



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 12:52 AM UTC

PDB ID : 7OIB / pdb_00007oib
EMDB ID : EMD-12924
Title : Cryo-EM structure of late human 39S mitoribosome assembly intermediates, state 3D
Authors : Cheng, J.; Berninghausen, O.; Beckmann, R.
Deposited on : 2021-05-11
Resolution : 3.30 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
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

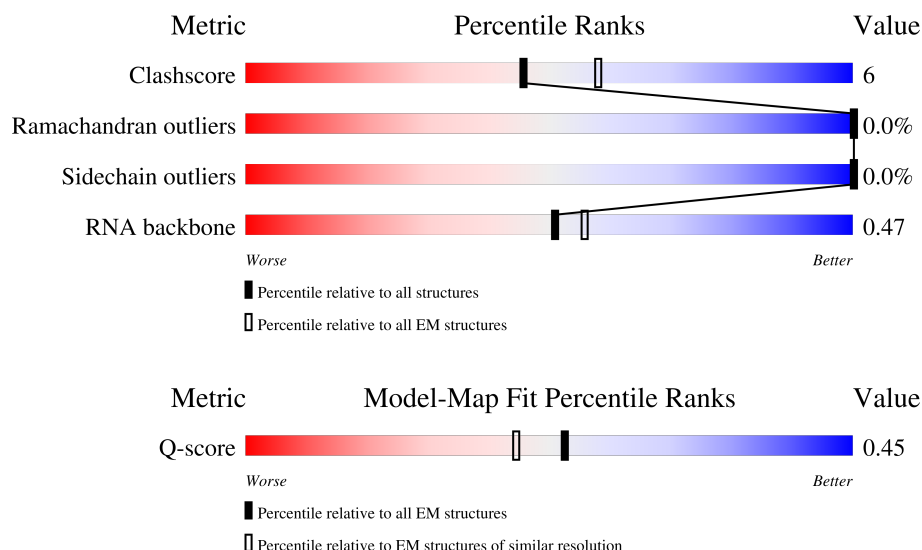
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	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	180	
13	Q	292	
14	R	149	
15	S	205	
16	T	206	
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	5	423	
28	6	380	

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Mol	Chain	Length	Quality of chain
29	7	338	
30	8	206	
31	9	137	
32	a	142	
33	b	215	
34	c	332	
35	d	306	
36	e	279	
37	f	212	
38	g	166	
39	h	158	
40	i	128	
41	j	123	
42	k	112	
43	l	138	
44	m	128	
45	o	102	
46	p	206	
47	q	222	
48	r	196	
49	s	439	
50	A	1559	
51	B	69	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 88360 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	220	Total	C	N	O	S	0	0
			1706	1059	339	299	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	285	Total	C	N	O	S	0	0
			2258	1457	384	406	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	S	0	0
			784	498	152	134			

- 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 39S ribosomal protein L18, mitochondrial.

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	159	Total	C	N	O	S	0	0
			1305	835	239	224	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	139	Total	C	N	O	S	0	0
			1154	734	220	197	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	192	Total	C	N	O	S	0	0
			1575	1003	281	283	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	43	Total	C	N	O	S	0	0
			351	218	76	56	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 L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	387	Total	C	N	O	S	0	0
			3156	2039	548	558	11		

- Molecule 28 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	324	Total	C	N	O	S	0	0
			2640	1694	470	468	8		

- Molecule 29 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	287	Total	C	N	O	S	0	0
			2334	1495	397	425	17		

- Molecule 30 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 31 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	117	Total	C	N	O	S	0	0
			947	614	163	168	2		

- Molecule 32 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 33 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L45, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L49, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 45 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	79	Total	C	N	O	S	0	0
			665	420	130	112	3		

- Molecule 46 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 47 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	120	Total	C	N	O	S	0	0
			1011	633	194	179	5		

- Molecule 48 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 49 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 50 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	A	1092	Total	C	N	O	P	0	0
			23184	10409	4202	7481	1092		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1437	U	UNK	conflict	GB 1025814679

- Molecule 51 is a RNA chain called mitochondrial Val tRNA.

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

- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	W	1	Total	Mg	0
			1	1	
52	g	1	Total	Mg	0
			1	1	
52	A	47	Total	Mg	0
			47	47	

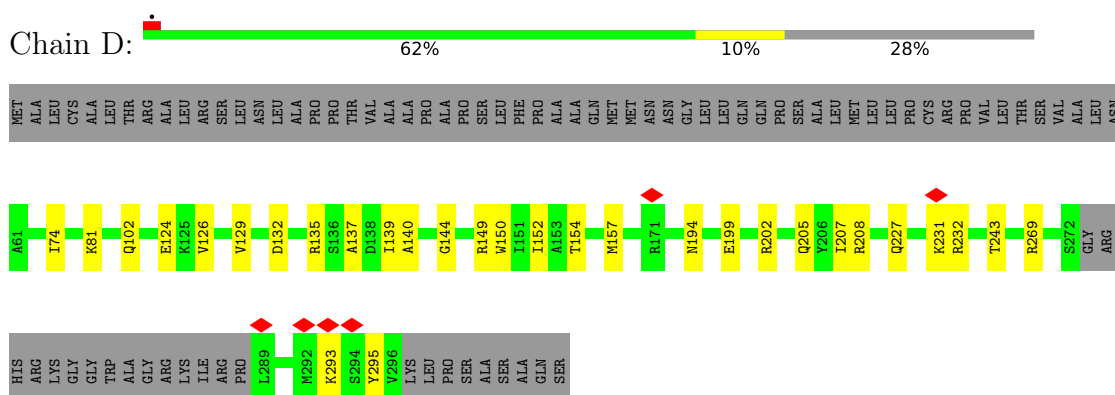
- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	0	1	Total	Zn	0
			1	1	
53	r	1	Total	Zn	0
			1	1	

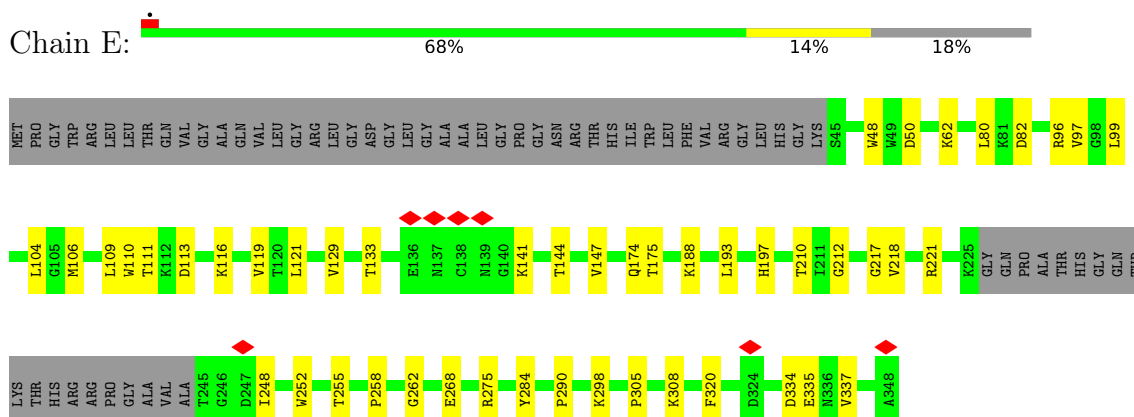
3 Residue-property plots [i](#)

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

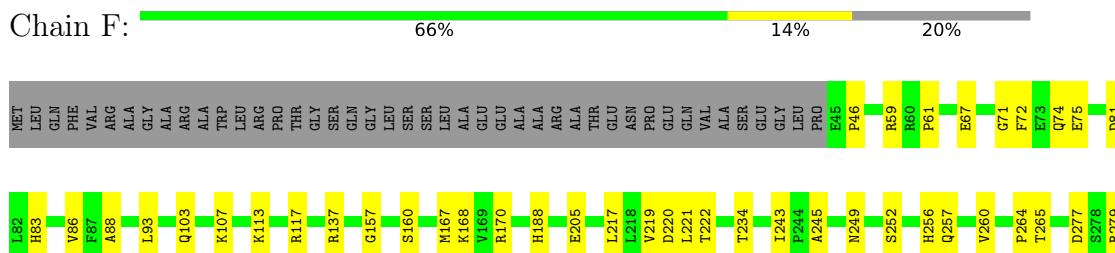
- Molecule 1: 39S ribosomal protein L2, mitochondrial



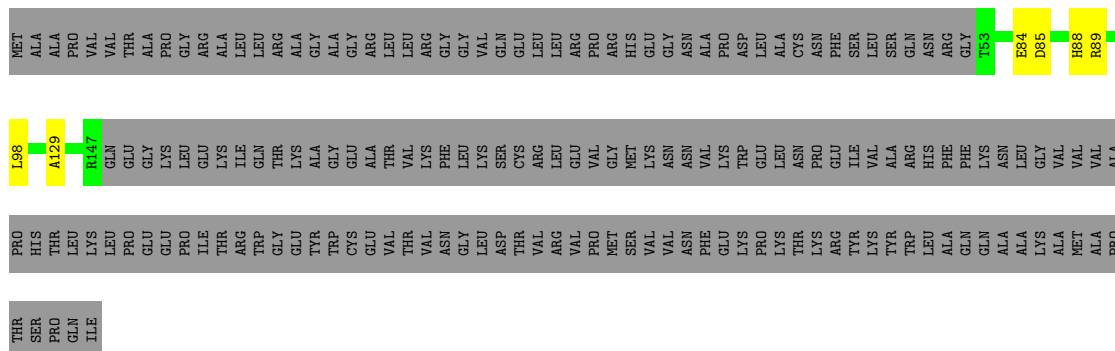
- Molecule 2: 39S ribosomal protein L3, mitochondrial



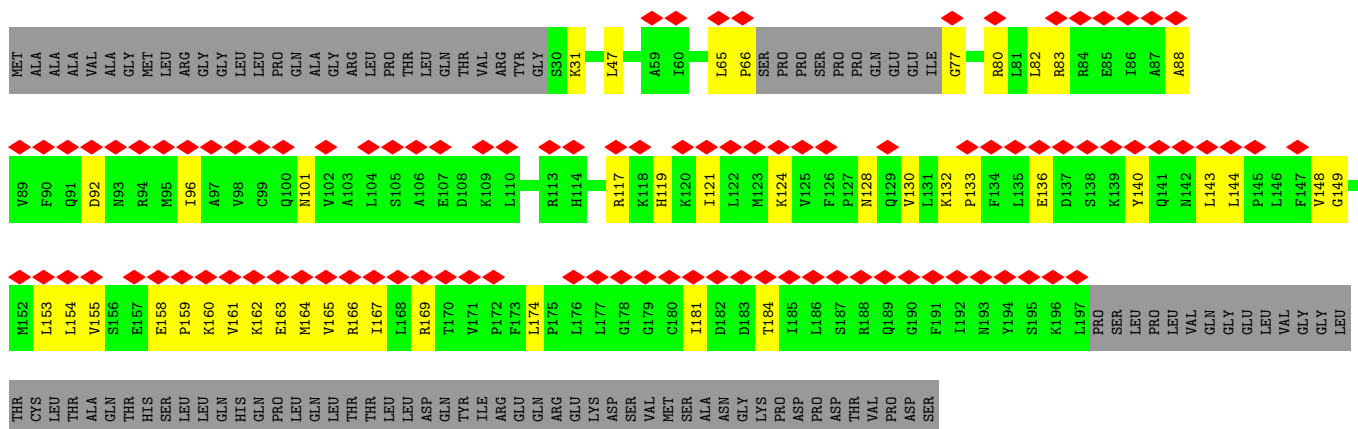
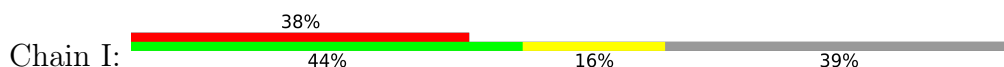
- Molecule 3: 39S ribosomal protein L4, mitochondrial



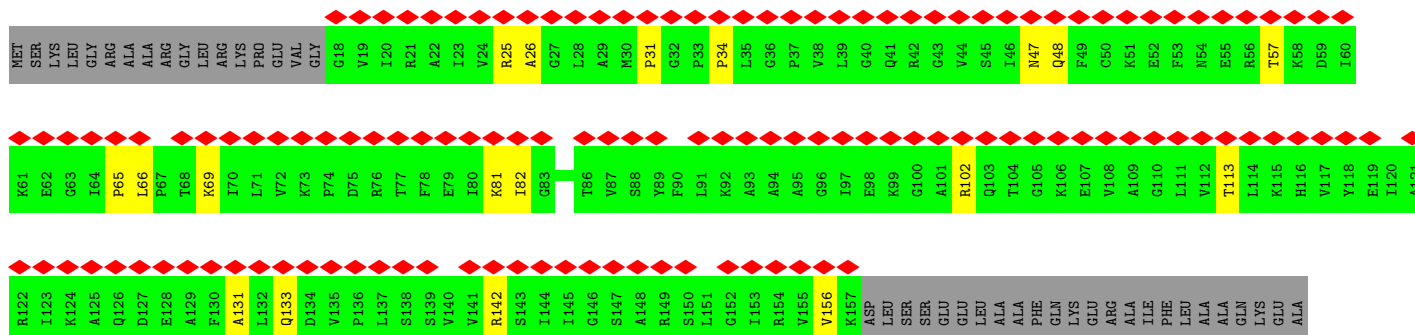
- Molecule 4: 39S ribosomal protein L9, mitochondrial



- Molecule 5: 39S ribosomal protein L10, mitochondrial



- Molecule 6: 39S ribosomal protein L11, mitochondrial



ASP
LEU
ALA
ALA
GLN
GLU
GLU
ALA
ALA
LYS
LYS

- Molecule 7: 39S ribosomal protein L13, mitochondrial

Chain K:  84% 15%

MET S2 S5 T13 F14 A15 R16 L20 Q25 Q26 A33 I37 D55 K71 Y77 R88 Q89 L95 I103 K114 R124 D136 N140 L141 V142 Q147 P148 R149 T171 E174 R177 L178

- Molecule 8: 39S ribosomal protein L14, mitochondrial

Chain L:  66% 13% 21%

MET ALA PHE PHE LEU GLY TRP GLY PRO PRO THR CYS VAL SER ARG VAL LEU SER HIS HIS CYS PHE SER THR THR GLY SER SER A31 I32 Q33 K34 M35 T36 R37 R53 A54 P55 R56 C57 V69 L75 K82 K83 V87 S102 I108 I123 K129

R130 E131 V137 I140 V145

- Molecule 9: 39S ribosomal protein L15, mitochondrial

Chain M:  81% 16%

MET ALA GLY PRO LEU GLN GLY GLY A10 D14 R17 R21 P31 R44 R45 K48 R51 E56 R62 E68 Q71 T72 P73 R77 I78 F83 K94 S97 P115 D135 V141 E142 E143 I154 E155 V156 I164 E168

V174 L195 K202 L205 V211 R220 E231 E235 L236 A237 L244 D250 M255 R263 V274 M277 K280 K281 L290 T295 S296

- Molecule 10: 39S ribosomal protein L16, mitochondrial

Chain N:  71% 10% 18%

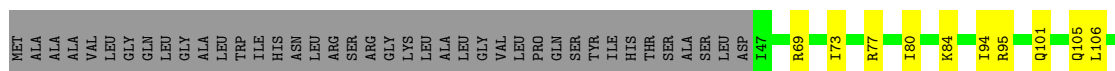
MET TRP ARG LEU LEU ARG ALA ARG ALA SER SER ALA PRO LEU LEU ARG VAL PRO LEU SER ASP SER TRP ALA LEU LEU PRO LEU VAL LYS THR LEU LEU PRO VAL PRO PRO SER SER PHE GLU ASP VAL ILE PRO K47 R55 F67 G94 N99 T108 R111

R123 I131 G137 H138 R139 V151 V154 E162 M163 G164 G165 F169 Q173 S191 R192 G193 T194 R205 T218 N222 M223 L224 G225 L226 T236 H237 K238 K249 R250 V251

- Molecule 11: 39S ribosomal protein L17, mitochondrial

Chain O:  73% 14% 13%

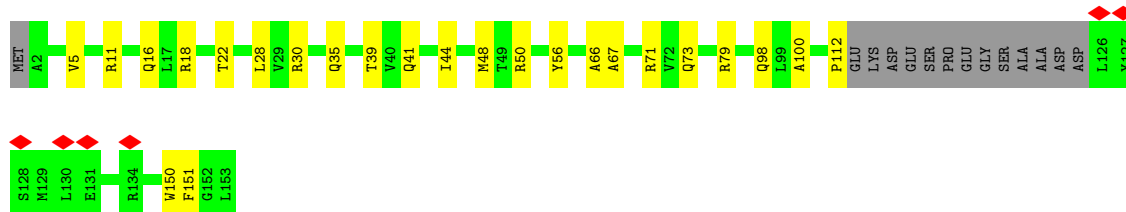
MET ARG LEU SER VAL ALA ALA I9 R17 M18 P22 R25 R38 R41 R45 P45 R48 V49 K58 L59 Y62 L65 N69 D84 Y92 R106 M107 L108 Q109 I110 A121 V122 I123 P131 P132 L133 P134 L135 L152 R157 Q158 S159





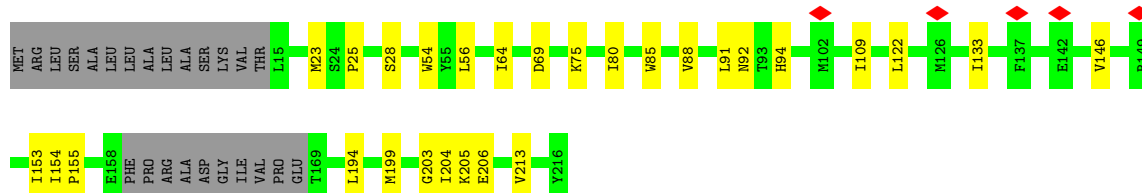
- Molecule 17: 39S ribosomal protein L23, mitochondrial

Chain U: 75% 16% 9%



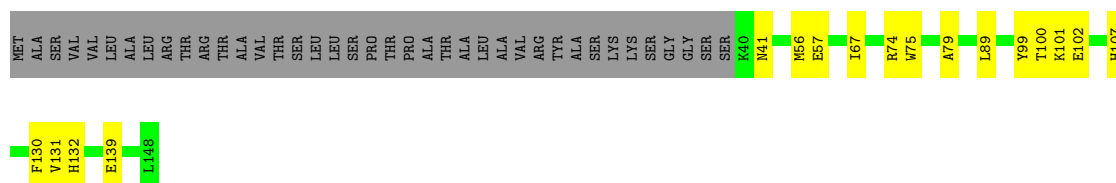
- Molecule 18: 39S ribosomal protein L24, mitochondrial

Chain V: 76% 13% 11%



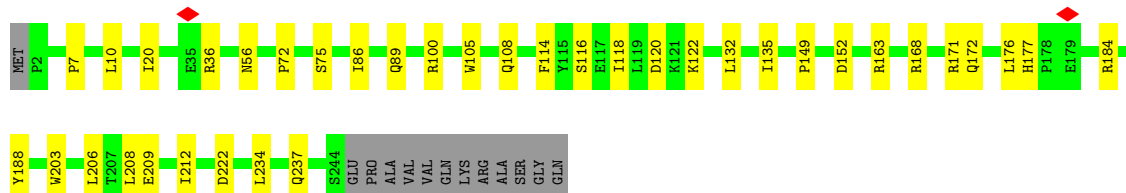
- Molecule 19: 39S ribosomal protein L27, mitochondrial

Chain W: 62% 11% 26%



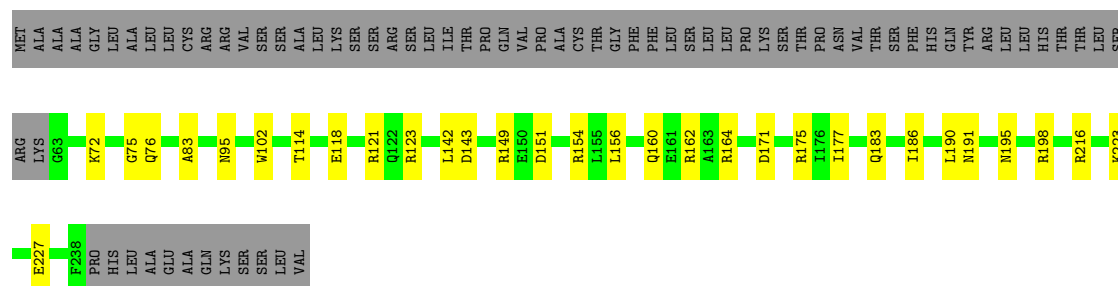
- Molecule 20: 39S ribosomal protein L28, mitochondrial

Chain X: 80% 14% 5%

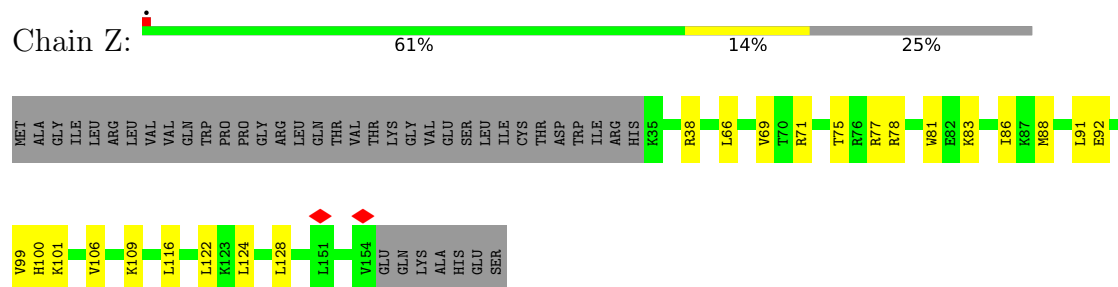


- Molecule 21: 39S ribosomal protein L47, mitochondrial

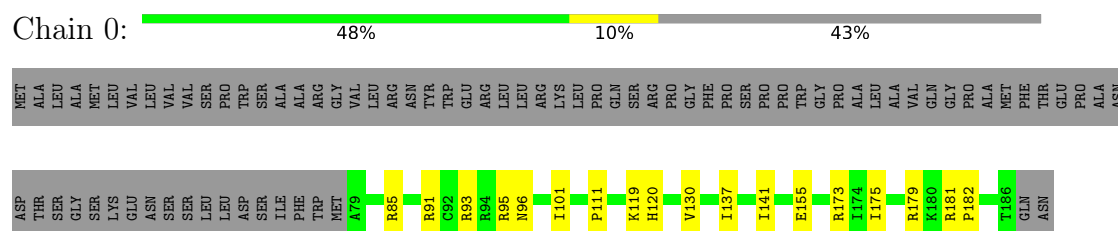
Chain Y: 58% 12% 30%



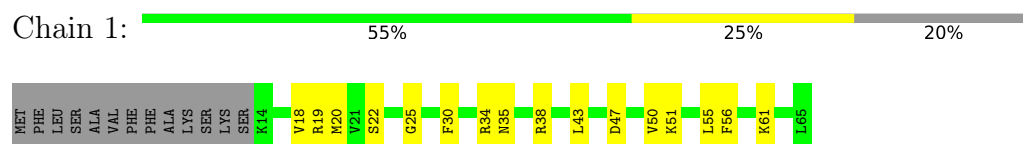
- Molecule 22: 39S ribosomal protein L30, mitochondrial



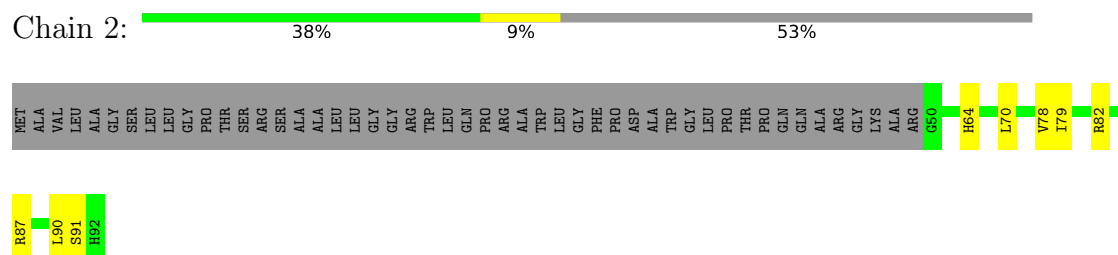
- Molecule 23: 39S ribosomal protein L32, mitochondrial



- Molecule 24: 39S ribosomal protein L33, mitochondrial

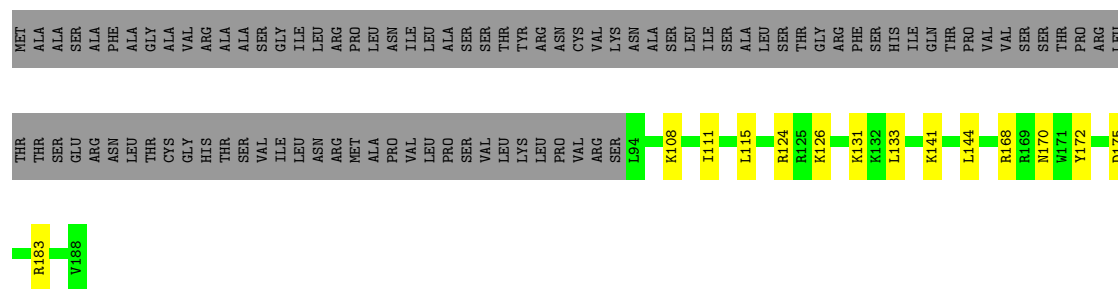


- Molecule 25: 39S ribosomal protein L34, mitochondrial

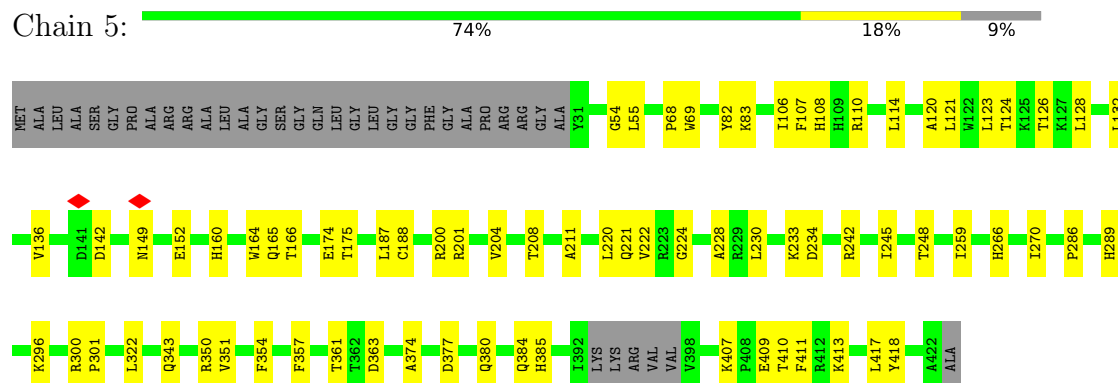


- Molecule 26: 39S ribosomal protein L35, mitochondrial

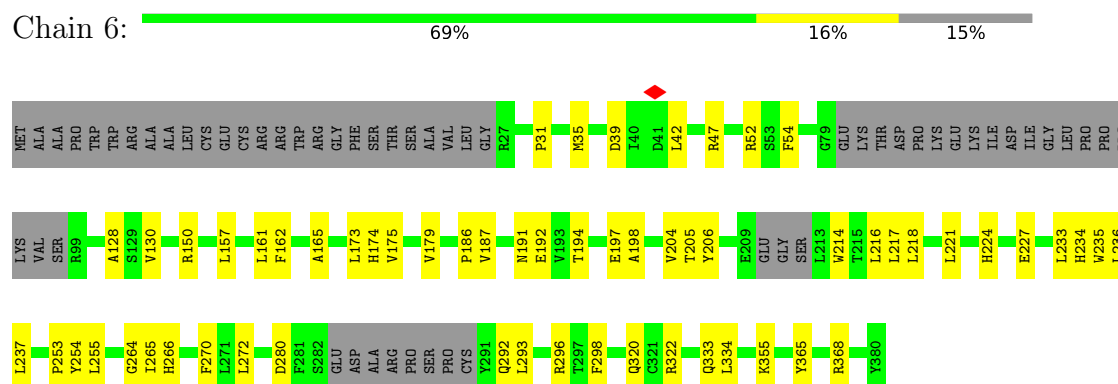




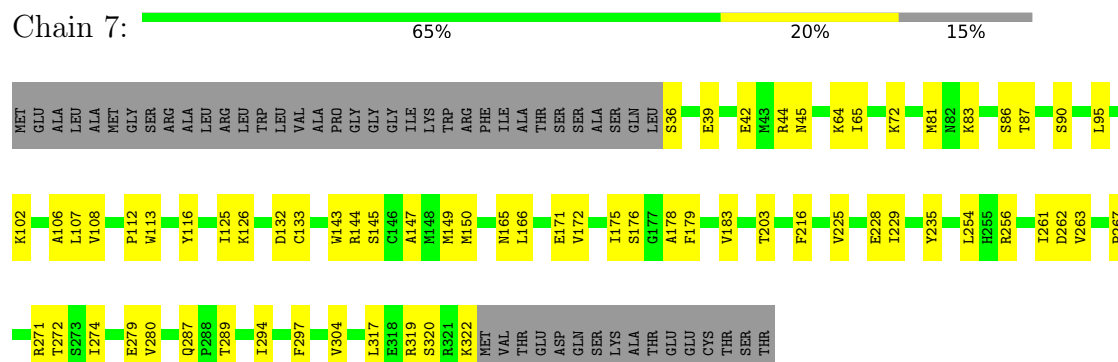
- Molecule 27: 39S ribosomal protein L37, mitochondrial

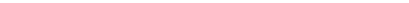


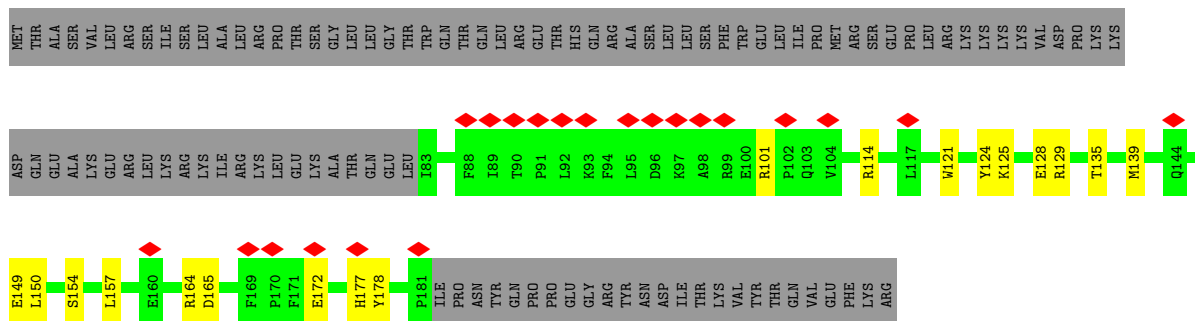
- Molecule 28: 39S ribosomal protein L38, mitochondrial



- Molecule 29: 39S ribosomal protein L39, mitochondrial

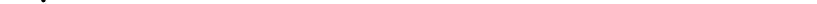


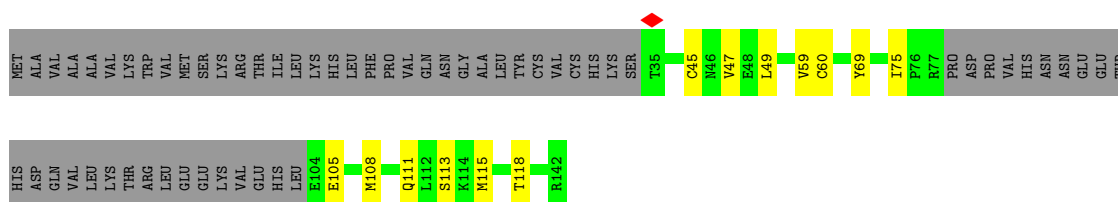
- Chain 8:  10% 39% 9% 52%

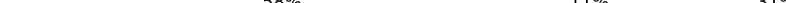


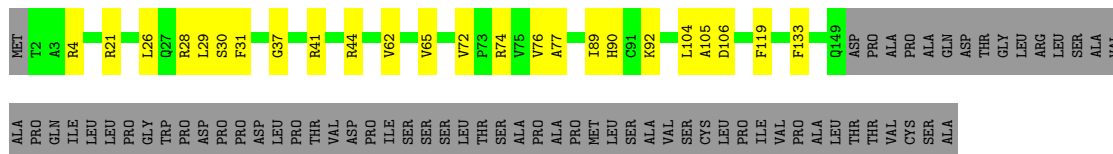
- Chain 9: 74% 11% 15%

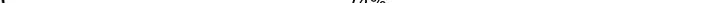


- Chain a:  49% 9% 42%

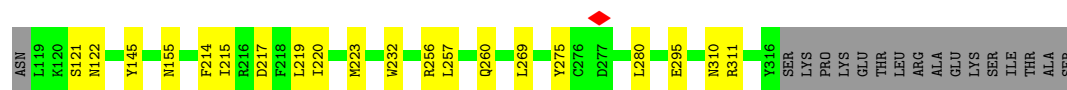


- Chain b:  58% 11% 31%

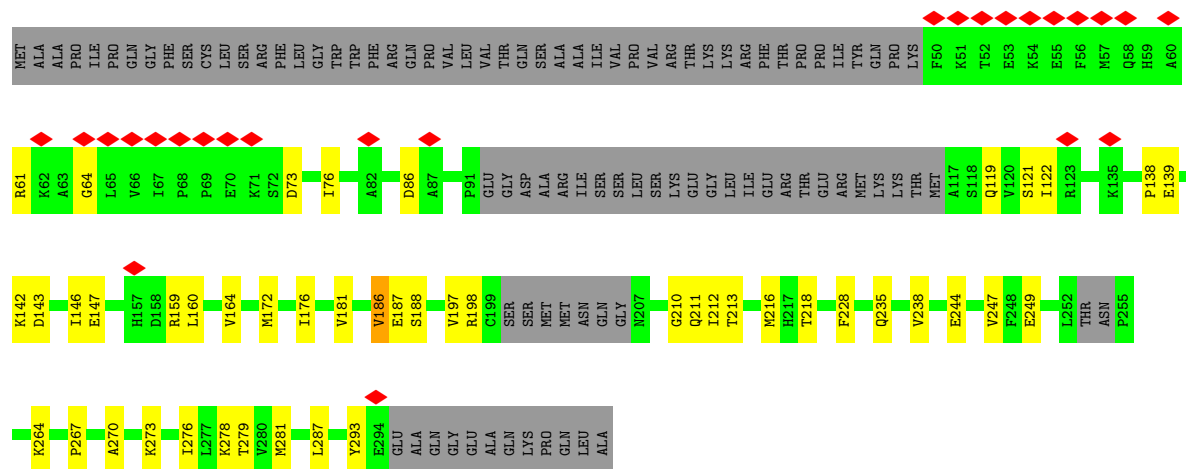


- Chain c:  74% 9% 17%

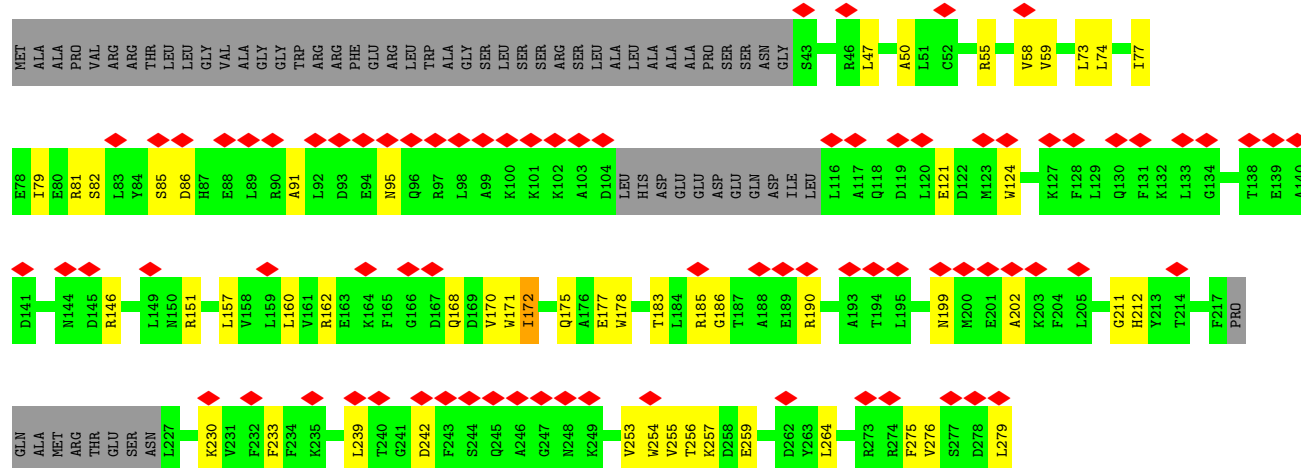




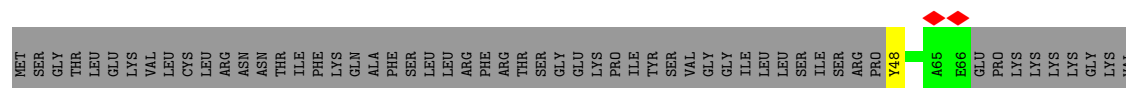
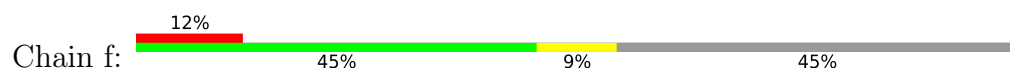
- Molecule 35: 39S ribosomal protein L45, mitochondrial

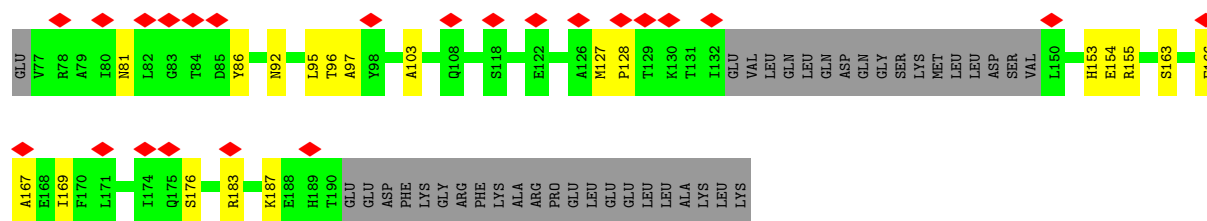


- Molecule 36: 39S ribosomal protein L46, mitochondrial



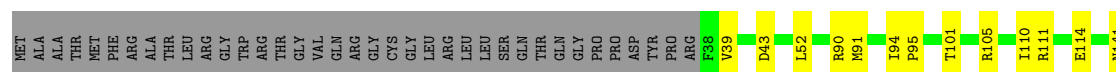
- Molecule 37: 39S ribosomal protein L48, mitochondrial





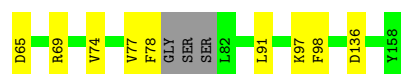
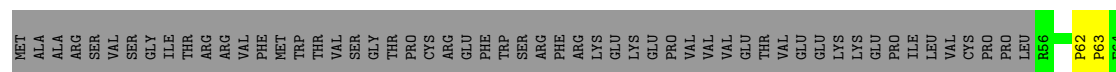
- Molecule 38: 39S ribosomal protein L49, mitochondrial

Chain g: 67% 10% 22%



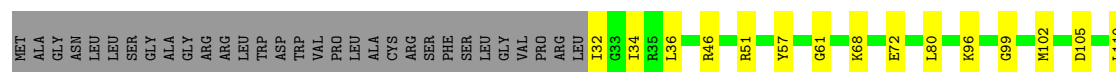
- Molecule 39: 39S ribosomal protein L50, mitochondrial

Chain h: 56% 7% 37%



- Molecule 40: 39S ribosomal protein L51, mitochondrial

Chain i: 63% 12% 24%



- Molecule 41: 39S ribosomal protein L52, mitochondrial

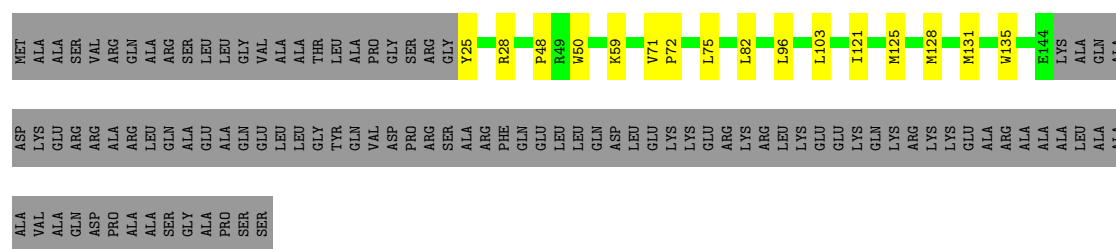
Chain j: 62% 7% 31%



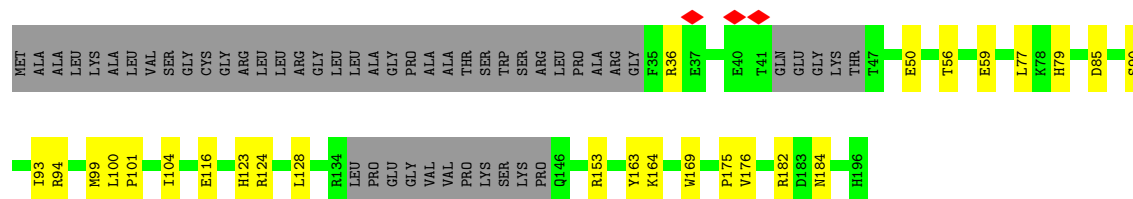
- Molecule 42: 39S ribosomal protein L53, mitochondrial

Chain k: 21% 49% 22% 29%

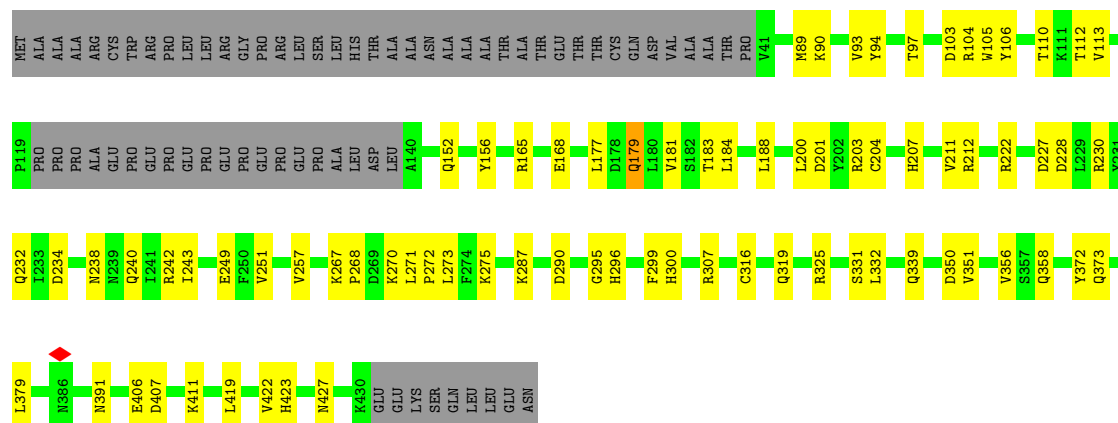
Chain q:



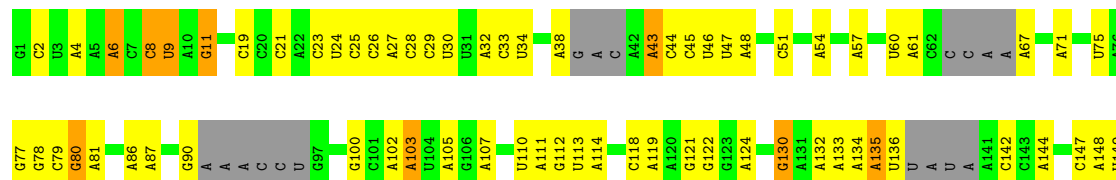
Chain r: 61% 13% 26%



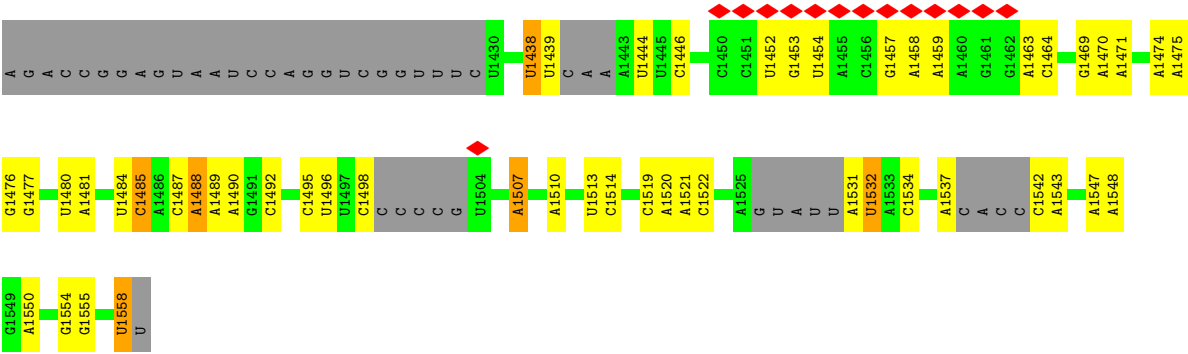
Chain s:



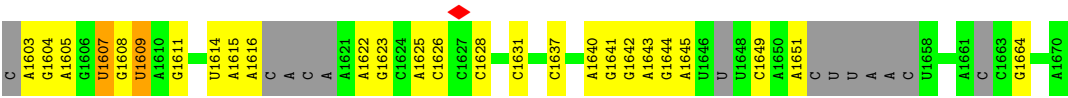
Chain A: 40% 25% 5% 30%







● Molecule 51: mitochondrial Val tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68090	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.869	Depositor
Minimum map value	-0.517	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	D	0.21	0/1736	0.57	0/2335
2	E	0.20	0/2322	0.55	0/3148
3	F	0.20	0/2071	0.50	0/2817
4	H	0.24	0/798	0.71	0/1073
5	I	0.24	0/1308	0.64	1/1761 (0.1%)
6	J	0.19	0/1077	0.51	0/1452
7	K	0.18	0/1495	0.47	0/2029
8	L	0.20	0/904	0.61	0/1218
9	M	0.21	0/2359	0.55	0/3185
10	N	0.24	1/1697 (0.1%)	0.49	0/2281
11	O	0.20	0/1269	0.54	0/1708
12	P	0.21	0/1173	0.61	2/1588 (0.1%)
13	Q	0.22	0/1846	0.54	0/2487
14	R	0.19	0/1174	0.44	0/1572
15	S	0.19	0/1276	0.52	0/1729
16	T	0.16	0/1335	0.44	0/1796
17	U	0.17	0/1183	0.48	0/1600
18	V	0.17	0/1616	0.46	0/2189
19	W	0.16	0/881	0.42	0/1188
20	X	0.18	0/2090	0.51	2/2825 (0.1%)
21	Y	0.18	0/1552	0.49	0/2079
22	Z	0.15	0/1003	0.40	0/1354
23	0	0.17	0/895	0.44	0/1201
24	1	0.25	0/438	0.71	0/583
25	2	0.16	0/357	0.47	0/475
26	3	0.15	0/852	0.40	0/1136
27	5	0.19	0/3250	0.51	0/4429
28	6	0.21	0/2726	0.54	0/3715
29	7	0.20	0/2391	0.57	2/3234 (0.1%)
30	8	0.27	0/855	0.68	0/1152
31	9	0.19	0/972	0.50	0/1306
32	a	0.16	0/709	0.45	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.20	0/1202	0.55	0/1626
34	c	0.19	0/2264	0.49	0/3059
35	d	0.20	0/1790	0.54	0/2423
36	e	0.22	0/1797	0.64	1/2422 (0.0%)
37	f	0.20	0/931	0.54	0/1259
38	g	0.20	0/1102	0.48	0/1503
39	h	0.18	0/847	0.47	0/1150
40	i	0.18	0/849	0.47	0/1135
41	j	0.15	0/698	0.37	0/940
42	k	0.18	0/635	0.49	0/855
43	l	0.19	0/226	0.55	0/299
44	m	0.26	0/379	0.75	1/510 (0.2%)
45	o	0.19	0/682	0.44	0/916
46	p	0.20	0/1071	0.58	1/1433 (0.1%)
47	q	0.20	0/1042	0.47	0/1413
48	r	0.17	0/1238	0.44	0/1676
49	s	0.18	0/3114	0.47	0/4225
50	A	0.14	0/25926	0.34	0/40305
51	B	0.14	0/1328	0.31	0/2056
All	All	0.18	1/92731 (0.0%)	0.47	10/130813 (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
35	d	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	151	VAL	C-N	6.16	1.46	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	83	ARG	CB-CG-CD	8.40	130.61	111.30
20	X	36	ARG	CA-C-N	7.24	130.37	120.67
20	X	36	ARG	C-N-CA	7.24	130.37	120.67
36	e	172	ILE	CG1-CB-CG2	-6.09	92.41	110.70
12	P	137	LEU	CA-C-N	5.70	128.39	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	137	LEU	C-N-CA	5.70	128.39	120.29
44	m	70	GLU	CA-CB-CG	5.67	125.43	114.10
29	7	287	GLN	CA-C-N	-5.26	113.54	120.96
29	7	287	GLN	C-N-CA	-5.26	113.54	120.96
46	p	181	GLU	N-CA-CB	5.12	118.74	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	d	186	VAL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1706	0	1755	21	0
2	E	2258	0	2264	32	0
3	F	2013	0	2044	31	0
4	H	784	0	832	3	0
5	I	1283	0	1369	27	0
6	J	1061	0	1141	12	0
7	K	1451	0	1448	22	0
8	L	889	0	941	14	0
9	M	2305	0	2378	38	0
10	N	1654	0	1681	18	0
11	O	1245	0	1283	19	0
12	P	1148	0	1148	26	0
13	Q	1805	0	1841	29	0
14	R	1153	0	1214	20	0
15	S	1251	0	1322	30	0
16	T	1305	0	1352	17	0
17	U	1154	0	1154	19	0
18	V	1575	0	1583	17	0
19	W	859	0	888	13	0
20	X	2035	0	2054	24	0
21	Y	1517	0	1561	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	Z	978	0	1030	15	0
23	0	880	0	902	14	0
24	1	433	0	475	13	0
25	2	351	0	375	6	0
26	3	831	0	883	10	0
27	5	3156	0	3138	52	0
28	6	2640	0	2464	45	0
29	7	2334	0	2343	43	0
30	8	836	0	844	21	0
31	9	947	0	949	14	0
32	a	686	0	658	12	0
33	b	1178	0	1180	23	0
34	c	2217	0	2220	25	0
35	d	1741	0	1727	36	0
36	e	1762	0	1767	39	0
37	f	915	0	917	14	0
38	g	1067	0	1056	17	0
39	h	827	0	806	7	0
40	i	827	0	857	14	0
41	j	684	0	673	8	0
42	k	627	0	636	19	0
43	l	221	0	227	5	0
44	m	372	0	387	14	0
45	o	665	0	664	10	0
46	p	1058	0	1083	9	0
47	q	1011	0	982	14	0
48	r	1203	0	1220	22	0
49	s	3036	0	3022	49	0
50	A	23184	0	11798	240	0
51	B	1191	0	607	9	0
52	A	47	0	0	0	0
52	W	1	0	0	0	0
52	g	1	0	0	0	0
53	0	1	0	0	0	0
53	r	1	0	0	0	0
All	All	88360	0	77143	1019	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 6.

All (1019) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:VAL:HA	1:D:139:ILE:O	1.19	1.26
2:E:106:MET:HA	2:E:119:VAL:O	1.07	1.22
50:A:1446:C:H42	50:A:1470:A:N6	1.48	1.12
50:A:1446:C:N4	50:A:1470:A:H61	1.47	1.12
28:6:216:LEU:O	28:6:236:LEU:HA	1.52	1.07
2:E:106:MET:CA	2:E:119:VAL:O	2.02	1.06
33:b:31:PHE:HA	33:b:74:ARG:O	1.58	1.02
51:B:1607:U:H3	51:B:1664:G:H1	1.06	0.99
50:A:662:C:H42	50:A:772:U:H3	1.12	0.96
1:D:129:VAL:CA	1:D:139:ILE:O	2.14	0.95
44:m:56:LEU:O	44:m:63:THR:HA	1.70	0.92
27:5:204:VAL:O	27:5:228:ALA:HA	1.73	0.88
35:d:197:VAL:HA	35:d:211:GLN:O	1.74	0.87
34:c:260:GLN:HA	34:c:269:LEU:O	1.75	0.86
50:A:1454:U:N3	50:A:1463:A:C8	2.45	0.83
44:m:69:ARG:HE	44:m:70:GLU:H	1.27	0.82
29:7:106:ALA:HA	29:7:126:LYS:O	1.81	0.81
50:A:662:C:N4	50:A:772:U:H3	1.86	0.72
7:K:15:ALA:HB3	34:c:269:LEU:HD12	1.73	0.70
14:R:47:ILE:HG12	15:S:172:MET:HE1	1.72	0.70
50:A:130:G:H22	50:A:133:A:H5'	1.56	0.70
28:6:186:PRO:HG3	46:p:191:LYS:HD3	1.73	0.70
42:k:15:GLN:HE22	42:k:17:ARG:HB2	1.56	0.70
33:b:29:LEU:HA	33:b:76:VAL:O	1.93	0.69
17:U:44:ILE:HG23	17:U:48:MET:HB3	1.74	0.69
42:k:34:LEU:HA	42:k:38:SER:HB2	1.74	0.69
37:f:96:THR:HA	37:f:153:HIS:O	1.92	0.69
44:m:51:LEU:HB3	44:m:67:ARG:HB3	1.75	0.69
12:P:52:ASN:HB3	12:P:55:ASN:HB2	1.73	0.68
9:M:164:ILE:HG12	9:M:174:VAL:HG11	1.76	0.68
29:7:81:MET:HG2	35:d:279:THR:HB	1.75	0.68
49:s:358:GLN:OE1	49:s:427:ASN:ND2	2.26	0.68
49:s:152:GLN:HA	49:s:156:TYR:HB2	1.75	0.67
2:E:104:LEU:HB2	2:E:121:LEU:HB2	1.76	0.67
42:k:18:VAL:HG11	42:k:34:LEU:HD21	1.76	0.67
9:M:141:VAL:HG12	9:M:143:GLU:H	1.58	0.67
22:Z:88:MET:SD	50:A:412:G:N2	2.68	0.67
35:d:197:VAL:HG12	35:d:212:ILE:HG12	1.76	0.67
3:F:221:LEU:HD22	3:F:264:PRO:HB2	1.77	0.66
7:K:171:THR:HG23	48:r:59:GLU:HG3	1.76	0.66
36:e:85:SER:OG	44:m:69:ARG:NH1	2.27	0.66
24:1:50:VAL:HG11	47:q:125:MET:HE3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:16:GLN:HE21	31:9:59:GLU:HB2	1.60	0.66
21:Y:151:ASP:OD1	21:Y:154:ARG:NH2	2.27	0.66
27:5:123:LEU:HD22	27:5:220:LEU:HD11	1.78	0.66
23:0:173:ARG:HD2	23:0:175:ILE:HD11	1.77	0.66
27:5:290:THR:HA	27:5:343:GLN:O	1.95	0.66
24:1:34:ARG:NH1	24:1:38:ARG:O	2.29	0.66
28:6:175:VAL:HB	28:6:187:VAL:HB	1.77	0.66
9:M:281:LYS:NZ	38:g:43:ASP:OD1	2.29	0.65
31:9:17:ARG:HH21	50:A:119:A:H5''	1.61	0.65
29:7:81:MET:HE2	29:7:86:SER:HB2	1.77	0.65
34:c:275:TYR:HA	34:c:280:LEU:HA	1.79	0.65
50:A:107:A:N6	50:A:110:U:OP2	2.29	0.65
9:M:94:LYS:NZ	9:M:135:ASP:OD2	2.29	0.65
13:Q:120:THR:HG22	13:Q:132:GLN:HG3	1.78	0.65
14:R:99:ARG:NH2	50:A:578:U:OP1	2.29	0.65
1:D:194:ASN:OD1	1:D:243:THR:OG1	2.15	0.64
3:F:257:GLN:OE1	9:M:21:ARG:NH1	2.30	0.64
35:d:213:THR:HG22	35:d:247:VAL:HG22	1.81	0.63
50:A:615:U:H2'	50:A:616:A:H8	1.62	0.63
9:M:14:ASP:OD1	9:M:17:ARG:NH2	2.32	0.63
25:2:87:ARG:NH2	50:A:122:G:N7	2.46	0.63
38:g:111:ARG:NH2	50:A:211:A:OP2	2.31	0.63
33:b:4:ARG:NH2	50:A:167:C:OP1	2.32	0.63
27:5:121:LEU:HD13	27:5:126:THR:HG23	1.80	0.62
50:A:214:G:H1'	50:A:225:C:H1'	1.81	0.62
12:P:142:ASN:OD1	46:p:184:ASN:ND2	2.31	0.62
46:p:183:MET:SD	46:p:187:ARG:NH2	2.72	0.62
39:h:65:ASP:OD1	39:h:69:ARG:NH1	2.33	0.62
15:S:142:THR:OG1	32:a:60:CYS:SG	2.56	0.62
50:A:495:C:O2	50:A:547:C:N4	2.33	0.62
50:A:1457:G:H2'	50:A:1458:A:H2'	1.82	0.62
10:N:87:PHE:HB2	10:N:163:MET:HB3	1.82	0.61
15:S:118:ASN:ND2	50:A:586:U:O2'	2.33	0.61
21:Y:198:ARG:NH2	25:2:70:LEU:O	2.34	0.61
36:e:50:ALA:HB2	36:e:175:GLN:HG3	1.81	0.61
36:e:183:THR:HG23	36:e:186:GLY:H	1.62	0.61
49:s:228:ASP:O	49:s:230:ARG:NH1	2.33	0.61
10:N:218:ILE:HG23	10:N:223:MET:HB2	1.81	0.61
37:f:166:PHE:HA	37:f:169:ILE:HG12	1.82	0.61
27:5:107:PHE:HB3	27:5:222:VAL:HG12	1.81	0.61
2:E:97:VAL:O	2:E:197:HIS:NE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:156:LEU:HD21	31:9:92:PHE:HB2	1.83	0.61
2:E:133:THR:OG1	2:E:144:THR:OG1	2.19	0.61
24:1:43:LEU:O	24:1:55:LEU:HA	2.01	0.61
12:P:54:ARG:NH2	12:P:140:GLY:O	2.34	0.60
23:0:119:LYS:O	23:0:120:HIS:ND1	2.34	0.60
49:s:103:ASP:OD1	49:s:325:ARG:NH1	2.34	0.60
50:A:669:G:HO2'	50:A:757:C:HO2'	1.48	0.60
1:D:199:GLU:HG2	1:D:202:ARG:HB2	1.83	0.60
50:A:1446:C:N3	50:A:1470:A:N1	2.49	0.60
5:I:140:TYR:HB3	5:I:143:LEU:HB2	1.82	0.60
42:k:66:VAL:HB	42:k:74:LEU:HB3	1.83	0.60
9:M:237:ALA:HB2	9:M:244:LEU:HD13	1.82	0.60
33:b:44:ARG:NH2	45:o:99:LYS:O	2.34	0.60
27:5:166:THR:O	49:s:287:LYS:NZ	2.34	0.60
28:6:191:ASN:OD1	28:6:192:GLU:N	2.35	0.60
14:R:48:ARG:NH2	50:A:174:A:OP2	2.35	0.60
7:K:114:LYS:HE2	50:A:1032:G:H5'	1.83	0.59
38:g:39:VAL:HG21	47:q:72:PRO:HB2	1.84	0.59
49:s:249:GLU:HA	49:s:356:VAL:HG21	1.84	0.59
8:L:33:GLN:NE2	50:A:800:G:N3	2.50	0.59
23:0:91:ARG:NH1	50:A:148:A:OP2	2.35	0.59
33:b:37:GLY:H	33:b:44:ARG:HH12	1.49	0.59
29:7:112:PRO:HB2	29:7:267:PRO:HG2	1.84	0.59
49:s:211:VAL:HG22	49:s:230:ARG:HG3	1.84	0.59
50:A:566:C:N4	50:A:1018:C:O2	2.35	0.59
16:T:129:VAL:HG21	16:T:137:ARG:HG2	1.84	0.59
3:F:160:SER:HB3	40:i:80:LEU:HD13	1.83	0.59
27:5:160:HIS:HA	27:5:164:TRP:HB2	1.83	0.59
10:N:123:ARG:NH1	10:N:162:GLU:OE2	2.36	0.59
50:A:1480:U:H2'	50:A:1481:A:H8	1.68	0.59
12:P:77:PHE:O	12:P:97:GLN:NE2	2.34	0.59
36:e:146:ARG:HA	36:e:151:ARG:HD2	1.83	0.59
50:A:1454:U:C2	50:A:1463:A:N7	2.71	0.59
36:e:85:SER:HB2	44:m:50:ARG:H	1.66	0.59
9:M:48:LYS:NZ	50:A:178:U:OP1	2.36	0.59
18:V:109:ILE:HD11	35:d:76:ILE:HG21	1.85	0.59
2:E:96:ARG:NH2	2:E:197:HIS:O	2.35	0.59
36:e:146:ARG:HB3	36:e:253:VAL:HG13	1.85	0.59
49:s:112:THR:HG22	49:s:391:ASN:HB2	1.83	0.59
50:A:77:G:N2	50:A:80:G:O2'	2.36	0.59
23:0:95:ARG:NH1	50:A:151:A:OP2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:e:211:GLY:O	36:e:233:PHE:HB2	2.02	0.58
26:3:172:TYR:HB2	26:3:175:ASP:HB2	1.85	0.58
43:l:120:ARG:NH1	50:A:520:C:OP1	2.35	0.58
49:s:179:GLN:HE21	49:s:179:GLN:HA	1.67	0.58
50:A:503:G:H2'	50:A:504:G:C8	2.38	0.58
39:h:91:LEU:HD23	39:h:97:LYS:HG3	1.85	0.58
10:N:108:THR:HA	10:N:111:ARG:HE	1.67	0.58
13:Q:121:THR:HA	13:Q:171:VAL:HA	1.85	0.58
15:S:101:PHE:HE2	41:j:49:TRP:HB3	1.68	0.58
21:Y:162:ARG:NH2	50:A:25:C:OP1	2.35	0.58
26:3:133:LEU:HD22	26:3:141:LYS:HG2	1.85	0.58
27:5:110:ARG:NH2	50:A:736:A:O2'	2.36	0.58
28:6:235:TRP:HE3	28:6:237:LEU:HD13	1.68	0.58
18:V:64:ILE:HD11	18:V:88:VAL:HG11	1.85	0.58
20:X:7:PRO:HD2	20:X:10:LEU:HD12	1.86	0.58
24:1:18:VAL:HG12	24:1:61:LYS:HA	1.85	0.58
27:5:201:ARG:NH1	27:5:418:TYR:O	2.37	0.58
14:R:65:ARG:NH1	50:A:579:G:OP2	2.37	0.58
50:A:1454:U:O2	50:A:1463:A:N7	2.37	0.58
42:k:64:VAL:HB	42:k:76:MET:HB2	1.84	0.57
3:F:59:ARG:NH1	38:g:114:GLU:OE2	2.37	0.57
22:Z:71:ARG:NH2	22:Z:92:GLU:O	2.36	0.57
49:s:165:ARG:O	49:s:307:ARG:NH2	2.36	0.57
38:g:101:THR:O	38:g:105:ARG:HB2	2.03	0.57
42:k:80:HIS:O	48:r:36:ARG:NH1	2.36	0.57
50:A:11:G:C6	50:A:102:A:N1	2.72	0.57
21:Y:123:ARG:NE	35:d:61:ARG:O	2.35	0.57
50:A:769:U:H2'	50:A:770:G:H8	1.69	0.57
14:R:23:GLU:HA	14:R:26:LYS:HE3	1.86	0.57
21:Y:143:ASP:OD1	31:9:137:ARG:NH2	2.34	0.57
28:6:333:GLN:HG3	28:6:334:LEU:HD12	1.87	0.57
9:M:77:ARG:NH1	50:A:1247:G:O6	2.37	0.57
13:Q:118:ARG:HE	13:Q:134:LEU:HD12	1.69	0.57
36:e:86:ASP:OD1	44:m:69:ARG:NH1	2.38	0.57
1:D:132:ASP:OD2	1:D:135:ARG:NH1	2.35	0.57
23:0:85:ARG:NH1	50:A:638:A:OP1	2.37	0.57
7:K:26:GLN:NE2	7:K:147:GLN:OE1	2.38	0.57
20:X:116:SER:O	20:X:120:ASP:HA	2.05	0.57
27:5:132:LEU:HD12	27:5:413:LYS:HD2	1.87	0.57
28:6:233:LEU:HB2	28:6:298:PHE:HE1	1.70	0.57
12:P:41:ASN:HD21	28:6:293:LEU:HD23	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:11:ARG:HH22	50:A:606:C:H1'	1.69	0.56
17:U:151:PHE:O	35:d:273:LYS:NZ	2.38	0.56
34:c:31:VAL:N	50:A:103:A:OP1	2.37	0.56
13:Q:112:TYR:HE2	13:Q:215:VAL:HG21	1.70	0.56
22:Z:101:LYS:HE3	41:j:80:LEU:HD22	1.86	0.56
29:7:262:ASP:OD2	29:7:263:VAL:N	2.38	0.56
48:r:99:MET:HG2	48:r:116:GLU:HG3	1.85	0.56
50:A:51:C:H42	50:A:60:U:H3	1.53	0.56
5:I:31:LYS:NZ	50:A:436:A:N7	2.53	0.56
20:X:177:HIS:O	20:X:184:ARG:NH1	2.36	0.56
48:r:153:ARG:HD3	48:r:175:PRO:HB2	1.86	0.56
5:I:47:LEU:HD12	10:N:226:ILE:HD13	1.87	0.56
5:I:164:MET:HA	5:I:167:ILE:HB	1.87	0.56
38:g:111:ARG:HD3	50:A:211:A:H62	1.70	0.56
3:F:252:SER:O	3:F:256:HIS:ND1	2.38	0.56
37:f:127:MET:HE3	37:f:128:PRO:HD2	1.86	0.56
2:E:212:GLY:HA2	2:E:262:GLY:HA3	1.87	0.56
13:Q:122:ALA:HB2	13:Q:172:GLN:HE22	1.70	0.56
22:Z:77:ARG:NH1	50:A:466:C:OP2	2.39	0.56
33:b:31:PHE:HB2	33:b:65:VAL:HG12	1.88	0.56
37:f:92:ASN:N	37:f:187:LYS:O	2.37	0.56
33:b:30:SER:H	33:b:76:VAL:H	1.54	0.56
48:r:169:TRP:O	50:A:485:A:N6	2.39	0.56
50:A:1070:A:N3	50:A:1251:A:O2'	2.36	0.56
1:D:81:LYS:HB2	50:A:254:U:H5''	1.87	0.56
13:Q:231:LYS:NZ	50:A:1484:U:OP1	2.39	0.56
16:T:94:ILE:HD13	16:T:106:LEU:HD11	1.86	0.56
15:S:173:ARG:NH1	50:A:592:C:OP1	2.39	0.56
35:d:210:GLY:O	35:d:249:GLU:HA	2.05	0.56
12:P:122:VAL:HG13	12:P:157:SER:HA	1.88	0.55
28:6:216:LEU:O	28:6:236:LEU:CA	2.43	0.55
33:b:77:ALA:HB2	33:b:104:LEU:HD13	1.87	0.55
50:A:27:A:N3	50:A:33:C:O2'	2.37	0.55
9:M:31:PRO:O	45:o:86:ARG:NH2	2.38	0.55
13:Q:102:ARG:HH21	13:Q:169:PRO:HA	1.71	0.55
26:3:108:LYS:NZ	50:A:75:U:O4	2.34	0.55
1:D:137:ALA:HB3	1:D:152:ILE:HD11	1.88	0.55
22:Z:99:VAL:O	41:j:76:ARG:NH1	2.38	0.55
48:r:124:ARG:NH1	48:r:153:ARG:O	2.40	0.55
49:s:207:HIS:ND1	49:s:234:ASP:OD1	2.39	0.55
7:K:20:LEU:HD12	7:K:141:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:186:ILE:HD12	21:Y:190:LEU:HD12	1.88	0.55
24:l:25:GLY:H	47:q:121:ILE:HD12	1.71	0.55
33:b:28:ARG:NH1	34:c:71:GLU:OE2	2.38	0.55
37:f:95:LEU:O	37:f:154:GLU:HA	2.07	0.55
49:s:204:CYS:SG	49:s:240:GLN:NE2	2.79	0.55
50:A:738:U:H2'	50:A:739:A:H8	1.71	0.55
7:K:16:ARG:HB2	7:K:55:ASP:HA	1.88	0.55
16:T:149:ARG:O	50:A:2:C:O2'	2.23	0.55
27:5:407:LYS:NZ	27:5:409:GLU:OE2	2.37	0.55
49:s:332:LEU:HD13	49:s:372:TYR:HB2	1.89	0.55
9:M:44:ARG:NH2	50:A:598:G:N7	2.44	0.55
21:Y:83:ALA:N	31:9:74:VAL:O	2.40	0.55
8:L:35:MET:HB2	8:L:56:ARG:HD3	1.87	0.55
27:5:110:ARG:NH1	50:A:736:A:N3	2.49	0.55
28:6:197:GLU:OE2	46:p:185:ARG:NH2	2.40	0.55
49:s:419:LEU:O	49:s:423:HIS:ND1	2.39	0.55
3:F:219:VAL:HA	3:F:243:ILE:O	2.07	0.54
3:F:221:LEU:HG	3:F:222:THR:HG23	1.89	0.54
15:S:129:ARG:NH2	15:S:154:VAL:O	2.41	0.54
27:5:211:ALA:HB1	27:5:322:LEU:HD22	1.89	0.54
36:e:91:ALA:O	36:e:95:ASN:ND2	2.39	0.54
5:I:77:GLY:O	5:I:80:ARG:NH1	2.40	0.54
13:Q:152:ARG:NH1	13:Q:190:LEU:O	2.41	0.54
34:c:220:ILE:HG23	34:c:223:MET:HE2	1.88	0.54
36:e:256:THR:OG1	36:e:257:LYS:N	2.40	0.54
50:A:573:A:H4'	50:A:574:U:H5'	1.89	0.54
15:S:173:ARG:NH2	50:A:473:G:OP1	2.41	0.54
29:7:150:MET:HE1	29:7:297:PHE:HB3	1.88	0.54
40:i:68:LYS:NZ	40:i:72:GLU:OE1	2.40	0.54
2:E:275:ARG:HH21	2:E:284:TYR:HE2	1.55	0.54
14:R:56:ALA:HA	14:R:59:LEU:HB2	1.90	0.54
28:6:214:TRP:HB3	28:6:272:LEU:HD11	1.90	0.54
32:a:69:TYR:OH	34:c:256:ARG:NH2	2.40	0.54
36:e:160:LEU:HD11	36:e:264:LEU:HD11	1.87	0.54
42:k:15:GLN:HB3	42:k:67:LEU:HB2	1.89	0.54
45:o:34:ASN:OD1	45:o:37:ARG:NH2	2.40	0.54
49:s:272:PRO:O	50:A:704:A:N6	2.33	0.54
50:A:411:U:H2'	50:A:412:G:C8	2.42	0.54
49:s:222:ARG:NH2	49:s:227:ASP:OD1	2.40	0.54
3:F:113:LYS:HD2	3:F:157:GLY:HA2	1.90	0.54
11:O:65:LEU:HB3	11:O:69:ASN:HD22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:216:ARG:NH1	50:A:21:C:O2	2.41	0.54
27:5:136:VAL:HG11	27:5:417:LEU:HD23	1.90	0.54
9:M:202:LYS:HB2	9:M:263:ARG:HB3	1.88	0.54
27:5:361:THR:OG1	27:5:363:ASP:OD1	2.25	0.54
48:r:79:HIS:HB3	48:r:184:ASN:HA	1.90	0.54
18:V:94:HIS:NE2	50:A:135:A:OP2	2.37	0.54
19:W:100:THR:OG1	19:W:132:HIS:NE2	2.35	0.54
31:9:53:ILE:HG22	31:9:55:GLU:H	1.72	0.54
41:j:63:GLN:OE1	41:j:66:ARG:NH1	2.41	0.54
33:b:30:SER:HB2	33:b:76:VAL:HB	1.90	0.54
42:k:77:ARG:NH2	48:r:50:GLU:OE2	2.41	0.54
50:A:405:U:O2'	50:A:1163:A:N7	2.40	0.54
6:J:131:ALA:HB3	50:A:499:A:H4'	1.90	0.53
15:S:162:GLU:HB3	15:S:192:VAL:HB	1.90	0.53
33:b:28:ARG:HG2	33:b:62:VAL:HB	1.89	0.53
49:s:350:ASP:OD1	49:s:351:VAL:N	2.40	0.53
19:W:101:LYS:NZ	50:A:394:A:OP1	2.41	0.53
30:8:101:ARG:NH1	36:e:79:ILE:O	2.41	0.53
5:I:101:ASN:HA	5:I:174:LEU:HD11	1.91	0.53
8:L:53:ARG:NH2	50:A:980:C:OP1	2.41	0.53
49:s:165:ARG:NH2	50:A:746:U:OP2	2.41	0.53
20:X:209:GLU:HG3	27:5:69:TRP:CD1	2.43	0.53
29:7:87:THR:O	29:7:90:SER:OG	2.26	0.53
36:e:162:ARG:HD3	36:e:171:TRP:HE3	1.73	0.53
5:I:128:ASN:ND2	5:I:149:GLY:O	2.41	0.53
16:T:69:ARG:NH1	35:d:228:PHE:O	2.41	0.53
30:8:164:ARG:NH1	37:f:81:ASN:OD1	2.41	0.53
19:W:79:ALA:HB3	19:W:132:HIS:HB3	1.90	0.53
20:X:89:GLN:OE1	20:X:100:ARG:NE	2.38	0.53
50:A:662:C:N4	50:A:772:U:N3	2.47	0.53
2:E:210:THR:HG22	2:E:290:PRO:HB3	1.91	0.53
17:U:66:ALA:HB2	17:U:100:ALA:HB2	1.90	0.53
18:V:69:ASP:HB3	18:V:91:LEU:HD12	1.91	0.53
22:Z:78:ARG:O	22:Z:83:LYS:NZ	2.41	0.53
2:E:221:ARG:NH2	50:A:1438:U:O4'	2.42	0.53
15:S:103:SER:OG	50:A:475:G:N2	2.42	0.53
20:X:108:GLN:NE2	50:A:1084:A:N3	2.57	0.53
20:X:116:SER:O	20:X:120:ASP:CA	2.57	0.53
20:X:116:SER:O	20:X:120:ASP:N	2.42	0.53
34:c:215:ILE:HG23	34:c:219:LEU:HD12	1.90	0.53
38:g:111:ARG:NH1	50:A:210:C:OP2	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:A:1152:C:O2'	50:A:1245:C:OP2	2.27	0.53
2:E:111:THR:OG1	2:E:113:ASP:OD1	2.27	0.53
19:W:67:ILE:HG21	19:W:131:VAL:HG11	1.91	0.53
21:Y:154:ARG:HG2	31:9:130:LEU:HB3	1.90	0.53
24:1:20:MET:HB2	24:1:30:PHE:O	2.09	0.53
30:8:165:ASP:OD2	36:e:185:ARG:NH1	2.42	0.53
36:e:81:ARG:NH1	44:m:48:TYR:OH	2.42	0.53
46:p:40:LYS:NZ	46:p:46:ASP:OD2	2.41	0.53
47:q:128:MET:HA	47:q:131:MET:HE3	1.91	0.53
50:A:130:G:N1	50:A:133:A:OP2	2.36	0.53
27:5:354:PHE:HB2	27:5:377:ASP:HB3	1.91	0.53
50:A:192:U:H2'	50:A:193:A:H8	1.74	0.53
6:J:25:ARG:HA	6:J:65:PRO:HA	1.89	0.52
7:K:174:GLU:HG3	48:r:56:THR:HG21	1.91	0.52
50:A:841:C:H3'	50:A:842:A:H8	1.74	0.52
35:d:197:VAL:CA	35:d:211:GLN:O	2.53	0.52
2:E:141:LYS:NZ	50:A:1532:U:OP2	2.42	0.52
16:T:84:LYS:HD3	16:T:149:ARG:HB3	1.90	0.52
20:X:163:ARG:HH21	27:5:55:LEU:HD13	1.73	0.52
49:s:212:ARG:HD3	49:s:379:LEU:HD12	1.92	0.52
49:s:307:ARG:NH1	50:A:746:U:O4	2.42	0.52
50:A:214:G:N3	50:A:225:C:O2'	2.42	0.52
12:P:73:PRO:HB2	12:P:147:GLN:HE21	1.73	0.52
15:S:127:ARG:HG2	15:S:159:THR:HG22	1.92	0.52
17:U:30:ARG:NH1	21:Y:118:GLU:OE2	2.42	0.52
36:e:170:VAL:HB	36:e:172:ILE:HD11	1.92	0.52
10:N:139:ARG:NH1	50:A:1145:G:N7	2.57	0.52
27:5:270:ILE:O	50:A:739:A:O2'	2.28	0.52
41:j:24:GLY:O	41:j:28:ARG:NH1	2.43	0.52
44:m:52:TYR:O	44:m:67:ARG:HA	2.10	0.52
15:S:97:ALA:HA	15:S:135:LEU:O	2.09	0.52
49:s:201:ASP:OD2	49:s:242:ARG:NH1	2.43	0.52
10:N:191:SER:N	10:N:194:THR:OG1	2.39	0.52
40:i:36:LEU:HD23	50:A:6:A:H1'	1.92	0.52
49:s:113:VAL:HG11	49:s:257:VAL:HG11	1.91	0.52
2:E:334:ASP:HB3	2:E:337:VAL:HG23	1.92	0.52
29:7:87:THR:HG23	29:7:90:SER:H	1.75	0.52
36:e:279:LEU:HD11	37:f:176:SER:HB2	1.92	0.52
50:A:385:U:H2'	50:A:386:G:H8	1.73	0.52
17:U:18:ARG:NH2	18:V:206:GLU:OE1	2.41	0.52
24:1:47:ASP:O	24:1:51:LYS:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:108:LYS:HD3	26:3:111:ILE:HD12	1.92	0.52
28:6:52:ARG:HB3	51:B:1637:C:H5'	1.92	0.52
8:L:37:ARG:HG3	8:L:56:ARG:HH12	1.74	0.52
15:S:52:PRO:HD2	48:r:77:LEU:HD21	1.92	0.52
23:0:179:ARG:HH12	23:0:182:PRO:HG3	1.74	0.51
34:c:94:ASN:OD1	34:c:122:ASN:ND2	2.40	0.51
2:E:305:PRO:HA	2:E:308:LYS:HE3	1.91	0.51
2:E:334:ASP:OD2	2:E:335:GLU:N	2.43	0.51
20:X:118:ILE:O	20:X:168:ARG:NH1	2.44	0.51
42:k:36:THR:HG23	42:k:37:VAL:HG13	1.92	0.51
42:k:39:SER:OG	42:k:40:GLU:N	2.41	0.51
12:P:144:MET:HE2	12:P:170:VAL:HG11	1.92	0.51
23:0:111:PRO:O	29:7:72:LYS:NZ	2.35	0.51
37:f:163:SER:O	37:f:167:ALA:N	2.40	0.51
50:A:669:G:H21	50:A:757:C:H5'	1.76	0.51
6:J:102:ARG:O	50:A:504:G:N2	2.44	0.51
7:K:25:MET:O	7:K:149:ARG:NH1	2.43	0.51
15:S:68:ASP:N	15:S:68:ASP:OD1	2.42	0.51
29:7:143:TRP:NE1	29:7:172:VAL:O	2.44	0.51
6:J:142:ARG:NH2	50:A:521:A:OP1	2.44	0.51
17:U:22:THR:HG21	17:U:56:TYR:HE2	1.76	0.51
19:W:56:MET:HG2	19:W:57:GLU:H	1.75	0.51
27:5:106:ILE:HB	27:5:266:HIS:HB3	1.92	0.51
48:r:101:PRO:HG2	48:r:104:ILE:HG12	1.92	0.51
50:A:237:A:N3	50:A:1260:U:O2'	2.40	0.51
2:E:62:LYS:HE2	50:A:1558:U:H5'	1.92	0.51
12:P:102:VAL:HG12	12:P:103:VAL:HG23	1.91	0.51
26:3:168:ARG:NH1	26:3:170:ASN:OD1	2.44	0.51
27:5:300:ARG:NH2	50:A:724:A:O2'	2.44	0.51
6:J:31:PRO:HB2	6:J:34:PRO:HG2	1.92	0.51
10:N:131:ILE:HD12	10:N:151:VAL:HG21	1.91	0.51
12:P:57:GLU:OE2	12:P:96:HIS:NE2	2.39	0.51
44:m:70:GLU:O	44:m:72:ARG:N	2.42	0.51
50:A:423:U:O2	50:A:596:U:O2'	2.29	0.51
1:D:295:TYR:OH	50:A:850:C:OP2	2.24	0.51
13:Q:117:LEU:O	13:Q:134:LEU:HA	2.11	0.51
29:7:203:THR:HG22	29:7:280:VAL:H	1.76	0.51
30:8:129:ARG:NH2	51:B:1626:C:O2'	2.40	0.51
29:7:289:THR:HG21	29:7:294:ILE:H	1.76	0.51
33:b:4:ARG:NH1	50:A:161:G:N7	2.57	0.51
20:X:203:TRP:HA	20:X:206:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:A:521:A:N6	50:A:528:A:OP2	2.45	0.50
27:5:233:LYS:HA	27:5:286:PRO:HD2	1.94	0.50
38:g:150:LYS:HE3	50:A:382:A:H5''	1.93	0.50
50:A:564:C:O2'	50:A:1018:C:O2'	2.26	0.50
11:O:59:LEU:HB2	13:Q:269:MET:HE1	1.93	0.50
17:U:41:GLN:NE2	50:A:700:A:OP1	2.33	0.50
19:W:57:GLU:HB2	19:W:99:TYR:HD1	1.76	0.50
29:7:116:TYR:OH	29:7:271:ARG:NH1	2.44	0.50
2:E:82:ASP:OD2	2:E:188:LYS:NZ	2.42	0.50
15:S:86:MET:HB3	15:S:91:GLN:HB2	1.92	0.50
30:8:172:GLU:HG2	37:f:183:ARG:HH12	1.76	0.50
44:m:57:VAL:HG13	44:m:62:SER:H	1.77	0.50
50:A:144:A:N3	50:A:192:U:O2'	2.40	0.50
50:A:991:U:H2'	50:A:992:A:H8	1.75	0.50
2:E:248:ILE:O	50:A:1045:A:O2'	2.30	0.50
4:H:98:LEU:HG	4:H:129:ALA:HB2	1.93	0.50
5:I:65:LEU:HD12	5:I:66:PRO:HD2	1.92	0.50
50:A:28:C:O2'	50:A:32:A:N3	2.39	0.50
50:A:1260:U:H2'	50:A:1261:A:H8	1.77	0.50
11:O:22:PRO:HA	11:O:25:ARG:HG2	1.92	0.50
18:V:122:LEU:HD12	18:V:133:ILE:HG13	1.94	0.50
5:I:148:VAL:O	42:k:31:ARG:NH1	2.44	0.50
27:5:245:ILE:O	27:5:248:THR:OG1	2.27	0.50
40:i:61:GLY:HA3	50:A:216:G:H1	1.76	0.50
43:l:123:LYS:HG2	50:A:527:G:H5'	1.93	0.50
15:S:104:ARG:NH2	50:A:475:G:N3	2.44	0.50
43:l:131:ARG:HH21	43:l:134:LYS:HZ2	1.59	0.50
9:M:56:GLU:OE1	50:A:370:G:O2'	2.29	0.50
22:Z:69:VAL:HG23	22:Z:91:LEU:HD21	1.93	0.50
36:e:199:ASN:HB2	36:e:242:ASP:O	2.12	0.50
43:l:114:SER:OG	43:l:115:ARG:N	2.45	0.50
51:B:1607:U:O4	51:B:1664:G:O6	2.30	0.50
13:Q:197:TYR:HE2	13:Q:223:LYS:H	1.59	0.49
50:A:118:C:C2	50:A:248:G:N2	2.80	0.49
3:F:217:LEU:HD11	3:F:243:ILE:HD12	1.94	0.49
5:I:117:ARG:NH2	6:J:133:GLN:O	2.45	0.49
11:O:18:MET:HE3	11:O:48:ARG:HG2	1.94	0.49
22:Z:100:HIS:HB3	22:Z:106:VAL:HG11	1.93	0.49
24:1:47:ASP:O	24:1:51:LYS:HA	2.12	0.49
5:I:133:PRO:HA	5:I:136:GLU:HG2	1.93	0.49
8:L:82:LYS:NZ	8:L:83:LYS:O	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:92:VAL:HG13	23:O:155:GLU:HG2	1.94	0.49
27:5:106:ILE:HA	27:5:221:GLN:O	2.12	0.49
35:d:198:ARG:HB2	35:d:211:GLN:HB3	1.93	0.49
38:g:91:MET:HE3	50:A:213:G:H5''	1.94	0.49
49:s:295:GLY:N	49:s:339:GLN:OE1	2.42	0.49
3:F:188:HIS:HB2	3:F:260:VAL:HG22	1.94	0.49
2:E:298:LYS:NZ	50:A:1534:C:OP1	2.40	0.49
27:5:107:PHE:O	27:5:222:VAL:HA	2.13	0.49
29:7:45:ASN:HD22	29:7:256:ARG:HH11	1.59	0.49
9:M:56:GLU:HG3	50:A:345:G:H5'	1.94	0.49
15:S:175:ARG:HB2	15:S:180:PHE:HB3	1.94	0.49
50:A:1176:G:O2'	50:A:1243:A:N6	2.45	0.49
5:I:101:ASN:HD22	5:I:174:LEU:HD21	1.77	0.49
13:Q:102:ARG:HH12	13:Q:106:LEU:HD13	1.78	0.49
28:6:218:LEU:HB2	28:6:234:HIS:HB2	1.94	0.49
2:E:268:GLU:OE2	50:A:1476:G:N2	2.46	0.49
10:N:94:GLY:HA2	10:N:154:VAL:O	2.11	0.49
16:T:137:ARG:NH2	29:7:95:LEU:O	2.46	0.49
29:7:178:ALA:HB2	29:7:320:SER:HB2	1.95	0.49
45:o:79:THR:OG1	50:A:383:U:OP2	2.30	0.49
28:6:198:ALA:O	28:6:254:TYR:OH	2.26	0.49
29:7:176:SER:O	29:7:319:ARG:NH1	2.46	0.49
1:D:269:ARG:NH1	50:A:320:G:OP1	2.46	0.49
7:K:177:ARG:NH2	50:A:1513:U:O2	2.45	0.49
25:2:70:LEU:HD12	50:A:29:C:H1'	1.95	0.49
46:p:77:THR:HB	46:p:102:ARG:HG3	1.95	0.49
50:A:241:C:H2'	50:A:242:A:H8	1.78	0.49
1:D:124:GLU:HG2	1:D:144:GLY:HA3	1.95	0.48
20:X:149:PRO:HD2	20:X:152:ASP:HB2	1.95	0.48
27:5:343:GLN:NE2	27:5:417:LEU:O	2.45	0.48
28:6:265:ILE:HG12	28:6:322:ARG:HG2	1.95	0.48
48:r:94:ARG:HE	48:r:100:LEU:HD23	1.78	0.48
11:O:38:ARG:NH2	11:O:84:ASP:OD1	2.46	0.48
14:R:71:ARG:HD3	14:R:107:ILE:HD11	1.95	0.48
35:d:176:ILE:HD11	35:d:181:VAL:HB	1.95	0.48
17:U:5:VAL:HG21	31:9:137:ARG:HD3	1.95	0.48
31:9:24:LYS:HG2	50:A:751:G:H5''	1.95	0.48
37:f:48:TYR:N	50:A:395:A:OP1	2.46	0.48
19:W:41:ASN:HD21	50:A:1171:U:H3'	1.77	0.48
50:A:214:G:O2'	50:A:225:C:O2	2.32	0.48
50:A:662:C:N4	50:A:772:U:C4	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:51:ARG:NH1	50:A:198:G:N7	2.59	0.48
13:Q:188:LEU:HD13	13:Q:191:ARG:HE	1.79	0.48
18:V:25:PRO:HG2	18:V:28:SER:HB3	1.96	0.48
27:5:230:LEU:HD13	27:5:289:HIS:HD2	1.78	0.48
44:m:69:ARG:HH21	44:m:71:PRO:HD3	1.78	0.48
50:A:158:A:H4'	50:A:159:A:C8	2.49	0.48
15:S:175:ARG:NH2	50:A:592:C:O2'	2.47	0.48
2:E:252:TRP:O	2:E:255:THR:OG1	2.29	0.48
9:M:168:GLU:OE1	9:M:220:ARG:NH2	2.46	0.48
28:6:194:THR:OG1	46:p:185:ARG:NH2	2.47	0.48
7:K:13:THR:HG21	16:T:208:ILE:HD11	1.95	0.48
34:c:145:TYR:OH	34:c:311:ARG:NH1	2.47	0.48
39:h:77:VAL:HG13	39:h:78:PHE:HD2	1.79	0.48
40:i:105:ASP:OD1	40:i:105:ASP:N	2.46	0.48
50:A:468:U:O2'	50:A:481:A:N3	2.47	0.48
5:I:121:ILE:HD11	5:I:154:LEU:HB3	1.95	0.48
8:L:102:SER:OG	13:Q:158:GLN:NE2	2.35	0.48
9:M:277:MET:HE2	9:M:277:MET:HB3	1.80	0.48
18:V:54:TRP:NE1	18:V:56:LEU:O	2.47	0.48
35:d:73:ASP:OD1	35:d:73:ASP:N	2.47	0.48
50:A:86:A:H2'	50:A:87:A:H8	1.78	0.48
27:5:68:PRO:O	50:A:43:A:N6	2.46	0.48
36:e:74:LEU:HA	36:e:77:ILE:HG22	1.96	0.48
36:e:255:VAL:HG13	36:e:259:GLU:HG2	1.96	0.48
50:A:77:G:OP2	50:A:79:C:N4	2.47	0.48
50:A:192:U:H2'	50:A:193:A:C8	2.48	0.48
50:A:381:A:H2'	50:A:382:A:C8	2.48	0.48
13:Q:102:ARG:NH2	13:Q:169:PRO:HA	2.28	0.47
16:T:95:ARG:NH1	50:A:149:U:OP1	2.47	0.47
27:5:121:LEU:HD11	27:5:128:LEU:HB2	1.96	0.47
32:a:49:LEU:HD13	32:a:60:CYS:HB3	1.95	0.47
49:s:203:ARG:NH1	49:s:238:ASN:OD1	2.47	0.47
15:S:163:LYS:HB2	33:b:106:ASP:HB3	1.96	0.47
20:X:56:ASN:ND2	50:A:75:U:OP1	2.46	0.47
20:X:86:ILE:HB	20:X:105:TRP:HB2	1.95	0.47
50:A:511:A:N6	50:A:536:C:O2'	2.47	0.47
8:L:83:LYS:HB3	8:L:108:ILE:HG23	1.95	0.47
14:R:115:SER:HA	32:a:47:VAL:HG21	1.96	0.47
15:S:174:PHE:HA	15:S:180:PHE:O	2.14	0.47
7:K:33:ALA:O	7:K:37:ILE:HG12	2.14	0.47
29:7:229:ILE:HG21	29:7:254:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:i:99:GLY:HA2	40:i:102:MET:HG3	1.95	0.47
16:T:77:ARG:HB3	16:T:80:ILE:HD11	1.96	0.47
20:X:172:GLN:HA	20:X:188:TYR:HE1	1.78	0.47
28:6:173:LEU:HA	28:6:206:TYR:HB3	1.97	0.47
50:A:416:A:H2'	50:A:417:U:C6	2.50	0.47
3:F:71:GLY:HA3	3:F:74:GLN:HB3	1.97	0.47
30:8:101:ARG:NH2	36:e:82:SER:OG	2.37	0.47
35:d:86:ASP:OD1	35:d:86:ASP:N	2.46	0.47
35:d:160:LEU:O	35:d:164:VAL:N	2.45	0.47
49:s:165:ARG:HG2	49:s:307:ARG:HH12	1.80	0.47
3:F:279:ARG:HH12	3:F:282:PRO:HD3	1.78	0.47
9:M:71:GLN:OE1	50:A:364:A:O2'	2.30	0.47
10:N:55:ARG:HG2	10:N:99:TRP:CD2	2.49	0.47
14:R:48:ARG:HG2	14:R:52:LYS:HE2	1.95	0.47
25:2:64:HIS:O	25:2:91:SER:OG	2.33	0.47
27:5:384:GLN:OE1	50:A:725:A:O2'	2.32	0.47
30:8:139:MET:HE1	37:f:169:ILE:HG22	1.95	0.47
35:d:121:SER:HB3	35:d:197:VAL:HG23	1.97	0.47
36:e:212:HIS:HB2	36:e:230:LYS:NZ	2.30	0.47
42:k:17:ARG:HH12	42:k:19:GLN:HB3	1.80	0.47
48:r:182:ARG:NH2	50:A:488:U:OP2	2.48	0.47
50:A:415:A:H2'	50:A:416:A:C8	2.50	0.47
5:I:124:LYS:HB2	5:I:153:LEU:HB3	1.97	0.47
17:U:112:PRO:HD2	21:Y:75:GLY:HA3	1.97	0.47
35:d:235:GLN:HE22	35:d:238:VAL:HB	1.80	0.47
49:s:181:VAL:HG12	49:s:200:LEU:HD11	1.97	0.47
49:s:300:HIS:NE2	49:s:331:SER:OG	2.47	0.47
50:A:159:A:H2'	50:A:160:G:C8	2.50	0.47
3:F:59:ARG:NH2	3:F:88:ALA:O	2.47	0.47
15:S:99:VAL:HG22	15:S:133:VAL:HG23	1.97	0.47
28:6:162:PHE:HB3	28:6:165:ALA:HB3	1.97	0.47
4:H:84:GLU:OE2	4:H:89:ARG:NH2	2.47	0.47
8:L:55:PRO:HB2	8:L:75:LEU:HD11	1.96	0.47
11:O:41:ARG:NH2	11:O:131:PRO:O	2.38	0.47
28:6:39:ASP:OD1	28:6:39:ASP:N	2.47	0.47
10:N:191:SER:OG	10:N:192:ARG:N	2.48	0.46
10:N:218:ILE:HG12	10:N:223:MET:HG3	1.96	0.46
12:P:158:MET:O	12:P:162:GLN:HG2	2.15	0.46
13:Q:182:ARG:HG3	13:Q:187:LEU:HD11	1.97	0.46
27:5:301:PRO:HD3	50:A:720:A:H4'	1.97	0.46
38:g:110:ILE:HD12	38:g:147:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:s:407:ASP:N	49:s:407:ASP:OD1	2.48	0.46
1:D:154:THR:H	1:D:157:MET:HE2	1.79	0.46
1:D:205:GLN:HA	1:D:208:ARG:HH11	1.81	0.46
12:P:80:ARG:O	12:P:94:VAL:HA	2.16	0.46
29:7:279:GLU:HG3	29:7:317:LEU:HD21	1.97	0.46
30:8:114:ARG:HE	36:e:73:LEU:HD11	1.79	0.46
33:b:31:PHE:CA	33:b:74:ARG:O	2.48	0.46
29:7:149:MET:HE2	29:7:272:THR:HG22	1.97	0.46
49:s:271:LEU:O	49:s:273:LEU:N	2.46	0.46
50:A:307:U:H2'	50:A:308:A:H8	1.81	0.46
3:F:137:ARG:NH1	50:A:1262:G:OP1	2.48	0.46
5:I:181:ILE:O	5:I:184:THR:OG1	2.26	0.46
8:L:35:MET:H	8:L:57:CYS:HB3	1.81	0.46
16:T:212:LEU:HA	33:b:119:PHE:HE2	1.81	0.46
34:c:94:ASN:HA	34:c:122:ASN:HB2	1.96	0.46
35:d:86:ASP:OD2	35:d:198:ARG:NE	2.49	0.46
36:e:58:VAL:HG13	36:e:59:VAL:HG23	1.98	0.46
43:l:123:LYS:NZ	50:A:521:A:N7	2.58	0.46
50:A:1070:A:H2'	50:A:1071:A:H8	1.80	0.46
3:F:72:PHE:HZ	3:F:205:GLU:HG3	1.79	0.46
6:J:25:ARG:HG2	6:J:65:PRO:HB3	1.98	0.46
9:M:295:THR:HG22	46:p:39:PHE:HE1	1.80	0.46
11:O:108:LEU:HD11	11:O:135:LEU:HD13	1.96	0.46
16:T:112:LYS:HE3	16:T:116:ILE:HD11	1.98	0.46
42:k:40:GLU:HA	42:k:43:ARG:HB2	1.96	0.46
50:A:241:C:H2'	50:A:242:A:C8	2.51	0.46
50:A:512:G:H1'	50:A:529:A:H2'	1.97	0.46
5:I:96:ILE:HD11	5:I:153:LEU:HD11	1.98	0.46
11:O:106:ARG:O	11:O:123:ILE:HA	2.14	0.46
14:R:10:LEU:N	50:A:105:A:HO2'	2.14	0.46
26:3:183:ARG:NH2	28:6:355:LYS:O	2.49	0.46
33:b:21:ARG:NH1	34:c:217:ASP:OD1	2.49	0.46
34:c:121:SER:OG	34:c:122:ASN:N	2.48	0.46
17:U:28:LEU:O	21:Y:114:THR:OG1	2.30	0.46
20:X:132:LEU:HA	20:X:135:ILE:HG22	1.98	0.46
24:1:47:ASP:O	24:1:51:LYS:CA	2.63	0.46
33:b:41:ARG:HH11	45:o:97:VAL:HA	1.79	0.46
40:i:51:ARG:NH1	50:A:608:A:OP1	2.48	0.46
49:s:267:LYS:HE3	49:s:270:LYS:HE3	1.98	0.46
50:A:641:U:H2'	50:A:642:A:H8	1.81	0.46
17:U:71:ARG:NH1	17:U:73:GLN:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:7:106:ALA:CA	29:7:126:LYS:O	2.60	0.46
35:d:139:GLU:O	35:d:142:LYS:HB3	2.16	0.46
35:d:276:ILE:HG22	35:d:278:LYS:H	1.80	0.46
41:j:87:GLY:HA3	45:o:62:HIS:HB2	1.98	0.46
49:s:168:GLU:OE2	49:s:307:ARG:NH2	2.49	0.46
30:8:125:LYS:HA	30:8:128:GLU:HB3	1.98	0.46
31:9:23:SER:OG	50:A:750:U:O2'	2.33	0.46
33:b:72:VAL:HG13	33:b:90:HIS:HB2	1.97	0.46
6:J:66:LEU:HD22	6:J:82:ILE:HD11	1.98	0.46
34:c:86:ASP:OD1	34:c:86:ASP:N	2.46	0.46
38:g:141:ASN:O	38:g:145:GLY:N	2.48	0.46
46:p:74:ASP:OD1	46:p:74:ASP:N	2.48	0.46
50:A:227:A:H2'	50:A:228:A:H8	1.81	0.46
7:K:88:ARG:HA	7:K:88:ARG:HD3	1.77	0.45
13:Q:100:LEU:HD21	13:Q:286:ILE:HD13	1.98	0.45
27:5:350:ARG:HG3	27:5:351:VAL:HG23	1.97	0.45
33:b:89:ILE:HA	33:b:92:LYS:NZ	2.31	0.45
36:e:202:ALA:HA	36:e:239:LEU:H	1.80	0.45
6:J:113:THR:HA	6:J:156:VAL:HB	1.97	0.45
27:5:230:LEU:HD22	27:5:289:HIS:HB3	1.98	0.45
6:J:69:LYS:HB3	6:J:81:LYS:HB3	1.99	0.45
9:M:97:SER:HA	9:M:141:VAL:HB	1.98	0.45
10:N:205:ARG:NH2	10:N:249:LYS:O	2.48	0.45
16:T:109:ASN:HD21	23:0:101:ILE:HD13	1.82	0.45
16:T:144:GLU:HB2	16:T:177:LYS:HB3	1.98	0.45
18:V:146:VAL:HG22	18:V:153:ILE:HG22	1.98	0.45
29:7:225:VAL:HA	29:7:228:GLU:HG3	1.97	0.45
50:A:8:C:H1'	50:A:9:U:H5'	1.98	0.45
50:A:1040:C:H2'	50:A:1041:A:H8	1.81	0.45
18:V:80:ILE:HB	18:V:85:TRP:HB2	1.98	0.45
42:k:78:GLY:HA2	42:k:81:LEU:HD13	1.99	0.45
1:D:124:GLU:OE2	1:D:149:ARG:NH1	2.49	0.45
3:F:103:GLN:HE22	3:F:249:ASN:HB2	1.82	0.45
5:I:163:GLU:O	5:I:166:ARG:HD3	2.17	0.45
9:M:44:ARG:HD3	9:M:45:ARG:HD3	1.99	0.45
28:6:174:HIS:HB2	28:6:205:THR:O	2.17	0.45
50:A:1542:C:H3'	50:A:1543:A:H8	1.82	0.45
51:B:1609:U:O2	51:B:1616:A:N6	2.50	0.45
13:Q:227:LYS:NZ	13:Q:234:GLU:OE1	2.50	0.45
16:T:137:ARG:HE	35:d:281:MET:HE1	1.81	0.45
17:U:79:ARG:NH1	50:A:696:G:OP1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:5:357:PHE:HD1	27:5:374:ALA:HB2	1.81	0.45
30:8:177:HIS:HD2	44:m:64:ILE:HD11	1.82	0.45
1:D:126:VAL:HG23	1:D:140:ALA:HB1	1.99	0.45
10:N:139:ARG:NH2	50:A:1145:G:O6	2.40	0.45
15:S:104:ARG:NE	50:A:477:G:OP1	2.49	0.45
27:5:108:HIS:CE1	27:5:110:ARG:HB3	2.51	0.45
27:5:149:ASN:HB3	27:5:152:GLU:HB3	1.99	0.45
27:5:174:GLU:HA	27:5:296:LYS:HB2	1.99	0.45
33:b:26:LEU:HD22	33:b:105:ALA:HA	1.98	0.45
38:g:150:LYS:NZ	45:o:79:THR:O	2.49	0.45
2:E:174:GLN:HG2	2:E:175:THR:HG23	1.99	0.45
3:F:234:THR:O	47:q:25:TYR:N	2.50	0.45
12:P:95:GLU:HG2	12:P:101:VAL:HA	1.99	0.45
50:A:1260:U:H2'	50:A:1261:A:C8	2.52	0.45
12:P:151:TRP:HH2	28:6:54:PHE:HB3	1.82	0.45
18:V:194:LEU:HG	21:Y:95:ASN:HB3	1.99	0.45
23:0:96:ASN:ND2	50:A:1039:A:O2'	2.46	0.45
24:1:55:LEU:HD21	47:q:135:TRP:HB2	1.99	0.45
27:5:188:CYS:HB3	27:5:418:TYR:CD2	2.52	0.45
48:r:164:LYS:HB2	48:r:164:LYS:HE2	1.78	0.45
50:A:607:U:H2'	50:A:608:A:H8	1.81	0.45
50:A:615:U:H2'	50:A:616:A:C8	2.48	0.45
50:A:1474:A:H2'	50:A:1475:A:H8	1.82	0.45
15:S:137:GLY:HA3	15:S:142:THR:HG22	1.97	0.44
20:X:222:ASP:OD1	20:X:222:ASP:N	2.47	0.44
27:5:165:GLN:NE2	27:5:175:THR:HG22	2.31	0.44
48:r:123:HIS:HB3	50:A:1521:A:H4'	1.98	0.44
49:s:228:ASP:OD1	49:s:228:ASP:N	2.51	0.44
50:A:159:A:H2'	50:A:160:G:H8	1.81	0.44
28:6:234:HIS:ND1	28:6:255:LEU:O	2.46	0.44
50:A:374:A:H2'	50:A:375:A:C8	2.52	0.44
50:A:640:G:O2'	50:A:1005:G:O6	2.34	0.44
50:A:1167:A:H2'	50:A:1168:A:C8	2.52	0.44
3:F:289:PRO:HD2	9:M:195:LEU:HD11	1.99	0.44
8:L:129:LYS:HB3	13:Q:125:TYR:HE1	1.82	0.44
21:Y:72:LYS:O	21:Y:76:GLN:NE2	2.50	0.44
30:8:135:THR:O	30:8:139:MET:HG3	2.17	0.44
35:d:287:LEU:HD11	35:d:293:TYR:HB2	1.99	0.44
40:i:46:ARG:NH1	50:A:609:U:OP2	2.42	0.44
42:k:19:GLN:HA	42:k:54:ASP:O	2.17	0.44
50:A:501:U:C2	50:A:503:G:H4'	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:6:42:LEU:HB3	28:6:47:ARG:HH22	1.83	0.44
28:6:217:LEU:HD12	28:6:236:LEU:HD22	2.00	0.44
29:7:65:ILE:HD13	29:7:83:LYS:HG3	2.00	0.44
49:s:97:THR:OG1	50:A:704:A:N1	2.43	0.44
50:A:1474:A:H2'	50:A:1475:A:C8	2.52	0.44
5:I:88:ALA:O	5:I:92:ASP:HB2	2.18	0.44
7:K:5:SER:OG	34:c:295:GLU:OE1	2.31	0.44
8:L:37:ARG:NH2	50:A:801:G:O5'	2.51	0.44
16:T:101:GLN:O	16:T:105:GLN:HG2	2.17	0.44
34:c:155:ASN:HD22	34:c:232:TRP:CD1	2.36	0.44
35:d:147:GLU:OE2	35:d:159:ARG:NH2	2.50	0.44
50:A:254:U:H2'	50:A:255:A:C8	2.53	0.44
12:P:130:ARG:HH22	28:6:130:VAL:H	1.65	0.44
15:S:143:LEU:HD22	32:a:59:VAL:HG22	1.99	0.44
18:V:199:MET:HG3	18:V:204:ILE:HB	2.00	0.44
25:2:78:VAL:O	25:2:82:ARG:HG2	2.17	0.44
29:7:150:MET:HG2	29:7:179:PHE:HE1	1.82	0.44
50:A:361:A:N6	50:A:374:A:O2'	2.50	0.44
3:F:61:PRO:HB2	3:F:81:ASP:HB2	2.00	0.44
12:P:40:GLU:OE2	28:6:292:GLN:NE2	2.51	0.44
17:U:30:ARG:O	21:Y:121:ARG:NH1	2.50	0.44
17:U:67:ALA:HB3	17:U:98:GLN:HB2	1.98	0.44
20:X:20:ILE:HG23	20:X:212:ILE:HD12	2.00	0.44
2:E:109:LEU:HD21	2:E:337:VAL:HG22	1.99	0.44
2:E:110:TRP:HE1	2:E:116:LYS:HZ3	1.66	0.44
12:P:104:SER:OG	28:6:150:ARG:NH2	2.47	0.44
42:k:82:THR:HB	48:r:36:ARG:HH22	1.81	0.44
49:s:316:CYS:HB2	49:s:319:GLN:HB2	1.98	0.44
50:A:783:G:O6	50:A:1002:A:N6	2.51	0.44
1:D:202:ARG:O	50:A:851:A:N6	2.50	0.44
3:F:107:LYS:HE2	3:F:107:LYS:HB3	1.82	0.44
10:N:222:ASN:HD21	10:N:225:GLY:HA2	1.82	0.44
30:8:139:MET:HB3	36:e:275:PHE:HA	1.99	0.44
32:a:105:GLU:HA	32:a:108:MET:HE3	2.00	0.44
50:A:362:G:O2'	50:A:1195:C:O2	2.35	0.44
2:E:80:LEU:HD11	2:E:320:PHE:HB3	1.99	0.43
7:K:25:MET:HE3	7:K:25:MET:HB3	1.88	0.43
7:K:136:ASP:O	7:K:140:ASN:ND2	2.51	0.43
13:Q:165:GLU:HB2	13:Q:168:ASN:HB2	2.00	0.43
21:Y:102:TRP:HE3	21:Y:142:LEU:HD22	1.82	0.43
31:9:97:ALA:O	31:9:101:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:113:SER:OG	32:a:118:THR:O	2.31	0.43
45:o:51:MET:HE2	45:o:51:MET:HB3	1.92	0.43
50:A:424:G:O2'	50:A:595:A:N3	2.49	0.43
9:M:250:ASP:OD2	9:M:250:ASP:N	2.51	0.43
12:P:64:LYS:HA	12:P:97:GLN:HE22	1.83	0.43
13:Q:124:PRO:HD3	13:Q:170:ARG:NH2	2.33	0.43
14:R:57:ARG:HH12	15:S:171:ILE:HG12	1.83	0.43
14:R:107:ILE:HG21	16:T:208:ILE:HG21	2.00	0.43
29:7:166:LEU:HA	29:7:183:VAL:HG23	1.99	0.43
36:e:55:ARG:HE	36:e:157:LEU:HD12	1.83	0.43
40:i:96:LYS:NZ	50:A:67:A:H5'	2.33	0.43
49:s:103:ASP:OD2	49:s:104:ARG:N	2.51	0.43
50:A:204:A:HO2'	50:A:420:A:HO2'	1.67	0.43
50:A:374:A:H2'	50:A:375:A:H8	1.84	0.43
50:A:1495:C:H2'	50:A:1496:U:C6	2.53	0.43
5:I:162:LYS:HA	5:I:165:VAL:HB	2.00	0.43
9:M:274:VAL:HG21	47:q:75:LEU:HD11	2.00	0.43
21:Y:123:ARG:HD2	35:d:64:GLY:HA2	1.99	0.43
21:Y:160:GLN:HG3	31:9:131:TYR:CG	2.53	0.43
50:A:132:A:N7	50:A:135:A:N6	2.65	0.43
2:E:129:VAL:HA	2:E:147:VAL:HG22	2.00	0.43
11:O:62:TYR:HE2	13:Q:269:MET:HG2	1.83	0.43
22:Z:66:LEU:HD12	22:Z:122:LEU:HD22	2.00	0.43
30:8:150:LEU:O	30:8:154:SER:OG	2.27	0.43
34:c:260:GLN:CA	34:c:269:LEU:O	2.56	0.43
36:e:212:HIS:HB2	36:e:230:LYS:HZ3	1.83	0.43
49:s:183:THR:HG23	49:s:184:LEU:HD12	1.99	0.43
50:A:227:A:H2'	50:A:228:A:C8	2.53	0.43
50:A:1007:A:H2'	50:A:1008:A:C8	2.54	0.43
3:F:83:HIS:HB3	3:F:86:VAL:HG12	2.00	0.43
5:I:153:LEU:HG	5:I:155:VAL:HG13	2.01	0.43
9:M:231:GLU:O	9:M:235:GLU:HG2	2.18	0.43
9:M:277:MET:HE1	38:g:52:LEU:HD11	2.00	0.43
11:O:49:VAL:HG21	11:O:121:ALA:HB3	2.01	0.43
14:R:98:ASN:HD22	50:A:477:G:H4'	1.83	0.43
21:Y:191:ASN:O	21:Y:195:ASN:ND2	2.40	0.43
28:6:253:PRO:O	28:6:296:ARG:NH2	2.45	0.43
29:7:102:LYS:HE2	29:7:102:LYS:HB2	1.85	0.43
37:f:97:ALA:HB3	37:f:103:ALA:HB2	2.00	0.43
49:s:243:ILE:HG13	49:s:296:HIS:HB2	2.01	0.43
50:A:988:U:H3'	50:A:989:C:H2'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:A:1554:G:H2'	50:A:1555:G:H8	1.84	0.43
1:D:102:GLN:NE2	50:A:732:A:OP1	2.47	0.43
1:D:232:ARG:HH12	1:D:293:LYS:HB3	1.82	0.43
5:I:160:LYS:HE3	5:I:163:GLU:HG2	1.99	0.43
34:c:74:ALA:O	34:c:78:ARG:HB2	2.19	0.43
35:d:267:PRO:HG2	35:d:270:ALA:HB2	2.01	0.43
36:e:121:GLU:HA	36:e:124:TRP:CE2	2.53	0.43
50:A:796:A:O2'	50:A:1485:C:OP1	2.37	0.43
51:B:1642:G:H2'	51:B:1643:A:C8	2.53	0.43
8:L:69:VAL:O	8:L:130:ARG:NH1	2.42	0.43
9:M:154:ILE:HG12	9:M:156:VAL:HG13	2.00	0.43
11:O:152:LEU:HD13	29:7:319:ARG:HB2	2.01	0.43
17:U:50:ARG:NH2	50:A:703:A:OP1	2.52	0.43
19:W:56:MET:HE1	50:A:393:G:H21	1.82	0.43
29:7:107:LEU:HD12	29:7:126:LYS:HE2	2.01	0.43
50:A:789:A:N6	50:A:998:A:O2'	2.52	0.43
50:A:991:U:H2'	50:A:992:A:C8	2.52	0.43
50:A:1488:A:H2'	50:A:1489:A:H8	1.84	0.43
3:F:93:LEU:HD12	45:o:91:GLN:HG2	2.00	0.43
6:J:26:ALA:HB1	6:J:57:THR:HG23	2.01	0.43
15:S:201:ALA:HA	15:S:202:PRO:HD3	1.89	0.43
20:X:176:LEU:HD23	20:X:177:HIS:CD2	2.54	0.43
28:6:173:LEU:HD12	28:6:272:LEU:HD22	2.01	0.43
28:6:224:HIS:CE1	28:6:227:GLU:H	2.37	0.43
38:g:154:ASP:OD1	38:g:154:ASP:N	2.50	0.43
50:A:187:U:H2'	50:A:188:G:C8	2.54	0.43
50:A:1454:U:N3	50:A:1463:A:H8	2.10	0.43
2:E:99:LEU:HD21	2:E:193:LEU:HB3	2.01	0.43
5:I:132:LYS:NZ	5:I:144:LEU:O	2.52	0.43
11:O:18:MET:HB2	11:O:25:ARG:HB2	2.01	0.43
15:S:129:ARG:HE	15:S:155:ARG:HG3	1.82	0.43
18:V:23:MET:HE3	18:V:23:MET:HB3	1.81	0.43
29:7:165:ASN:HD22	29:7:235:TYR:HE1	1.65	0.43
48:r:123:HIS:CE1	48:r:128:LEU:HD12	2.54	0.43
15:S:152:ASP:OD1	15:S:152:ASP:N	2.48	0.43
28:6:179:VAL:HG22	28:6:197:GLU:HG2	2.00	0.43
29:7:317:LEU:HD23	29:7:317:LEU:HA	1.86	0.43
30:8:121:TRP:HA	30:8:124:TYR:HB3	2.00	0.43
34:c:41:PHE:HE2	40:i:36:LEU:HD13	1.84	0.43
11:O:108:LEU:HD12	11:O:133:LEU:HD13	2.01	0.42
12:P:110:TRP:HA	12:P:113:LYS:HE3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:74:ARG:HG3	50:A:395:A:C4	2.53	0.42
21:Y:149:ARG:HG2	31:9:86:LEU:HD13	2.00	0.42
21:Y:175:ARG:HE	21:Y:177:ILE:HD11	1.84	0.42
28:6:157:LEU:O	28:6:161:LEU:CB	2.67	0.42
30:8:139:MET:HE2	30:8:139:MET:HB2	1.88	0.42
35:d:138:PRO:O	35:d:142:LYS:N	2.40	0.42
36:e:257:LYS:NZ	36:e:276:VAL:O	2.52	0.42
50:A:67:A:N6	50:A:90:G:H1'	2.34	0.42
9:M:68:GLU:OE2	9:M:71:GLN:NE2	2.49	0.42
9:M:211:VAL:HG13	47:q:103:LEU:HD11	2.01	0.42
14:R:111:LYS:HG2	32:a:45:CYS:HB3	2.00	0.42
26:3:126:LYS:HD3	26:3:144:LEU:HA	2.01	0.42
26:3:131:LYS:NZ	50:A:1239:G:N7	2.66	0.42
32:a:111:GLN:HE22	32:a:115:MET:HE2	1.83	0.42
36:e:47:LEU:HB3	36:e:178:TRP:CE2	2.54	0.42
50:A:750:U:H2'	50:A:751:G:H8	1.83	0.42
3:F:220:ASP:O	3:F:245:ALA:N	2.53	0.42
22:Z:78:ARG:HD2	22:Z:116:LEU:HD21	2.02	0.42
22:Z:124:LEU:HD21	22:Z:128:LEU:HD23	2.01	0.42
34:c:59:ARG:HG3	34:c:61:SER:H	1.83	0.42
37:f:103:ALA:HB1	37:f:155:ARG:CZ	2.49	0.42
40:i:32:ILE:HG22	40:i:34:ILE:HG22	2.01	0.42
50:A:212:A:N6	50:A:223:A:O4'	2.52	0.42
2:E:129:VAL:HG23	2:E:193:LEU:HD21	2.00	0.42
10:N:236:THR:O	10:N:238:LYS:NZ	2.52	0.42
13:Q:154:VAL:HA	13:Q:159:GLY:HA2	2.00	0.42
17:U:11:ARG:HD3	27:5:82:TYR:CZ	2.55	0.42
24:1:34:ARG:HD2	24:1:35:ASN:O	2.19	0.42
30:8:114:ARG:HG3	36:e:73:LEU:HD21	2.01	0.42
50:A:162:A:N6	50:A:167:C:OP2	2.46	0.42
50:A:1070:A:H2'	50:A:1071:A:C8	2.54	0.42
1:D:227:GLN:NE2	1:D:231:LYS:HA	2.35	0.42
7:K:77:TYR:HD2	7:K:95:LEU:HD13	1.84	0.42
14:R:32:ARG:HE	14:R:32:ARG:HB3	1.71	0.42
28:6:175:VAL:HG13	28:6:204:VAL:HG22	2.01	0.42
29:7:106:ALA:HB1	29:7:125:ILE:HG23	2.00	0.42
29:7:322:LYS:HA	29:7:322:LYS:HD3	1.77	0.42
36:e:81:ARG:NH2	44:m:46:GLN:OE1	2.52	0.42
36:e:177:GLU:O	36:e:190:ARG:NH1	2.52	0.42
49:s:94:TYR:O	49:s:106:TYR:OH	2.32	0.42
1:D:202:ARG:NH2	50:A:851:A:OP2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:168:LYS:NZ	38:g:90:ARG:HE	2.18	0.42
9:M:62:ARG:HB3	40:i:128:ARG:HH11	1.84	0.42
14:R:114:LYS:HD3	32:a:45:CYS:SG	2.59	0.42
28:6:365:TYR:HA	28:6:368:ARG:HD3	2.01	0.42
30:8:121:TRP:HD1	30:8:121:TRP:O	2.03	0.42
32:a:75:ILE:HG22	34:c:257:LEU:HB2	2.02	0.42
44:m:55:LEU:HD22	44:m:63:THR:HB	2.02	0.42
11:O:133:LEU:HD23	23:0:130:VAL:HG11	2.02	0.42
27:5:200:ARG:NH2	27:5:234:ASP:OD1	2.53	0.42
27:5:380:GLN:HB3	27:5:410:THR:HG22	2.01	0.42
33:b:133:PHE:CE2	34:c:269:LEU:HD22	2.55	0.42
49:s:106:TYR:O	49:s:110:THR:OG1	2.19	0.42
10:N:169:PHE:CD1	10:N:191:SER:HB2	2.55	0.42
12:P:59:LEU:HD11	28:6:264:GLY:HA2	2.01	0.42
14:R:34:ARG:NH2	50:A:1012:A:OP1	2.47	0.42
16:T:73:ILE:HB	16:T:178:LEU:HB2	2.02	0.42
20:X:171:ARG:NH2	27:5:54:GLY:O	2.45	0.42
21:Y:164:ARG:NH1	50:A:27:A:OP2	2.41	0.42
21:Y:171:ASP:OD1	21:Y:171:ASP:N	2.50	0.42
35:d:119:GLN:HA	35:d:122:ILE:HD12	2.02	0.42
35:d:186:VAL:HG22	35:d:187:GLU:H	1.85	0.42
36:e:168:GLN:HB3	36:e:170:VAL:HG23	2.01	0.42
14:R:10:LEU:N	50:A:105:A:O2'	2.53	0.42
21:Y:223:LYS:O	21:Y:227:GLU:HG2	2.20	0.42
29:7:132:ASP:OD1	29:7:133:CYS:N	2.51	0.42
48:r:85:ASP:N	48:r:85:ASP:OD2	2.51	0.42
50:A:118:C:N4	50:A:246:G:O2'	2.53	0.42
50:A:242:A:H2'	50:A:243:G:C8	2.54	0.42
1:D:208:ARG:HB2	50:A:859:U:H2'	2.01	0.42
3:F:277:ASP:HA	38:g:90:ARG:HH12	1.84	0.42
7:K:124:ARG:HH21	32:a:118:THR:HG22	1.85	0.42
15:S:161:ILE:HG22	15:S:162:GLU:HB2	2.01	0.42
17:U:35:GLN:HE21	17:U:39:THR:HG21	1.85	0.42
19:W:102:GLU:HB2	19:W:130:PHE:CD2	2.55	0.42
27:5:83:LYS:HA	27:5:83:LYS:HD3	1.75	0.42
27:5:114:LEU:HD11	27:5:259:ILE:HD13	2.01	0.42
35:d:122:ILE:HG13	35:d:197:VAL:HG21	2.02	0.42
36:e:199:ASN:HB2	36:e:242:ASP:HB2	2.02	0.42
50:A:48:A:N3	50:A:241:C:O2'	2.46	0.42
50:A:632:U:H2'	50:A:633:A:C8	2.55	0.42
7:K:71:LYS:HE3	48:r:176:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:83:PHE:HB3	26:3:115:LEU:HD13	2.02	0.41
11:O:58:LYS:HB2	11:O:58:LYS:HE2	1.89	0.41
12:P:72:PHE:HB2	19:W:107:HIS:HA	2.02	0.41
15:S:151:LYS:HE2	15:S:151:LYS:HB3	1.73	0.41
23:O:137:ILE:O	23:O:141:ILE:HG12	2.20	0.41
30:8:164:ARG:CZ	37:f:86:TYR:HB3	2.50	0.41
34:c:79:LEU:HD13	34:c:214:PHE:HE1	1.85	0.41
34:c:220:ILE:O	34:c:223:MET:HG2	2.20	0.41
47:q:71:VAL:HA	47:q:72:PRO:HD3	1.91	0.41
49:s:90:LYS:HD2	49:s:232:GLN:HB2	2.01	0.41
50:A:345:G:H22	50:A:367:U:H5''	1.85	0.41
50:A:1134:A:H2'	50:A:1135:A:H8	1.83	0.41
50:A:1507:A:H61	50:A:1522:C:H42	1.68	0.41
51:B:1622:A:H2'	51:B:1623:G:C8	2.55	0.41
2:E:217:GLY:HA2	2:E:258:PRO:HB3	2.01	0.41
3:F:220:ASP:OD1	3:F:221:LEU:N	2.49	0.41
10:N:169:PHE:O	10:N:173:GLN:HG2	2.20	0.41
11:O:45:PRO:HG2	11:O:48:ARG:HD2	2.02	0.41
20:X:114:PHE:O	20:X:122:LYS:HA	2.19	0.41
24:1:22:SER:HB3	24:1:56:PHE:CE2	2.55	0.41
29:7:39:GLU:HA	29:7:42:GLU:HG2	2.01	0.41
29:7:145:SER:HB3	29:7:216:PHE:HE2	1.84	0.41
36:e:157:LEU:HD22	36:e:254:TRP:HB3	2.03	0.41
49:s:251:VAL:O	49:s:373:GLN:NE2	2.53	0.41
50:A:357:A:O2'	50:A:378:U:OP1	2.28	0.41
3:F:117:ARG:NH1	50:A:235:C:OP1	2.53	0.41
4:H:85:ASP:HB3	4:H:88:HIS:HD2	1.85	0.41
18:V:154:ILE:HD12	18:V:155:PRO:HD2	2.02	0.41
48:r:90:SER:HA	48:r:93:ILE:HD12	2.02	0.41
50:A:431:C:H2'	50:A:432:A:H8	1.85	0.41
50:A:472:A:C8	50:A:591:C:H5'	2.55	0.41
2:E:218:VAL:HB	2:E:258:PRO:HD3	2.01	0.41
9:M:290:LEU:HD23	47:q:82:LEU:HD22	2.02	0.41
30:8:149:GLU:OE1	36:e:212:HIS:NE2	2.52	0.41
35:d:143:ASP:HA	35:d:146:ILE:HG22	2.03	0.41
36:e:121:GLU:HA	36:e:124:TRP:NE1	2.36	0.41
49:s:89:MET:HG2	49:s:275:LYS:HD3	2.02	0.41
49:s:406:GLU:OE2	49:s:411:LYS:NZ	2.41	0.41
50:A:113:U:H2'	50:A:114:A:H8	1.86	0.41
50:A:539:G:H3'	50:A:540:C:H5''	2.02	0.41
5:I:166:ARG:HA	5:I:169:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:77:TYR:HE2	7:K:103:ILE:HG12	1.85	0.41
7:K:142:VAL:HG11	33:b:133:PHE:HE1	1.85	0.41
28:6:218:LEU:O	28:6:233:LEU:HA	2.21	0.41
29:7:36:SER:HB2	29:7:39:GLU:HG2	2.02	0.41
29:7:64:LYS:HE3	35:d:276:ILE:HB	2.02	0.41
29:7:274:ILE:O	29:7:304:VAL:N	2.53	0.41
47:q:48:PRO:HB2	47:q:50:TRP:CD1	2.55	0.41
49:s:242:ARG:NH2	49:s:290:ASP:OD2	2.52	0.41
49:s:356:VAL:HG22	49:s:373:GLN:HG2	2.02	0.41
2:E:121:LEU:HD22	2:E:284:TYR:CE1	2.55	0.41
5:I:119:HIS:HB3	5:I:121:ILE:HG22	2.02	0.41
6:J:47:ASN:OD1	6:J:48:GLN:N	2.54	0.41
8:L:137:VAL:HA	8:L:140:ILE:HD12	2.03	0.41
18:V:75:LYS:HE3	18:V:75:LYS:HB3	1.88	0.41
27:5:208:THR:HA	27:5:224:GLY:O	2.20	0.41
28:6:280:ASP:OD1	28:6:280:ASP:N	2.54	0.41
29:7:147:ALA:O	29:7:150:MET:HG3	2.20	0.41
42:k:54:ASP:OD1	42:k:54:ASP:N	2.53	0.41
50:A:403:A:C5	50:A:404:A:H1'	2.56	0.41
50:A:722:U:H2'	50:A:724:A:H62	1.86	0.41
13:Q:132:GLN:OE1	13:Q:132:GLN:N	2.53	0.41
22:Z:38:ARG:HG2	22:Z:81:TRP:CE2	2.56	0.41
23:0:93:ARG:NH2	50:A:640:G:OP2	2.50	0.41
29:7:44:ARG:HB3	29:7:261:ILE:HD12	2.02	0.41
30:8:154:SER:HB2	30:8:157:LEU:HB2	2.02	0.41
49:s:105:TRP:HZ3	49:s:268:PRO:HA	1.86	0.41
27:5:187:LEU:HD22	27:5:411:PHE:HZ	1.86	0.41
38:g:94:ILE:HD12	38:g:95:PRO:HD2	2.03	0.41
50:A:193:A:H2'	50:A:194:A:C8	2.56	0.41
50:A:679:G:H2'	50:A:680:A:C8	2.56	0.41
51:B:1604:G:H2'	51:B:1605:A:H8	1.86	0.41
2:E:48:TRP:CD1	2:E:50:ASP:H	2.39	0.41
3:F:46:PRO:HB3	39:h:98:PHE:CE2	2.55	0.41
8:L:87:VAL:HG21	8:L:123:ILE:HD12	2.03	0.41
9:M:280:LYS:HE3	9:M:280:LYS:HB3	1.93	0.41
11:O:110:ILE:HD13	11:O:110:ILE:HG21	1.83	0.41
12:P:51:ARG:NH2	28:6:221:LEU:O	2.54	0.41
13:Q:139:GLN:HB3	13:Q:150:ILE:HG22	2.02	0.41
13:Q:154:VAL:HG13	13:Q:199:THR:HB	2.02	0.41
13:Q:205:LYS:HE2	13:Q:206:PRO:HD2	2.03	0.41
14:R:29:ARG:HD3	14:R:29:ARG:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:150:TRP:CD1	35:d:172:MET:HG3	2.56	0.41
22:Z:75:THR:HG21	22:Z:86:ILE:HG21	2.03	0.41
27:5:165:GLN:NE2	27:5:175:THR:O	2.40	0.41
28:6:175:VAL:HG11	28:6:270:PHE:CZ	2.56	0.41
31:9:22:THR:HG23	31:9:24:LYS:H	1.86	0.41
35:d:188:SER:HA	35:d:218:THR:HA	2.03	0.41
35:d:197:VAL:O	35:d:198:ARG:NH1	2.43	0.41
35:d:216:MET:HE3	35:d:216:MET:HB2	1.92	0.41
47:q:59:LYS:HE3	47:q:59:LYS:HB3	1.79	0.41
48:r:153:ARG:NH2	50:A:489:U:OP2	2.54	0.41
49:s:188:LEU:HD21	49:s:422:VAL:HG13	2.03	0.41
50:A:542:C:H2'	50:A:543:A:H8	1.85	0.41
3:F:67:GLU:HG2	3:F:75:GLU:HB2	2.03	0.41
9:M:205:LEU:HD13	47:q:96:LEU:HD13	2.03	0.41
11:O:17:ARG:H	11:O:17:ARG:HG2	1.72	0.41
18:V:203:GLY:O	18:V:205:LYS:NZ	2.52	0.41
18:V:213:VAL:HG21	21:Y:183:GLN:HG2	2.03	0.41
19:W:75:TRP:HB2	19:W:89:LEU:HD11	2.02	0.41
22:Z:109:LYS:NZ	50:A:411:U:O2	2.53	0.41
24:1:19:ARG:NH1	50:A:1235:A:N1	2.69	0.41
29:7:108:VAL:HB	29:7:113:TRP:CD1	2.55	0.41
29:7:144:ARG:NH1	29:7:171:GLU:OE1	2.53	0.41
39:h:62:PRO:HA	39:h:63:PRO:HD3	1.93	0.41
39:h:136:ASP:OD1	39:h:136:ASP:N	2.53	0.41
40:i:102:MET:HE1	40:i:110:LEU:HD13	2.03	0.41
42:k:70:ASP:OD1	42:k:71:GLY:N	2.51	0.41
45:o:65:VAL:HG22	45:o:68:ARG:HH22	1.86	0.41
49:s:93:VAL:HA	49:s:273:LEU:HD11	2.03	0.41
3:F:167:MET:HA	3:F:170:ARG:HE	1.86	0.40
3:F:219:VAL:HG12	3:F:265:THR:HG21	2.03	0.40
5:I:82:LEU:HD13	5:I:130:VAL:HG11	2.03	0.40
9:M:72:THR:HA	9:M:73:PRO:HD3	1.90	0.40
12:P:130:ARG:NH2	28:6:130:VAL:H	2.19	0.40
20:X:234:LEU:HA	20:X:237:GLN:HG2	2.03	0.40
23:0:181:ARG:HD3	23:0:182:PRO:HD2	2.03	0.40
12:P:63:ARG:NH1	19:W:139:GLU:OE1	2.54	0.40
13:Q:246:ASP:OD1	13:Q:246:ASP:N	2.54	0.40
15:S:139:ASP:OD1	34:c:310:ASN:ND2	2.54	0.40
20:X:208:LEU:O	20:X:212:ILE:HG12	2.21	0.40
27:5:120:ALA:O	27:5:124:THR:CB	2.69	0.40
27:5:385:HIS:HB2	50:A:725:A:H1'	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:6:266:HIS:O	28:6:320:GLN:HA	2.21	0.40
1:D:74:ILE:O	1:D:150:TRP:NE1	2.45	0.40
5:I:158:GLU:HA	5:I:159:PRO:HD3	1.91	0.40
9:M:115:PRO:HD3	9:M:255:MET:HG2	2.02	0.40
12:P:79:HIS:HA	12:P:95:GLU:O	2.21	0.40
27:5:142:ASP:OD1	27:5:142:ASP:N	2.53	0.40
27:5:242:ARG:HA	27:5:245:ILE:HD12	2.03	0.40
28:6:204:VAL:HG21	28:6:216:LEU:HD21	2.02	0.40
33:b:30:SER:O	33:b:74:ARG:O	2.40	0.40
35:d:244:GLU:HG2	35:d:264:LYS:HD3	2.03	0.40
39:h:74:VAL:HA	39:h:77:VAL:HG12	2.03	0.40
50:A:367:U:H4'	50:A:370:G:C6	2.57	0.40
50:A:457:A:H4'	50:A:581:A:C5	2.56	0.40
7:K:71:LYS:NZ	50:A:570:C:OP2	2.43	0.40
7:K:89:GLN:NE2	48:r:163:TYR:O	2.55	0.40
9:M:78:ILE:HD13	26:3:124:ARG:HD2	2.04	0.40
12:P:123:VAL:HG11	28:6:128:ALA:HB3	2.04	0.40
20:X:72:PRO:O	20:X:75:SER:OG	2.34	0.40
22:Z:99:VAL:HG12	41:j:80:LEU:HD12	2.02	0.40
29:7:175:ILE:O	29:7:319:ARG:NH2	2.54	0.40
30:8:177:HIS:CG	30:8:178:TYR:H	2.40	0.40
40:i:57:TYR:OH	47:q:28:ARG:O	2.29	0.40
41:j:93:LEU:HD23	41:j:93:LEU:HA	1.91	0.40
42:k:18:VAL:HG23	42:k:64:VAL:HG22	2.03	0.40
49:s:177:LEU:HD21	49:s:299:PHE:HB3	2.03	0.40
50:A:658:C:H1'	50:A:781:A:H61	1.87	0.40
50:A:1131:A:H2'	50:A:1132:A:C8	2.56	0.40
51:B:1603:A:H2'	51:B:1604:G:C8	2.57	0.40
5:I:161:VAL:HA	5:I:164:MET:SD	2.61	0.40
9:M:77:ARG:O	50:A:1227:A:O2'	2.39	0.40
13:Q:284:LYS:HE3	13:Q:284:LYS:HB3	1.87	0.40
25:2:79:ILE:HG23	25:2:90:LEU:HD23	2.03	0.40
28:6:31:PRO:HB3	28:6:35:MET:HE3	2.03	0.40
50:A:26:C:H2'	50:A:27:A:C8	2.56	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	216/305 (71%)	210 (97%)	5 (2%)	1 (0%)	24	55
2	E	281/348 (81%)	272 (97%)	9 (3%)	0	100	100
3	F	248/311 (80%)	240 (97%)	8 (3%)	0	100	100
4	H	93/267 (35%)	90 (97%)	3 (3%)	0	100	100
5	I	154/261 (59%)	143 (93%)	11 (7%)	0	100	100
6	J	138/192 (72%)	128 (93%)	10 (7%)	0	100	100
7	K	175/178 (98%)	170 (97%)	5 (3%)	0	100	100
8	L	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
9	M	285/296 (96%)	276 (97%)	9 (3%)	0	100	100
10	N	203/251 (81%)	198 (98%)	5 (2%)	0	100	100
11	O	150/175 (86%)	146 (97%)	4 (3%)	0	100	100
12	P	139/180 (77%)	130 (94%)	9 (6%)	0	100	100
13	Q	215/292 (74%)	207 (96%)	8 (4%)	0	100	100
14	R	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
15	S	154/205 (75%)	149 (97%)	5 (3%)	0	100	100
16	T	155/206 (75%)	152 (98%)	3 (2%)	0	100	100
17	U	135/153 (88%)	127 (94%)	8 (6%)	0	100	100
18	V	188/216 (87%)	181 (96%)	7 (4%)	0	100	100
19	W	107/148 (72%)	105 (98%)	2 (2%)	0	100	100
20	X	241/256 (94%)	235 (98%)	6 (2%)	0	100	100
21	Y	174/250 (70%)	170 (98%)	4 (2%)	0	100	100
22	Z	118/161 (73%)	112 (95%)	6 (5%)	0	100	100
23	0	106/188 (56%)	103 (97%)	3 (3%)	0	100	100
24	1	50/65 (77%)	48 (96%)	2 (4%)	0	100	100
25	2	41/92 (45%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	3	93/188 (50%)	89 (96%)	4 (4%)	0	100	100
27	5	383/423 (90%)	367 (96%)	16 (4%)	0	100	100
28	6	316/380 (83%)	305 (96%)	11 (4%)	0	100	100
29	7	285/338 (84%)	270 (95%)	15 (5%)	0	100	100
30	8	97/206 (47%)	91 (94%)	6 (6%)	0	100	100
31	9	113/137 (82%)	109 (96%)	4 (4%)	0	100	100
32	a	78/142 (55%)	75 (96%)	3 (4%)	0	100	100
33	b	146/215 (68%)	136 (93%)	10 (7%)	0	100	100
34	c	271/332 (82%)	262 (97%)	9 (3%)	0	100	100
35	d	203/306 (66%)	196 (97%)	7 (3%)	0	100	100
36	e	211/279 (76%)	195 (92%)	16 (8%)	0	100	100
37	f	110/212 (52%)	103 (94%)	7 (6%)	0	100	100
38	g	127/166 (76%)	123 (97%)	4 (3%)	0	100	100
39	h	96/158 (61%)	92 (96%)	4 (4%)	0	100	100
40	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
41	j	83/123 (68%)	83 (100%)	0	0	100	100
42	k	76/112 (68%)	72 (95%)	4 (5%)	0	100	100
43	l	21/138 (15%)	21 (100%)	0	0	100	100
44	m	43/128 (34%)	36 (84%)	7 (16%)	0	100	100
45	o	77/102 (76%)	75 (97%)	2 (3%)	0	100	100
46	p	119/206 (58%)	117 (98%)	2 (2%)	0	100	100
47	q	118/222 (53%)	118 (100%)	0	0	100	100
48	r	140/196 (71%)	135 (96%)	5 (4%)	0	100	100
49	s	366/439 (83%)	354 (97%)	12 (3%)	0	100	100
All	All	7684/10566 (73%)	7394 (96%)	289 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	207	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	179/245 (73%)	179 (100%)	0	100	100
2	E	246/290 (85%)	246 (100%)	0	100	100
3	F	217/262 (83%)	217 (100%)	0	100	100
4	H	86/228 (38%)	86 (100%)	0	100	100
5	I	145/232 (62%)	145 (100%)	0	100	100
6	J	113/150 (75%)	113 (100%)	0	100	100
7	K	155/156 (99%)	155 (100%)	0	100	100
8	L	98/124 (79%)	98 (100%)	0	100	100
9	M	245/249 (98%)	245 (100%)	0	100	100
10	N	172/211 (82%)	172 (100%)	0	100	100
11	O	133/150 (89%)	133 (100%)	0	100	100
12	P	123/155 (79%)	123 (100%)	0	100	100
13	Q	199/256 (78%)	199 (100%)	0	100	100
14	R	118/126 (94%)	118 (100%)	0	100	100
15	S	141/180 (78%)	141 (100%)	0	100	100
16	T	141/176 (80%)	141 (100%)	0	100	100
17	U	124/135 (92%)	124 (100%)	0	100	100
18	V	172/191 (90%)	171 (99%)	1 (1%)	78	81
19	W	89/119 (75%)	89 (100%)	0	100	100
20	X	219/229 (96%)	219 (100%)	0	100	100
21	Y	159/223 (71%)	159 (100%)	0	100	100
22	Z	111/147 (76%)	111 (100%)	0	100	100
23	0	97/164 (59%)	97 (100%)	0	100	100
24	1	49/60 (82%)	49 (100%)	0	100	100
25	2	38/72 (53%)	38 (100%)	0	100	100
26	3	88/166 (53%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	5	348/368 (95%)	348 (100%)	0	100	100
28	6	265/332 (80%)	265 (100%)	0	100	100
29	7	263/303 (87%)	263 (100%)	0	100	100
30	8	91/190 (48%)	91 (100%)	0	100	100
31	9	99/112 (88%)	99 (100%)	0	100	100
32	a	78/133 (59%)	78 (100%)	0	100	100
33	b	130/186 (70%)	130 (100%)	0	100	100
34	c	241/288 (84%)	241 (100%)	0	100	100
35	d	193/274 (70%)	193 (100%)	0	100	100
36	e	188/236 (80%)	188 (100%)	0	100	100
37	f	101/188 (54%)	101 (100%)	0	100	100
38	g	119/148 (80%)	119 (100%)	0	100	100
39	h	95/148 (64%)	95 (100%)	0	100	100
40	i	86/110 (78%)	86 (100%)	0	100	100
41	j	68/97 (70%)	68 (100%)	0	100	100
42	k	71/90 (79%)	71 (100%)	0	100	100
43	l	23/116 (20%)	23 (100%)	0	100	100
44	m	40/113 (35%)	40 (100%)	0	100	100
45	o	68/87 (78%)	68 (100%)	0	100	100
46	p	117/181 (65%)	117 (100%)	0	100	100
47	q	104/178 (58%)	104 (100%)	0	100	100
48	r	133/169 (79%)	133 (100%)	0	100	100
49	s	326/381 (86%)	325 (100%)	1 (0%)	86	86
All	All	6904/9124 (76%)	6902 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	V	92	ASN
49	s	179	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	165	ASN
1	D	195	ASN
1	D	205	GLN
1	D	227	GLN
2	E	52	HIS
2	E	117	HIS
3	F	103	GLN
3	F	130	GLN
3	F	188	HIS
3	F	228	GLN
4	H	121	ASN
4	H	126	GLN
6	J	133	GLN
7	K	40	GLN
7	K	94	GLN
7	K	96	HIS
8	L	72	GLN
8	L	89	HIS
8	L	142	GLN
9	M	26	ASN
10	N	98	HIS
10	N	138	HIS
10	N	222	ASN
12	P	115	HIS
13	Q	175	GLN
14	R	149	HIS
15	S	75	HIS
15	S	118	ASN
16	T	132	HIS
17	U	16	GLN
17	U	35	GLN
18	V	92	ASN
19	W	41	ASN
20	X	215	GLN
21	Y	76	GLN
21	Y	122	GLN
21	Y	225	ASN
22	Z	150	HIS
24	1	31	ASN
24	1	52	GLN
25	2	54	GLN
25	2	57	ASN
27	5	109	HIS

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Mol	Chain	Res	Type
28	6	200	GLN
28	6	266	HIS
28	6	292	GLN
28	6	320	GLN
28	6	354	GLN
29	7	45	ASN
30	8	144	GLN
31	9	134	ASN
35	d	154	ASN
35	d	251	GLN
39	h	99	ASN
40	i	120	HIS
41	j	26	GLN
42	k	15	GLN
42	k	72	HIS
44	m	59	GLN
45	o	94	HIS
46	p	96	ASN
47	q	138	GLN
47	q	142	ASN
48	r	96	HIS
49	s	179	GLN
49	s	192	ASN
49	s	240	GLN
49	s	358	GLN
49	s	427	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	A	1071/1559 (68%)	251 (23%)	11 (1%)
51	B	51/69 (73%)	15 (29%)	1 (1%)
All	All	1122/1628 (68%)	266 (23%)	12 (1%)

All (266) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	A	4	A
50	A	6	A
50	A	8	C
50	A	9	U

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Mol	Chain	Res	Type
50	A	11	G
50	A	19	C
50	A	23	C
50	A	24	U
50	A	30	U
50	A	34	U
50	A	38	A
50	A	43	A
50	A	44	C
50	A	45	C
50	A	46	U
50	A	47	U
50	A	54	A
50	A	57	A
50	A	61	A
50	A	71	A
50	A	78	G
50	A	80	G
50	A	81	A
50	A	100	G
50	A	103	A
50	A	111	A
50	A	112	G
50	A	121	G
50	A	124	A
50	A	130	G
50	A	134	A
50	A	135	A
50	A	136	U
50	A	142	C
50	A	147	C
50	A	153	A
50	A	154	U
50	A	157	C
50	A	158	A
50	A	159	A
50	A	162	A
50	A	166	A
50	A	174	A
50	A	197	A
50	A	199	A
50	A	200	A

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Mol	Chain	Res	Type
50	A	201	A
50	A	202	U
50	A	208	U
50	A	212	A
50	A	213	G
50	A	218	G
50	A	222	A
50	A	223	A
50	A	231	C
50	A	233	C
50	A	248	G
50	A	257	G
50	A	315	G
50	A	316	A
50	A	317	G
50	A	322	C
50	A	324	A
50	A	330	C
50	A	331	C
50	A	332	G
50	A	345	G
50	A	351	U
50	A	352	G
50	A	360	U
50	A	361	A
50	A	362	G
50	A	366	C
50	A	367	U
50	A	369	A
50	A	390	A
50	A	395	A
50	A	404	A
50	A	409	C
50	A	413	U
50	A	415	A
50	A	423	U
50	A	427	A
50	A	435	G
50	A	441	C
50	A	443	G
50	A	454	A
50	A	455	C

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Mol	Chain	Res	Type
50	A	456	U
50	A	461	A
50	A	472	A
50	A	477	G
50	A	484	A
50	A	488	U
50	A	489	U
50	A	493	A
50	A	496	C
50	A	498	U
50	A	501	U
50	A	502	A
50	A	503	G
50	A	504	G
50	A	510	A
50	A	511	A
50	A	512	G
50	A	513	C
50	A	514	A
50	A	517	C
50	A	520	C
50	A	523	U
50	A	524	U
50	A	525	A
50	A	527	G
50	A	528	A
50	A	530	A
50	A	534	U
50	A	540	C
50	A	546	A
50	A	567	A
50	A	569	A
50	A	571	A
50	A	573	A
50	A	574	U
50	A	575	A
50	A	589	C
50	A	590	A
50	A	592	C
50	A	593	C
50	A	594	A
50	A	613	C

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Mol	Chain	Res	Type
50	A	614	C
50	A	615	U
50	A	627	A
50	A	629	U
50	A	630	G
50	A	652	C
50	A	662	C
50	A	675	G
50	A	701	U
50	A	704	A
50	A	711	A
50	A	717	U
50	A	718	A
50	A	720	A
50	A	723	C
50	A	726	C
50	A	731	A
50	A	734	U
50	A	735	C
50	A	736	A
50	A	737	U
50	A	745	C
50	A	746	U
50	A	756	C
50	A	761	C
50	A	765	G
50	A	771	C
50	A	773	C
50	A	774	A
50	A	776	A
50	A	779	G
50	A	788	A
50	A	798	A
50	A	838	C
50	A	841	C
50	A	842	A
50	A	850	C
50	A	851	A
50	A	852	U
50	A	853	C
50	A	854	A
50	A	857	A

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Mol	Chain	Res	Type
50	A	866	G
50	A	985	G
50	A	986	U
50	A	990	U
50	A	1013	C
50	A	1014	C
50	A	1016	G
50	A	1036	A
50	A	1037	A
50	A	1038	C
50	A	1039	A
50	A	1055	A
50	A	1061	U
50	A	1062	G
50	A	1070	A
50	A	1080	U
50	A	1134	A
50	A	1140	G
50	A	1144	G
50	A	1161	G
50	A	1162	A
50	A	1163	A
50	A	1174	G
50	A	1177	C
50	A	1181	A
50	A	1182	C
50	A	1183	A
50	A	1184	U
50	A	1189	A
50	A	1191	A
50	A	1194	U
50	A	1195	C
50	A	1200	G
50	A	1201	U
50	A	1209	A
50	A	1222	A
50	A	1223	A
50	A	1225	U
50	A	1231	A
50	A	1236	C
50	A	1240	A
50	A	1242	C

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Mol	Chain	Res	Type
50	A	1243	A
50	A	1245	C
50	A	1246	G
50	A	1247	G
50	A	1249	A
50	A	1252	A
50	A	1253	G
50	A	1256	A
50	A	1258	C
50	A	1262	G
50	A	1438	U
50	A	1439	U
50	A	1444	U
50	A	1452	U
50	A	1453	G
50	A	1459	A
50	A	1464	C
50	A	1469	G
50	A	1471	A
50	A	1477	G
50	A	1485	C
50	A	1487	C
50	A	1488	A
50	A	1490	A
50	A	1492	C
50	A	1498	C
50	A	1507	A
50	A	1510	A
50	A	1514	C
50	A	1519	C
50	A	1520	A
50	A	1532	U
50	A	1537	A
50	A	1547	A
50	A	1548	A
50	A	1550	A
50	A	1558	U
51	B	1607	U
51	B	1608	G
51	B	1609	U
51	B	1611	G
51	B	1614	U

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Mol	Chain	Res	Type
51	B	1615	A
51	B	1625	A
51	B	1628	C
51	B	1631	C
51	B	1640	A
51	B	1641	G
51	B	1644	G
51	B	1645	A
51	B	1649	C
51	B	1651	A

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	A	43	A
50	A	135	A
50	A	153	A
50	A	360	U
50	A	502	A
50	A	516	C
50	A	573	A
50	A	787	A
50	A	837	A
50	A	1235	A
50	A	1531	A
51	B	1607	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 51 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

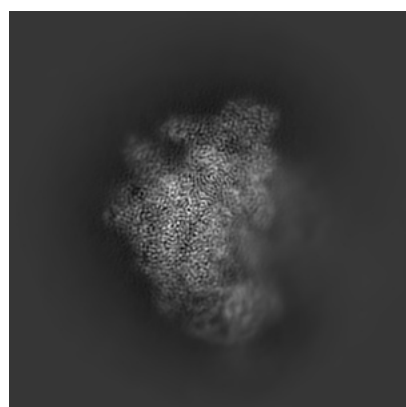
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12924. These allow visual inspection of the internal detail of the map and identification of artifacts.

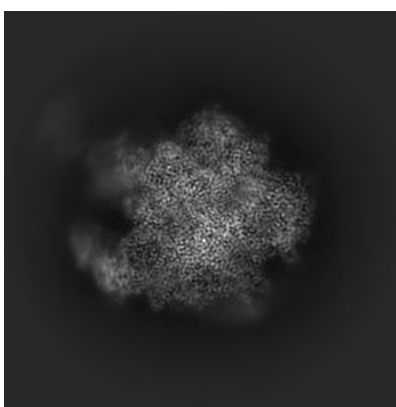
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

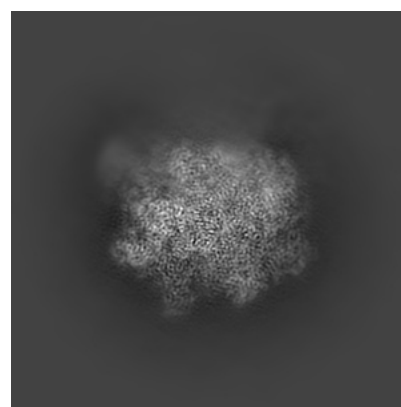
6.1.1 Primary map



X



Y

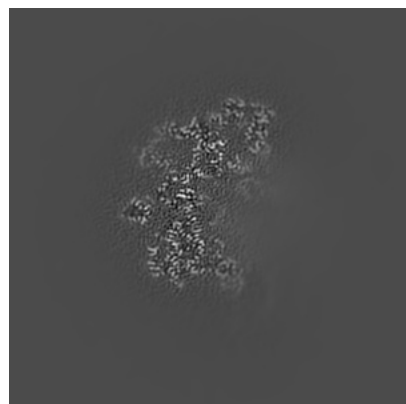


Z

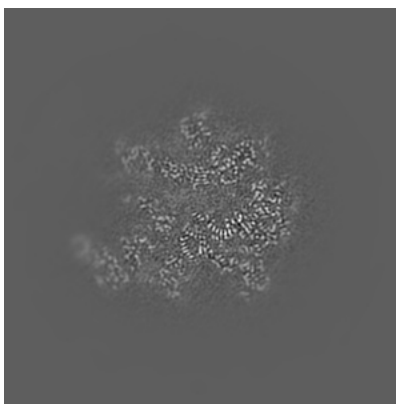
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

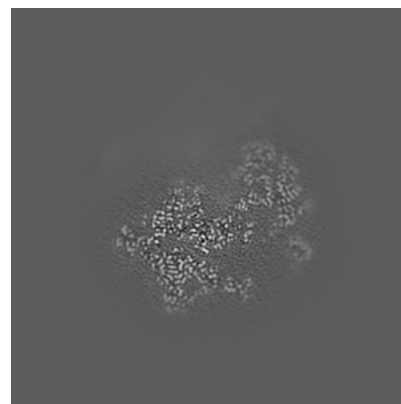
6.2.1 Primary map



X Index: 180



Y Index: 180

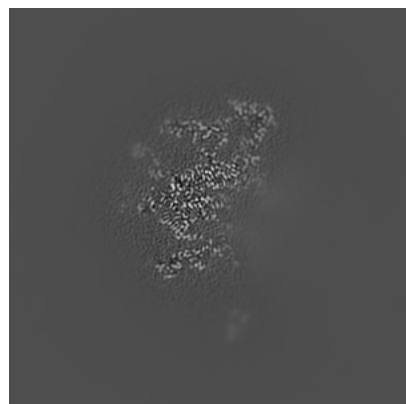


Z Index: 180

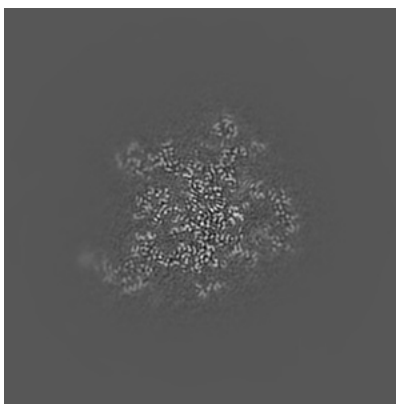
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

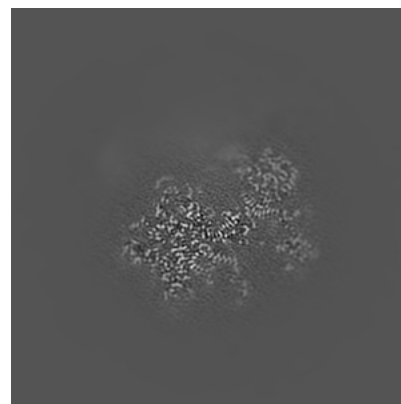
6.3.1 Primary map



X Index: 168



Y Index: 161

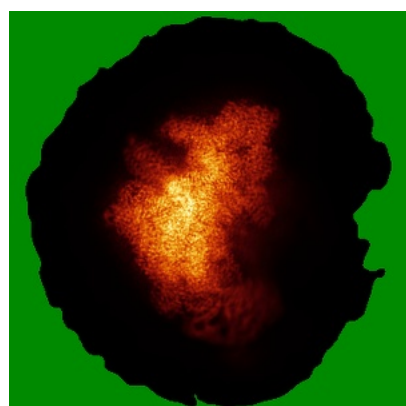


Z Index: 188

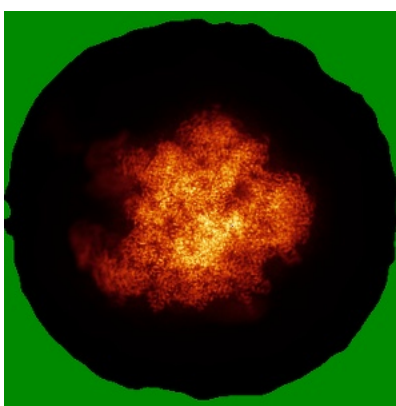
The images above show the largest variance slices of the map in three orthogonal directions.

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

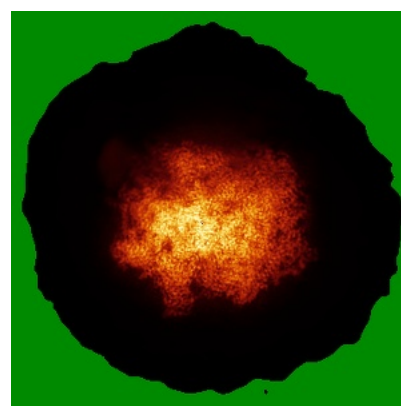
6.4.1 Primary map



X



Y

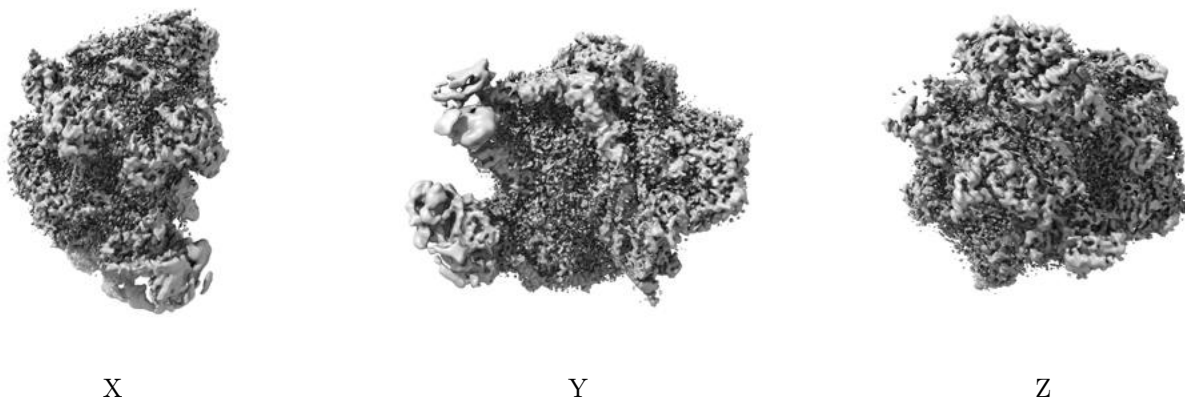


Z

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

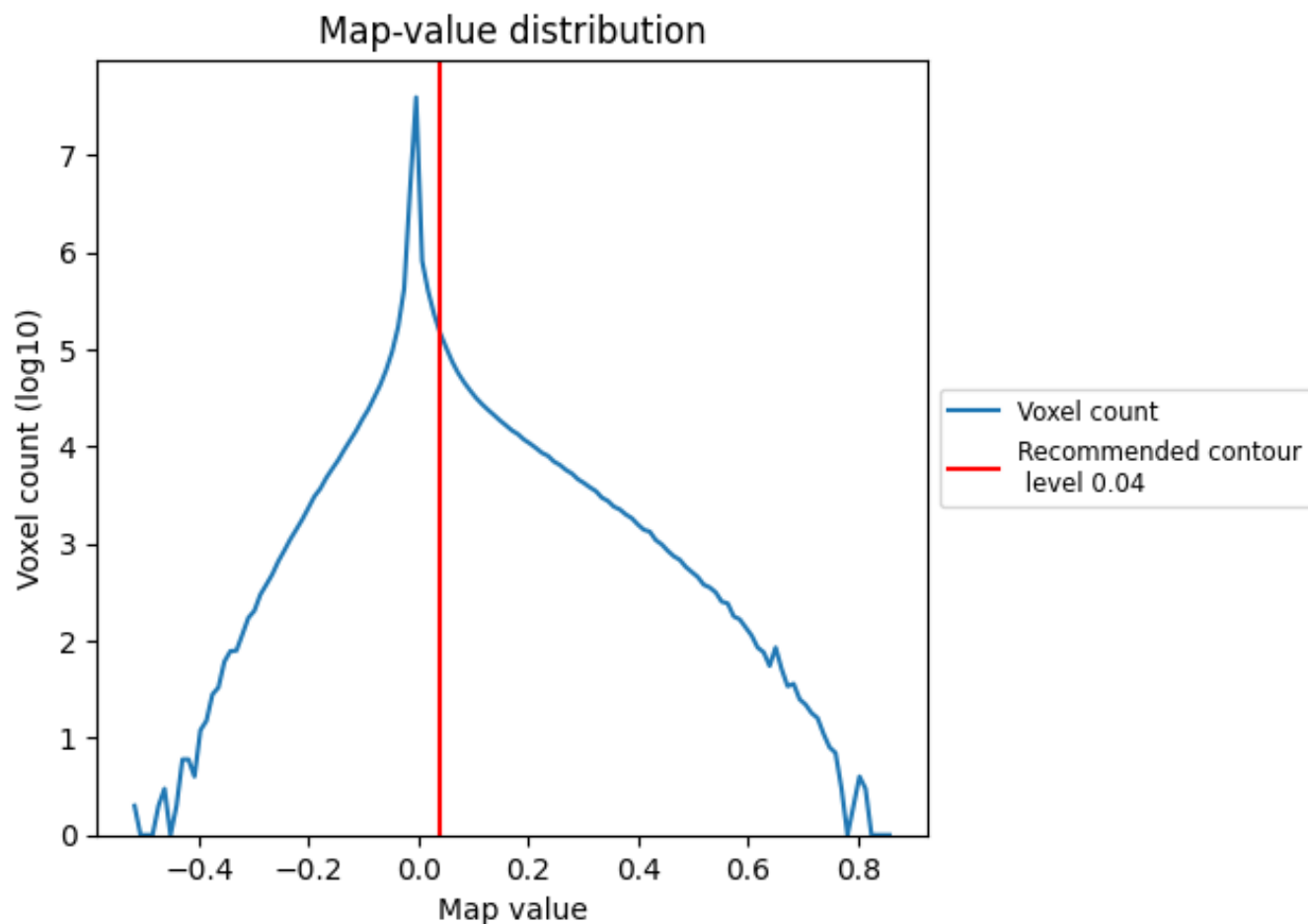
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

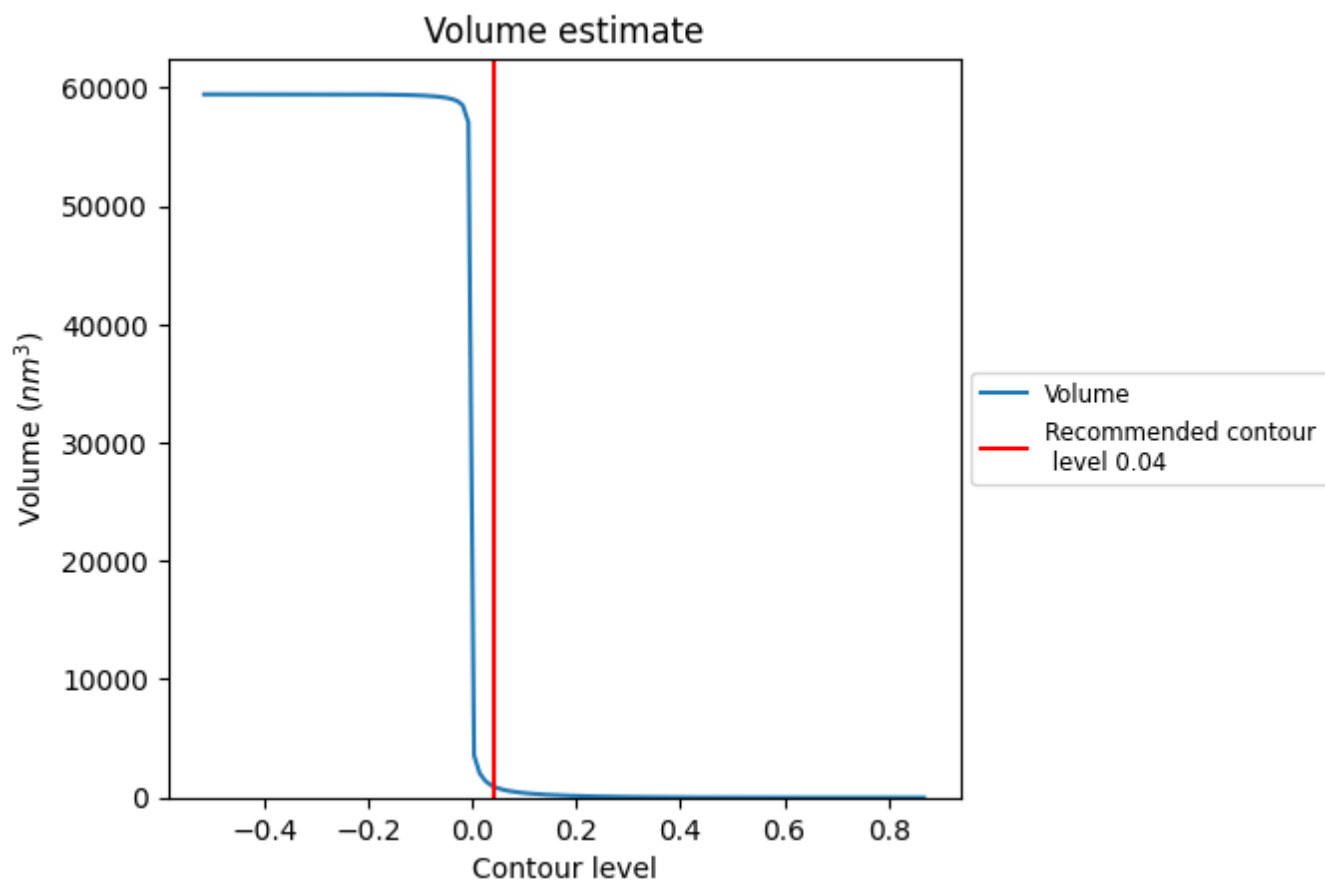
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

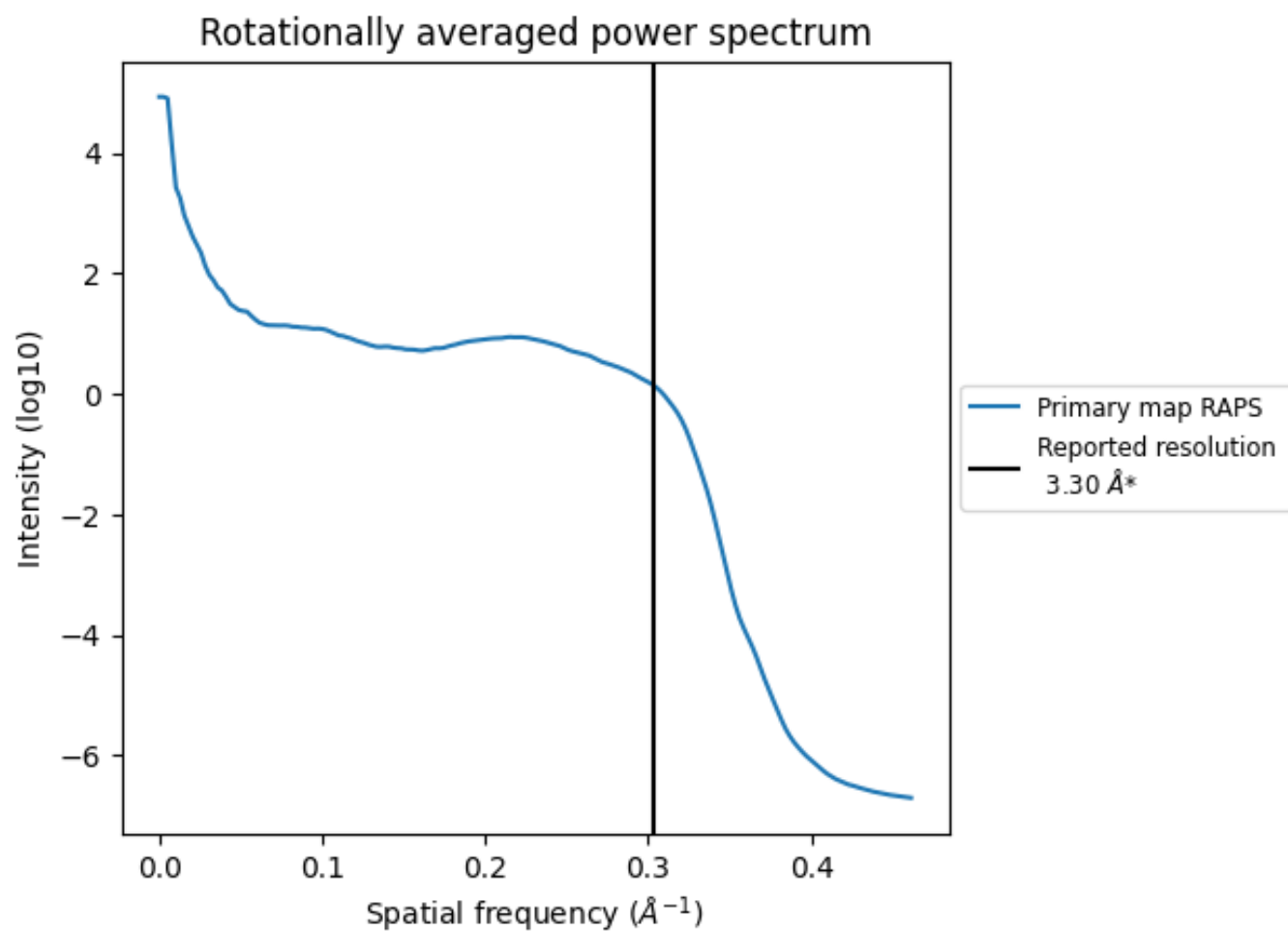
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 956 nm^3 ; this corresponds to an approximate mass of 863 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 [i](#)

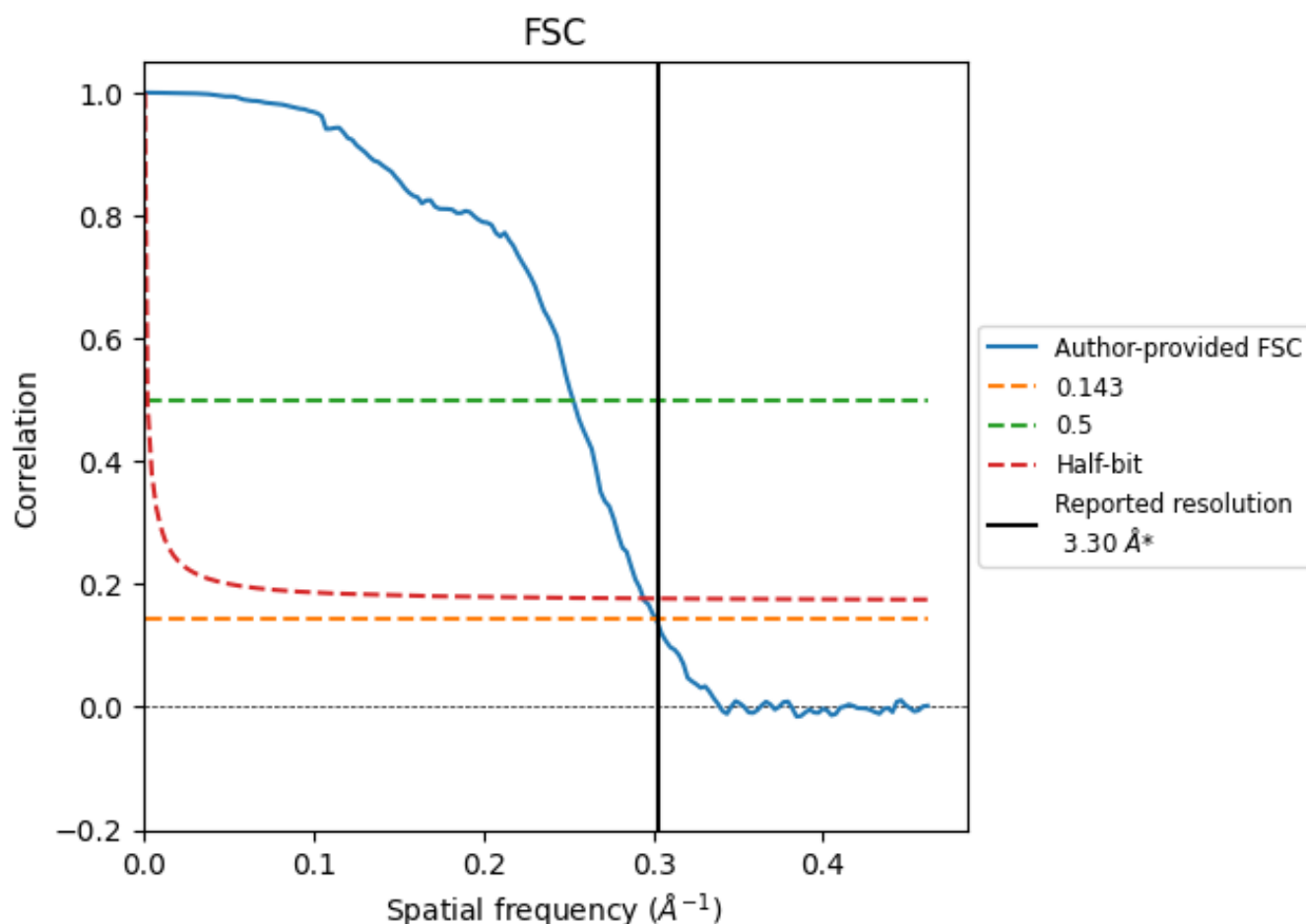


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

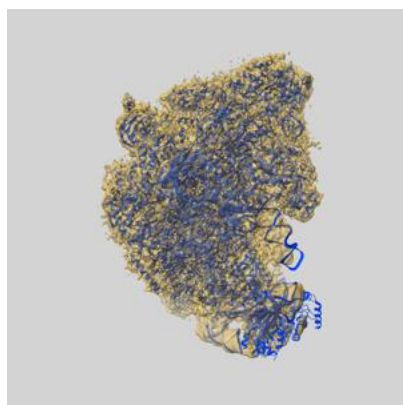
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.95	3.40
Unmasked-calculated*	-	-	-

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

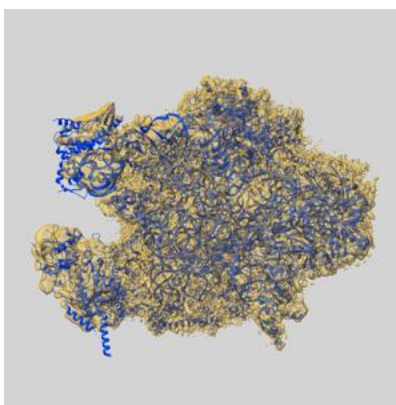
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12924 and PDB model 7OIB. Per-residue inclusion information can be found in section [3](#) on page [13](#).

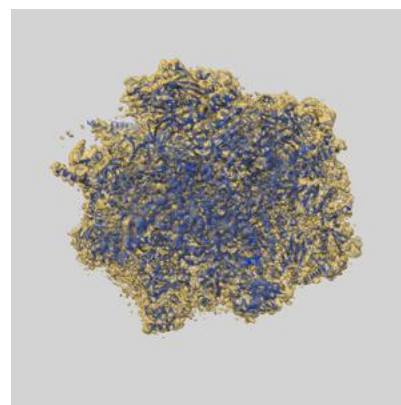
9.1 Map-model overlay [i](#)



X



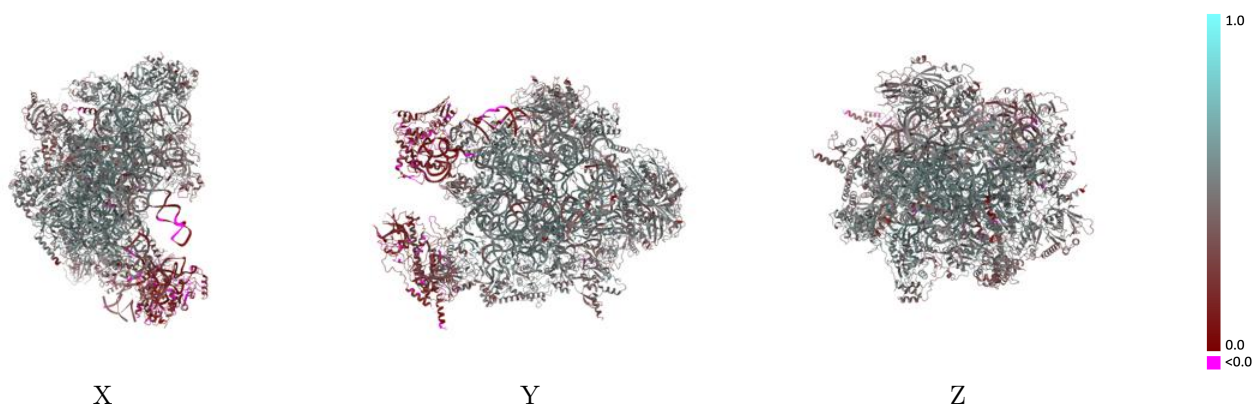
Y



Z

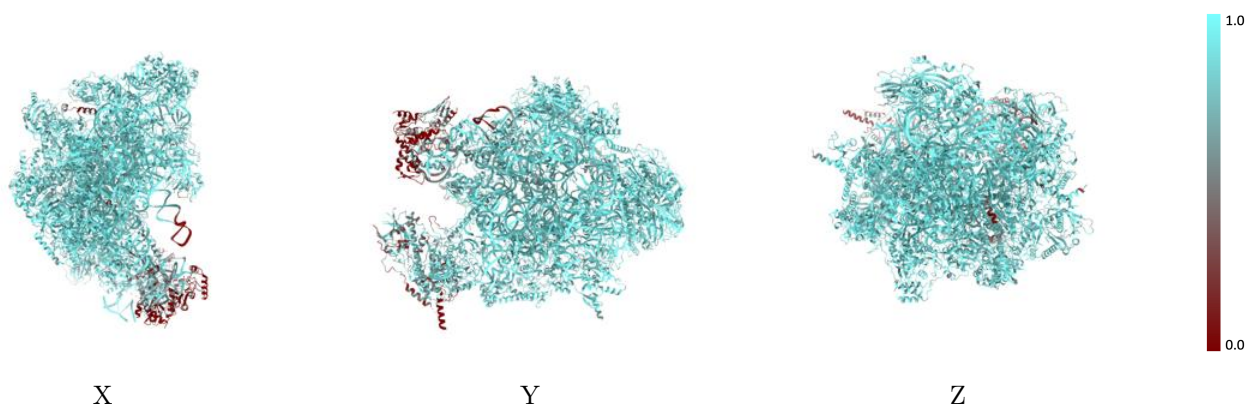
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



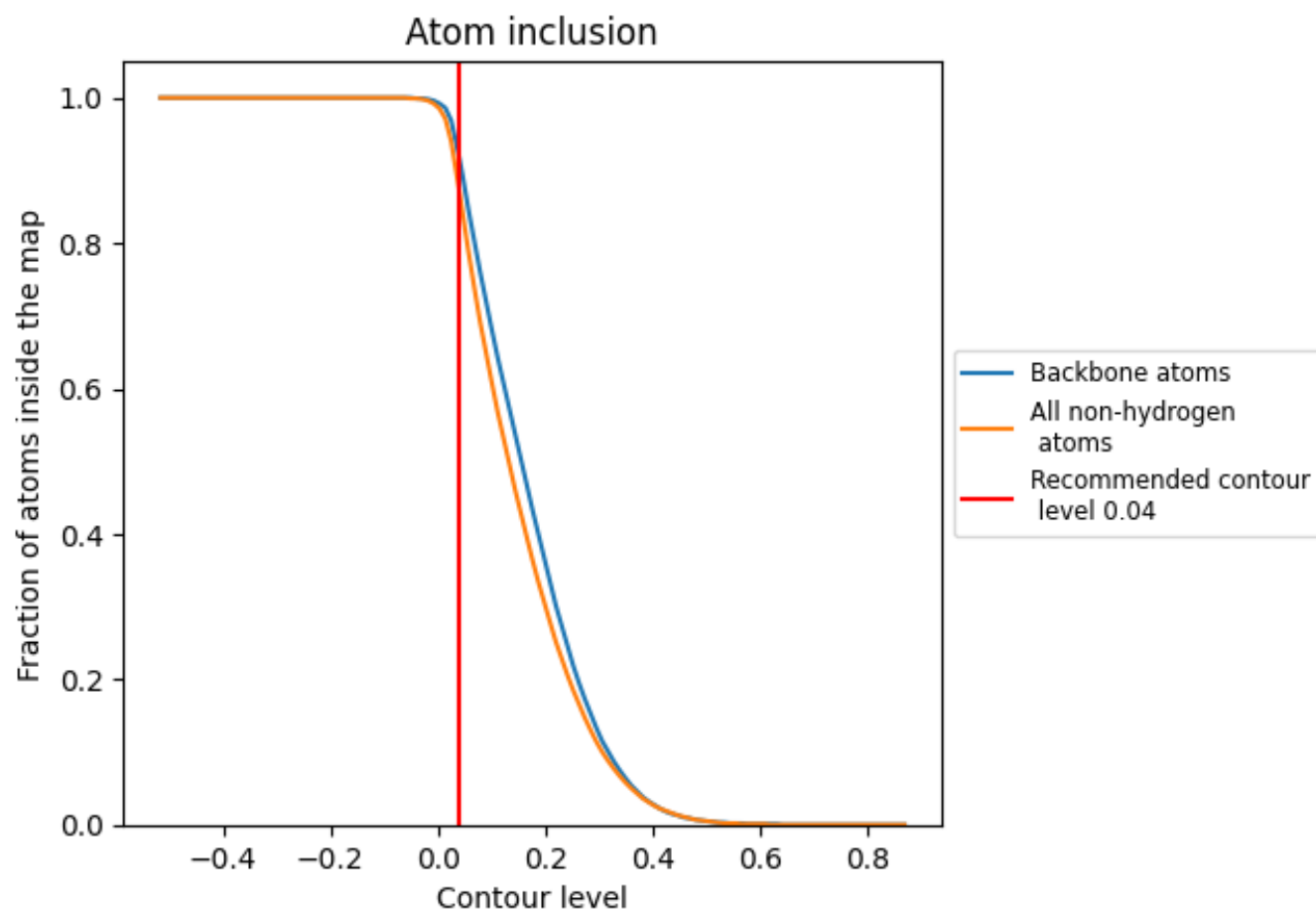
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8700	 0.4500
0	 0.9060	 0.4960
1	 0.8860	 0.4690
2	 0.9640	 0.5750
3	 0.9510	 0.5650
5	 0.8990	 0.4600
6	 0.8870	 0.4200
7	 0.8610	 0.4280
8	 0.5830	 0.2110
9	 0.9050	 0.4800
A	 0.9340	 0.4780
B	 0.9070	 0.2730
D	 0.8490	 0.4420
E	 0.8820	 0.4550
F	 0.9440	 0.5370
H	 0.8810	 0.4500
I	 0.3370	 0.2120
J	 0.0570	 0.0890
K	 0.9220	 0.5090
L	 0.8180	 0.3630
M	 0.9350	 0.5250
N	 0.8570	 0.4340
O	 0.9090	 0.4990
P	 0.8940	 0.4510
Q	 0.8680	 0.4270
R	 0.9100	 0.5260
S	 0.9120	 0.5020
T	 0.9350	 0.5280
U	 0.8880	 0.4820
V	 0.8560	 0.4430
W	 0.9260	 0.5240
X	 0.9130	 0.4910
Y	 0.9160	 0.5060
Z	 0.9170	 0.5100
a	 0.8950	 0.4910



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Chain	Atom inclusion	Q-score
b	 0.9320	 0.5220
c	 0.9090	 0.4820
d	 0.7710	 0.3760
e	 0.4860	 0.1660
f	 0.6480	 0.2690
g	 0.9350	 0.5140
h	 0.8810	 0.4330
i	 0.9470	 0.5560
j	 0.8820	 0.4740
k	 0.5120	 0.1950
l	 0.6750	 0.1940
m	 0.5890	 0.2120
o	 0.9240	 0.5260
p	 0.8860	 0.4550
q	 0.8870	 0.4420
r	 0.8710	 0.4140
s	 0.9100	 0.4970