE:O	5:I:184:THR:OG1	2.23	0.57
10:N:206:GLU:HG2	10:N:251:VAL:HG13	1.87	0.57
45:m:57:VAL:HG13	45:m:62:SER:H	1.70	0.57
5:I:186:LEU:HB3	5:I:190:GLY:HA3	1.87	0.57
31:8:143:GLN:HG2	38:f:165:THR:HG22	1.86	0.57
20:X:156:LYS:NZ	20:X:205:GLY:O	2.38	0.57
56:A:1962:A:OP2	56:A:2501:C:N4	2.37	0.57
3:F:137:ARG:NH1	56:A:2932:G:OP1	2.34	0.56
35:c:50:LEU:HD22	35:c:55:PRO:HD3	1.87	0.56
1:D:194:ASN:OD1	1:D:243:THR:OG1	2.24	0.56
9:M:47:ARG:NH1	56:A:1847:U:OP1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:101:LYS:NZ	56:A:2064:A:OP1	2.34	0.56
24:1:34:ARG:NH2	24:1:58:GLU:OE2	2.38	0.56
24:1:45:HIS:ND1	56:A:2852:C:O2'	2.36	0.56
56:A:2765:A:H5''	56:A:2767:A:H5''	1.86	0.56
7:K:8:PRO:HG2	35:c:295:GLU:HG3	1.88	0.56
12:P:80:ARG:NH1	12:P:95:GLU:OE2	2.32	0.56
55:n:156:ILE:HA	55:n:160:ARG:HB3	1.87	0.56
8:L:145:VAL:O	52:u:119:ARG:NH2	2.39	0.56
2:E:344:SER:OG	13:Q:102:ARG:NH2	2.39	0.56
12:P:85:ARG:HD2	12:P:158:MET:HE3	1.86	0.56
37:e:179:GLN:HG3	37:e:181:GLY:H	1.71	0.56
9:M:57:ARG:NH1	56:A:2096:U:O4	2.39	0.56
28:5:251:HIS:O	28:5:371:LYS:NZ	2.38	0.56
59:G:25:G:N2	59:G:42:C:O2	2.37	0.56
8:L:55:PRO:HB3	8:L:77:ILE:HG12	1.88	0.56
17:U:65:VAL:HG13	17:U:97:VAL:HG13	1.88	0.56
49:r:182:ARG:NH2	56:A:2158:U:OP2	2.37	0.56
53:v:3:PRO:HD3	53:v:51:ARG:HH11	1.71	0.56
7:K:21:LEU:HD12	7:K:145:LEU:HD12	1.89	0.55
13:Q:81:ILE:O	13:Q:143:ARG:NH2	2.39	0.55
28:5:33:TRP:O	28:5:39:ARG:NH2	2.39	0.55
34:b:4:ARG:NH2	56:A:1837:C:OP1	2.39	0.55
5:I:132:LYS:NZ	5:I:147:PHE:O	2.39	0.55
14:R:57:ARG:NH2	15:S:170:ILE:O	2.35	0.55
15:S:181:LYS:NZ	56:A:2296:U:O4	2.39	0.55
38:f:48:TYR:N	56:A:2065:A:OP1	2.39	0.55
6:J:73:LYS:HE2	6:J:74:PRO:HD2	1.89	0.55
17:U:144:ARG:HH22	36:d:273:LYS:HB2	1.71	0.55
3:F:165:LEU:O	3:F:170:ARG:NH1	2.40	0.55
11:O:38:ARG:NH2	11:O:82:GLU:OE1	2.40	0.55
28:5:343:GLN:NE2	28:5:417:LEU:O	2.39	0.55
30:7:41:THR:O	30:7:45:ASN:ND2	2.39	0.55
7:K:25:MET:O	7:K:149:ARG:NH1	2.38	0.55
22:Z:99:VAL:HG12	42:j:80:LEU:HD12	1.89	0.55
1:D:132:ASP:OD2	1:D:135:ARG:NH1	2.36	0.55
9:M:168:GLU:OE1	9:M:220:ARG:NH2	2.39	0.55
10:N:191:SER:OG	10:N:192:ARG:N	2.39	0.55
16:T:109:ASN:HD21	23:0:101:ILE:HD13	1.71	0.55
23:0:93:ARG:NH2	56:A:2310:G:OP2	2.37	0.55
28:5:208:THR:HG21	50:s:160:ARG:HD3	1.88	0.55
53:v:51:ARG:HA	54:w:112:4HH:HS3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:226:MET:SD	48:q:26:ARG:NH1	2.80	0.55
14:R:11:ARG:HB2	56:A:2292:G:C8	2.41	0.55
28:5:127:LYS:HD3	28:5:248:THR:HG22	1.88	0.55
1:D:135:ARG:NH2	56:A:2528:G:OP1	2.40	0.54
26:3:104:ARG:NH1	26:3:160:LYS:O	2.39	0.54
31:8:173:LYS:NZ	31:8:174:GLU:O	2.40	0.54
10:N:205:ARG:NH2	10:N:249:LYS:O	2.41	0.54
14:R:114:LYS:HD2	33:a:44:ASN:HB3	1.89	0.54
20:X:238:LEU:HD11	32:9:101:GLU:HG2	1.89	0.54
39:g:90:ARG:N	56:A:1881:A:OP1	2.41	0.54
49:r:132:ARG:HD3	49:r:133:PRO:HD2	1.89	0.54
55:n:223:ARG:NH1	55:n:224:ILE:O	2.40	0.54
56:A:1788:C:N3	56:A:1916:G:O2'	2.39	0.54
56:A:2579:C:O2	56:A:2580:U:N3	2.41	0.54
2:E:311:GLY:HA2	2:E:314:LEU:HD12	1.88	0.54
7:K:36:SER:O	7:K:40:GLN:NE2	2.37	0.54
18:V:94:HIS:NE2	56:A:1805:A:OP2	2.36	0.54
21:Y:165:PRO:HD3	32:9:132:PRO:HB3	1.90	0.54
50:s:310:ARG:NH1	56:A:2417:C:O2	2.41	0.54
56:A:3063:G:O2'	56:A:3066:C:OP2	2.24	0.54
36:d:84:ILE:HA	36:d:211:GLN:HE22	1.72	0.54
2:E:276:ILE:HD11	2:E:332:LEU:HD12	1.89	0.54
49:r:182:ARG:NH1	56:A:2157:U:OP1	2.41	0.54
55:n:127:LEU:HD23	55:n:131:LEU:HD11	1.90	0.54
4:C:214:THR:HG23	4:C:215:ARG:HG3	1.89	0.54
56:A:1990:G:O2'	56:A:1993:A:N6	2.40	0.54
7:K:119:ARG:NH1	56:A:2705:U:OP2	2.39	0.54
8:L:141:ALA:O	52:u:197:ARG:NH2	2.41	0.54
34:b:80:LEU:HD11	35:c:78:ARG:HD3	1.90	0.54
56:A:2694:A:O2'	56:A:2941:G:N2	2.36	0.54
12:P:118:SER:OG	12:P:121:ASN:ND2	2.41	0.54
45:m:56:LEU:HD12	45:m:75:LEU:HD23	1.90	0.54
59:G:6:U:H3	59:G:64:A:H61	1.56	0.54
37:e:59:VAL:HG11	37:e:136:ARG:HG3	1.90	0.54
1:D:192:LEU:HB3	1:D:213:CYS:HB2	1.89	0.53
8:L:53:ARG:HE	8:L:56:ARG:HH12	1.55	0.53
10:N:85:GLY:O	10:N:192:ARG:NH1	2.41	0.53
56:A:2332:C:H42	56:A:2442:U:H3	1.56	0.53
2:E:260:LYS:NZ	56:A:3220:A:OP1	2.41	0.53
9:M:123:ASN:O	9:M:125:ARG:NH1	2.41	0.53
11:O:77:ASP:O	11:O:83:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:84:ARG:O	56:A:3157:C:O2'	2.21	0.53
26:3:175:ASP:HB3	26:3:178:GLN:HB2	1.90	0.53
55:n:149:ILE:HA	55:n:152:ILE:HD12	1.89	0.53
32:9:24:LYS:HG2	56:A:2421:G:H5''	1.89	0.53
35:c:121:SER:OG	35:c:122:ASN:N	2.42	0.53
10:N:61:LYS:NZ	10:N:128:PHE:O	2.40	0.53
18:V:138:THR:OG1	18:V:141:GLY:O	2.26	0.53
37:e:123:MET:O	37:e:127:LYS:NZ	2.42	0.53
4:H:64:LEU:HD12	20:X:61:ARG:HH21	1.73	0.53
23:0:96:ASN:ND2	56:A:2708:C:O2'	2.37	0.53
40:h:91:LEU:HD13	40:h:97:LYS:HG3	1.90	0.53
50:s:419:LEU:O	50:s:423:HIS:ND1	2.41	0.53
12:P:63:ARG:HG2	12:P:177:ARG:HH11	1.74	0.53
21:Y:95:ASN:OD1	21:Y:149:ARG:NH1	2.42	0.53
30:7:62:THR:OG1	30:7:64:LYS:NZ	2.42	0.53
37:e:126:GLN:OE1	37:e:130:GLN:NE2	2.42	0.53
2:E:292:HIS:ND1	2:E:293:LYS:O	2.38	0.52
16:T:69:ARG:NH1	36:d:228:PHE:O	2.41	0.52
43:k:36:THR:HG21	43:k:87:LEU:HD11	1.89	0.52
56:A:2770:C:H42	56:A:2777:G:H1	1.56	0.52
4:C:184:LEU:HD11	4:C:189:VAL:HB	1.90	0.52
17:U:8:PRO:HA	21:Y:183:GLN:HE22	1.74	0.52
23:0:94:ARG:NH2	56:A:2310:G:OP2	2.38	0.52
26:3:124:ARG:NH1	56:A:2869:A:OP1	2.38	0.52
48:q:41:ASP:OD1	48:q:41:ASP:N	2.42	0.52
50:s:247:LEU:HD11	50:s:296:HIS:HD2	1.73	0.52
59:x:6:U:H3	59:x:64:A:H61	1.56	0.52
7:K:63:ARG:NH1	7:K:130:ASP:OD1	2.42	0.52
37:e:192:LEU:O	37:e:196:SER:OG	2.27	0.52
48:q:137:GLN:HG2	48:q:140:ARG:HH22	1.73	0.52
12:P:63:ARG:HA	12:P:177:ARG:HE	1.75	0.52
22:Z:71:ARG:NH1	22:Z:73:LYS:O	2.40	0.52
56:A:2330:U:H3	56:A:2447:A:H61	1.58	0.52
21:Y:123:ARG:HD2	36:d:64:GLY:HA2	1.92	0.52
34:b:72:VAL:HG13	34:b:90:HIS:HB2	1.92	0.52
50:s:228:ASP:OD1	50:s:228:ASP:N	2.41	0.52
14:R:24:VAL:HG11	14:R:43:VAL:HG22	1.91	0.52
53:v:43:GLN:HE21	54:w:112:4HH:HR	1.54	0.52
54:w:102:SER:OG	54:w:107:ASP:OD2	2.28	0.52
56:A:2632:A:O2'	56:A:2635:G:N3	2.39	0.52
3:F:237:LEU:O	48:q:25:TYR:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:216:TYR:OH	21:Y:191:ASN:ND2	2.42	0.52
6:J:32:GLY:O	6:J:36:GLY:N	2.41	0.52
49:r:94:ARG:NH2	56:A:3181:U:OP1	2.43	0.52
50:s:362:THR:OG1	50:s:363:ASP:N	2.42	0.52
52:u:159:ILE:HB	52:u:162:LYS:HD3	1.92	0.52
59:x:29:G:N2	59:x:37:A:N1	2.58	0.52
1:D:164:LEU:HD23	1:D:182:HIS:HE1	1.74	0.52
42:j:45:GLU:OE2	42:j:70:ARG:NH2	2.40	0.52
50:s:239:ASN:OD1	50:s:239:ASN:N	2.41	0.52
7:K:10:GLN:NE2	16:T:206:ARG:O	2.42	0.51
28:5:223:ARG:HH22	28:5:274:LYS:HD3	1.75	0.51
28:5:355:LEU:HD12	28:5:376:VAL:HG12	1.92	0.51
36:d:217:HIS:HD2	36:d:243:LEU:HD13	1.75	0.51
2:E:236:THR:HG22	2:E:239:ARG:HD3	1.92	0.51
3:F:160:SER:HB2	41:i:80:LEU:HD13	1.92	0.51
9:M:133:LYS:NZ	56:A:1889:C:OP1	2.42	0.51
23:0:156:THR:HG22	23:0:173:ARG:HE	1.75	0.51
1:D:169:ILE:HA	1:D:186:ALA:HB2	1.92	0.51
7:K:59:ILE:HB	7:K:127:LEU:HD23	1.93	0.51
2:E:123:GLN:OE1	2:E:125:GLN:NE2	2.43	0.51
2:E:150:LYS:HD2	2:E:296:LEU:HD11	1.91	0.51
7:K:5:SER:HB2	7:K:8:PRO:HD2	1.92	0.51
8:L:101:ASP:OD1	13:Q:152:ARG:NH2	2.44	0.51
9:M:229:PHE:HE2	9:M:259:ARG:HH12	1.58	0.51
25:2:89:SER:OG	32:9:17:ARG:NH1	2.41	0.51
37:e:67:GLN:O	37:e:71:ALA:N	2.43	0.51
2:E:294:ASN:ND2	56:A:3217:A:N1	2.58	0.51
10:N:123:ARG:NH2	10:N:162:GLU:OE2	2.44	0.51
30:7:107:LEU:HD13	30:7:128:LEU:HD11	1.91	0.51
40:h:122:ARG:HG3	40:h:124:ARG:HH21	1.75	0.51
50:s:177:LEU:HD12	50:s:301:LEU:HD23	1.91	0.51
53:v:54:GLN:HA	53:v:57:LYS:HG2	1.92	0.51
55:n:11:LEU:HA	55:n:14:VAL:HG12	1.93	0.51
29:6:222:ASP:OD1	29:6:222:ASP:N	2.41	0.51
56:A:3011:A:O2'	56:A:3173:G:N2	2.44	0.51
5:I:181:ILE:HG12	5:I:186:LEU:HD11	1.93	0.51
29:6:183:ASP:HA	47:p:192:ARG:HA	1.93	0.51
43:k:66:VAL:HB	43:k:74:LEU:HB3	1.93	0.51
9:M:45:ARG:NH2	56:A:2269:G:O6	2.44	0.51
18:V:122:LEU:HD12	18:V:133:ILE:HG13	1.93	0.51
30:7:148:MET:HG2	30:7:257:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:7:186:ASP:N	30:7:186:ASP:OD1	2.43	0.51
45:m:51:LEU:HB3	45:m:67:ARG:HB3	1.93	0.51
54:w:97:LYS:O	54:w:102:SER:OG	2.27	0.51
16:T:61:PRO:HD3	36:d:180:THR:HG21	1.93	0.51
28:5:236:LEU:HB2	28:5:341:VAL:HB	1.92	0.51
50:s:181:VAL:HG12	50:s:200:LEU:HD11	1.92	0.51
8:L:108:ILE:HA	8:L:114:PRO:HA	1.92	0.51
37:e:255:VAL:HG23	37:e:259:GLU:HB3	1.93	0.51
59:G:29:G:N2	59:G:37:A:N1	2.58	0.51
43:k:16:VAL:HG22	43:k:66:VAL:HG13	1.92	0.50
44:l:120:ARG:NH2	56:A:2190:C:OP2	2.35	0.50
9:M:75:TYR:O	26:3:113:ARG:NH1	2.44	0.50
35:c:215:ILE:HG23	35:c:219:LEU:HD12	1.92	0.50
43:k:18:VAL:HG21	43:k:34:LEU:HD13	1.91	0.50
49:r:150:TYR:OH	56:A:2241:A:OP1	2.29	0.50
50:s:232:GLN:HE22	50:s:281:HIS:H	1.60	0.50
56:A:2643:G:O2'	56:A:2645:G:OP2	2.28	0.50
10:N:70:SER:HA	10:N:73:ARG:HG2	1.93	0.50
16:T:157:ARG:HB2	16:T:167:MET:HE3	1.93	0.50
18:V:105:ARG:NH2	36:d:171:ASP:OD1	2.45	0.50
37:e:256:THR:OG1	37:e:257:LYS:N	2.44	0.50
10:N:218:ILE:HA	10:N:223:MET:HG3	1.93	0.50
19:W:102:GLU:OE2	29:6:74:TYR:N	2.45	0.50
54:w:138:LEU:HD13	54:w:144:ILE:HG12	1.94	0.50
12:P:66:ARG:NH2	56:A:2874:A:O3'	2.40	0.50
15:S:142:THR:HG22	33:a:60:CYS:HB2	1.94	0.50
37:e:85:SER:HB3	45:m:50:ARG:H	1.76	0.50
37:e:95:ASN:HD21	37:e:118:GLN:HE22	1.59	0.50
56:A:2299:U:H5''	56:A:2300:G:H5''	1.94	0.50
17:U:37:GLU:HB3	17:U:104:THR:HG23	1.93	0.50
17:U:50:ARG:HG3	17:U:68:VAL:HB	1.93	0.50
50:s:221:HIS:ND1	56:A:2425:A:OP1	2.45	0.50
1:D:125:LYS:HB2	28:5:258:PRO:HD2	1.94	0.50
41:i:123:ARG:O	41:i:128:ARG:NH2	2.44	0.50
55:n:215:THR:OG1	55:n:216:THR:N	2.44	0.50
56:A:2032:G:O2'	56:A:2865:C:O2	2.30	0.50
59:x:50:A:H61	59:x:59:G:H1	1.59	0.50
11:O:79:TRP:NE1	13:Q:267:PHE:O	2.39	0.50
50:s:169:SER:HA	50:s:173:SER:HB2	1.94	0.50
11:O:9:ILE:N	56:A:2458:A:OP1	2.45	0.49
29:6:196:THR:HG22	29:6:326:SER:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:21:LEU:HD21	7:K:31:LEU:HD22	1.94	0.49
13:Q:120:THR:HG23	13:Q:132:GLN:HG2	1.94	0.49
28:5:245:ILE:O	28:5:248:THR:OG1	2.28	0.49
31:8:129:ARG:NH1	57:B:1627:C:OP1	2.45	0.49
56:A:2695:G:OP1	56:A:2941:G:O2'	2.29	0.49
1:D:206:TYR:O	1:D:208:ARG:N	2.34	0.49
2:E:108:PRO:HB3	2:E:116:LYS:HE2	1.95	0.49
10:N:204:GLU:OE1	10:N:207:ARG:NH2	2.46	0.49
33:a:52:THR:OG1	33:a:54:ASP:OD2	2.26	0.49
56:A:1850:U:O2'	56:A:2134:A:N1	2.41	0.49
17:U:11:ARG:HH21	21:Y:185:VAL:HG13	1.78	0.49
56:A:1953:A:O2'	56:A:2463:A:OP1	2.31	0.49
39:g:111:ARG:HD3	56:A:1881:A:H62	1.78	0.49
43:k:40:GLU:HB3	43:k:43:ARG:HH21	1.78	0.49
22:Z:134:MET:HE1	42:j:78:VAL:HG21	1.95	0.49
37:e:55:ARG:HD3	37:e:157:LEU:HD12	1.93	0.49
5:I:160:LYS:HG2	5:I:163:GLU:HB2	1.95	0.49
9:M:274:VAL:HG11	48:q:75:LEU:HD13	1.95	0.49
50:s:111:LYS:NZ	50:s:384:ASP:OD2	2.42	0.49
56:A:2575:U:O2'	56:A:2581:A:N6	2.46	0.49
59:G:50:A:H61	59:G:59:G:H1	1.59	0.49
13:Q:100:LEU:HD11	13:Q:286:ILE:HD13	1.95	0.49
15:S:132:LYS:NZ	42:j:43:LEU:O	2.38	0.49
18:V:54:TRP:NE1	18:V:56:LEU:O	2.43	0.49
22:Z:35:LYS:HB3	56:A:2119:U:H1'	1.95	0.49
28:5:385:HIS:HB2	56:A:2395:A:H1'	1.95	0.49
10:N:72:ILE:HD11	10:N:96:TYR:CZ	2.48	0.48
31:8:119:LYS:NZ	57:B:1641:G:O2'	2.44	0.48
36:d:164:VAL:HG22	36:d:261:MET:HB2	1.95	0.48
39:g:86:VAL:HG22	39:g:113:VAL:HG22	1.95	0.48
56:A:3068:G:OP2	56:A:3068:G:N2	2.40	0.48
1:D:146:SER:O	1:D:146:SER:OG	2.30	0.48
3:F:223:HIS:HA	3:F:226:MET:HE3	1.94	0.48
6:J:26:ALA:HB1	6:J:57:THR:HG23	1.94	0.48
8:L:85:LEU:HD11	8:L:134:TYR:HE1	1.78	0.48
23:0:123:CYS:HB3	23:0:126:CYS:HB2	1.95	0.48
28:5:310:ARG:HA	28:5:313:MET:HE2	1.94	0.48
37:e:127:LYS:HA	37:e:130:GLN:HB2	1.95	0.48
3:F:278:SER:O	3:F:278:SER:OG	2.31	0.48
28:5:201:ARG:NH1	28:5:418:TYR:O	2.39	0.48
36:d:188:SER:HB3	36:d:218:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:52:GLU:O	10:N:211:ASN:ND2	2.39	0.48
21:Y:83:ALA:N	32:9:74:VAL:O	2.46	0.48
34:b:77:ALA:HB2	34:b:104:LEU:HD13	1.96	0.48
9:M:37:GLU:OE1	56:A:2293:A:N6	2.36	0.48
12:P:39:VAL:HG12	12:P:41:ASN:H	1.79	0.48
32:9:24:LYS:NZ	56:A:2422:U:OP2	2.46	0.48
49:r:121:MET:HE3	49:r:151:LEU:HA	1.96	0.48
50:s:159:ARG:NH2	50:s:171:VAL:O	2.45	0.48
20:X:92:ALA:HB3	20:X:98:SER:HB3	1.94	0.48
52:u:95:ASP:N	52:u:95:ASP:OD1	2.46	0.48
56:A:1749:C:OP2	56:A:2899:C:O2'	2.32	0.48
56:A:2537:G:O2'	56:A:2634:U:OP2	2.31	0.48
2:E:298:LYS:NZ	56:A:3205:C:OP2	2.44	0.48
6:J:66:LEU:HD13	6:J:82:ILE:HD11	1.94	0.48
9:M:263:ARG:HD2	47:p:43:TYR:HD2	1.79	0.48
12:P:104:SER:HB3	29:6:150:ARG:HH12	1.78	0.48
55:n:130:ILE:HG13	55:n:134:ARG:HH12	1.77	0.48
3:F:49:ARG:HD3	3:F:263:LEU:HD22	1.95	0.48
7:K:114:LYS:HE2	56:A:2702:G:H5'	1.95	0.48
12:P:63:ARG:NH1	19:W:137:LYS:O	2.35	0.48
22:Z:101:LYS:HE3	42:j:80:LEU:HD22	1.96	0.48
52:u:118:MET:HE1	52:u:197:ARG:HG3	1.96	0.48
16:T:84:LYS:HD3	16:T:149:ARG:HB3	1.96	0.47
28:5:276:ASP:OD1	50:s:158:ARG:NH2	2.47	0.47
6:J:67:PRO:HG3	6:J:86:THR:HG22	1.95	0.47
11:O:108:LEU:HD13	23:0:122:LEU:HD21	1.96	0.47
40:h:66:LEU:HD21	40:h:131:ASN:HB3	1.96	0.47
43:k:46:ASN:ND2	43:k:49:CYS:SG	2.87	0.47
49:r:182:ARG:HH22	56:A:2157:U:H5'	1.79	0.47
56:A:2655:G:N2	56:A:2659:C:O2'	2.48	0.47
8:L:127:LEU:HB2	8:L:138:LEU:HD21	1.96	0.47
21:Y:172:ILE:HG12	21:Y:198:ARG:HG3	1.95	0.47
29:6:233:LEU:HB3	29:6:298:PHE:HE1	1.79	0.47
31:8:101:ARG:HH22	37:e:82:SER:HB2	1.80	0.47
2:E:251:VAL:HG11	2:E:257:MET:HE1	1.97	0.47
32:9:28:ARG:O	56:A:2377:G:O2'	2.31	0.47
52:u:121:THR:HG21	52:u:176:VAL:HG13	1.96	0.47
56:A:2459:A:N6	56:A:2668:A:O2'	2.47	0.47
1:D:207:ILE:O	1:D:212:THR:OG1	2.27	0.47
20:X:177:HIS:O	20:X:184:ARG:NH2	2.47	0.47
29:6:187:VAL:HG13	29:6:319:PHE:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:s:89:MET:O	50:s:230:ARG:NH2	2.41	0.47
56:A:2392:U:H2'	56:A:2394:A:H62	1.80	0.47
30:7:276:PHE:HB2	30:7:304:VAL:HG22	1.96	0.47
54:w:83:VAL:HA	54:w:86:VAL:HG22	1.96	0.47
1:D:180:ASP:OD1	1:D:180:ASP:N	2.46	0.47
1:D:194:ASN:HD22	1:D:247:VAL:HG22	1.78	0.47
11:O:145:LEU:H	30:7:306:LEU:HD23	1.79	0.47
16:T:211:THR:O	34:b:117:LYS:NZ	2.39	0.47
23:0:84:ARG:NH2	56:A:2306:A:O2'	2.48	0.47
28:5:360:ASN:N	28:5:372:ASN:OD1	2.45	0.47
36:d:250:LYS:NZ	36:d:257:GLY:O	2.44	0.47
54:w:141:PRO:HA	54:w:144:ILE:HD12	1.97	0.47
1:D:204:ALA:O	1:D:208:ARG:NH1	2.47	0.47
9:M:277:MET:HE1	39:g:52:LEU:HD21	1.97	0.47
17:U:128:SER:OG	17:U:129:MET:SD	2.73	0.47
22:Z:99:VAL:HG21	42:j:77:VAL:HG22	1.97	0.47
28:5:212:THR:HG21	28:5:273:VAL:HG13	1.97	0.47
1:D:181:ALA:HB2	1:D:243:THR:HG22	1.97	0.47
50:s:307:ARG:HG3	50:s:310:ARG:H	1.80	0.47
56:A:2310:G:O2'	56:A:2675:G:O6	2.31	0.47
2:E:55:GLU:OE2	11:O:137:ARG:NH1	2.48	0.47
5:I:86:ILE:HD13	5:I:131:LEU:HD13	1.96	0.47
28:5:149:ASN:HB3	28:5:152:GLU:HB2	1.96	0.47
37:e:58:VAL:HG13	37:e:59:VAL:HG23	1.97	0.47
50:s:332:LEU:HD13	50:s:372:TYR:HB2	1.96	0.47
8:L:111:ASN:HB3	52:u:164:THR:HB	1.96	0.46
11:O:128:ASN:OD1	11:O:128:ASN:N	2.45	0.46
15:S:119:GLU:HG3	15:S:189:PRO:HB2	1.98	0.46
31:8:97:LYS:HE3	37:e:89:LEU:HD13	1.97	0.46
37:e:230:LYS:HE3	37:e:230:LYS:HB2	1.75	0.46
9:M:165:ALA:HB2	9:M:236:LEU:HD13	1.98	0.46
26:3:105:LYS:NZ	56:A:1754:G:N7	2.56	0.46
3:F:241:ASN:OD1	3:F:256:HIS:NE2	2.33	0.46
14:R:48:ARG:NH2	56:A:1844:A:OP1	2.48	0.46
15:S:143:LEU:HD22	33:a:59:VAL:HG22	1.97	0.46
30:7:103:SER:HB2	30:7:127:PHE:HB3	1.98	0.46
36:d:83:GLY:O	36:d:262:HIS:NE2	2.41	0.46
56:A:2191:A:N6	56:A:2198:A:OP2	2.48	0.46
41:i:61:GLY:HA3	56:A:1886:G:H1	1.80	0.46
50:s:401:LEU:HD23	50:s:402:TYR:HD1	1.81	0.46
57:B:1628:C:H2'	57:B:1629:A:H8	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:101:ALA:HB3	6:J:104:THR:HG22	1.97	0.46
31:8:129:ARG:HD2	57:B:1627:C:H5'	1.96	0.46
39:g:110:ILE:HD11	39:g:157:LEU:HD13	1.98	0.46
56:A:2822:C:O2'	56:A:2915:C:OP2	2.33	0.46
3:F:253:MET:HE3	3:F:259:LEU:HD22	1.98	0.46
19:W:100:THR:OG1	19:W:132:HIS:NE2	2.42	0.46
31:8:171:PHE:O	38:f:187:LYS:NZ	2.48	0.46
38:f:91:LEU:N	38:f:159:ILE:O	2.42	0.46
48:q:61:PHE:HB2	48:q:70:VAL:HG22	1.98	0.46
56:A:2138:U:O2'	56:A:2151:A:N3	2.47	0.46
4:C:197:LEU:HB2	4:C:199:VAL:HG22	1.97	0.46
6:J:25:ARG:HA	6:J:65:PRO:HA	1.96	0.46
10:N:214:THR:HG23	10:N:217:ARG:H	1.81	0.46
19:W:49:ARG:HH22	19:W:71:ARG:HD3	1.80	0.46
50:s:310:ARG:HE	50:s:310:ARG:HB2	1.46	0.46
56:A:3008:C:O2'	56:A:3051:A:N3	2.41	0.46
10:N:104:MET:HB3	10:N:104:MET:HE3	1.79	0.46
13:Q:221:LYS:NZ	13:Q:241:LYS:O	2.49	0.46
19:W:61:VAL:HG13	19:W:65:ASN:HB2	1.98	0.46
28:5:239:ILE:HD11	28:5:420:HIS:HE2	1.81	0.46
31:8:164:ARG:NH2	38:f:163:SER:O	2.47	0.46
50:s:94:TYR:O	50:s:106:TYR:OH	2.29	0.46
10:N:224:LEU:HD22	46:o:35:MET:HE2	1.98	0.46
37:e:141:ASP:OD1	37:e:141:ASP:N	2.48	0.46
55:n:79:LYS:HB3	55:n:79:LYS:HE3	1.76	0.46
8:L:98:PRO:HA	13:Q:162:ILE:HG13	1.97	0.46
20:X:159:MET:HB3	20:X:205:GLY:HA3	1.98	0.46
36:d:90:PRO:HG2	36:d:267:PRO:HB3	1.98	0.46
36:d:244:GLU:OE2	36:d:264:LYS:NZ	2.49	0.46
41:i:79:TRP:HH2	56:A:1685:C:H5'	1.80	0.46
3:F:211:ARG:HH11	40:h:58:ARG:HE	1.65	0.45
13:Q:129:LYS:HD2	52:u:116:PRO:HB3	1.97	0.45
14:R:54:THR:HG21	15:S:172:MET:H	1.80	0.45
17:U:30:ARG:O	21:Y:121:ARG:NH1	2.45	0.45
21:Y:194:TYR:OH	28:5:64:MET:O	2.30	0.45
24:1:20:MET:HE3	24:1:20:MET:HB3	1.85	0.45
28:5:166:THR:OG1	28:5:167:THR:N	2.48	0.45
10:N:244:LYS:HD2	56:A:2110:A:H2	1.82	0.45
15:S:164:THR:HG22	34:b:107:GLN:HB2	1.98	0.45
34:b:144:ARG:NH2	34:b:147:GLU:OE1	2.50	0.45
36:d:245:TYR:HB2	36:d:265:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:s:300:HIS:HB2	50:s:361:ILE:HB	1.97	0.45
56:A:1742:G:O2'	56:A:1754:G:O6	2.29	0.45
17:U:28:LEU:HA	17:U:42:PHE:HA	1.99	0.45
20:X:28:TYR:O	20:X:31:SER:OG	2.32	0.45
21:Y:69:ASP:OD1	21:Y:69:ASP:N	2.36	0.45
50:s:104:ARG:HH21	50:s:262:PRO:HG3	1.82	0.45
50:s:237:PRO:HB3	50:s:300:HIS:CE1	2.51	0.45
26:3:169:ARG:NH2	56:A:1892:A:N7	2.64	0.45
36:d:180:THR:HG23	36:d:225:TYR:HB2	1.98	0.45
55:n:39:GLU:O	55:n:178:ALA:N	2.49	0.45
56:A:2506:A:H1'	56:A:2601:A:H61	1.81	0.45
3:F:96:LEU:HD21	3:F:177:ALA:HB2	1.99	0.45
11:O:131:PRO:HB2	23:0:130:VAL:HG13	1.97	0.45
14:R:34:ARG:NH2	56:A:2682:A:OP1	2.41	0.45
15:S:96:PHE:HB3	34:b:126:ILE:HD13	1.97	0.45
21:Y:171:ASP:OD1	21:Y:171:ASP:N	2.49	0.45
28:5:270:ILE:O	56:A:2409:A:O2'	2.30	0.45
30:7:221:VAL:HG21	30:7:254:LEU:HD12	1.99	0.45
37:e:213:TYR:OH	37:e:271:GLN:O	2.28	0.45
40:h:66:LEU:HA	40:h:69:ARG:HB2	1.98	0.45
46:o:12:ILE:HG12	46:o:23:ARG:HB3	1.99	0.45
53:v:4:TRP:HB3	53:v:55:LEU:HD23	1.99	0.45
55:n:195:ALA:O	55:n:199:HIS:ND1	2.49	0.45
3:F:68:SER:O	3:F:210:ARG:NH2	2.47	0.45
21:Y:150:GLU:HG2	32:9:133:ARG:HH21	1.81	0.45
54:w:87:LEU:HD21	54:w:98:LEU:HD22	1.99	0.45
5:I:134:PHE:HA	5:I:137:ASP:HB2	1.99	0.45
6:J:24:VAL:HG21	6:J:35:LEU:HD11	1.97	0.45
17:U:80:ARG:NH2	17:U:84:ASN:O	2.50	0.45
28:5:184:LEU:HD23	28:5:184:LEU:HA	1.87	0.45
28:5:228:ALA:HB3	28:5:292:TYR:HB2	1.99	0.45
36:d:158:ASP:N	36:d:158:ASP:OD1	2.50	0.45
26:3:138:PRO:HG2	56:A:2854:U:H4'	1.99	0.45
37:e:124:TRP:CD1	37:e:127:LYS:HZ1	2.34	0.45
59:G:9:A:O2'	59:G:10:G:N7	2.41	0.45
5:I:142:ASN:HD22	5:I:185:ILE:HB	1.82	0.44
56:A:1822:U:O2	56:A:2707:A:O2'	2.31	0.44
56:A:2512:A:O2'	56:A:2541:C:OP1	2.28	0.44
2:E:97:VAL:HG22	2:E:181:ILE:HD11	1.98	0.44
6:J:113:THR:HG23	6:J:116:HIS:H	1.83	0.44
16:T:81:LYS:HD2	16:T:81:LYS:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:295:ASP:HB2	28:5:348:ASP:HA	1.99	0.44
51:t:18:UNK:O	51:t:22:UNK:N	2.50	0.44
56:A:3009:C:O2'	56:A:3115:U:OP1	2.32	0.44
16:T:47:ILE:N	56:A:1674:A:N7	2.65	0.44
18:V:191:LEU:HD12	32:9:118:GLY:HA3	2.00	0.44
39:g:90:ARG:HA	39:g:90:ARG:HD3	1.76	0.44
41:i:97:MET:HE2	41:i:97:MET:HB3	1.76	0.44
56:A:1781:A:N6	56:A:1795:A:OP2	2.49	0.44
2:E:143:ALA:O	2:E:181:ILE:N	2.50	0.44
31:8:143:GLN:HE21	38:f:165:THR:HA	1.83	0.44
4:H:84:GLU:OE2	20:X:44:ARG:NH2	2.41	0.44
30:7:56:LEU:O	30:7:59:THR:OG1	2.34	0.44
31:8:88:PHE:HA	45:m:45:ARG:HH22	1.81	0.44
38:f:96:THR:HG22	38:f:154:GLU:HB3	1.99	0.44
53:v:6:ARG:HH12	54:w:112:4HH:HJ2	1.82	0.44
6:J:99:LYS:HD3	6:J:99:LYS:HA	1.80	0.44
9:M:14:ASP:OD2	9:M:17:ARG:NH2	2.50	0.44
18:V:103:ASP:OD1	18:V:103:ASP:N	2.46	0.44
21:Y:223:LYS:HB3	21:Y:223:LYS:HE2	1.73	0.44
50:s:66:TRP:O	50:s:69:THR:OG1	2.31	0.44
13:Q:195:PRO:O	13:Q:199:THR:OG1	2.33	0.44
15:S:162:GLU:HG2	15:S:192:VAL:HB	2.00	0.44
17:U:35:GLN:NE2	56:A:2372:U:O4	2.50	0.44
28:5:118:LYS:HD2	28:5:254:GLU:HG2	1.99	0.44
34:b:21:ARG:HH12	35:c:81:GLU:CD	2.25	0.44
49:r:90:SER:HA	49:r:93:ILE:HD12	1.99	0.44
59:x:48:U:H2'	59:x:49:G:C8	2.53	0.44
5:I:44:ARG:NH1	10:N:234:ASP:OD2	2.48	0.44
19:W:62:HIS:HA	19:W:94:GLU:HG3	2.00	0.44
55:n:5:LYS:HG3	55:n:8:ARG:HE	1.81	0.44
56:A:2194:U:O2'	56:A:2195:A:O4'	2.36	0.44
59:G:46:G:O2'	59:G:56:A:O2'	2.33	0.44
59:x:46:G:O2'	59:x:56:A:O2'	2.33	0.44
5:I:165:VAL:O	5:I:169:ARG:N	2.51	0.44
9:M:30:ASN:ND2	56:A:1877:U:O3'	2.51	0.44
15:S:184:ARG:NH2	56:A:2261:C:O2'	2.51	0.44
29:6:186:PRO:HG3	47:p:191:LYS:HD3	1.98	0.44
31:8:114:ARG:HG3	37:e:73:LEU:HD21	2.00	0.44
50:s:85:LYS:NZ	56:A:2443:C:OP1	2.51	0.44
17:U:9:LEU:HD12	17:U:9:LEU:HA	1.84	0.43
18:V:81:ARG:NH1	18:V:81:ARG:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:136:VAL:HG22	28:5:420:HIS:HD2	1.83	0.43
33:a:62:HIS:O	33:a:62:HIS:ND1	2.50	0.43
38:f:81:ASN:HA	38:f:86:TYR:HA	2.00	0.43
44:l:133:SER:HA	44:l:136:LYS:HD2	1.99	0.43
59:x:9:A:O2'	59:x:10:G:N7	2.41	0.43
12:P:122:VAL:HG13	12:P:157:SER:HA	2.00	0.43
28:5:333:ALA:HB1	28:5:363:ASP:HA	1.99	0.43
56:A:2003:A:OP2	56:A:2734:A:O2'	2.34	0.43
1:D:140:ALA:HB2	1:D:153:ALA:HB2	2.00	0.43
3:F:107:LYS:HG2	41:i:74:ILE:HG22	1.99	0.43
14:R:12:ASN:OD1	14:R:12:ASN:N	2.50	0.43
15:S:178:LYS:HD3	15:S:178:LYS:HA	1.86	0.43
17:U:3:ARG:O	17:U:23:ASN:ND2	2.48	0.43
5:I:123:MET:HG3	5:I:154:LEU:HD13	1.99	0.43
10:N:234:ASP:HA	10:N:237:HIS:HB2	2.00	0.43
26:3:110:VAL:HG13	26:3:158:LEU:HD22	1.99	0.43
28:5:187:LEU:HD23	28:5:187:LEU:HA	1.91	0.43
28:5:262:ILE:HD12	28:5:262:ILE:HA	1.73	0.43
37:e:168:GLN:HB3	37:e:170:VAL:HG23	2.00	0.43
48:q:44:ASP:HB3	48:q:47:THR:HG23	2.00	0.43
55:n:76:ALA:HB3	55:n:94:VAL:HG13	2.00	0.43
59:G:48:U:H2'	59:G:49:G:C8	2.53	0.43
5:I:101:ASN:HD22	5:I:152:MET:HB3	1.83	0.43
29:6:73:THR:OG1	29:6:74:TYR:N	2.51	0.43
50:s:174:LEU:HD23	50:s:301:LEU:HD21	2.00	0.43
6:J:33:PRO:HA	6:J:37:PRO:HD2	2.00	0.43
11:O:17:ARG:HD2	56:A:2457:A:C6	2.54	0.43
15:S:161:ILE:HG23	34:b:17:ASN:HD22	1.83	0.43
52:u:175:MET:HE2	52:u:175:MET:HB3	1.86	0.43
56:A:2456:U:O4	56:A:2457:A:N6	2.52	0.43
11:O:144:LEU:HD23	30:7:302:LEU:HD23	1.99	0.43
21:Y:198:ARG:NH1	25:2:70:LEU:O	2.51	0.43
29:6:27:ARG:N	56:A:2073:A:OP2	2.52	0.43
30:7:112:PRO:HB2	30:7:267:PRO:HG2	2.01	0.43
36:d:51:LYS:HB3	36:d:51:LYS:HE2	1.87	0.43
38:f:100:MET:SD	38:f:155:ARG:NH2	2.91	0.43
49:r:54:THR:O	49:r:54:THR:OG1	2.37	0.43
4:C:177:LYS:HD3	4:C:178:ASN:H	1.84	0.43
7:K:3:SER:HA	35:c:309:GLU:HG3	2.01	0.43
14:R:54:THR:HG21	15:S:171:ILE:HA	2.01	0.43
14:R:101:VAL:O	14:R:105:LEU:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:222:ASP:OD1	20:X:222:ASP:N	2.48	0.43
28:5:106:ILE:HD11	28:5:223:ARG:HE	1.83	0.43
28:5:136:VAL:HG11	28:5:417:LEU:HD23	2.00	0.43
50:s:89:MET:HG3	50:s:275:LYS:HE3	2.01	0.43
50:s:106:TYR:O	50:s:110:THR:OG1	2.26	0.43
55:n:175:VAL:HG22	55:n:188:ASN:HB3	2.00	0.43
1:D:184:LEU:HD23	1:D:184:LEU:HA	1.85	0.43
3:F:63:GLN:HA	3:F:81:ASP:HA	2.00	0.43
3:F:221:LEU:HD22	3:F:264:PRO:HB2	1.99	0.43
10:N:114:ASP:H	10:N:118:MET:HE3	1.83	0.43
30:7:152:CYS:SG	30:7:156:ARG:NH1	2.91	0.43
30:7:166:LEU:HD23	30:7:183:VAL:HG23	2.01	0.43
36:d:181:VAL:HG23	36:d:224:ILE:HG12	2.01	0.43
37:e:162:ARG:HB3	37:e:251:HIS:CD2	2.54	0.43
5:l:123:MET:HB3	5:l:152:MET:HE3	2.01	0.43
9:M:62:ARG:NH1	41:i:126:LYS:O	2.33	0.43
14:R:64:MET:HE1	16:T:210:HIS:HB3	2.01	0.43
26:3:104:ARG:NH2	56:A:1871:A:N3	2.67	0.43
50:s:324:PHE:HA	50:s:361:ILE:HD11	2.00	0.43
10:N:111:ARG:NH1	56:A:2956:A:O2'	2.50	0.42
16:T:97:MET:HE1	16:T:105:GLN:HG3	2.00	0.42
20:X:192:LYS:HE3	20:X:192:LYS:HB3	1.87	0.42
28:5:391:VAL:HG13	28:5:398:VAL:HB	2.00	0.42
29:6:302:ASP:OD2	29:6:302:ASP:N	2.44	0.42
1:D:102:GLN:HG2	1:D:133:PRO:HB2	2.00	0.42
3:F:252:SER:O	3:F:256:HIS:ND1	2.53	0.42
8:L:119:ILE:HB	8:L:141:ALA:HA	2.01	0.42
9:M:72:THR:HA	9:M:73:PRO:HD3	1.84	0.42
11:O:143:THR:HG1	11:O:146:ASN:HD22	1.62	0.42
18:V:177:THR:HG22	32:9:74:VAL:HA	2.00	0.42
18:V:206:GLU:OE1	18:V:208:ARG:NE	2.42	0.42
30:7:156:ARG:NH2	30:7:259:ASP:O	2.52	0.42
37:e:164:LYS:HE2	37:e:164:LYS:HB3	1.78	0.42
56:A:1851:G:H2'	56:A:2693:A:N7	2.34	0.42
4:C:226:ASN:OD1	4:C:226:ASN:N	2.51	0.42
10:N:127:PRO:HA	10:N:152:THR:HG23	2.01	0.42
12:P:64:LYS:HA	12:P:97:GLN:HE22	1.84	0.42
17:U:24:PHE:HB2	17:U:45:PRO:HG3	2.02	0.42
32:9:128:PHE:HD1	32:9:135:PHE:HB3	1.83	0.42
42:j:48:ASP:HB2	42:j:60:MET:HE3	2.01	0.42
57:B:1642:G:H2'	57:B:1643:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:95:MET:HE1	5:I:161:VAL:HG11	2.01	0.42
12:P:49:THR:HG21	29:6:228:PRO:HB3	2.02	0.42
13:Q:249:LEU:HD12	13:Q:249:LEU:HA	1.89	0.42
17:U:153:LEU:HD22	36:d:222:LEU:HB2	2.02	0.42
30:7:170:PRO:HG2	30:7:180:CYS:HB2	2.01	0.42
35:c:33:LYS:NZ	56:A:1771:C:OP1	2.53	0.42
56:A:2387:U:O2'	56:A:2406:A:N6	2.49	0.42
3:F:113:LYS:HG3	3:F:157:GLY:H	1.83	0.42
13:Q:84:ARG:HG3	56:A:3157:C:H1'	2.02	0.42
26:3:183:ARG:NH1	29:6:355:LYS:O	2.52	0.42
44:l:123:LYS:HG3	56:A:2197:G:H5'	2.01	0.42
56:A:2976:G:O2'	56:A:3005:A:N6	2.53	0.42
11:O:113:ARG:HG2	11:O:115:LEU:H	1.83	0.42
20:X:11:TRP:HA	20:X:14:LEU:HD12	2.01	0.42
21:Y:218:ARG:NH2	41:i:105:ASP:OD1	2.53	0.42
29:6:219:THR:HB	29:6:231:GLU:HG3	2.01	0.42
37:e:264:LEU:HD23	37:e:269:LEU:HB3	2.02	0.42
32:9:100:ILE:HD13	32:9:100:ILE:HA	1.93	0.42
4:C:179:ASN:HB3	4:C:182:TRP:CD1	2.55	0.42
4:H:58:ARG:NH2	20:X:66:PRO:O	2.52	0.42
6:J:81:LYS:HE2	6:J:129:ALA:HB2	2.02	0.42
13:Q:185:ASP:N	13:Q:185:ASP:OD1	2.51	0.42
26:3:179:LYS:HB2	29:6:370:ARG:HH12	1.84	0.42
28:5:127:LYS:HG3	28:5:251:HIS:CD2	2.55	0.42
30:7:254:LEU:HD23	30:7:254:LEU:HA	1.82	0.42
41:i:45:ASP:O	41:i:51:ARG:NH1	2.53	0.42
49:r:40:GLU:HG3	49:r:49:ILE:HG12	2.01	0.42
54:w:85:TYR:O	54:w:89:LEU:N	2.51	0.42
56:A:2900:C:O2'	56:A:2901:A:O4'	2.35	0.42
3:F:113:LYS:HD2	3:F:157:GLY:HA2	2.02	0.42
11:O:134:PRO:HG2	23:0:122:LEU:HD13	2.01	0.42
28:5:275:ASN:HD21	28:5:326:ARG:HH11	1.67	0.42
29:6:306:LYS:HA	29:6:306:LYS:HD3	1.91	0.42
40:h:87:GLN:HB3	40:h:124:ARG:HG3	2.01	0.42
42:j:39:GLY:O	42:j:44:THR:OG1	2.37	0.42
7:K:69:GLY:HA2	49:r:152:THR:HA	2.01	0.42
9:M:244:LEU:HD12	9:M:245:PRO:HD2	2.01	0.42
18:V:121:LYS:HD3	18:V:130:PRO:HB2	2.00	0.42
34:b:36:ASP:HA	46:o:100:LYS:HG3	2.01	0.42
40:h:138:SER:OG	40:h:141:ASP:OD2	2.38	0.42
49:r:123:HIS:HB3	56:A:3191:A:H4'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:s:403:GLU:CD	50:s:404:THR:HG1	2.27	0.42
7:K:27:PRO:HD3	7:K:149:ARG:HD2	2.02	0.41
8:L:74:LEU:HD12	8:L:74:LEU:HA	1.92	0.41
8:L:87:VAL:HG12	8:L:127:LEU:HD11	2.01	0.41
10:N:92:LEU:HD11	10:N:188:LYS:HD2	2.02	0.41
16:T:149:ARG:O	56:A:1672:C:O2'	2.37	0.41
18:V:25:PRO:HA	18:V:26:PRO:HD3	1.85	0.41
20:X:234:LEU:HA	20:X:237:GLN:HB3	2.01	0.41
28:5:136:VAL:HG22	28:5:420:HIS:CD2	2.55	0.41
30:7:69:HIS:HB3	30:7:77:THR:HG23	2.01	0.41
30:7:79:PHE:HB3	30:7:81:MET:HE3	2.02	0.41
37:e:273:ARG:HA	37:e:276:VAL:HG22	2.02	0.41
52:u:128:SER:OG	52:u:185:ARG:NH2	2.44	0.41
56:A:1985:G:OP1	56:A:1987:G:O2'	2.36	0.41
56:A:2694:A:C6	56:A:2985:C:H1'	2.54	0.41
1:D:254:LYS:HA	1:D:254:LYS:HD3	1.92	0.41
11:O:131:PRO:HB3	23:0:184:TRP:HZ3	1.84	0.41
12:P:165:MET:HE3	12:P:165:MET:HB3	1.87	0.41
20:X:189:ASP:HA	20:X:192:LYS:HB2	2.02	0.41
53:v:3:PRO:HD3	54:w:112:4HH:HP3	2.02	0.41
1:D:198:SER:HB2	1:D:206:TYR:HE1	1.84	0.41
12:P:137:LEU:HD11	12:P:169:GLY:HA3	2.01	0.41
15:S:167:TRP:HE1	15:S:169:ARG:HH21	1.67	0.41
17:U:83:ARG:HB2	17:U:85:VAL:HG22	2.02	0.41
24:1:61:LYS:HE3	24:1:61:LYS:HB2	1.92	0.41
56:A:2116:C:O2'	56:A:2837:A:N3	2.50	0.41
4:C:184:LEU:HB3	4:C:213:ILE:HG12	2.02	0.41
10:N:76:SER:HB2	10:N:155:LYS:HB2	2.03	0.41
13:Q:223:LYS:HE2	13:Q:244:ARG:HH21	1.86	0.41
14:R:119:LEU:HD11	33:a:58:ILE:HD13	2.03	0.41
20:X:167:LEU:HD23	20:X:167:LEU:HA	1.92	0.41
52:u:170:VAL:HB	52:u:177:ILE:HG22	2.02	0.41
56:A:2483:U:O2	56:A:2652:G:N2	2.53	0.41
56:A:2627:G:O2'	56:A:2630:U:OP2	2.28	0.41
4:C:189:VAL:HA	4:C:192:HIS:HB3	2.03	0.41
20:X:56:ASN:OD1	20:X:56:ASN:N	2.53	0.41
26:3:131:LYS:HB3	26:3:131:LYS:HE3	1.94	0.41
37:e:97:ARG:HG3	37:e:101:LYS:HZ2	1.85	0.41
41:i:126:LYS:HE2	56:A:2093:U:H4'	2.02	0.41
48:q:41:ASP:HA	48:q:42:PRO:HD3	1.96	0.41
48:q:150:LYS:HA	48:q:150:LYS:HD2	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:85:ASP:OD2	56:A:2796:G:O2'	2.28	0.41
5:I:179:GLY:H	5:I:191:PHE:HE2	1.69	0.41
26:3:106:THR:HB	26:3:162:THR:HA	2.03	0.41
28:5:40:LYS:HA	28:5:40:LYS:HD3	1.86	0.41
30:7:94:HIS:ND1	36:d:281:MET:HB2	2.35	0.41
36:d:173:THR:HA	36:d:176:ILE:HG22	2.02	0.41
37:e:257:LYS:HE3	37:e:278:ASP:HA	2.03	0.41
38:f:94:HIS:CE1	38:f:187:LYS:HB2	2.56	0.41
38:f:177:SER:HB2	45:m:37:ARG:HD3	2.01	0.41
49:r:99:MET:HE3	49:r:99:MET:HB3	1.91	0.41
55:n:212:VAL:HG21	55:n:226:PRO:HB3	2.01	0.41
1:D:199:GLU:HB2	1:D:202:ARG:HB2	2.02	0.41
14:R:81:LEU:HD23	14:R:81:LEU:HA	1.95	0.41
16:T:74:TYR:CE2	16:T:177:LYS:HD3	2.56	0.41
28:5:384:GLN:HG2	28:5:405:GLY:HA3	2.03	0.41
32:9:28:ARG:HD3	56:A:2337:A:H5''	2.02	0.41
40:h:67:GLN:HE22	40:h:87:GLN:NE2	2.18	0.41
48:q:95:SER:O	48:q:98:THR:OG1	2.37	0.41
4:H:115:LYS:HE3	4:H:115:LYS:HB3	1.81	0.41
6:J:29:ALA:HB2	6:J:54:ASN:HD21	1.85	0.41
14:R:111:LYS:NZ	15:S:139:ASP:OD2	2.50	0.41
23:0:168:GLN:H	23:0:168:GLN:HG2	1.71	0.41
30:7:146:CYS:HB3	30:7:278:TYR:HE2	1.86	0.41
52:u:109:ILE:HD13	52:u:127:VAL:HG22	2.03	0.41
55:n:39:GLU:HB2	55:n:178:ALA:HB2	2.02	0.41
56:A:2017:U:O2'	56:A:2723:A:N1	2.45	0.41
4:C:164:VAL:HG13	4:C:231:VAL:HG12	2.01	0.41
6:J:58:LYS:HD2	6:J:58:LYS:HA	1.79	0.41
7:K:116:LEU:HD23	7:K:116:LEU:HA	1.86	0.41
12:P:61:VAL:HG13	29:6:346:ARG:HH22	1.85	0.41
29:6:45:LEU:O	29:6:50:LYS:NZ	2.51	0.41
37:e:46:ARG:HB3	37:e:229:ALA:HB2	2.03	0.41
37:e:50:ALA:HB2	37:e:175:GLN:HG2	2.03	0.41
38:f:112:ASN:HD21	57:B:1635:C:H5''	1.85	0.41
43:k:65:ASP:OD1	43:k:73:ARG:NE	2.37	0.41
50:s:214:GLU:HA	50:s:228:ASP:HA	2.03	0.41
56:A:1782:G:O2'	56:A:1793:G:O6	2.33	0.41
10:N:226:ILE:HD12	10:N:226:ILE:HA	1.92	0.41
36:d:135:LYS:HE3	36:d:135:LYS:HB3	1.79	0.41
56:A:2740:A:N3	56:A:2921:A:O2'	2.46	0.41
18:V:59:GLY:O	18:V:75:LYS:NZ	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:r:160:LYS:HE2	49:r:160:LYS:HB3	1.91	0.40
54:w:100:VAL:HB	54:w:142:GLN:HB2	2.03	0.40
4:C:178:ASN:HB2	4:C:216:TRP:CZ3	2.57	0.40
33:a:104:GLU:HB2	33:a:107:PRO:HD2	2.02	0.40
56:A:1911:C:H2'	56:A:1912:A:C8	2.56	0.40
56:A:2588:C:H2'	56:A:2589:A:C8	2.56	0.40
56:A:2756:C:N3	56:A:2789:C:O2'	2.37	0.40
59:G:69:C:N4	59:G:70:A:N7	2.69	0.40
59:x:69:C:N4	59:x:70:A:N7	2.69	0.40
5:I:162:LYS:N	5:I:195:SER:OG	2.54	0.40
12:P:125:CYS:HB3	12:P:161:LEU:HD12	2.03	0.40
30:7:81:MET:HG2	36:d:279:THR:HB	2.03	0.40
31:8:131:MET:HE3	31:8:131:MET:HB3	1.96	0.40
56:A:1800:G:N1	56:A:1803:A:OP2	2.53	0.40
56:A:2127:A:H4'	56:A:2251:A:C5	2.56	0.40
56:A:2131:A:O2'	56:A:2132:A:O4'	2.40	0.40
3:F:224:GLU:OE1	48:q:32:ARG:NH2	2.49	0.40
7:K:20:LEU:HB2	7:K:141:LEU:HD13	2.03	0.40
8:L:38:VAL:HG11	8:L:75:LEU:HD11	2.04	0.40
9:M:210:LEU:HD23	9:M:210:LEU:HA	1.94	0.40
20:X:2:PRO:HB2	20:X:3:LEU:H	1.56	0.40
21:Y:102:TRP:HE3	21:Y:142:LEU:HD22	1.87	0.40
52:u:163:ASP:OD1	52:u:163:ASP:N	2.49	0.40
52:u:197:ARG:HA	52:u:197:ARG:HD2	1.88	0.40
4:C:208:LEU:HD22	4:C:212:PRO:HG3	2.03	0.40
14:R:25:LEU:O	14:R:29:ARG:NE	2.54	0.40
22:Z:101:LYS:NZ	42:j:83:GLU:OE1	2.43	0.40
34:b:58:ASN:OD1	34:b:58:ASN:N	2.55	0.40
36:d:226:ASP:HB3	36:d:228:PHE:H	1.87	0.40
38:f:129:THR:HB	38:f:151:THR:HB	2.02	0.40
54:w:151:LYS:HB2	54:w:151:LYS:HE3	1.91	0.40
55:n:18:LYS:NZ	4:C:196:ASN:HB2	2.37	0.40
56:A:1874:A:O2'	56:A:2090:A:O2'	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	234/305 (77%)	223 (95%)	9 (4%)	2 (1%)	14	44
2	E	302/348 (87%)	286 (95%)	16 (5%)	0	100	100
3	F	248/311 (80%)	234 (94%)	14 (6%)	0	100	100
4	C	78/267 (29%)	66 (85%)	12 (15%)	0	100	100
4	H	93/267 (35%)	88 (95%)	5 (5%)	0	100	100
5	I	154/261 (59%)	142 (92%)	12 (8%)	0	100	100
6	J	138/192 (72%)	125 (91%)	13 (9%)	0	100	100
7	K	175/178 (98%)	170 (97%)	5 (3%)	0	100	100
8	L	113/145 (78%)	105 (93%)	8 (7%)	0	100	100
9	M	285/296 (96%)	277 (97%)	8 (3%)	0	100	100
10	N	203/251 (81%)	198 (98%)	5 (2%)	0	100	100
11	O	150/175 (86%)	147 (98%)	3 (2%)	0	100	100
12	P	139/179 (78%)	133 (96%)	6 (4%)	0	100	100
13	Q	215/292 (74%)	204 (95%)	11 (5%)	0	100	100
14	R	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
15	S	154/205 (75%)	148 (96%)	6 (4%)	0	100	100
16	T	164/212 (77%)	158 (96%)	6 (4%)	0	100	100
17	U	148/153 (97%)	134 (90%)	12 (8%)	2 (1%)	9	34
18	V	200/216 (93%)	186 (93%)	13 (6%)	1 (0%)	24	57
19	W	107/148 (72%)	103 (96%)	4 (4%)	0	100	100
20	X	241/256 (94%)	230 (95%)	11 (5%)	0	100	100
21	Y	174/250 (70%)	167 (96%)	7 (4%)	0	100	100
22	Z	118/161 (73%)	111 (94%)	7 (6%)	0	100	100
23	0	106/188 (56%)	99 (93%)	7 (7%)	0	100	100
24	1	50/65 (77%)	50 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	2	43/92 (47%)	42 (98%)	1 (2%)	0	100	100
26	3	93/188 (50%)	87 (94%)	6 (6%)	0	100	100
27	4	35/103 (34%)	35 (100%)	0	0	100	100
28	5	383/423 (90%)	363 (95%)	20 (5%)	0	100	100
29	6	316/380 (83%)	305 (96%)	11 (4%)	0	100	100
30	7	285/338 (84%)	266 (93%)	19 (7%)	0	100	100
31	8	108/206 (52%)	92 (85%)	11 (10%)	5 (5%)	2	12
32	9	113/137 (82%)	106 (94%)	7 (6%)	0	100	100
33	a	78/142 (55%)	75 (96%)	3 (4%)	0	100	100
34	b	146/155 (94%)	132 (90%)	14 (10%)	0	100	100
35	c	271/332 (82%)	266 (98%)	5 (2%)	0	100	100
36	d	203/306 (66%)	191 (94%)	12 (6%)	0	100	100
37	e	211/279 (76%)	196 (93%)	14 (7%)	1 (0%)	24	57
38	f	110/194 (57%)	96 (87%)	13 (12%)	1 (1%)	14	44
39	g	127/166 (76%)	122 (96%)	5 (4%)	0	100	100
40	h	96/158 (61%)	92 (96%)	4 (4%)	0	100	100
41	i	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
42	j	83/123 (68%)	80 (96%)	3 (4%)	0	100	100
43	k	76/112 (68%)	70 (92%)	6 (8%)	0	100	100
44	l	21/138 (15%)	20 (95%)	1 (5%)	0	100	100
45	m	43/128 (34%)	32 (74%)	11 (26%)	0	100	100
46	o	89/102 (87%)	85 (96%)	3 (3%)	1 (1%)	11	39
47	p	119/206 (58%)	114 (96%)	5 (4%)	0	100	100
48	q	126/222 (57%)	124 (98%)	2 (2%)	0	100	100
49	r	140/196 (71%)	133 (95%)	7 (5%)	0	100	100
50	s	366/439 (83%)	353 (96%)	13 (4%)	0	100	100
52	u	109/234 (47%)	100 (92%)	9 (8%)	0	100	100
53	v	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
54	w	76/156 (49%)	71 (93%)	5 (7%)	0	100	100
55	n	230/229 (100%)	213 (93%)	17 (7%)	0	100	100
All	All	8385/11552 (73%)	7937 (95%)	435 (5%)	13 (0%)	44	73

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	207	ILE
17	U	117	SER
31	8	186	GLN
31	8	187	PRO
31	8	188	PRO
17	U	118	PRO
1	D	208	ARG
18	V	160	PRO
37	e	256	THR
31	8	181	PRO
46	o	16	GLN
38	f	179	PRO
31	8	182	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	190/245 (78%)	190 (100%)	0	100	100
2	E	259/290 (89%)	253 (98%)	6 (2%)	44	70
3	F	217/262 (83%)	216 (100%)	1 (0%)	81	85
4	C	73/228 (32%)	72 (99%)	1 (1%)	59	76
4	H	86/228 (38%)	85 (99%)	1 (1%)	63	78
5	I	145/232 (62%)	144 (99%)	1 (1%)	76	82
6	J	113/150 (75%)	113 (100%)	0	100	100
7	K	155/156 (99%)	154 (99%)	1 (1%)	78	83
8	L	98/124 (79%)	96 (98%)	2 (2%)	48	72
9	M	245/249 (98%)	242 (99%)	3 (1%)	63	78
10	N	172/211 (82%)	172 (100%)	0	100	100
11	O	133/150 (89%)	133 (100%)	0	100	100
12	P	123/154 (80%)	121 (98%)	2 (2%)	55	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	Q	199/256 (78%)	197 (99%)	2 (1%)	68	79
14	R	118/126 (94%)	117 (99%)	1 (1%)	73	81
15	S	141/180 (78%)	139 (99%)	2 (1%)	59	76
16	T	146/182 (80%)	145 (99%)	1 (1%)	76	82
17	U	124/135 (92%)	123 (99%)	1 (1%)	73	81
18	V	172/191 (90%)	170 (99%)	2 (1%)	63	78
19	W	89/119 (75%)	89 (100%)	0	100	100
20	X	219/229 (96%)	217 (99%)	2 (1%)	70	80
21	Y	159/223 (71%)	158 (99%)	1 (1%)	78	83
22	Z	111/147 (76%)	111 (100%)	0	100	100
23	0	97/164 (59%)	96 (99%)	1 (1%)	68	79
24	1	49/60 (82%)	49 (100%)	0	100	100
25	2	39/72 (54%)	39 (100%)	0	100	100
26	3	88/166 (53%)	88 (100%)	0	100	100
27	4	36/89 (40%)	36 (100%)	0	100	100
28	5	348/368 (95%)	347 (100%)	1 (0%)	86	87
29	6	265/332 (80%)	263 (99%)	2 (1%)	73	81
30	7	263/303 (87%)	261 (99%)	2 (1%)	73	81
31	8	91/190 (48%)	89 (98%)	2 (2%)	45	71
32	9	99/112 (88%)	98 (99%)	1 (1%)	68	79
33	a	78/133 (59%)	78 (100%)	0	100	100
34	b	130/135 (96%)	128 (98%)	2 (2%)	57	75
35	c	241/288 (84%)	240 (100%)	1 (0%)	84	86
36	d	193/274 (70%)	189 (98%)	4 (2%)	47	71
37	e	188/236 (80%)	186 (99%)	2 (1%)	65	78
38	f	101/173 (58%)	101 (100%)	0	100	100
39	g	119/148 (80%)	115 (97%)	4 (3%)	32	63
40	h	95/148 (64%)	95 (100%)	0	100	100
41	i	86/110 (78%)	86 (100%)	0	100	100
42	j	68/97 (70%)	68 (100%)	0	100	100
43	k	71/90 (79%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	l	23/116 (20%)	23 (100%)	0	100	100
45	m	40/113 (35%)	40 (100%)	0	100	100
46	o	78/87 (90%)	78 (100%)	0	100	100
47	p	117/181 (65%)	116 (99%)	1 (1%)	70	80
48	q	110/178 (62%)	109 (99%)	1 (1%)	70	80
49	r	133/169 (79%)	132 (99%)	1 (1%)	73	81
50	s	326/381 (86%)	322 (99%)	4 (1%)	63	78
52	u	105/200 (52%)	105 (100%)	0	100	100
53	v	59/60 (98%)	59 (100%)	0	100	100
54	w	72/135 (53%)	72 (100%)	0	100	100
55	n	184/181 (102%)	177 (96%)	7 (4%)	29	60
All	All	7479/9956 (75%)	7413 (99%)	66 (1%)	70	80

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	97	VAL
2	E	152	VAL
2	E	181	ILE
2	E	204	VAL
2	E	285	VAL
2	E	289	VAL
3	F	77	VAL
4	H	102	VAL
5	I	47	LEU
7	K	73	GLU
8	L	38	VAL
8	L	105	VAL
9	M	141	VAL
9	M	158	LEU
9	M	248	THR
12	P	49	THR
12	P	147	GLN
13	Q	136	ILE
13	Q	226	PRO
14	R	45	THR
15	S	159	THR
15	S	195	ILE

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Mol	Chain	Res	Type
16	T	209	VAL
17	U	47	GLU
18	V	45	VAL
18	V	79	VAL
20	X	97	LEU
20	X	124	THR
21	Y	172	ILE
23	0	169	ASP
28	5	98	LEU
29	6	250	VAL
29	6	251	THR
30	7	73	THR
30	7	77	THR
31	8	150	LEU
31	8	153	GLU
32	9	66	THR
34	b	62	VAL
34	b	112	VAL
35	c	93	VAL
36	d	67	ILE
36	d	84	ILE
36	d	180	THR
36	d	246	VAL
37	e	51	LEU
37	e	255	VAL
39	g	43	ASP
39	g	57	ILE
39	g	137	VAL
39	g	140	VAL
47	p	186	GLU
48	q	46	LEU
49	r	85	ASP
50	s	239	ASN
50	s	257	VAL
50	s	360	VAL
50	s	401	LEU
55	n	53[A]	ARG
55	n	53[B]	ARG
55	n	63[A]	SER
55	n	63[B]	SER
55	n	75	LEU
55	n	202[A]	GLU

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Mol	Chain	Res	Type
55	n	202[B]	GLU
4	C	233	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	195	ASN
1	D	205	GLN
2	E	52	HIS
2	E	57	ASN
2	E	72	GLN
2	E	313	ASN
3	F	58	HIS
3	F	184	GLN
4	H	121	ASN
5	I	36	HIS
5	I	101	ASN
5	I	129	GLN
5	I	151	ASN
6	J	54	ASN
7	K	9	GLN
7	K	64	HIS
7	K	70	ASN
7	K	89	GLN
7	K	117	HIS
8	L	43	ASN
8	L	48	ASN
8	L	104	ASN
9	M	58	GLN
10	N	98	HIS
10	N	210	GLN
11	O	39	HIS
11	O	91	GLN
11	O	147	GLN
11	O	150	GLN
12	P	87	GLN
12	P	97	GLN
12	P	142	ASN
13	Q	237	ASN
14	R	22	GLN
14	R	30	HIS
14	R	77	GLN

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Mol	Chain	Res	Type
14	R	79	HIS
15	S	140	ASN
17	U	4	ASN
17	U	55	ASN
17	U	82	HIS
17	U	103	GLN
19	W	76	HIS
19	W	80	HIS
20	X	15	GLN
20	X	237	GLN
21	Y	88	GLN
21	Y	117	GLN
21	Y	191	ASN
21	Y	195	ASN
21	Y	225	ASN
22	Z	107	ASN
23	0	118	GLN
23	0	170	GLN
25	2	54	GLN
26	3	178	GLN
28	5	206	ASN
28	5	250	ASN
28	5	275	ASN
28	5	289	HIS
28	5	302	HIS
28	5	353	HIS
28	5	367	ASN
28	5	385	HIS
29	6	243	ASN
29	6	266	HIS
29	6	359	HIS
30	7	45	ASN
30	7	49	ASN
30	7	207	HIS
30	7	298	GLN
31	8	103	GLN
31	8	127	GLN
31	8	167	ASN
32	9	113	ASN
32	9	123	GLN
33	a	46	ASN
34	b	17	ASN

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Mol	Chain	Res	Type
34	b	24	GLN
34	b	27	GLN
34	b	123	ASN
35	c	155	ASN
35	c	222	GLN
36	d	59	HIS
36	d	77	HIS
36	d	167	HIS
36	d	207	ASN
36	d	217	HIS
37	e	95	ASN
37	e	130	GLN
37	e	212	HIS
37	e	251	HIS
38	f	112	ASN
40	h	87	GLN
40	h	99	ASN
40	h	135	GLN
41	i	59	ASN
41	i	120	HIS
42	j	30	GLN
42	j	95	GLN
42	j	102	GLN
42	j	107	ASN
43	k	35	GLN
43	k	46	ASN
44	l	135	ASN
47	p	104	HIS
47	p	125	ASN
47	p	184	ASN
48	q	134	ASN
48	q	139	GLN
49	r	112	HIS
49	r	130	ASN
49	r	148	ASN
49	r	184	ASN
50	s	315	ASN
50	s	319	GLN
50	s	358	GLN
53	v	19	GLN
53	v	42	ASN
53	v	43	GLN

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Mol	Chain	Res	Type
53	v	63	ASN
54	w	101	ASN
54	w	115	GLN
54	w	142	GLN
55	n	3	HIS
55	n	17	ASN
55	n	56	GLN
4	C	196	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
56	A	1477/1559 (94%)	388 (26%)	21 (1%)
57	B	51/69 (73%)	14 (27%)	1 (1%)
59	G	73/73 (100%)	30 (41%)	2 (2%)
59	x	72/73 (98%)	30 (41%)	0
All	All	1673/1774 (94%)	462 (27%)	24 (1%)

All (462) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
56	A	1676	A
56	A	1678	C
56	A	1680	A
56	A	1681	G
56	A	1685	C
56	A	1689	C
56	A	1699	C
56	A	1700	U
56	A	1703	C
56	A	1704	U
56	A	1708	A
56	A	1713	A
56	A	1714	C
56	A	1715	C
56	A	1716	U
56	A	1724	A
56	A	1727	A
56	A	1728	U
56	A	1741	A
56	A	1748	G

Continued on next page...

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Mol	Chain	Res	Type
56	A	1750	G
56	A	1751	A
56	A	1770	G
56	A	1780	U
56	A	1791	G
56	A	1794	A
56	A	1795	A
56	A	1803	A
56	A	1804	A
56	A	1805	A
56	A	1812	C
56	A	1817	C
56	A	1821	A
56	A	1823	A
56	A	1824	U
56	A	1827	C
56	A	1828	A
56	A	1829	A
56	A	1832	A
56	A	1836	A
56	A	1839	C
56	A	1844	A
56	A	1849	C
56	A	1852	C
56	A	1854	U
56	A	1856	A
56	A	1867	A
56	A	1868	G
56	A	1869	A
56	A	1872	U
56	A	1878	U
56	A	1882	A
56	A	1883	G
56	A	1887	A
56	A	1888	G
56	A	1892	A
56	A	1893	A
56	A	1901	C
56	A	1903	C
56	A	1909	A
56	A	1918	G
56	A	1927	G

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Mol	Chain	Res	Type
56	A	1935	A
56	A	1940	A
56	A	1944	C
56	A	1968	G
56	A	1974	A
56	A	1985	G
56	A	1987	G
56	A	1992	C
56	A	1993	A
56	A	1994	A
56	A	1995	A
56	A	2001	C
56	A	2010	U
56	A	2015	G
56	A	2020	U
56	A	2021	U
56	A	2022	G
56	A	2029	A
56	A	2030	U
56	A	2031	A
56	A	2032	G
56	A	2034	A
56	A	2036	C
56	A	2037	U
56	A	2039	A
56	A	2053	U
56	A	2060	A
56	A	2065	A
56	A	2074	A
56	A	2079	C
56	A	2083	U
56	A	2085	A
56	A	2097	A
56	A	2098	G
56	A	2113	G
56	A	2124	A
56	A	2125	C
56	A	2132	A
56	A	2136	C
56	A	2141	U
56	A	2142	A
56	A	2147	G

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Mol	Chain	Res	Type
56	A	2154	A
56	A	2157	U
56	A	2159	U
56	A	2160	A
56	A	2163	A
56	A	2168	U
56	A	2171	U
56	A	2172	A
56	A	2173	G
56	A	2174	G
56	A	2180	A
56	A	2181	A
56	A	2182	G
56	A	2183	C
56	A	2187	C
56	A	2193	U
56	A	2194	U
56	A	2195	A
56	A	2197	G
56	A	2198	A
56	A	2200	A
56	A	2204	U
56	A	2210	C
56	A	2211	U
56	A	2215	C
56	A	2216	A
56	A	2230	A
56	A	2237	A
56	A	2239	A
56	A	2241	A
56	A	2242	U
56	A	2243	A
56	A	2244	U
56	A	2245	A
56	A	2246	A
56	A	2252	C
56	A	2261	C
56	A	2262	C
56	A	2263	C
56	A	2264	A
56	A	2284	C
56	A	2285	U

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Mol	Chain	Res	Type
56	A	2290	A
56	A	2297	A
56	A	2299	U
56	A	2300	G
56	A	2316	U
56	A	2322	C
56	A	2324	U
56	A	2332	C
56	A	2345	G
56	A	2371	U
56	A	2372	U
56	A	2374	A
56	A	2381	A
56	A	2387	U
56	A	2388	A
56	A	2390	A
56	A	2393	C
56	A	2401	A
56	A	2404	U
56	A	2405	C
56	A	2406	A
56	A	2407	U
56	A	2414	C
56	A	2416	U
56	A	2426	C
56	A	2427	C
56	A	2434	A
56	A	2444	A
56	A	2446	A
56	A	2451	A
56	A	2452	A
56	A	2458	A
56	A	2478	G
56	A	2493	C
56	A	2500	A
56	A	2502	C
56	A	2507	A
56	A	2508	C
56	A	2511	C
56	A	2520	C
56	A	2521	A
56	A	2523	C

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Mol	Chain	Res	Type
56	A	2524	A
56	A	2527	A
56	A	2531	U
56	A	2536	G
56	A	2540	C
56	A	2550	A
56	A	2557	C
56	A	2558	A
56	A	2559	U
56	A	2560	G
56	A	2563	U
56	A	2570	C
56	A	2571	G
56	A	2573	G
56	A	2574	G
56	A	2575	U
56	A	2576	A
56	A	2577	C
56	A	2578	C
56	A	2579	C
56	A	2580	U
56	A	2582	A
56	A	2583	C
56	A	2584	C
56	A	2587	G
56	A	2588	C
56	A	2592	G
56	A	2593	G
56	A	2594	U
56	A	2601	A
56	A	2603	C
56	A	2607	U
56	A	2618	U
56	A	2626	U
56	A	2627	G
56	A	2629	A
56	A	2630	U
56	A	2632	A
56	A	2633	A
56	A	2634	U
56	A	2635	G
56	A	2645	G

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Mol	Chain	Res	Type
56	A	2654	U
56	A	2655	G
56	A	2656	U
56	A	2660	U
56	A	2683	C
56	A	2684	C
56	A	2686	G
56	A	2694	A
56	A	2695	G
56	A	2696	A
56	A	2706	A
56	A	2708	C
56	A	2709	A
56	A	2718	C
56	A	2719	G
56	A	2723	A
56	A	2724	G
56	A	2732	G
56	A	2739	U
56	A	2743	U
56	A	2744	U
56	A	2745	A
56	A	2747	U
56	A	2750	U
56	A	2757	A
56	A	2758	G
56	A	2759	U
56	A	2761	C
56	A	2762	C
56	A	2763	U
56	A	2764	A
56	A	2765	A
56	A	2766	C
56	A	2767	A
56	A	2768	A
56	A	2771	C
56	A	2773	A
56	A	2774	C
56	A	2775	A
56	A	2776	G
56	A	2777	G
56	A	2778	U

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Mol	Chain	Res	Type
56	A	2779	C
56	A	2780	C
56	A	2781	U
56	A	2782	A
56	A	2784	A
56	A	2785	C
56	A	2786	U
56	A	2787	A
56	A	2788	C
56	A	2789	C
56	A	2790	A
56	A	2791	A
56	A	2792	A
56	A	2804	A
56	A	2810	G
56	A	2814	G
56	A	2831	G
56	A	2832	A
56	A	2833	A
56	A	2844	G
56	A	2847	C
56	A	2852	C
56	A	2854	U
56	A	2859	A
56	A	2861	A
56	A	2864	U
56	A	2865	C
56	A	2869	A
56	A	2871	U
56	A	2879	A
56	A	2880	A
56	A	2895	U
56	A	2896	G
56	A	2900	C
56	A	2901	A
56	A	2903	U
56	A	2906	C
56	A	2910	A
56	A	2912	C
56	A	2913	A
56	A	2917	G
56	A	2918	A

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Mol	Chain	Res	Type
56	A	2919	A
56	A	2921	A
56	A	2922	A
56	A	2926	A
56	A	2928	C
56	A	2932	G
56	A	2935	A
56	A	2939	C
56	A	2955	U
56	A	2956	A
56	A	2963	A
56	A	2971	A
56	A	2978	U
56	A	2985	C
56	A	2989	G
56	A	2990	A
56	A	2991	U
56	A	2992	G
56	A	2993	U
56	A	2994	U
56	A	3000	A
56	A	3005	A
56	A	3016	G
56	A	3022	G
56	A	3041	U
56	A	3042	U
56	A	3051	A
56	A	3053	A
56	A	3054	G
56	A	3056	C
56	A	3060	C
56	A	3063	G
56	A	3065	U
56	A	3069	A
56	A	3072	U
56	A	3073	C
56	A	3077	C
56	A	3086	U
56	A	3089	A
56	A	3090	G
56	A	3093	C
56	A	3098	U

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Mol	Chain	Res	Type
56	A	3099	C
56	A	3100	U
56	A	3102	U
56	A	3108	U
56	A	3109	U
56	A	3114	U
56	A	3122	U
56	A	3123	G
56	A	3131	G
56	A	3141	A
56	A	3150	U
56	A	3155	C
56	A	3157	C
56	A	3158	A
56	A	3160	A
56	A	3162	C
56	A	3168	C
56	A	3169	C
56	A	3172	C
56	A	3176	A
56	A	3180	A
56	A	3184	C
56	A	3189	C
56	A	3190	A
56	A	3196	G
56	A	3202	U
56	A	3206	C
56	A	3207	A
56	A	3217	A
56	A	3218	A
56	A	3220	A
56	A	3228	U
57	B	1607	U
57	B	1608	G
57	B	1611	G
57	B	1614	U
57	B	1615	A
57	B	1631	C
57	B	1632	U
57	B	1641	G
57	B	1644	G
57	B	1645	A

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Mol	Chain	Res	Type
57	B	1646	U
57	B	1649	C
57	B	1650	A
57	B	1669	G
59	G	2	U
59	G	3	U
59	G	7	G
59	G	9	A
59	G	10	G
59	G	13	U
59	G	14	A
59	G	16	A
59	G	17	U
59	G	18	U
59	G	19	A
59	G	20	U
59	G	21	C
59	G	38	A
59	G	40	U
59	G	45	A
59	G	46	G
59	G	47	A
59	G	50	A
59	G	52	C
59	G	55	C
59	G	56	A
59	G	57	C
59	G	58	A
59	G	59	G
59	G	62	C
59	G	70	A
59	G	71	C
59	G	72	C
59	G	73	A
59	x	2	U
59	x	3	U
59	x	7	G
59	x	9	A
59	x	10	G
59	x	13	U
59	x	14	A
59	x	16	A

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Mol	Chain	Res	Type
59	x	17	U
59	x	18	U
59	x	19	A
59	x	20	U
59	x	21	C
59	x	38	A
59	x	40	U
59	x	45	A
59	x	46	G
59	x	47	A
59	x	50	A
59	x	52	C
59	x	55	C
59	x	56	A
59	x	57	C
59	x	58	A
59	x	59	G
59	x	62	C
59	x	70	A
59	x	71	C
59	x	72	C
59	x	73	A

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
56	A	1703	C
56	A	1713	A
56	A	1811	A
56	A	1823	A
56	A	1871	A
56	A	2030	U
56	A	2186	C
56	A	2243	A
56	A	2245	A
56	A	2457	A
56	A	2507	A
56	A	2530	A
56	A	2559	U
56	A	2653	C
56	A	2757	A
56	A	2784	A

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Mol	Chain	Res	Type
56	A	2900	C
56	A	2905	A
56	A	2989	G
56	A	3041	U
56	A	3092	U
57	B	1607	U
59	G	1	G
59	G	70	A

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	4HH	w	112	53,54	22,26,27	1.77	3 (13%)	27,35,37	3.00	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	4HH	w	112	53,54	-	9/33/35/37	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	w	112	4HH	CL3-NN	5.05	1.45	1.33
54	w	112	4HH	CQ-NR	5.05	1.45	1.33
54	w	112	4HH	ON-CL3	-2.24	1.19	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	w	112	4HH	P-OG-CB	-8.75	71.20	121.35
54	w	112	4HH	O1P-P-OG	-8.68	68.22	107.57
54	w	112	4HH	OG-P-O2P	6.94	136.44	108.94
54	w	112	4HH	OG-CB-CA	3.12	111.18	108.14
54	w	112	4HH	CL2-CK-CM	3.10	114.05	108.77
54	w	112	4HH	CO-NN-CL3	-2.36	118.30	122.55

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	w	112	4HH	CB-OG-P-O2P
54	w	112	4HH	CJ-CK-CM-CL3
54	w	112	4HH	CJ-CK-CM-OM
54	w	112	4HH	CL1-CK-CM-CL3
54	w	112	4HH	CL1-CK-CM-OM
54	w	112	4HH	CL2-CK-CM-CL3
54	w	112	4HH	CL2-CK-CM-OM
54	w	112	4HH	CJ-O3P-P-OG
54	w	112	4HH	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	w	112	4HH	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 101 ligands modelled in this entry, 101 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
56	A	1
17	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2585:G	O3'	2586:U	P	8.18
1	U	124:ASP	C	125:ASP	N	6.70

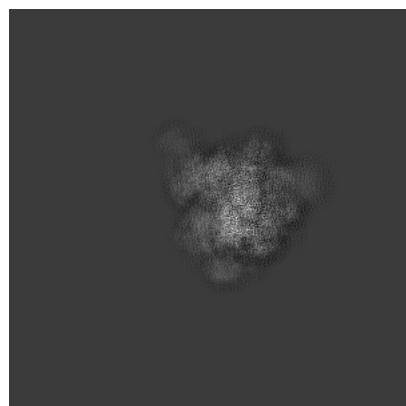
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11645. These allow visual inspection of the internal detail of the map and identification of artifacts.

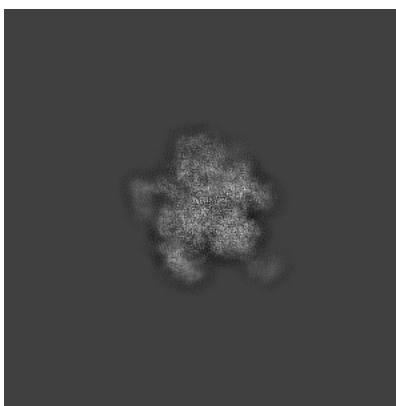
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

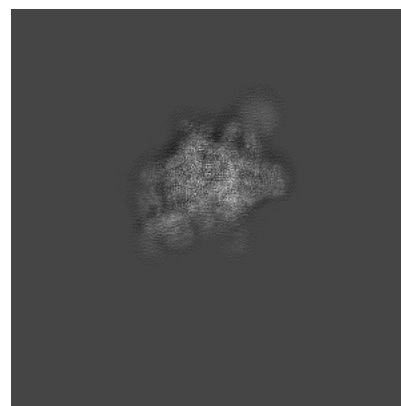
6.1.1 Primary map



X

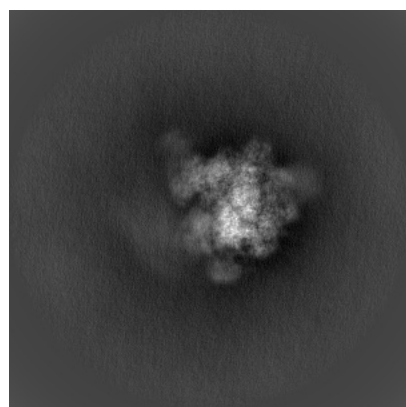


Y

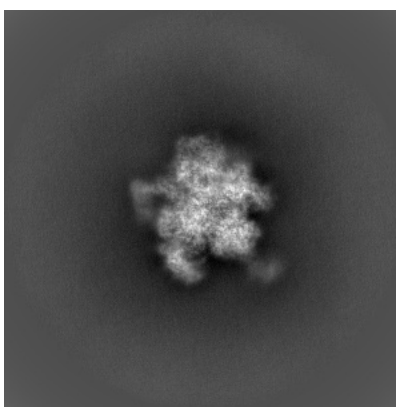


Z

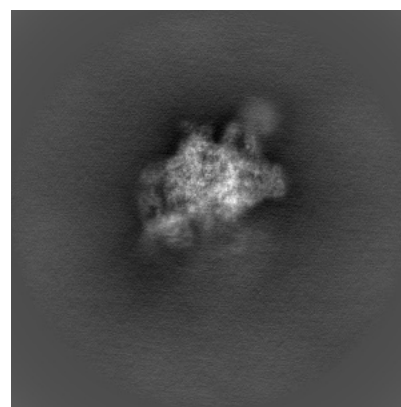
6.1.2 Raw map



X



Y

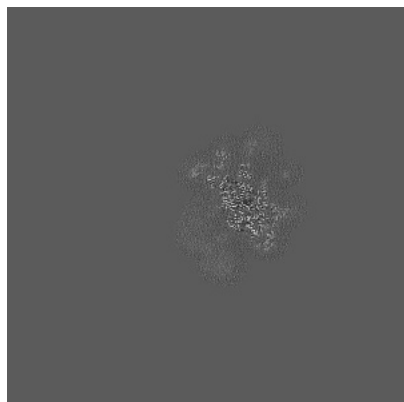


Z

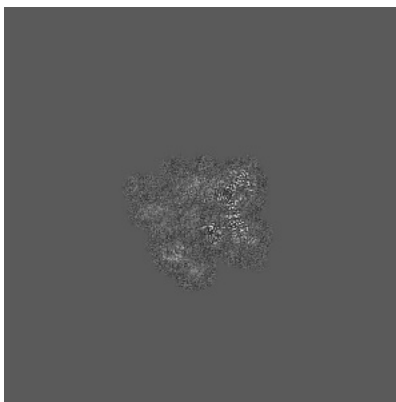
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

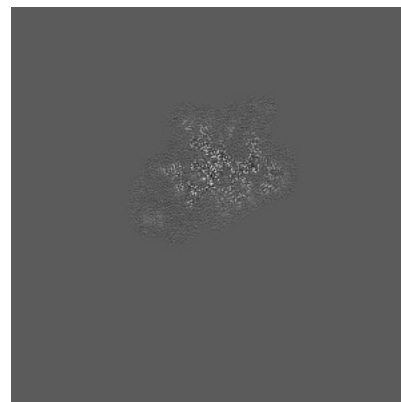
6.2.1 Primary map



X Index: 256

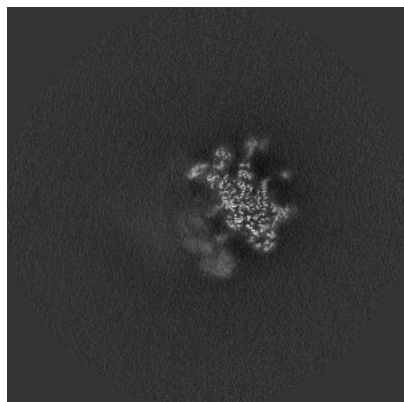


Y Index: 256

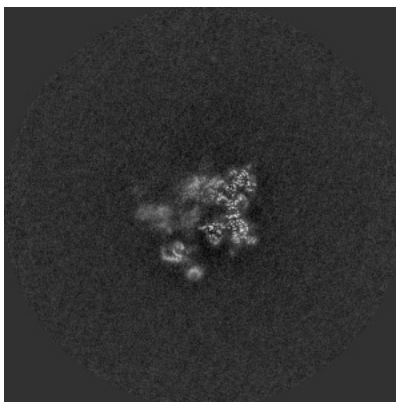


Z Index: 256

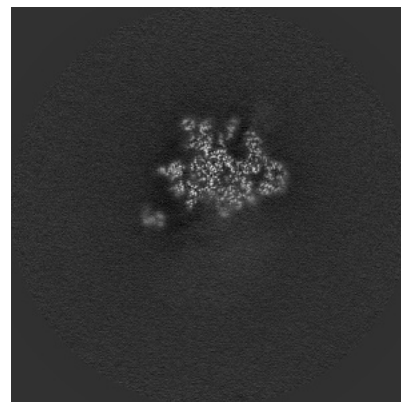
6.2.2 Raw map



X Index: 256



Y Index: 256

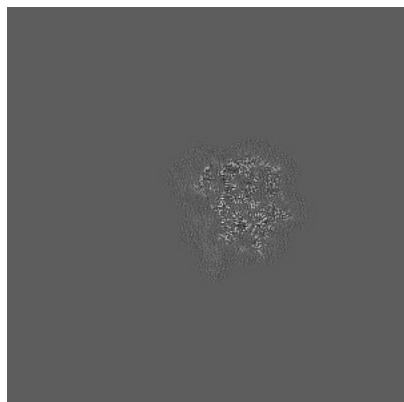


Z Index: 256

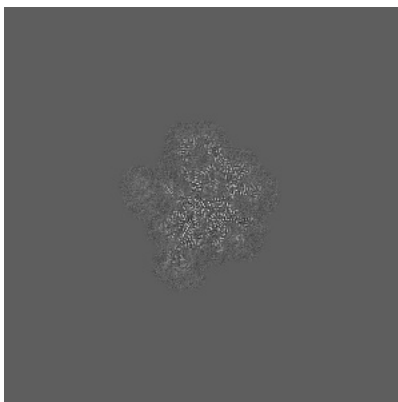
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

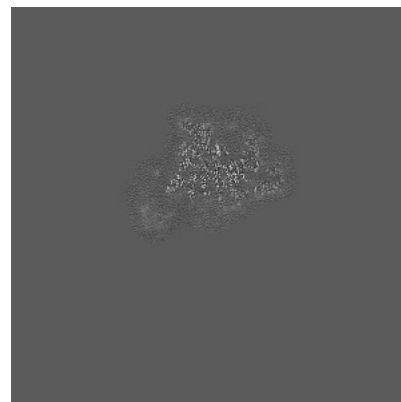
6.3.1 Primary map



X Index: 236

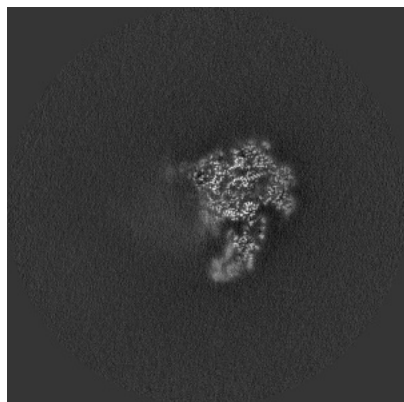


Y Index: 291

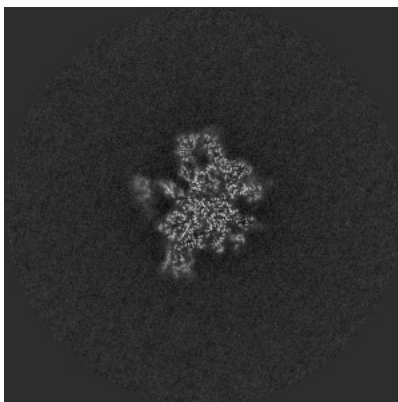


Z Index: 248

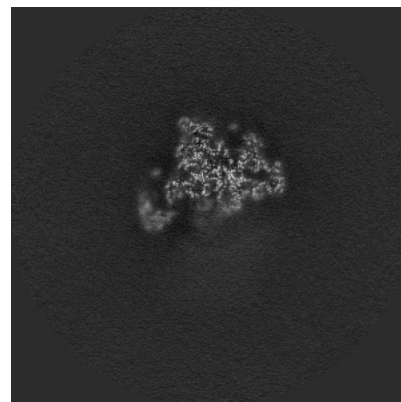
6.3.2 Raw map



X Index: 281



Y Index: 291

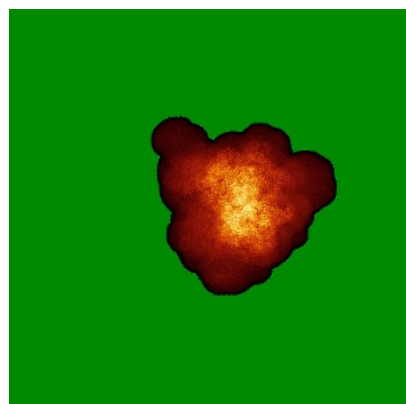


Z Index: 246

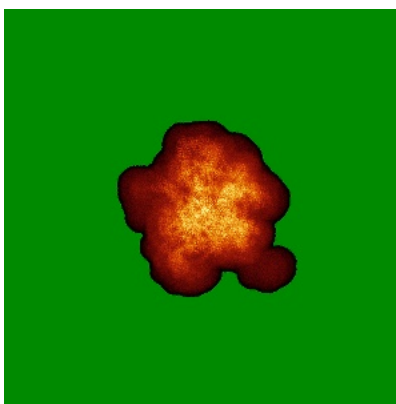
The images above show the largest variance slices of the map in three orthogonal directions.

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

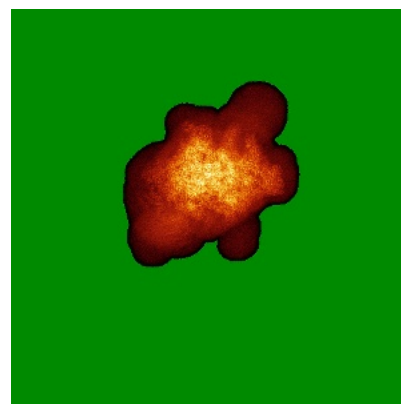
6.4.1 Primary map



X

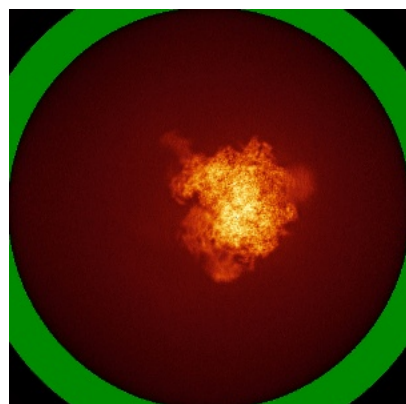


Y

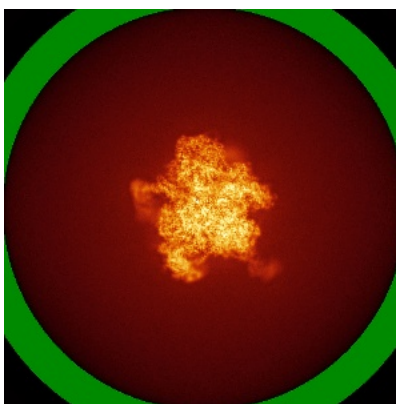


Z

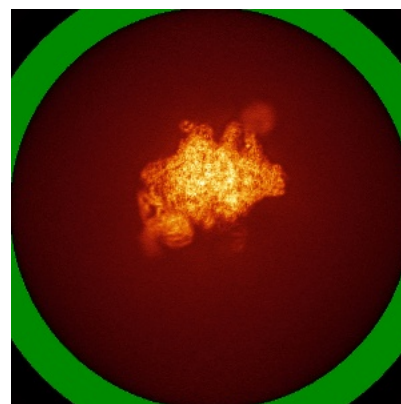
6.4.2 Raw map



X



Y

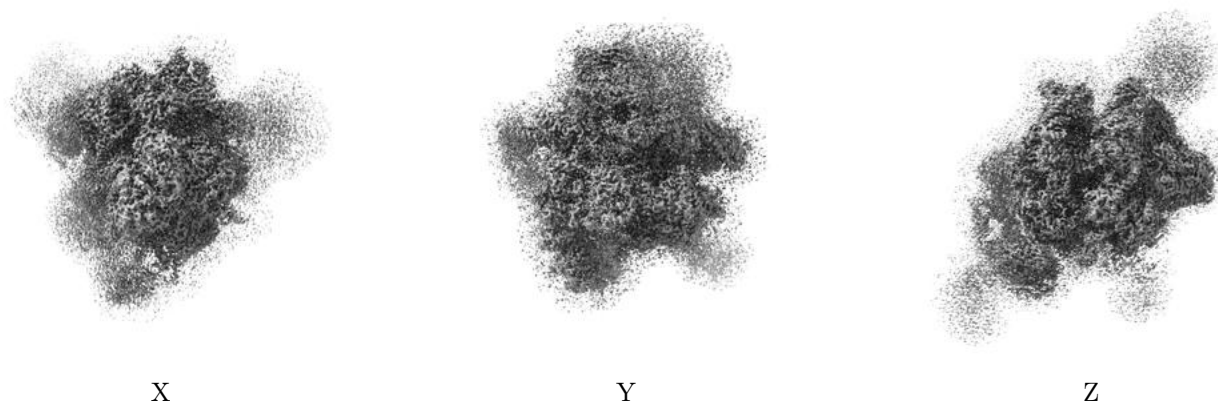


Z

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 0.1. 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.

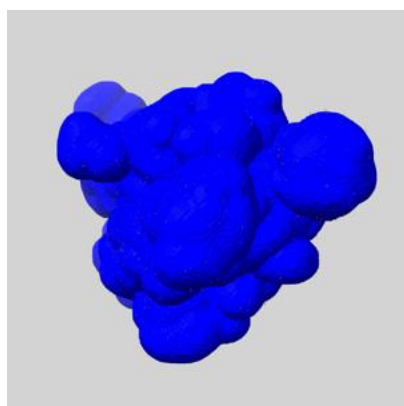
6.6 Mask visualisation [i](#)

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

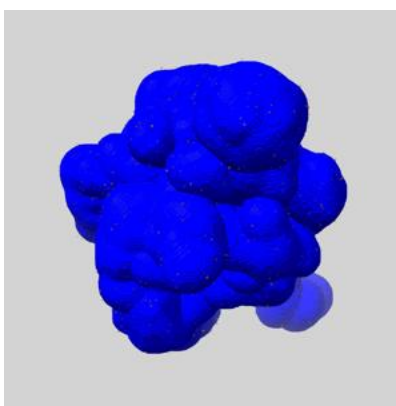
A mask typically either:

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

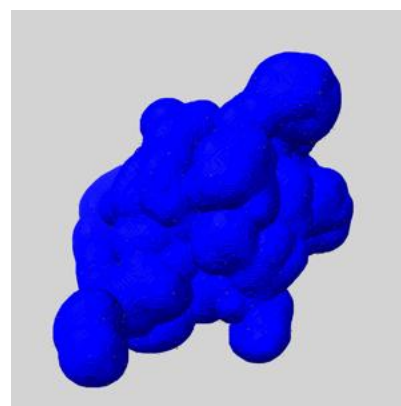
6.6.1 emd_11645_msk_1.map [i](#)



X



Y

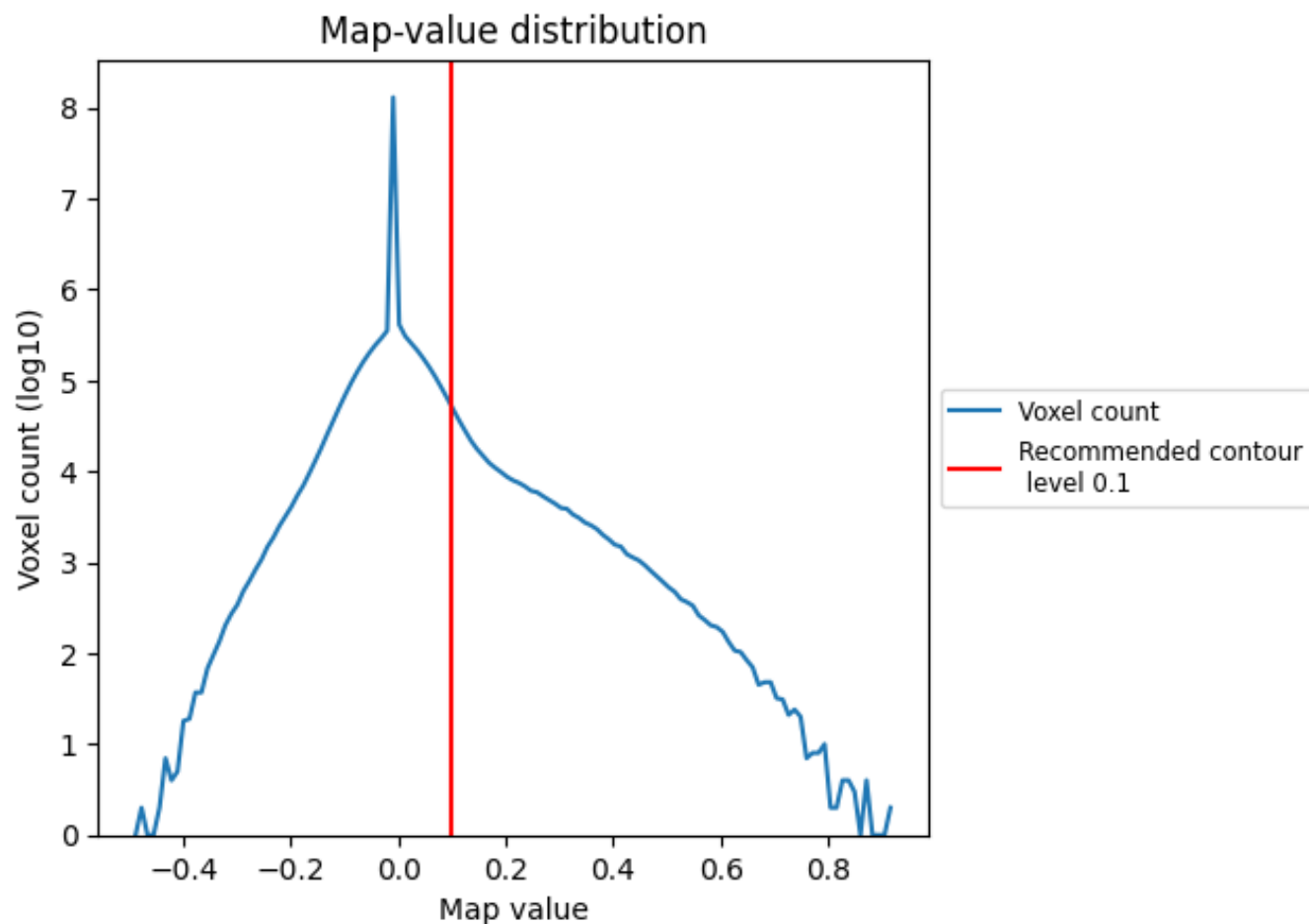


Z

7 Map analysis [i](#)

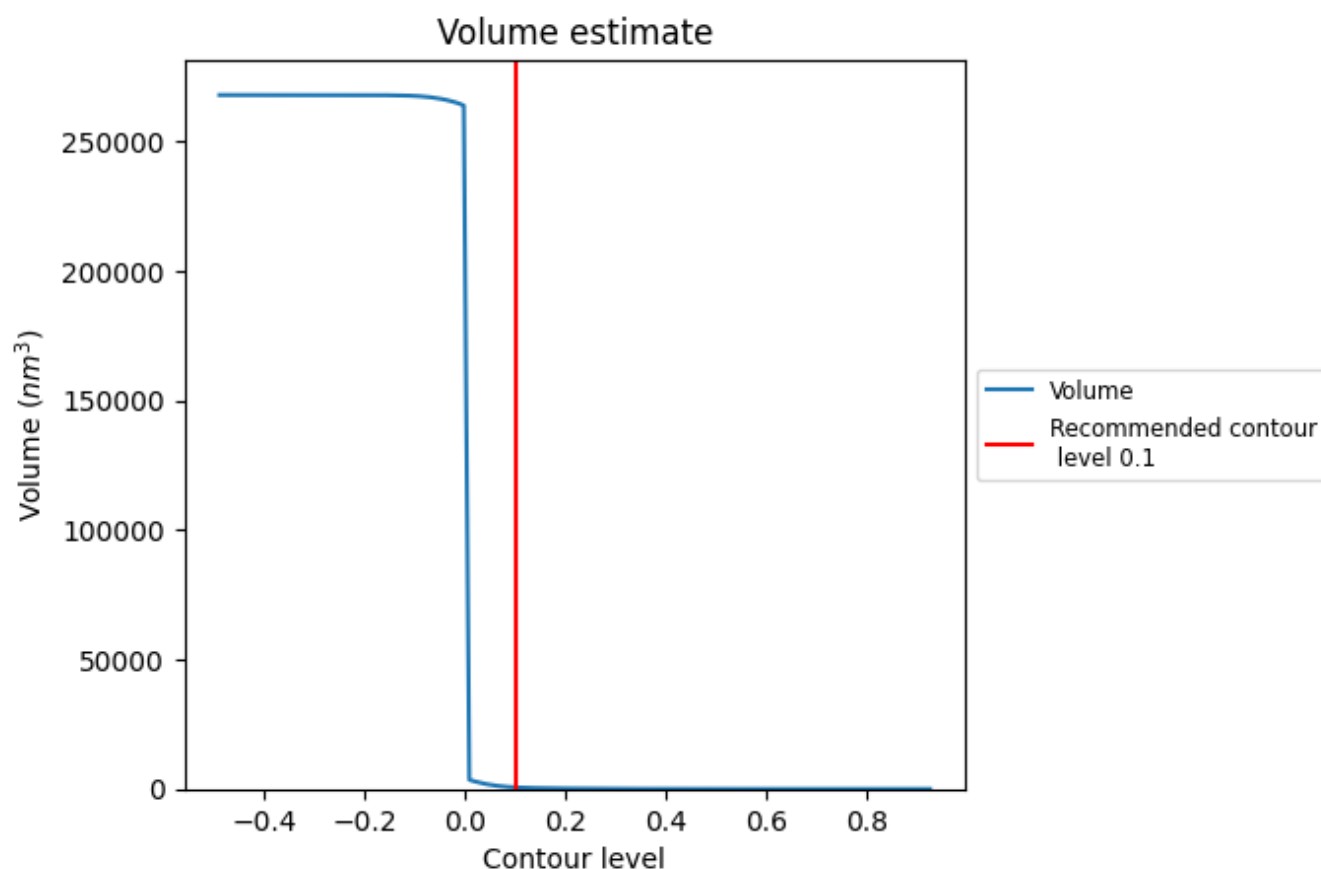
This section contains the results of statistical analysis of the map.

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.

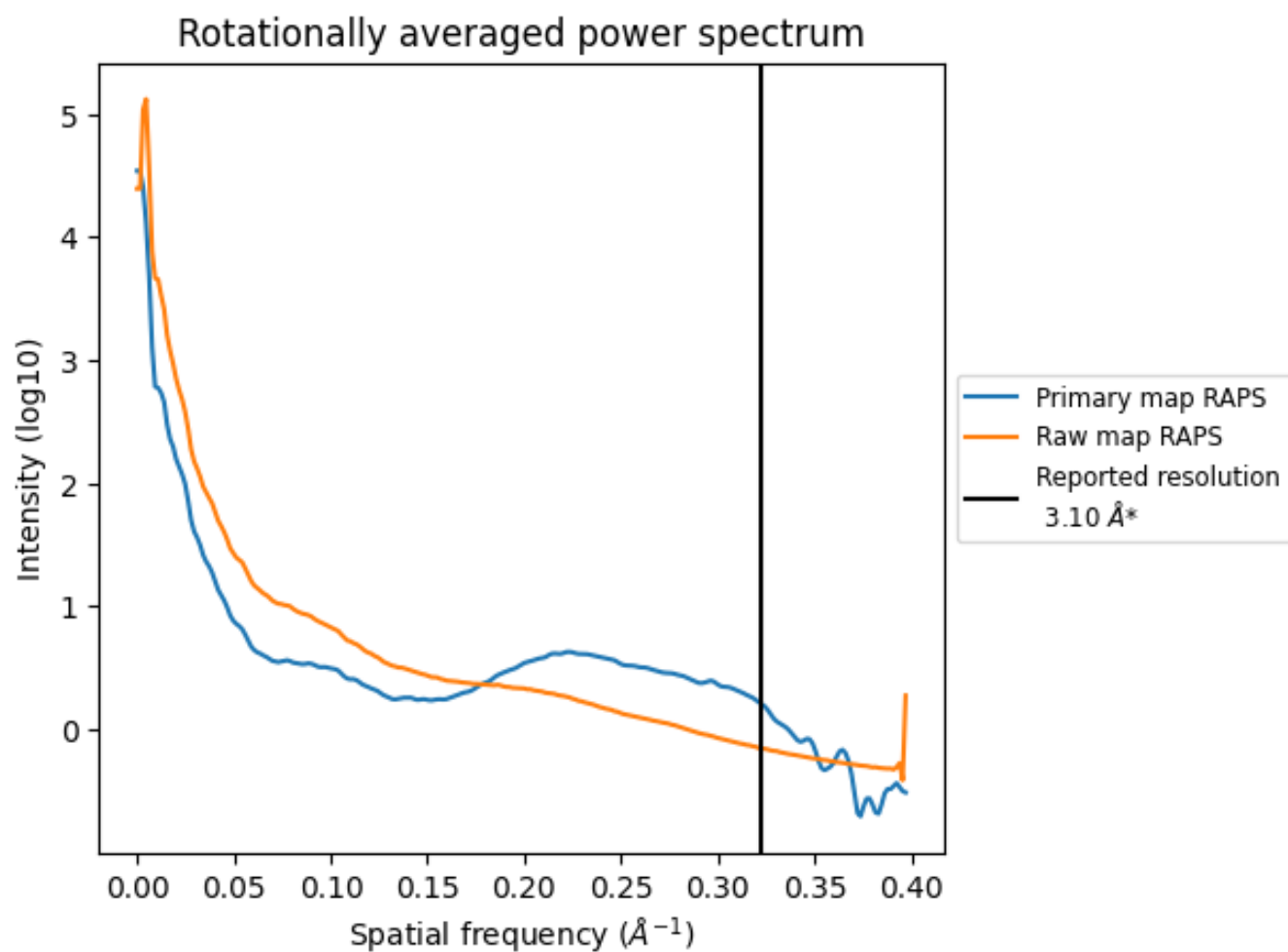
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 618 nm³; this corresponds to an approximate mass of 558 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

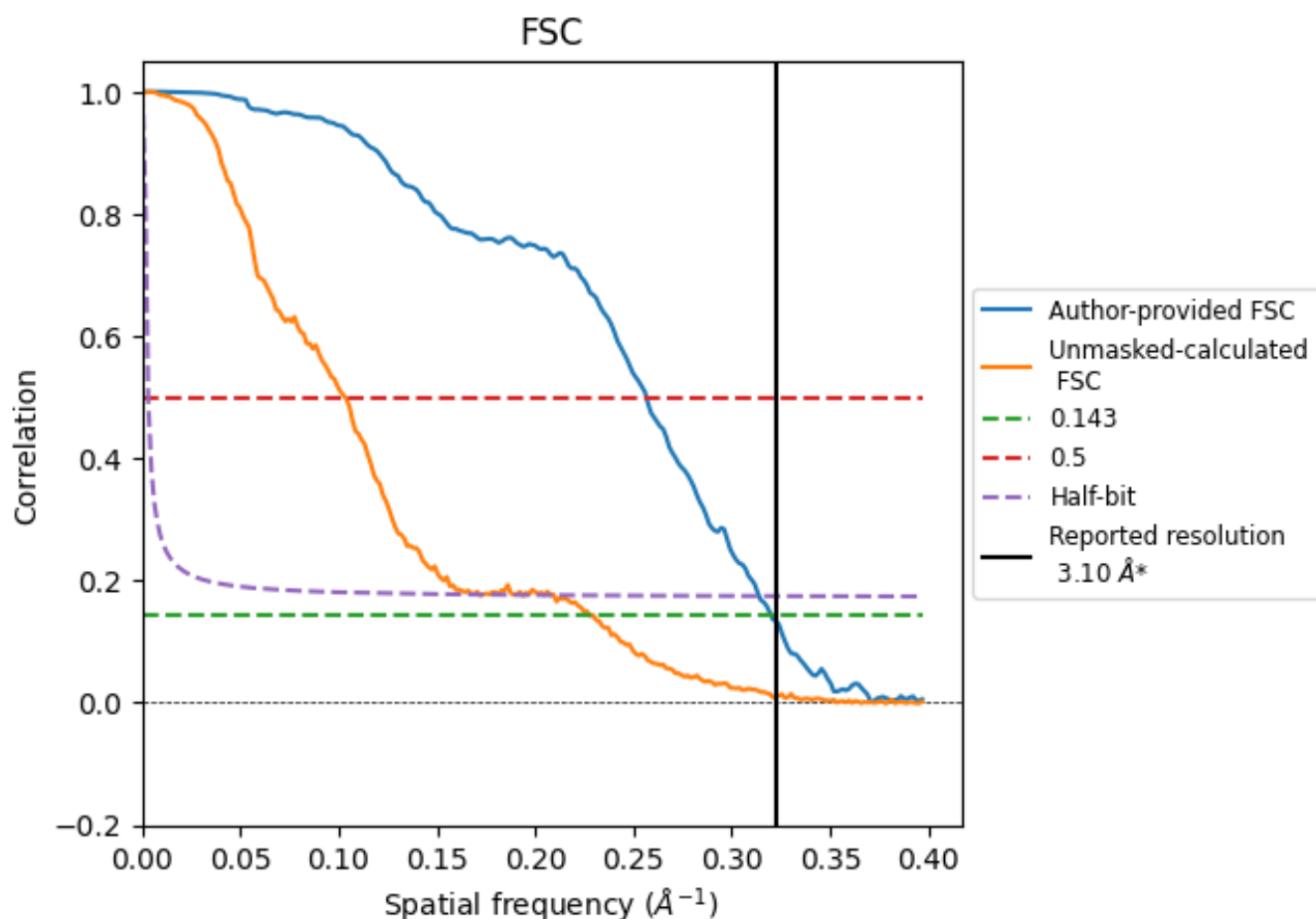


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

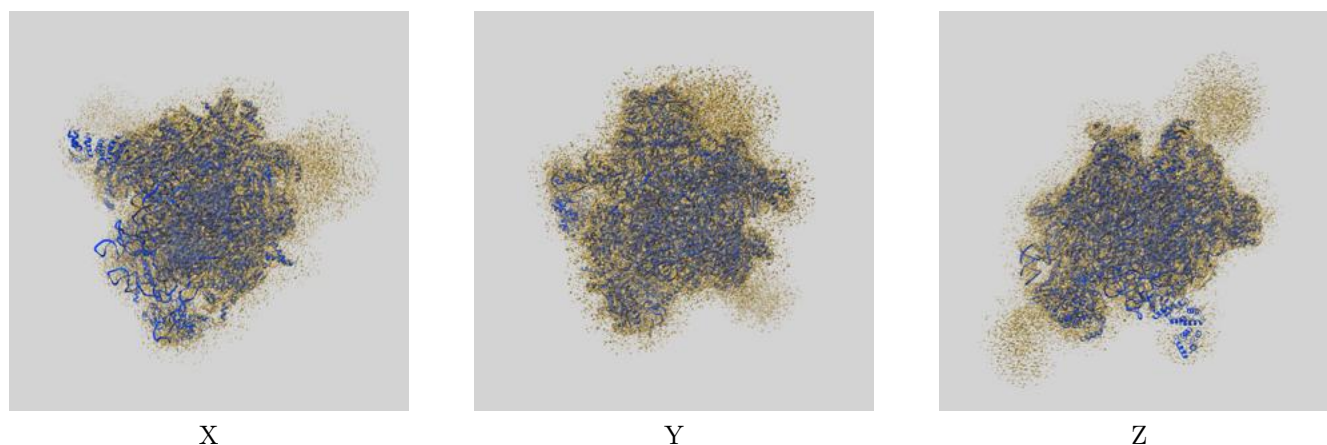
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.90	3.18
Unmasked-calculated*	4.39	9.70	5.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.39 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

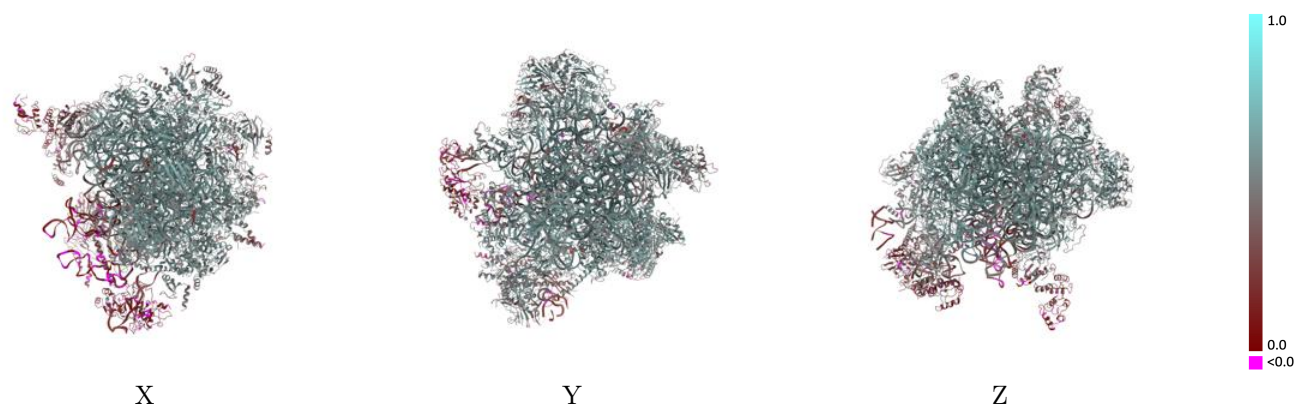
This section contains information regarding the fit between EMDB map EMD-11645 and PDB model 7A5J. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



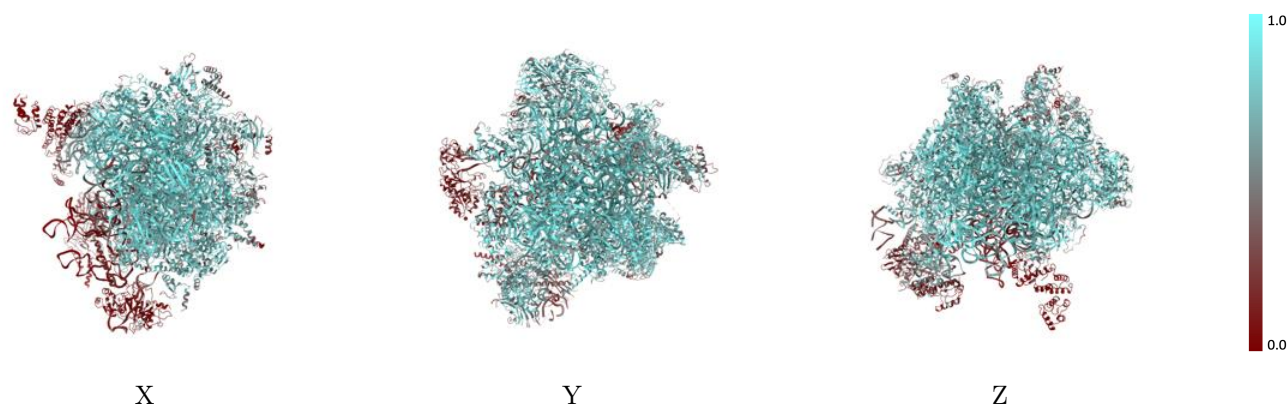
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



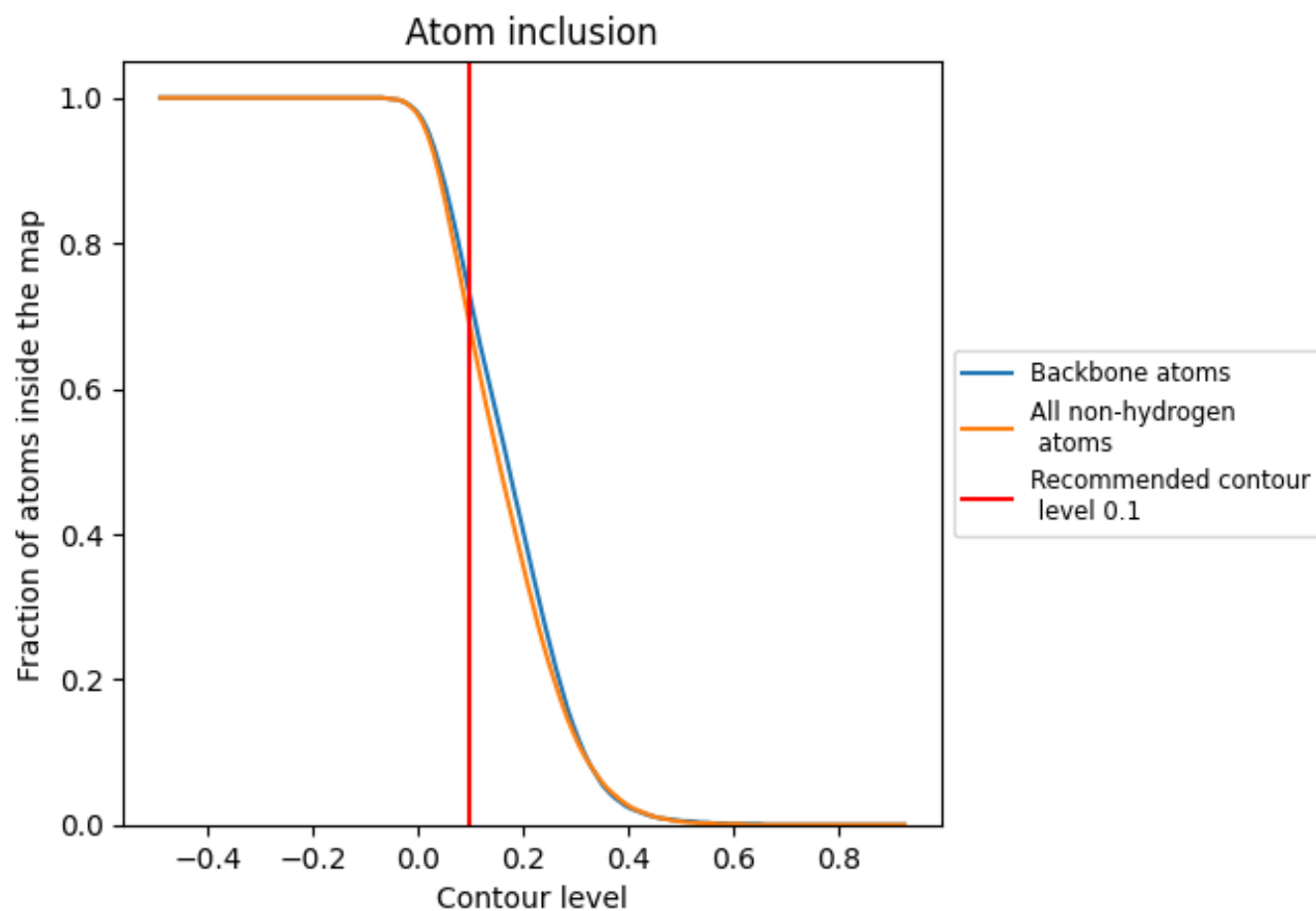
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 69% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6860	 0.4970
0	 0.7350	 0.5330
1	 0.7450	 0.5370
2	 0.9030	 0.6090
3	 0.8760	 0.5990
4	 0.8370	 0.5950
5	 0.7300	 0.5220
6	 0.6930	 0.4980
7	 0.6310	 0.4940
8	 0.2400	 0.2830
9	 0.6870	 0.5150
A	 0.8270	 0.5520
B	 0.5360	 0.3280
C	 0.0860	 0.1370
D	 0.7090	 0.5280
E	 0.7820	 0.5520
F	 0.8180	 0.5750
G	 0.0390	 0.1030
H	 0.6730	 0.5110
I	 0.4770	 0.3960
J	 0.2370	 0.2780
K	 0.8230	 0.5780
L	 0.7060	 0.5310
M	 0.8220	 0.5710
N	 0.7930	 0.5670
O	 0.8060	 0.5610
P	 0.7400	 0.5350
Q	 0.7110	 0.5230
R	 0.8490	 0.5820
S	 0.8040	 0.5720
T	 0.7850	 0.5750
U	 0.6610	 0.5050
V	 0.5880	 0.4850
W	 0.8320	 0.5830
X	 0.7300	 0.5270



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Chain	Atom inclusion	Q-score
Y	 0.7620	 0.5620
Y2	 0.0760	 0.1870
Z	 0.8060	 0.5700
a	 0.7670	 0.5510
b	 0.8240	 0.5720
c	 0.7270	 0.5390
d	 0.5670	 0.4820
e	 0.1410	 0.2160
f	 0.3610	 0.3600
g	 0.8070	 0.5600
h	 0.6400	 0.4910
i	 0.8370	 0.5880
j	 0.7490	 0.5320
k	 0.5300	 0.4280
l	 0.6700	 0.5090
m	 0.2320	 0.2940
n	 0.0600	 0.1760
o	 0.8460	 0.5810
p	 0.6520	 0.4940
q	 0.6310	 0.4850
r	 0.8020	 0.5560
s	 0.7740	 0.5470
t	 0.1290	 0.2100
u	 0.1290	 0.3340
v	 0.0450	 0.2670
w	 0.0320	 0.1850
x	 0.0740	 0.0900
y	 0.0500	 0.1040
z	 0.1000	 0.1620