



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 09:26 PM UTC

PDB ID : 8QU5 / pdb_00008qu5
EMDB ID : EMD-18461
Title : mt-LSU assembly intermediate in GTPBP8 knock-out cells, state 2
Authors : Valentin Gese, G.; Cipullo, M.; Rorbach, J.; Hallberg, B.M.
Deposited on : 2023-10-13
Resolution : 2.42 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

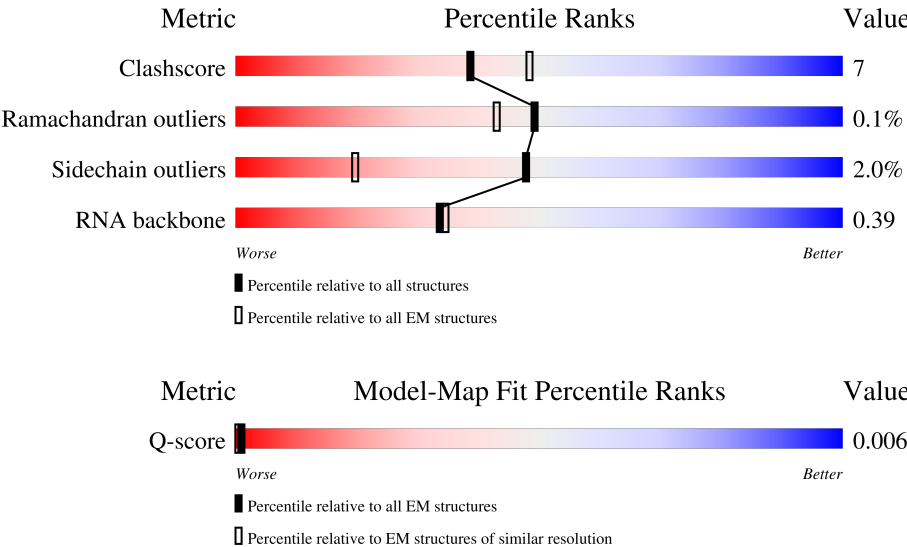
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.42 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	5729 (1.92 - 2.92)

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	0	188	47% 48% 10% 43%
2	1	65	66% 63% 17% 20%
3	2	92	29% 33% 12% 53%

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Mol	Chain	Length	Quality of chain
4	3	188	
5	7	338	
6	8	206	
7	F	311	
8	H	267	
9	J	192	
10	K	178	
11	L	145	
12	M	296	
13	N	251	
14	O	175	
15	P	180	
16	Q	292	
17	R	149	
18	S	205	
19	W	148	
20	X	256	
21	Y	250	
22	Z	161	
23	b	215	
24	g	166	
25	i	128	
26	j	123	
27	l	138	
28	m	128	

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Mol	Chain	Length	Quality of chain
29	o	102	
30	q	222	
31	t	28	
32	u	234	
33	v	70	
34	w	156	
35	5	423	
36	6	380	
37	9	137	
38	A	1559	
39	B	69	
40	D	305	
41	E	348	
42	I	261	
43	T	206	
44	U	153	
45	V	216	
46	a	142	
47	c	332	
48	d	306	
49	e	279	
50	f	212	
51	h	158	
52	k	112	
53	p	206	

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Mol	Chain	Length	Quality of chain
54	r	196	63%
			60%15%26%
55	s	439	70%
			67%17%16%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 89817 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 L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 2 is a protein called 39S ribosomal protein L33, mitochondrial.

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

- Molecule 3 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	43	Total	C	N	O	S	0	0
			351	218	76	56	1		

- Molecule 4 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 5 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	287	Total	C	N	O	S	0	0
			2334	1495	397	425	17		

- Molecule 6 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 7 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 8 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	95	Total	C	N	O	S	0	0
			784	498	152	134			

- Molecule 9 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 10 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 11 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 12 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 13 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 14 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 17 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 18 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- 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 L43, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 25 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 26 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 28 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 29 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 30 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

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

- Molecule 31 is a protein called Unknown protein or protein extension.

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

- Molecule 32 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

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

- Molecule 33 is a protein called MIEF1 upstream open reading frame protein.

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

- Molecule 34 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	w	79	Total	C	N	O	S	0	0
			638	410	95	128	5		

- Molecule 35 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	5	387	Total	C	N	O	S	0	0
			3156	2039	548	558	11		

- Molecule 36 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	6	324	Total	C	N	O	S	0	0
			2640	1694	470	468	8		

- Molecule 37 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	9	117	Total	C	N	O	S	0	0
			947	614	163	168	2		

- Molecule 38 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A	1049	Total	C	N	O	P	0	0
			22263	9996	4029	7189	1049		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 39 is a RNA chain called mitochondrial tRNA^{Val}.

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

- Molecule 40 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	D	220	Total	C	N	O	S	0	0
			1706	1059	339	299	9		

- Molecule 41 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	E	285	Total	C	N	O	S	0	0
			2258	1457	384	406	11		

- Molecule 42 is a protein called 39S ribosomal protein L10, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	T	159	Total	C	N	O	S	0	0
			1305	835	239	224	7		

- Molecule 44 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 45 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	V	192	Total	C	N	O	S	0	0
			1575	1003	281	283	8		

- Molecule 46 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 47 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 48 is a protein called 39S ribosomal protein L45, mitochondrial.

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

- Molecule 49 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 50 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 51 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 52 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 53 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 54 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 55 is a protein called 39S ribosomal protein S30, mitochondrial.

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

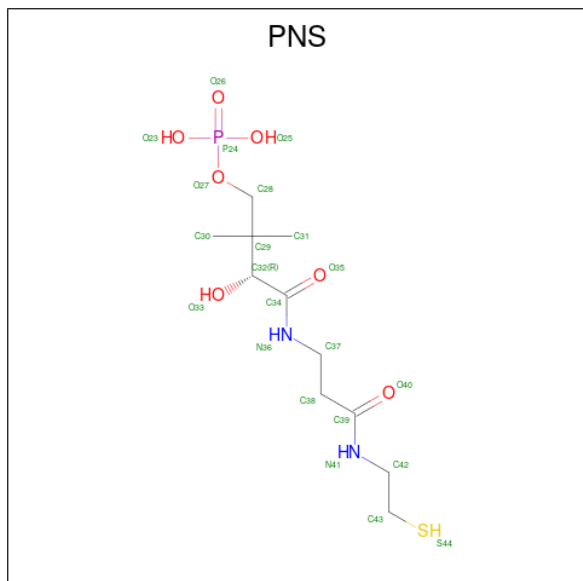
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	0	1	Total	Zn	0
			1	1	
56	r	1	Total	Zn	0
			1	1	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 58 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C₁₁H₂₃N₂O₇PS).

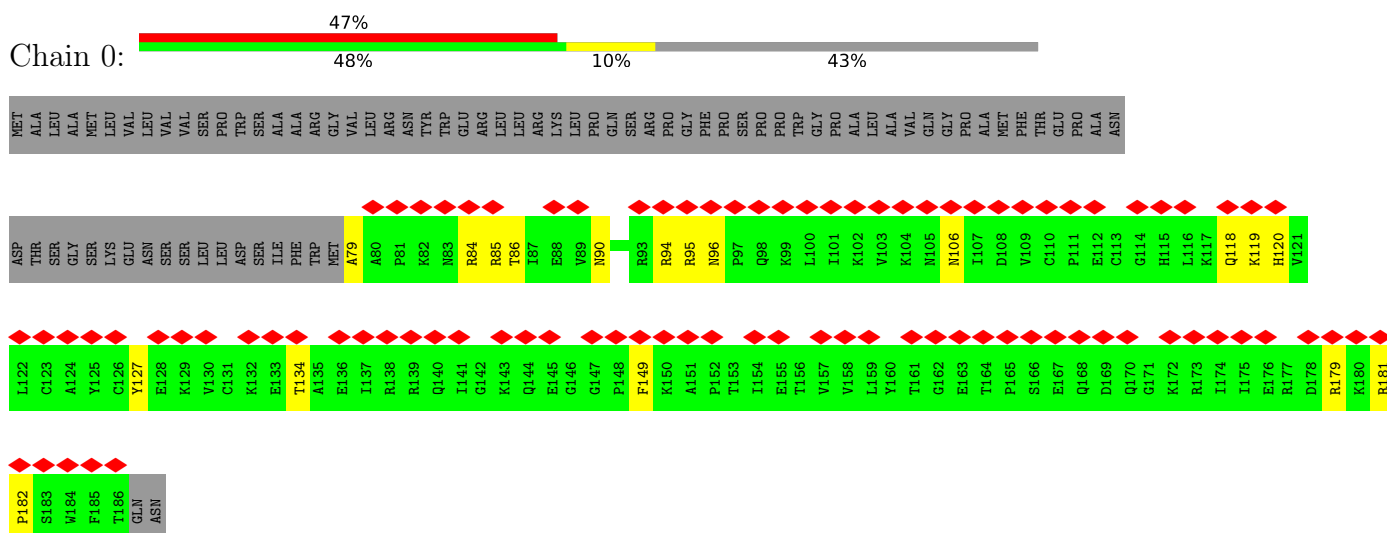


Mol	Chain	Residues	Atoms						AltConf
58	v	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

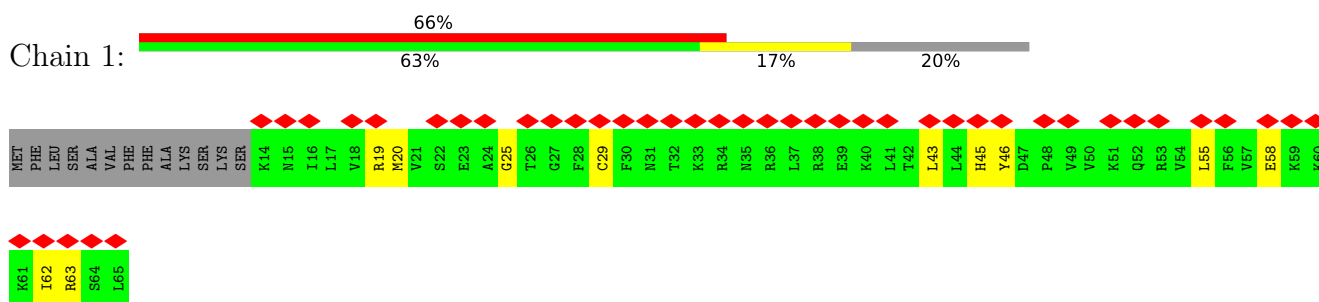
3 Residue-property plots [i](#)

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.

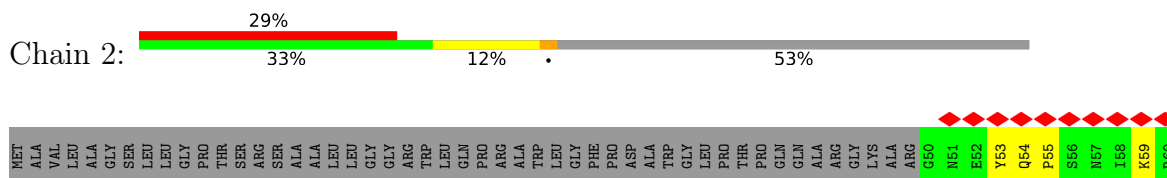
- Molecule 1: 39S ribosomal protein L32, mitochondrial

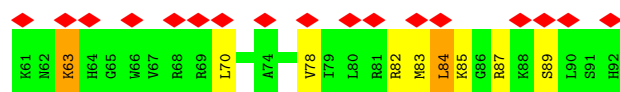


- Molecule 2: 39S ribosomal protein L33, mitochondrial



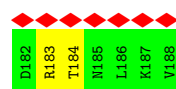
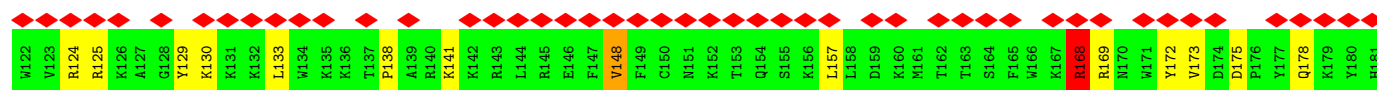
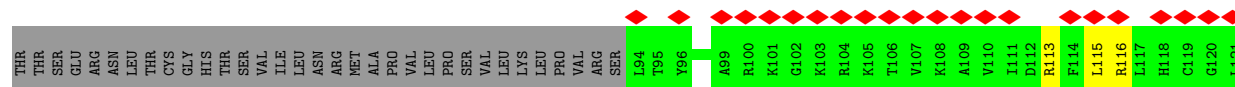
- Molecule 3: 39S ribosomal protein L34, mitochondrial





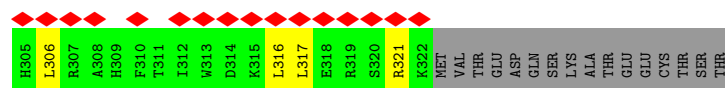
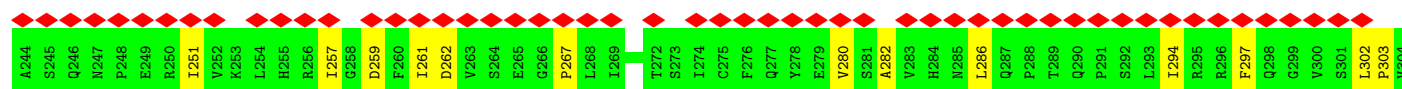
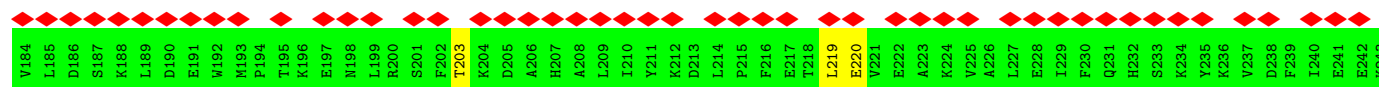
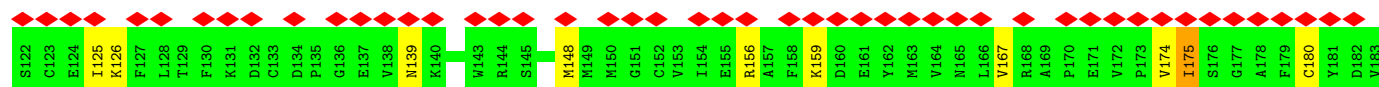
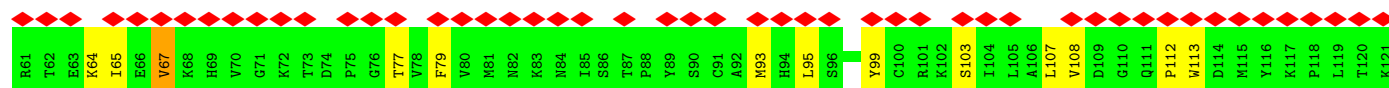
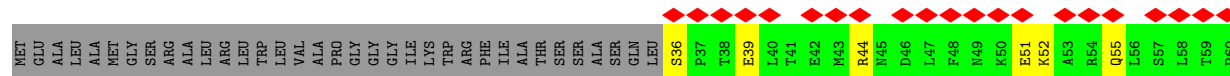
- Molecule 4: 39S ribosomal protein L35, mitochondrial

Chain 3: 41% 40% 10% 49%



- Molecule 5: 39S ribosomal protein L39, mitochondrial

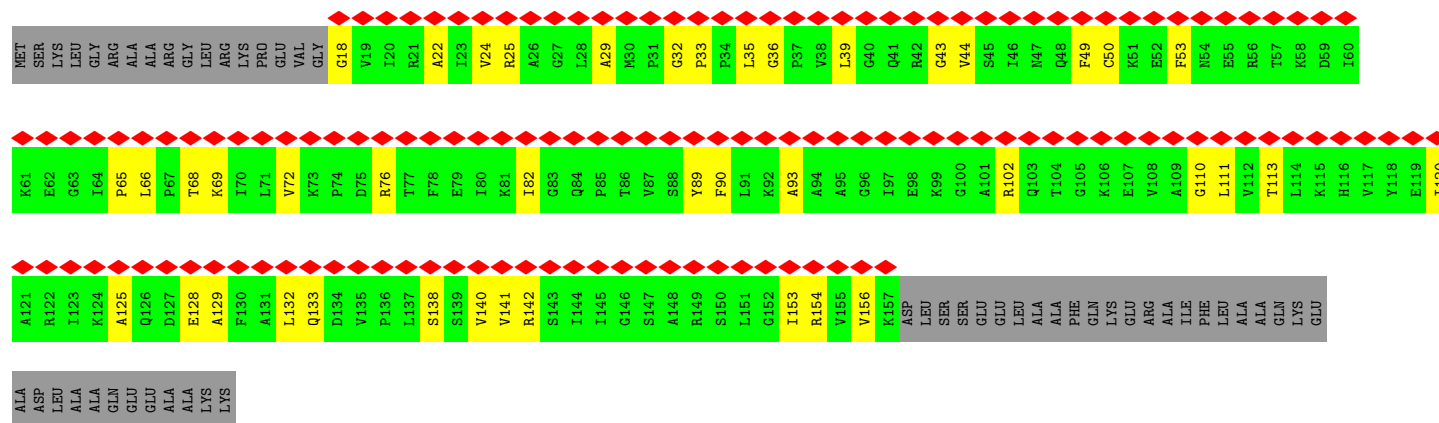
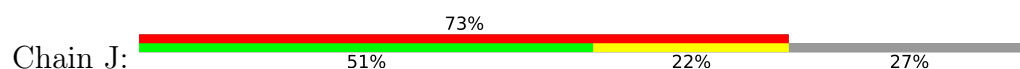
Chain 7: 70% 70% 14% 15%



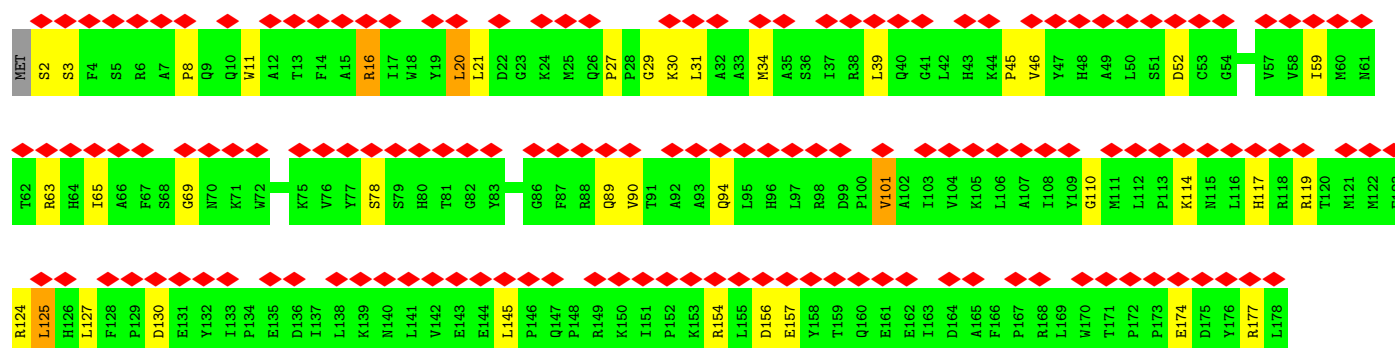
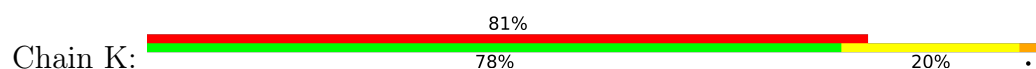
- Molecule 6: 39S ribosomal protein L40, mitochondrial

Chain 8: 47% 39% 9% 52%

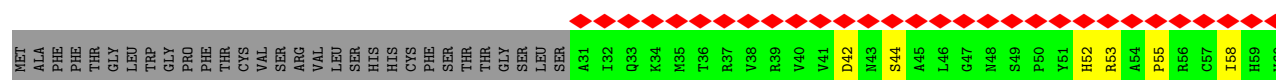
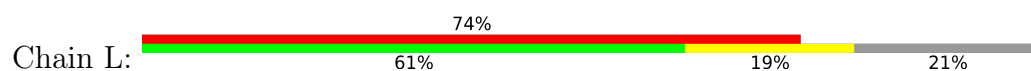
- Molecule 9: 39S ribosomal protein L11, mitochondrial

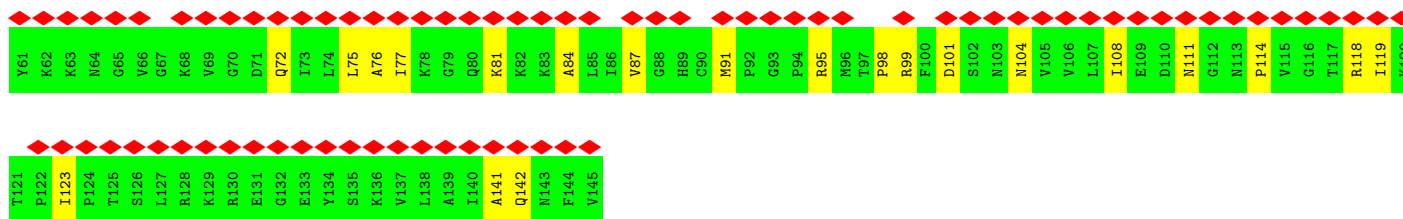


- Molecule 10: 39S ribosomal protein L13, mitochondrial

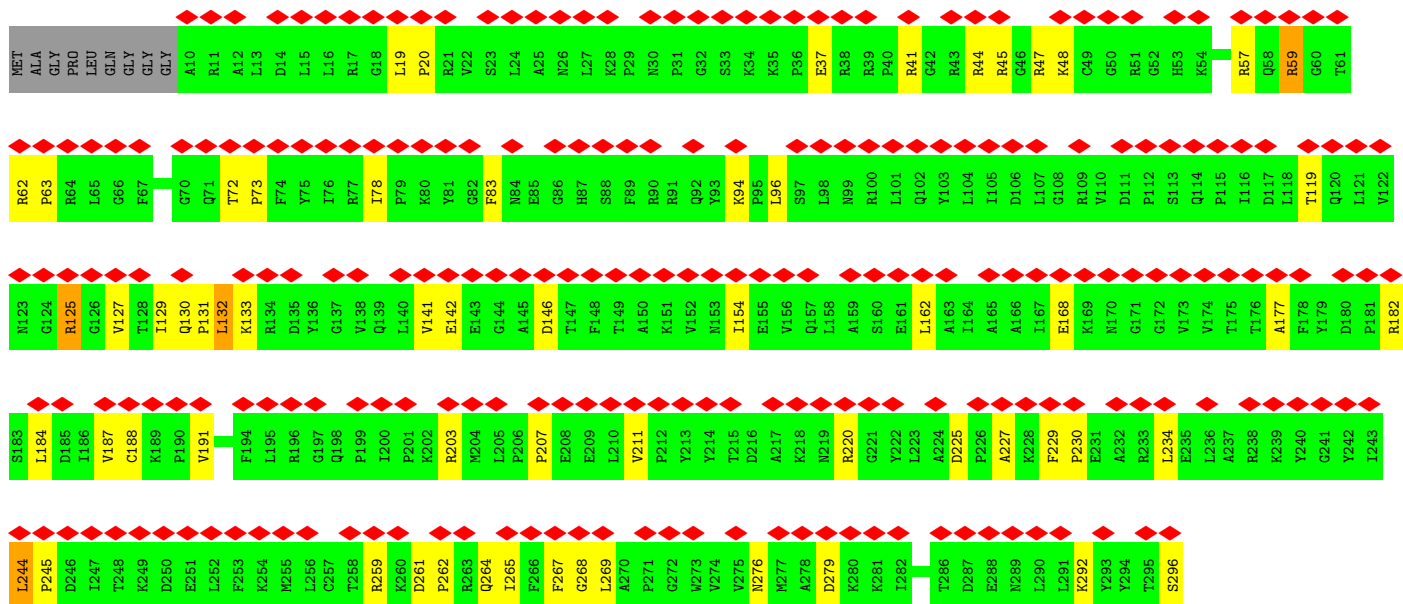
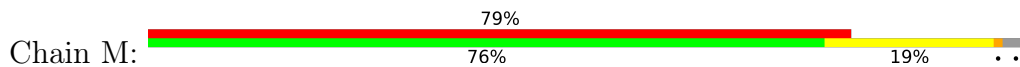


- Molecule 11: 39S ribosomal protein L14, mitochondrial

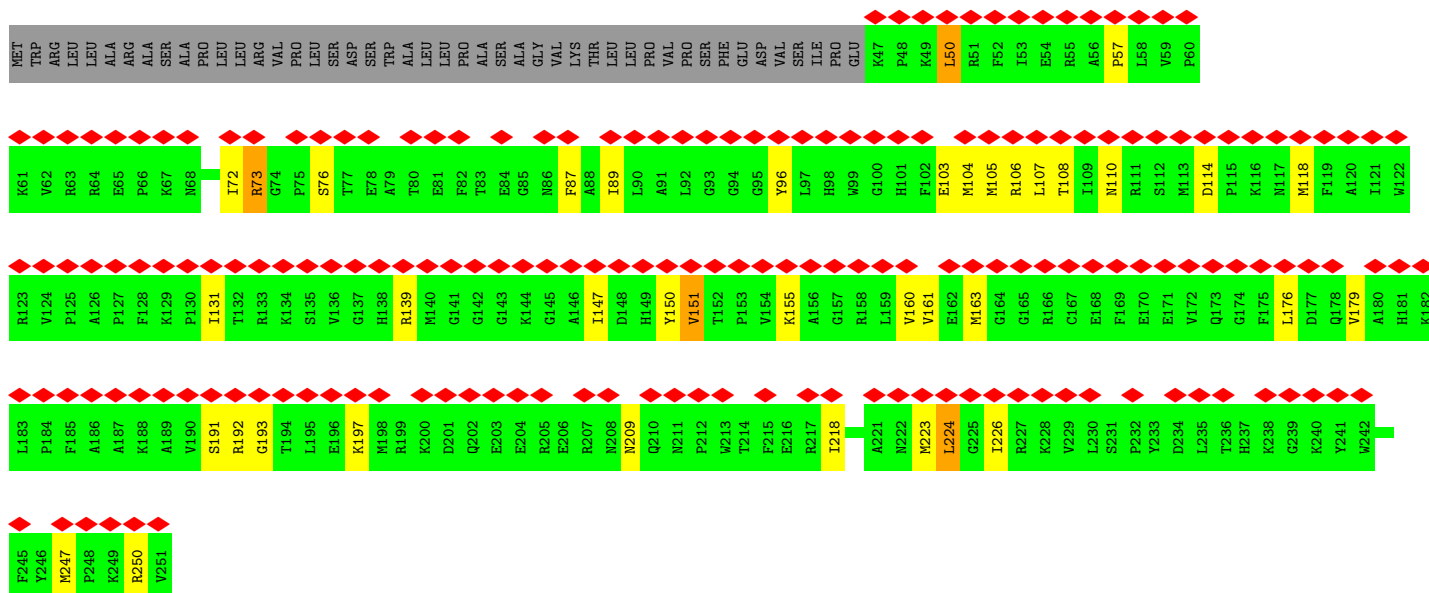




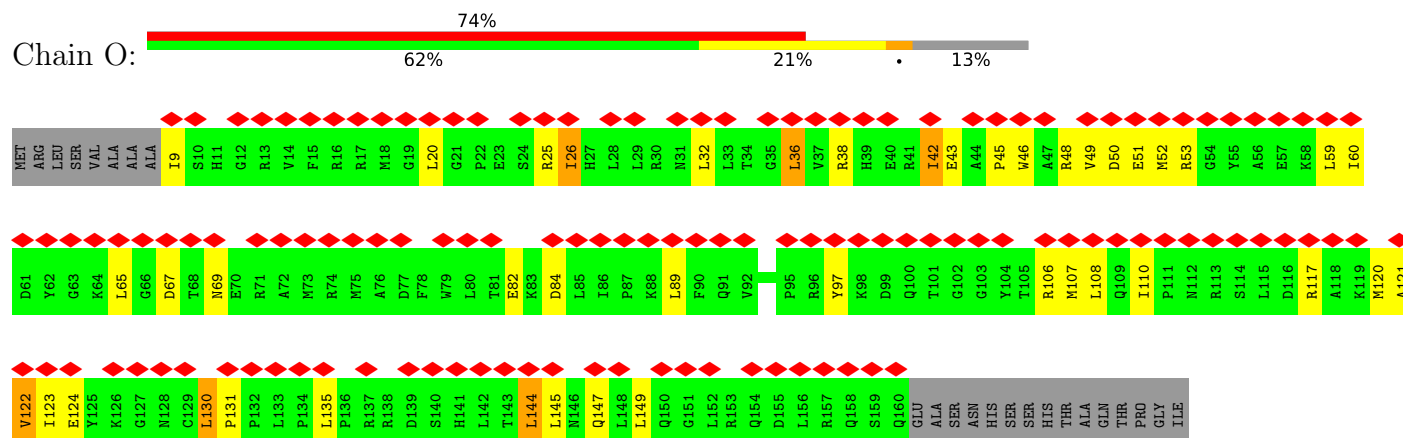
• Molecule 12: 39S ribosomal protein L15, mitochondrial



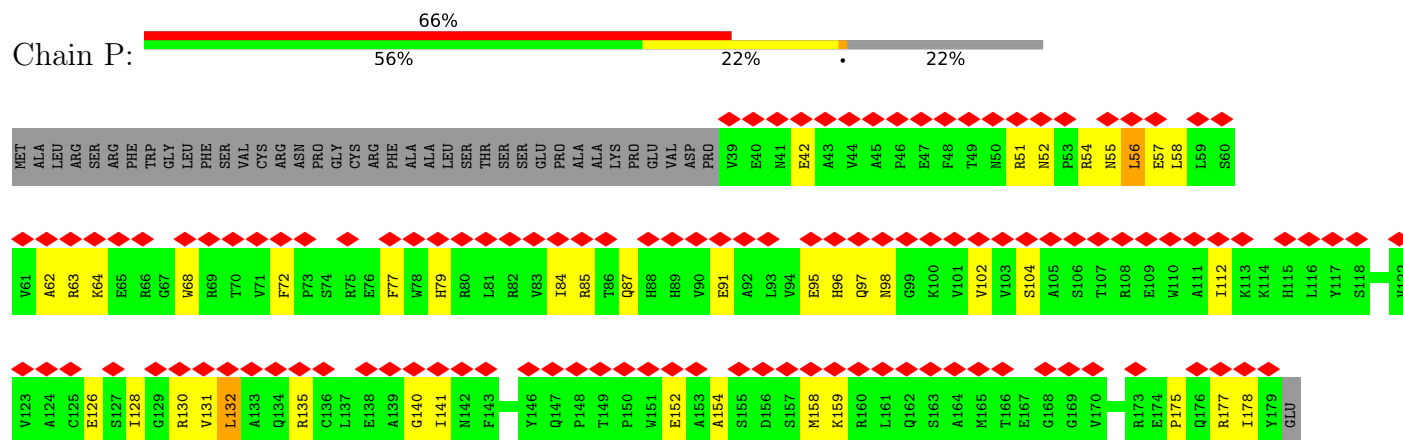
• Molecule 13: 39S ribosomal protein L16, mitochondrial



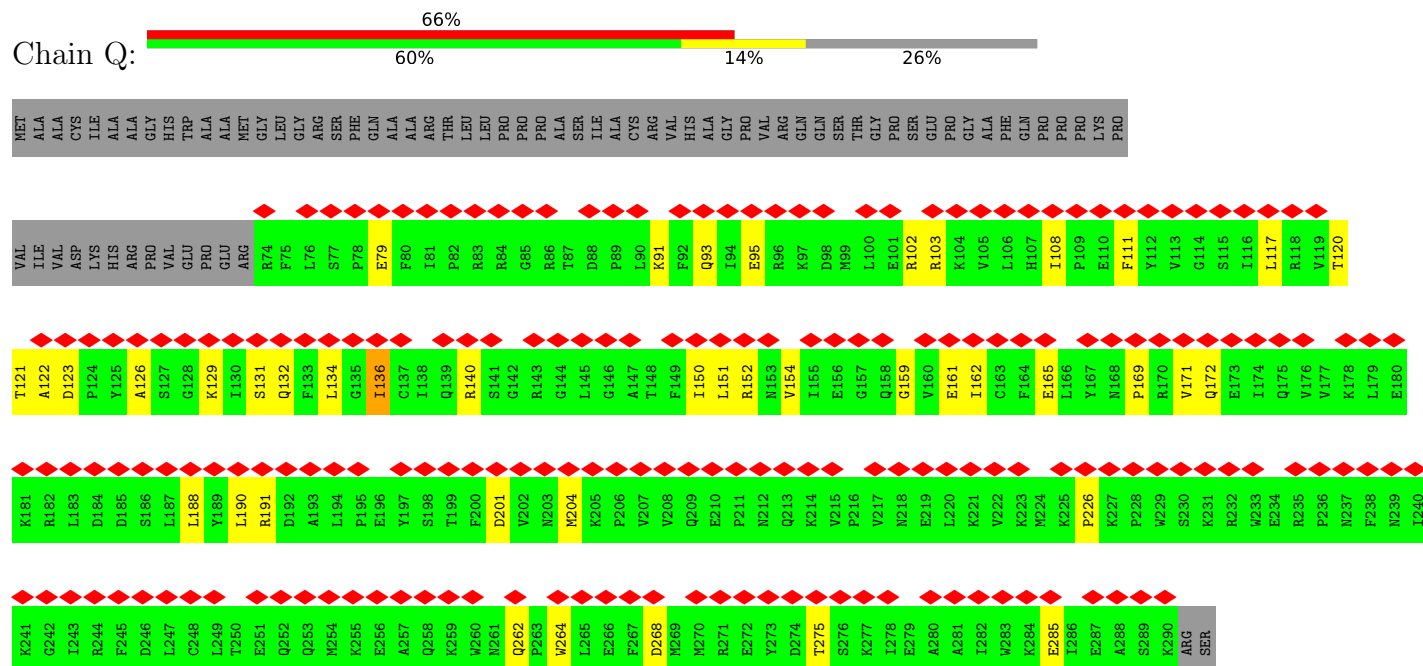
Chain O:



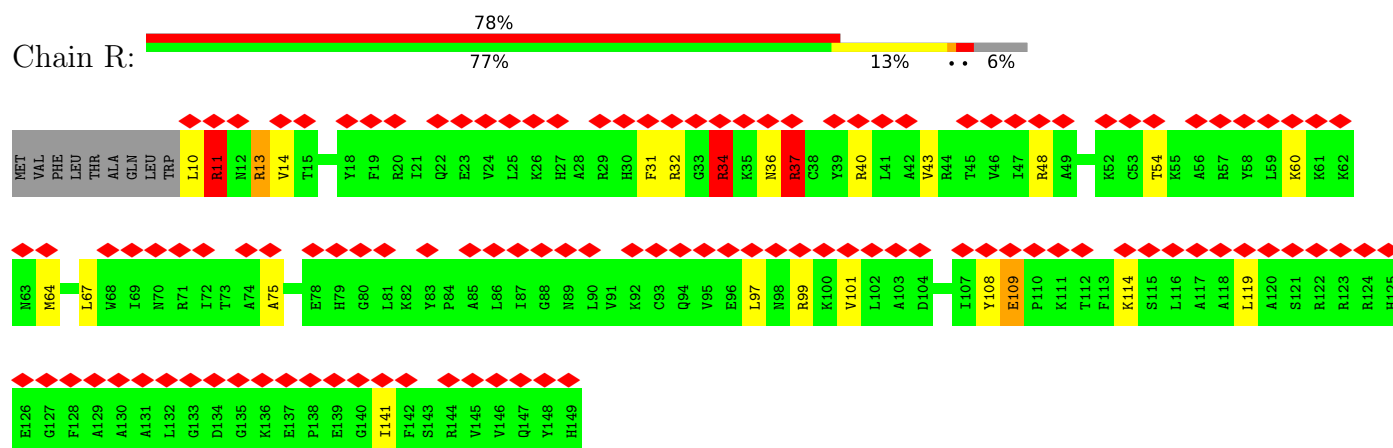
Chain P:



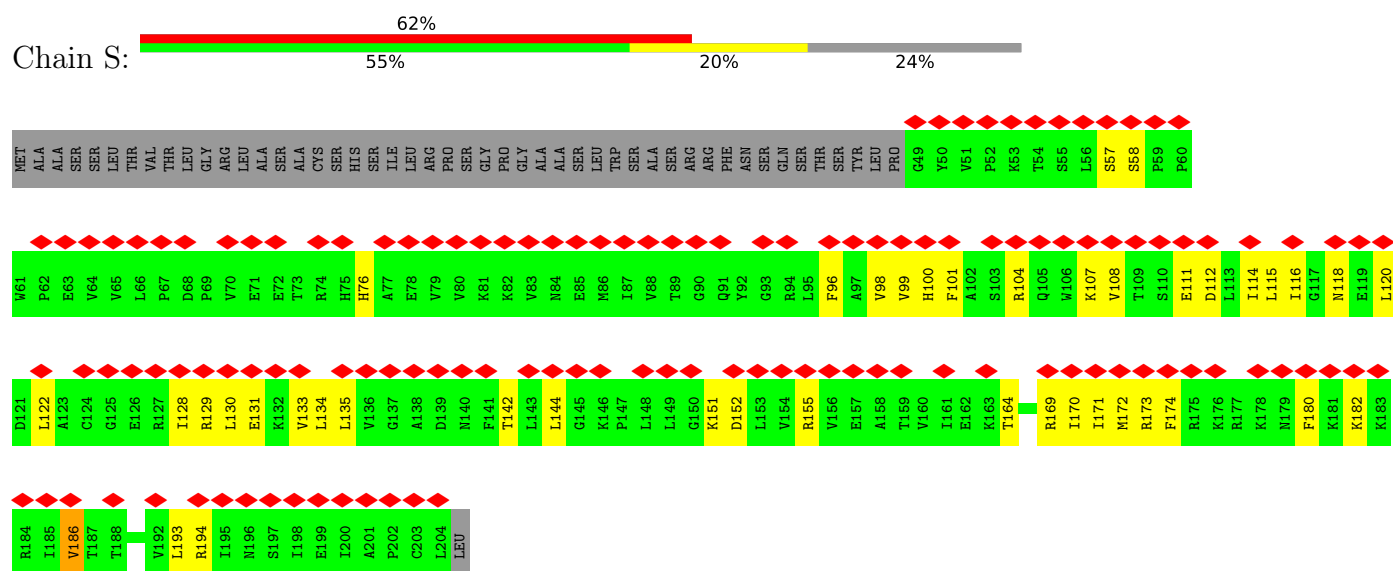
Chain Q:



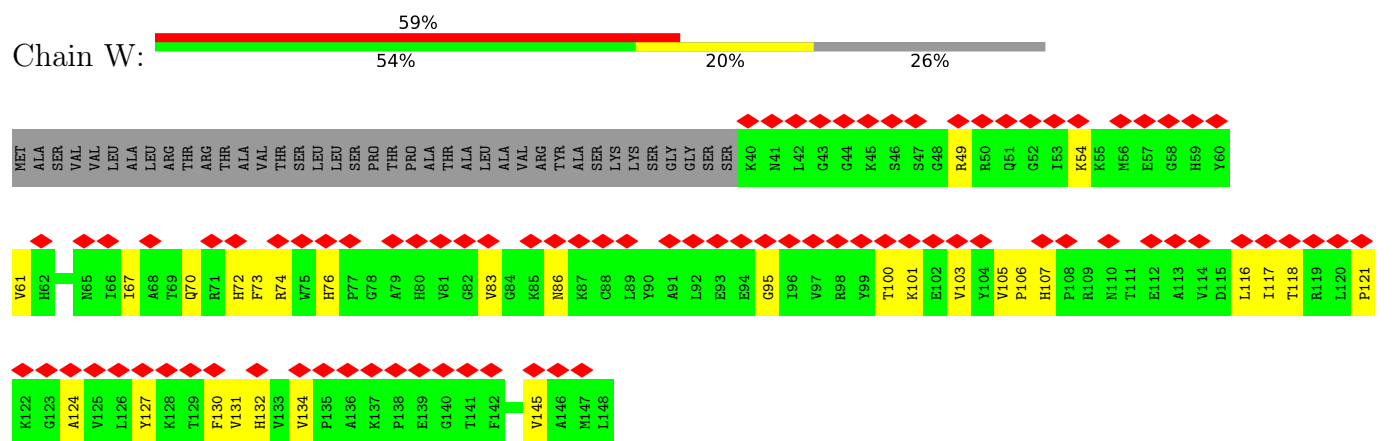
- Molecule 17: 39S ribosomal protein L20, mitochondrial



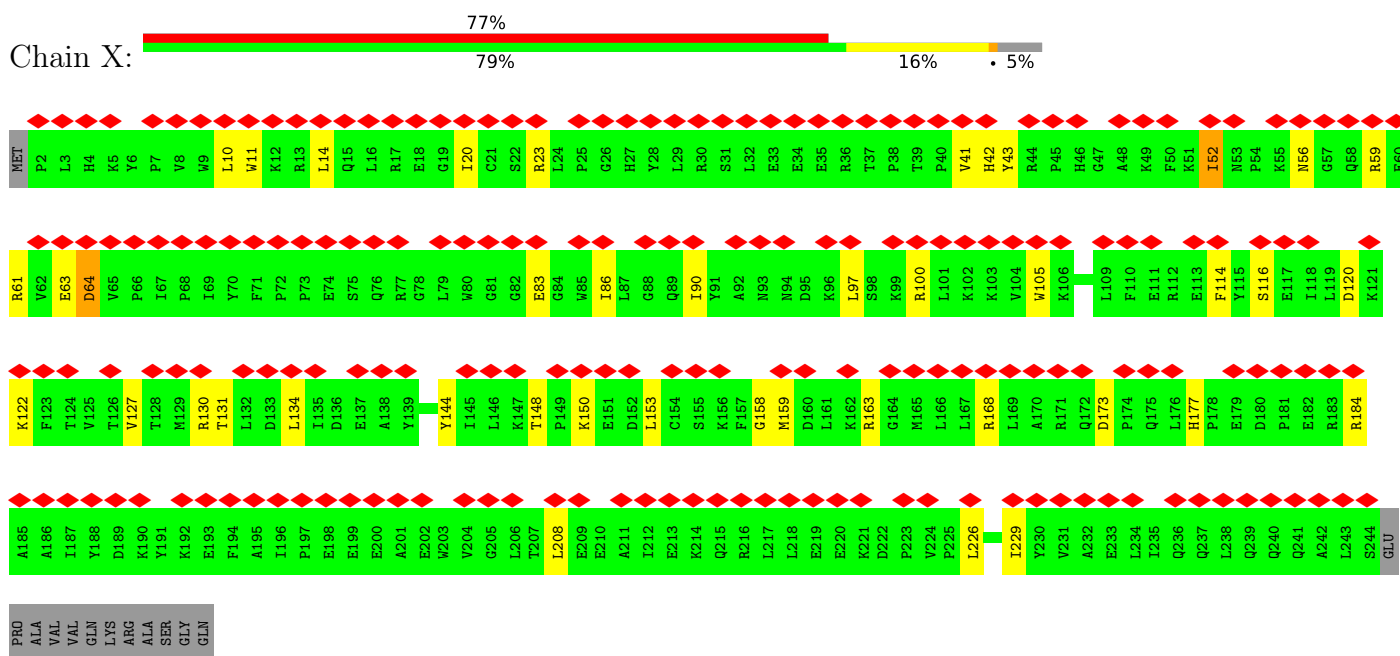
- Molecule 18: 39S ribosomal protein L21, mitochondrial



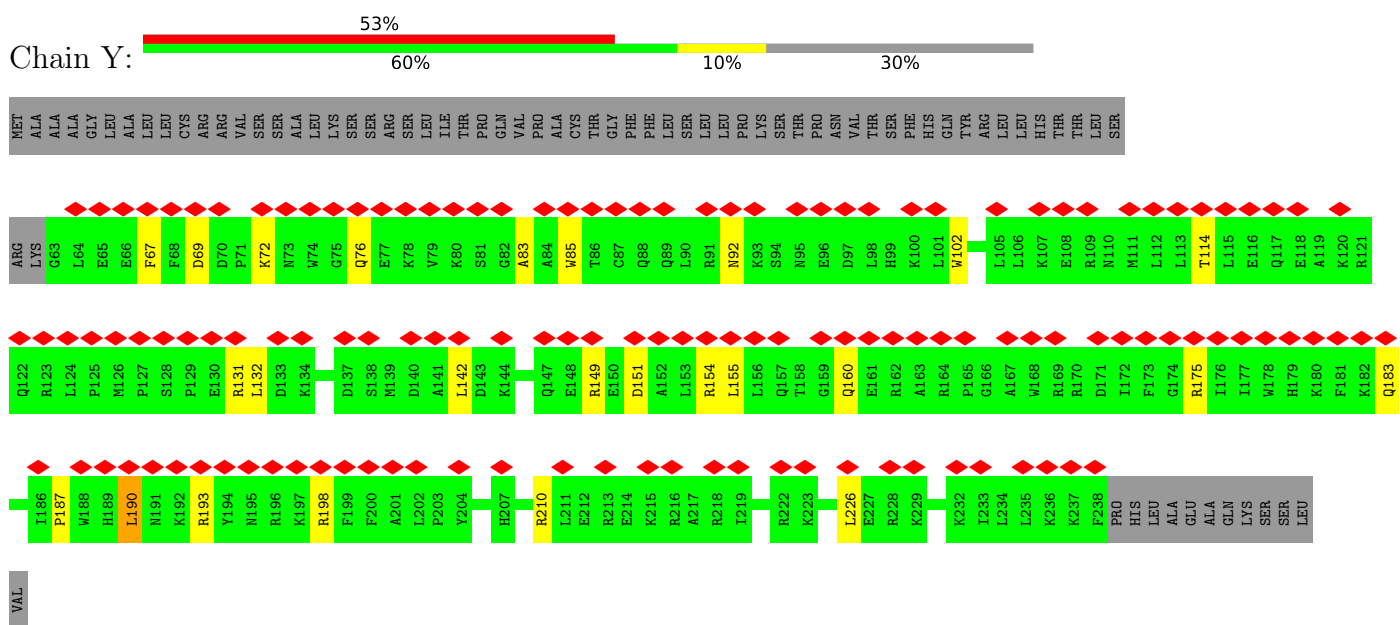
- Molecule 19: 39S ribosomal protein L27, mitochondrial



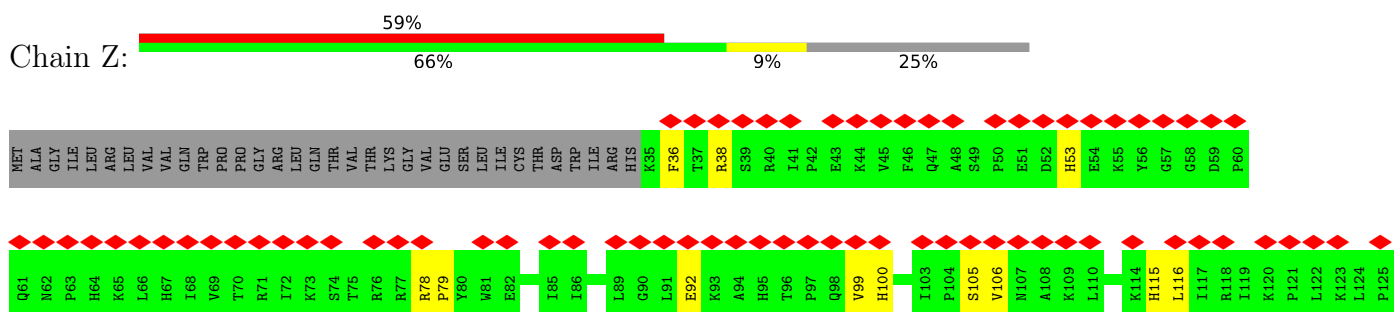
- Molecule 20: 39S ribosomal protein L28, mitochondrial

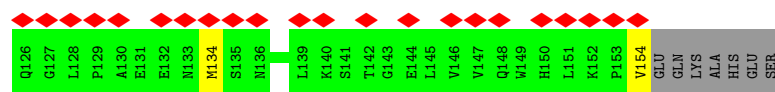


- Molecule 21: 39S ribosomal protein L47, mitochondrial

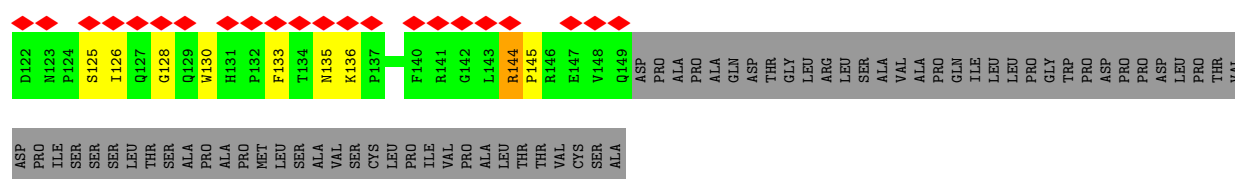
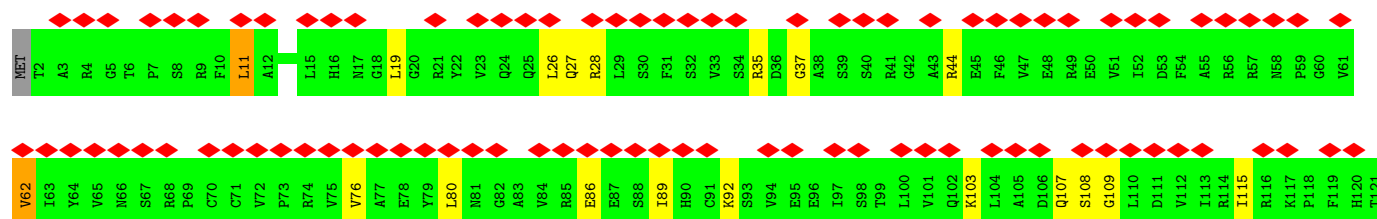


- Molecule 22: 39S ribosomal protein L30, mitochondrial

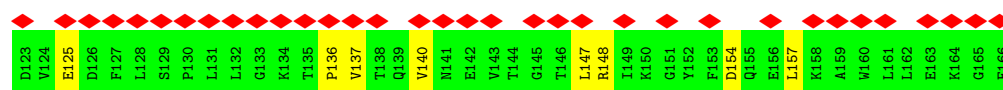
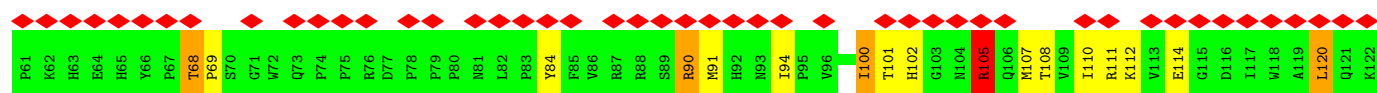
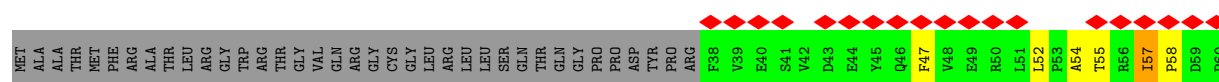




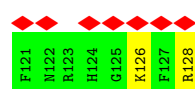
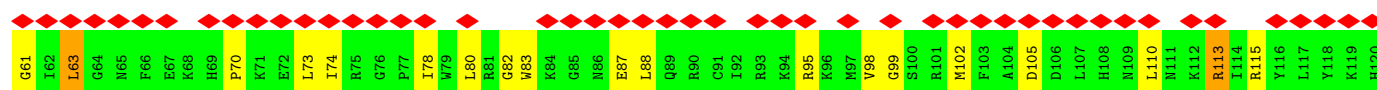
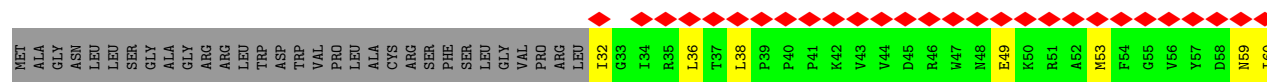
• Molecule 23: 39S ribosomal protein L43, mitochondrial



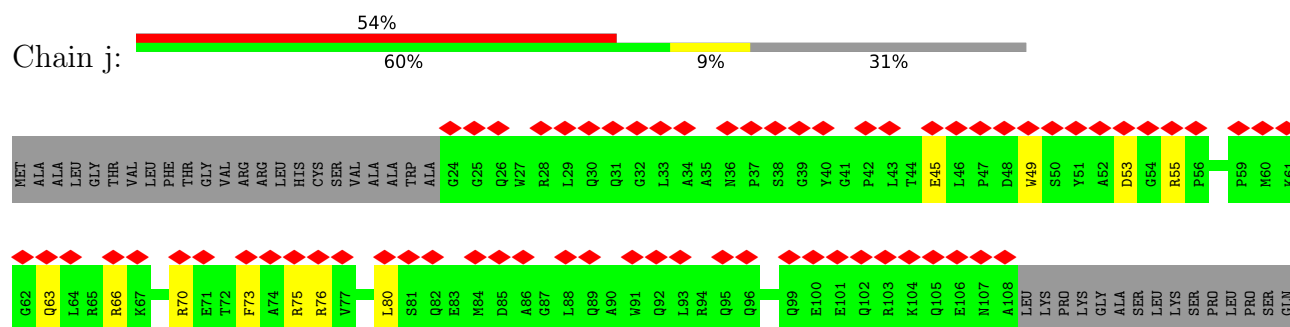
• Molecule 24: 39S ribosomal protein L49, mitochondrial



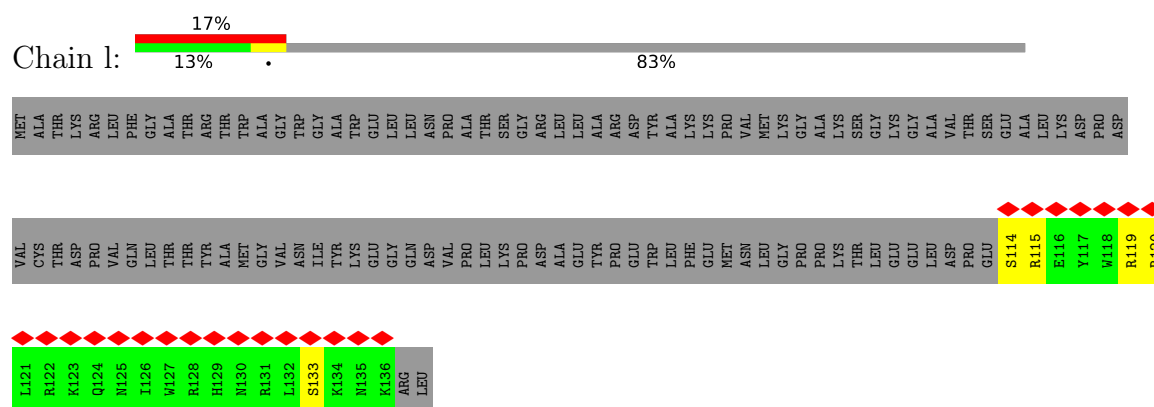
• Molecule 25: 39S ribosomal protein L51, mitochondrial



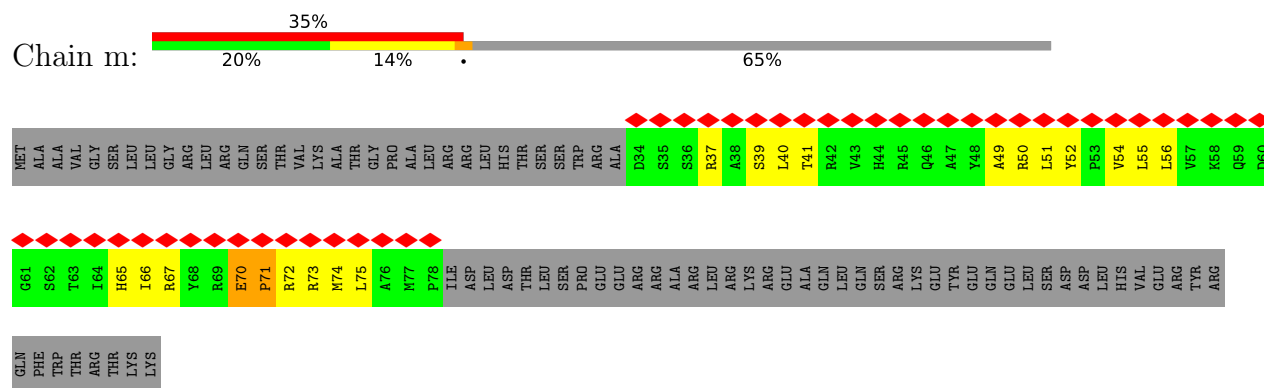
- Molecule 26: 39S ribosomal protein L52, mitochondrial



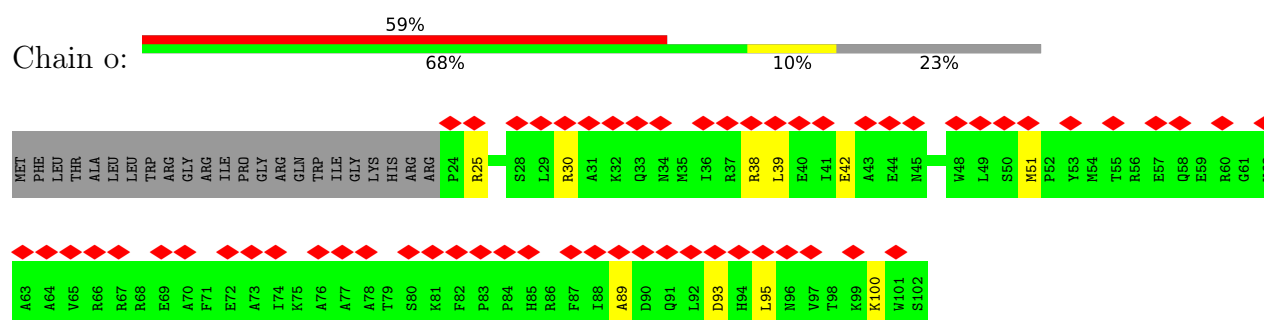
- Molecule 27: 39S ribosomal protein L54, mitochondrial



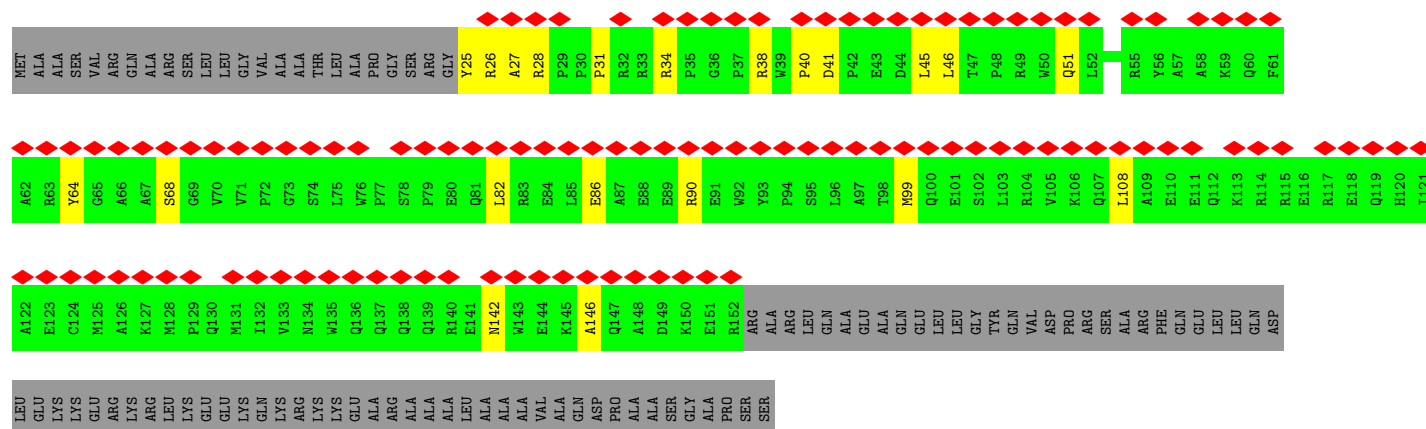
- Molecule 28: 39S ribosomal protein L55, mitochondrial



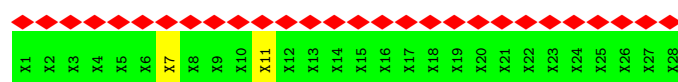
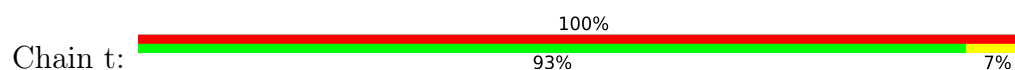
- Molecule 29: Ribosomal protein 63, mitochondrial



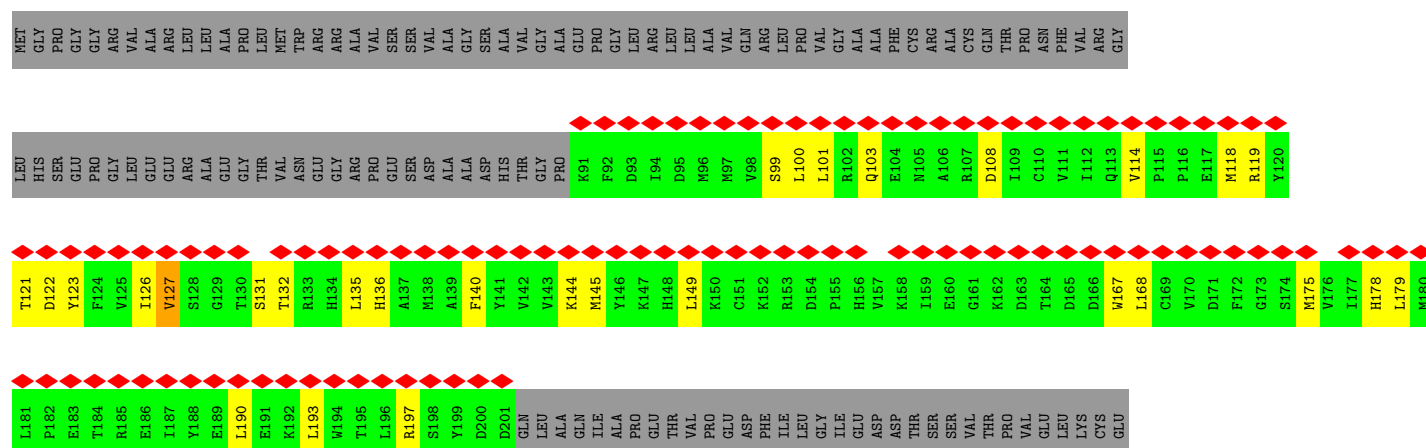
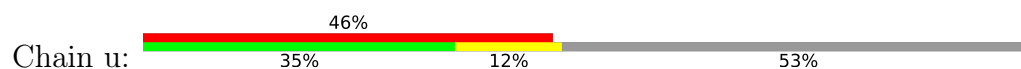
- Molecule 30: Growth arrest and DNA damage-inducible proteins-interacting protein 1



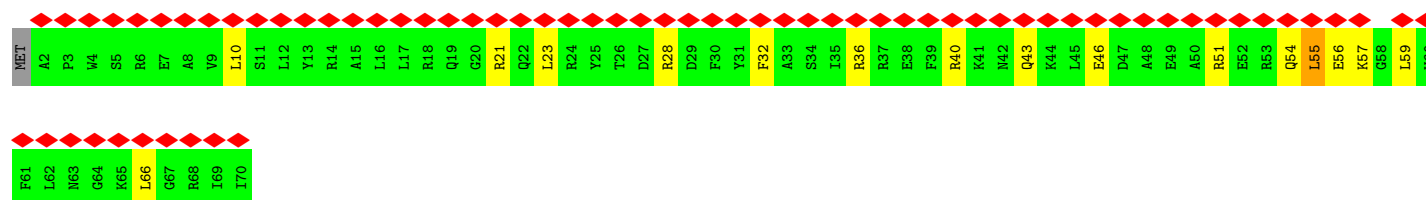
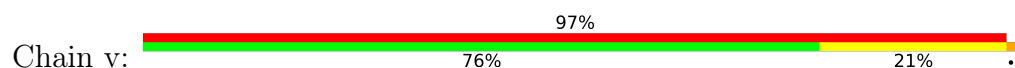
- Molecule 31: Unknown protein or protein extension



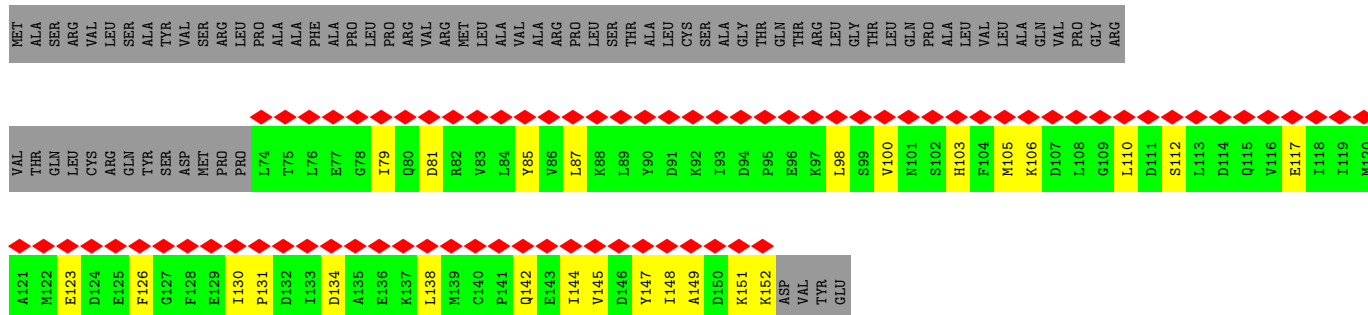
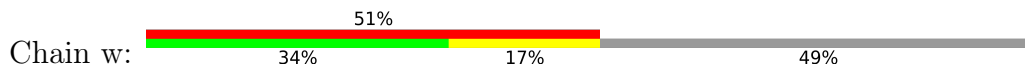
- Molecule 32: Mitochondrial assembly of ribosomal large subunit protein 1



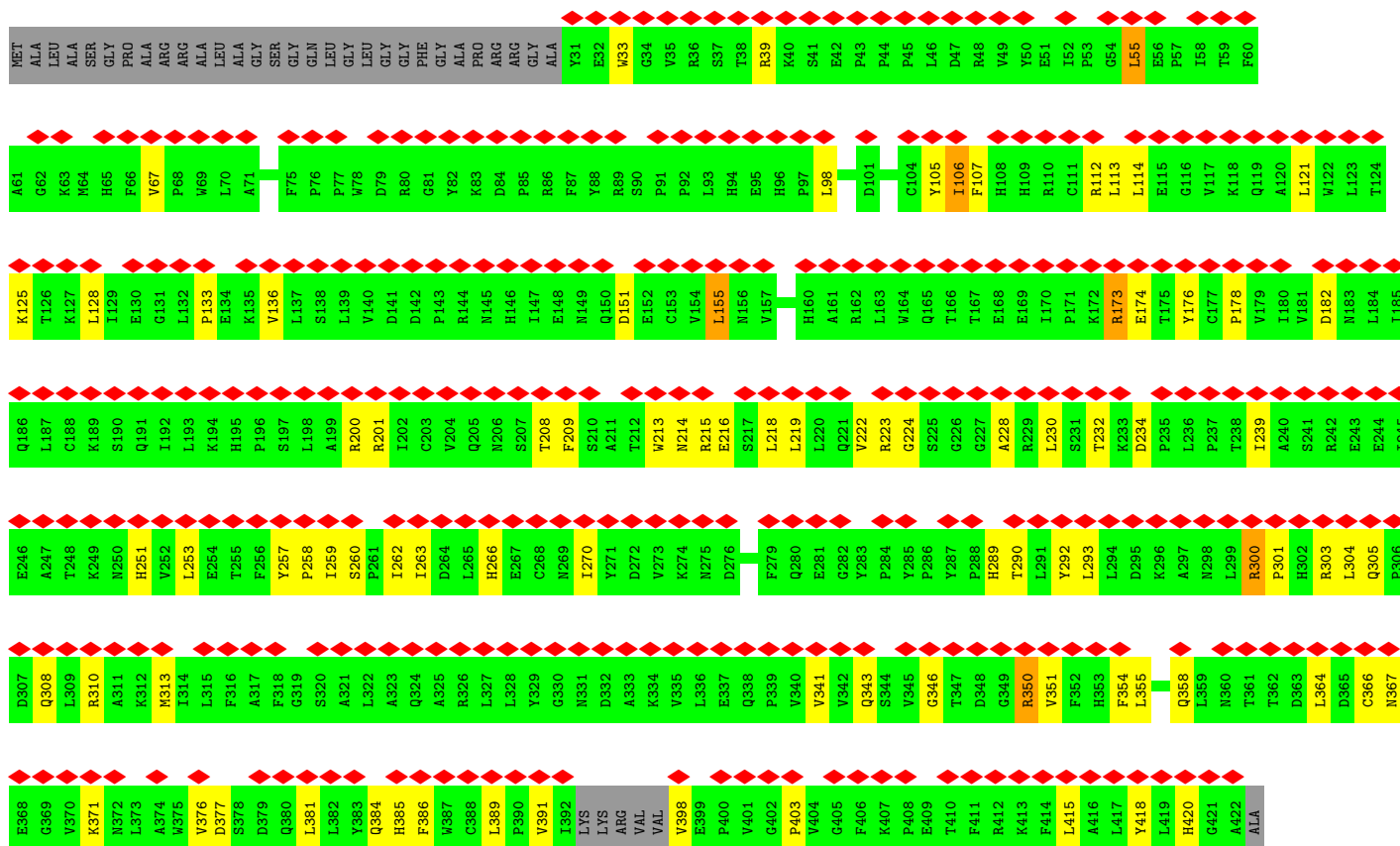
- Molecule 33: MIEF1 upstream open reading frame protein



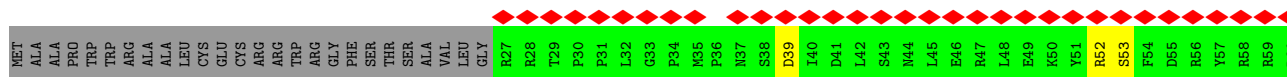
- Molecule 34: Acyl carrier protein, mitochondrial

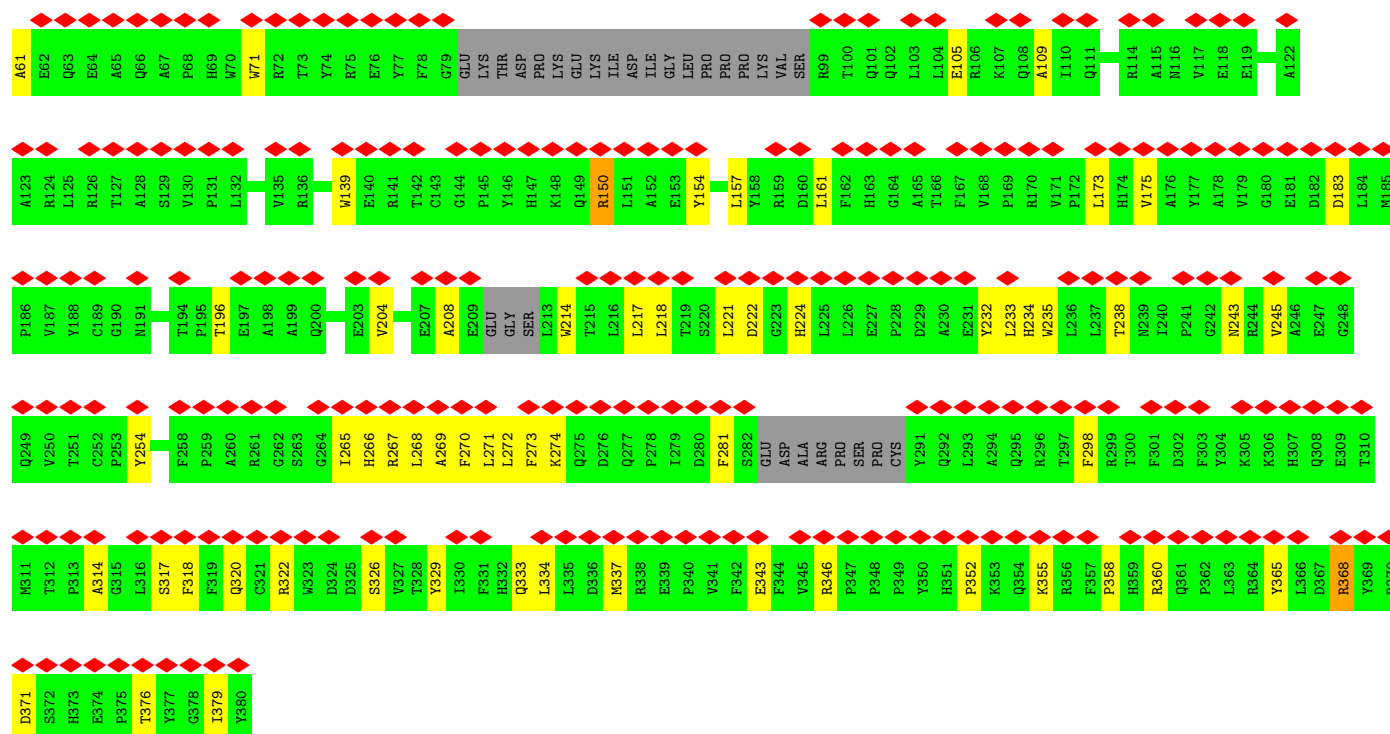


- Molecule 35: 39S ribosomal protein L37, mitochondrial

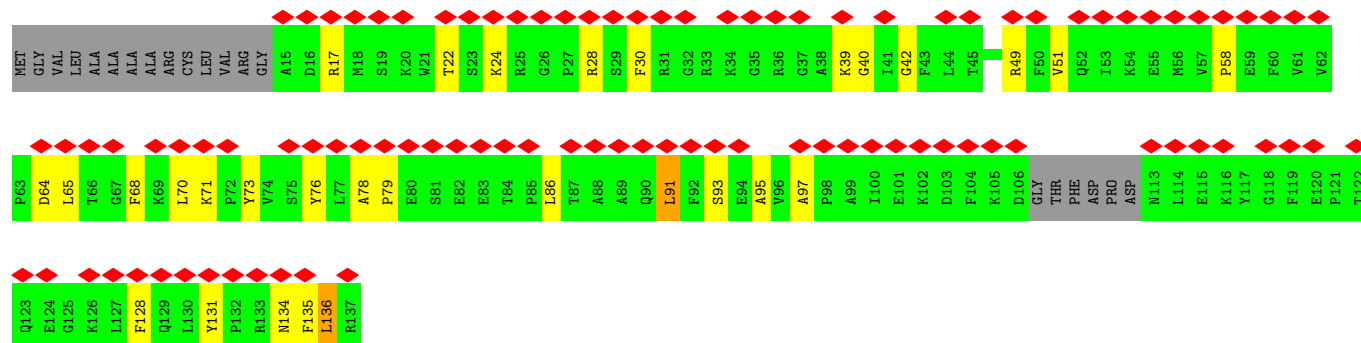


- Molecule 36: 39S ribosomal protein L38, mitochondrial

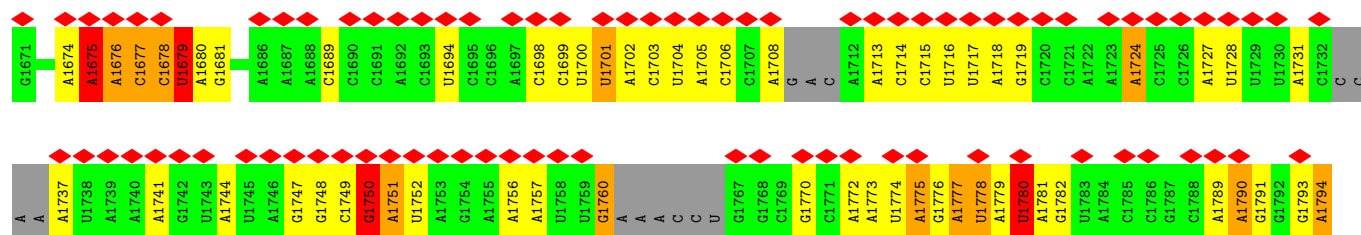
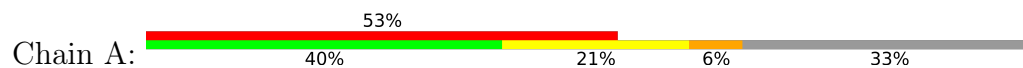




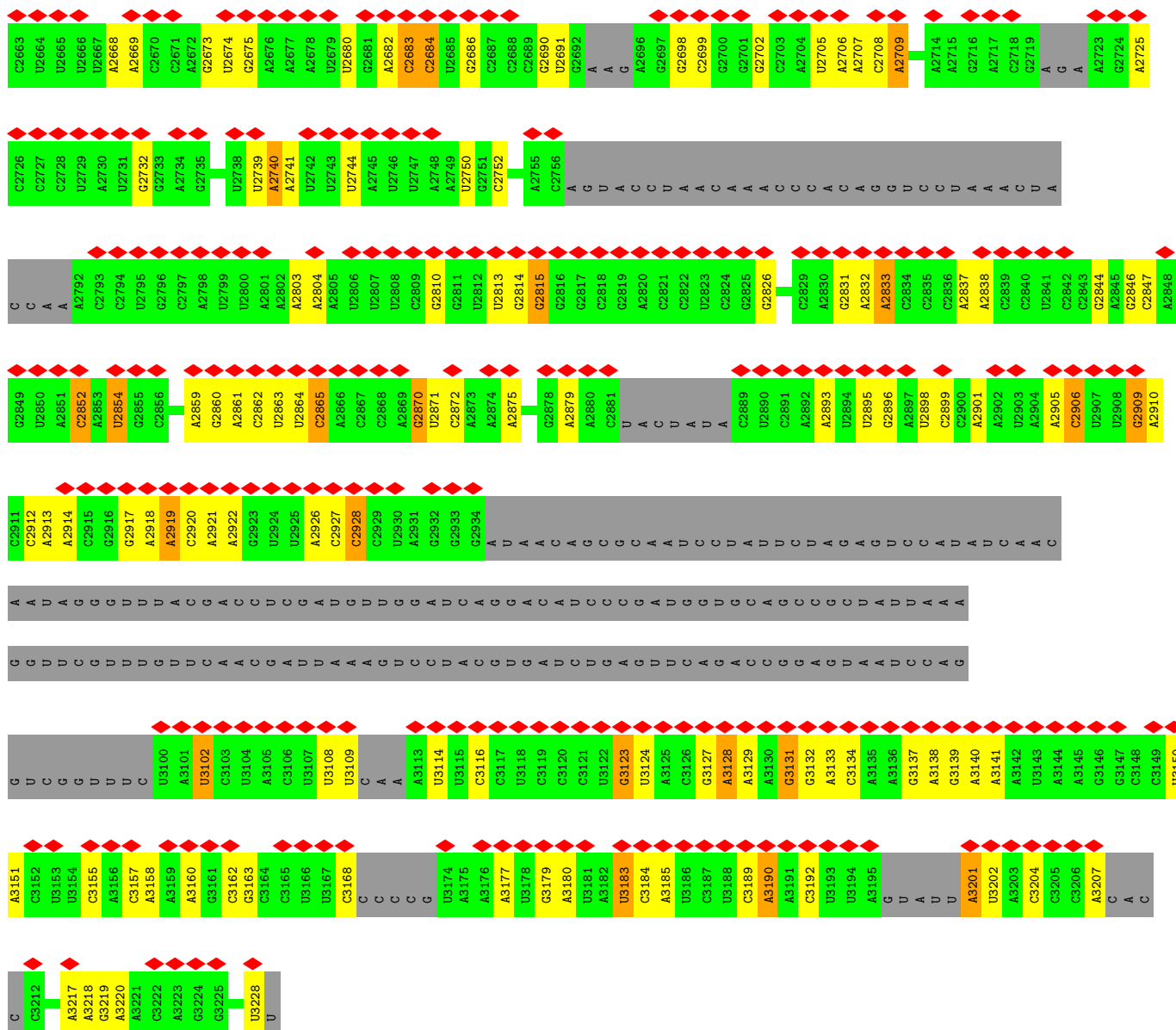
• Molecule 37: 39S ribosomal protein L41, mitochondrial



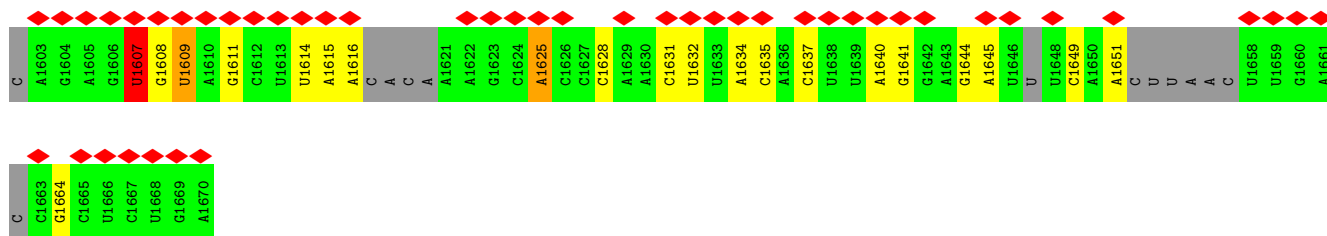
• Molecule 38: 16S ribosomal RNA





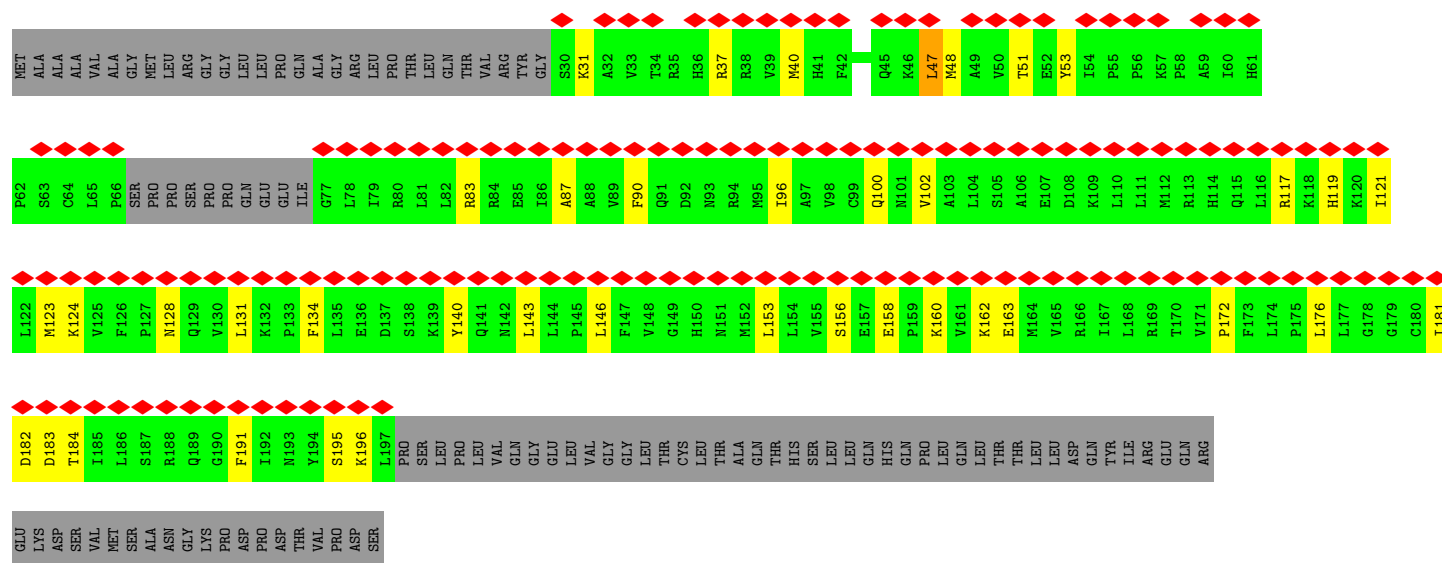


• Molecule 39: mitochondrial tRNAVal

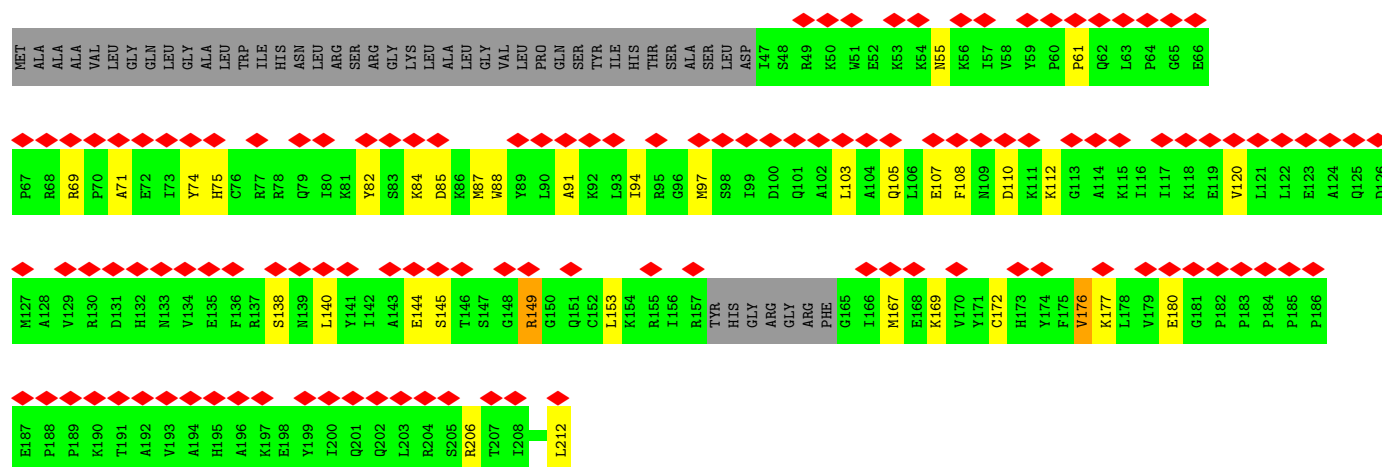


• Molecule 40: 39S ribosomal protein L2, mitochondrial





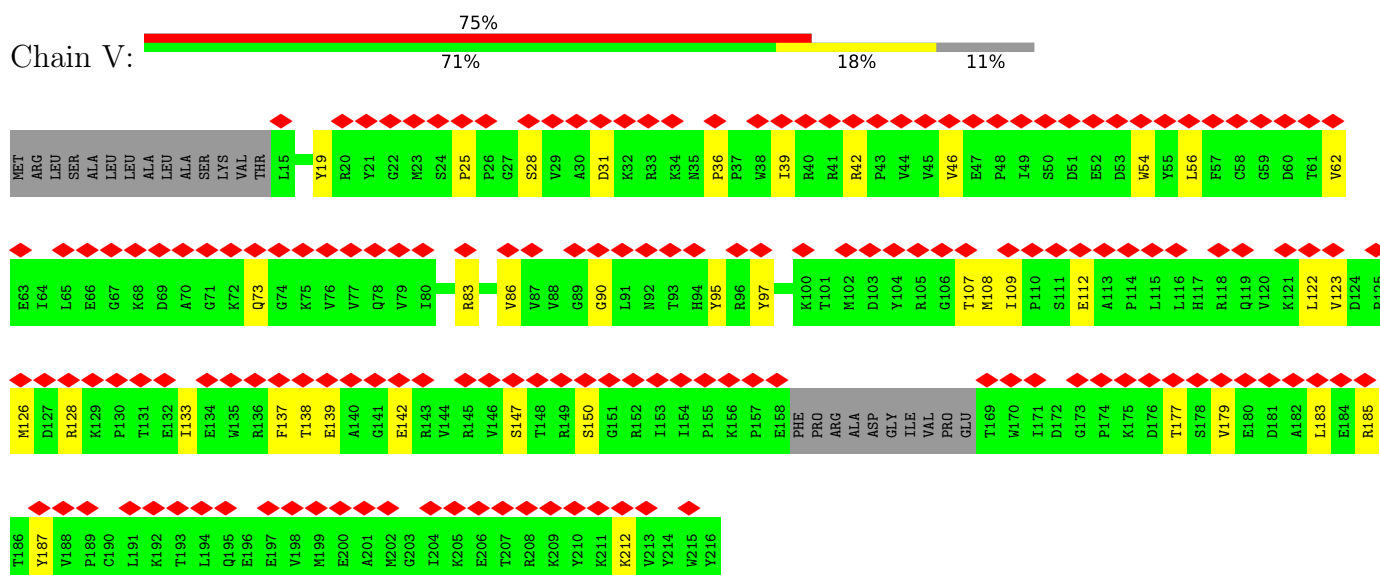
• Molecule 43: 39S ribosomal protein L22, mitochondrial



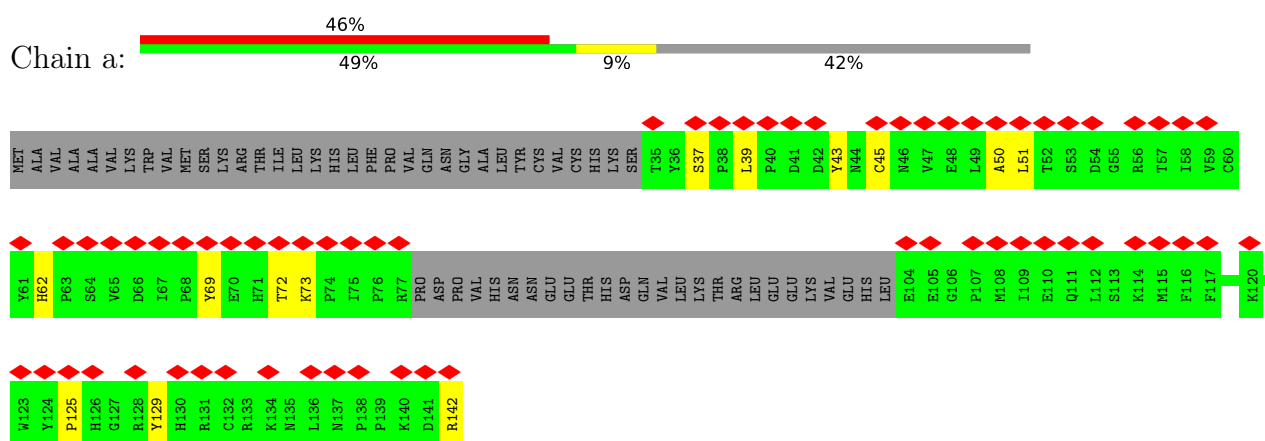
• Molecule 44: 39S ribosomal protein L23, mitochondrial



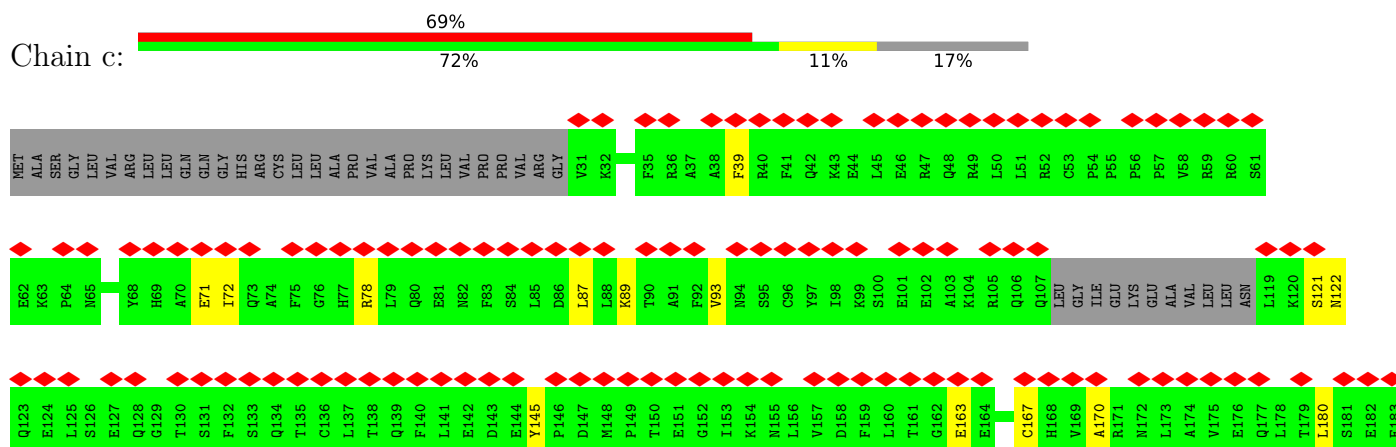
- Molecule 45: 39S ribosomal protein L24, mitochondrial

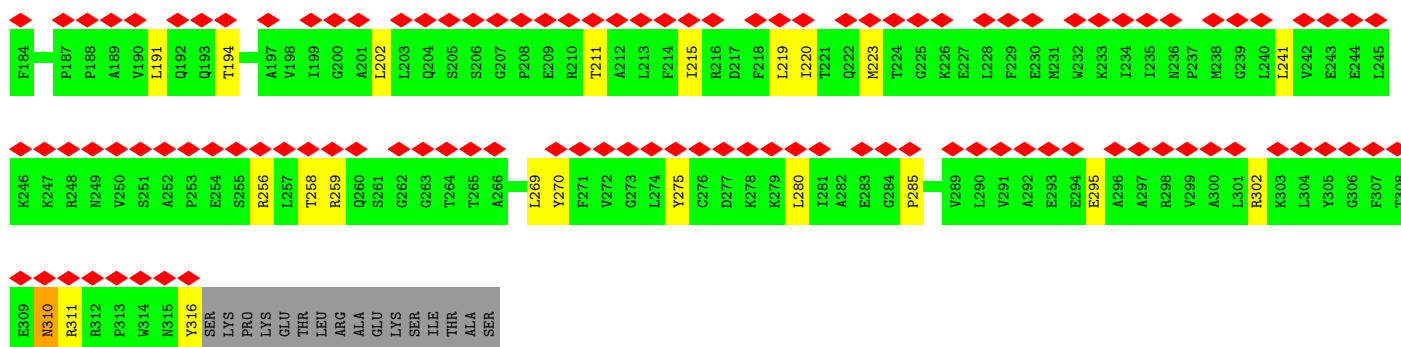


- Molecule 46: 39S ribosomal protein L42, mitochondrial

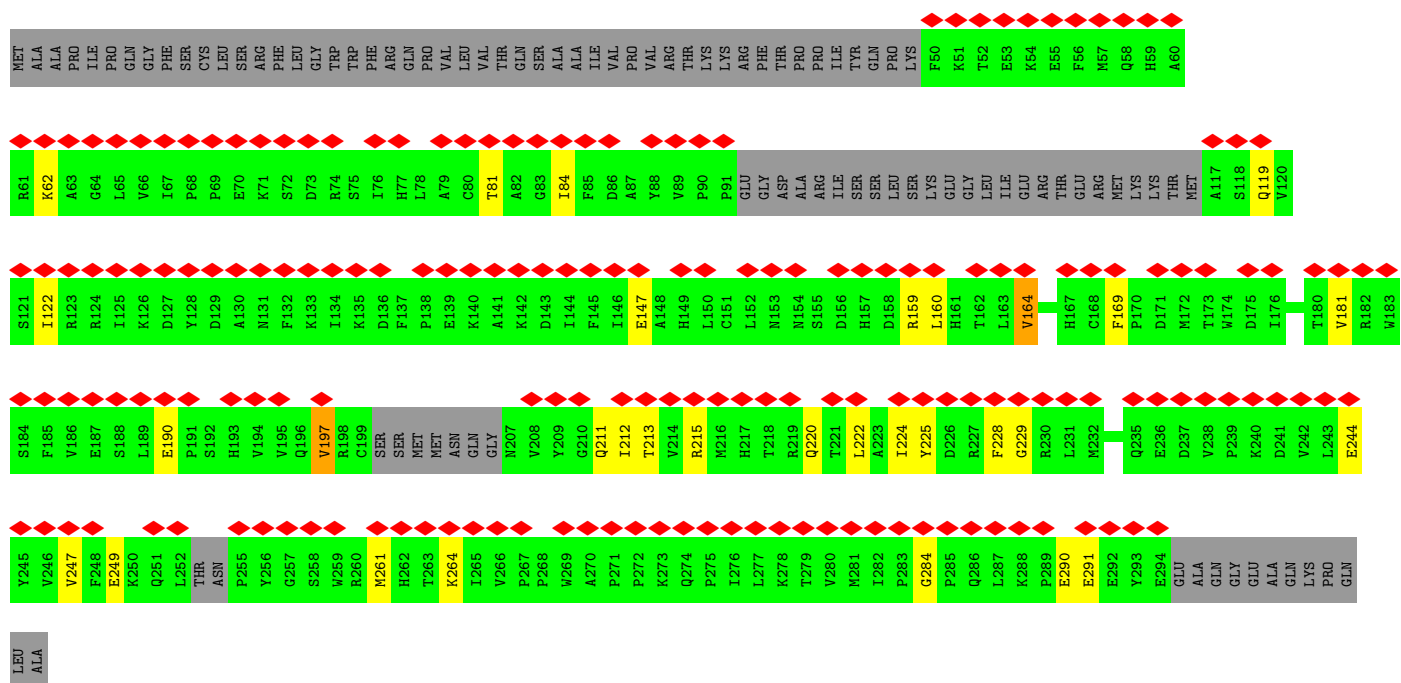


- Molecule 47: 39S ribosomal protein L44, mitochondrial

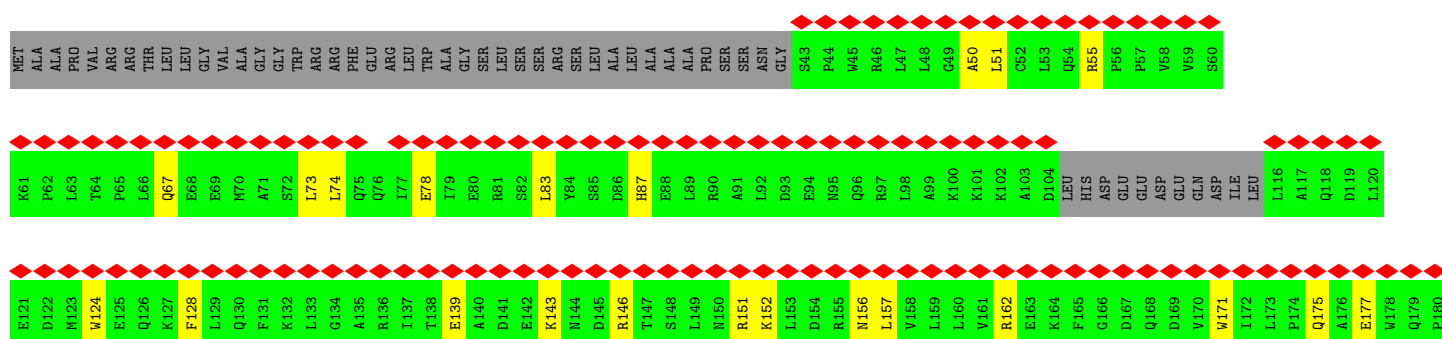
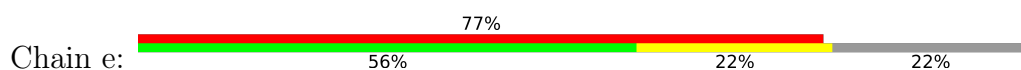




- Molecule 48: 39S ribosomal protein L45, mitochondrial

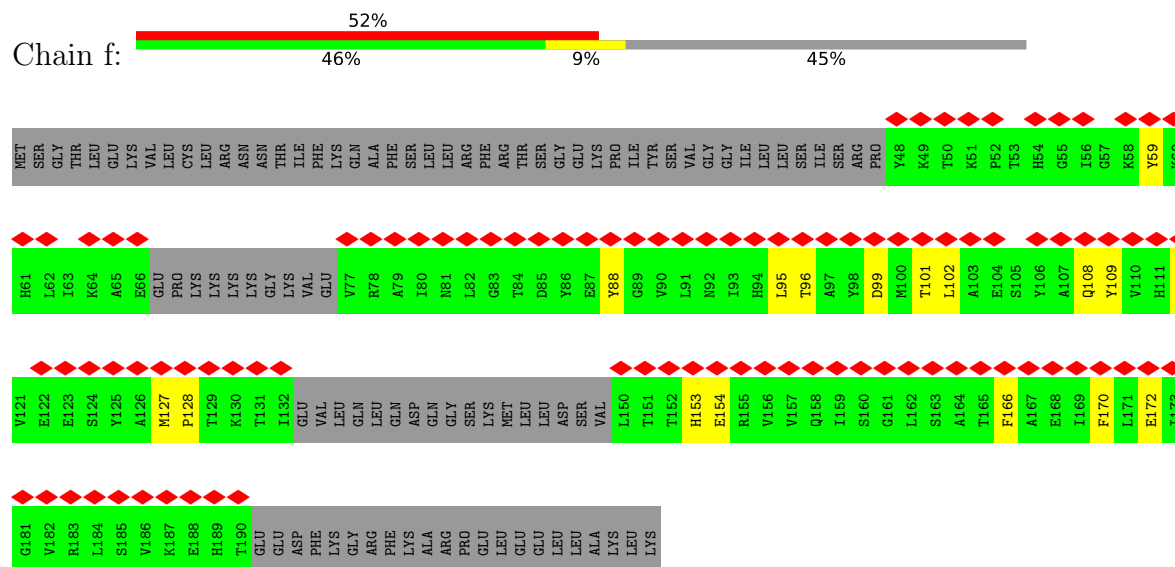


- Molecule 49: 39S ribosomal protein L46, mitochondrial

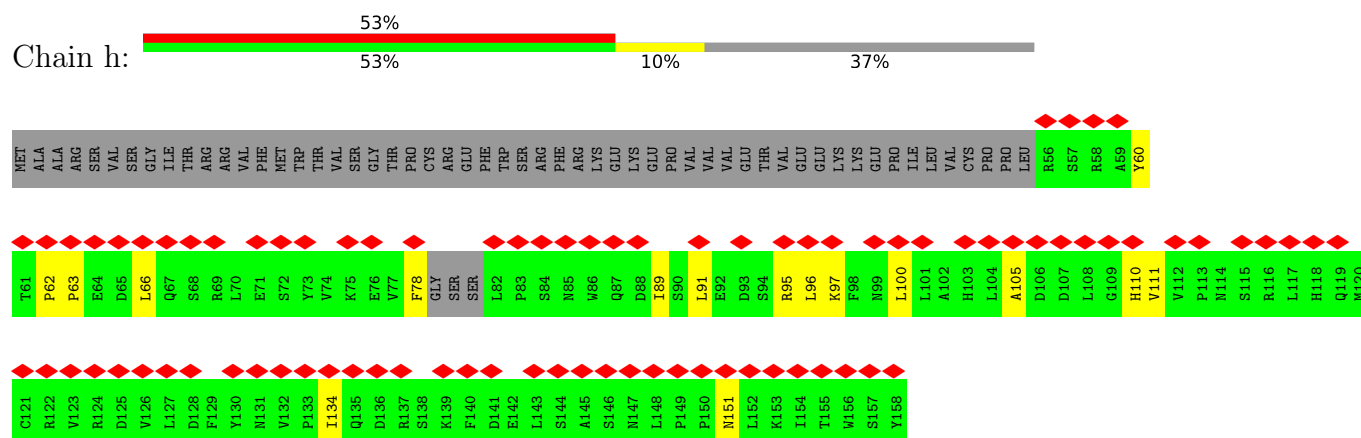




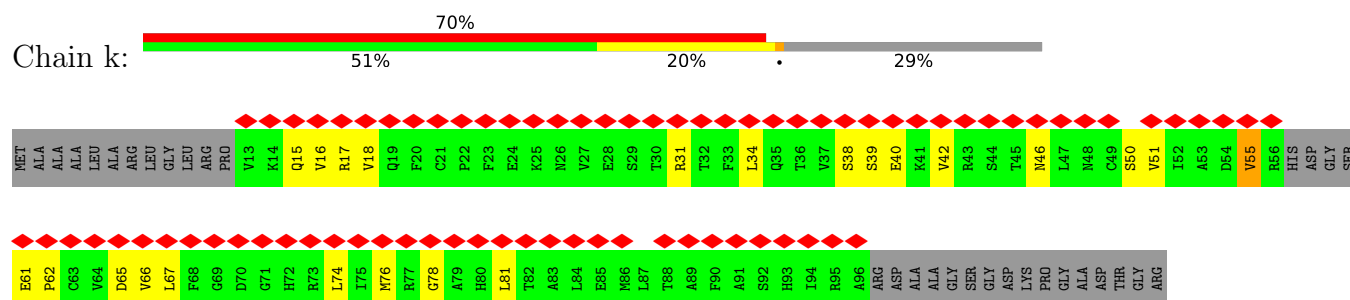
• Molecule 50: 39S ribosomal protein L48, mitochondrial



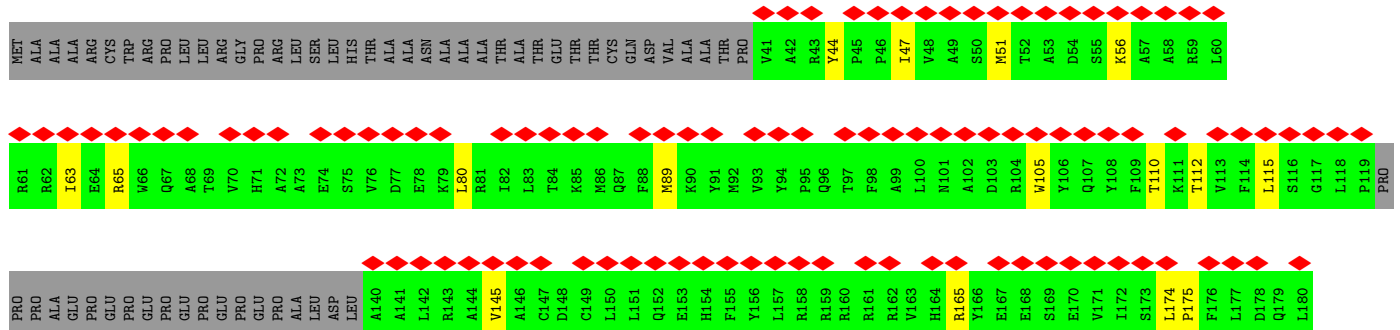
• Molecule 51: 39S ribosomal protein L50, mitochondrial



• Molecule 52: 39S ribosomal protein L53, mitochondrial



Chain p:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76796	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.129	Depositor
Minimum map value	-1.129	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	606.0, 606.0, 606.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0	0.50	0/895	0.91	1/1201 (0.1%)
2	1	0.44	0/438	0.83	0/583
3	2	0.66	0/357	0.98	0/475
4	3	0.58	0/852	0.98	3/1136 (0.3%)
5	7	0.48	0/2391	0.77	0/3234
6	8	0.41	0/855	0.66	0/1152
7	F	0.58	0/2071	0.93	0/2817
8	H	0.44	0/798	0.83	0/1073
9	J	0.45	0/1077	0.72	1/1452 (0.1%)
10	K	0.56	0/1495	0.84	0/2029
11	L	0.43	0/904	0.73	0/1218
12	M	0.55	0/2359	0.93	0/3185
13	N	0.45	0/1697	0.75	0/2281
14	O	0.53	0/1269	0.94	2/1708 (0.1%)
15	P	0.51	0/1173	0.82	0/1588
16	Q	0.43	0/1846	0.80	0/2487
17	R	0.60	0/1174	1.00	4/1572 (0.3%)
18	S	0.57	0/1276	0.92	0/1729
19	W	0.56	0/881	0.83	0/1188
20	X	0.47	0/2090	0.81	0/2825
21	Y	0.50	0/1552	0.81	0/2079
22	Z	0.56	0/1003	0.90	0/1354
23	b	0.60	0/1202	0.95	0/1626
24	g	0.60	0/1102	0.97	3/1503 (0.2%)
25	i	0.57	0/849	0.95	0/1135
26	j	0.54	0/698	0.80	0/940
27	l	0.37	0/226	0.65	0/299
28	m	0.47	0/379	0.87	2/510 (0.4%)
29	o	0.58	0/682	0.86	1/916 (0.1%)
30	q	0.46	0/1107	0.76	0/1498
32	u	0.41	0/949	0.72	0/1281
33	v	0.38	0/597	0.73	0/796

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	w	0.39	0/647	0.71	0/871
35	5	0.47	0/3250	0.77	0/4429
36	6	0.48	0/2726	0.79	1/3715 (0.0%)
37	9	0.48	0/972	0.80	0/1306
38	A	0.55	2/24893 (0.0%)	0.95	61/38695 (0.2%)
39	B	0.53	0/1328	0.73	1/2056 (0.0%)
40	D	0.47	0/1736	0.73	0/2335
41	E	0.49	0/2322	0.80	2/3148 (0.1%)
42	I	0.44	0/1308	0.80	3/1761 (0.2%)
43	T	0.62	0/1335	0.88	1/1796 (0.1%)
44	U	0.51	0/1183	0.90	1/1600 (0.1%)
45	V	0.47	0/1616	0.76	0/2189
46	a	0.53	0/709	0.82	0/963
47	c	0.51	0/2264	0.84	1/3059 (0.0%)
48	d	0.47	0/1790	0.75	0/2423
49	e	0.41	0/1797	0.68	0/2422
50	f	0.45	0/931	0.65	0/1259
51	h	0.51	0/847	0.77	0/1150
52	k	0.43	0/635	0.70	0/855
53	p	0.47	0/1071	0.69	0/1433
54	r	0.49	0/1238	0.83	0/1676
55	s	0.51	0/3114	0.83	0/4225
All	All	0.51	2/93956 (0.0%)	0.86	88/132236 (0.1%)

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
2	1	0	1
4	3	0	1
5	7	0	1
12	M	0	3
13	N	0	1
16	Q	0	1
17	R	0	5
21	Y	0	1
24	g	0	2
35	5	0	4
36	6	0	1
41	E	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
43	T	0	1
53	p	0	1
55	s	0	1
All	All	0	25

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A	2875	A	P-O5'	5.51	1.68	1.59
38	A	1779	A	O5'-C5'	5.42	1.50	1.42

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A	1778	U	O5'-P-OP1	-20.33	47.00	108.00
38	A	2317	G	O5'-P-OP1	16.31	156.94	108.00
38	A	2451	A	OP1-P-O3'	15.98	155.95	108.00
38	A	2317	G	OP1-P-OP2	-13.20	80.01	119.60
38	A	2452	A	OP1-P-OP2	-12.81	81.17	119.60
38	A	2691	U	O5'-P-OP2	12.79	146.37	108.00
38	A	2691	U	O5'-P-OP1	-12.36	70.93	108.00
38	A	2690	G	OP1-P-O3'	11.88	143.65	108.00
38	A	1779	A	O5'-P-OP1	11.78	143.34	108.00
38	A	1823	A	C2'-C3'-O3'	11.74	127.12	109.50
38	A	2451	A	O3'-P-O5'	-9.70	89.44	104.00
38	A	1777	A	OP1-P-O3'	9.62	136.85	108.00
38	A	2875	A	P-O5'-C5'	-8.93	107.51	120.90
38	A	2165	C	C2'-C3'-O3'	8.84	122.77	109.50
38	A	1776	G	OP1-P-OP2	-8.80	93.18	119.60
38	A	2691	U	OP1-P-OP2	-8.79	93.23	119.60
38	A	1778	U	O5'-P-OP2	8.65	133.95	108.00
38	A	2690	G	O3'-P-O5'	-8.58	91.13	104.00
38	A	1777	A	O3'-P-O5'	-8.42	91.37	104.00
38	A	2014	A	O3'-P-O5'	8.29	116.44	104.00
38	A	2457	A	C2'-C3'-O3'	8.15	121.72	109.50
38	A	2243	A	C2'-C3'-O3'	7.79	121.19	109.50
38	A	2690	G	OP2-P-O3'	-7.78	84.67	108.00
38	A	1780	U	C2'-C3'-O3'	7.46	120.69	109.50
38	A	2451	A	OP2-P-O3'	-7.40	85.80	108.00
17	R	34	ARG	CB-CG-CD	-7.39	94.30	111.30
38	A	2014	A	OP1-P-O3'	-7.12	86.64	108.00
38	A	2875	A	O5'-P-OP1	7.08	129.25	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A	1776	G	O5'-P-OP1	6.84	128.52	108.00
38	A	1779	A	O5'-P-OP2	-6.84	87.49	108.00
38	A	1795	A	O5'-P-OP1	6.82	128.45	108.00
38	A	1679	U	O3'-P-O5'	-6.59	94.11	104.00
41	E	266	ARG	NE-CZ-NH1	-6.38	115.11	121.50
38	A	2317	G	P-O5'-C5'	-6.37	111.35	120.90
24	g	90	ARG	CB-CA-C	-6.36	99.87	110.68
38	A	1750	G	C4'-C3'-C2'	-6.22	96.38	102.60
17	R	37	ARG	CB-CA-C	-6.20	101.03	109.28
9	J	33	PRO	N-CA-C	6.10	118.14	110.70
38	A	2863	U	OP1-P-O3'	6.06	126.18	108.00
17	R	13	ARG	CB-CG-CD	-6.05	97.39	111.30
38	A	1674	A	O3'-P-O5'	-6.01	94.98	104.00
38	A	2316	U	OP2-P-O3'	5.99	125.98	108.00
41	E	266	ARG	NE-CZ-NH2	5.89	124.50	119.20
38	A	1675	A	O3'-P-O5'	-5.87	95.20	104.00
42	I	182	ASP	CA-CB-CG	5.87	118.47	112.60
42	I	183	ASP	CA-CB-CG	5.85	118.45	112.60
38	A	2030	U	C2'-C3'-O3'	5.83	118.25	109.50
38	A	1780	U	P-O3'-C3'	5.81	128.92	120.20
17	R	11	ARG	CG-CD-NE	-5.71	99.45	112.00
38	A	1699	C	C4'-C3'-O3'	-5.71	104.44	113.00
42	I	102	VAL	N-CA-C	-5.66	107.75	113.47
38	A	1823	A	P-O3'-C3'	5.66	128.69	120.20
38	A	1805	A	C2'-C3'-O3'	5.60	122.11	113.70
38	A	2453	G	O5'-P-OP2	-5.58	91.27	108.00
38	A	1778	U	O3'-P-O5'	-5.56	95.66	104.00
38	A	3201	A	C2'-C3'-O3'	5.55	117.82	109.50
38	A	2690	G	C4'-C3'-O3'	5.51	121.27	113.00
38	A	2015	G	O5'-P-OP1	-5.49	91.53	108.00
4	3	116	ARG	CG-CD-NE	-5.44	100.02	112.00
38	A	2451	A	C2'-C3'-O3'	5.42	121.83	113.70
38	A	1678	C	P-O5'-C5'	-5.41	112.78	120.90
29	o	30	ARG	CB-CG-CD	-5.41	98.86	111.30
38	A	2909	G	O3'-P-O5'	-5.41	95.89	104.00
39	B	1607	U	C2'-C3'-O3'	5.41	121.81	113.70
38	A	1778	U	OP1-P-OP2	-5.40	103.40	119.60
4	3	168	ARG	N-CA-CB	-5.40	102.21	110.85
14	O	122	VAL	CA-C-N	-5.30	116.26	123.10
14	O	122	VAL	C-N-CA	-5.30	116.26	123.10
36	6	150	ARG	CB-CG-CD	-5.27	99.19	111.30
38	A	1680	A	P-O5'-C5'	-5.26	113.01	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A	2468	A	O5'-P-OP1	-5.21	92.36	108.00
38	A	2870	G	P-O5'-C5'	-5.19	113.12	120.90
38	A	1790	A	O3'-P-O5'	5.17	111.76	104.00
4	3	169	ARG	CB-CA-C	-5.15	100.84	109.65
38	A	1677	C	O3'-P-O5'	-5.15	96.27	104.00
47	c	310	ASN	CB-CA-C	-5.13	102.47	110.94
24	g	94	ILE	CB-CA-C	5.13	115.71	110.94
44	U	50	ARG	N-CA-CB	-5.06	102.67	110.16
1	0	85	ARG	CB-CG-CD	-5.05	99.68	111.30
38	A	1680	A	C5'-C4'-C3'	-5.05	108.42	116.00
38	A	1744	A	O3'-P-O5'	-5.05	96.43	104.00
24	g	105	ARG	CG-CD-NE	-5.04	100.90	112.00
38	A	2317	G	C4'-C3'-C2'	-5.03	97.57	102.60
43	T	108	PHE	CA-CB-CG	-5.03	108.77	113.80
38	A	1778	U	P-O5'-C5'	-5.03	113.36	120.90
38	A	2469	A	OP1-P-OP2	-5.01	104.56	119.60
28	m	70	GLU	CA-C-N	5.00	126.09	119.84
28	m	70	GLU	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	25	GLY	Peptide
4	3	184	THR	Peptide
35	5	173	ARG	Sidechain
35	5	300	ARG	Sidechain
35	5	303	ARG	Sidechain
35	5	350	ARG	Sidechain
36	6	368	ARG	Sidechain
5	7	159	LYS	Peptide
41	E	266	ARG	Sidechain
12	M	125	ARG	Sidechain
12	M	41	ARG	Sidechain
12	M	59	ARG	Sidechain
13	N	73	ARG	Sidechain
16	Q	226	PRO	Peptide
17	R	11	ARG	Sidechain
17	R	34	ARG	Sidechain
17	R	37	ARG	Sidechain
17	R	40	ARG	Sidechain
17	R	48	ARG	Sidechain

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Mol	Chain	Res	Type	Group
43	T	149	ARG	Sidechain
21	Y	210	ARG	Sidechain
24	g	105	ARG	Sidechain
24	g	90	ARG	Sidechain
53	p	145	ARG	Sidechain
55	s	357	SER	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	0	880	0	902	16	0
2	1	433	0	475	8	0
3	2	351	0	375	11	0
4	3	831	0	883	11	0
5	7	2334	0	2343	34	0
6	8	836	0	844	24	0
7	F	2013	0	2044	58	0
8	H	784	0	832	14	0
9	J	1061	0	1141	25	0
10	K	1451	0	1448	33	0
11	L	889	0	941	19	0
12	M	2305	0	2378	46	0
13	N	1654	0	1681	32	0
14	O	1245	0	1283	35	0
15	P	1148	0	1148	30	0
16	Q	1805	0	1841	33	0
17	R	1153	0	1214	26	0
18	S	1251	0	1322	37	0
19	W	859	0	888	24	0
20	X	2035	0	2054	30	0
21	Y	1517	0	1561	21	0
22	Z	978	0	1030	13	0
23	b	1178	0	1180	24	0
24	g	1067	0	1056	23	0
25	i	827	0	857	23	0
26	j	684	0	673	10	0
27	l	221	0	227	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	m	372	0	387	34	0
29	o	665	0	664	12	0
30	q	1076	0	1049	17	0
31	t	140	0	30	1	0
32	u	927	0	921	22	0
33	v	588	0	604	20	0
34	w	638	0	637	20	0
35	5	3156	0	3138	72	0
36	6	2640	0	2464	51	0
37	9	947	0	949	25	0
38	A	22263	0	11334	177	0
39	B	1191	0	607	10	0
40	D	1706	0	1755	57	0
41	E	2258	0	2264	32	0
42	I	1283	0	1369	30	0
43	T	1305	0	1352	30	0
44	U	1154	0	1154	30	0
45	V	1575	0	1583	28	0
46	a	686	0	658	12	0
47	c	2217	0	2220	26	0
48	d	1741	0	1727	21	0
49	e	1762	0	1767	53	0
50	f	915	0	917	16	0
51	h	827	0	806	8	0
52	k	627	0	636	15	0
53	p	1058	0	1083	11	0
54	r	1203	0	1220	21	0
55	s	3036	0	3022	47	0
56	0	1	0	0	0	0
56	r	1	0	0	0	0
57	A	47	0	0	0	0
57	g	1	0	0	0	0
58	v	21	0	21	8	0
All	All	89817	0	78959	1217	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 7.

All (1217) 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)
35:5:105:TYR:CE2	35:5:218:LEU:HD22	1.71	1.23
28:m:72:ARG:HH21	28:m:75:LEU:HD11	1.19	1.06
28:m:51:LEU:HB3	28:m:67:ARG:HB3	1.41	0.99
33:v:51:ARG:CD	58:v:101:PNS:O40	2.13	0.97
35:5:105:TYR:HE2	35:5:218:LEU:HD22	1.11	0.96
38:A:3116:C:N4	38:A:3140:A:H61	1.64	0.95
39:B:1607:U:H3	39:B:1664:G:H1	0.94	0.94
38:A:3116:C:H42	38:A:3140:A:N6	1.64	0.94
28:m:50:ARG:HD3	28:m:52:TYR:OH	1.70	0.92
33:v:51:ARG:HD2	58:v:101:PNS:O40	1.71	0.89
20:X:144:TYR:O	20:X:148:THR:HG23	1.72	0.89
50:f:96:THR:HA	50:f:153:HIS:O	1.76	0.85
49:e:213:TYR:O	49:e:231:VAL:HB	1.76	0.84
1:0:179:ARG:HH12	1:0:182:PRO:HG3	1.43	0.84
17:R:11:ARG:HB2	38:A:2292:G:C8	2.12	0.84
36:6:157:LEU:O	36:6:161:LEU:HB3	1.78	0.83
38:A:3116:C:H42	38:A:3140:A:H61	0.87	0.83
38:A:1747:G:N2	38:A:1750:G:O2'	2.13	0.82
35:5:290:THR:HA	35:5:343:GLN:O	1.80	0.82
42:I:123:MET:HA	42:I:153:LEU:O	1.80	0.82
33:v:51:ARG:HD3	58:v:101:PNS:O40	1.78	0.81
49:e:211:GLY:O	49:e:233:PHE:HB2	1.80	0.80
9:J:102:ARG:O	38:A:2174:G:N2	2.14	0.80
14:O:26:ILE:HD11	16:Q:268:ASP:HB3	1.64	0.79
35:5:293:LEU:O	35:5:346:GLY:HA2	1.83	0.79
23:b:126:ILE:O	47:c:310:ASN:ND2	2.16	0.79
45:V:137:PHE:HD2	45:V:142:GLU:O	1.66	0.78
49:e:279:LEU:HD11	50:f:176:SER:HB2	1.64	0.77
35:5:301:PRO:HD3	38:A:2390:A:H4'	1.66	0.77
35:5:105:TYR:CE2	35:5:218:LEU:CD2	2.64	0.76
34:w:81:ASP:O	34:w:85:TYR:HB2	1.84	0.76
16:Q:123:ASP:OD2	16:Q:126:ALA:N	2.19	0.76
33:v:43:GLN:HG2	58:v:101:PNS:N41	2.02	0.75
7:F:268:PHE:HE2	25:i:63:LEU:HD12	1.50	0.75
38:A:2123:C:H2'	38:A:2124:A:H5''	1.69	0.75
16:Q:120:THR:HG22	16:Q:132:GLN:HG2	1.68	0.74
24:g:68:THR:HG22	24:g:69:PRO:HD2	1.68	0.74
36:6:266:HIS:O	36:6:320:GLN:HA	1.88	0.74
15:P:104:SER:OG	36:6:150:ARG:NH1	2.19	0.74
42:I:140:TYR:HB3	42:I:143:LEU:HB2	1.70	0.73
55:s:271:LEU:O	55:s:273:LEU:N	2.22	0.73
18:S:101:PHE:CE2	18:S:116:ILE:HD13	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:2521:A:OP2	40:D:202:ARG:NH2	2.20	0.73
14:O:32:LEU:HB3	14:O:52:MET:HE2	1.72	0.72
16:Q:152:ARG:NH1	16:Q:190:LEU:O	2.23	0.72
5:7:77:THR:HG22	48:d:284:GLY:H	1.55	0.72
17:R:10:LEU:HG	17:R:13:ARG:HD3	1.72	0.71
36:6:270:PHE:HB2	36:6:317:SER:O	1.89	0.71
28:m:55:LEU:HD21	28:m:65:HIS:CD2	2.26	0.71
35:5:106:ILE:HG22	35:5:266:HIS:HB3	1.71	0.71
6:8:178:TYR:HE2	28:m:65:HIS:ND1	1.88	0.71
16:Q:129:LYS:NZ	32:u:121:THR:O	2.23	0.70
55:s:243:ILE:HG22	55:s:245:LYS:H	1.54	0.70
35:5:106:ILE:HD11	35:5:223:ARG:HE	1.56	0.70
7:F:281:ARG:NH1	38:A:1883:G:N7	2.39	0.70
7:F:275:TRP:HZ2	24:g:55:THR:HG21	1.57	0.70
25:i:38:LEU:HD23	25:i:38:LEU:H	1.56	0.70
45:V:139:GLU:CD	45:V:139:GLU:H	1.99	0.70
6:8:178:TYR:CE2	28:m:65:HIS:ND1	2.60	0.70
23:b:28:ARG:NH2	47:c:71:GLU:OE2	2.23	0.70
7:F:221:LEU:HD23	7:F:222:THR:HG23	1.73	0.70
48:d:197:VAL:HG12	48:d:212:ILE:HG12	1.74	0.70
7:F:107:LYS:HG2	25:i:74:ILE:HG22	1.73	0.69
32:u:145:MET:O	32:u:149:LEU:HB2	1.92	0.69
35:5:114:LEU:HD21	40:D:127:ILE:HD11	1.74	0.69
50:f:95:LEU:O	50:f:154:GLU:HA	1.92	0.69
19:W:127:TYR:HE2	36:6:71:TRP:CZ2	2.10	0.69
3:2:82:ARG:NH1	38:A:1790:A:OP1	2.25	0.69
17:R:54:THR:HG21	18:S:172:MET:H	1.56	0.69
47:c:270:TYR:O	47:c:285:PRO:HA	1.92	0.69
35:5:218:LEU:HD12	35:5:218:LEU:O	1.93	0.69
38:A:2529:U:O2'	40:D:206:TYR:HA	1.92	0.69
14:O:9:ILE:N	38:A:2458:A:OP1	2.26	0.69
44:U:143:ARG:HH21	44:U:143:ARG:HG2	1.56	0.69
23:b:27:GLN:HE21	23:b:80:LEU:HD23	1.57	0.69
19:W:101:LYS:NZ	38:A:2064:A:OP1	2.26	0.68
52:k:17:ARG:HB3	52:k:65:ASP:HB3	1.74	0.68
8:H:64:LEU:HB2	20:X:63:GLU:OE1	1.93	0.68
5:7:203:THR:HG22	5:7:280:VAL:H	1.59	0.68
45:V:137:PHE:CD2	45:V:142:GLU:O	2.46	0.68
18:S:101:PHE:CD1	18:S:130:LEU:HD22	2.29	0.68
13:N:250:ARG:NH2	42:I:51:THR:OG1	2.27	0.68
58:v:101:PNS:P24	34:w:112:SER:OG	2.52	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:m:72:ARG:NH2	28:m:75:LEU:HD11	2.03	0.68
9:J:142:ARG:HG3	38:A:2191:A:H4'	1.74	0.67
55:s:321:GLU:OE1	55:s:325:ARG:NH2	2.27	0.67
6:8:122:SER:HB3	39:B:1628:C:H1'	1.76	0.67
18:S:122:LEU:HD12	18:S:128:ILE:HD11	1.77	0.67
6:8:128:GLU:HB3	28:m:37:ARG:HH12	1.60	0.67
6:8:143:GLN:HG2	49:e:210:CYS:HA	1.76	0.67
35:5:114:LEU:HD21	40:D:127:ILE:CD1	2.24	0.67
6:8:150:LEU:HB2	49:e:212:HIS:HE1	1.59	0.67
9:J:89:TYR:O	9:J:93:ALA:HB3	1.96	0.66
10:K:21:LEU:HD21	10:K:31:LEU:HD22	1.76	0.66
38:A:2511:C:H3'	38:A:2512:A:H8	1.61	0.66
28:m:67:ARG:NH1	50:f:101:THR:OG1	2.28	0.66
38:A:2127:A:H4'	38:A:2251:A:C5	2.30	0.66
48:d:84:ILE:HA	48:d:211:GLN:HE22	1.61	0.66
11:L:58:ILE:HD11	11:L:76:ALA:HB2	1.76	0.66
16:Q:201:ASP:HB3	16:Q:204:MET:HB3	1.77	0.66
18:S:129:ARG:HE	18:S:155:ARG:HG3	1.61	0.66
7:F:280:TYR:CD1	12:M:125:ARG:HD2	2.31	0.65
18:S:99:VAL:HG22	18:S:133:VAL:HG12	1.78	0.65
35:5:258:PRO:HG3	40:D:123:GLU:HB3	1.78	0.65
4:3:148:VAL:HG13	36:6:360:ARG:HA	1.77	0.65
5:7:107:LEU:HB2	5:7:126:LYS:HB2	1.76	0.65
20:X:61:ARG:NH2	20:X:63:GLU:OE2	2.30	0.65
37:9:93:SER:O	37:9:97:ALA:HB3	1.96	0.65
21:Y:114:THR:HG22	44:U:28:LEU:H	1.60	0.65
34:w:147:TYR:O	34:w:151:LYS:HB2	1.97	0.65
28:m:72:ARG:HG2	49:e:124:TRP:CE2	2.32	0.65
55:s:51:MET:HE3	55:s:65:ARG:HD2	1.77	0.65
38:A:3228:U:OP2	41:E:156:ARG:NH2	2.30	0.64
33:v:43:GLN:HG2	58:v:101:PNS:H41	1.62	0.64
52:k:34:LEU:HA	52:k:38:SER:HB2	1.79	0.64
25:i:99:GLY:HA2	25:i:102:MET:HE3	1.78	0.64
3:2:70:LEU:O	21:Y:198:ARG:NH2	2.30	0.64
18:S:104:ARG:NH1	38:A:2147:G:OP1	2.31	0.64
49:e:55:ARG:HD2	49:e:157:LEU:HD13	1.79	0.64
15:P:77:PHE:O	15:P:97:GLN:NE2	2.31	0.64
42:I:119:HIS:NE2	42:I:158:GLU:O	2.31	0.63
45:V:139:GLU:OE1	45:V:139:GLU:N	2.28	0.63
16:Q:120:THR:HA	16:Q:131:SER:O	1.98	0.63
35:5:386:PHE:HA	35:5:403:PRO:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:110:GLY:O	9:J:153:ILE:HA	1.98	0.63
37:9:40:GLY:O	38:A:1705:A:N6	2.31	0.63
1:0:96:ASN:HD21	38:A:2709:A:H1'	1.63	0.63
35:5:300:ARG:HB3	38:A:2390:A:H5'	1.80	0.63
34:w:138:LEU:HD13	34:w:144:ILE:HG12	1.80	0.63
42:I:172:PRO:HB2	52:k:51:VAL:O	1.99	0.63
37:9:79:PRO:HD2	45:V:183:LEU:HD11	1.81	0.63
49:e:199:ASN:O	49:e:242:ASP:HB2	1.99	0.63
20:X:20:ILE:HA	20:X:23:ARG:HH11	1.64	0.63
35:5:208:THR:HA	35:5:224:GLY:O	1.98	0.63
1:0:119:LYS:O	1:0:120:HIS:ND1	2.32	0.63
7:F:103:GLN:HE22	7:F:250:VAL:H	1.47	0.63
20:X:114:PHE:O	20:X:122:LYS:HA	1.99	0.63
22:Z:99:VAL:O	26:j:76:ARG:NH2	2.31	0.63
15:P:63:ARG:HG2	15:P:177:ARG:HH11	1.64	0.62
13:N:247:MET:HE3	42:I:37:ARG:HH22	1.64	0.62
35:5:308:GLN:HE22	38:A:2389:C:H42	1.47	0.62
40:D:132:ASP:OD2	40:D:135:ARG:NH1	2.27	0.62
32:u:99:SER:O	32:u:103:GLN:HB2	1.99	0.62
3:2:83:MET:HE1	21:Y:175:ARG:HH22	1.64	0.62
20:X:41:VAL:HG11	20:X:83:GLU:HB3	1.82	0.62
21:Y:193:ARG:NH2	38:A:1706:C:OP1	2.32	0.62
26:j:45:GLU:OE2	26:j:70:ARG:NH2	2.30	0.62
36:6:157:LEU:O	36:6:161:LEU:CB	2.48	0.62
11:L:55:PRO:HB3	11:L:77:ILE:HG12	1.81	0.62
23:b:37:GLY:O	23:b:44:ARG:NH2	2.33	0.62
7:F:226:MET:HE3	30:q:26:ARG:NH1	2.15	0.62
20:X:226:LEU:HD12	21:Y:155:LEU:HB3	1.81	0.62
23:b:35:ARG:O	23:b:44:ARG:NH1	2.32	0.62
26:j:63:GLN:OE1	26:j:66:ARG:NH2	2.32	0.62
35:5:230:LEU:O	35:5:289:HIS:HB3	2.00	0.61
7:F:165:LEU:HB2	7:F:170:ARG:HD3	1.82	0.61
33:v:10:LEU:HD11	34:w:112:SER:HB3	1.82	0.61
35:5:351:VAL:HG22	35:5:381:LEU:HB3	1.82	0.61
20:X:153:LEU:HD11	20:X:158:GLY:HA3	1.82	0.61
35:5:216:GLU:HA	35:5:216:GLU:OE1	2.00	0.61
50:f:96:THR:HG22	50:f:154:GLU:HG2	1.82	0.61
24:g:57:ILE:HD12	24:g:91:MET:SD	2.40	0.61
7:F:63:GLN:HG2	7:F:81:ASP:HB3	1.83	0.61
7:F:95:ILE:HD13	7:F:172:LEU:HD22	1.80	0.61
13:N:87:PHE:HB2	13:N:163:MET:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:6:218:LEU:HD22	36:6:234:HIS:HB2	1.82	0.61
55:s:249:GLU:HA	55:s:356:VAL:HG21	1.82	0.61
6:8:117:LEU:O	6:8:121:TRP:HB2	2.01	0.61
15:P:52:ASN:HB3	15:P:55:ASN:HB2	1.81	0.61
42:I:124:LYS:HB2	42:I:153:LEU:HB2	1.83	0.61
12:M:129:ILE:HD11	12:M:188:CYS:SG	2.40	0.61
39:B:1607:U:O4	39:B:1664:G:O6	2.19	0.61
7:F:275:TRP:HZ2	24:g:55:THR:CG2	2.14	0.61
29:o:25:ARG:HG3	29:o:25:ARG:HH11	1.66	0.61
25:i:115:ARG:NH1	38:A:2010:U:OP2	2.33	0.60
6:8:150:LEU:HB2	49:e:212:HIS:CE1	2.37	0.60
9:J:111:LEU:HG	9:J:154:ARG:HB3	1.83	0.60
40:D:194:ASN:OD1	40:D:243:THR:OG1	2.20	0.60
38:A:2029:A:N6	38:A:2124:A:H2'	2.16	0.60
10:K:174:GLU:HG3	54:r:56:THR:HG21	1.82	0.60
14:O:117:ARG:HD2	43:T:110:ASP:OD1	2.02	0.60
18:S:100:HIS:ND1	18:S:100:HIS:O	2.34	0.60
36:6:173:LEU:HD21	36:6:175:VAL:HG23	1.82	0.60
28:m:56:LEU:HD13	28:m:66:ILE:HD12	1.82	0.60
35:5:105:TYR:HE2	35:5:218:LEU:CD2	2.01	0.60
35:5:114:LEU:HD12	40:D:148:LYS:HD3	1.82	0.60
12:M:127:VAL:HG12	12:M:129:ILE:HG23	1.84	0.60
38:A:1777:A:N6	38:A:1780:U:OP2	2.34	0.60
38:A:2123:C:C2'	38:A:2124:A:H5''	2.32	0.60
23:b:136:LYS:O	47:c:259:ARG:NH2	2.35	0.59
35:5:300:ARG:N	35:5:301:PRO:HD2	2.17	0.59
18:S:101:PHE:HZ	18:S:120:LEU:HD11	1.66	0.59
49:e:213:TYR:HB3	49:e:268:TYR:HD1	1.67	0.59
40:D:235:GLN:HB3	40:D:294:SER:HA	1.84	0.59
23:b:133:PHE:CG	47:c:259:ARG:HD3	2.37	0.59
12:M:177:ALA:HB1	12:M:203:ARG:HH12	1.68	0.59
35:5:112:ARG:HE	35:5:304:LEU:HD22	1.66	0.59
40:D:227:GLN:HE21	40:D:231:LYS:HG2	1.67	0.59
38:A:2927:C:H2'	38:A:2928:C:H4'	1.84	0.59
10:K:52:ASP:O	43:T:206:ARG:NH1	2.36	0.59
47:c:145:TYR:OH	47:c:311:ARG:NH1	2.36	0.59
3:2:59:LYS:O	3:2:63:LYS:HB2	2.02	0.59
35:5:300:ARG:HH11	35:5:300:ARG:HG2	1.66	0.59
36:6:329:TYR:O	36:6:333:GLN:HB2	2.03	0.59
43:T:84:LYS:HD3	43:T:149:ARG:HB3	1.85	0.59
12:M:168:GLU:OE1	12:M:220:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:5:341:VAL:HG22	35:5:358:GLN:HG2	1.85	0.58
1:0:79:ALA:HB3	38:A:3102:U:O4	2.04	0.58
9:J:32:GLY:O	9:J:36:GLY:N	2.34	0.58
17:R:109:GLU:OE1	18:S:107:LYS:HE3	2.04	0.58
18:S:101:PHE:HD1	18:S:130:LEU:HD22	1.65	0.58
45:V:142:GLU:OE1	45:V:142:GLU:HA	2.02	0.58
36:6:217:LEU:HD22	36:6:271:LEU:HD12	1.86	0.58
14:O:25:ARG:NH2	14:O:51:GLU:OE2	2.36	0.58
21:Y:160:GLN:HG3	37:9:131:TYR:CG	2.38	0.58
38:A:2032:G:O2'	38:A:2865:C:O2	2.20	0.58
41:E:207:THR:HG22	41:E:298:LYS:HB3	1.85	0.58
7:F:253:MET:HG2	7:F:259:LEU:HD13	1.86	0.58
10:K:29:GLY:HA3	38:A:2239:A:O3'	2.02	0.58
14:O:38:ARG:NH2	14:O:82:GLU:OE1	2.36	0.58
14:O:50:ASP:HB3	14:O:107:MET:HE1	1.85	0.58
19:W:106:PRO:HD2	19:W:117:ILE:HD11	1.85	0.58
33:v:46:GLU:HB2	33:v:51:ARG:HE	1.68	0.58
10:K:63:ARG:NH1	10:K:130:ASP:OD1	2.36	0.58
44:U:24:PHE:HB2	44:U:45:PRO:HG3	1.86	0.58
1:0:106:ASN:HD22	1:0:118:GLN:HE21	1.52	0.58
18:S:135:LEU:HD23	18:S:144:LEU:HB3	1.86	0.58
40:D:194:ASN:HA	40:D:207:ILE:CG2	2.33	0.58
48:d:220:GLN:NE2	48:d:244:GLU:OE2	2.35	0.58
1:0:134:THR:HG22	14:O:131:PRO:HD2	1.85	0.57
7:F:121:ARG:HG2	38:A:1778:U:C6	2.39	0.57
32:u:123:TYR:HB2	32:u:175:MET:HB3	1.84	0.57
4:3:168:ARG:NH2	38:A:1890:C:OP2	2.37	0.57
22:Z:99:VAL:HG12	26:j:80:LEU:HD12	1.85	0.57
35:5:105:TYR:CD2	35:5:218:LEU:HD22	2.37	0.57
37:9:136:LEU:HD12	44:U:17:LEU:HD21	1.86	0.57
15:P:104:SER:CB	36:6:150:ARG:HH12	2.16	0.57
29:o:89:ALA:O	29:o:93:ASP:HB2	2.05	0.57
35:5:258:PRO:HD2	40:D:125:LYS:HB2	1.85	0.57
45:V:108:MET:HE3	48:d:169:PHE:HD2	1.69	0.57
55:s:105:TRP:HZ3	55:s:268:PRO:HA	1.69	0.57
55:s:246:GLN:OE1	55:s:353:ARG:NH1	2.38	0.57
17:R:10:LEU:HD22	38:A:1775:A:H4'	1.85	0.57
17:R:34:ARG:HH12	38:A:2682:A:H5''	1.69	0.57
20:X:177:HIS:O	20:X:184:ARG:NH2	2.38	0.57
38:A:2191:A:N6	38:A:2198:A:OP2	2.38	0.57
48:d:119:GLN:HA	48:d:122:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:m:51:LEU:HB3	28:m:67:ARG:CB	2.24	0.57
49:e:156:ASN:ND2	49:e:277:SER:O	2.38	0.57
12:M:225:ASP:HB3	12:M:227:ALA:H	1.69	0.57
4:3:113:ARG:NH2	38:A:1750:G:OP2	2.34	0.57
6:8:178:TYR:CE2	28:m:65:HIS:CE1	2.93	0.57
40:D:124:GLU:HG2	40:D:144:GLY:HA3	1.87	0.57
43:T:55:ASN:ND2	43:T:74:TYR:O	2.33	0.57
18:S:180:PHE:CZ	18:S:182:LYS:HE3	2.40	0.57
34:w:148:ILE:HG22	34:w:152:LYS:HE2	1.87	0.57
45:V:97:TYR:HA	45:V:107:THR:O	2.04	0.57
5:7:174:VAL:HG11	14:O:144:LEU:HD22	1.86	0.56
17:R:99:ARG:NH2	38:A:2248:U:OP1	2.36	0.56
32:u:101:LEU:HD13	32:u:127:VAL:HG11	1.86	0.56
32:u:167:TRP:HH2	32:u:190:LEU:HD11	1.70	0.56
40:D:199:GLU:HB2	40:D:202:ARG:HB2	1.87	0.56
48:d:147:GLU:OE2	48:d:159:ARG:NH1	2.38	0.56
49:e:151:ARG:HD3	49:e:152:LYS:HG2	1.87	0.56
54:r:79:HIS:HB3	54:r:184:ASN:HA	1.86	0.56
7:F:147:ARG:HG3	38:A:1774:U:H1'	1.88	0.56
21:Y:183:GLN:HE22	44:U:8:PRO:HA	1.69	0.56
40:D:187:LEU:HD21	40:D:244:VAL:HG12	1.88	0.56
40:D:194:ASN:HA	40:D:207:ILE:HG21	1.87	0.56
44:U:128:SER:O	44:U:132:GLU:HB2	2.06	0.56
54:r:72:ILE:HD11	54:r:115:ILE:HD11	1.87	0.56
4:3:172:TYR:HB2	4:3:175:ASP:HB2	1.86	0.56
10:K:117:HIS:ND1	38:A:1839:C:H5'	2.19	0.56
28:m:54:VAL:N	28:m:66:ILE:O	2.39	0.56
19:W:49:ARG:HD2	38:A:2826:G:OP1	2.05	0.56
25:i:105:ASP:OD1	25:i:105:ASP:N	2.37	0.56
28:m:50:ARG:HD3	28:m:52:TYR:HH	1.65	0.56
40:D:130:ARG:NH1	40:D:131:TYR:O	2.38	0.56
50:f:127:MET:HB2	50:f:154:GLU:HB2	1.87	0.56
13:N:193:GLY:O	13:N:197:LYS:HB2	2.06	0.56
13:N:218:ILE:HA	13:N:223:MET:HG3	1.88	0.56
37:9:128:PHE:HD1	37:9:135:PHE:HB3	1.71	0.56
47:c:170:ALA:HB3	47:c:191:LEU:HD21	1.88	0.56
8:H:64:LEU:HD23	8:H:64:LEU:H	1.70	0.56
15:P:87:GLN:HE22	39:B:1625:A:H62	1.54	0.56
25:i:95:ARG:HB2	25:i:110:LEU:HD21	1.87	0.56
2:1:43:LEU:O	2:1:55:LEU:HA	2.05	0.55
4:3:124:ARG:HD2	12:M:78:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:64:LYS:HA	15:P:97:GLN:HE22	1.72	0.55
16:Q:79:GLU:OE2	16:Q:103:ARG:NH2	2.40	0.55
1:O:181:ARG:HD3	1:O:182:PRO:HD2	1.88	0.55
8:H:75:ARG:NH2	20:X:100:ARG:HH22	2.04	0.55
22:Z:99:VAL:HG23	26:j:73:PHE:CZ	2.42	0.55
35:5:385:HIS:HB2	38:A:2395:A:H1'	1.88	0.55
30:q:28:ARG:HH12	30:q:31:PRO:HD3	1.71	0.55
30:q:86:GLU:OE2	30:q:90:ARG:NH2	2.39	0.55
39:B:1635:C:H5''	50:f:112:ASN:HD21	1.71	0.55
45:V:108:MET:HE3	48:d:169:PHE:CD2	2.42	0.55
35:5:201:ARG:NH1	35:5:418:TYR:O	2.39	0.55
5:7:51:GLU:O	5:7:55:GLN:HB2	2.06	0.55
7:F:275:TRP:CZ2	24:g:55:THR:HG21	2.40	0.55
36:6:204:VAL:HB	36:6:245:VAL:HG21	1.89	0.55
7:F:133:THR:HG21	7:F:135:ARG:HE	1.72	0.55
8:H:107:VAL:HG12	8:H:108:ARG:H	1.70	0.55
44:U:3:ARG:O	44:U:23:ASN:ND2	2.39	0.55
5:7:77:THR:HG22	48:d:284:GLY:N	2.22	0.55
35:5:350:ARG:NH2	35:5:384:GLN:O	2.40	0.55
32:u:168:LEU:HD22	32:u:179:LEU:HD12	1.87	0.55
37:9:71:LYS:H	45:V:177:THR:HG22	1.71	0.55
9:J:29:ALA:HB1	9:J:50:CYS:HB2	1.89	0.55
11:L:98:PRO:HA	16:Q:162:ILE:HG13	1.89	0.55
10:K:27:PRO:HG2	10:K:30:LYS:HB3	1.88	0.54
18:S:173:ARG:NH2	38:A:2143:G:OP1	2.40	0.54
38:A:2194:U:O2'	38:A:2195:A:O4'	2.25	0.54
53:p:75:ARG:HG2	53:p:110:TRP:HE1	1.71	0.54
7:F:289:PRO:HG2	12:M:191:VAL:CG1	2.38	0.54
25:i:53:MET:HE2	30:q:27:ALA:HA	1.89	0.54
44:U:44:ILE:HG23	44:U:48:MET:HB3	1.89	0.54
17:R:36:ASN:OD1	17:R:37:ARG:HG3	2.07	0.54
40:D:228:LEU:HD11	40:D:234:MET:HE3	1.88	0.54
37:9:91:LEU:O	37:9:95:ALA:HB3	2.08	0.54
39:B:1634:A:H4'	50:f:108:GLN:HG2	1.89	0.54
44:U:46:MET:HE1	44:U:72:VAL:HG13	1.90	0.54
55:s:419:LEU:O	55:s:423:HIS:ND1	2.37	0.54
15:P:128:ILE:O	15:P:132:LEU:HB2	2.08	0.54
15:P:152:GLU:HG3	15:P:158:MET:HG3	1.90	0.54
40:D:207:ILE:HG22	40:D:207:ILE:O	2.05	0.54
4:3:183:ARG:NH1	36:6:355:LYS:O	2.40	0.54
7:F:217:LEU:HD11	7:F:243:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:72:PHE:HB2	19:W:107:HIS:HA	1.89	0.54
35:5:173:ARG:HA	35:5:176:TYR:CE2	2.43	0.54
38:A:2108:G:O6	42:I:31:LYS:HE2	2.08	0.54
44:U:37:GLU:CD	44:U:37:GLU:H	2.15	0.54
21:Y:114:THR:HG22	44:U:28:LEU:N	2.22	0.54
24:g:105:ARG:HB3	24:g:107:MET:HE2	1.89	0.54
35:5:308:GLN:HE22	38:A:2389:C:N4	2.05	0.54
36:6:218:LEU:HA	36:6:269:ALA:O	2.07	0.54
44:U:33:VAL:HG23	44:U:35:GLN:HE21	1.71	0.54
40:D:180:ASP:OD1	40:D:180:ASP:N	2.41	0.54
42:I:128:ASN:HA	42:I:131:LEU:HB3	1.90	0.54
44:U:30:ARG:HH11	44:U:107:PHE:HD2	1.54	0.54
55:s:165:ARG:O	55:s:307:ARG:NH2	2.39	0.54
13:N:250:ARG:HG2	13:N:250:ARG:HH11	1.72	0.54
20:X:163:ARG:HE	35:5:55:LEU:HD22	1.73	0.54
41:E:292:HIS:ND1	41:E:293:LYS:O	2.34	0.54
42:I:83:ARG:HG2	42:I:134:PHE:HE1	1.73	0.54
54:r:85:ASP:OD1	54:r:85:ASP:N	2.33	0.54
16:Q:131:SER:HB3	32:u:119:ARG:HD3	1.90	0.53
20:X:64:ASP:OD1	20:X:64:ASP:N	2.37	0.53
36:6:322:ARG:NH1	53:p:181:GLU:OE1	2.42	0.53
16:Q:117:LEU:O	16:Q:134:LEU:HA	2.08	0.53
22:Z:134:MET:HG2	26:j:75:ARG:HE	1.74	0.53
23:b:108:SER:OG	23:b:109:GLY:N	2.41	0.53
35:5:251:HIS:O	35:5:371:LYS:NZ	2.38	0.53
7:F:245:ALA:O	25:i:63:LEU:HD11	2.07	0.53
16:Q:121:THR:HG22	16:Q:171:VAL:HG12	1.89	0.53
16:Q:152:ARG:HG3	16:Q:161:GLU:HG2	1.89	0.53
33:v:21:ARG:HH12	34:w:123:GLU:C	2.15	0.53
40:D:226:ILE:O	40:D:233:GLN:HA	2.08	0.53
5:7:156:ARG:NH2	5:7:259:ASP:O	2.42	0.53
47:c:121:SER:OG	47:c:122:ASN:N	2.38	0.53
15:P:56:LEU:HB3	15:P:62:ALA:HB2	1.91	0.53
30:q:40:PRO:HG3	30:q:51:GLN:HB3	1.90	0.53
55:s:211:VAL:HG22	55:s:230:ARG:HG3	1.91	0.53
10:K:114:LYS:HE2	38:A:2702:G:H5'	1.91	0.53
38:A:2212:C:H2'	38:A:2213:A:H8	1.74	0.53
52:k:66:VAL:HB	52:k:74:LEU:HB3	1.89	0.53
5:7:108:VAL:HG22	5:7:125:ILE:HG12	1.90	0.53
9:J:89:TYR:O	9:J:93:ALA:CB	2.57	0.53
21:Y:72:LYS:O	21:Y:76:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:q:41:ASP:OD1	30:q:41:ASP:N	2.41	0.53
32:u:108:ASP:O	32:u:127:VAL:HA	2.09	0.53
41:E:208:ALA:HB2	41:E:297:VAL:HG12	1.91	0.53
41:E:268:GLU:HB3	41:E:271:LEU:HD11	1.91	0.53
43:T:97:MET:HE1	43:T:105:GLN:HG3	1.90	0.53
54:r:70:CYS:SG	54:r:73:CYS:HB2	2.48	0.53
33:v:23:LEU:HD23	33:v:28:ARG:HG2	1.90	0.53
42:I:87:ALA:HA	42:I:90:PHE:HD2	1.74	0.53
7:F:70:ARG:NH1	7:F:194:GLU:OE1	2.42	0.53
37:9:30:PHE:HA	38:A:1701:U:O4	2.09	0.53
32:u:127:VAL:HG23	32:u:179:LEU:HD23	1.91	0.52
40:D:166:SER:OG	40:D:182:HIS:ND1	2.39	0.52
45:V:122:LEU:HD12	45:V:133:ILE:HG13	1.91	0.52
49:e:266:PRO:HD2	49:e:269:LEU:HB2	1.91	0.52
11:L:108:ILE:HA	11:L:114:PRO:HA	1.90	0.52
42:I:191:PHE:O	42:I:195:SER:CB	2.57	0.52
14:O:49:VAL:HG12	14:O:107:MET:HE2	1.91	0.52
15:P:58:LEU:HD23	53:p:177:ARG:HH21	1.74	0.52
27:l:119:ARG:NH1	38:A:2192:A:OP2	2.43	0.52
38:A:2531:U:O4	40:D:246:ARG:NH2	2.42	0.52
12:M:264:GLN:NE2	12:M:269:LEU:O	2.43	0.52
22:Z:36:PHE:HE2	22:Z:79:PRO:HG3	1.74	0.52
37:9:134:ASN:O	44:U:8:PRO:HG3	2.09	0.52
40:D:248:SER:OG	40:D:249:ASN:N	2.42	0.52
55:s:51:MET:HE3	55:s:65:ARG:CD	2.38	0.52
6:8:122:SER:CB	39:B:1628:C:H1'	2.38	0.52
12:M:207:PRO:C	30:q:99:MET:HE1	2.34	0.52
1:0:179:ARG:NH1	1:0:182:PRO:HG3	2.21	0.52
36:6:52:ARG:HB3	39:B:1637:C:H5'	1.91	0.52
45:V:36:PRO:HG2	45:V:39:ILE:HG23	1.91	0.52
10:K:21:LEU:HD11	10:K:34:MET:HE3	1.92	0.52
28:m:71:PRO:HD2	49:e:87:HIS:CG	2.44	0.52
41:E:106:MET:HG2	41:E:120:THR:HG22	1.92	0.52
41:E:331:ASP:N	41:E:331:ASP:OD1	2.42	0.52
35:5:178:PRO:O	35:5:182:ASP:HB2	2.10	0.52
38:A:2348:A:H5'	48:d:62:LYS:HB3	1.91	0.52
42:I:162:LYS:HD2	42:I:196:LYS:HA	1.90	0.52
9:J:138:SER:HA	9:J:141:VAL:HG12	1.91	0.52
36:6:105:GLU:O	36:6:109:ALA:HB2	2.10	0.52
45:V:123:VAL:HG13	45:V:128:ARG:HA	1.92	0.52
4:3:175:ASP:HB3	4:3:178:GLN:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:6:365:TYR:HA	36:6:368:ARG:HD3	1.92	0.51
41:E:104:LEU:HB2	41:E:121:LEU:HB2	1.91	0.51
41:E:133:THR:OG1	41:E:144:THR:OG1	2.27	0.51
5:7:148:MET:HE2	5:7:262:ASP:HB3	1.92	0.51
15:P:79:HIS:HA	15:P:95:GLU:O	2.10	0.51
23:b:80:LEU:HD11	47:c:78:ARG:HD3	1.92	0.51
1:0:95:ARG:HG2	43:T:88:TRP:CH2	2.46	0.51
7:F:116:THR:HG23	7:F:118:ALA:H	1.75	0.51
7:F:143:SER:HG	7:F:146:TRP:CD1	2.29	0.51
18:S:116:ILE:HD11	18:S:193:LEU:HD12	1.93	0.51
37:9:22:THR:HG23	37:9:24:LYS:H	1.75	0.51
49:e:143:LYS:O	49:e:146:ARG:NH1	2.44	0.51
9:J:128:GLU:HA	9:J:133:GLN:HE21	1.76	0.51
14:O:42:ILE:O	14:O:122:VAL:HA	2.10	0.51
18:S:174:PHE:HA	18:S:180:PHE:O	2.10	0.51
36:6:233:LEU:HB3	36:6:298:PHE:CE1	2.45	0.51
42:I:40:MET:HE1	42:I:48:MET:HE2	1.91	0.51
55:s:184:LEU:O	55:s:188:LEU:HB2	2.10	0.51
55:s:207:HIS:ND1	55:s:234:ASP:OD1	2.43	0.51
55:s:362:THR:OG1	55:s:363:ASP:N	2.42	0.51
3:2:82:ARG:HE	3:2:87:ARG:HD2	1.75	0.51
6:8:117:LEU:O	6:8:121:TRP:CB	2.58	0.51
7:F:187:LEU:HD12	7:F:259:LEU:HD23	1.92	0.51
18:S:142:THR:HG23	46:a:62:HIS:NE2	2.26	0.51
34:w:100:VAL:HB	34:w:142:GLN:HB2	1.91	0.51
41:E:119:VAL:HG11	41:E:284:TYR:HB3	1.92	0.51
42:I:191:PHE:O	42:I:195:SER:HB2	2.11	0.51
43:T:75:HIS:HD2	43:T:120:VAL:HG13	1.75	0.51
51:h:78:PHE:HE2	51:h:89:ILE:HD13	1.75	0.51
51:h:91:LEU:HD23	51:h:97:LYS:HG3	1.92	0.51
7:F:89:THR:H	7:F:179:THR:HG21	1.75	0.51
13:N:105:MET:HE2	13:N:179:VAL:HG13	1.93	0.51
32:u:99:SER:O	32:u:103:GLN:CB	2.57	0.51
35:5:151:ASP:O	35:5:155:LEU:HB2	2.10	0.51
38:A:2180:A:H1'	38:A:2206:C:H4'	1.93	0.51
8:H:98:LEU:HD22	8:H:102:VAL:HG21	1.93	0.51
19:W:74:ARG:NH1	38:A:2833:A:OP1	2.40	0.51
35:5:305:GLN:NE2	38:A:2389:C:O2'	2.44	0.51
38:A:3123:G:N2	38:A:3133:A:OP2	2.43	0.51
55:s:110:THR:HG23	55:s:333:PHE:CG	2.46	0.51
2:1:19:ARG:HB3	2:1:62:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:66:LEU:HB3	9:J:82:ILE:HD11	1.92	0.51
20:X:150:LYS:HG3	20:X:159:MET:HE2	1.93	0.51
53:p:100:GLU:OE2	53:p:102:ARG:NH2	2.39	0.51
54:r:94:ARG:HE	54:r:100:LEU:HD23	1.75	0.51
55:s:105:TRP:HH2	55:s:266:CYS:SG	2.33	0.51
7:F:230:ILE:HG23	7:F:242:LEU:HD11	1.93	0.51
16:Q:111:PHE:O	16:Q:140:ARG:NH1	2.43	0.51
17:R:54:THR:HG21	18:S:171:ILE:HA	1.93	0.51
18:S:111:GLU:HG2	23:b:19:LEU:HD21	1.92	0.51
47:c:220:ILE:O	47:c:223:MET:HG2	2.10	0.51
48:d:164:VAL:HG23	48:d:261:MET:HB2	1.92	0.51
10:K:16:ARG:HH22	10:K:124:ARG:HH21	1.59	0.51
14:O:45:PRO:HG2	14:O:48:ARG:HD2	1.93	0.51
35:5:213:TRP:O	35:5:219:LEU:HD12	2.11	0.51
42:I:83:ARG:O	42:I:87:ALA:CB	2.59	0.51
55:s:324:PHE:HA	55:s:361:ILE:HD11	1.92	0.51
7:F:275:TRP:CZ2	24:g:55:THR:CG2	2.94	0.50
10:K:154:ARG:NH1	10:K:157:GLU:OE2	2.43	0.50
38:A:1724:A:H2'	38:A:1724:A:N3	2.26	0.50
54:r:93:ILE:HG22	54:r:94:ARG:O	2.11	0.50
11:L:72:GLN:HA	11:L:84:ALA:O	2.10	0.50
13:N:226:ILE:HD13	42:I:47:LEU:HG	1.93	0.50
15:P:102:VAL:HG11	15:P:141:ILE:HD11	1.92	0.50
30:q:34:ARG:HG3	30:q:38:ARG:HD3	1.92	0.50
36:6:376:THR:HG23	38:A:1892:A:N1	2.27	0.50
38:A:2673:G:H5''	43:T:112:LYS:HB2	1.92	0.50
43:T:153:LEU:HB2	43:T:169:LYS:HB2	1.92	0.50
52:k:42:VAL:O	52:k:46:ASN:N	2.41	0.50
10:K:69:GLY:HA2	54:r:152:THR:HA	1.93	0.50
16:Q:103:ARG:NH1	16:Q:108:ILE:HB	2.27	0.50
18:S:173:ARG:NH1	38:A:2262:C:OP1	2.45	0.50
55:s:325:ARG:O	55:s:328:ALA:HB3	2.11	0.50
6:8:165:ASP:OD2	49:e:185:ARG:NH1	2.45	0.50
20:X:127:VAL:HG22	20:X:131:THR:HB	1.93	0.50
32:u:140:PHE:O	32:u:144:LYS:HB2	2.12	0.50
52:k:15:GLN:HB3	52:k:67:LEU:HB2	1.94	0.50
7:F:280:TYR:CG	12:M:125:ARG:HD2	2.46	0.50
12:M:146:ASP:N	12:M:146:ASP:OD1	2.42	0.50
13:N:160:VAL:HG12	13:N:161:VAL:HG23	1.94	0.50
40:D:154:THR:H	40:D:157:MET:HE3	1.76	0.50
40:D:257:ILE:HG23	40:D:262:ARG:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:e:198:ASN:HD22	49:e:243:PHE:HD1	1.59	0.50
12:M:94:LYS:HG3	12:M:129:ILE:HG22	1.92	0.50
38:A:2182:G:H1'	38:A:2199:A:H2'	1.91	0.50
38:A:2342:U:H5''	44:U:78:LYS:HB3	1.94	0.50
40:D:206:TYR:N	40:D:206:TYR:CD2	2.80	0.50
4:3:138:PRO:HG2	38:A:2854:U:H4'	1.94	0.50
7:F:285:PRO:HD3	38:A:1887:A:O4'	2.12	0.50
8:H:103:GLU:HG2	8:H:104:ASN:H	1.76	0.50
10:K:3:SER:O	47:c:302:ARG:NH1	2.45	0.50
11:L:101:ASP:OD2	16:Q:152:ARG:NH2	2.31	0.50
11:L:123:ILE:HD12	11:L:141:ALA:HB2	1.93	0.50
13:N:224:LEU:HD12	29:o:38:ARG:HH11	1.76	0.50
18:S:152:ASP:OD1	18:S:152:ASP:N	2.44	0.50
23:b:133:PHE:CD1	47:c:259:ARG:HD3	2.46	0.50
48:d:190:GLU:OE1	48:d:215:ARG:NH1	2.37	0.50
49:e:139:GLU:HG2	49:e:152:LYS:HA	1.93	0.50
53:p:133:LEU:HD21	53:p:157:MET:HE1	1.92	0.50
15:P:96:HIS:ND1	15:P:98:ASN:OD1	2.45	0.50
16:Q:136:ILE:O	16:Q:151:LEU:HA	2.11	0.50
20:X:144:TYR:O	20:X:148:THR:CG2	2.53	0.50
35:5:228:ALA:HB3	35:5:292:TYR:HB2	1.93	0.50
35:5:354:PHE:HB2	35:5:377:ASP:HB2	1.93	0.50
40:D:198:SER:HB2	40:D:206:TYR:OH	2.12	0.50
55:s:332:LEU:HD21	55:s:359:ALA:HB2	1.93	0.50
22:Z:53:HIS:CE1	29:o:51:MET:HE1	2.47	0.50
22:Z:99:VAL:HG23	26:j:73:PHE:CE1	2.47	0.50
30:q:64:TYR:HB3	30:q:68:SER:HB2	1.94	0.50
36:6:175:VAL:HG22	36:6:204:VAL:HG22	1.92	0.50
37:9:68:PHE:CE2	37:9:70:LEU:HB2	2.47	0.50
7:F:167:MET:HA	7:F:170:ARG:HE	1.77	0.49
35:5:136:VAL:HG22	35:5:420:HIS:CD2	2.46	0.49
40:D:207:ILE:HG12	40:D:229:PRO:HD3	1.94	0.49
41:E:252:TRP:O	41:E:255:THR:OG1	2.26	0.49
46:a:73:LYS:O	47:c:256:ARG:HD3	2.12	0.49
55:s:242:ARG:NH2	55:s:292:CYS:O	2.45	0.49
6:8:94:PHE:HB3	49:e:83:LEU:HD23	1.94	0.49
28:m:71:PRO:HD2	49:e:87:HIS:CD2	2.48	0.49
41:E:102:LEU:O	41:E:122:LEU:HA	2.12	0.49
49:e:51:LEU:HD12	49:e:188:ALA:HB1	1.93	0.49
10:K:59:ILE:HB	10:K:127:LEU:HD23	1.94	0.49
13:N:57:PRO:HD2	13:N:150:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:6:268:LEU:O	36:6:318:PHE:HA	2.12	0.49
55:s:89:MET:HG3	55:s:275:LYS:HE3	1.93	0.49
55:s:112:THR:HG22	55:s:391:ASN:HB2	1.94	0.49
2:1:20:MET:SD	2:1:58:GLU:HB3	2.52	0.49
2:1:20:MET:O	2:1:29:CYS:HA	2.11	0.49
9:J:49:PHE:O	9:J:53:PHE:HB2	2.12	0.49
12:M:44:ARG:NH1	38:A:2268:G:N7	2.57	0.49
12:M:62:ARG:NH1	25:i:126:LYS:O	2.45	0.49
41:E:171:PRO:O	41:E:173:LYS:NZ	2.45	0.49
11:L:87:VAL:HG11	11:L:123:ILE:HG12	1.93	0.49
27:l:133:SER:O	38:A:2200:A:O2'	2.31	0.49
7:F:142:ARG:NH2	38:A:1794:A:OP1	2.40	0.49
14:O:49:VAL:HG13	14:O:123:ILE:HG12	1.94	0.49
25:i:87:GLU:OE2	25:i:113:ARG:NH1	2.45	0.49
38:A:1874:A:O2'	38:A:2090:A:O2'	2.30	0.49
38:A:2123:C:HO2'	38:A:2134:A:HO2'	1.60	0.49
40:D:66:TRP:HA	40:D:80:ARG:HH11	1.78	0.49
6:8:132:GLU:OE1	50:f:109:TYR:OH	2.30	0.49
7:F:160:SER:OG	25:i:83:TRP:O	2.26	0.49
13:N:191:SER:OG	13:N:192:ARG:N	2.44	0.49
14:O:65:LEU:HB3	14:O:69:ASN:HD22	1.77	0.49
24:g:91:MET:HE3	38:A:1883:G:H5''	1.94	0.49
38:A:3127:G:H2'	38:A:3128:A:H2'	1.94	0.49
40:D:138:ASP:OD1	40:D:138:ASP:N	2.43	0.49
49:e:198:ASN:HD21	49:e:200:MET:HE2	1.77	0.49
7:F:249:ASN:N	7:F:249:ASN:OD1	2.42	0.49
33:v:46:GLU:H	33:v:51:ARG:HH21	1.60	0.49
7:F:226:MET:HE3	30:q:26:ARG:HH12	1.74	0.49
10:K:39:LEU:HD11	10:K:125:LEU:HB2	1.95	0.49
15:P:54:ARG:NH1	15:P:140:GLY:O	2.45	0.49
15:P:85:ARG:HD2	15:P:158:MET:HE3	1.95	0.49
28:m:41:THR:OG1	28:m:67:ARG:NH2	2.46	0.49
38:A:1747:G:OP2	38:A:1749:C:N4	2.44	0.49
12:M:132:LEU:O	12:M:133:LYS:HB2	2.12	0.49
41:E:97:VAL:O	41:E:197:HIS:NE2	2.38	0.49
55:s:165:ARG:HG2	55:s:307:ARG:HH12	1.77	0.49
55:s:240:GLN:HB3	55:s:298:GLN:HG3	1.95	0.49
10:K:101:VAL:HG13	10:K:127:LEU:HD13	1.95	0.48
10:K:117:HIS:CE1	38:A:1839:C:H5'	2.48	0.48
36:6:221:LEU:HD12	36:6:267:ARG:HG3	1.94	0.48
40:D:220:VAL:HG12	40:D:221:ASN:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:e:146:ARG:HB3	49:e:253:VAL:HG13	1.94	0.48
5:7:112:PRO:HB2	5:7:267:PRO:HG2	1.95	0.48
6:8:114:ARG:HG3	49:e:73:LEU:HD21	1.95	0.48
35:5:259:ILE:HD11	40:D:125:LYS:HB3	1.96	0.48
38:A:2529:U:OP2	40:D:208:ARG:NE	2.44	0.48
10:K:8:PRO:HG2	47:c:295:GLU:HG3	1.95	0.48
27:l:114:SER:OG	27:l:115:ARG:N	2.45	0.48
38:A:2173:G:H2'	38:A:2174:G:C8	2.47	0.48
44:U:44:ILE:HG22	44:U:93:LYS:HB3	1.94	0.48
18:S:122:LEU:HD21	26:j:49:TRP:CH2	2.47	0.48
47:c:275:TYR:HA	47:c:280:LEU:HA	1.96	0.48
10:K:21:LEU:HD12	10:K:145:LEU:HD12	1.95	0.48
12:M:264:GLN:NE2	12:M:267:PHE:O	2.47	0.48
38:A:2318:A:H2'	38:A:2319:A:C8	2.48	0.48
44:U:52:ASP:O	44:U:56:TYR:HB2	2.14	0.48
45:V:46:VAL:HG11	45:V:83:ARG:HA	1.96	0.48
54:r:72:ILE:HD12	54:r:111:GLU:HB3	1.94	0.48
28:m:73:ARG:CB	49:e:128:PHE:HB2	2.44	0.48
36:6:161:LEU:HD13	36:6:221:LEU:HD21	1.94	0.48
41:E:207:THR:HG22	41:E:298:LYS:HD2	1.94	0.48
49:e:203:LYS:N	49:e:237:LEU:O	2.46	0.48
22:Z:100:HIS:HB3	22:Z:106:VAL:HG11	1.94	0.48
35:5:258:PRO:HB3	40:D:123:GLU:HB2	1.96	0.48
38:A:3179:G:O2'	38:A:3190:A:N6	2.42	0.48
43:T:91:ALA:O	43:T:145:SER:OG	2.30	0.48
11:L:42:ASP:HB3	11:L:44:SER:H	1.78	0.48
11:L:119:ILE:HG21	11:L:123:ILE:HD11	1.95	0.48
14:O:67:ASP:OD2	55:s:44:TYR:OH	2.26	0.48
15:P:175:PRO:HG2	53:p:177:ARG:NH1	2.29	0.48
42:I:160:LYS:HG2	42:I:163:GLU:HB3	1.96	0.48
2:1:19:ARG:NH2	38:A:2906:C:O2	2.47	0.48
12:M:182:ARG:HH21	12:M:182:ARG:HG3	1.78	0.48
38:A:2521:A:N6	40:D:202:ARG:O	2.46	0.48
43:T:94:ILE:HA	43:T:97:MET:HE2	1.95	0.48
2:1:63:ARG:HD3	38:A:2909:G:H5'	1.96	0.48
9:J:22:ALA:H	9:J:68:THR:HG22	1.78	0.48
9:J:113:THR:HA	9:J:156:VAL:HB	1.95	0.48
38:A:2387:U:H3'	40:D:75:THR:HB	1.96	0.48
38:A:2397:C:H2'	38:A:2398:A:O4'	2.14	0.48
51:h:151:ASN:OD1	51:h:151:ASN:N	2.47	0.48
5:7:52:LYS:HG3	5:7:219:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:42:HIS:CG	20:X:86:ILE:HD11	2.49	0.47
38:A:1718:A:N3	38:A:1911:C:O2'	2.39	0.47
38:A:1737:A:H61	38:A:1760:G:H1'	1.79	0.47
45:V:147:SER:OG	45:V:150:SER:O	2.31	0.47
47:c:163:GLU:O	47:c:167:CYS:HB2	2.14	0.47
7:F:278:SER:OG	7:F:278:SER:O	2.32	0.47
12:M:276:ASN:ND2	12:M:279:ASP:OD1	2.47	0.47
18:S:128:ILE:HG23	26:j:49:TRP:HB2	1.96	0.47
25:i:70:PRO:O	25:i:73:LEU:HB2	2.14	0.47
28:m:72:ARG:HG2	49:e:124:TRP:CZ2	2.49	0.47
55:s:271:LEU:O	55:s:272:PRO:C	2.56	0.47
3:2:85:LYS:HG2	38:A:1782:G:C8	2.49	0.47
8:H:98:LEU:HD23	8:H:129:ALA:HB2	1.97	0.47
9:J:39:LEU:HB3	9:J:44:VAL:HG11	1.97	0.47
21:Y:67:PHE:CG	44:U:28:LEU:HD23	2.50	0.47
22:Z:53:HIS:HE1	29:o:51:MET:HE1	1.78	0.47
52:k:39:SER:OG	52:k:40:GLU:N	2.47	0.47
54:r:90:SER:HA	54:r:93:ILE:HD12	1.96	0.47
1:0:90:ASN:O	1:0:94:ARG:HG2	2.14	0.47
5:7:302:LEU:HD23	14:O:144:LEU:HD12	1.97	0.47
6:8:164:ARG:HD3	50:f:88:TYR:CE1	2.49	0.47
34:w:81:ASP:O	34:w:85:TYR:CB	2.59	0.47
35:5:270:ILE:O	38:A:2409:A:O2'	2.33	0.47
36:6:235:TRP:HB3	36:6:254:TYR:HA	1.97	0.47
43:T:69:ARG:NH1	48:d:228:PHE:O	2.48	0.47
12:M:227:ALA:HB2	53:p:52:SER:HB3	1.96	0.47
14:O:106:ARG:HG2	14:O:124:GLU:HG2	1.97	0.47
16:Q:154:VAL:HG12	16:Q:159:GLY:HA2	1.96	0.47
36:6:222:ASP:OD1	36:6:222:ASP:N	2.44	0.47
49:e:74:LEU:O	49:e:78:GLU:HB2	2.15	0.47
7:F:217:LEU:HD23	7:F:259:LEU:HD12	1.96	0.47
7:F:268:PHE:CE2	25:i:63:LEU:HD12	2.40	0.47
18:S:112:ASP:O	18:S:194:ARG:HA	2.14	0.47
21:Y:92:ASN:HB3	45:V:185:ARG:HA	1.96	0.47
25:i:36:LEU:HD23	38:A:1676:A:H1'	1.97	0.47
34:w:131:PRO:HG2	34:w:134:ASP:HB2	1.96	0.47
35:5:107:PHE:HB3	35:5:222:VAL:HG12	1.95	0.47
46:a:37:SER:OG	46:a:39:LEU:O	2.32	0.47
49:e:171:TRP:CD1	49:e:263:TYR:HB3	2.50	0.47
49:e:183:THR:O	49:e:187:THR:N	2.46	0.47
55:s:188:LEU:HD21	55:s:422:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:90:PHE:HE2	9:J:120:ILE:HD13	1.80	0.47
12:M:37:GLU:HG3	38:A:1901:C:OP1	2.15	0.47
12:M:191:VAL:CG2	24:g:52:LEU:HD23	2.45	0.47
12:M:268:GLY:HA3	24:g:47:PHE:CG	2.50	0.47
20:X:97:LEU:HD23	38:A:2919:A:C2	2.49	0.47
28:m:39:SER:HA	50:f:102:LEU:HD22	1.97	0.47
35:5:33:TRP:O	35:5:39:ARG:NH2	2.48	0.47
7:F:138:HIS:CD2	7:F:146:TRP:HE1	2.33	0.47
38:A:1800:G:N1	38:A:1803:A:OP2	2.47	0.47
38:A:2030:U:H5	38:A:2124:A:N1	2.13	0.47
38:A:2123:C:C3'	38:A:2124:A:H5''	2.45	0.47
38:A:2284:C:H5''	47:c:39:PHE:CE2	2.49	0.47
38:A:2668:A:H2'	38:A:2669:A:C8	2.49	0.47
44:U:44:ILE:HD11	44:U:53:LEU:HG	1.96	0.47
15:P:84:ILE:HB	15:P:91:GLU:HB3	1.97	0.47
36:6:371:ASP:OD1	36:6:371:ASP:N	2.45	0.47
38:A:2037:U:H4'	38:A:2040:G:N1	2.30	0.47
6:8:114:ARG:HE	49:e:73:LEU:HD11	1.79	0.46
8:H:58:ARG:NH1	8:H:77:HIS:O	2.47	0.46
15:P:68:TRP:HZ3	19:W:130:PHE:CE2	2.33	0.46
19:W:67:ILE:HG21	19:W:131:VAL:HG11	1.96	0.46
19:W:118:THR:HG22	36:6:53:SER:O	2.14	0.46
28:m:54:VAL:HG13	28:m:54:VAL:O	2.14	0.46
38:A:3131:G:H3'	38:A:3132:G:H8	1.81	0.46
6:8:154:SER:HB3	49:e:230:LYS:HZ1	1.80	0.46
8:H:59:TRP:CZ3	8:H:81:LYS:HD3	2.50	0.46
12:M:59:ARG:NH1	38:A:2016:C:OP2	2.41	0.46
13:N:76:SER:HB3	13:N:155:LYS:HB2	1.96	0.46
42:I:83:ARG:O	42:I:87:ALA:HB3	2.15	0.46
43:T:85:ASP:OD1	43:T:85:ASP:N	2.42	0.46
6:8:169:PHE:HB2	6:8:170:PRO:HD3	1.96	0.46
18:S:118:ASN:ND2	38:A:2256:U:O2'	2.49	0.46
19:W:116:LEU:HD11	50:f:59:TYR:CE2	2.50	0.46
24:g:107:MET:SD	24:g:148:ARG:HD3	2.56	0.46
25:i:60:ILE:HD13	30:q:31:PRO:HG2	1.97	0.46
38:A:1814:A:H2'	38:A:1815:A:C8	2.50	0.46
54:r:99:MET:HG3	54:r:116:GLU:HG2	1.98	0.46
55:s:214:GLU:HA	55:s:228:ASP:HA	1.98	0.46
9:J:43:GLY:HA3	9:J:76:ARG:HH12	1.80	0.46
12:M:229:PHE:HE2	12:M:259:ARG:HH12	1.64	0.46
16:Q:102:ARG:NH1	16:Q:169:PRO:HA	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:9:42:GLY:HA3	37:9:51:VAL:O	2.16	0.46
40:D:202:ARG:HE	40:D:205:GLN:NE2	2.13	0.46
44:U:66:ALA:HB2	44:U:100:ALA:HB2	1.98	0.46
15:P:178:ILE:O	36:6:346:ARG:NH2	2.49	0.46
25:i:49:GLU:OE1	30:q:25:TYR:CD1	2.69	0.46
39:B:1609:U:O2	39:B:1616:A:N6	2.48	0.46
41:E:148:GLY:HA2	41:E:175:THR:O	2.15	0.46
19:W:127:TYR:CE2	36:6:71:TRP:CZ2	2.99	0.46
21:Y:69:ASP:OD1	21:Y:69:ASP:N	2.46	0.46
24:g:100:ILE:HA	24:g:105:ARG:O	2.14	0.46
38:A:2181:A:N6	38:A:2206:C:O2'	2.48	0.46
43:T:61:PRO:HB3	48:d:225:TYR:CG	2.50	0.46
48:d:213:THR:HG22	48:d:247:VAL:HG22	1.97	0.46
5:7:282:ALA:HB2	5:7:321:ARG:HG2	1.98	0.46
5:7:316:LEU:HD21	14:O:149:LEU:HD23	1.98	0.46
10:K:177:ARG:NH1	38:A:3183:U:O2	2.48	0.46
26:j:53:ASP:OD2	26:j:55:ARG:NH2	2.48	0.46
40:D:184:LEU:HD13	40:D:226:ILE:HD11	1.98	0.46
45:V:95:TYR:HB3	45:V:108:MET:SD	2.55	0.46
13:N:50:LEU:HB2	13:N:110:ASN:HD21	1.80	0.46
15:P:154:ALA:HA	15:P:159:LYS:HE3	1.97	0.46
20:X:10:LEU:CD2	30:q:45:LEU:HB3	2.46	0.46
32:u:135:LEU:HD22	32:u:179:LEU:HB3	1.97	0.46
36:6:265:ILE:HG12	36:6:322:ARG:HG2	1.97	0.46
47:c:215:ILE:HG23	47:c:219:LEU:HD12	1.98	0.46
7:F:291:SER:HB3	24:g:54:ALA:HA	1.97	0.46
12:M:261:ASP:HB2	12:M:262:PRO:HD2	1.97	0.46
18:S:164:THR:HG22	23:b:107:GLN:HB2	1.97	0.46
19:W:145:VAL:HG21	36:6:343:GLU:HB2	1.98	0.46
20:X:130:ARG:HE	20:X:134:LEU:HD11	1.81	0.46
20:X:144:TYR:CE1	20:X:148:THR:HG21	2.51	0.46
23:b:11:LEU:HD23	23:b:115:ILE:HD13	1.98	0.46
23:b:19:LEU:HD22	47:c:316:TYR:CE2	2.50	0.46
36:6:274:LYS:HG3	36:6:314:ALA:HB2	1.98	0.46
38:A:1871:A:H61	38:A:1901:C:H5'	1.81	0.46
38:A:2349:G:H2'	38:A:2350:A:C8	2.50	0.46
38:A:2740:A:H2'	38:A:2741:A:C8	2.51	0.46
45:V:19:TYR:OH	45:V:31:ASP:OD2	2.32	0.46
45:V:25:PRO:HG2	45:V:28:SER:HB3	1.96	0.46
55:s:405:ILE:HG12	55:s:410:VAL:HG12	1.97	0.46
1:0:84:ARG:HB2	38:A:2680:U:O2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:120:LYS:HA	6:8:123:LEU:HD12	1.98	0.46
17:R:10:LEU:CD2	38:A:1775:A:H4'	2.46	0.46
18:S:98:VAL:HB	18:S:135:LEU:HB3	1.98	0.46
44:U:71:ARG:NH2	44:U:96:TYR:OH	2.48	0.46
49:e:256:THR:OG1	49:e:257:LYS:N	2.41	0.46
52:k:76:MET:HG2	54:r:49:ILE:HB	1.98	0.46
55:s:110:THR:HG22	55:s:112:THR:HG23	1.97	0.46
5:7:44:ARG:HB3	5:7:261:ILE:HD12	1.96	0.45
10:K:21:LEU:CD2	10:K:31:LEU:HD22	2.44	0.45
13:N:139:ARG:NH1	38:A:2815:G:N7	2.63	0.45
15:P:42:GLU:HB3	36:6:337:MET:HB2	1.98	0.45
15:P:112:ILE:HD13	15:P:131:VAL:HG21	1.98	0.45
36:6:238:THR:HG21	36:6:281:PHE:HD2	1.80	0.45
8:H:97:ILE:HG21	8:H:140:PHE:CD2	2.52	0.45
17:R:43:VAL:HG11	38:A:2296:U:C5	2.51	0.45
17:R:141:ILE:HG22	46:a:51:LEU:HD12	1.98	0.45
25:i:59:ASN:HB3	25:i:63:LEU:HD23	1.97	0.45
33:v:32:PHE:HZ	34:w:117:GLU:HG3	1.81	0.45
43:T:74:TYR:CE2	43:T:177:LYS:HD3	2.51	0.45
5:7:175:ILE:HG12	14:O:147:GLN:HE21	1.81	0.45
10:K:2:SER:HB2	23:b:128:GLY:HA2	1.97	0.45
13:N:104:MET:HE3	13:N:108:THR:HG21	1.98	0.45
18:S:100:HIS:O	18:S:100:HIS:CG	2.69	0.45
35:5:200:ARG:NH2	35:5:234:ASP:OD1	2.49	0.45
35:5:260:SER:CB	40:D:145:GLY:HA2	2.46	0.45
51:h:105:ALA:HB1	51:h:111:VAL:HG22	1.99	0.45
55:s:174:LEU:HB3	55:s:175:PRO:HD3	1.98	0.45
55:s:249:GLU:HB3	55:s:354:PRO:HG2	1.97	0.45
7:F:83:HIS:HB3	7:F:86:VAL:HG12	1.98	0.45
10:K:90:VAL:HG13	10:K:94:GLN:HB2	1.99	0.45
32:u:114:VAL:N	32:u:122:ASP:O	2.45	0.45
42:I:119:HIS:HB3	42:I:121:ILE:HG22	1.98	0.45
3:2:89:SER:OG	37:9:17:ARG:NH1	2.50	0.45
19:W:103:VAL:HG11	36:6:61:ALA:HB1	1.98	0.45
50:f:127:MET:HE3	50:f:128:PRO:HD2	1.98	0.45
7:F:223:HIS:HA	7:F:226:MET:HE2	1.99	0.45
17:R:31:PHE:CD1	38:A:1829:A:H5'	2.52	0.45
49:e:157:LEU:HD23	49:e:254:TRP:HB3	1.99	0.45
49:e:162:ARG:HH11	49:e:171:TRP:HB2	1.81	0.45
55:s:105:TRP:CZ3	55:s:268:PRO:HA	2.50	0.45
4:3:115:LEU:HB2	12:M:83:PHE:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:114:ILE:HG22	18:S:116:ILE:HG13	1.98	0.45
22:Z:115:HIS:HA	29:o:42:GLU:OE1	2.17	0.45
43:T:212:LEU:O	46:a:142:ARG:NH2	2.50	0.45
50:f:166:PHE:O	50:f:170:PHE:CB	2.65	0.45
12:M:142:GLU:HB2	12:M:162:LEU:HD22	1.99	0.45
13:N:103:GLU:OE1	13:N:106:ARG:NH2	2.42	0.45
13:N:114:ASP:H	13:N:118:MET:HE3	1.81	0.45
13:N:209:ASN:HB3	42:I:53:TYR:CD1	2.52	0.45
13:N:224:LEU:HD11	29:o:38:ARG:HB3	1.98	0.45
19:W:76:HIS:HB2	19:W:130:PHE:CD1	2.52	0.45
21:Y:83:ALA:HB2	37:9:76:TYR:CE1	2.51	0.45
4:3:133:LEU:HD22	4:3:141:LYS:HG2	1.99	0.45
11:L:99:ARG:NH1	16:Q:161:GLU:OE1	2.50	0.45
16:Q:122:ALA:HB2	16:Q:172:GLN:HE22	1.82	0.45
38:A:2312:A:H2'	38:A:2313:A:O4'	2.17	0.45
44:U:80:ARG:HD3	44:U:84:ASN:OD1	2.16	0.45
19:W:54:LYS:HE2	38:A:2862:C:O3'	2.17	0.45
19:W:74:ARG:HD2	38:A:2065:A:C5	2.52	0.45
33:v:43:GLN:HA	58:v:101:PNS:H432	1.99	0.45
40:D:74:ILE:HD13	40:D:148:LYS:HB2	1.99	0.45
40:D:205:GLN:HB2	40:D:206:TYR:CE2	2.51	0.45
45:V:54:TRP:NE1	45:V:56:LEU:O	2.50	0.45
55:s:237:PRO:HG3	55:s:298:GLN:HE21	1.82	0.45
7:F:282:PRO:HB3	7:F:286:PHE:CZ	2.53	0.44
13:N:224:LEU:CD1	29:o:38:ARG:HH11	2.30	0.44
16:Q:188:LEU:HD22	16:Q:191:ARG:HH12	1.82	0.44
25:i:32:ILE:HD12	38:A:1675:A:H4'	1.98	0.44
28:m:40:LEU:HD11	49:e:67:GLN:HG2	1.99	0.44
34:w:87:LEU:HD13	34:w:98:LEU:HD11	1.99	0.44
35:5:257:TYR:HE2	40:D:123:GLU:HG3	1.82	0.44
38:A:2142:A:O2'	38:A:2261:C:H3'	2.17	0.44
42:I:100:GLN:NE2	52:k:31:ARG:HG3	2.32	0.44
43:T:74:TYR:CZ	43:T:177:LYS:HD3	2.53	0.44
28:m:70:GLU:HA	49:e:87:HIS:ND1	2.32	0.44
35:5:133:PRO:HG3	35:5:239:ILE:HD13	1.99	0.44
38:A:2675:G:O3'	43:T:167:MET:HG3	2.17	0.44
42:I:181:ILE:O	42:I:184:THR:OG1	2.28	0.44
49:e:50:ALA:HA	49:e:175:GLN:HA	1.99	0.44
55:s:63:ILE:HG21	55:s:382:GLN:HE22	1.82	0.44
5:7:139:ASN:HB3	5:7:174:VAL:HG21	1.99	0.44
11:L:111:ASN:OD1	11:L:111:ASN:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:72:ILE:HD11	13:N:96:TYR:CZ	2.53	0.44
28:m:55:LEU:HD21	28:m:65:HIS:NE2	2.31	0.44
35:5:355:LEU:HD23	35:5:376:VAL:HG12	1.99	0.44
38:A:2674:U:H2'	38:A:2675:G:O4'	2.17	0.44
41:E:54:SER:O	41:E:58:VAL:HG23	2.17	0.44
45:V:62:VAL:O	45:V:73:GLN:HA	2.17	0.44
13:N:224:LEU:HD23	29:o:39:LEU:CD2	2.46	0.44
38:A:1782:G:O2'	38:A:1793:G:O6	2.30	0.44
43:T:140:LEU:HD23	43:T:180:GLU:HA	1.98	0.44
52:k:61:GLU:HB3	52:k:62:PRO:HD3	1.99	0.44
12:M:19:LEU:HD23	29:o:95:LEU:HD12	1.99	0.44
28:m:54:VAL:HG21	28:m:72:ARG:HB2	1.99	0.44
38:A:2740:A:N3	38:A:2921:A:O2'	2.46	0.44
40:D:121:PRO:HB3	40:D:166:SER:HA	2.00	0.44
5:7:36:SER:HB2	5:7:39:GLU:HB2	2.00	0.44
9:J:25:ARG:HA	9:J:65:PRO:HA	2.00	0.44
13:N:247:MET:HE3	42:I:37:ARG:NH2	2.31	0.44
37:9:39:LYS:HG3	44:U:7:TYR:CE2	2.52	0.44
37:9:58:PRO:HB3	44:U:17:LEU:CD1	2.48	0.44
42:I:96:ILE:HD11	42:I:153:LEU:HD22	1.98	0.44
45:V:90:GLY:N	45:V:112:GLU:OE2	2.46	0.44
47:c:89:LYS:O	47:c:93:VAL:HG23	2.17	0.44
48:d:81:THR:OG1	48:d:249:GLU:OE2	2.27	0.44
49:e:200:MET:HA	49:e:241:GLY:HA2	2.00	0.44
5:7:303:PRO:HG2	5:7:306:LEU:H	1.83	0.44
9:J:132:LEU:HD11	38:A:2170:G:H4'	1.99	0.44
31:t:7:UNK:O	31:t:11:UNK:CB	2.65	0.44
34:w:123:GLU:HG2	34:w:130:ILE:HD12	1.99	0.44
38:A:2158:U:OP2	54:r:195:TYR:OH	2.31	0.44
38:A:2187:C:H2'	38:A:2188:A:C8	2.53	0.44
55:s:244:SER:HA	55:s:292:CYS:HA	2.00	0.44
5:7:99:TYR:O	5:7:103:SER:OG	2.28	0.44
5:7:220:GLU:HB3	5:7:251:ILE:HD11	2.00	0.44
7:F:243:ILE:HG22	7:F:244:PRO:O	2.18	0.44
11:L:142:GLN:NE2	32:u:197:ARG:O	2.51	0.44
15:P:79:HIS:CE1	36:6:154:TYR:OH	2.71	0.44
16:Q:165:GLU:OE2	41:E:116:LYS:HD2	2.17	0.44
24:g:154:ASP:OD1	24:g:154:ASP:N	2.50	0.44
28:m:55:LEU:O	28:m:74:MET:HA	2.18	0.44
5:7:148:MET:HG2	5:7:257:ILE:HD11	1.99	0.44
5:7:303:PRO:HG2	5:7:306:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:119:THR:HG22	12:M:187:VAL:O	2.18	0.44
19:W:95:GLY:HA3	19:W:134:VAL:O	2.18	0.44
35:5:366:CYS:SG	35:5:367:ASN:N	2.91	0.44
36:6:355:LYS:HE3	36:6:358:PRO:HA	2.00	0.44
38:A:1751:A:C5	38:A:1752:U:H1'	2.53	0.44
38:A:2519:G:C5	40:D:228:LEU:HD13	2.53	0.44
43:T:87:MET:HG3	43:T:172:CYS:SG	2.58	0.44
7:F:249:ASN:OD1	7:F:252:SER:OG	2.31	0.43
8:H:103:GLU:O	8:H:105:VAL:N	2.51	0.43
12:M:230:PRO:O	12:M:234:LEU:HB2	2.18	0.43
21:Y:131:ARG:HB2	37:9:73:TYR:OH	2.18	0.43
22:Z:78:ARG:HD2	22:Z:116:LEU:HD21	1.99	0.43
34:w:134:ASP:OD2	34:w:147:TYR:OH	2.33	0.43
38:A:1679:U:C4'	45:V:42:ARG:HG2	2.48	0.43
38:A:2837:A:H2'	38:A:2838:A:C8	2.53	0.43
45:V:126:MET:SD	45:V:126:MET:N	2.90	0.43
55:s:243:ILE:HG13	55:s:296:HIS:HB2	2.00	0.43
5:7:67:VAL:HG21	5:7:125:ILE:HG13	1.99	0.43
13:N:224:LEU:HD13	13:N:224:LEU:HA	1.85	0.43
16:Q:275:THR:O	16:Q:275:THR:OG1	2.29	0.43
24:g:111:ARG:NH2	24:g:112:LYS:HD3	2.33	0.43
42:I:121:ILE:HG13	42:I:156:SER:HB2	2.00	0.43
42:I:172:PRO:O	52:k:51:VAL:HG13	2.18	0.43
43:T:82:TYR:CD1	43:T:112:LYS:HD3	2.53	0.43
12:M:244:LEU:HD22	12:M:245:PRO:HD2	2.00	0.43
14:O:110:ILE:HD12	14:O:120:MET:HB3	1.99	0.43
16:Q:93:GLN:NE2	16:Q:285:GLU:OE1	2.43	0.43
21:Y:187:PRO:HD2	21:Y:190:LEU:HD11	2.01	0.43
33:v:21:ARG:HH12	34:w:123:GLU:CB	2.31	0.43
34:w:79:ILE:HG12	34:w:126:PHE:HZ	1.83	0.43
37:9:64:ASP:OD1	37:9:64:ASP:N	2.47	0.43
38:A:1789:A:N3	38:A:1915:C:O2'	2.46	0.43
40:D:202:ARG:HH21	40:D:205:GLN:HE22	1.67	0.43
44:U:143:ARG:HH21	44:U:143:ARG:CG	2.25	0.43
1:O:127:TYR:OH	14:O:43:GLU:HG2	2.18	0.43
2:1:45:HIS:CD2	2:1:46:TYR:H	2.37	0.43
4:3:129:TYR:CZ	4:3:130:LYS:HE3	2.53	0.43
7:F:263:LEU:HA	7:F:263:LEU:HD23	1.82	0.43
16:Q:152:ARG:NH1	16:Q:191:ARG:HA	2.33	0.43
17:R:97:LEU:HD22	17:R:101:VAL:HG11	2.00	0.43
41:E:99:LEU:HD12	41:E:198:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:130:GLN:HA	12:M:131:PRO:HD3	1.84	0.43
17:R:97:LEU:HD23	18:S:134:LEU:CD1	2.48	0.43
18:S:96:PHE:HB3	23:b:126:ILE:HD12	2.00	0.43
20:X:86:ILE:HB	20:X:105:TRP:HB2	1.99	0.43
34:w:103:HIS:CE1	34:w:105:MET:HG2	2.54	0.43
53:p:38:GLU:HB3	53:p:39:PHE:H	1.72	0.43
12:M:62:ARG:O	25:i:128:ARG:NH1	2.51	0.43
21:Y:149:ARG:HG2	37:9:86:LEU:HD22	2.00	0.43
24:g:110:ILE:HD11	24:g:157:LEU:HD13	2.00	0.43
33:v:36:ARG:O	33:v:40:ARG:N	2.35	0.43
35:5:232:THR:HG23	35:5:289:HIS:HB2	2.00	0.43
35:5:258:PRO:HG2	40:D:124:GLU:C	2.43	0.43
41:E:99:LEU:HD12	41:E:198:PHE:HE2	1.84	0.43
47:c:122:ASN:HD21	47:c:194:THR:HG22	1.84	0.43
49:e:264:LEU:HD23	49:e:269:LEU:HB3	2.01	0.43
10:K:45:PRO:HD2	23:b:130:TRP:CZ2	2.54	0.43
10:K:119:ARG:NH1	38:A:2705:U:OP2	2.44	0.43
12:M:72:THR:HA	12:M:73:PRO:HD3	1.85	0.43
12:M:132:LEU:H	12:M:132:LEU:HD22	1.84	0.43
19:W:86:ASN:OD1	38:A:2872:C:H5'	2.18	0.43
28:m:55:LEU:CD2	28:m:65:HIS:CD2	3.00	0.43
32:u:145:MET:O	32:u:149:LEU:CB	2.65	0.43
34:w:145:VAL:O	34:w:149:ALA:HB2	2.18	0.43
35:5:112:ARG:HH12	38:A:2389:C:H5	1.57	0.43
42:I:176:LEU:O	52:k:55:VAL:HG21	2.19	0.43
54:r:40:GLU:HA	54:r:48:ILE:O	2.19	0.43
1:0:149:PHE:HB3	55:s:47:ILE:CG2	2.49	0.43
12:M:211:VAL:HG21	30:q:99:MET:HE3	2.01	0.43
15:P:57:GLU:OE2	15:P:96:HIS:NE2	2.52	0.43
18:S:76:HIS:ND1	46:a:50:ALA:HA	2.33	0.43
32:u:100:LEU:HD21	32:u:145:MET:HB2	2.01	0.43
33:v:56:GLU:HA	33:v:59:LEU:HD12	2.00	0.43
38:A:1884:G:N3	38:A:1895:C:O2'	2.51	0.43
54:r:112:HIS:O	54:r:116:GLU:HB2	2.19	0.43
7:F:63:GLN:HA	7:F:81:ASP:HA	2.01	0.43
7:F:147:ARG:NH2	38:A:1795:A:H5''	2.34	0.43
14:O:107:MET:HA	14:O:122:VAL:O	2.18	0.43
17:R:108:TYR:CE2	43:T:212:LEU:HB2	2.54	0.43
28:m:70:GLU:HB3	49:e:124:TRP:HH2	1.83	0.43
44:U:11:ARG:NH1	45:V:212:LYS:O	2.52	0.43
48:d:181:VAL:HG23	48:d:224:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:e:235:LYS:NZ	50:f:172:GLU:OE1	2.52	0.43
51:h:110:HIS:NE2	51:h:134:ILE:HD12	2.34	0.43
2:l:45:HIS:ND1	38:A:2852:C:O2'	2.22	0.43
3:2:84:LEU:O	3:2:84:LEU:HD22	2.18	0.43
5:7:286:LEU:HD12	5:7:294:ILE:HB	2.01	0.43
28:m:49:ALA:HA	49:e:83:LEU:H	1.84	0.43
38:A:2093:U:O2	38:A:2266:U:O2'	2.37	0.43
38:A:2919:A:H2'	38:A:2920:C:C6	2.53	0.43
41:E:85:TRP:HB3	41:E:86:PRO:HD2	2.01	0.43
41:E:112:LYS:NZ	41:E:335:GLU:O	2.43	0.43
43:T:103:LEU:O	43:T:107:GLU:HG3	2.19	0.43
55:s:145:VAL:HG21	55:s:187:LEU:HD11	2.01	0.43
10:K:78:SER:HB3	10:K:89:GLN:HG2	2.01	0.42
18:S:131:GLU:HG2	18:S:151:LYS:HE2	2.01	0.42
23:b:76:VAL:HG22	23:b:86:GLU:HG3	2.00	0.42
27:l:120:ARG:HH22	38:A:2190:C:P	2.42	0.42
36:6:208:ALA:H	36:6:243:ASN:HD21	1.67	0.42
38:A:2529:U:HO2'	40:D:206:TYR:HA	1.84	0.42
6:8:125:LYS:HG2	39:B:1628:C:H5'	2.00	0.42
7:F:116:THR:HG22	7:F:119:GLU:CD	2.44	0.42
13:N:73:ARG:NH2	38:A:2104:A:OP1	2.52	0.42
17:R:14:VAL:HG21	38:A:2294:A:H4'	1.99	0.42
20:X:56:ASN:OD1	20:X:56:ASN:N	2.50	0.42
38:A:2126:U:H2'	38:A:2127:A:C8	2.54	0.42
38:A:2511:C:OP1	40:D:263:ASN:ND2	2.52	0.42
46:a:72:THR:HG22	47:c:258:THR:HA	2.01	0.42
51:h:62:PRO:HA	51:h:63:PRO:HD3	1.87	0.42
55:s:253:LEU:HB2	55:s:354:PRO:HD3	2.01	0.42
49:e:177:GLU:O	49:e:190:ARG:NH2	2.51	0.42
49:e:264:LEU:HB3	49:e:269:LEU:HB3	2.01	0.42
6:8:154:SER:HB3	49:e:230:LYS:NZ	2.34	0.42
7:F:252:SER:O	7:F:256:HIS:ND1	2.52	0.42
12:M:45:ARG:HH11	12:M:45:ARG:HG2	1.84	0.42
22:Z:38:ARG:HE	22:Z:38:ARG:HB2	1.38	0.42
32:u:118:MET:HE1	33:v:66:LEU:HD22	2.02	0.42
33:v:54:GLN:HA	33:v:57:LYS:HG2	2.00	0.42
35:5:125:LYS:HA	35:5:253:LEU:HD21	2.00	0.42
36:6:196:THR:HG22	36:6:326:SER:HB3	2.01	0.42
38:A:2357:C:H2'	38:A:2358:A:C8	2.54	0.42
49:e:255:VAL:HG13	49:e:259:GLU:HB2	2.00	0.42
8:H:55:ILE:HG22	8:H:83:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:118:ARG:CZ	32:u:193:LEU:HD12	2.49	0.42
14:O:53:ARG:HD2	14:O:107:MET:HE3	2.01	0.42
15:P:68:TRP:CZ3	19:W:130:PHE:CD2	3.07	0.42
20:X:150:LYS:CG	20:X:159:MET:HE2	2.49	0.42
24:g:101:THR:HG23	24:g:102:HIS:ND1	2.35	0.42
35:5:114:LEU:HD21	40:D:127:ILE:HD12	2.00	0.42
38:A:3219:G:H2'	38:A:3220:A:H5''	2.01	0.42
41:E:56:GLU:OE1	41:E:57:ASN:ND2	2.52	0.42
41:E:100:ILE:HA	41:E:297:VAL:O	2.20	0.42
3:2:54:GLN:N	38:A:1918:G:O2'	2.49	0.42
5:7:306:LEU:HD23	14:O:145:LEU:H	1.84	0.42
7:F:110:SER:O	7:F:158:PRO:HA	2.19	0.42
8:H:116:LYS:HD3	8:H:120:ARG:HH22	1.84	0.42
12:M:129:ILE:HD12	12:M:184:LEU:HD11	2.00	0.42
13:N:147:ILE:HG21	13:N:150:TYR:HE1	1.85	0.42
14:O:60:ILE:HD13	14:O:97:TYR:HD2	1.84	0.42
21:Y:85:TRP:HH2	37:9:70:LEU:HD12	1.85	0.42
35:5:232:THR:OG1	35:5:234:ASP:O	2.33	0.42
36:6:183:ASP:HA	53:p:192:ARG:HA	2.01	0.42
36:6:233:LEU:HB3	36:6:298:PHE:HE1	1.84	0.42
41:E:207:THR:CG2	41:E:298:LYS:HD2	2.49	0.42
55:s:228:ASP:OD1	55:s:228:ASP:N	2.46	0.42
6:8:160:GLU:OE1	49:e:207:ASN:ND2	2.46	0.42
11:L:52:HIS:CE1	11:L:53:ARG:HG3	2.54	0.42
20:X:168:ARG:HD3	20:X:173:ASP:HB2	2.02	0.42
21:Y:85:TRP:CH2	37:9:70:LEU:HD12	2.55	0.42
23:b:89:ILE:HA	23:b:92:LYS:HD2	2.02	0.42
25:i:53:MET:HE2	30:q:27:ALA:CA	2.49	0.42
35:5:300:ARG:HH11	35:5:300:ARG:CG	2.32	0.42
41:E:144:THR:HA	41:E:179:PHE:O	2.20	0.42
41:E:334:ASP:HB3	41:E:337:VAL:HG23	2.02	0.42
44:U:3:ARG:H	44:U:23:ASN:HB3	1.84	0.42
21:Y:151:ASP:OD1	21:Y:154:ARG:NH1	2.48	0.42
25:i:61:GLY:HA3	38:A:1886:G:H1	1.85	0.42
28:m:66:ILE:HG23	50:f:99:ASP:OD1	2.19	0.42
38:A:1839:C:H2'	38:A:1840:C:C6	2.55	0.42
40:D:66:TRP:HB3	40:D:80:ARG:HE	1.84	0.42
41:E:276:ILE:HG13	41:E:332:LEU:HB2	2.02	0.42
11:L:91:MET:HE3	11:L:91:MET:HB2	1.96	0.42
12:M:62:ARG:HA	12:M:63:PRO:HD3	1.93	0.42
17:R:34:ARG:NH1	38:A:2682:A:H5''	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:144:ARG:HB2	23:b:145:PRO:HD2	1.99	0.42
32:u:126:ILE:HD13	32:u:178:HIS:HB2	2.01	0.42
38:A:1882:A:N1	38:A:1891:A:O2'	2.47	0.42
38:A:2094:G:O2'	38:A:2095:U:H5'	2.20	0.42
38:A:3116:C:N3	38:A:3140:A:N1	2.68	0.42
38:A:3151:A:N1	38:A:3163:G:O2'	2.45	0.42
3:2:78:VAL:O	3:2:82:ARG:HG2	2.19	0.42
21:Y:102:TRP:HE3	21:Y:142:LEU:HD22	1.84	0.42
24:g:57:ILE:HG13	24:g:58:PRO:HD2	2.02	0.42
24:g:125:GLU:HG3	24:g:136:PRO:HD2	2.00	0.42
28:m:70:GLU:O	28:m:72:ARG:N	2.53	0.42
30:q:142:ASN:O	30:q:146:ALA:CB	2.68	0.42
37:9:49:ARG:HH12	38:A:2415:C:N4	2.17	0.42
38:A:2171:U:C2	38:A:2173:G:H4'	2.54	0.42
45:V:56:LEU:HD13	45:V:86:VAL:HG21	2.02	0.42
51:h:60:TYR:N	51:h:134:ILE:O	2.43	0.42
52:k:78:GLY:HA2	52:k:81:LEU:HD13	2.02	0.42
54:r:41:THR:O	54:r:47:THR:HA	2.20	0.42
7:F:86:VAL:HG11	7:F:270:GLU:HG2	2.02	0.41
12:M:225:ASP:OD1	53:p:49:TYR:CD1	2.73	0.41
38:A:2165:C:O2'	38:A:2166:C:O4'	2.34	0.41
55:s:371:CYS:HB2	55:s:394:TRP:HB2	2.02	0.41
1:0:96:ASN:ND2	38:A:2709:A:H1'	2.34	0.41
5:7:79:PHE:HZ	5:7:95:LEU:HD11	1.85	0.41
12:M:187:VAL:HG23	12:M:265:ILE:HG23	2.02	0.41
15:P:135:ARG:HH12	36:6:139:TRP:NE1	2.18	0.41
16:Q:188:LEU:HD22	16:Q:191:ARG:NH1	2.35	0.41
16:Q:262:GLN:HG2	16:Q:264:TRP:CH2	2.55	0.41
18:S:169:ARG:HB3	18:S:186:VAL:O	2.20	0.41
20:X:42:HIS:ND1	20:X:86:ILE:HD11	2.36	0.41
23:b:44:ARG:NH1	29:o:100:LYS:HA	2.35	0.41
25:i:74:ILE:HD11	25:i:82:GLY:H	1.85	0.41
30:q:142:ASN:O	30:q:146:ALA:HB2	2.20	0.41
35:5:121:LEU:HD21	35:5:128:LEU:HD13	2.02	0.41
38:A:2075:U:O2'	38:A:2833:A:N7	2.41	0.41
49:e:266:PRO:O	49:e:270:ALA:N	2.41	0.41
6:8:114:ARG:NE	49:e:73:LEU:HD11	2.35	0.41
7:F:48:LEU:HD11	51:h:95:ARG:HG2	2.02	0.41
7:F:69:LEU:HB3	7:F:195:LEU:HD23	2.01	0.41
35:5:114:LEU:HD13	35:5:263:ILE:HG12	2.02	0.41
35:5:258:PRO:CG	40:D:123:GLU:HB3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:6:379:ILE:HG12	38:A:1882:A:C5	2.56	0.41
1:0:86:THR:HG21	38:A:2683:C:H5'	2.01	0.41
5:7:108:VAL:HB	5:7:113:TRP:CD1	2.55	0.41
9:J:69:LYS:HD3	9:J:129:ALA:HB1	2.03	0.41
12:M:229:PHE:N	12:M:230:PRO:HD2	2.35	0.41
17:R:108:TYR:HD1	23:b:125:SER:HB2	1.84	0.41
32:u:131:SER:OG	32:u:132:THR:N	2.52	0.41
35:5:107:PHE:HE1	35:5:113:LEU:HD11	1.84	0.41
35:5:215:ARG:NH2	35:5:366:CYS:O	2.53	0.41
36:6:224:HIS:HA	36:6:232:TYR:CE2	2.55	0.41
38:A:1756:A:H2'	38:A:1757:A:H8	1.85	0.41
41:E:106:MET:HE2	41:E:118:VAL:HG12	2.02	0.41
43:T:144:GLU:O	43:T:176:VAL:HA	2.20	0.41
48:d:160:LEU:HD23	48:d:160:LEU:HA	1.92	0.41
49:e:190:ARG:O	49:e:194:THR:OG1	2.33	0.41
55:s:236:LYS:HA	55:s:237:PRO:HD2	1.94	0.41
9:J:125:ALA:HB2	9:J:140:VAL:HG21	2.02	0.41
10:K:45:PRO:HB3	17:R:75:ALA:HB2	2.02	0.41
12:M:48:LYS:NZ	38:A:1848:U:OP1	2.54	0.41
12:M:292:LYS:O	12:M:296:SER:OG	2.35	0.41
13:N:250:ARG:HG2	13:N:250:ARG:NH1	2.35	0.41
14:O:36:LEU:HD13	14:O:123:ILE:HG13	2.02	0.41
14:O:46:TRP:CD1	14:O:121:ALA:HB2	2.55	0.41
15:P:68:TRP:HZ3	19:W:130:PHE:CD2	2.39	0.41
16:Q:102:ARG:HA	16:Q:102:ARG:HD2	1.95	0.41
44:U:143:ARG:CG	44:U:143:ARG:NH2	2.83	0.41
13:N:131:ILE:HD12	13:N:151:VAL:HG21	2.01	0.41
18:S:57:SER:OG	18:S:58:SER:N	2.53	0.41
20:X:226:LEU:HD23	20:X:229:ILE:HD12	2.02	0.41
35:5:209:PHE:CE1	35:5:224:GLY:HA3	2.55	0.41
38:A:2898:U:H2'	38:A:2899:C:O4'	2.21	0.41
47:c:93:VAL:HG22	47:c:180:LEU:HD22	2.02	0.41
5:7:67:VAL:HG13	5:7:79:PHE:HB2	2.02	0.41
10:K:69:GLY:O	54:r:152:THR:HG22	2.20	0.41
11:L:75:LEU:O	11:L:81:LYS:HA	2.21	0.41
11:L:95:ARG:HG3	16:Q:165:GLU:OE2	2.19	0.41
13:N:89:ILE:HD11	13:N:176:LEU:HD22	2.01	0.41
14:O:26:ILE:HG21	16:Q:264:TRP:HB2	2.02	0.41
14:O:52:MET:HE1	14:O:123:ILE:HD11	2.02	0.41
16:Q:91:LYS:NZ	16:Q:95:GLU:OE2	2.31	0.41
16:Q:150:ILE:HA	16:Q:162:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:54:THR:HG22	18:S:170:ILE:O	2.20	0.41
24:g:101:THR:O	24:g:105:ARG:HB2	2.21	0.41
28:m:52:TYR:CD2	28:m:71:PRO:HD3	2.55	0.41
34:w:105:MET:HA	34:w:110:LEU:H	1.85	0.41
52:k:15:GLN:HA	52:k:50:SER:O	2.20	0.41
7:F:165:LEU:HB2	7:F:170:ARG:CD	2.50	0.41
7:F:263:LEU:N	7:F:264:PRO:HD2	2.36	0.41
10:K:20:LEU:HD22	10:K:21:LEU:H	1.86	0.41
10:K:156:ASP:OD1	54:r:130:ASN:ND2	2.54	0.41
15:P:126:GLU:OE2	15:P:130:ARG:NE	2.50	0.41
17:R:109:GLU:OE1	18:S:107:LYS:CE	2.68	0.41
33:v:21:ARG:HH22	34:w:123:GLU:HB2	1.85	0.41
36:6:39:ASP:OD1	36:6:39:ASP:N	2.52	0.41
36:6:352:PRO:HD3	38:A:2860:G:H5''	2.01	0.41
37:9:28:ARG:HG3	38:A:2338:A:OP1	2.21	0.41
38:A:2116:C:O2'	38:A:2837:A:N3	2.45	0.41
43:T:61:PRO:HA	48:d:229:GLY:CA	2.50	0.41
1:0:134:THR:HG22	14:O:130:LEU:HD12	2.03	0.41
5:7:93:MET:O	43:T:138:SER:HB3	2.21	0.41
5:7:180:CYS:HA	5:7:297:PHE:O	2.21	0.41
7:F:59:ARG:HD2	24:g:114:GLU:OE2	2.21	0.41
7:F:191:ASP:N	7:F:191:ASP:OD1	2.48	0.41
7:F:253:MET:HG2	7:F:259:LEU:CD1	2.50	0.41
9:J:138:SER:O	9:J:142:ARG:HB2	2.20	0.41
13:N:103:GLU:O	13:N:107:LEU:CB	2.69	0.41
13:N:218:ILE:HG23	13:N:223:MET:HB2	2.02	0.41
14:O:84:ASP:OD1	14:O:84:ASP:N	2.52	0.41
17:R:32:ARG:HG2	46:a:129:TYR:CZ	2.56	0.41
19:W:121:PRO:HG2	19:W:124:ALA:HB2	2.03	0.41
21:Y:114:THR:CG2	44:U:28:LEU:H	2.32	0.41
22:Z:92:GLU:H	22:Z:92:GLU:CD	2.29	0.41
23:b:135:ASN:HA	46:a:43:TYR:CD1	2.56	0.41
24:g:105:ARG:HG2	38:A:2052:A:H5'	2.03	0.41
33:v:43:GLN:CG	58:v:101:PNS:H41	2.30	0.41
35:5:214:ASN:OD1	35:5:219:LEU:HD13	2.21	0.41
35:5:258:PRO:HG3	40:D:123:GLU:CB	2.46	0.41
38:A:1698:C:O2'	38:A:1702:A:N3	2.51	0.41
38:A:1828:A:O2'	38:A:2684:C:N3	2.51	0.41
38:A:2123:C:O2'	38:A:2134:A:O2'	2.36	0.41
40:D:83:GLY:O	40:D:85:ARG:NH1	2.47	0.41
41:E:73:LEU:HD11	41:E:151:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:I:191:PHE:O	42:I:195:SER:OG	2.36	0.41
43:T:71:ALA:H	43:T:180:GLU:HB3	1.85	0.41
47:c:275:TYR:CE2	47:c:280:LEU:HB3	2.56	0.41
54:r:70:CYS:SG	54:r:73:CYS:CB	3.09	0.41
55:s:80:LEU:HD21	55:s:341:MET:HB3	2.02	0.41
3:2:53:TYR:CZ	3:2:55:PRO:HB3	2.56	0.41
5:7:65:ILE:H	5:7:65:ILE:HG13	1.70	0.41
11:L:87:VAL:O	11:L:104:ASN:HB2	2.21	0.41
12:M:20:PRO:HG2	29:o:95:LEU:O	2.21	0.41
14:O:50:ASP:CB	14:O:107:MET:HE1	2.49	0.41
17:R:114:LYS:HD3	46:a:45:CYS:SG	2.61	0.41
19:W:70:GLN:HG3	19:W:72:HIS:O	2.20	0.41
19:W:100:THR:OG1	19:W:132:HIS:NE2	2.43	0.41
24:g:84:TYR:CE2	24:g:120:LEU:HD23	2.56	0.41
35:5:300:ARG:N	35:5:301:PRO:CD	2.84	0.41
36:6:183:ASP:HB3	53:p:192:ARG:HG2	2.02	0.41
36:6:214:TRP:HA	36:6:273:PHE:O	2.21	0.41
37:9:78:ALA:HA	45:V:179:VAL:HG13	2.01	0.41
38:A:2371:U:H2'	44:U:71:ARG:HD3	2.01	0.41
38:A:3228:U:O4	41:E:65:VAL:HG12	2.21	0.41
43:T:144:GLU:HB2	43:T:177:LYS:HB3	2.03	0.41
48:d:290:GLU:HG2	48:d:291:GLU:HG3	2.03	0.41
49:e:162:ARG:HD3	49:e:171:TRP:HE3	1.84	0.41
54:r:161:PRO:HG2	54:r:163:TYR:CZ	2.56	0.41
14:O:52:MET:SD	14:O:123:ILE:HD11	2.61	0.40
14:O:108:LEU:HD11	14:O:135:LEU:HD23	2.03	0.40
17:R:34:ARG:HG3	38:A:2683:C:OP1	2.21	0.40
20:X:116:SER:O	20:X:120:ASP:N	2.54	0.40
23:b:28:ARG:HA	23:b:62:VAL:O	2.21	0.40
35:5:310:ARG:HA	35:5:313:MET:HE2	2.03	0.40
38:A:2310:G:O2'	38:A:2675:G:O6	2.34	0.40
49:e:202:ALA:HA	49:e:238:LEU:HA	2.03	0.40
8:H:55:ILE:HG23	20:X:43:TYR:HA	2.02	0.40
10:K:30:LYS:NZ	38:A:2240:C:O3'	2.54	0.40
20:X:11:TRP:HA	20:X:14:LEU:HD12	2.04	0.40
33:v:55:LEU:HD13	33:v:55:LEU:HA	1.90	0.40
35:5:257:TYR:CE2	40:D:123:GLU:HG3	2.56	0.40
36:6:238:THR:HG21	36:6:281:PHE:CD2	2.55	0.40
40:D:225:ILE:HA	40:D:234:MET:O	2.20	0.40
45:V:185:ARG:NH2	45:V:187:TYR:O	2.54	0.40
54:r:155:ALA:HA	54:r:156:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:s:115:LEU:HD11	55:s:257:VAL:HG21	2.03	0.40
9:J:18:GLY:N	9:J:72:VAL:O	2.54	0.40
10:K:110:GLY:O	10:K:114:LYS:NZ	2.48	0.40
17:R:60:LYS:O	17:R:64:MET:HG2	2.22	0.40
28:m:72:ARG:NE	28:m:75:LEU:HD21	2.37	0.40
32:u:132:THR:O	32:u:136:HIS:CB	2.70	0.40
35:5:112:ARG:HG2	35:5:304:LEU:HD11	2.03	0.40
38:A:1834:U:C4	43:T:206:ARG:HA	2.55	0.40
41:E:94:SER:HA	41:E:182:THR:HG21	2.03	0.40
43:T:75:HIS:CD2	43:T:120:VAL:HG13	2.56	0.40
48:d:222:LEU:HD23	48:d:222:LEU:HA	1.92	0.40
52:k:18:VAL:HG11	52:k:34:LEU:HD13	2.04	0.40
55:s:366:TYR:HA	55:s:400:PRO:HA	2.03	0.40
5:7:317:LEU:HD23	5:7:317:LEU:HA	1.92	0.40
9:J:24:VAL:HG21	9:J:35:LEU:HD21	2.03	0.40
9:J:133:GLN:HB3	42:I:117:ARG:CZ	2.51	0.40
14:O:123:ILE:HD13	14:O:123:ILE:HG21	1.91	0.40
19:W:103:VAL:HG22	19:W:127:TYR:CE1	2.56	0.40
20:X:52:ILE:HA	20:X:59:ARG:HA	2.03	0.40
35:5:391:VAL:HG13	35:5:398:VAL:HB	2.03	0.40
38:A:2402:A:H3'	40:D:133:PRO:HG3	2.04	0.40
55:s:422:VAL:O	55:s:426:LEU:HB2	2.21	0.40
5:7:107:LEU:HD12	5:7:126:LYS:HD2	2.04	0.40
10:K:11:TRP:CD1	47:c:269:LEU:HD23	2.56	0.40
38:A:1823:A:C6	46:a:125:PRO:HG2	2.56	0.40
38:A:2055:U:H2'	38:A:2056:G:H8	1.86	0.40
46:a:69:TYR:OH	47:c:256:ARG:NH2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	106/188 (56%)	102 (96%)	4 (4%)	0	100	100
2	1	50/65 (77%)	50 (100%)	0	0	100	100
3	2	41/92 (45%)	40 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	89 (96%)	4 (4%)	0	100	100
5	7	285/338 (84%)	259 (91%)	26 (9%)	0	100	100
6	8	97/206 (47%)	90 (93%)	7 (7%)	0	100	100
7	F	248/311 (80%)	232 (94%)	16 (6%)	0	100	100
8	H	93/267 (35%)	84 (90%)	8 (9%)	1 (1%)	11	16
9	J	138/192 (72%)	122 (88%)	16 (12%)	0	100	100
10	K	175/178 (98%)	166 (95%)	9 (5%)	0	100	100
11	L	113/145 (78%)	104 (92%)	9 (8%)	0	100	100
12	M	285/296 (96%)	274 (96%)	11 (4%)	0	100	100
13	N	203/251 (81%)	191 (94%)	12 (6%)	0	100	100
14	O	150/175 (86%)	144 (96%)	6 (4%)	0	100	100
15	P	139/180 (77%)	131 (94%)	8 (6%)	0	100	100
16	Q	215/292 (74%)	201 (94%)	14 (6%)	0	100	100
17	R	138/149 (93%)	132 (96%)	6 (4%)	0	100	100
18	S	154/205 (75%)	147 (96%)	7 (4%)	0	100	100
19	W	107/148 (72%)	103 (96%)	3 (3%)	1 (1%)	14	20
20	X	241/256 (94%)	236 (98%)	5 (2%)	0	100	100
21	Y	174/250 (70%)	169 (97%)	5 (3%)	0	100	100
22	Z	118/161 (73%)	111 (94%)	7 (6%)	0	100	100
23	b	146/215 (68%)	131 (90%)	15 (10%)	0	100	100
24	g	127/166 (76%)	115 (91%)	12 (9%)	0	100	100
25	i	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
26	j	83/123 (68%)	82 (99%)	1 (1%)	0	100	100
27	l	21/138 (15%)	21 (100%)	0	0	100	100
28	m	43/128 (34%)	38 (88%)	4 (9%)	1 (2%)	5	5
29	o	77/102 (76%)	77 (100%)	0	0	100	100
30	q	126/222 (57%)	124 (98%)	2 (2%)	0	100	100
32	u	109/234 (47%)	100 (92%)	9 (8%)	0	100	100
33	v	67/70 (96%)	66 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	w	77/156 (49%)	69 (90%)	8 (10%)	0	100	100
35	5	383/423 (90%)	359 (94%)	24 (6%)	0	100	100
36	6	316/380 (83%)	300 (95%)	16 (5%)	0	100	100
37	9	113/137 (82%)	108 (96%)	5 (4%)	0	100	100
40	D	216/305 (71%)	203 (94%)	13 (6%)	0	100	100
41	E	281/348 (81%)	269 (96%)	11 (4%)	1 (0%)	30	42
42	I	154/261 (59%)	142 (92%)	12 (8%)	0	100	100
43	T	155/206 (75%)	153 (99%)	2 (1%)	0	100	100
44	U	135/153 (88%)	128 (95%)	7 (5%)	0	100	100
45	V	188/216 (87%)	182 (97%)	6 (3%)	0	100	100
46	a	78/142 (55%)	74 (95%)	4 (5%)	0	100	100
47	c	271/332 (82%)	264 (97%)	7 (3%)	0	100	100
48	d	203/306 (66%)	192 (95%)	11 (5%)	0	100	100
49	e	211/279 (76%)	181 (86%)	29 (14%)	1 (0%)	24	35
50	f	110/212 (52%)	99 (90%)	10 (9%)	1 (1%)	14	20
51	h	96/158 (61%)	91 (95%)	5 (5%)	0	100	100
52	k	76/112 (68%)	69 (91%)	7 (9%)	0	100	100
53	p	119/206 (58%)	115 (97%)	4 (3%)	0	100	100
54	r	140/196 (71%)	133 (95%)	7 (5%)	0	100	100
55	s	366/439 (83%)	350 (96%)	15 (4%)	1 (0%)	36	49
All	All	7945/11026 (72%)	7503 (94%)	435 (6%)	7 (0%)	49	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	m	71	PRO
8	H	103	GLU
55	s	272	PRO
49	e	256	THR
50	f	179	PRO
19	W	73	PHE
41	E	317	PRO

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	0	97/164 (59%)	97 (100%)	0	100	100
2	1	49/60 (82%)	49 (100%)	0	100	100
3	2	38/72 (53%)	36 (95%)	2 (5%)	20	34
4	3	88/166 (53%)	83 (94%)	5 (6%)	18	31
5	7	263/303 (87%)	259 (98%)	4 (2%)	57	75
6	8	91/190 (48%)	91 (100%)	0	100	100
7	F	217/262 (83%)	211 (97%)	6 (3%)	38	58
8	H	86/228 (38%)	86 (100%)	0	100	100
9	J	113/150 (75%)	113 (100%)	0	100	100
10	K	155/156 (99%)	149 (96%)	6 (4%)	28	46
11	L	98/124 (79%)	98 (100%)	0	100	100
12	M	245/249 (98%)	238 (97%)	7 (3%)	37	57
13	N	172/211 (82%)	169 (98%)	3 (2%)	53	73
14	O	133/150 (89%)	125 (94%)	8 (6%)	17	29
15	P	123/155 (79%)	120 (98%)	3 (2%)	43	63
16	Q	199/256 (78%)	198 (100%)	1 (0%)	81	90
17	R	118/126 (94%)	115 (98%)	3 (2%)	42	62
18	S	141/180 (78%)	138 (98%)	3 (2%)	47	67
19	W	89/119 (75%)	86 (97%)	3 (3%)	32	52
20	X	219/229 (96%)	215 (98%)	4 (2%)	51	71
21	Y	159/223 (71%)	156 (98%)	3 (2%)	50	70
22	Z	111/147 (76%)	109 (98%)	2 (2%)	51	71
23	b	130/186 (70%)	125 (96%)	5 (4%)	29	47
24	g	119/148 (80%)	111 (93%)	8 (7%)	15	24
25	i	86/110 (78%)	80 (93%)	6 (7%)	14	22
26	j	68/97 (70%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	l	23/116 (20%)	23 (100%)	0	100	100
28	m	40/113 (35%)	40 (100%)	0	100	100
29	o	68/87 (78%)	68 (100%)	0	100	100
30	q	110/178 (62%)	107 (97%)	3 (3%)	39	60
32	u	105/200 (52%)	104 (99%)	1 (1%)	68	82
33	v	59/60 (98%)	58 (98%)	1 (2%)	53	73
34	w	73/136 (54%)	72 (99%)	1 (1%)	59	77
35	5	348/368 (95%)	338 (97%)	10 (3%)	37	57
36	6	265/332 (80%)	263 (99%)	2 (1%)	73	85
37	9	99/112 (88%)	96 (97%)	3 (3%)	36	56
40	D	179/245 (73%)	177 (99%)	2 (1%)	65	81
41	E	246/290 (85%)	242 (98%)	4 (2%)	55	74
42	I	145/232 (62%)	143 (99%)	2 (1%)	59	77
43	T	141/176 (80%)	140 (99%)	1 (1%)	76	87
44	U	124/135 (92%)	116 (94%)	8 (6%)	15	25
45	V	172/191 (90%)	170 (99%)	2 (1%)	63	79
46	a	78/133 (59%)	78 (100%)	0	100	100
47	c	241/288 (84%)	236 (98%)	5 (2%)	47	67
48	d	193/274 (70%)	190 (98%)	3 (2%)	55	74
49	e	188/236 (80%)	188 (100%)	0	100	100
50	f	101/188 (54%)	101 (100%)	0	100	100
51	h	95/148 (64%)	92 (97%)	3 (3%)	34	54
52	k	71/90 (79%)	69 (97%)	2 (3%)	38	58
53	p	117/181 (65%)	117 (100%)	0	100	100
54	r	133/169 (79%)	132 (99%)	1 (1%)	73	85
55	s	326/381 (86%)	320 (98%)	6 (2%)	51	71
All	All	7147/9520 (75%)	7005 (98%)	142 (2%)	48	68

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	63	LYS
3	2	84	LEU

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Mol	Chain	Res	Type
4	3	125	ARG
4	3	148	VAL
4	3	157	LEU
4	3	168	ARG
4	3	173	VAL
5	7	64	LYS
5	7	67	VAL
5	7	167	VAL
5	7	175	ILE
7	F	125	ARG
7	F	147	ARG
7	F	203	LEU
7	F	259	LEU
7	F	277	ASP
7	F	281	ARG
10	K	16	ARG
10	K	20	LEU
10	K	46	VAL
10	K	65	ILE
10	K	101	VAL
10	K	125	LEU
12	M	47	ARG
12	M	57	ARG
12	M	96	LEU
12	M	132	LEU
12	M	141	VAL
12	M	154	ILE
12	M	244	LEU
13	N	50	LEU
13	N	151	VAL
13	N	224	LEU
14	O	20	LEU
14	O	26	ILE
14	O	36	LEU
14	O	42	ILE
14	O	59	LEU
14	O	89	LEU
14	O	130	LEU
14	O	144	LEU
15	P	51	ARG
15	P	56	LEU
15	P	132	LEU

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Mol	Chain	Res	Type
16	Q	136	ILE
17	R	67	LEU
17	R	109	GLU
17	R	119	LEU
18	S	108	VAL
18	S	115	LEU
18	S	186	VAL
19	W	61	VAL
19	W	83	VAL
19	W	105	VAL
20	X	52	ILE
20	X	64	ASP
20	X	90	ILE
20	X	208	LEU
21	Y	132	LEU
21	Y	190	LEU
21	Y	226	LEU
22	Z	105	SER
22	Z	154	VAL
23	b	11	LEU
23	b	26	LEU
23	b	62	VAL
23	b	103	LYS
23	b	144	ARG
24	g	57	ILE
24	g	68	THR
24	g	100	ILE
24	g	108	THR
24	g	120	LEU
24	g	137	VAL
24	g	140	VAL
24	g	147	LEU
25	i	63	LEU
25	i	78	ILE
25	i	80	LEU
25	i	88	LEU
25	i	98	VAL
25	i	113	ARG
30	q	46	LEU
30	q	82	LEU
30	q	108	LEU
32	u	127	VAL

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Mol	Chain	Res	Type
33	v	55	LEU
34	w	106	LYS
35	5	55	LEU
35	5	67	VAL
35	5	98	LEU
35	5	106	ILE
35	5	155	LEU
35	5	174	GLU
35	5	262	ILE
35	5	364	LEU
35	5	389	LEU
35	5	415	LEU
36	6	272	LEU
36	6	334	LEU
37	9	65	LEU
37	9	91	LEU
37	9	136	LEU
40	D	206	TYR
40	D	236	VAL
41	E	97	VAL
41	E	204	VAL
41	E	266	ARG
41	E	284	TYR
42	I	47	LEU
42	I	146	LEU
43	T	176	VAL
44	U	6	VAL
44	U	12	LEU
44	U	17	LEU
44	U	28	LEU
44	U	44	ILE
44	U	53	LEU
44	U	71	ARG
44	U	143	ARG
45	V	109	ILE
45	V	138	THR
47	c	72	ILE
47	c	87	LEU
47	c	202	LEU
47	c	211	THR
47	c	241	LEU
48	d	164	VAL

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Mol	Chain	Res	Type
48	d	197	VAL
48	d	264	LYS
51	h	66	LEU
51	h	96	LEU
51	h	100	LEU
52	k	16	VAL
52	k	55	VAL
54	r	86	VAL
55	s	56	LYS
55	s	251	VAL
55	s	306	LEU
55	s	360	VAL
55	s	361	ILE
55	s	379	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	96	ASN
1	0	106	ASN
1	0	168	GLN
5	7	55	GLN
6	8	144	GLN
7	F	105	ASN
7	F	188	HIS
7	F	223	HIS
8	H	121	ASN
9	J	126	GLN
10	K	160	GLN
11	L	59	HIS
11	L	80	GLN
11	L	142	GLN
12	M	130	GLN
13	N	86	ASN
14	O	147	GLN
15	P	79	HIS
15	P	87	GLN
17	R	30	HIS
17	R	77	GLN
17	R	89	ASN
17	R	125	HIS
18	S	118	ASN

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Mol	Chain	Res	Type
18	S	140	ASN
19	W	70	GLN
19	W	80	HIS
20	X	237	GLN
20	X	240	GLN
21	Y	117	GLN
22	Z	107	ASN
23	b	27	GLN
23	b	66	ASN
23	b	102	GLN
24	g	93	ASN
25	i	108	HIS
25	i	120	HIS
26	j	105	GLN
30	q	139	GLN
30	q	142	ASN
32	u	136	HIS
33	v	63	ASN
34	w	115	GLN
35	5	109	HIS
35	5	266	HIS
35	5	269	ASN
35	5	275	ASN
35	5	302	HIS
35	5	305	GLN
35	5	308	GLN
35	5	353	HIS
35	5	384	GLN
36	6	243	ASN
36	6	277	GLN
36	6	359	HIS
40	D	205	GLN
40	D	227	GLN
41	E	184	ASN
42	I	141	GLN
42	I	189	GLN
43	T	75	HIS
44	U	35	GLN
44	U	55	ASN
44	U	82	HIS
44	U	101	HIS
45	V	92	ASN

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Mol	Chain	Res	Type
46	a	111	GLN
47	c	122	ASN
49	e	198	ASN
49	e	212	HIS
50	f	112	ASN
51	h	87	GLN
52	k	15	GLN
52	k	26	ASN
54	r	112	HIS
55	s	179	GLN
55	s	298	GLN
55	s	315	ASN
55	s	343	GLN
55	s	382	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
38	A	1028/1559 (65%)	289 (28%)	25 (2%)
39	B	51/69 (73%)	15 (29%)	1 (1%)
All	All	1079/1628 (66%)	304 (28%)	26 (2%)

All (304) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
38	A	1675	A
38	A	1676	A
38	A	1677	C
38	A	1678	C
38	A	1679	U
38	A	1681	G
38	A	1689	C
38	A	1694	U
38	A	1700	U
38	A	1701	U
38	A	1703	C
38	A	1704	U
38	A	1708	A
38	A	1713	A
38	A	1714	C
38	A	1715	C

Continued on next page...

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Mol	Chain	Res	Type
38	A	1716	U
38	A	1717	U
38	A	1719	G
38	A	1724	A
38	A	1727	A
38	A	1728	U
38	A	1731	A
38	A	1741	A
38	A	1748	G
38	A	1750	G
38	A	1751	A
38	A	1760	G
38	A	1770	G
38	A	1773	A
38	A	1775	A
38	A	1780	U
38	A	1781	A
38	A	1791	G
38	A	1794	A
38	A	1803	A
38	A	1804	A
38	A	1805	A
38	A	1806	U
38	A	1812	C
38	A	1817	C
38	A	1820	A
38	A	1823	A
38	A	1824	U
38	A	1827	C
38	A	1828	A
38	A	1829	A
38	A	1832	A
38	A	1836	A
38	A	1844	A
38	A	1849	C
38	A	1867	A
38	A	1869	A
38	A	1870	A
38	A	1871	A
38	A	1872	U
38	A	1874	A
38	A	1875	C

Continued on next page...

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Mol	Chain	Res	Type
38	A	1878	U
38	A	1882	A
38	A	1883	G
38	A	1887	A
38	A	1888	G
38	A	1890	C
38	A	1892	A
38	A	1893	A
38	A	1901	C
38	A	1903	C
38	A	1914	A
38	A	1918	G
38	A	2012	A
38	A	2015	G
38	A	2020	U
38	A	2021	U
38	A	2022	G
38	A	2027	A
38	A	2028	G
38	A	2029	A
38	A	2030	U
38	A	2031	A
38	A	2032	G
38	A	2036	C
38	A	2037	U
38	A	2039	A
38	A	2041	U
38	A	2053	U
38	A	2055	U
38	A	2060	A
38	A	2065	A
38	A	2074	A
38	A	2079	C
38	A	2083	U
38	A	2085	A
38	A	2095	U
38	A	2105	G
38	A	2113	G
38	A	2124	A
38	A	2125	C
38	A	2126	U
38	A	2132	A

Continued on next page...

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Mol	Chain	Res	Type
38	A	2134	A
38	A	2141	U
38	A	2142	A
38	A	2147	G
38	A	2154	A
38	A	2156	A
38	A	2157	U
38	A	2158	U
38	A	2159	U
38	A	2161	A
38	A	2163	A
38	A	2166	C
38	A	2168	U
38	A	2171	U
38	A	2172	A
38	A	2173	G
38	A	2174	G
38	A	2180	A
38	A	2181	A
38	A	2182	G
38	A	2183	C
38	A	2187	C
38	A	2190	C
38	A	2193	U
38	A	2194	U
38	A	2195	A
38	A	2197	G
38	A	2198	A
38	A	2200	A
38	A	2204	U
38	A	2207	A
38	A	2210	C
38	A	2216	A
38	A	2237	A
38	A	2239	A
38	A	2241	A
38	A	2243	A
38	A	2244	U
38	A	2245	A
38	A	2257	C
38	A	2259	C
38	A	2261	C

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Mol	Chain	Res	Type
38	A	2262	C
38	A	2263	C
38	A	2264	A
38	A	2283	C
38	A	2284	C
38	A	2285	U
38	A	2290	A
38	A	2297	A
38	A	2299	U
38	A	2300	G
38	A	2321	A
38	A	2324	U
38	A	2332	C
38	A	2335	A
38	A	2342	U
38	A	2345	G
38	A	2371	U
38	A	2374	A
38	A	2375	C
38	A	2381	A
38	A	2387	U
38	A	2389	C
38	A	2390	A
38	A	2393	C
38	A	2394	A
38	A	2396	C
38	A	2397	C
38	A	2401	A
38	A	2405	C
38	A	2406	A
38	A	2407	U
38	A	2414	C
38	A	2415	C
38	A	2417	C
38	A	2418	A
38	A	2426	C
38	A	2427	C
38	A	2431	C
38	A	2435	G
38	A	2443	C
38	A	2444	A
38	A	2445	U

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Mol	Chain	Res	Type
38	A	2446	A
38	A	2449	G
38	A	2457	A
38	A	2458	A
38	A	2468	A
38	A	2508	C
38	A	2511	C
38	A	2512	A
38	A	2520	C
38	A	2521	A
38	A	2522	U
38	A	2523	C
38	A	2524	A
38	A	2526	C
38	A	2527	A
38	A	2655	G
38	A	2656	U
38	A	2659	C
38	A	2660	U
38	A	2683	C
38	A	2684	C
38	A	2686	G
38	A	2698	G
38	A	2699	C
38	A	2706	A
38	A	2707	A
38	A	2708	C
38	A	2709	A
38	A	2725	A
38	A	2732	G
38	A	2739	U
38	A	2740	A
38	A	2744	U
38	A	2750	U
38	A	2752	C
38	A	2803	A
38	A	2804	A
38	A	2810	G
38	A	2813	U
38	A	2814	G
38	A	2815	G
38	A	2831	G

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Mol	Chain	Res	Type
38	A	2832	A
38	A	2833	A
38	A	2844	G
38	A	2846	G
38	A	2847	C
38	A	2852	C
38	A	2854	U
38	A	2859	A
38	A	2861	A
38	A	2864	U
38	A	2865	C
38	A	2870	G
38	A	2871	U
38	A	2879	A
38	A	2893	A
38	A	2895	U
38	A	2896	G
38	A	2901	A
38	A	2906	C
38	A	2910	A
38	A	2912	C
38	A	2913	A
38	A	2914	A
38	A	2917	G
38	A	2918	A
38	A	2919	A
38	A	2922	A
38	A	2926	A
38	A	2928	C
38	A	3102	U
38	A	3108	U
38	A	3109	U
38	A	3114	U
38	A	3123	G
38	A	3124	U
38	A	3128	A
38	A	3129	A
38	A	3131	G
38	A	3134	C
38	A	3137	G
38	A	3138	A
38	A	3139	G

Continued on next page...

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Mol	Chain	Res	Type
38	A	3141	A
38	A	3150	U
38	A	3155	C
38	A	3157	C
38	A	3158	A
38	A	3160	A
38	A	3162	C
38	A	3168	C
38	A	3177	A
38	A	3180	A
38	A	3183	U
38	A	3184	C
38	A	3185	A
38	A	3189	C
38	A	3190	A
38	A	3192	C
38	A	3202	U
38	A	3204	C
38	A	3207	A
38	A	3217	A
38	A	3218	A
39	B	1607	U
39	B	1608	G
39	B	1609	U
39	B	1611	G
39	B	1614	U
39	B	1615	A
39	B	1625	A
39	B	1631	C
39	B	1632	U
39	B	1640	A
39	B	1641	G
39	B	1644	G
39	B	1645	A
39	B	1649	C
39	B	1651	A

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
38	A	1678	C
38	A	1703	C

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Mol	Chain	Res	Type
38	A	1713	A
38	A	1727	A
38	A	1772	A
38	A	1780	U
38	A	1805	A
38	A	1823	A
38	A	2030	U
38	A	2036	C
38	A	2125	C
38	A	2141	U
38	A	2165	C
38	A	2172	A
38	A	2186	C
38	A	2243	A
38	A	2321	A
38	A	2373	A
38	A	2444	A
38	A	2457	A
38	A	2507	A
38	A	2744	U
38	A	2905	A
38	A	3108	U
38	A	3201	A
39	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, 50 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	PNS	v	101	-	14,20,21	0.20	0	18,26,29	0.94	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PNS	v	101	-	-	7/24/26/27	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	v	101	PNS	C28-C29-C32-O33
58	v	101	PNS	C28-C29-C32-C34
58	v	101	PNS	C31-C29-C32-O33
58	v	101	PNS	C31-C29-C32-C34
58	v	101	PNS	N41-C42-C43-S44
58	v	101	PNS	C30-C29-C32-O33
58	v	101	PNS	C30-C29-C32-C34

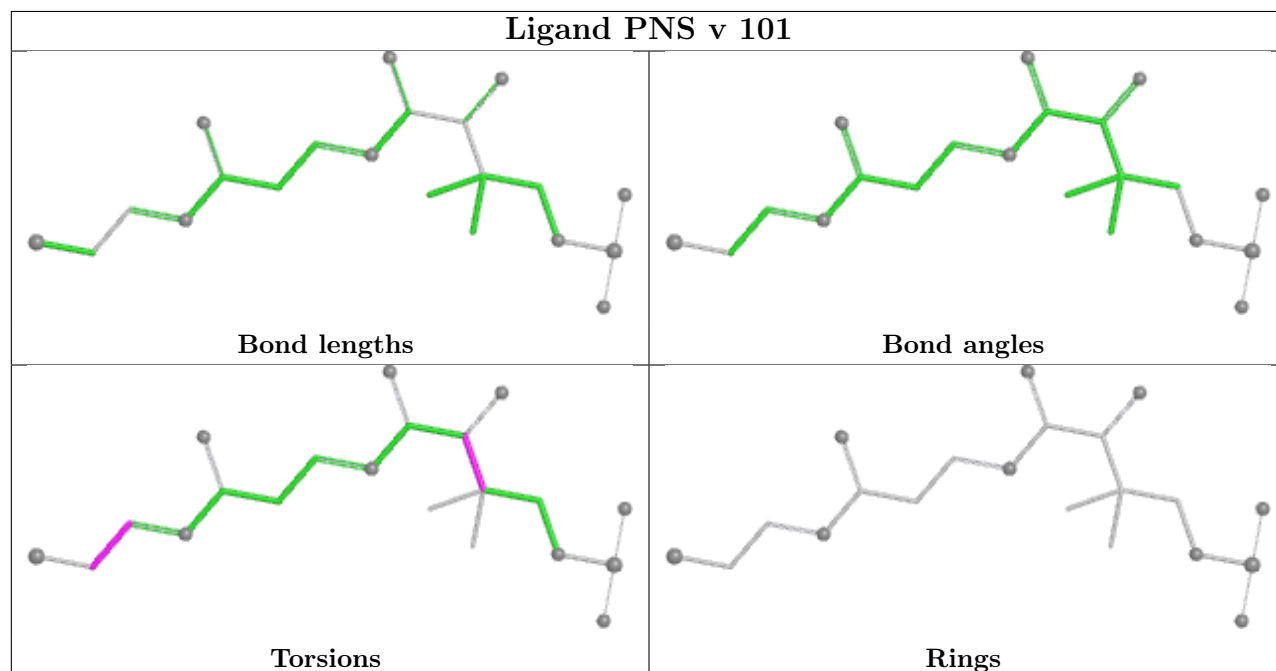
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	v	101	PNS	8	0

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

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

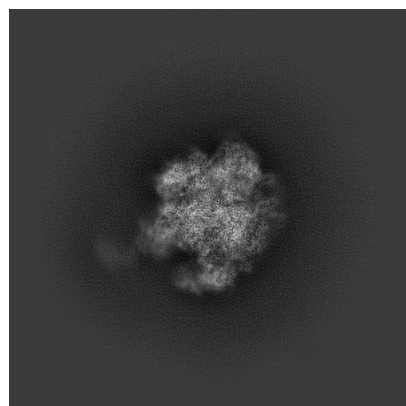
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18461. These allow visual inspection of the internal detail of the map and identification of artifacts.

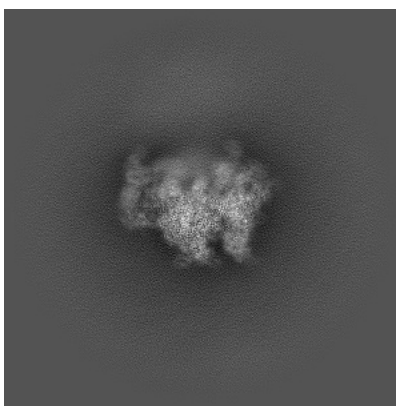
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

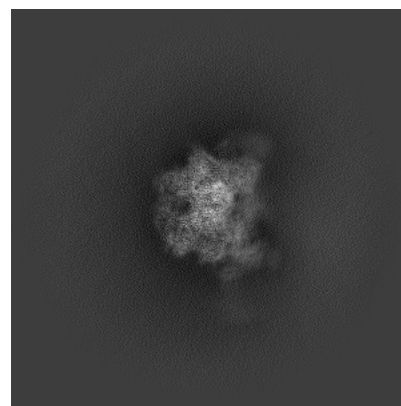
6.1.1 Primary map



X

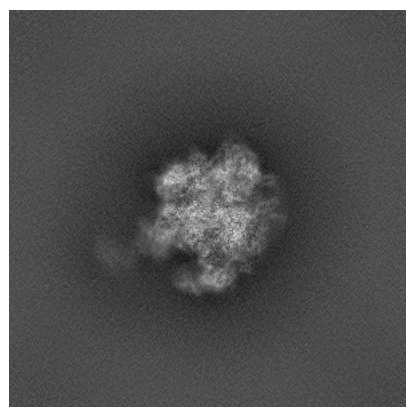


Y

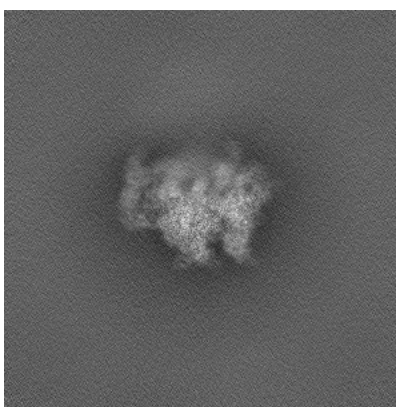


Z

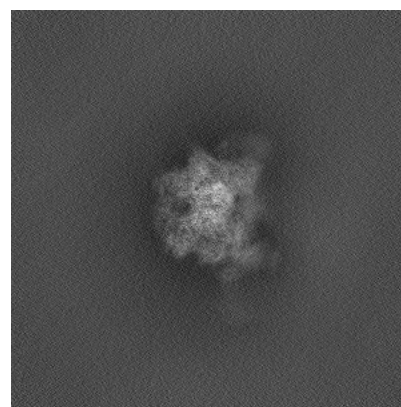
6.1.2 Raw map



X



Y

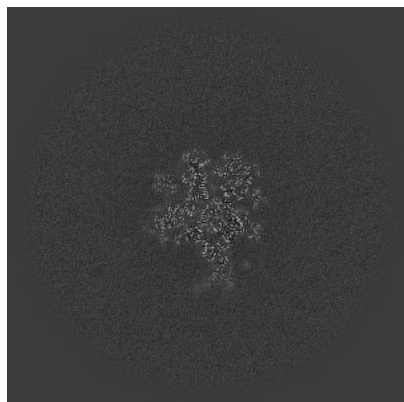


Z

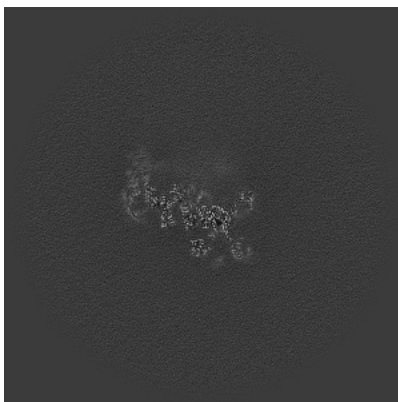
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

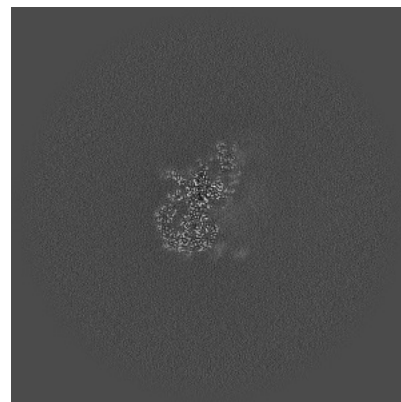
6.2.1 Primary map



X Index: 300

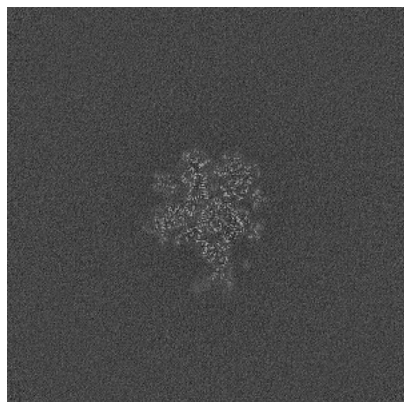


Y Index: 300

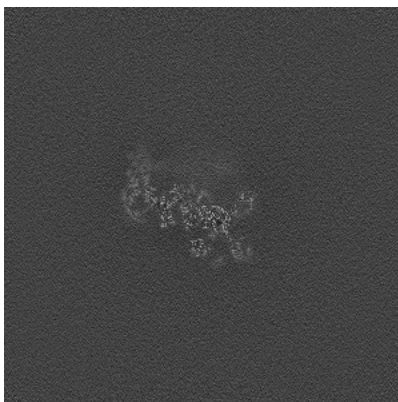


Z Index: 300

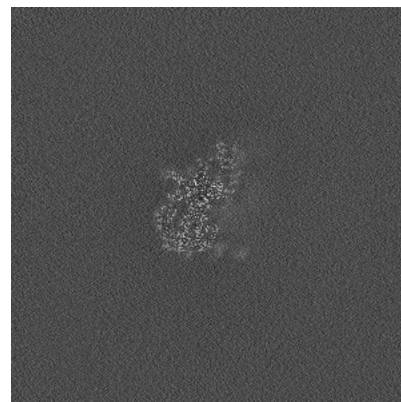
6.2.2 Raw map



X Index: 300



Y Index: 300

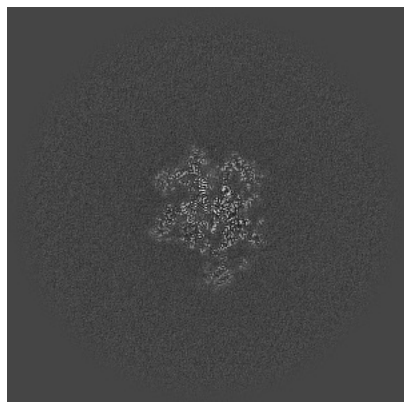


Z Index: 300

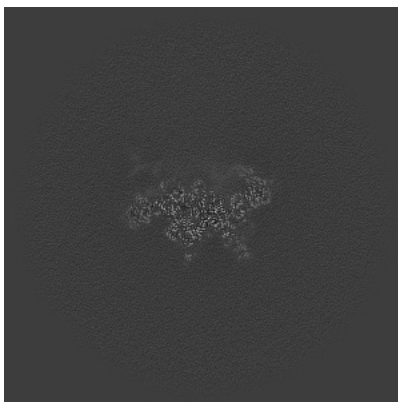
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

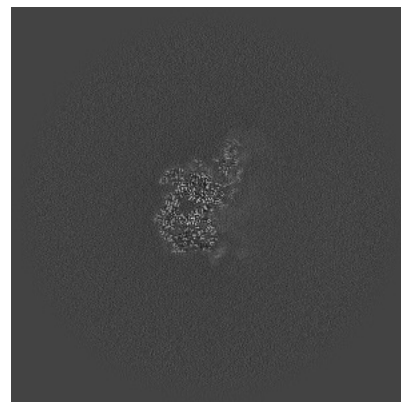
6.3.1 Primary map



X Index: 293

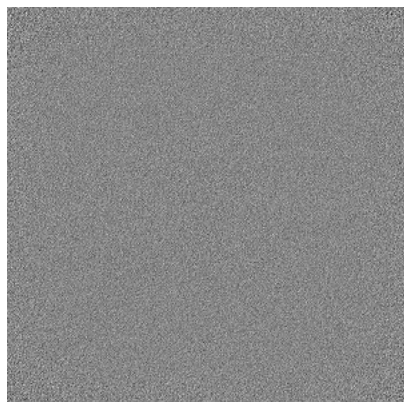


Y Index: 326

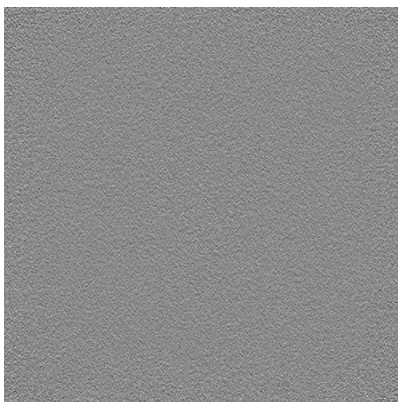


Z Index: 294

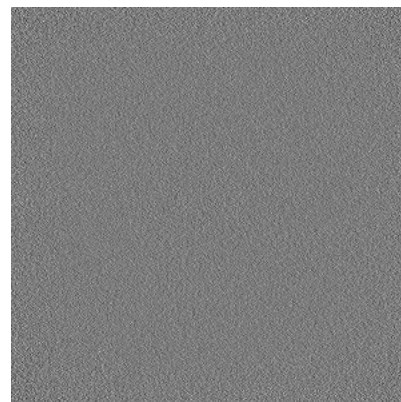
6.3.2 Raw map



X Index: 0



Y Index: 0

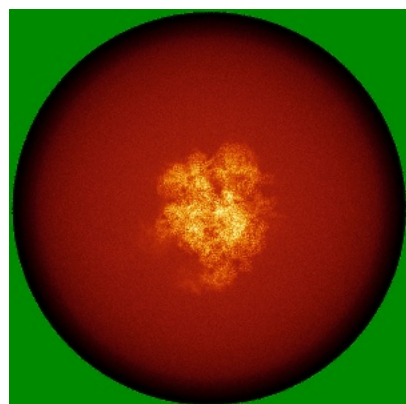


Z Index: 0

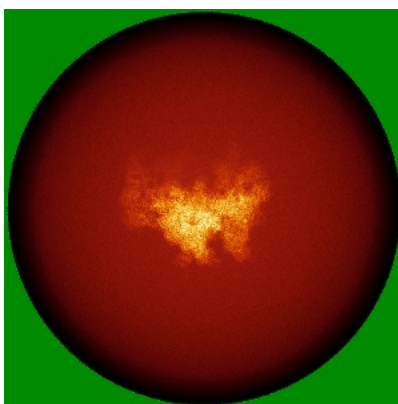
The images above show the largest variance slices of the map in three orthogonal directions.

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

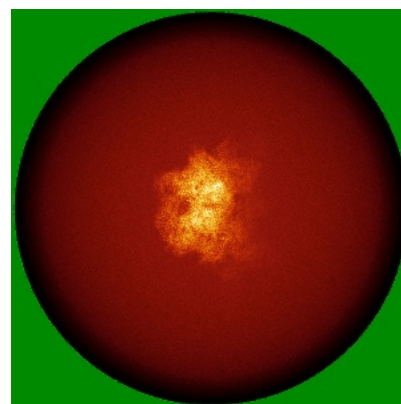
6.4.1 Primary map



X

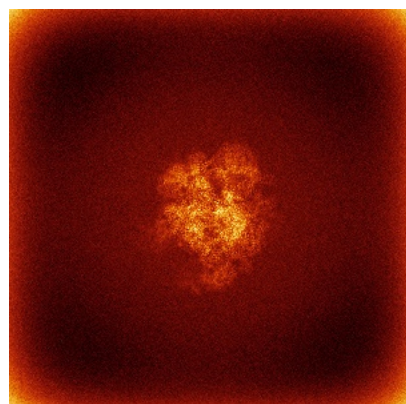


Y

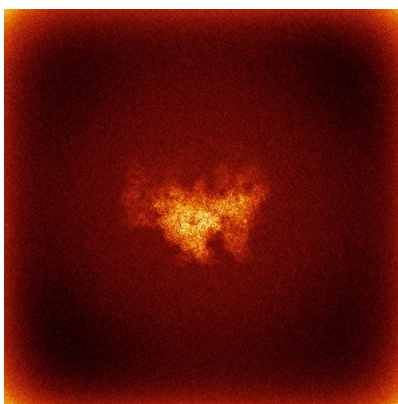


Z

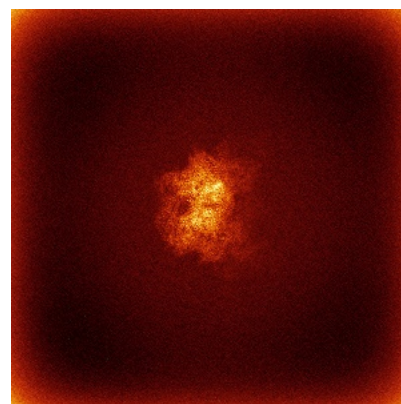
6.4.2 Raw map



X



Y

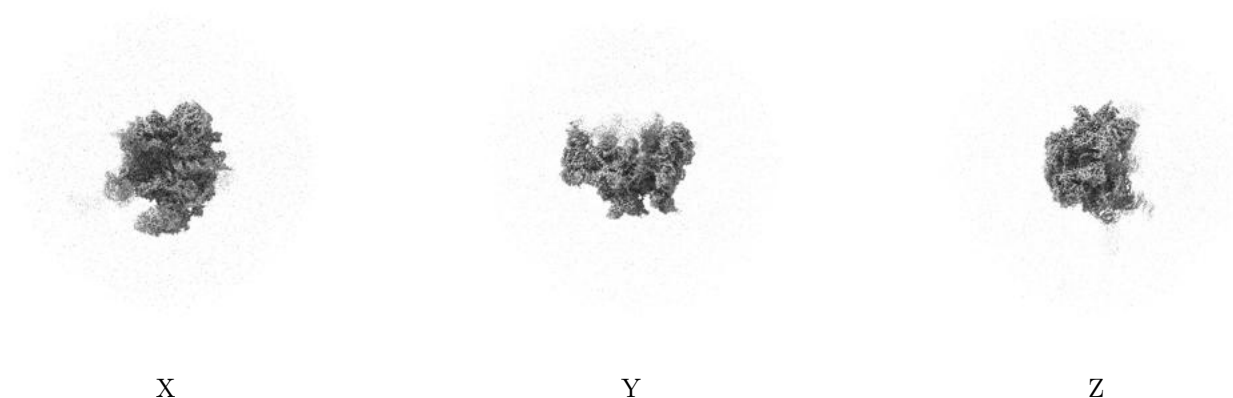


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

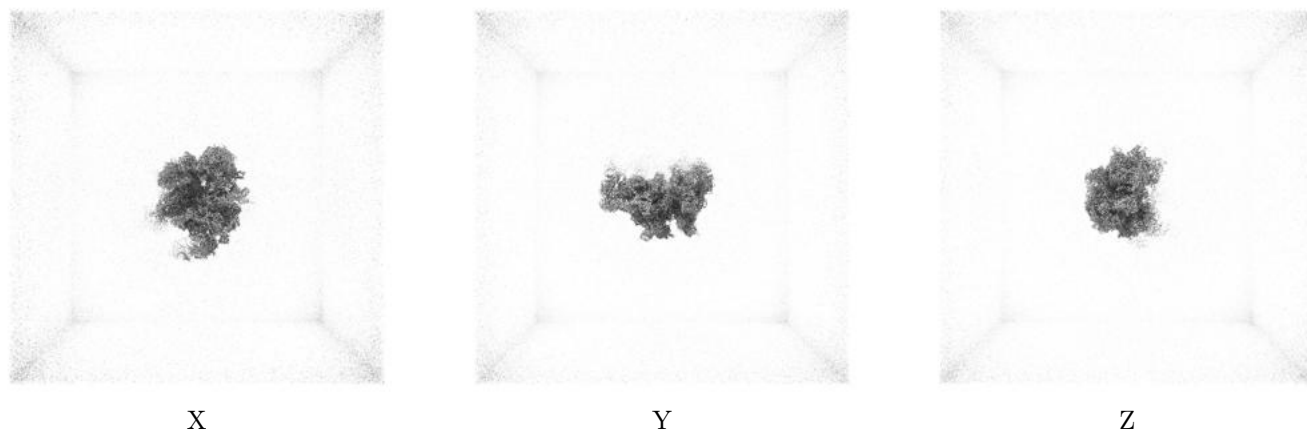
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

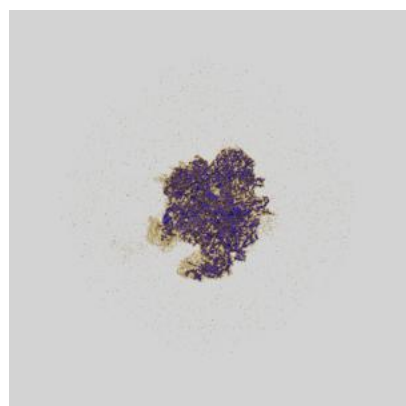
6.6 Mask visualisation [i](#)

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

A mask typically either:

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

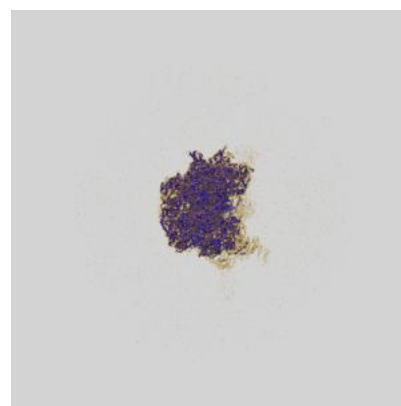
6.6.1 emd_18461_msk_1.map [i](#)



X



Y

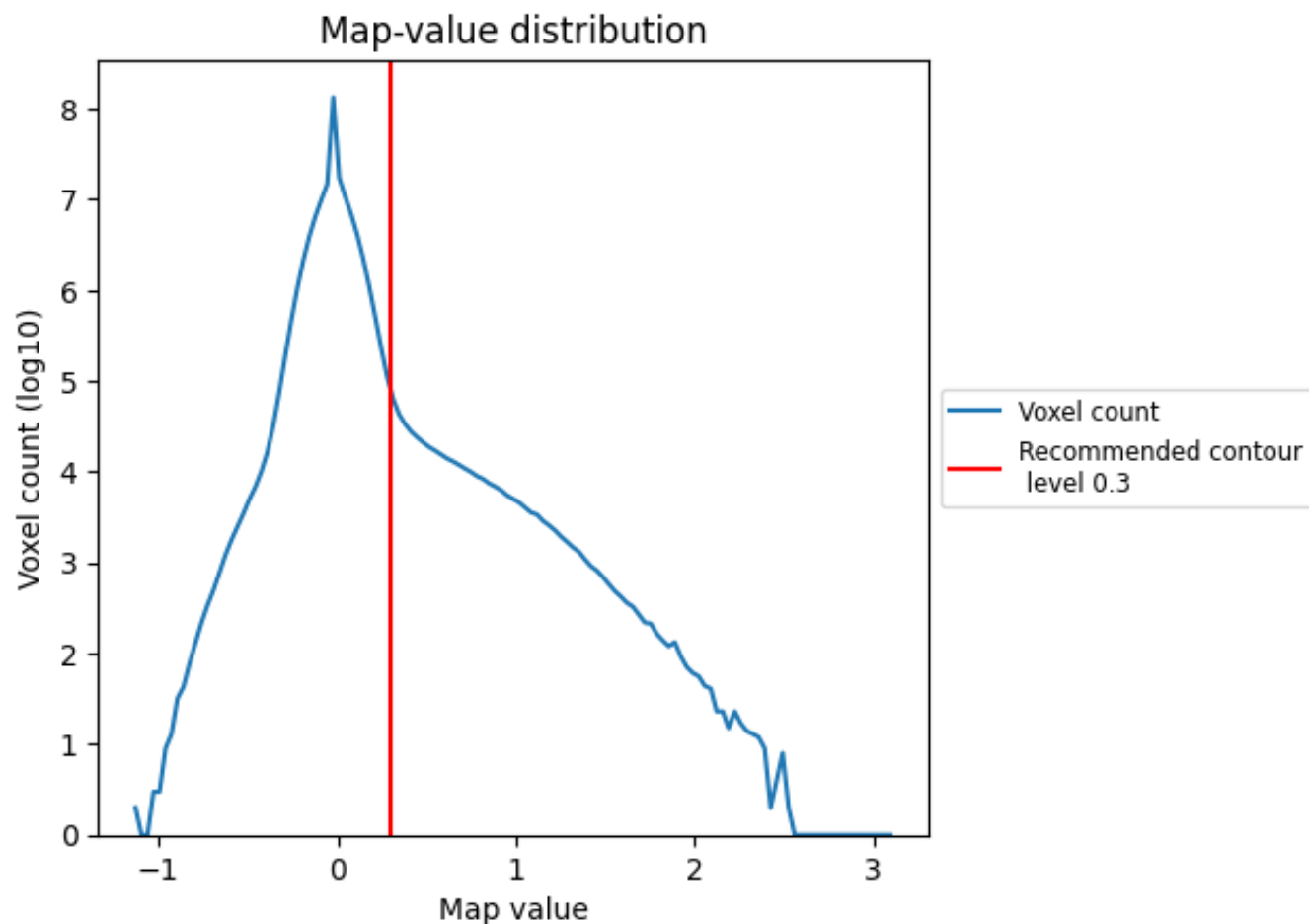


Z

7 Map analysis [i](#)

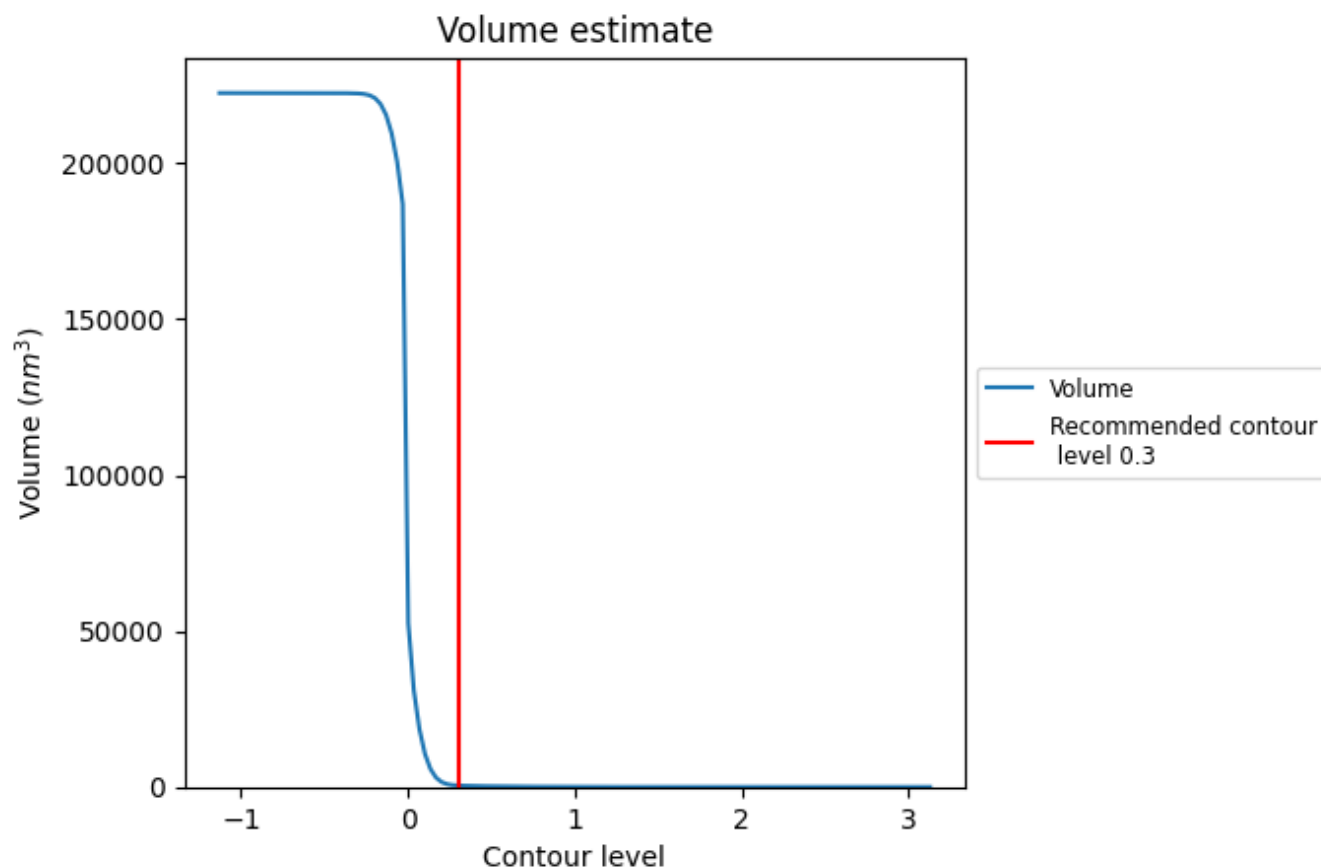
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

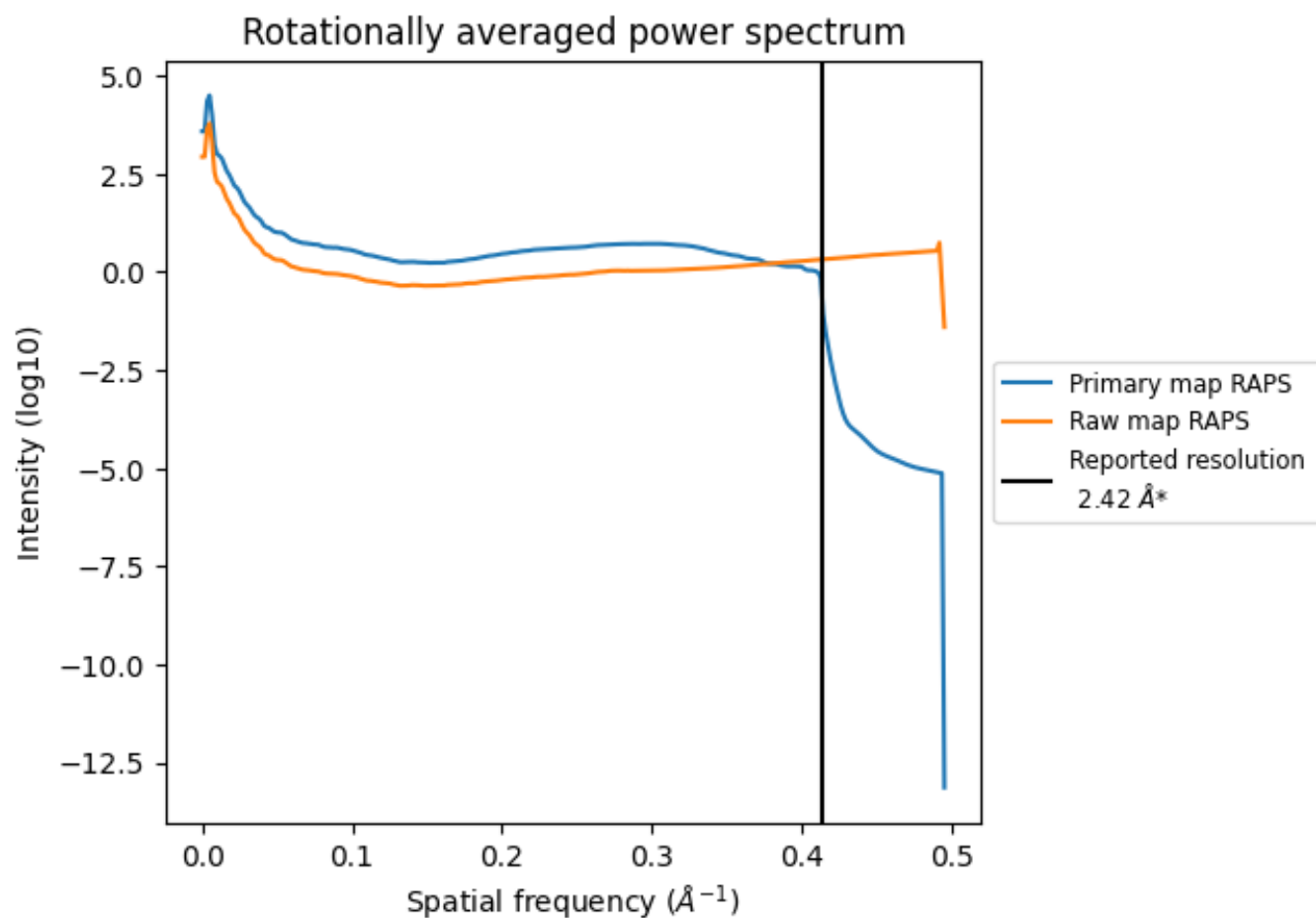
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 458 nm^3 ; this corresponds to an approximate mass of 414 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

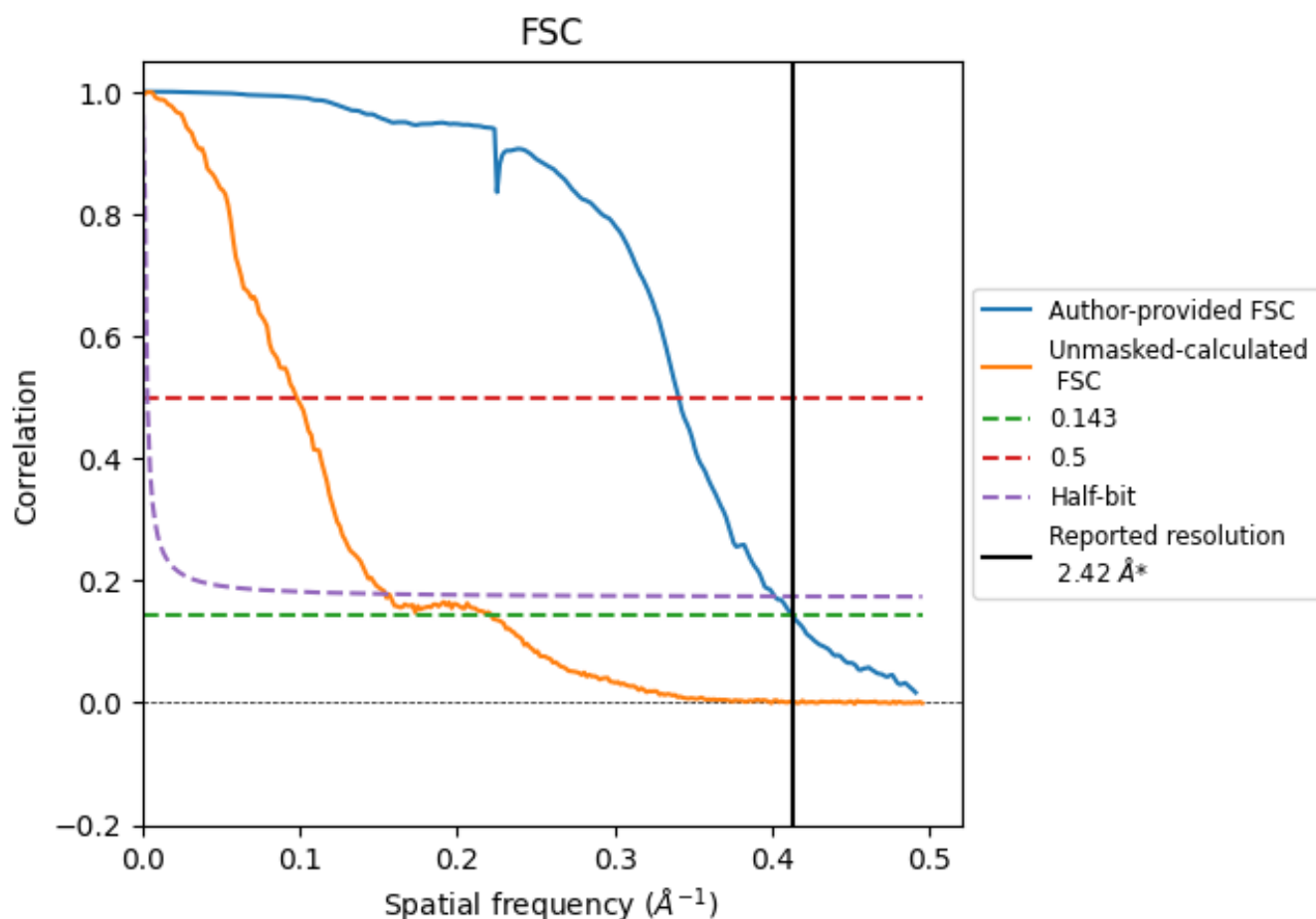


*Reported resolution corresponds to spatial frequency of 0.413 Å⁻¹

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 0.413 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

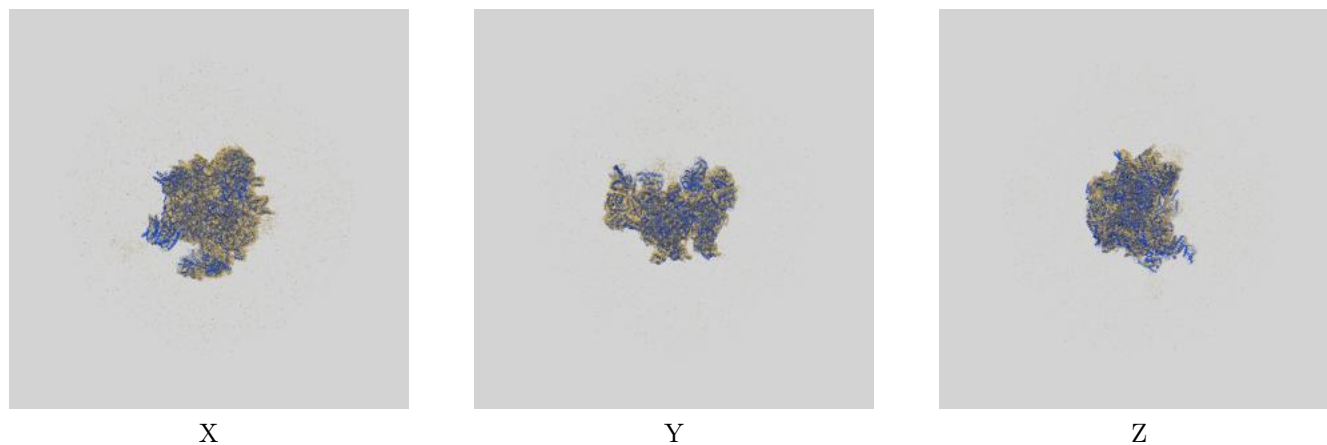
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.42	2.94	2.49
Unmasked-calculated*	4.51	10.21	6.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.51 differs from the reported value 2.42 by more than 10 %

9 Map-model fit [i](#)

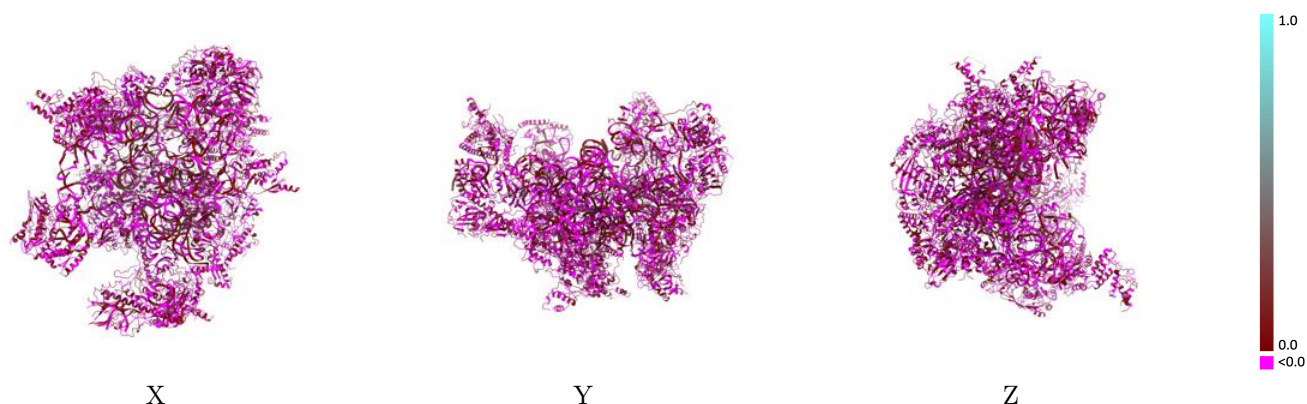
This section contains information regarding the fit between EMDB map EMD-18461 and PDB model 8QU5. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



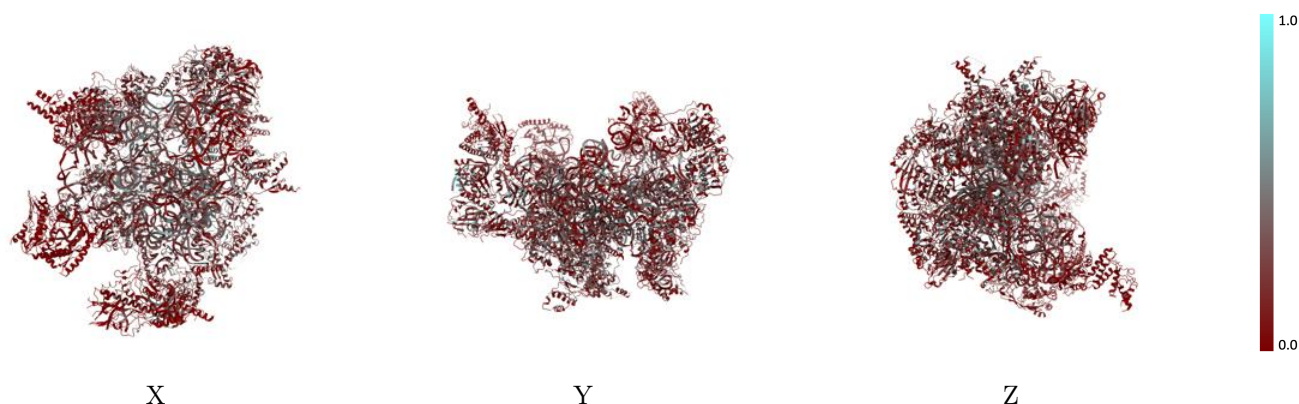
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



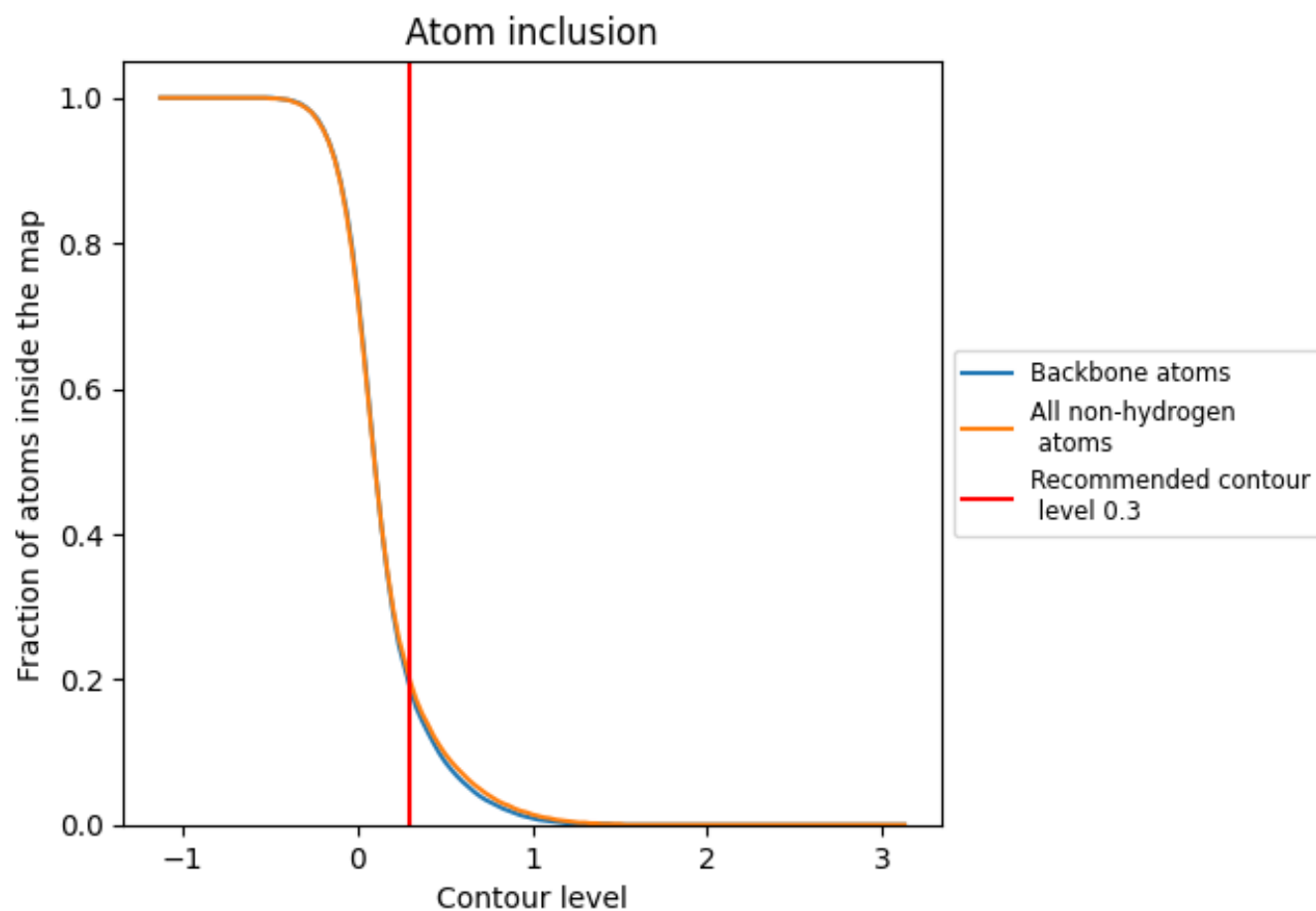
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 19% of all backbone atoms, 20% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1970	0.0060
0	0.1960	-0.0140
1	0.2020	-0.0110
2	0.2820	0.0440
3	0.2320	0.0000
5	0.1690	0.0150
6	0.2110	0.0060
7	0.1930	0.0130
8	0.0730	0.0040
9	0.1970	0.0150
A	0.2580	0.0320
B	0.2290	0.0200
D	0.0220	0.0070
E	0.1980	-0.0250
F	0.2600	-0.0090
H	0.1460	-0.0190
I	0.0560	0.0040
J	0.0070	0.0030
K	0.2150	-0.0060
L	0.1020	-0.0640
M	0.2250	-0.0310
N	0.1640	-0.0080
O	0.2070	-0.0520
P	0.1900	-0.0150
Q	0.1660	-0.0370
R	0.2270	-0.0420
S	0.2050	-0.0190
T	0.2510	-0.0010
U	0.2230	0.0390
V	0.1770	0.0240
W	0.2290	-0.0200
X	0.1950	-0.0000
Y	0.2480	0.0210
Z	0.2190	0.0210
a	0.1970	0.0260



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Chain	Atom inclusion	Q-score
b	 0.2510	 -0.0080
c	 0.2040	 0.0070
d	 0.1610	 0.0150
e	 0.0390	 0.0270
f	 0.0920	 0.0030
g	 0.2280	 0.0070
h	 0.1590	 -0.0190
i	 0.2210	 -0.0350
j	 0.2090	 -0.0090
k	 0.0700	 0.0420
l	 0.0580	 0.0410
m	 0.0110	 0.0130
o	 0.2200	 0.0320
p	 0.1640	 -0.0030
q	 0.1510	 -0.0160
r	 0.1930	 -0.0190
s	 0.2120	 -0.0100
t	 0.0000	 0.0050
u	 0.0810	 -0.0080
v	 0.0400	 -0.0020
w	 0.0170	 0.0150