



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 08:56 PM UTC

PDB ID : 5OOL / pdb_00005ool
EMDB ID : EMD-3842
Title : Structure of a native assembly intermediate of the human mitochondrial ribosome with unfolded interfacial rRNA
Authors : Brown, A.; Rathore, S.; Kimanius, D.; Aibara, S.; Bai, X.C.; Rorbach, J.; Amunts, A.; Ramakrishnan, V.
Deposited on : 2017-08-08
Resolution : 3.06 Å (reported)
Based on initial model : 3J9M

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

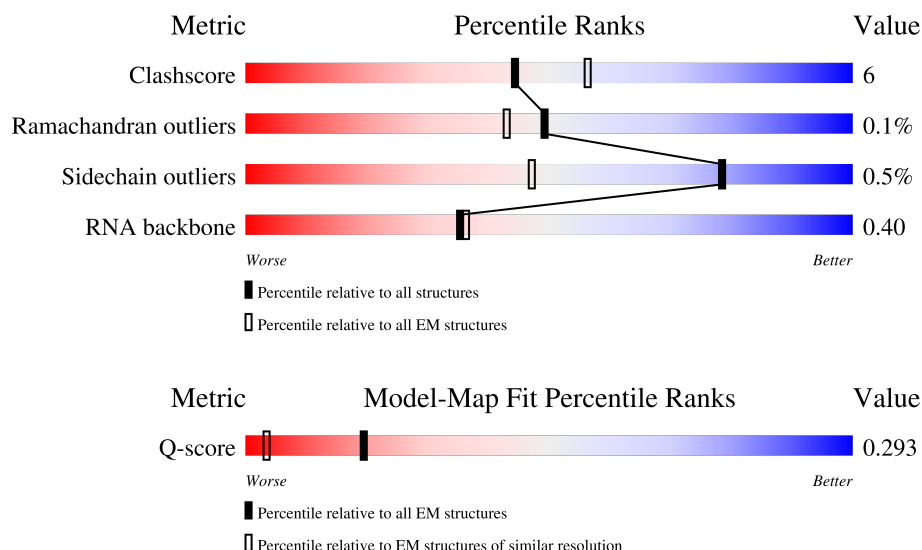
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 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	13976 (2.56 - 3.56)

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

Mol	Chain	Length	Quality of chain
1	A	1559	9% 56% 31% 5% 8%
2	B	69	14% 48% 30% • 19%

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Mol	Chain	Length	Quality of chain
3	D	305	
4	E	348	
5	F	311	
6	H	267	
7	I	261	
8	J	192	
9	K	178	
10	L	145	
11	M	296	
12	N	251	
13	O	175	
14	P	180	
15	Q	292	
16	R	149	
17	S	205	
18	T	206	
19	U	153	
20	V	216	
21	W	148	
22	X	256	
23	Y	250	
24	Z	161	
25	0	188	
26	1	65	
27	2	92	

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Mol	Chain	Length	Quality of chain
28	3	188	
29	4	103	
30	5	423	
31	6	380	
32	7	338	
33	8	206	
34	9	137	
35	a	142	
36	b	215	
37	c	332	
38	d	306	
39	e	279	
40	f	212	
41	g	166	
42	h	158	
43	i	128	
44	j	123	
45	k	112	
46	l	138	
47	m	128	
48	o	102	
49	p	206	
50	q	222	
51	r	196	
52	s	439	

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Mol	Chain	Length	Quality of chain
53	t	28	68% 93% 7%
54	u	234	12% 33% 14% 53%
55	v	70	54% 74% 24% .
56	w	156	46% 38% 12% 49%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 98998 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1441	Total	C	N	O	P	0	0
			30607	13732	5531	9903	1441		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a RNA chain called mitochondrial tRNAVal.

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

- Molecule 3 is a protein called 39S ribosomal protein L2, mitochondrial.

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

- Molecule 4 is a protein called 39S ribosomal protein L3, mitochondrial.

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

- Molecule 5 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 6 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 7 is a protein called 39S ribosomal protein L10, mitochondrial.

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

- Molecule 8 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 9 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 10 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 11 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 12 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 13 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 14 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 17 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 18 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 19 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 25 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 26 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 27 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	45	Total	C	N	O	S	0	0
			367	227	81	58	1		

- Molecule 28 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 29 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	37	Total	C	N	O	S	0	0
			333	212	71	47	3		

- Molecule 30 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	387	Total	C	N	O	S	0	0
			3156	2039	548	558	11		

- Molecule 31 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	324	Total	C	N	O	S	0	0
			2640	1694	470	468	8		

- Molecule 32 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7	287	Total	C	N	O	S	0	0
			2334	1495	397	425	17		

- Molecule 33 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	8	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 34 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	9	117	Total	C	N	O	S	0	0
			947	614	163	168	2		

- Molecule 35 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L45, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 45 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 46 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 47 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 48 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 49 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 50 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

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

- Molecule 51 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 52 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 53 is a protein called Unknown protein or protein extension.

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

- Molecule 54 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

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

- Molecule 55 is a protein called MIEF1 upstream open reading frame protein.

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

- Molecule 56 is a protein called Acyl carrier protein, mitochondrial.

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

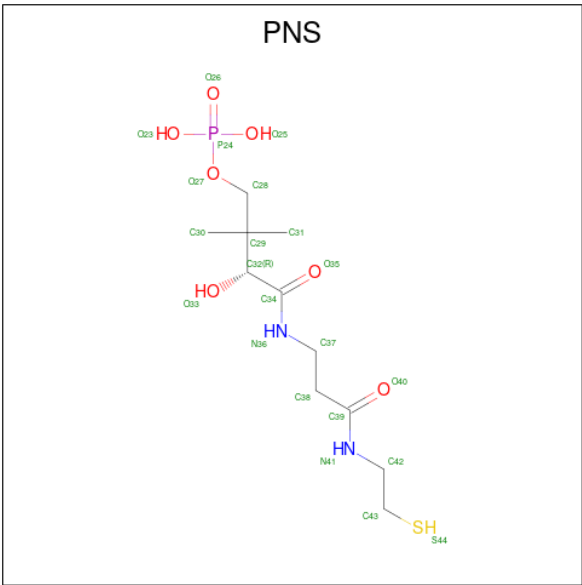
- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	A	84	Total	Mg	0
			84	84	
57	D	1	Total	Mg	0
			1	1	
57	E	1	Total	Mg	0
			1	1	
57	M	1	Total	Mg	0
			1	1	
57	R	1	Total	Mg	0
			1	1	
57	T	1	Total	Mg	0
			1	1	
57	W	1	Total	Mg	0
			1	1	
57	g	1	Total	Mg	0
			1	1	
57	o	1	Total	Mg	0
			1	1	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	0	1	Total	Zn	0
			1	1	
58	4	1	Total	Zn	0
			1	1	
58	r	1	Total	Zn	0
			1	1	

- Molecule 59 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C₁₁H₂₃N₂O₇PS).

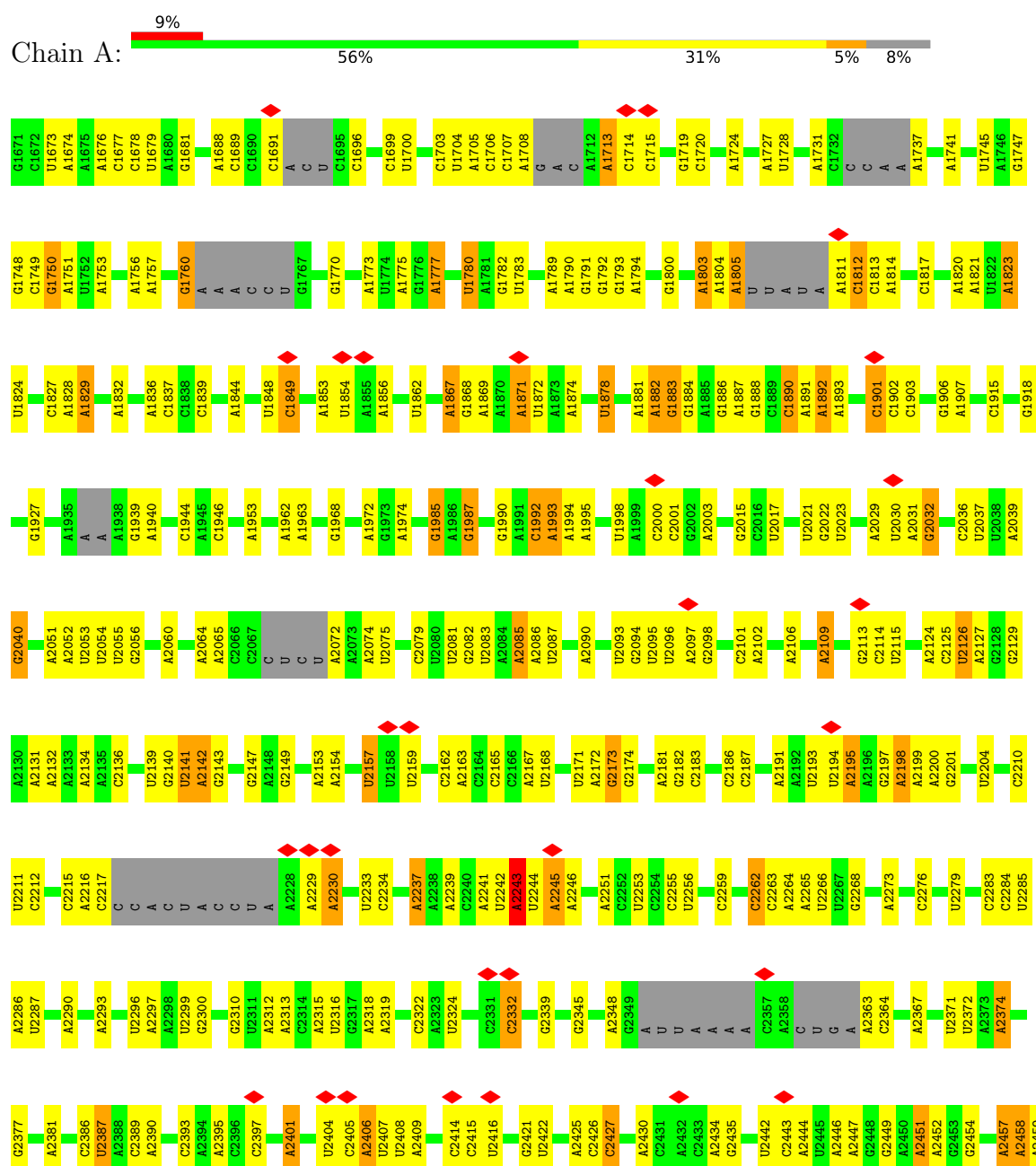


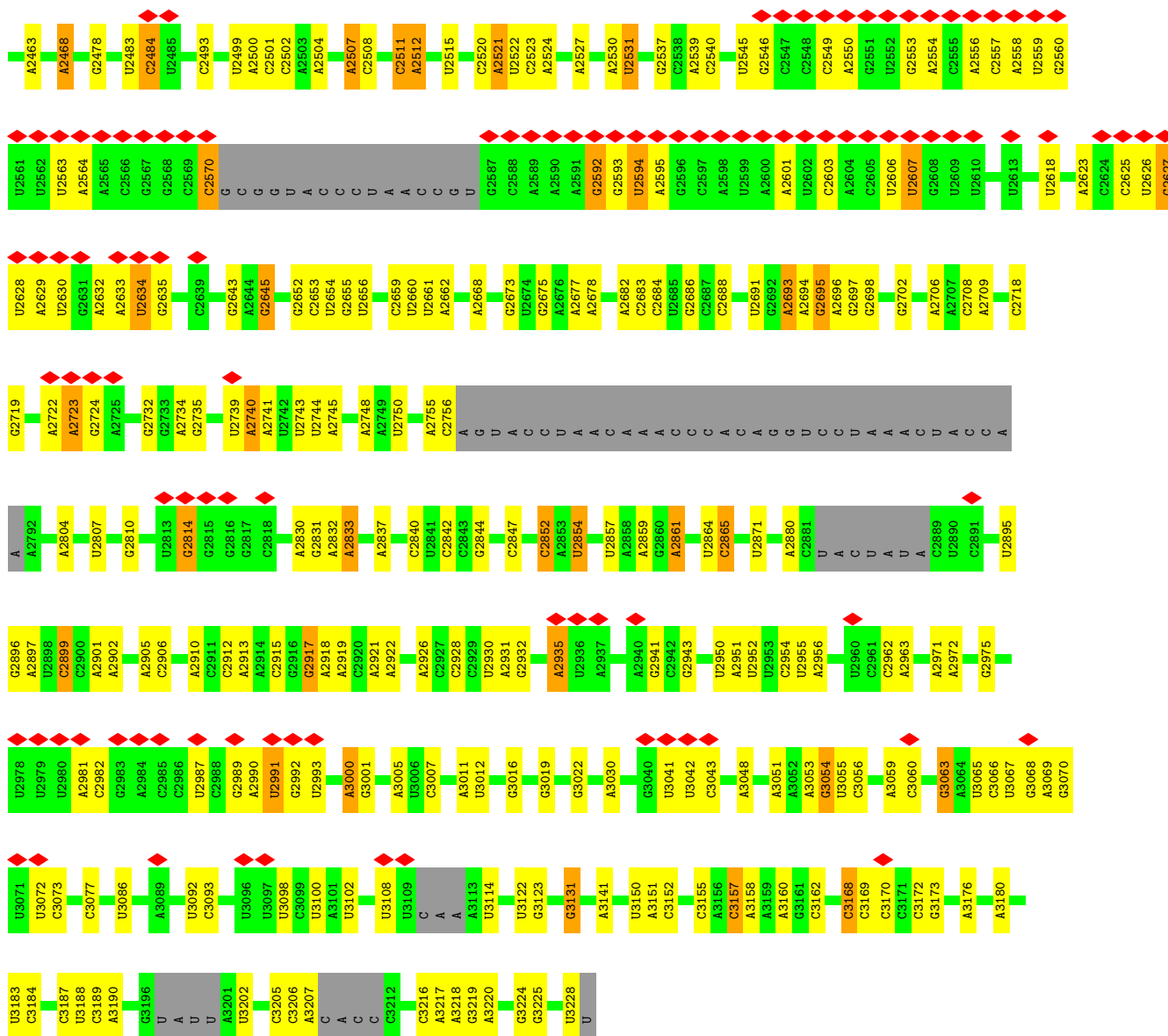
Mol	Chain	Residues	Atoms						AltConf
59	v	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

3 Residue-property plots

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

• Molecule 1: 16S ribosomal RNA

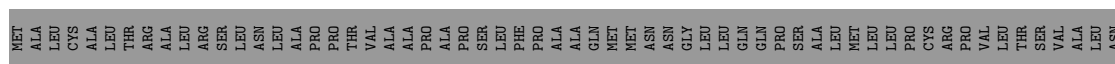


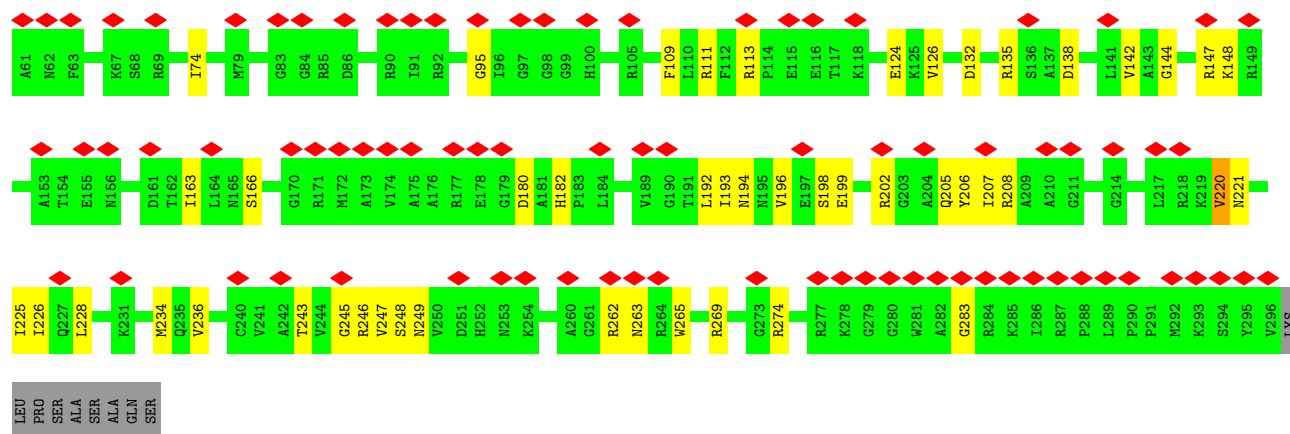


- Molecule 2: mitochondrial tRNA^{Val}

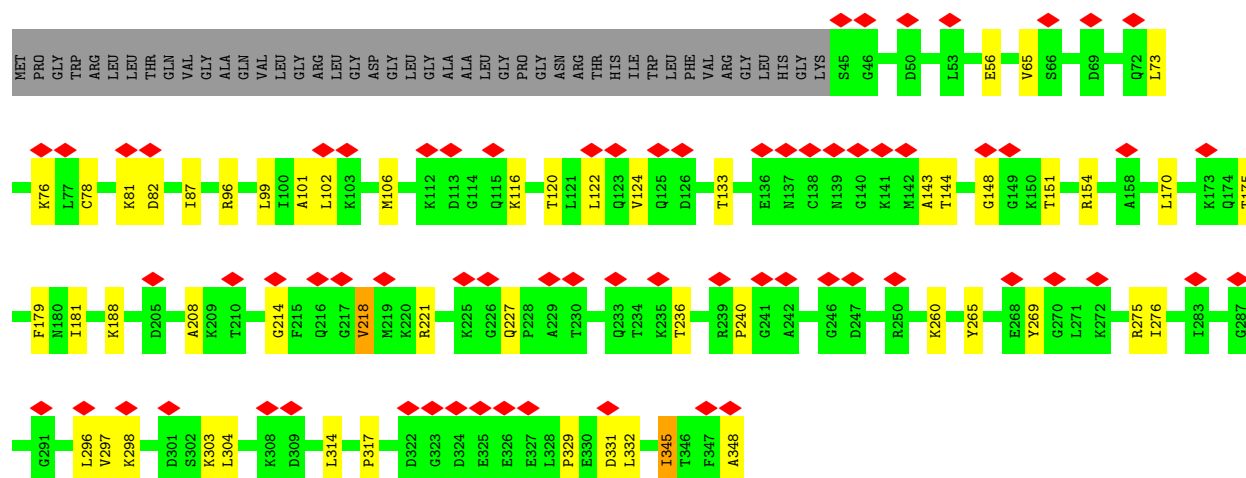


- Molecule 3: 39S ribosomal protein L2, mitochondrial

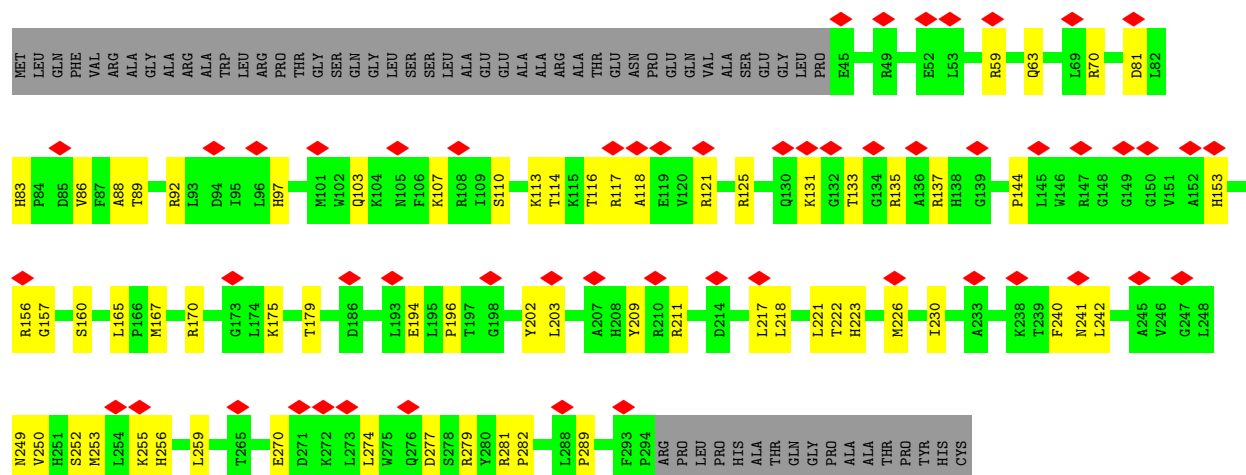


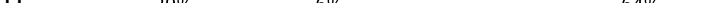


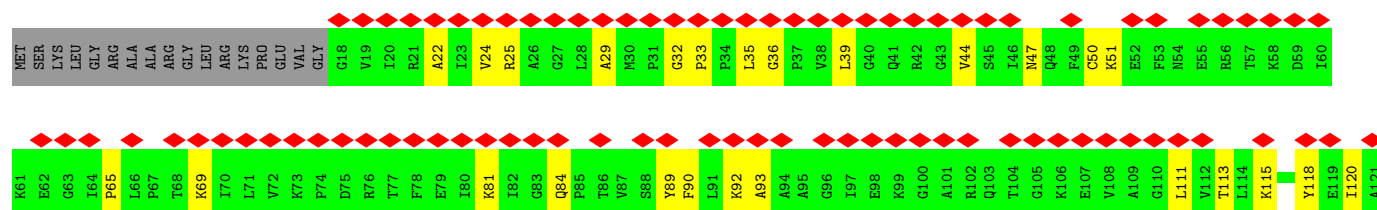
• Molecule 4: 39S ribosomal protein L3, mitochondrial

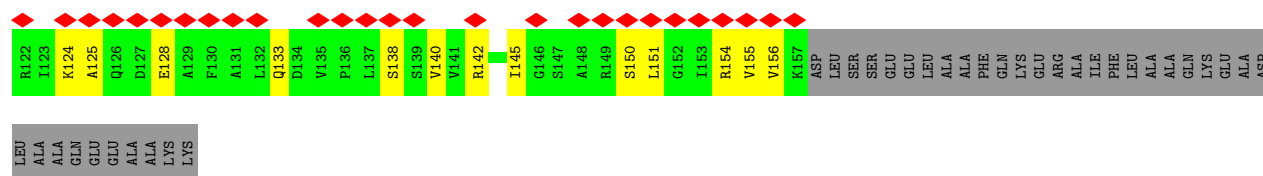


• Molecule 5: 39S ribosomal protein L4, mitochondrial

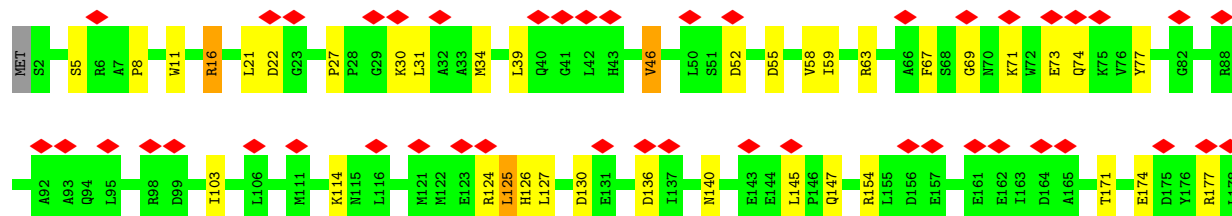
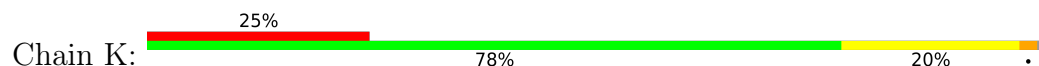


- Chain H: 

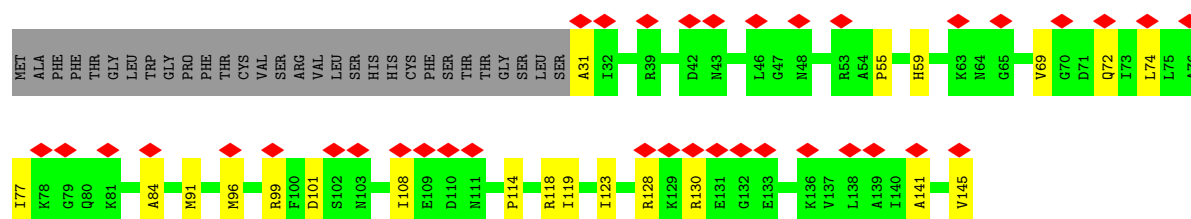




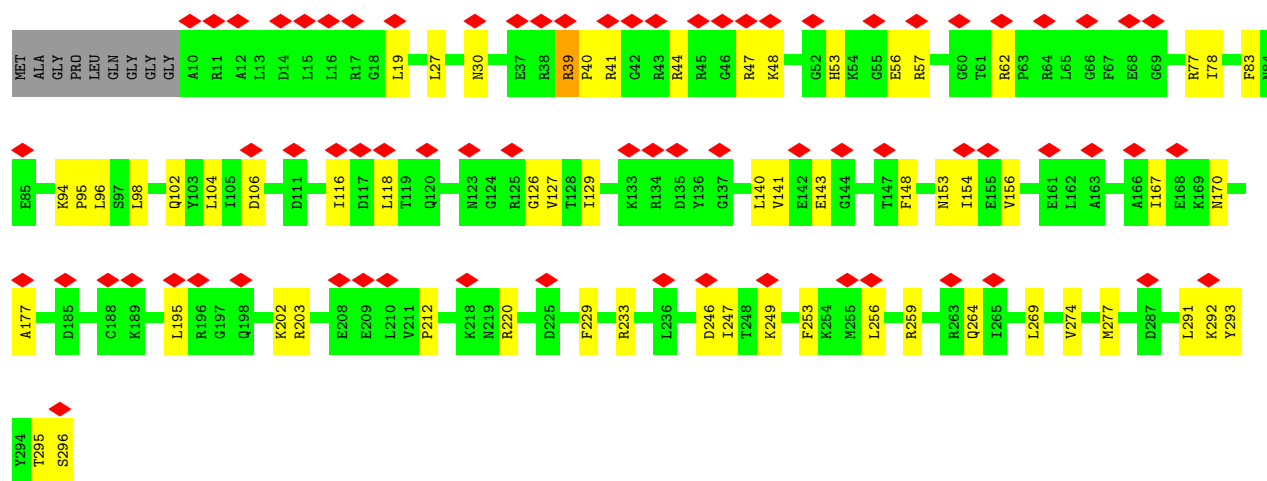
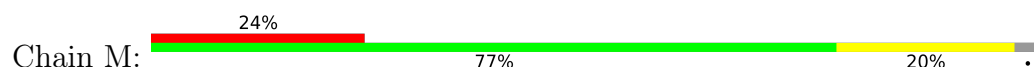
- Molecule 9: 39S ribosomal protein L13, mitochondrial



- Molecule 10: 39S ribosomal protein L14, mitochondrial

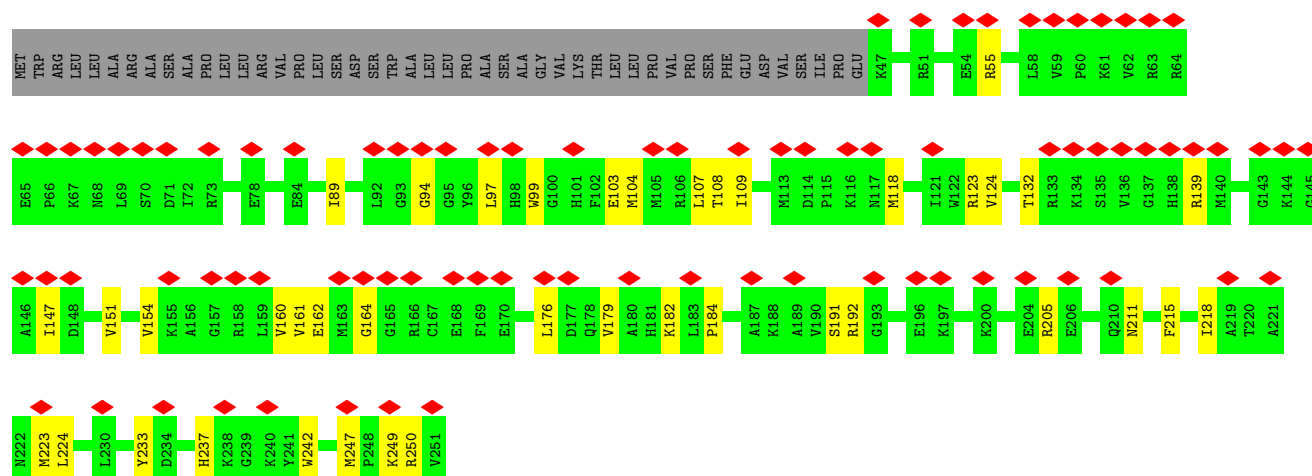


- Molecule 11: 39S ribosomal protein L15, mitochondrial

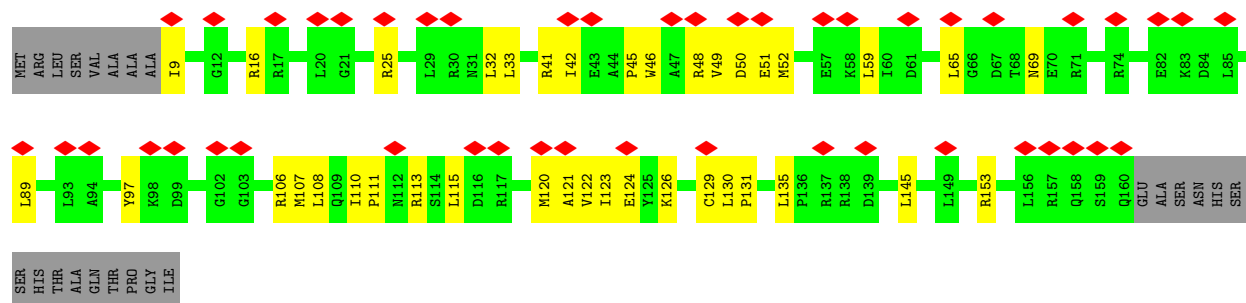


- Molecule 12: 39S ribosomal protein L16, mitochondrial

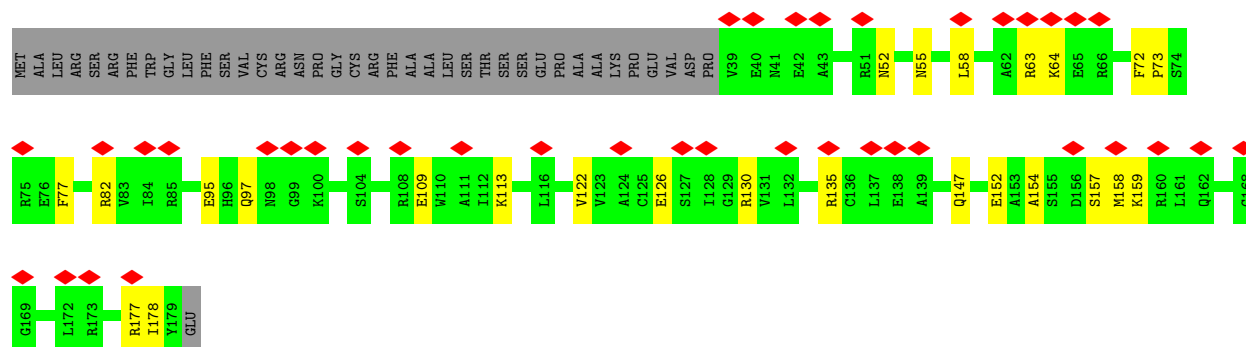




- Molecule 13: 39S ribosomal protein L17, mitochondrial

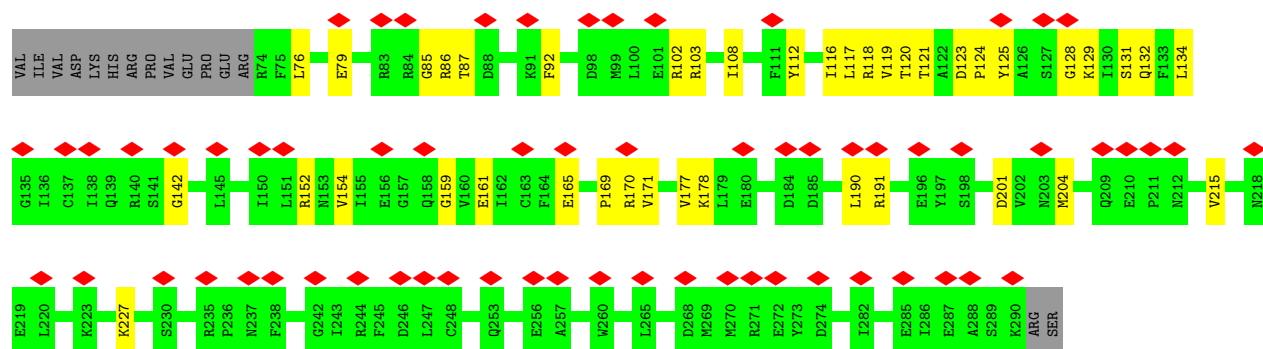


- Molecule 14: 39S ribosomal protein L18, mitochondrial

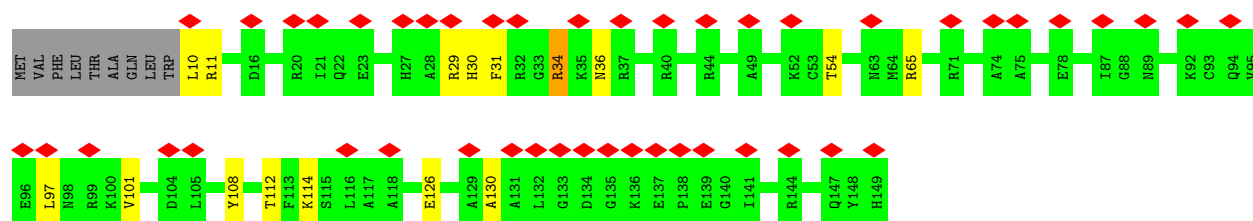
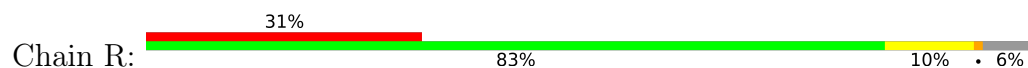


- Molecule 15: 39S ribosomal protein L19, mitochondrial

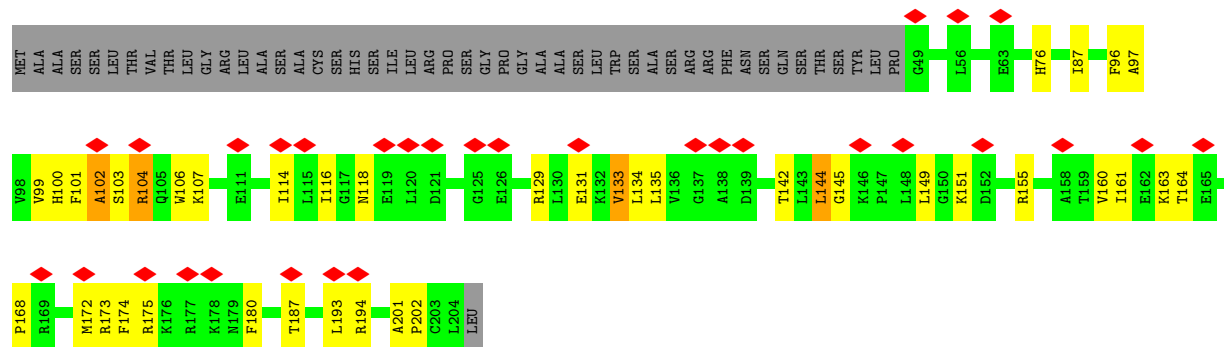




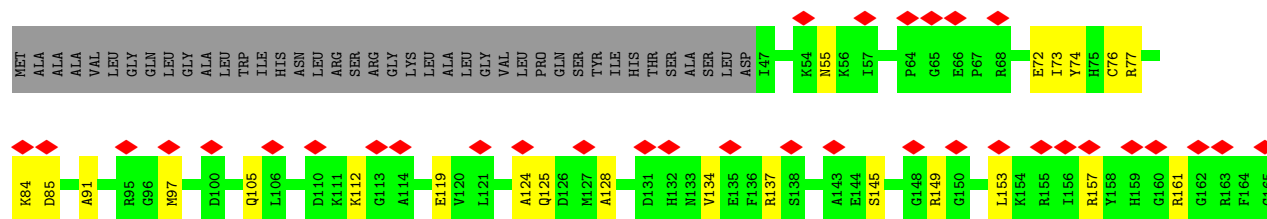
- Molecule 16: 39S ribosomal protein L20, mitochondrial

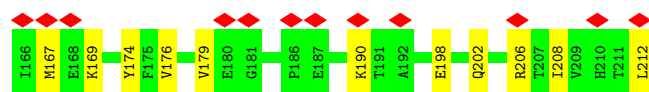


- Molecule 17: 39S ribosomal protein L21, mitochondrial

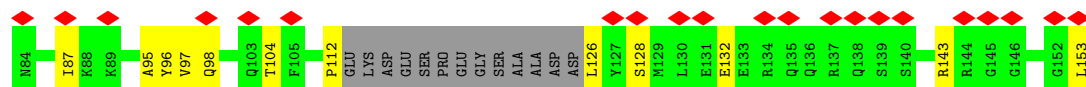


- Molecule 18: 39S ribosomal protein L22, mitochondrial

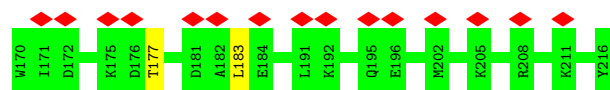
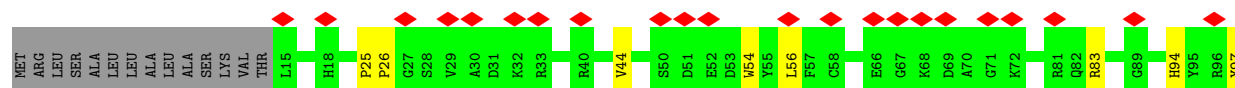
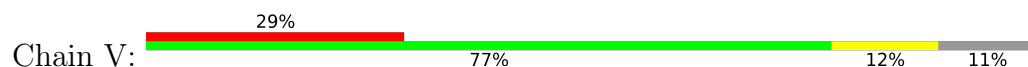




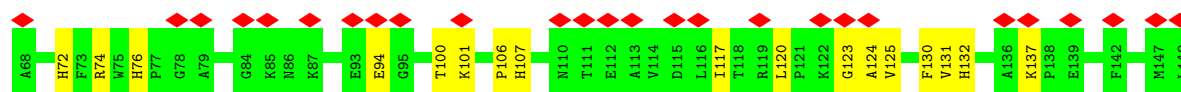
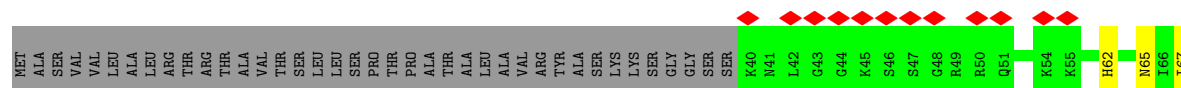
- Molecule 19: 39S ribosomal protein L23, mitochondrial



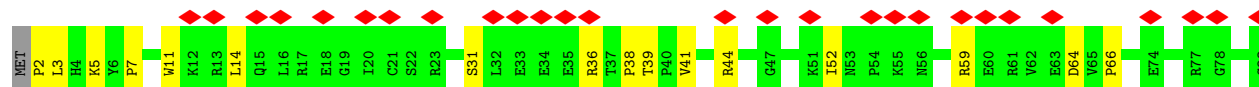
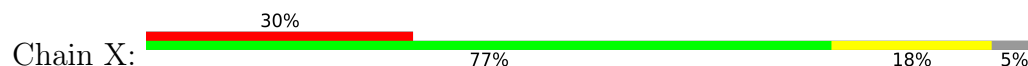
- Molecule 20: 39S ribosomal protein L24, mitochondrial

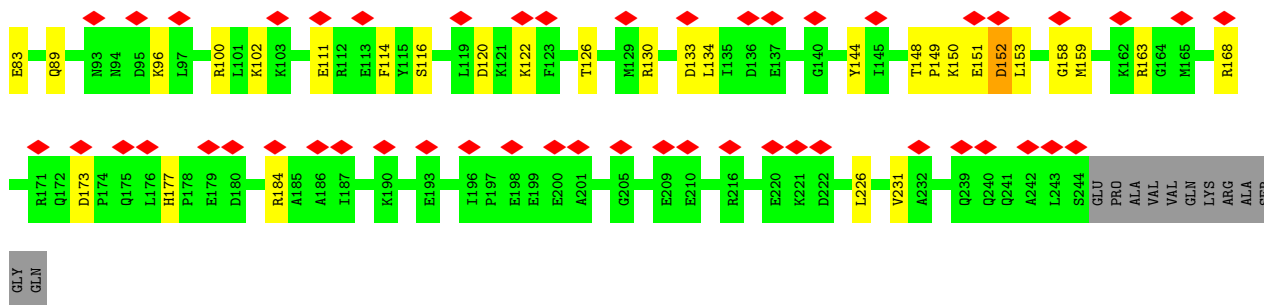


- Molecule 21: 39S ribosomal protein L27, mitochondrial

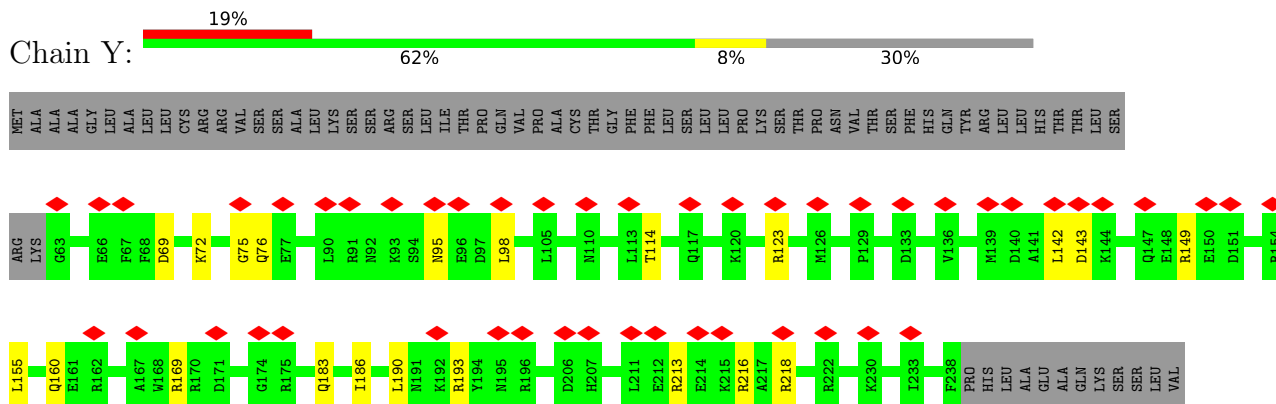


- Molecule 22: 39S ribosomal protein L28, mitochondrial

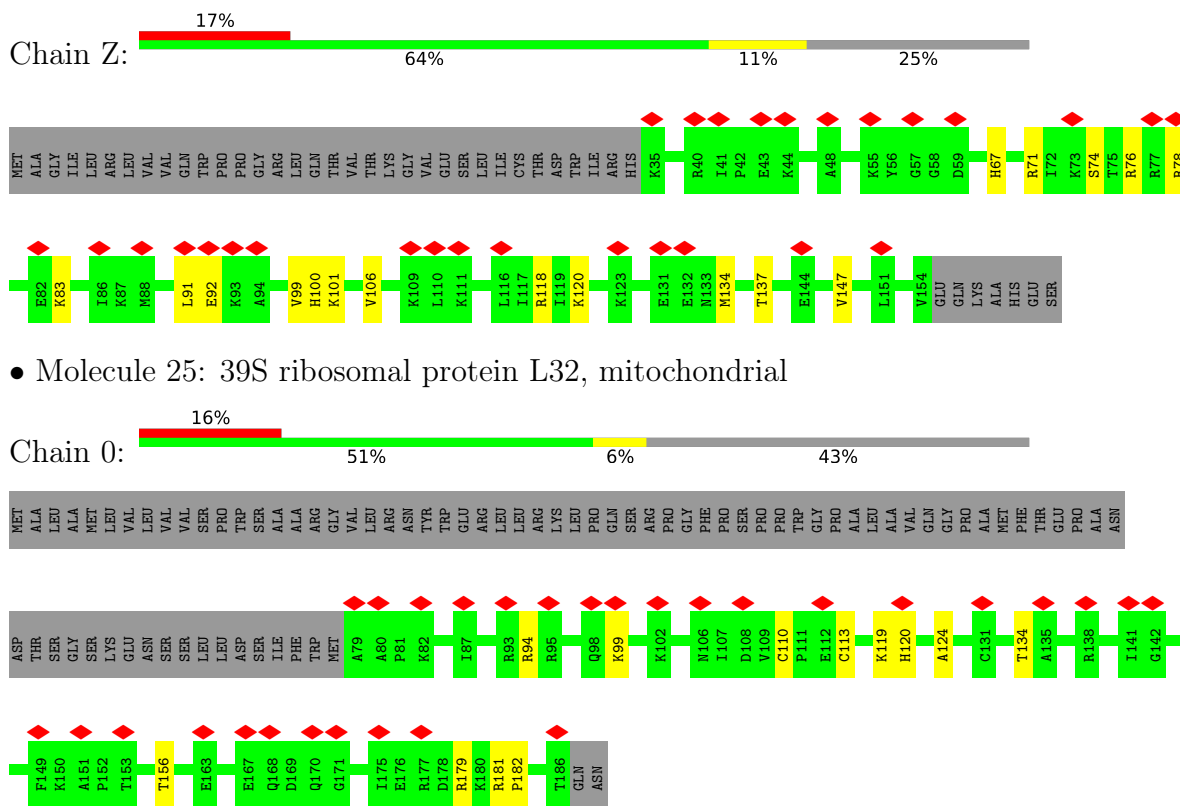




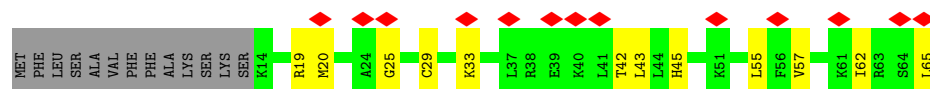
- Molecule 23: 39S ribosomal protein L47, mitochondrial



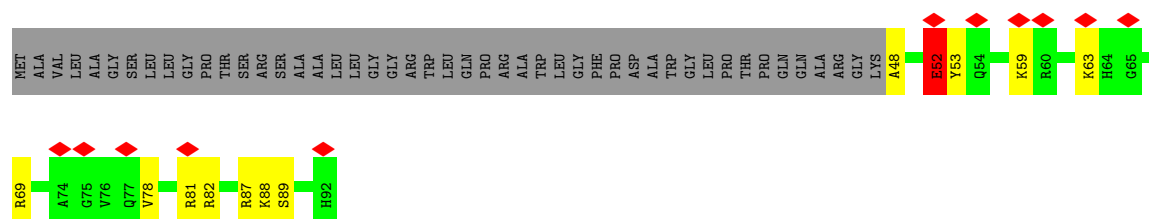
- Molecule 24: 39S ribosomal protein L30, mitochondrial

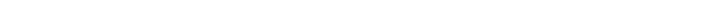


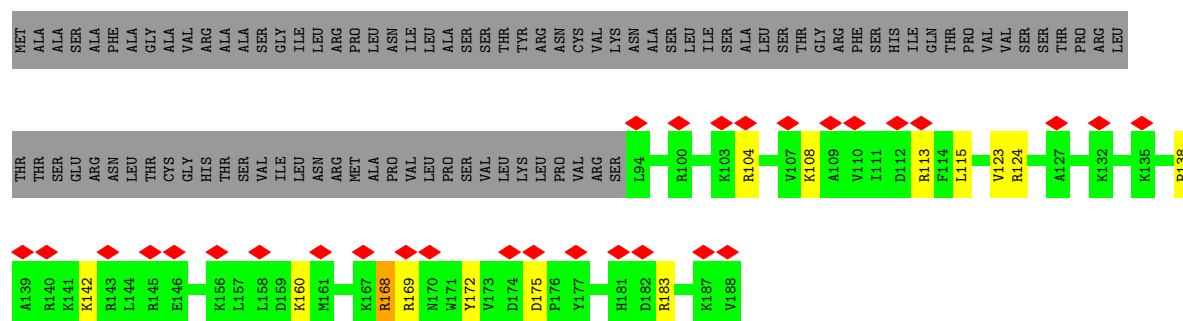
- Molecule 26: 39S ribosomal protein L33, mitochondrial

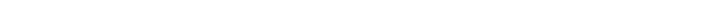


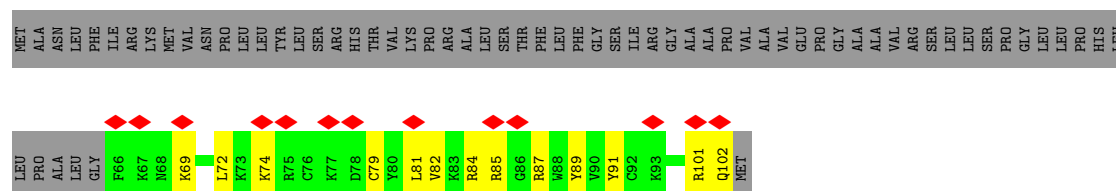
- Chain 2:

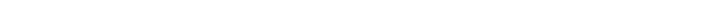


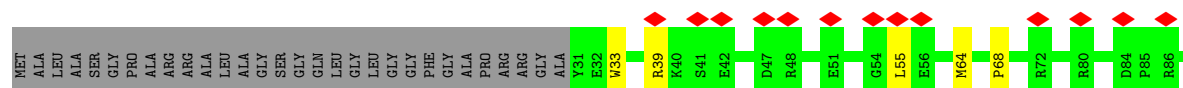
- Chain 3:  16% 43% 7% 49%

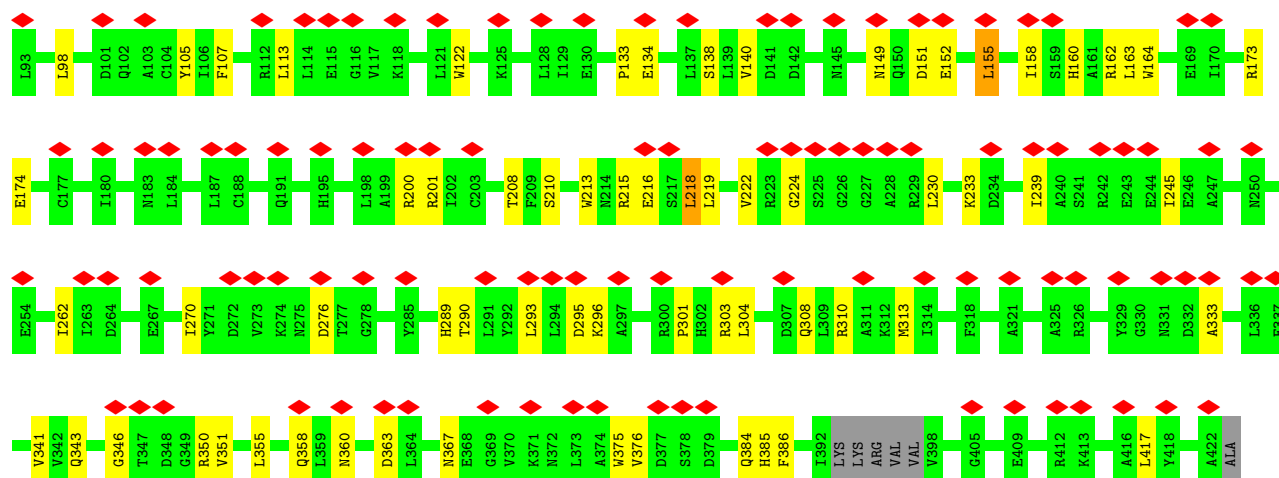


- Chain 4:  13% 23% 13% 64%

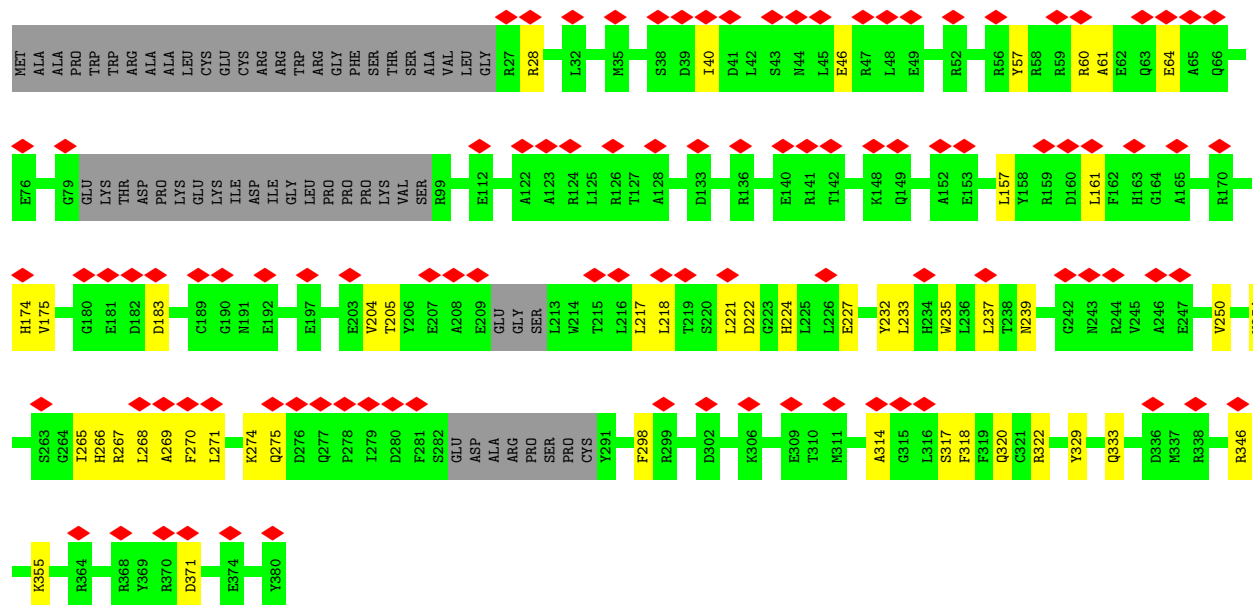
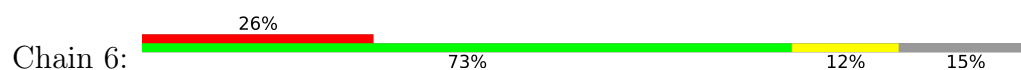


- Chain 5:  28% 75% 16% 9%

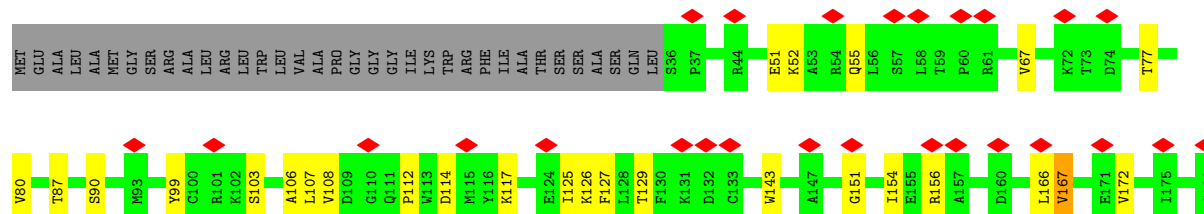
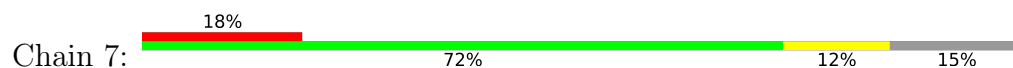


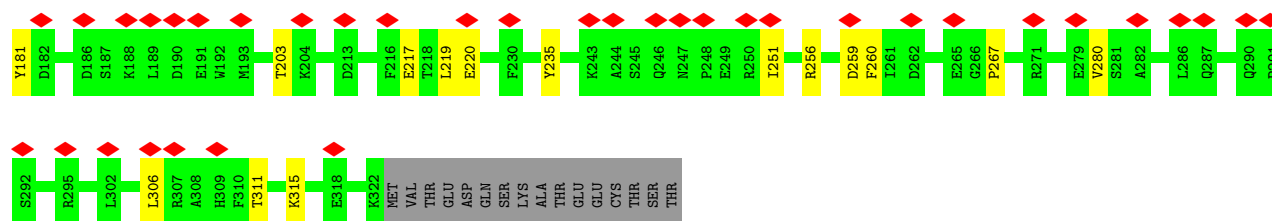


• Molecule 31: 39S ribosomal protein L38, mitochondrial



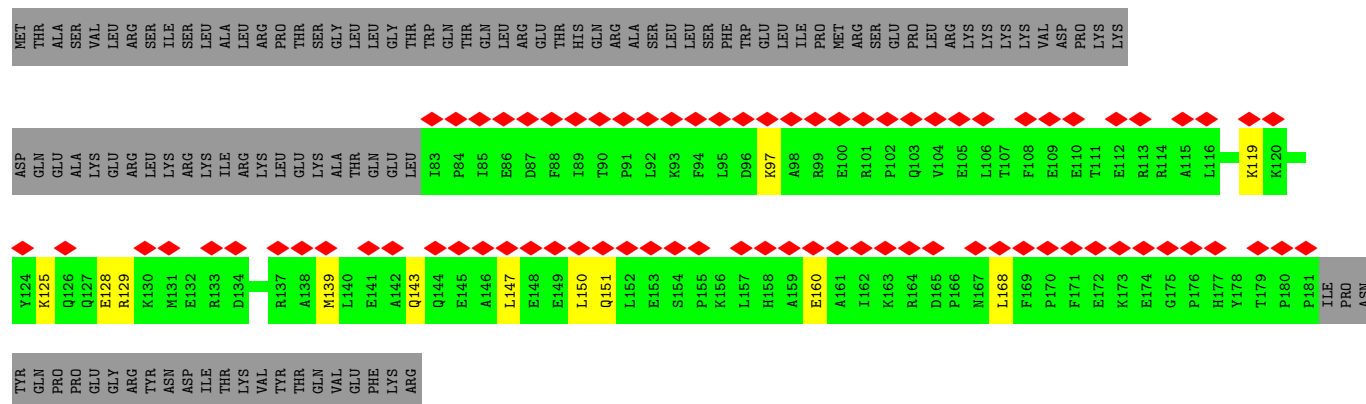
• Molecule 32: 39S ribosomal protein L39, mitochondrial





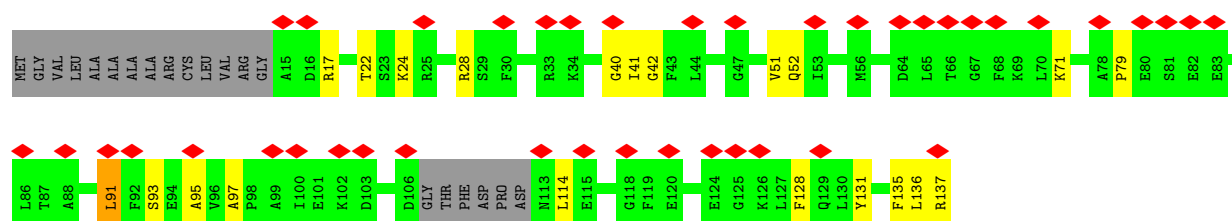
- Molecule 33: 39S ribosomal protein L40, mitochondrial

Chain 8: 38%
42% 6% 52%



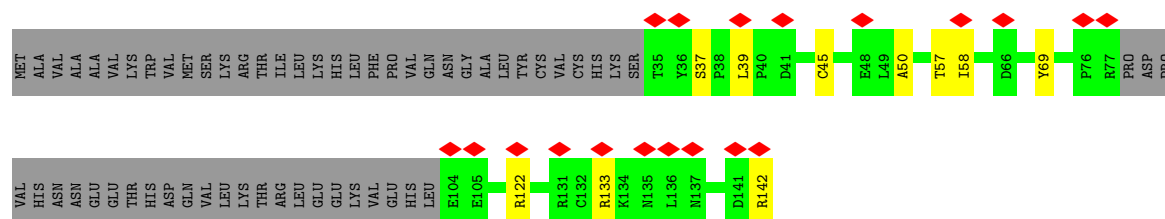
- Molecule 34: 39S ribosomal protein L41, mitochondrial

Chain 9: 30%
70% 15% 15%



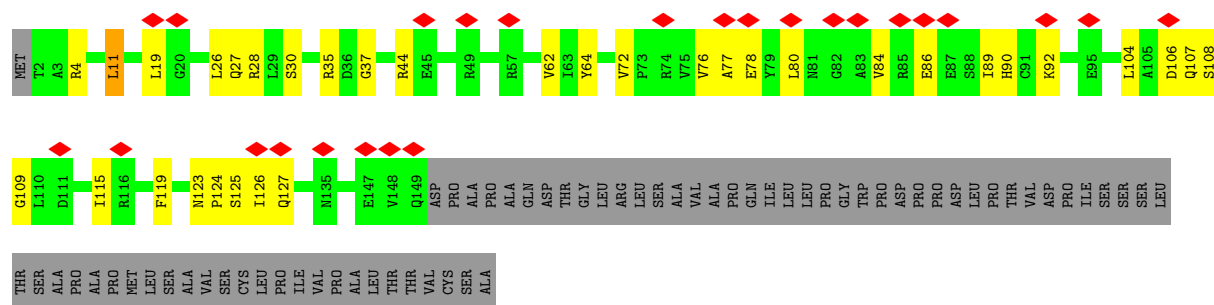
- Molecule 35: 39S ribosomal protein L42, mitochondrial

Chain a: 13%
51% 7% 42%

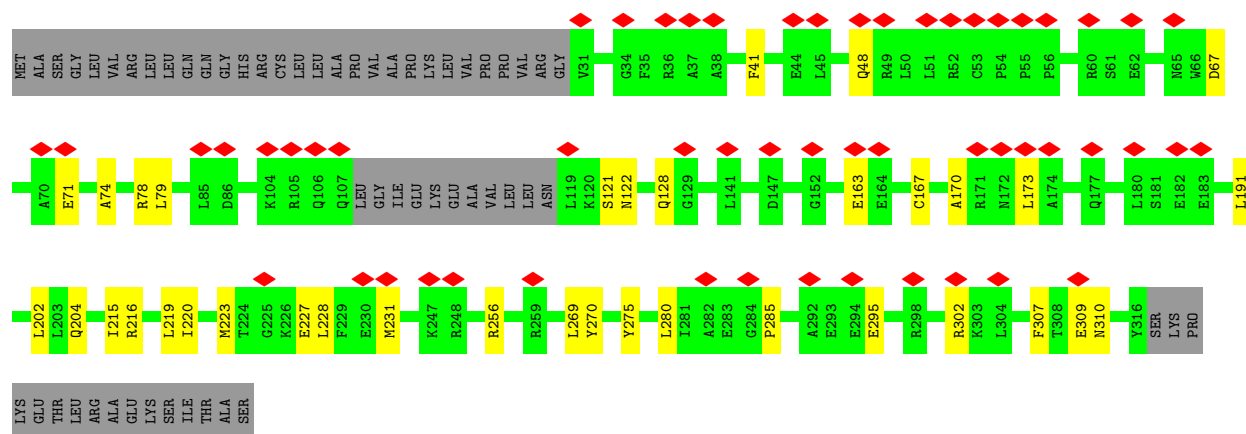


- Molecule 36: 39S ribosomal protein L43, mitochondrial

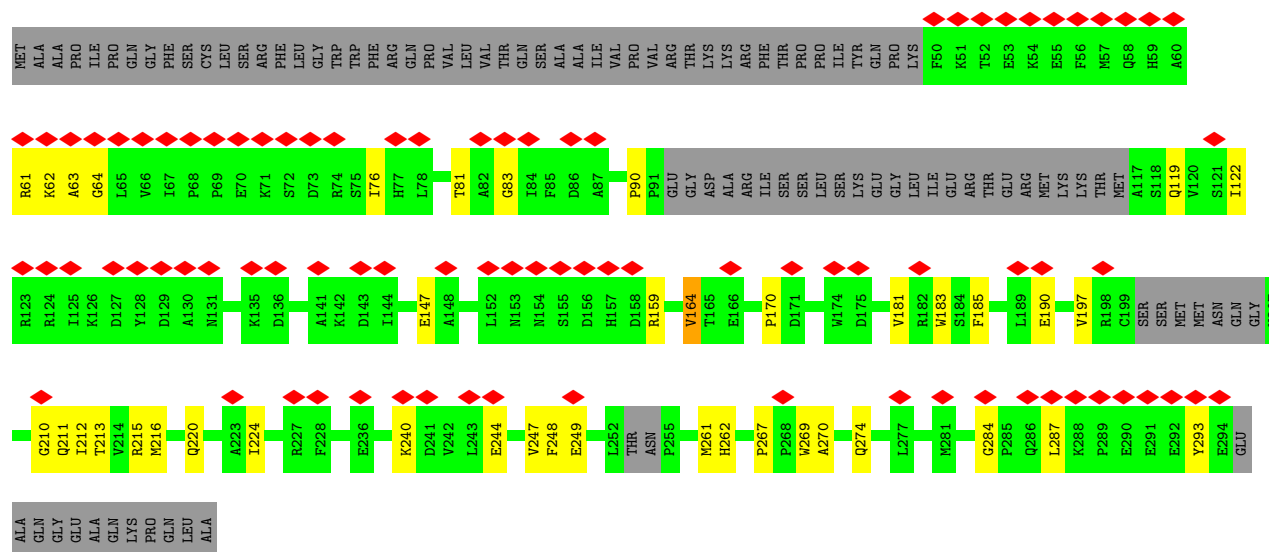
Chain b: 12%
53% 15% 31%



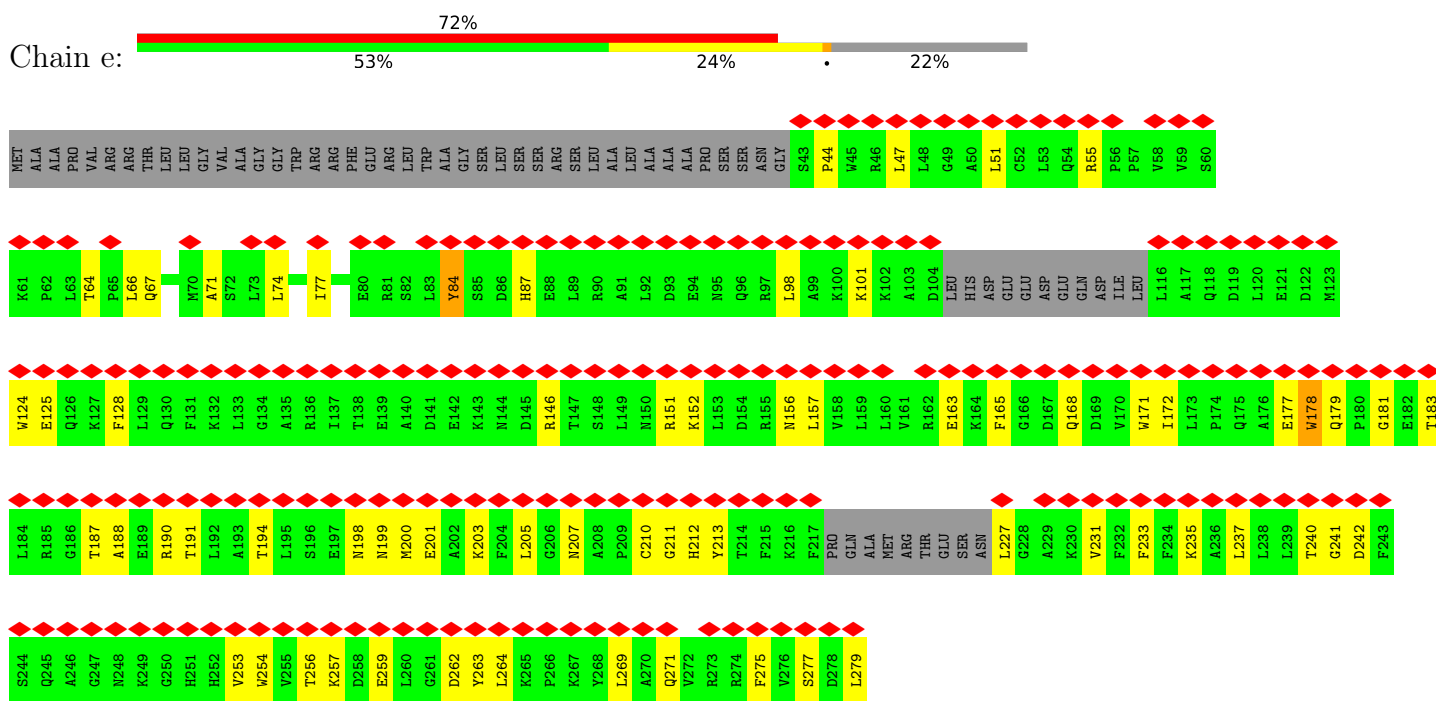
- Molecule 37: 39S ribosomal protein L44, mitochondrial



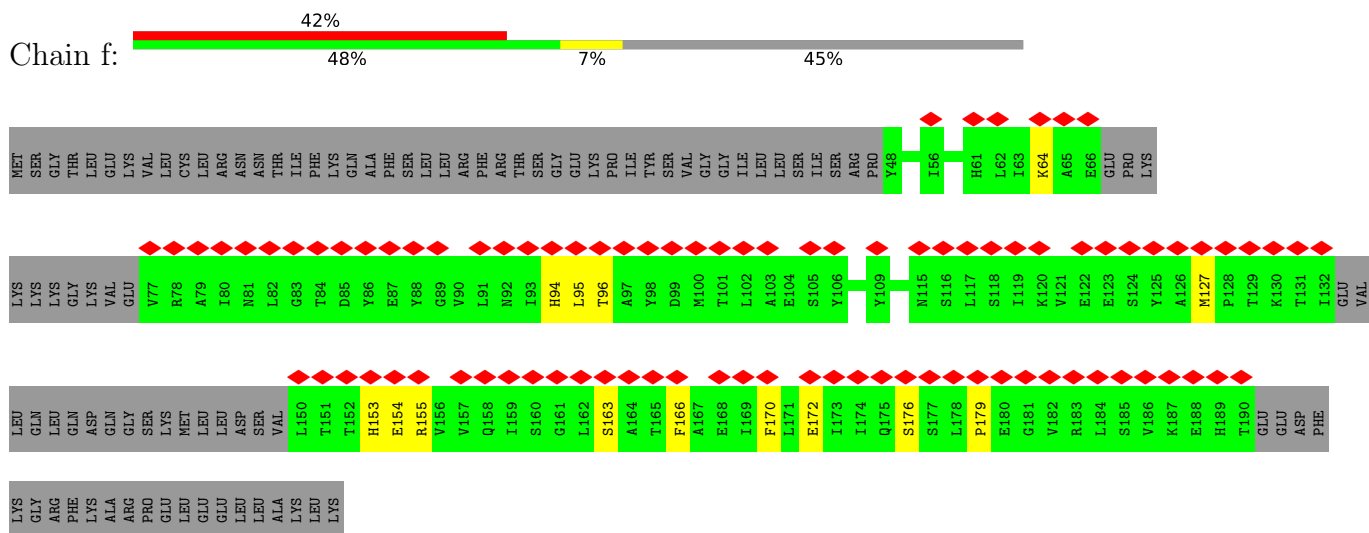
- Molecule 38: 39S ribosomal protein L45, mitochondrial



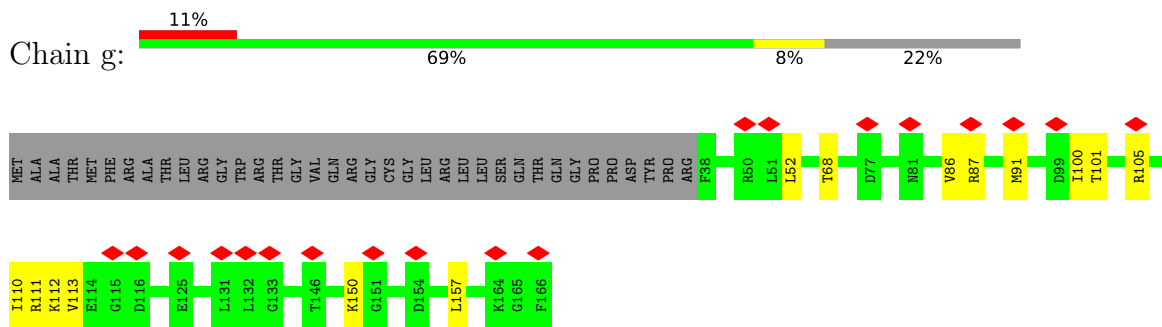
- Molecule 39: 39S ribosomal protein L46, mitochondrial



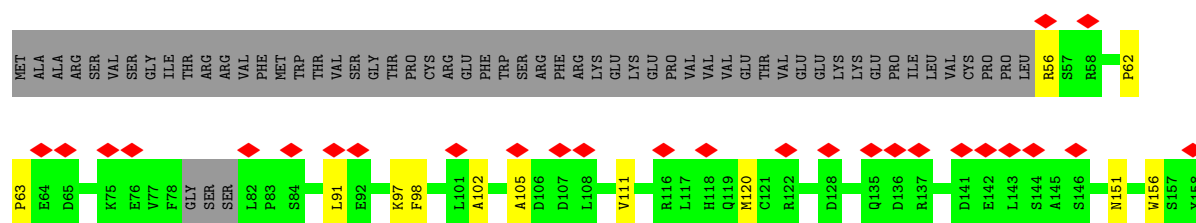
- Molecule 40: 39S ribosomal protein L48, mitochondrial



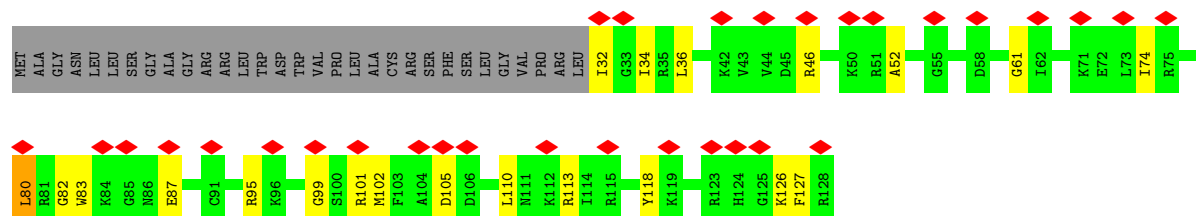
- Molecule 41: 39S ribosomal protein L49, mitochondrial



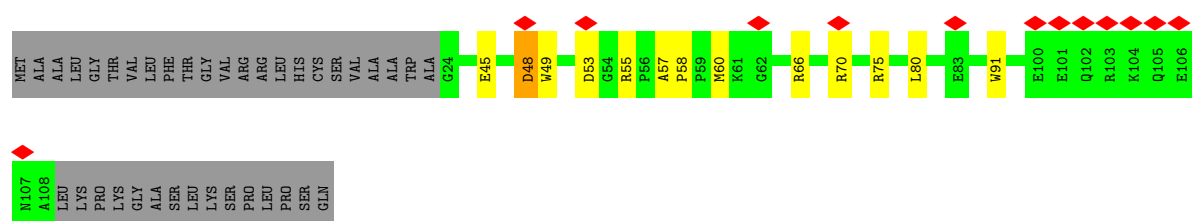
- Molecule 42: 39S ribosomal protein L50, mitochondrial



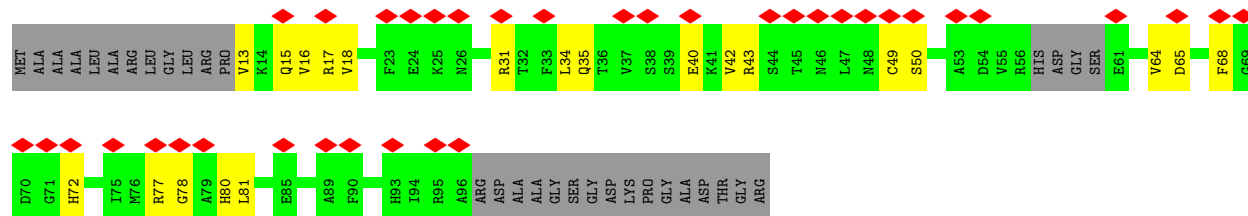
- Molecule 43: 39S ribosomal protein L51, mitochondrial



- Molecule 44: 39S ribosomal protein L52, mitochondrial

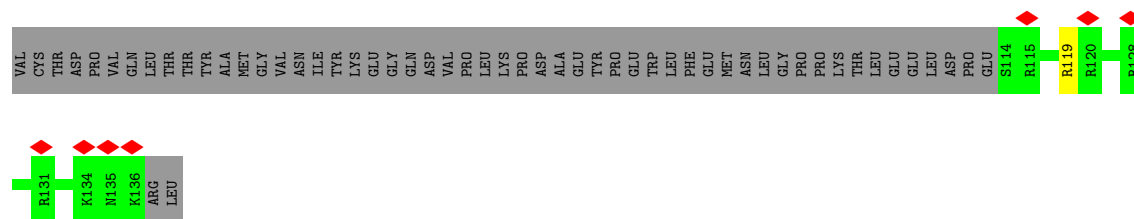


- Molecule 45: 39S ribosomal protein L53, mitochondrial

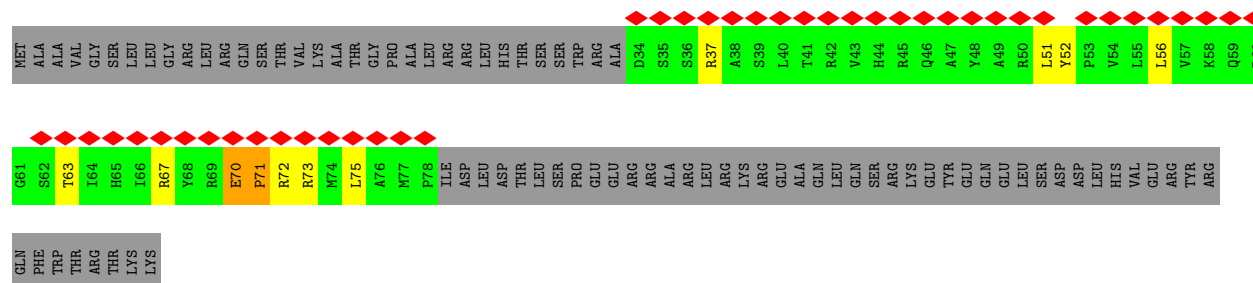


- Molecule 46: 39S ribosomal protein L54, mitochondrial

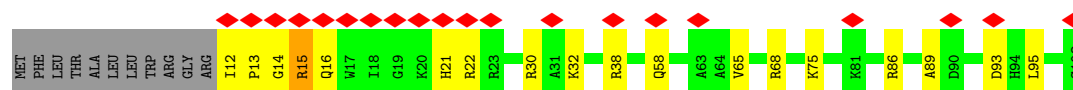




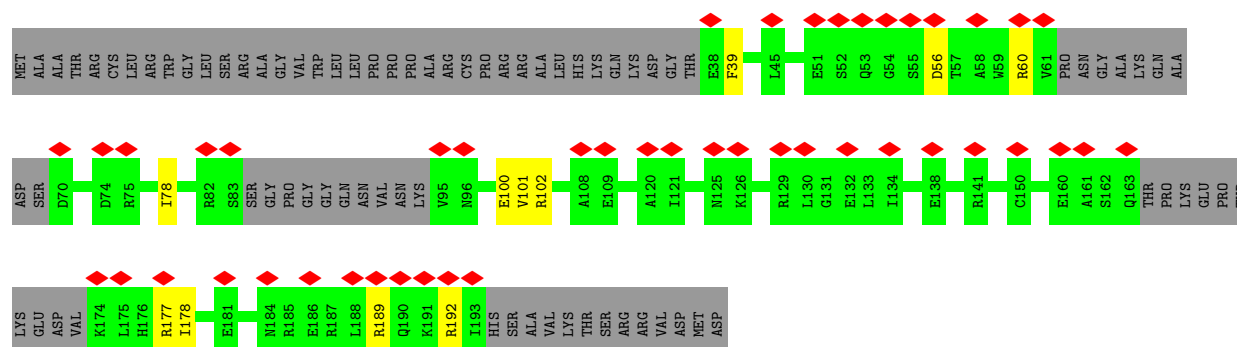
- Molecule 47: 39S ribosomal protein L55, mitochondrial



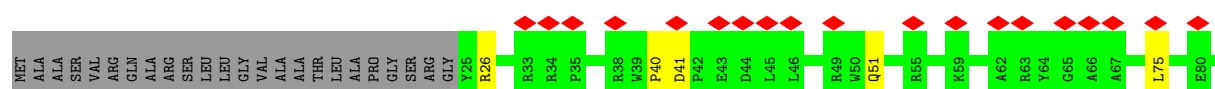
- Molecule 48: Ribosomal protein 63, mitochondrial

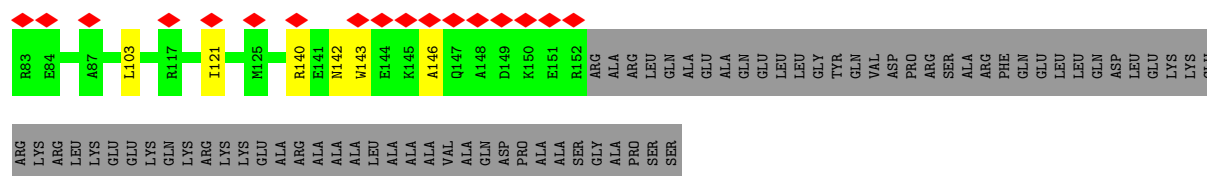


- Molecule 49: Peptidyl-tRNA hydrolase ICT1, mitochondrial

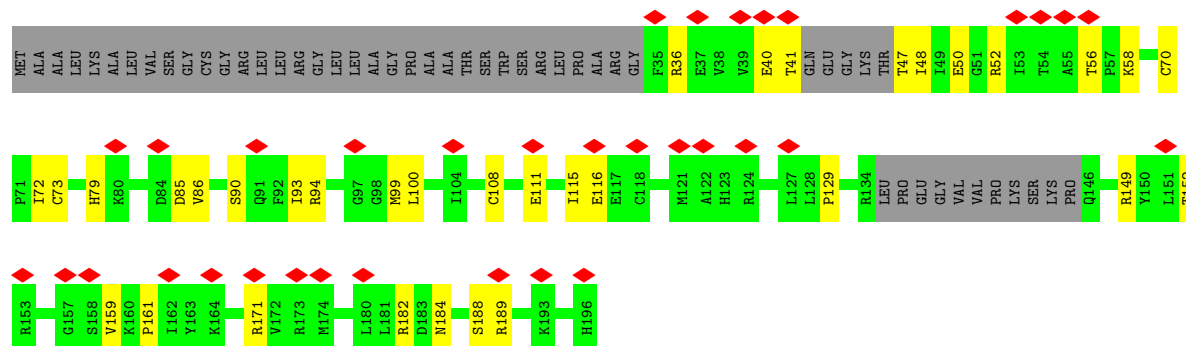


- Molecule 50: Growth arrest and DNA damage-inducible proteins-interacting protein 1

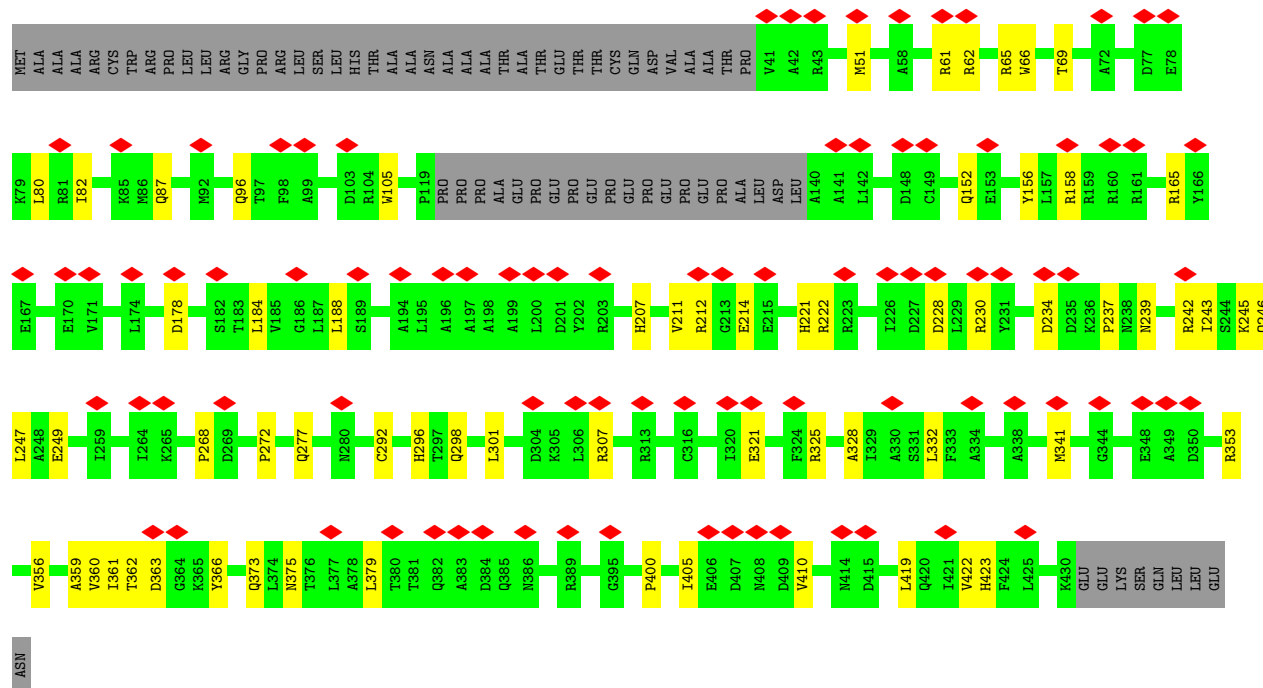




- Molecule 51: 39S ribosomal protein S18a, mitochondrial

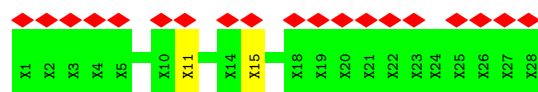


- Molecule 52: 39S ribosomal protein S30, mitochondrial

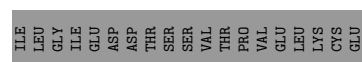
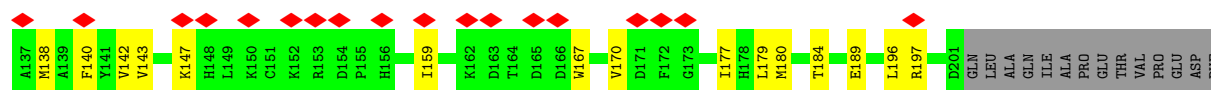
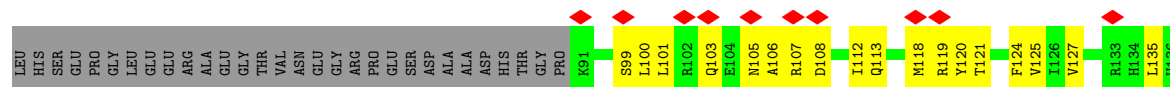
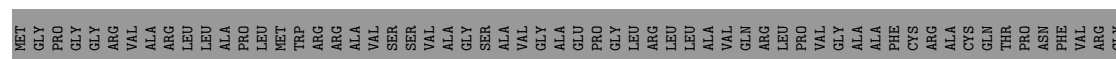
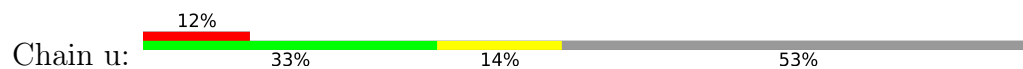


- Molecule 53: Unknown protein or protein extension

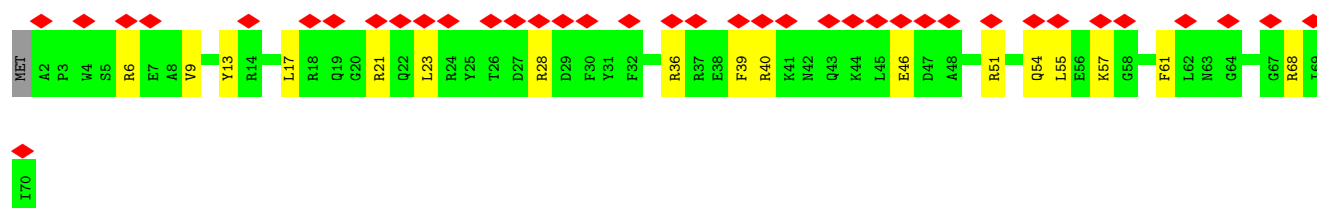
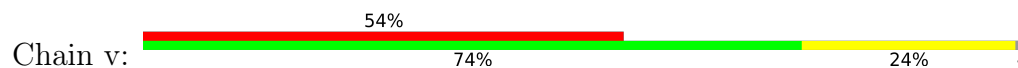




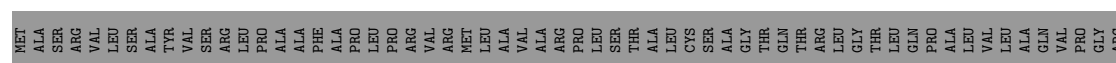
- Molecule 54: Mitochondrial assembly of ribosomal large subunit protein 1



- Molecule 55: MIEF1 upstream open reading frame protein



- Molecule 56: Acyl carrier protein, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	134685	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130841	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.349	Depositor
Minimum map value	-0.151	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.0853	Depositor
Map size (Å)	373.12, 373.12, 373.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PNS, ZN, 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	A	0.45	0/34235	0.49	5/53263 (0.0%)
2	B	0.22	0/1328	0.40	0/2056
3	D	0.37	0/1879	0.60	0/2527
4	E	0.44	0/2465	0.63	0/3344
5	F	0.49	0/2071	0.68	0/2817
6	H	0.33	0/798	0.67	0/1073
7	I	0.28	0/1308	0.63	2/1761 (0.1%)
8	J	0.24	0/1077	0.60	0/1452
9	K	0.48	0/1495	0.65	2/2029 (0.1%)
10	L	0.40	0/904	0.62	0/1218
11	M	0.48	0/2359	0.69	0/3185
12	N	0.36	0/1697	0.57	0/2281
13	O	0.45	0/1269	0.68	0/1708
14	P	0.34	0/1173	0.58	0/1588
15	Q	0.39	0/1846	0.62	0/2487
16	R	0.52	0/1174	0.71	1/1572 (0.1%)
17	S	0.52	0/1276	0.71	1/1729 (0.1%)
18	T	0.46	0/1402	0.61	0/1886
19	U	0.40	0/1183	0.65	0/1600
20	V	0.34	0/1616	0.52	0/2189
21	W	0.46	0/881	0.52	0/1188
22	X	0.35	0/2090	0.59	1/2825 (0.0%)
23	Y	0.40	0/1552	0.55	0/2079
24	Z	0.46	0/1003	0.61	0/1354
25	0	0.42	0/895	0.61	0/1201
26	1	0.38	0/438	0.67	0/583
27	2	0.51	0/373	0.67	0/496
28	3	0.54	0/852	0.64	0/1136
29	4	0.47	0/341	0.63	0/451
30	5	0.34	0/3250	0.59	0/4429
31	6	0.33	0/2726	0.57	0/3715
32	7	0.35	0/2391	0.57	0/3234

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	8	0.20	0/855	0.45	0/1152
34	9	0.37	0/972	0.58	0/1306
35	a	0.41	0/709	0.53	0/963
36	b	0.50	0/1202	0.65	0/1626
37	c	0.39	0/2264	0.57	0/3059
38	d	0.31	0/1790	0.56	0/2423
39	e	0.21	0/1797	0.58	3/2422 (0.1%)
40	f	0.25	0/931	0.48	0/1259
41	g	0.47	0/1102	0.64	0/1503
42	h	0.34	0/847	0.56	0/1150
43	i	0.51	0/849	0.66	0/1135
44	j	0.35	0/698	0.55	0/940
45	k	0.25	0/635	0.66	1/855 (0.1%)
46	l	0.23	0/226	0.45	0/299
47	m	0.27	0/379	0.88	2/510 (0.4%)
48	o	0.41	0/792	0.66	0/1064
49	p	0.27	0/1071	0.50	0/1433
50	q	0.29	0/1107	0.51	0/1498
51	r	0.40	0/1238	0.57	0/1676
52	s	0.39	0/3114	0.63	0/4225
54	u	0.30	0/949	0.60	0/1281
55	v	0.24	0/597	0.57	0/796
56	w	0.20	0/647	0.57	0/871
All	All	0.41	0/104118	0.56	18/147902 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	m	70	GLU	CA-C-N	8.33	130.26	119.84
47	m	70	GLU	C-N-CA	8.33	130.26	119.84
17	S	103	SER	N-CA-C	7.24	119.17	111.28
16	R	34	ARG	CB-CG-CD	-6.68	95.94	111.30
1	A	2243	A	C2'-C3'-O3'	6.06	118.59	109.50
1	A	2243	A	P-O3'-C3'	5.86	128.99	120.20
9	K	46	VAL	CB-CA-C	5.59	120.46	111.29
39	e	178	TRP	CA-C-N	5.48	142.44	121.95
39	e	178	TRP	C-N-CA	5.48	142.44	121.95
9	K	46	VAL	N-CA-CB	-5.44	102.26	111.23
22	X	152	ASP	N-CA-C	5.37	117.22	111.36
7	I	182	ASP	CA-C-N	5.22	129.82	122.46
7	I	182	ASP	C-N-CA	5.22	129.82	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1823	A	P-O3'-C3'	5.12	127.88	120.20
39	e	84	TYR	CA-CB-CG	5.08	123.05	113.90
1	A	2457	A	P-O3'-C3'	5.06	127.79	120.20
1	A	2507	A	C2'-C3'-O3'	5.05	121.28	113.70
45	k	42	VAL	N-CA-C	-5.05	107.47	111.81

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30607	0	15549	215	0
2	B	1191	0	607	8	0
3	D	1842	0	1891	47	0
4	E	2396	0	2402	37	0
5	F	2013	0	2044	48	0
6	H	784	0	832	12	0
7	I	1283	0	1368	36	0
8	J	1061	0	1141	24	0
9	K	1451	0	1448	29	0
10	L	889	0	941	17	0
11	M	2305	0	2378	42	0
12	N	1654	0	1681	25	0
13	O	1245	0	1283	23	0
14	P	1148	0	1148	16	0
15	Q	1805	0	1841	34	0
16	R	1153	0	1214	16	0
17	S	1251	0	1322	44	0
18	T	1368	0	1410	22	0
19	U	1154	0	1154	24	0
20	V	1575	0	1583	21	0
21	W	859	0	888	13	0
22	X	2035	0	2054	51	0
23	Y	1517	0	1561	18	0
24	Z	978	0	1030	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	0	880	0	902	9	0
26	1	433	0	475	8	0
27	2	367	0	393	14	0
28	3	831	0	883	12	0
29	4	333	0	352	9	0
30	5	3156	0	3138	50	0
31	6	2640	0	2464	36	0
32	7	2334	0	2343	27	0
33	8	836	0	844	12	0
34	9	947	0	949	18	0
35	a	686	0	658	9	0
36	b	1178	0	1180	28	0
37	c	2217	0	2220	22	0
38	d	1741	0	1727	27	0
39	e	1762	0	1767	49	0
40	f	915	0	917	11	0
41	g	1067	0	1056	10	0
42	h	827	0	806	10	0
43	i	827	0	857	17	0
44	j	684	0	673	17	0
45	k	627	0	636	15	0
46	l	221	0	227	1	0
47	m	372	0	387	12	0
48	o	771	0	774	26	0
49	p	1058	0	1083	8	0
50	q	1076	0	1049	8	0
51	r	1203	0	1220	27	0
52	s	3036	0	3022	39	0
53	t	140	0	30	1	0
54	u	927	0	921	24	0
55	v	588	0	604	13	0
56	w	638	0	636	15	0
57	A	84	0	0	0	0
57	D	1	0	0	0	0
57	E	1	0	0	0	0
57	M	1	0	0	0	0
57	R	1	0	0	0	0
57	T	1	0	0	0	0
57	W	1	0	0	0	0
57	g	1	0	0	0	0
57	o	1	0	0	0	0
58	0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	4	1	0	0	0	0
58	r	1	0	0	0	0
59	v	21	0	21	2	0
All	All	98998	0	83984	1143	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1143) 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)
3:D:109:PHE:CD1	3:D:208:ARG:NH1	1.70	1.59
3:D:109:PHE:CG	3:D:208:ARG:NH1	1.71	1.59
3:D:109:PHE:CD2	3:D:208:ARG:NH1	2.11	1.19
3:D:109:PHE:CE1	3:D:208:ARG:NH1	2.13	1.17
27:2:52:GLU:HG2	27:2:53:TYR:N	1.55	1.14
48:o:12:ILE:CD1	48:o:16:GLN:HA	1.79	1.11
48:o:12:ILE:HD12	48:o:16:GLN:HA	1.27	1.11
27:2:52:GLU:HG2	27:2:53:TYR:H	1.08	1.10
22:X:144:TYR:O	22:X:148:THR:HG23	1.53	1.06
22:X:36:ARG:HD2	22:X:151:GLU:OE2	1.56	1.06
44:j:49:TRP:CZ3	44:j:57:ALA:HB2	1.93	1.04
22:X:150:LYS:HG2	22:X:159:MET:HE1	1.38	1.03
48:o:13:PRO:HG3	48:o:21:HIS:HB2	1.40	1.03
3:D:109:PHE:CE1	3:D:208:ARG:CZ	2.42	1.03
22:X:31:SER:HB2	22:X:150:LYS:NZ	1.74	1.03
3:D:109:PHE:CZ	3:D:208:ARG:CZ	2.42	1.02
22:X:36:ARG:HD2	22:X:151:GLU:CD	1.89	0.96
2:B:1607:U:H3	2:B:1664:G:H1	1.15	0.95
22:X:31:SER:HB2	22:X:150:LYS:HZ2	1.32	0.94
3:D:109:PHE:CZ	3:D:208:ARG:NH2	2.37	0.93
44:j:49:TRP:CZ3	44:j:57:ALA:CB	2.52	0.92
3:D:109:PHE:CE2	3:D:208:ARG:NH2	2.38	0.90
48:o:13:PRO:HG3	48:o:21:HIS:CB	2.02	0.89
30:5:290:THR:HA	30:5:343:GLN:O	1.72	0.89
22:X:36:ARG:O	22:X:151:GLU:OE1	1.91	0.87
40:f:95:LEU:O	40:f:154:GLU:HA	1.76	0.86
30:5:218:LEU:HD11	30:5:262:ILE:CD1	2.06	0.86
27:2:59:LYS:O	27:2:63:LYS:HB2	1.75	0.85
27:2:52:GLU:CG	27:2:53:TYR:N	2.41	0.84
31:6:218:LEU:HA	31:6:269:ALA:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:j:49:TRP:CH2	44:j:57:ALA:HB1	2.13	0.83
39:e:211:GLY:O	39:e:233:PHE:HB2	1.78	0.83
3:D:198:SER:HB2	3:D:206:TYR:CE2	2.14	0.83
48:o:89:ALA:O	48:o:93:ASP:HB2	1.79	0.83
27:2:52:GLU:CG	27:2:53:TYR:H	1.89	0.83
30:5:218:LEU:HD11	30:5:262:ILE:HD12	1.61	0.83
3:D:109:PHE:CE2	3:D:208:ARG:NH1	2.46	0.82
17:S:104:ARG:HD2	17:S:104:ARG:N	1.94	0.82
20:V:136:ARG:HD2	20:V:146:VAL:HG11	1.60	0.82
39:e:213:TYR:O	39:e:231:VAL:HB	1.80	0.81
15:Q:129:LYS:NZ	54:u:121:THR:O	2.13	0.81
3:D:109:PHE:CZ	3:D:208:ARG:NH1	2.46	0.81
7:I:191:PHE:O	7:I:195:SER:HB2	1.80	0.81
48:o:12:ILE:CD1	48:o:16:GLN:CA	2.57	0.81
44:j:49:TRP:CE3	44:j:57:ALA:HB2	2.17	0.79
22:X:150:LYS:HG2	22:X:159:MET:CE	2.13	0.79
40:f:96:THR:HA	40:f:153:HIS:O	1.83	0.79
30:5:213:TRP:O	30:5:219:LEU:HD12	1.83	0.79
55:v:36:ARG:NH2	56:w:117:GLU:OE2	2.15	0.78
51:r:70:CYS:HB3	51:r:108:CYS:SG	2.23	0.78
31:6:174:HIS:HB2	31:6:205:THR:O	1.83	0.78
22:X:36:ARG:CD	22:X:151:GLU:CD	2.57	0.77
47:m:72:ARG:HD3	47:m:75:LEU:HD21	1.65	0.77
6:H:117:SER:O	6:H:121:ASN:HB2	1.85	0.76
3:D:198:SER:HB2	3:D:206:TYR:HE2	1.48	0.75
17:S:160:VAL:HG22	17:S:193:LEU:HD21	1.68	0.74
20:V:139:GLU:OE1	20:V:139:GLU:N	2.18	0.74
31:6:157:LEU:O	31:6:161:LEU:HB3	1.87	0.74
37:c:270:TYR:O	37:c:285:PRO:HA	1.88	0.74
30:5:218:LEU:HD23	30:5:218:LEU:H	1.53	0.74
44:j:48:ASP:OD2	44:j:60:MET:HE2	1.88	0.73
1:A:1747:G:N2	1:A:1750:G:O2'	2.22	0.73
1:A:2140:G:N3	24:Z:76:ARG:NH2	2.37	0.72
3:D:109:PHE:CE2	3:D:208:ARG:CZ	2.71	0.72
10:L:99:ARG:HH12	15:Q:191:ARG:HE	1.38	0.72
1:A:1792:G:N7	27:2:87:ARG:NH2	2.38	0.72
8:J:84:GLN:HE22	8:J:124:LYS:HG3	1.56	0.71
48:o:14:GLY:O	48:o:15:ARG:C	2.33	0.70
15:Q:79:GLU:OE2	15:Q:103:ARG:NH2	2.23	0.70
20:V:139:GLU:H	20:V:139:GLU:CD	1.99	0.70
44:j:49:TRP:CH2	44:j:57:ALA:CB	2.75	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:96:LEU:O	6:H:111:LEU:HA	1.92	0.70
31:6:329:TYR:O	31:6:333:GLN:HB2	1.92	0.69
47:m:56:LEU:O	47:m:63:THR:HA	1.92	0.69
22:X:149:PRO:HG2	22:X:152:ASP:HB2	1.74	0.69
1:A:2521:A:C2	3:D:205:GLN:HG2	2.27	0.69
31:6:266:HIS:O	31:6:320:GLN:HA	1.92	0.69
15:Q:120:THR:HG22	15:Q:132:GLN:HG2	1.75	0.68
33:8:147:LEU:O	33:8:151:GLN:HB2	1.93	0.68
31:6:270:PHE:HB2	31:6:317:SER:O	1.93	0.68
56:w:147:TYR:O	56:w:151:LYS:HB2	1.93	0.68
15:Q:152:ARG:NH1	15:Q:190:LEU:O	2.27	0.67
22:X:114:PHE:O	22:X:122:LYS:HA	1.95	0.67
40:f:96:THR:HG22	40:f:154:GLU:HG2	1.77	0.67
1:A:2521:A:C2	3:D:205:GLN:NE2	2.55	0.67
3:D:132:ASP:OD2	3:D:135:ARG:NH1	2.27	0.67
30:5:218:LEU:HD23	30:5:218:LEU:N	2.08	0.67
30:5:293:LEU:O	30:5:346:GLY:HA2	1.94	0.66
8:J:47:ASN:O	8:J:51:LYS:HB2	1.95	0.66
34:9:91:LEU:O	34:9:95:ALA:HB3	1.95	0.66
17:S:160:VAL:HA	17:S:193:LEU:HD23	1.78	0.66
1:A:2451:A:OP2	1:A:2452:A:OP2	2.13	0.66
22:X:31:SER:CB	22:X:150:LYS:NZ	2.54	0.66
54:u:101:LEU:HD13	54:u:127:VAL:HG11	1.78	0.66
37:c:163:GLU:O	37:c:167:CYS:HB2	1.95	0.65
14:P:73:PRO:HB2	14:P:147:GLN:HE21	1.61	0.65
1:A:2917:G:O6	11:M:77:ARG:NH1	2.29	0.65
39:e:151:ARG:HD3	39:e:152:LYS:HG2	1.79	0.65
1:A:2313:A:OP2	1:A:2668:A:OP1	2.15	0.65
1:A:2234:C:HO2'	1:A:2688:C:HO2'	1.43	0.64
17:S:135:LEU:HD23	17:S:144:LEU:HB3	1.79	0.64
39:e:163:GLU:HB2	39:e:172:ILE:HD12	1.79	0.64
48:o:14:GLY:O	48:o:15:ARG:O	2.14	0.64
7:I:128:ASN:ND2	7:I:149:GLY:O	2.30	0.64
41:g:101:THR:O	41:g:105:ARG:HB2	1.97	0.64
1:A:2389:C:H5''	30:5:301:PRO:HB3	1.79	0.64
1:A:2606:U:H4'	1:A:2607:U:H3'	1.80	0.64
11:M:62:ARG:NH1	43:i:126:LYS:O	2.31	0.64
5:F:107:LYS:HG2	43:i:74:ILE:HG22	1.80	0.64
5:F:221:LEU:HD23	5:F:222:THR:HG23	1.79	0.64
38:d:90:PRO:HG2	38:d:269:TRP:HE1	1.63	0.64
1:A:1874:A:HO2'	1:A:2090:A:HO2'	1.44	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:59:ARG:NH1	5:F:88:ALA:O	2.31	0.63
26:1:43:LEU:O	26:1:55:LEU:HA	1.99	0.63
51:r:41:THR:O	51:r:47:THR:HA	1.97	0.63
1:A:2256:U:O2'	17:S:118:ASN:ND2	2.31	0.63
1:A:2468:A:H61	1:A:2659:C:H42	1.46	0.63
31:6:233:LEU:HB3	31:6:298:PHE:HE1	1.64	0.63
7:I:98:VAL:HG13	7:I:177:LEU:HB3	1.79	0.63
13:O:32:LEU:HB3	13:O:52:MET:HE2	1.81	0.63
30:5:201:ARG:HD3	30:5:230:LEU:HD21	1.78	0.63
19:U:126:LEU:HD11	38:d:76:ILE:HD12	1.81	0.63
22:X:163:ARG:HE	30:5:55:LEU:HD22	1.64	0.62
55:v:46:GLU:HB2	55:v:51:ARG:HE	1.63	0.62
56:w:81:ASP:O	56:w:85:TYR:HB2	1.98	0.62
1:A:2484:C:OP2	15:Q:227:LYS:NZ	2.33	0.62
32:7:220:GLU:HB3	32:7:251:ILE:HD11	1.80	0.62
7:I:148:VAL:O	45:k:31:ARG:NH2	2.32	0.62
22:X:31:SER:HB2	22:X:150:LYS:HZ1	1.62	0.62
22:X:111:GLU:HG2	22:X:126:THR:HG22	1.82	0.62
1:A:2064:A:OP1	21:W:101:LYS:NZ	2.32	0.61
1:A:2401:A:OP1	3:D:262:ARG:NH2	2.33	0.61
17:S:104:ARG:HH21	17:S:104:ARG:HG3	1.64	0.61
45:k:15:GLN:HE22	45:k:17:ARG:HB2	1.64	0.61
45:k:17:ARG:HB3	45:k:65:ASP:HB3	1.83	0.61
32:7:107:LEU:HB2	32:7:126:LYS:HB2	1.82	0.61
1:A:2126:U:O4	24:Z:76:ARG:NH1	2.34	0.61
17:S:104:ARG:HG3	17:S:104:ARG:NH2	2.14	0.61
18:T:125:GLN:HE21	18:T:137:ARG:HB3	1.65	0.61
51:r:99:MET:HG3	51:r:116:GLU:HG2	1.83	0.61
1:A:2143:G:OP1	17:S:173:ARG:NH2	2.34	0.61
30:5:158:ILE:O	30:5:162:ARG:HB3	2.01	0.61
31:6:322:ARG:HH22	49:p:178:ILE:HG12	1.65	0.61
52:s:321:GLU:OE1	52:s:325:ARG:NH2	2.33	0.61
4:E:275:ARG:HA	4:E:332:LEU:O	2.01	0.60
3:D:207:ILE:HG22	3:D:207:ILE:O	2.01	0.60
19:U:3:ARG:O	19:U:23:ASN:ND2	2.34	0.60
30:5:200:ARG:HE	30:5:233:LYS:HD2	1.64	0.60
31:6:217:LEU:HD22	31:6:271:LEU:HD12	1.82	0.60
1:A:1849:C:OP1	1:A:2935:A:N6	2.33	0.60
12:N:160:VAL:HG12	12:N:161:VAL:HG23	1.84	0.60
43:i:87:GLU:OE2	43:i:113:ARG:NH1	2.35	0.60
3:D:74:ILE:HD13	3:D:148:LYS:HE3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:108:ILE:HA	10:L:114:PRO:HA	1.83	0.60
17:S:99:VAL:HG22	17:S:133:VAL:HG12	1.84	0.60
36:b:28:ARG:NH2	37:c:71:GLU:OE2	2.35	0.60
3:D:228:LEU:HD11	3:D:234:MET:HE3	1.83	0.60
44:j:45:GLU:OE2	44:j:70:ARG:NH2	2.34	0.59
45:k:77:ARG:HB2	51:r:50:GLU:HG2	1.84	0.59
29:4:89:TYR:HE1	29:4:101:ARG:HG3	1.67	0.59
1:A:2395:A:OP1	30:5:173:ARG:NH2	2.34	0.59
1:A:2458:A:OP1	13:O:9:ILE:N	2.35	0.59
10:L:55:PRO:HB3	10:L:77:ILE:HG12	1.84	0.59
19:U:8:PRO:HA	23:Y:183:GLN:HE22	1.67	0.59
1:A:2702:G:H5'	9:K:114:LYS:HE2	1.83	0.59
6:H:95:GLU:HA	6:H:112:VAL:O	2.02	0.59
7:I:150:HIS:H	45:k:35:GLN:HE22	1.50	0.59
19:U:46:MET:HE1	19:U:72:VAL:HG13	1.84	0.59
1:A:2256:U:H4'	17:S:102:ALA:HB1	1.84	0.59
20:V:105:ARG:HE	38:d:170:PRO:HB2	1.67	0.59
36:b:126:ILE:O	37:c:310:ASN:ND2	2.35	0.59
5:F:114:THR:O	5:F:156:ARG:NH2	2.36	0.59
7:I:51:THR:OG1	12:N:250:ARG:NH2	2.36	0.59
22:X:177:HIS:O	22:X:184:ARG:NH2	2.34	0.59
25:0:110:CYS:HB3	25:0:113:CYS:SG	2.41	0.59
1:A:1892:A:N7	28:3:169:ARG:NH2	2.51	0.59
18:T:190:LYS:NZ	18:T:198:GLU:OE1	2.33	0.59
28:3:183:ARG:NH1	31:6:355:LYS:O	2.35	0.59
48:o:12:ILE:HD11	48:o:16:GLN:CA	2.32	0.59
19:U:44:ILE:HG23	19:U:48:MET:HB3	1.85	0.59
1:A:1848:U:OP1	11:M:48:LYS:NZ	2.36	0.59
1:A:1881:A:OP2	41:g:111:ARG:NH2	2.31	0.59
22:X:231:VAL:HG11	34:9:114:LEU:HD11	1.84	0.59
39:e:98:LEU:HD23	39:e:101:LYS:HD2	1.85	0.59
51:r:70:CYS:CB	51:r:108:CYS:SG	2.89	0.59
4:E:154:ARG:HB3	32:7:311:THR:HG21	1.85	0.58
14:P:52:ASN:HB3	14:P:55:ASN:HB2	1.84	0.58
12:N:89:ILE:HD11	12:N:176:LEU:HD22	1.85	0.58
54:u:99:SER:O	54:u:103:GLN:HB2	2.03	0.58
5:F:167:MET:HA	5:F:170:ARG:HE	1.67	0.58
51:r:79:HIS:HB3	51:r:184:ASN:HA	1.85	0.58
6:H:58:ARG:NH1	6:H:77:HIS:O	2.36	0.58
32:7:112:PRO:HB2	32:7:267:PRO:HG2	1.86	0.58
39:e:152:LYS:HB2	39:e:157:LEU:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:69:LYS:HB3	8:J:81:LYS:HB3	1.85	0.58
13:O:45:PRO:HG2	13:O:48:ARG:HD2	1.85	0.58
30:5:341:VAL:HG22	30:5:358:GLN:HG2	1.84	0.58
36:b:37:GLY:O	36:b:44:ARG:NH2	2.37	0.58
1:A:2312:A:N1	18:T:157:ARG:NH2	2.51	0.58
1:A:2531:U:O4	3:D:246:ARG:NH2	2.37	0.58
28:3:172:TYR:HB2	28:3:175:ASP:HB2	1.86	0.58
31:6:183:ASP:OD2	49:p:189:ARG:NH1	2.37	0.58
32:7:156:ARG:HH12	32:7:260:PHE:HB2	1.69	0.58
1:A:1705:A:N6	34:9:40:GLY:O	2.37	0.57
56:w:145:VAL:O	56:w:149:ALA:HB2	2.04	0.57
6:H:75:ARG:HH21	22:X:100:ARG:HH22	1.52	0.57
10:L:99:ARG:NH1	15:Q:161:GLU:OE1	2.34	0.57
10:L:101:ASP:OD2	15:Q:152:ARG:NH2	2.37	0.57
14:P:77:PHE:O	14:P:97:GLN:NE2	2.34	0.57
31:6:161:LEU:HD13	31:6:221:LEU:HD21	1.85	0.57
33:8:143:GLN:HG2	39:e:210:CYS:HA	1.86	0.57
54:u:127:VAL:O	54:u:179:LEU:HA	2.04	0.57
16:R:29:ARG:NH2	16:R:36:ASN:O	2.38	0.57
32:7:51:GLU:O	32:7:55:GLN:HB2	2.04	0.57
48:o:13:PRO:CG	48:o:21:HIS:HB2	2.25	0.57
1:A:3187:C:O2	29:4:85:ARG:NH2	2.34	0.57
32:7:151:GLY:HA2	32:7:154:ILE:HD12	1.87	0.57
34:9:128:PHE:HD1	34:9:135:PHE:HB3	1.69	0.57
45:k:80:HIS:O	51:r:36:ARG:NH1	2.37	0.57
1:A:1745:U:O4	28:3:108:LYS:NZ	2.37	0.57
18:T:84:LYS:HD3	18:T:149:ARG:HB3	1.86	0.57
39:e:179:GLN:HG2	39:e:181:GLY:H	1.70	0.57
4:E:56:GLU:OE2	13:O:153:ARG:NH2	2.38	0.57
3:D:109:PHE:CD1	3:D:208:ARG:CZ	2.67	0.57
3:D:111:ARG:HH21	3:D:163:ILE:HG21	1.69	0.57
19:U:42:PHE:HB2	19:U:95:ALA:HB3	1.87	0.57
20:V:136:ARG:HD2	20:V:146:VAL:CG1	2.32	0.57
4:E:269:TYR:HB3	4:E:304:LEU:HD21	1.85	0.57
39:e:55:ARG:HD2	39:e:157:LEU:HD13	1.86	0.57
41:g:100:ILE:HA	41:g:105:ARG:O	2.04	0.57
8:J:25:ARG:HA	8:J:65:PRO:HA	1.86	0.57
15:Q:121:THR:HG22	15:Q:171:VAL:HG12	1.87	0.57
32:7:203:THR:HG22	32:7:280:VAL:H	1.70	0.57
5:F:70:ARG:NH1	5:F:194:GLU:OE1	2.37	0.56
11:M:177:ALA:HB1	11:M:203:ARG:HH12	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:142:GLU:OE1	20:V:142:GLU:HA	2.05	0.56
54:u:135:LEU:HD22	54:u:179:LEU:HB3	1.87	0.56
1:A:2852:C:O2'	26:1:45:HIS:ND1	2.36	0.56
3:D:194:ASN:OD1	3:D:243:THR:OG1	2.22	0.56
10:L:31:ALA:N	10:L:91:MET:SD	2.79	0.56
18:T:55:ASN:ND2	18:T:74:TYR:O	2.37	0.56
24:Z:101:LYS:HE3	44:j:80:LEU:HD22	1.86	0.56
1:A:1871:A:N7	1:A:1901:C:N4	2.53	0.56
1:A:2545:U:H5''	1:A:2546:G:H5'	1.87	0.56
1:A:2982:C:H5''	12:N:139:ARG:HA	1.87	0.56
7:I:81:LEU:O	7:I:85:GLU:HB2	2.06	0.56
17:S:129:ARG:HE	17:S:155:ARG:HG3	1.70	0.56
22:X:36:ARG:HG2	22:X:151:GLU:OE1	2.06	0.56
55:v:21:ARG:HH22	56:w:123:GLU:HB2	1.71	0.56
7:I:166:ARG:HH11	7:I:169:ARG:HH11	1.53	0.56
9:K:63:ARG:NH1	9:K:130:ASP:OD1	2.38	0.56
22:X:11:TRP:HA	22:X:14:LEU:HD12	1.88	0.56
1:A:2521:A:N6	3:D:202:ARG:O	2.39	0.56
13:O:108:LEU:HD11	13:O:135:LEU:HD23	1.87	0.56
36:b:35:ARG:O	36:b:44:ARG:NH1	2.39	0.56
1:A:2987:U:O2'	1:A:2991:U:OP1	2.24	0.56
15:Q:87:THR:HG21	15:Q:92:PHE:HE2	1.71	0.56
22:X:150:LYS:HB3	22:X:159:MET:HE2	1.85	0.56
13:O:33:LEU:HD21	13:O:59:LEU:HG	1.86	0.56
15:Q:120:THR:HA	15:Q:131:SER:O	2.05	0.56
52:s:211:VAL:HG22	52:s:230:ARG:HG3	1.88	0.56
52:s:51:MET:HG3	52:s:61:ARG:HE	1.70	0.56
11:M:202:LYS:NZ	11:M:293:TYR:O	2.39	0.56
45:k:49:CYS:SG	45:k:50:SER:N	2.79	0.56
1:A:1775:A:HO2'	16:R:10:LEU:N	2.04	0.55
5:F:175:LYS:NZ	5:F:277:ASP:OD2	2.39	0.55
23:Y:218:ARG:NH2	43:i:105:ASP:OD1	2.38	0.55
38:d:211:GLN:HA	38:d:248:PHE:O	2.06	0.55
45:k:15:GLN:HA	45:k:50:SER:O	2.06	0.55
56:w:138:LEU:HD13	56:w:144:ILE:HG12	1.88	0.55
32:7:156:ARG:NH2	32:7:259:ASP:O	2.39	0.55
37:c:128:GLN:OE1	37:c:204:GLN:NE2	2.38	0.55
38:d:216:MET:HB2	38:d:244:GLU:HB2	1.88	0.55
13:O:42:ILE:O	13:O:122:VAL:HA	2.06	0.55
14:P:82:ARG:NH2	14:P:95:GLU:OE2	2.39	0.55
1:A:3220:A:OP1	4:E:260:LYS:NZ	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:129:ARG:NH2	17:S:151:LYS:O	2.39	0.55
1:A:1814:A:N3	1:A:1862:U:O2'	2.37	0.55
1:A:2017:U:O2'	1:A:2723:A:N1	2.40	0.55
7:I:40:MET:HE1	7:I:48:MET:HE2	1.88	0.55
1:A:2422:U:OP2	34:9:24:LYS:NZ	2.40	0.55
19:U:39:THR:HA	19:U:97:VAL:O	2.06	0.55
41:g:110:ILE:HD11	41:g:157:LEU:HD13	1.89	0.55
12:N:205:ARG:NH2	12:N:249:LYS:O	2.40	0.55
54:u:108:ASP:O	54:u:127:VAL:HA	2.06	0.55
24:Z:78:ARG:O	24:Z:83:LYS:NZ	2.40	0.55
21:W:125:VAL:HG21	31:6:64:GLU:HG3	1.89	0.55
1:A:1790:A:OP1	27:2:82:ARG:NH1	2.40	0.55
1:A:3063:G:O2'	1:A:3066:C:OP2	2.22	0.55
33:8:160:GLU:O	39:e:207:ASN:ND2	2.40	0.55
38:d:147:GLU:OE2	38:d:159:ARG:NH1	2.39	0.55
1:A:2191:A:OP1	8:J:142:ARG:NH2	2.40	0.54
9:K:69:GLY:HA2	51:r:152:THR:HA	1.89	0.54
13:O:65:LEU:HB3	13:O:69:ASN:HD22	1.72	0.54
19:U:79:ARG:HG3	19:U:87:ILE:HB	1.89	0.54
29:4:87:ARG:HB2	29:4:102:GLN:HB3	1.87	0.54
13:O:25:ARG:NH2	13:O:51:GLU:OE2	2.40	0.54
34:9:42:GLY:HA3	34:9:51:VAL:O	2.07	0.54
1:A:2032:G:O2'	1:A:2865:C:O2	2.25	0.54
3:D:166:SER:OG	3:D:182:HIS:ND1	2.40	0.54
12:N:104:MET:HE2	12:N:182:LYS:HE3	1.89	0.54
18:T:202:GLN:OE1	35:a:122:ARG:NH1	2.41	0.54
30:5:343:GLN:NE2	30:5:417:LEU:O	2.41	0.54
45:k:13:VAL:HG13	45:k:49:CYS:HB2	1.89	0.54
49:p:78:ILE:HG12	49:p:101:VAL:HG22	1.90	0.54
1:A:3151:A:H5'	15:Q:142:GLY:HA2	1.88	0.54
5:F:270:GLU:O	5:F:274:LEU:HB2	2.08	0.54
20:V:97:TYR:HA	20:V:107:THR:O	2.07	0.54
1:A:1812:C:O2'	37:c:48:GLN:OE1	2.26	0.54
1:A:2157:U:H5'	51:r:182:ARG:HH22	1.71	0.54
8:J:138:SER:O	8:J:142:ARG:HB2	2.08	0.54
13:O:130:LEU:HD12	25:0:134:THR:HG22	1.90	0.54
19:U:44:ILE:HD11	19:U:53:LEU:HG	1.90	0.54
19:U:67:ALA:HB3	19:U:98:GLN:HB2	1.89	0.54
32:7:114:ASP:HB2	32:7:117:LYS:HB2	1.89	0.54
37:c:227:GLU:OE2	37:c:302:ARG:NE	2.40	0.54
43:i:99:GLY:HA2	43:i:102:MET:HE3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:178:ASP:OD1	52:s:239:ASN:ND2	2.41	0.54
1:A:2191:A:N6	1:A:2198:A:OP2	2.41	0.54
1:A:2409:A:O2'	30:5:270:ILE:O	2.24	0.54
7:I:94:ARG:HB3	7:I:157:GLU:HA	1.89	0.54
9:K:8:PRO:HG2	37:c:295:GLU:HG3	1.90	0.54
39:e:128:PHE:CD1	47:m:73:ARG:HB3	2.43	0.54
39:e:200:MET:HA	39:e:241:GLY:HA2	1.90	0.54
55:v:17:LEU:HD13	56:w:120:MET:HB2	1.90	0.54
1:A:1706:C:OP1	23:Y:193:ARG:NH2	2.41	0.54
5:F:103:GLN:HE22	5:F:250:VAL:H	1.56	0.54
7:I:191:PHE:O	7:I:195:SER:CB	2.53	0.54
22:X:38:PRO:CB	22:X:152:ASP:OD1	2.55	0.54
24:Z:71:ARG:NH2	24:Z:92:GLU:O	2.41	0.54
39:e:156:ASN:ND2	39:e:277:SER:OG	2.41	0.54
5:F:117:ARG:HD2	5:F:144:PRO:HD3	1.90	0.54
51:r:70:CYS:SG	51:r:73:CYS:N	2.80	0.54
31:6:239:ASN:OD1	31:6:275:GLN:NE2	2.35	0.53
52:s:165:ARG:O	52:s:307:ARG:NH2	2.40	0.53
3:D:206:TYR:CE1	3:D:234:MET:HE1	2.43	0.53
5:F:160:SER:OG	43:i:83:TRP:O	2.26	0.53
28:3:104:ARG:NH1	28:3:160:LYS:O	2.39	0.53
39:e:67:GLN:O	39:e:71:ALA:HB2	2.08	0.53
54:u:118:MET:SD	54:u:197:ARG:NE	2.79	0.53
1:A:1906:G:H1'	5:F:137:ARG:HD3	1.90	0.53
7:I:82:LEU:HD13	7:I:130:VAL:HG11	1.90	0.53
1:A:1953:A:O2'	1:A:2463:A:OP1	2.26	0.53
17:S:160:VAL:HG22	17:S:193:LEU:CD2	2.36	0.53
31:6:157:LEU:O	31:6:161:LEU:CB	2.55	0.53
39:e:183:THR:O	39:e:187:THR:N	2.42	0.53
43:i:74:ILE:HD11	43:i:82:GLY:H	1.73	0.53
1:A:1713:A:N6	30:5:68:PRO:O	2.42	0.53
18:T:153:LEU:HB2	18:T:169:LYS:HB2	1.89	0.53
22:X:168:ARG:HD3	22:X:173:ASP:HB2	1.89	0.53
30:5:208:THR:HA	30:5:224:GLY:O	2.08	0.53
30:5:350:ARG:NH2	30:5:384:GLN:O	2.41	0.53
51:r:40:GLU:HA	51:r:48:ILE:O	2.09	0.53
51:r:90:SER:HA	51:r:93:ILE:HD12	1.90	0.53
54:u:106:ALA:HB2	54:u:138:MET:HE1	1.90	0.53
1:A:1688:A:OP2	22:X:5:LYS:NZ	2.42	0.53
1:A:2367:A:OP2	19:U:79:ARG:NH1	2.42	0.53
1:A:3019:G:N2	1:A:3131:G:O2'	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:134:MET:HG2	44:j:75:ARG:HE	1.74	0.53
50:q:41:ASP:OD1	50:q:41:ASP:N	2.42	0.53
1:A:1878:U:O3'	5:F:92:ARG:NH2	2.41	0.53
34:9:22:THR:HG23	34:9:24:LYS:H	1.74	0.53
42:h:91:LEU:HD23	42:h:97:LYS:HG3	1.90	0.53
1:A:1753:A:OP1	43:i:118:TYR:OH	2.26	0.53
4:E:133:THR:OG1	4:E:144:THR:OG1	2.26	0.53
7:I:39:VAL:O	48:o:22:ARG:NH2	2.42	0.53
32:7:108:VAL:HG22	32:7:125:ILE:HG12	1.90	0.53
38:d:197:VAL:HG12	38:d:212:ILE:HG12	1.90	0.53
55:v:36:ARG:O	55:v:40:ARG:N	2.42	0.53
1:A:2003:A:OP2	1:A:2734:A:O2'	2.25	0.52
1:A:2814:G:N2	1:A:2840:C:OP1	2.38	0.52
4:E:102:LEU:O	4:E:122:LEU:HA	2.09	0.52
52:s:242:ARG:NH2	52:s:292:CYS:O	2.38	0.52
1:A:1837:C:OP1	36:b:4:ARG:NH2	2.42	0.52
9:K:21:LEU:HD22	9:K:59:ILE:HG12	1.89	0.52
26:l:19:ARG:HB3	26:l:62:ILE:HD11	1.91	0.52
1:A:1907:A:N3	1:A:2930:U:O2'	2.37	0.52
3:D:124:GLU:HG2	3:D:144:GLY:HA3	1.92	0.52
4:E:96:ARG:HH21	4:E:314:LEU:HD13	1.73	0.52
10:L:119:ILE:HG21	10:L:123:ILE:HD11	1.91	0.52
11:M:19:LEU:HD23	48:o:95:LEU:HD12	1.91	0.52
22:X:41:VAL:HG11	22:X:83:GLU:HB3	1.91	0.52
25:0:119:LYS:O	25:0:120:HIS:ND1	2.42	0.52
52:s:246:GLN:OE1	52:s:353:ARG:NH1	2.42	0.52
52:s:332:LEU:HD21	52:s:359:ALA:HB2	1.91	0.52
54:u:196:LEU:HD21	55:v:61:PHE:HB2	1.90	0.52
6:H:98:LEU:HD23	6:H:129:ALA:HB2	1.91	0.52
30:5:174:GLU:HA	30:5:296:LYS:HB2	1.92	0.52
1:A:2055:U:H2'	1:A:2056:G:H8	1.75	0.52
9:K:136:ASP:O	9:K:140:ASN:ND2	2.43	0.52
10:L:99:ARG:NH1	15:Q:191:ARG:HH11	2.07	0.52
11:M:30:ASN:OD1	48:o:86:ARG:NH2	2.43	0.52
1:A:2943:G:H5''	48:o:13:PRO:O	2.10	0.52
6:H:120:ARG:NH2	22:X:133:ASP:OD1	2.43	0.52
32:7:217:GLU:HB2	32:7:256:ARG:HB3	1.91	0.52
31:6:222:ASP:OD1	31:6:222:ASP:N	2.43	0.52
6:H:84:GLU:OE1	22:X:44:ARG:NH2	2.41	0.52
11:M:116:ILE:HB	11:M:154:ILE:HA	1.91	0.52
17:S:194:ARG:HH11	36:b:19:LEU:HG	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:b:30:SER:HB2	36:b:76:VAL:HB	1.92	0.52
51:r:94:ARG:HE	51:r:100:LEU:HD23	1.75	0.52
52:s:80:LEU:HD21	52:s:341:MET:HB3	1.92	0.52
12:N:94:GLY:HA2	12:N:154:VAL:O	2.10	0.52
20:V:143:ARG:O	20:V:144:VAL:HB	2.08	0.52
31:6:265:ILE:HG12	31:6:322:ARG:HG2	1.91	0.52
39:e:55:ARG:HB3	39:e:157:LEU:H	1.75	0.52
52:s:362:THR:OG1	52:s:363:ASP:N	2.42	0.52
1:A:2237:A:OP1	51:r:171:ARG:NH1	2.42	0.51
4:E:82:ASP:OD2	4:E:188:LYS:NZ	2.42	0.51
4:E:214:GLY:O	4:E:260:LYS:HA	2.10	0.51
9:K:21:LEU:HD21	9:K:31:LEU:HD22	1.91	0.51
18:T:91:ALA:O	18:T:145:SER:OG	2.29	0.51
19:U:19:VAL:HG22	34:9:136:LEU:HD22	1.91	0.51
38:d:119:GLN:HA	38:d:122:ILE:HD12	1.93	0.51
52:s:325:ARG:O	52:s:328:ALA:HB3	2.10	0.51
1:A:2421:G:H5''	34:9:24:LYS:HG2	1.92	0.51
18:T:77:ARG:NH1	18:T:119:GLU:OE1	2.38	0.51
20:V:122:LEU:HD12	20:V:133:ILE:HG13	1.91	0.51
26:1:20:MET:O	26:1:29:CYS:HA	2.10	0.51
36:b:78:GLU:HG2	36:b:84:VAL:HG22	1.92	0.51
36:b:89:ILE:HA	36:b:92:LYS:HD2	1.91	0.51
1:A:1902:C:O2	43:i:127:PHE:N	2.42	0.51
9:K:154:ARG:HD3	51:r:129:PRO:HG3	1.92	0.51
15:Q:117:LEU:O	15:Q:134:LEU:HA	2.11	0.51
25:0:94:ARG:HA	25:0:99:LYS:HD2	1.92	0.51
30:5:218:LEU:N	30:5:218:LEU:CD2	2.73	0.51
33:8:128:GLU:HB3	47:m:37:ARG:HH12	1.75	0.51
1:A:1805:A:OP2	20:V:94:HIS:NE2	2.40	0.51
1:A:2468:A:H61	1:A:2659:C:N4	2.08	0.51
47:m:52:TYR:CD2	47:m:71:PRO:HD3	2.45	0.51
52:s:228:ASP:O	52:s:230:ARG:NH1	2.44	0.51
31:6:175:VAL:HG22	31:6:204:VAL:HG22	1.91	0.51
1:A:1985:G:OP1	1:A:1987:G:O2'	2.27	0.51
1:A:2141:U:OP1	1:A:2253:U:OP2	2.29	0.51
1:A:2537:G:O2'	1:A:2634:U:OP2	2.28	0.51
3:D:194:ASN:HD22	3:D:247:VAL:HG22	1.76	0.51
30:5:160:HIS:HA	30:5:164:TRP:HB2	1.93	0.51
44:j:49:TRP:CE3	44:j:49:TRP:C	2.89	0.51
8:J:145:ILE:HG23	8:J:155:VAL:HG21	1.93	0.51
31:6:274:LYS:HG3	31:6:314:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1691:C:O2	23:Y:216:ARG:NH1	2.43	0.51
5:F:253:MET:HE3	5:F:259:LEU:HD13	1.93	0.51
47:m:51:LEU:HB3	47:m:67:ARG:HB3	1.93	0.51
2:B:1607:U:O4	2:B:1664:G:O6	2.28	0.51
31:6:235:TRP:HB3	31:6:254:TYR:HA	1.93	0.51
1:A:1883:G:H5''	41:g:91:MET:HE3	1.93	0.51
13:O:111:PRO:HG2	25:0:124:ALA:HB2	1.93	0.51
36:b:123:ASN:ND2	37:c:309:GLU:OE2	2.39	0.51
56:w:147:TYR:O	56:w:151:LYS:CB	2.58	0.51
1:A:2273:A:N1	1:A:2293:A:O2'	2.43	0.50
14:P:63:ARG:NH1	21:W:137:LYS:O	2.39	0.50
38:d:240:LYS:HG3	38:d:274:GLN:HE21	1.76	0.50
52:s:96:GLN:NE2	52:s:301:LEU:O	2.44	0.50
1:A:2459:A:N6	1:A:2668:A:O2'	2.43	0.50
4:E:227:GLN:HE21	4:E:236:THR:HB	1.76	0.50
17:S:101:PHE:CE2	17:S:116:ILE:HD13	2.46	0.50
17:S:106:TRP:CZ3	17:S:114:ILE:HG23	2.46	0.50
43:i:95:ARG:HB2	43:i:110:LEU:HD21	1.93	0.50
1:A:1789:A:H5''	34:9:17:ARG:HH21	1.76	0.50
8:J:125:ALA:HB2	8:J:140:VAL:HG21	1.94	0.50
35:a:37:SER:OG	35:a:39:LEU:O	2.27	0.50
52:s:249:GLU:HA	52:s:356:VAL:HG21	1.92	0.50
1:A:2279:U:OP2	43:i:46:ARG:NH2	2.39	0.50
7:I:37:ARG:HH22	12:N:247:MET:HE3	1.76	0.50
11:M:274:VAL:HG11	50:q:75:LEU:HD13	1.94	0.50
1:A:2570:C:O5'	1:A:2592:G:O2'	2.30	0.50
7:I:52:GLU:O	12:N:211:ASN:ND2	2.43	0.50
11:M:153:ASN:HB2	11:M:256:LEU:HD23	1.93	0.50
21:W:123:GLY:HA3	31:6:40:ILE:HG21	1.93	0.50
34:9:91:LEU:O	34:9:95:ALA:CB	2.58	0.50
1:A:1747:G:OP2	1:A:1749:C:N4	2.45	0.50
1:A:2051:A:H2'	1:A:2052:A:C8	2.46	0.50
1:A:2483:U:O2	1:A:2652:G:N2	2.45	0.50
23:Y:123:ARG:HD2	38:d:64:GLY:HA2	1.94	0.50
39:e:264:LEU:HD23	39:e:269:LEU:HB3	1.93	0.50
1:A:3068:G:OP2	1:A:3068:G:N2	2.42	0.50
5:F:289:PRO:HD2	11:M:195:LEU:HD11	1.94	0.50
6:H:58:ARG:NH2	22:X:66:PRO:O	2.45	0.50
9:K:22:ASP:HB3	9:K:147:GLN:HE21	1.77	0.50
11:M:148:PHE:O	11:M:170:ASN:ND2	2.45	0.50
16:R:114:LYS:HZ3	35:a:45:CYS:H	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:104:ARG:HH21	17:S:104:ARG:CG	2.23	0.50
36:b:11:LEU:HD23	36:b:115:ILE:HD13	1.94	0.50
52:s:188:LEU:HD21	52:s:422:VAL:HG13	1.94	0.50
1:A:2740:A:N3	1:A:2921:A:O2'	2.40	0.50
7:I:124:LYS:HB2	7:I:153:LEU:HB2	1.93	0.50
33:8:150:LEU:HB2	39:e:212:HIS:HE1	1.77	0.50
1:A:1884:G:O6	5:F:281:ARG:NH2	2.45	0.49
1:A:2276:C:H1'	16:R:11:ARG:HH22	1.77	0.49
30:5:355:LEU:HD23	30:5:376:VAL:HG12	1.93	0.49
7:I:128:ASN:OD1	7:I:151:ASN:ND2	2.42	0.49
15:Q:103:ARG:NH1	15:Q:108:ILE:HB	2.27	0.49
16:R:54:THR:HG21	17:S:172:MET:H	1.77	0.49
18:T:85:ASP:OD1	18:T:85:ASP:N	2.45	0.49
22:X:150:LYS:CG	22:X:159:MET:CE	2.88	0.49
38:d:267:PRO:HG2	38:d:270:ALA:HB2	1.93	0.49
1:A:2854:U:H4'	28:3:138:PRO:HG2	1.94	0.49
5:F:249:ASN:OD1	5:F:252:SER:OG	2.26	0.49
10:L:123:ILE:HD12	10:L:141:ALA:HB2	1.93	0.49
17:S:174:PHE:HA	17:S:180:PHE:O	2.12	0.49
21:W:67:ILE:HG21	21:W:131:VAL:HG11	1.93	0.49
22:X:130:ARG:HE	22:X:134:LEU:HD11	1.77	0.49
30:5:133:PRO:HG3	30:5:239:ILE:HD13	1.94	0.49
30:5:216:GLU:HA	30:5:216:GLU:OE1	2.13	0.49
54:u:105:ASN:O	54:u:107:ARG:NH1	2.45	0.49
1:A:1871:A:N7	1:A:1902:C:N4	2.60	0.49
1:A:2332:C:H42	1:A:2442:U:H3	1.60	0.49
1:A:2677:A:H2'	1:A:2678:A:C8	2.47	0.49
10:L:69:VAL:O	10:L:130:ARG:NH2	2.43	0.49
17:S:161:ILE:HD11	17:S:194:ARG:HB2	1.95	0.49
30:5:107:PHE:HB3	30:5:222:VAL:HG12	1.94	0.49
1:A:1867:A:H5'	5:F:153:HIS:HD2	1.78	0.49
5:F:133:THR:HG21	5:F:135:ARG:HE	1.78	0.49
8:J:32:GLY:O	8:J:36:GLY:N	2.45	0.49
10:L:145:VAL:O	54:u:119:ARG:NH2	2.46	0.49
12:N:123:ARG:NH2	12:N:162:GLU:OE2	2.46	0.49
38:d:287:LEU:HD11	38:d:293:TYR:HB2	1.94	0.49
52:s:247:LEU:HD11	52:s:296:HIS:HD2	1.75	0.49
7:I:119:HIS:NE2	7:I:158:GLU:O	2.35	0.49
8:J:138:SER:O	8:J:142:ARG:CB	2.61	0.49
15:Q:152:ARG:NH1	15:Q:191:ARG:HA	2.27	0.49
16:R:112:THR:OG1	36:b:127:GLN:NE2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:100:HIS:ND1	17:S:100:HIS:O	2.46	0.49
17:S:107:LYS:NZ	36:b:124:PRO:O	2.45	0.49
19:U:153:LEU:HD11	38:d:220:GLN:HB2	1.95	0.49
20:V:147:SER:OG	20:V:150:SER:O	2.29	0.49
1:A:1756:A:H2'	1:A:1757:A:H8	1.77	0.49
5:F:116:THR:HG23	5:F:118:ALA:H	1.77	0.49
6:H:98:LEU:HD22	6:H:102:VAL:HG21	1.95	0.49
48:o:13:PRO:HG3	48:o:21:HIS:HB3	1.90	0.49
7:I:119:HIS:HB3	7:I:121:ILE:HG22	1.95	0.49
10:L:72:GLN:HA	10:L:84:ALA:O	2.13	0.49
30:5:113:LEU:O	30:5:308:GLN:NE2	2.46	0.49
1:A:2198:A:N1	8:J:150:SER:OG	2.37	0.48
23:Y:95:ASN:OD1	23:Y:149:ARG:NH1	2.44	0.48
30:5:33:TRP:O	30:5:39:ARG:NH2	2.46	0.48
36:b:72:VAL:HG13	36:b:90:HIS:HB2	1.95	0.48
38:d:220:GLN:NE2	38:d:244:GLU:OE2	2.46	0.48
1:A:2141:U:OP1	1:A:2253:U:P	2.71	0.48
4:E:143:ALA:HB3	4:E:181:ILE:O	2.13	0.48
34:9:93:SER:O	34:9:97:ALA:HB3	2.12	0.48
1:A:2195:A:OP2	46:l:119:ARG:NH2	2.37	0.48
1:A:2511:C:H3'	1:A:2512:A:H8	1.78	0.48
1:A:2643:G:O2'	1:A:2645:G:OP2	2.26	0.48
11:M:229:PHE:HE2	11:M:259:ARG:HH22	1.61	0.48
30:5:105:TYR:CD2	30:5:218:LEU:HD12	2.48	0.48
1:A:1747:G:H5''	22:X:96:LYS:HZ2	1.78	0.48
1:A:2377:G:O2'	34:9:28:ARG:O	2.31	0.48
8:J:111:LEU:HG	8:J:154:ARG:HB3	1.96	0.48
24:Z:137:THR:HG22	24:Z:147:VAL:HA	1.95	0.48
29:4:79:CYS:HA	29:4:91:TYR:O	2.14	0.48
32:7:103:SER:HA	32:7:129:THR:HG22	1.95	0.48
51:r:85:ASP:OD1	51:r:85:ASP:N	2.41	0.48
1:A:2072:A:OP2	31:6:28:ARG:NH1	2.47	0.48
1:A:2142:A:O2'	1:A:2262:C:OP1	2.31	0.48
4:E:208:ALA:HB2	4:E:297:VAL:HG12	1.95	0.48
4:E:329:PRO:HD2	4:E:332:LEU:HD21	1.94	0.48
27:2:82:ARG:NH2	27:2:89:SER:O	2.47	0.48
45:k:18:VAL:HG11	45:k:34:LEU:HD13	1.95	0.48
8:J:92:LYS:HE2	8:J:151:LEU:HD13	1.95	0.48
19:U:52:ASP:O	19:U:56:TYR:HB2	2.14	0.48
5:F:209:TYR:OH	42:h:56:ARG:NH2	2.43	0.48
8:J:113:THR:HA	8:J:156:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:58:VAL:HG22	9:K:126:HIS:HB2	1.95	0.48
14:P:177:ARG:NH2	14:P:178:ILE:O	2.46	0.48
39:e:235:LYS:NZ	40:f:172:GLU:OE1	2.44	0.48
52:s:207:HIS:ND1	52:s:234:ASP:OD1	2.43	0.48
5:F:83:HIS:HB3	5:F:86:VAL:HG12	1.95	0.48
13:O:16:ARG:NH1	13:O:50:ASP:OD1	2.43	0.48
20:V:177:THR:HG22	34:9:71:LYS:H	1.79	0.48
24:Z:99:VAL:HG12	44:j:80:LEU:HD12	1.95	0.48
39:e:157:LEU:HB3	39:e:254:TRP:HB3	1.96	0.48
54:u:140:PHE:HA	54:u:143:VAL:HG12	1.96	0.48
1:A:3168:C:N3	4:E:303:LYS:NZ	2.62	0.48
4:E:276:ILE:HG13	4:E:332:LEU:HB2	1.95	0.48
7:I:192:ILE:O	7:I:196:LYS:HB2	2.14	0.48
10:L:118:ARG:HH12	54:u:189:GLU:HG3	1.78	0.48
10:L:128:ARG:NH2	54:u:120:TYR:O	2.47	0.48
14:P:58:LEU:HA	49:p:177:ARG:HH21	1.79	0.48
25:0:179:ARG:HH12	25:0:182:PRO:HG3	1.78	0.48
30:5:245:ILE:HG12	30:5:360:ASN:HD22	1.78	0.48
39:e:256:THR:OG1	39:e:257:LYS:N	2.47	0.48
1:A:2468:A:N6	1:A:2659:C:H42	2.10	0.48
3:D:163:ILE:HG23	3:D:180:ASP:HA	1.96	0.48
5:F:160:SER:HB3	43:i:80:LEU:HD13	1.94	0.48
7:I:147:PHE:HD1	7:I:151:ASN:HD22	1.62	0.48
8:J:89:TYR:O	8:J:93:ALA:CB	2.62	0.48
12:N:242:TRP:HB3	12:N:247:MET:HE1	1.96	0.48
30:5:151:ASP:O	30:5:155:LEU:HB2	2.14	0.48
1:A:2268:G:N7	11:M:44:ARG:NH1	2.44	0.47
1:A:2931:A:OP2	5:F:131:LYS:NZ	2.39	0.47
5:F:70:ARG:HA	5:F:196:PRO:HD3	1.95	0.47
21:W:62:HIS:HA	21:W:94:GLU:HG2	1.95	0.47
38:d:181:VAL:HG23	38:d:224:ILE:HG12	1.96	0.47
52:s:419:LEU:O	52:s:423:HIS:ND1	2.39	0.47
1:A:1886:G:H1	43:i:61:GLY:HA3	1.79	0.47
18:T:212:LEU:HA	36:b:119:PHE:HE1	1.78	0.47
22:X:36:ARG:HD2	22:X:151:GLU:OE1	2.13	0.47
1:A:2165:C:O2'	1:A:2216:A:N1	2.46	0.47
9:K:39:LEU:HD11	9:K:125:LEU:HB2	1.95	0.47
9:K:77:TYR:HE2	9:K:103:ILE:HG12	1.79	0.47
22:X:36:ARG:CD	22:X:151:GLU:OE2	2.45	0.47
56:w:100:VAL:HB	56:w:142:GLN:HB2	1.96	0.47
39:e:152:LYS:H	39:e:157:LEU:HD21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:p:56:ASP:HB3	49:p:60:ARG:HG3	1.95	0.47
38:d:213:THR:HG22	38:d:247:VAL:HG22	1.95	0.47
4:E:144:THR:HA	4:E:179:PHE:O	2.15	0.47
11:M:246:ASP:OD2	11:M:249:LYS:NZ	2.35	0.47
22:X:226:LEU:HD12	23:Y:155:LEU:HB3	1.94	0.47
52:s:214:GLU:HA	52:s:228:ASP:HA	1.97	0.47
1:A:1789:A:N3	1:A:1915:C:O2'	2.41	0.47
1:A:2395:A:H1'	30:5:385:HIS:HB2	1.96	0.47
7:I:49:ALA:HB1	48:o:32:LYS:HE2	1.97	0.47
8:J:39:LEU:HB3	8:J:44:VAL:HG11	1.96	0.47
8:J:128:GLU:HA	8:J:133:GLN:HE21	1.79	0.47
9:K:21:LEU:HD11	9:K:34:MET:HE3	1.97	0.47
11:M:78:ILE:HD13	28:3:124:ARG:HD2	1.96	0.47
11:M:95:PRO:HB3	11:M:141:VAL:HG21	1.96	0.47
13:O:49:VAL:HG12	13:O:107:MET:HE2	1.96	0.47
16:R:108:TYR:HD1	36:b:125:SER:HB2	1.79	0.47
17:S:104:ARG:HD3	17:S:106:TRP:CE2	2.50	0.47
24:Z:71:ARG:HB2	24:Z:91:LEU:HB3	1.97	0.47
36:b:108:SER:OG	36:b:109:GLY:N	2.48	0.47
45:k:40:GLU:HA	45:k:43:ARG:HB2	1.96	0.47
52:s:373:GLN:NE2	52:s:375:ASN:OD1	2.48	0.47
1:A:1800:G:N1	1:A:1803:A:OP2	2.39	0.47
1:A:2075:U:O2'	1:A:2833:A:N7	2.46	0.47
1:A:2162:C:OP1	29:4:74:LYS:NZ	2.39	0.47
12:N:132:THR:HG22	12:N:147:ILE:HA	1.95	0.47
15:Q:152:ARG:HH12	15:Q:191:ARG:HA	1.80	0.47
51:r:36:ARG:HA	51:r:52:ARG:O	2.15	0.47
1:A:2673:G:H5''	18:T:112:LYS:HB2	1.96	0.47
3:D:196:VAL:O	3:D:206:TYR:HD2	1.97	0.47
17:S:163:LYS:HB2	36:b:106:ASP:HB3	1.96	0.47
52:s:66:TRP:O	52:s:69:THR:OG1	2.30	0.47
3:D:198:SER:HB2	3:D:206:TYR:CZ	2.50	0.47
9:K:52:ASP:O	18:T:206:ARG:NH1	2.43	0.47
19:U:28:LEU:H	23:Y:114:THR:HG22	1.80	0.47
29:4:74:LYS:HD2	29:4:81:LEU:HG	1.97	0.47
30:5:276:ASP:OD1	52:s:158:ARG:NH2	2.47	0.47
37:c:215:ILE:HG23	37:c:219:LEU:HD12	1.96	0.47
39:e:213:TYR:OH	39:e:271:GLN:O	2.31	0.47
39:e:279:LEU:HD11	40:f:176:SER:HB2	1.96	0.47
42:h:120:MET:HE3	42:h:120:MET:HB3	1.84	0.47
54:u:113:GLN:N	55:v:68:ARG:O	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1642:G:H4'	33:8:119:LYS:HG3	1.97	0.46
17:S:145:GLY:HA2	35:a:57:THR:HA	1.96	0.46
30:5:210:SER:HA	30:5:222:VAL:O	2.15	0.46
49:p:100:GLU:OE2	49:p:102:ARG:NH2	2.48	0.46
54:u:100:LEU:HD23	54:u:142:VAL:HG12	1.97	0.46
56:w:148:ILE:HA	56:w:151:LYS:HB3	1.97	0.46
1:A:1673:U:O2'	18:T:149:ARG:NH2	2.48	0.46
22:X:36:ARG:CD	22:X:151:GLU:OE1	2.63	0.46
23:Y:143:ASP:OD1	34:9:137:ARG:NH2	2.48	0.46
1:A:1890:C:OP2	28:3:168:ARG:NH2	2.49	0.46
1:A:2499:U:OP2	1:A:2504:A:N6	2.36	0.46
27:2:78:VAL:HG22	27:2:81:ARG:HH21	1.81	0.46
38:d:83:GLY:O	38:d:262:HIS:NE2	2.45	0.46
10:L:96:MET:HB2	15:Q:170:ARG:HH21	1.80	0.46
21:W:76:HIS:HB2	21:W:130:PHE:CD1	2.50	0.46
23:Y:72:LYS:O	23:Y:76:GLN:NE2	2.48	0.46
31:6:268:LEU:O	31:6:318:PHE:HA	2.16	0.46
38:d:164:VAL:HG23	38:d:261:MET:HB2	1.97	0.46
1:A:1990:G:O2'	1:A:1993:A:N6	2.49	0.46
1:A:2230:A:N7	1:A:2975:G:O2'	2.48	0.46
1:A:2734:A:H2'	1:A:2735:G:H8	1.81	0.46
8:J:89:TYR:O	8:J:93:ALA:HB3	2.16	0.46
15:Q:124:PRO:HG3	15:Q:170:ARG:HH12	1.80	0.46
23:Y:98:LEU:HD22	23:Y:142:LEU:HG	1.98	0.46
37:c:275:TYR:HA	37:c:280:LEU:HA	1.97	0.46
1:A:2127:A:H4'	1:A:2251:A:C5	2.51	0.46
15:Q:102:ARG:NH1	15:Q:169:PRO:HA	2.30	0.46
32:7:107:LEU:HD12	32:7:126:LYS:HD2	1.98	0.46
39:e:51:LEU:HD12	39:e:188:ALA:HB1	1.97	0.46
40:f:166:PHE:O	40:f:170:PHE:CB	2.64	0.46
1:A:1696:C:H1'	19:U:4:ASN:HD22	1.81	0.46
4:E:73:LEU:HD11	4:E:151:THR:HG21	1.97	0.46
5:F:63:GLN:HG2	5:F:81:ASP:HB3	1.98	0.46
5:F:211:ARG:NH2	42:h:56:ARG:O	2.49	0.46
5:F:223:HIS:HA	5:F:226:MET:HE2	1.97	0.46
7:I:83:ARG:O	7:I:87:ALA:CB	2.64	0.46
21:W:106:PRO:HD2	21:W:117:ILE:HD11	1.97	0.46
30:5:218:LEU:HD11	30:5:262:ILE:HD11	1.93	0.46
38:d:190:GLU:OE1	38:d:215:ARG:NH1	2.43	0.46
42:h:105:ALA:HB1	42:h:111:VAL:HG22	1.97	0.46
8:J:29:ALA:HB1	8:J:50:CYS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:97:MET:HE1	18:T:105:GLN:HG3	1.97	0.46
55:v:13:TYR:HD1	55:v:39:PHE:HD2	1.64	0.46
55:v:54:GLN:HA	55:v:57:LYS:HG2	1.97	0.46
1:A:1777:A:N6	1:A:1780:U:OP2	2.37	0.46
1:A:1782:G:N7	5:F:121:ARG:NH1	2.64	0.46
1:A:3000:A:H2'	1:A:3001:G:C8	2.51	0.46
7:I:83:ARG:HG2	7:I:134:PHE:HE1	1.81	0.46
17:S:100:HIS:HB2	17:S:134:LEU:HD21	1.97	0.46
38:d:81:THR:OG1	38:d:249:GLU:OE2	2.30	0.46
54:u:112:ILE:HB	54:u:124:PHE:HB3	1.98	0.46
1:A:2109:A:H61	1:A:2981:A:H2	1.64	0.46
1:A:2173:G:H2'	1:A:2174:G:C8	2.51	0.46
4:E:148:GLY:HA2	4:E:175:THR:O	2.16	0.46
26:l:25:GLY:H	50:q:121:ILE:HG23	1.80	0.46
7:I:81:LEU:O	7:I:85:GLU:CB	2.64	0.45
22:X:116:SER:O	22:X:120:ASP:N	2.50	0.45
23:Y:213:ARG:HA	23:Y:216:ARG:HH21	1.81	0.45
48:o:89:ALA:O	48:o:93:ASP:CB	2.58	0.45
1:A:2279:U:OP1	5:F:255:LYS:NZ	2.46	0.45
1:A:3054:G:H2'	1:A:3055:U:C6	2.51	0.45
2:B:1610:A:H5'	2:B:1645:A:H1'	1.99	0.45
9:K:74:GLN:HA	51:r:161:PRO:HA	1.98	0.45
52:s:405:ILE:HG12	52:s:410:VAL:HG12	1.99	0.45
53:t:11:UNK:O	53:t:15:UNK:CB	2.64	0.45
1:A:3183:U:H3	9:K:177:ARG:HB3	1.81	0.45
15:Q:118:ARG:HE	15:Q:134:LEU:HD12	1.81	0.45
31:6:57:TYR:O	31:6:61:ALA:HB2	2.16	0.45
34:9:41:ILE:HG22	34:9:52:GLN:HG3	1.99	0.45
35:a:142:ARG:HD2	36:b:124:PRO:HG3	1.98	0.45
52:s:243:ILE:HG22	52:s:245:LYS:H	1.81	0.45
1:A:1747:G:H5''	22:X:96:LYS:NZ	2.32	0.45
1:A:2447:A:O3'	52:s:222:ARG:NH2	2.48	0.45
5:F:218:LEU:HD13	5:F:230:ILE:HD11	1.98	0.45
37:c:216:ARG:HA	37:c:220:ILE:HD12	1.97	0.45
39:e:177:GLU:O	39:e:190:ARG:NH2	2.50	0.45
39:e:190:ARG:O	39:e:194:THR:OG1	2.31	0.45
1:A:2339:G:O2'	1:A:2427:C:O2'	2.34	0.45
11:M:118:LEU:HD21	11:M:129:ILE:HD11	1.99	0.45
17:S:144:LEU:HG	35:a:58:ILE:HB	1.99	0.45
30:5:149:ASN:HB3	30:5:152:GLU:HB3	1.97	0.45
30:5:333:ALA:HB1	30:5:363:ASP:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:k:78:GLY:HA2	45:k:81:LEU:HB2	1.99	0.45
12:N:97:LEU:HD12	12:N:124:VAL:HG11	1.97	0.45
17:S:104:ARG:HD3	17:S:106:TRP:NE1	2.32	0.45
29:4:69:LYS:HB2	29:4:72:LEU:HD23	1.99	0.45
50:q:40:PRO:HG3	50:q:51:GLN:HB3	1.99	0.45
1:A:2262:C:O2'	17:S:175:ARG:NH2	2.50	0.45
11:M:78:ILE:O	28:3:113:ARG:NH1	2.46	0.45
11:M:102:GLN:NE2	11:M:106:ASP:OD2	2.42	0.45
14:P:177:ARG:HH22	31:6:346:ARG:HH12	1.64	0.45
30:5:210:SER:HB3	30:5:276:ASP:HB3	1.98	0.45
42:h:151:ASN:OD1	42:h:151:ASN:N	2.46	0.45
1:A:2682:A:H5''	16:R:34:ARG:NH1	2.31	0.45
1:A:2740:A:H2'	1:A:2741:A:C8	2.52	0.45
1:A:2861:A:H4'	21:W:65:ASN:HD22	1.82	0.45
9:K:74:GLN:HE21	51:r:159:VAL:HG11	1.82	0.45
12:N:191:SER:OG	12:N:192:ARG:N	2.49	0.45
13:O:129:CYS:SG	25:0:156:THR:OG1	2.63	0.45
21:W:120:LEU:HB3	21:W:124:ALA:HB3	1.99	0.45
22:X:144:TYR:O	22:X:148:THR:CG2	2.44	0.45
30:5:134:GLU:O	30:5:138:SER:HB3	2.16	0.45
39:e:87:HIS:HB2	47:m:70:GLU:HG3	1.99	0.45
52:s:66:TRP:HE1	52:s:82:ILE:HG22	1.82	0.45
1:A:2095:U:H5''	11:M:53:HIS:HD2	1.82	0.45
1:A:2255:C:H5''	44:j:66:ARG:HH11	1.82	0.45
1:A:2549:C:H4'	1:A:2550:A:H5'	1.99	0.45
1:A:2594:U:H2'	1:A:2595:A:C8	2.52	0.45
1:A:2972:A:H5''	12:N:184:PRO:HA	1.99	0.45
4:E:345:ILE:H	4:E:345:ILE:HG13	1.58	0.45
12:N:109:ILE:HG13	12:N:179:VAL:HG21	1.98	0.45
18:T:124:ALA:O	18:T:128:ALA:HB2	2.17	0.45
37:c:79:LEU:HD21	37:c:173:LEU:HD22	1.99	0.45
50:q:142:ASN:O	50:q:146:ALA:HB2	2.17	0.45
1:A:2950:U:H2'	1:A:2951:A:H8	1.82	0.45
15:Q:177:VAL:HG11	15:Q:204:MET:HG3	1.99	0.45
22:X:153:LEU:HD11	22:X:158:GLY:HA3	1.98	0.45
2:B:1621:A:OP2	14:P:113:LYS:NZ	2.44	0.44
19:U:22:THR:HG21	19:U:56:TYR:HE1	1.82	0.44
23:Y:123:ARG:HB2	38:d:61:ARG:HG3	2.00	0.44
24:Z:67:HIS:O	24:Z:99:VAL:HA	2.16	0.44
32:7:52:LYS:HG3	32:7:219:LEU:HD11	1.99	0.44
41:g:86:VAL:HG22	41:g:113:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2040:G:O2'	11:M:56:GLU:OE1	2.34	0.44
31:6:371:ASP:OD1	31:6:371:ASP:N	2.49	0.44
52:s:165:ARG:HG2	52:s:307:ARG:HH22	1.83	0.44
54:u:159:ILE:HA	54:u:170:VAL:HG22	1.98	0.44
1:A:1963:A:OP1	27:2:48:ALA:N	2.50	0.44
5:F:217:LEU:HD23	5:F:259:LEU:HD12	1.98	0.44
13:O:131:PRO:HD2	25:0:134:THR:HG22	1.98	0.44
14:P:122:VAL:HG22	14:P:157:SER:HB3	1.99	0.44
17:S:100:HIS:O	17:S:100:HIS:CG	2.70	0.44
19:U:143:ARG:HG3	32:7:80:VAL:HG21	2.00	0.44
25:0:181:ARG:HD3	25:0:182:PRO:HD2	2.00	0.44
54:u:125:VAL:HB	54:u:177:ILE:HG22	2.00	0.44
1:A:2149:G:OP2	16:R:65:ARG:NH2	2.50	0.44
5:F:89:THR:H	5:F:179:THR:HG21	1.81	0.44
22:X:89:GLN:HA	22:X:102:LYS:HA	1.98	0.44
27:2:82:ARG:NE	27:2:87:ARG:HD2	2.32	0.44
31:6:183:ASP:HA	49:p:192:ARG:HA	1.99	0.44
48:o:12:ILE:HD11	48:o:16:GLN:HG2	2.00	0.44
1:A:2081:U:H2'	1:A:2082:G:C8	2.52	0.44
1:A:2139:U:H3'	24:Z:74:SER:HB2	1.99	0.44
1:A:2153:A:H2'	48:o:30:ARG:HH11	1.83	0.44
1:A:2167:A:N6	1:A:2212:C:OP2	2.48	0.44
4:E:99:LEU:HD13	4:E:124:VAL:HG21	1.99	0.44
4:E:101:ALA:O	4:E:296:LEU:HA	2.16	0.44
13:O:110:ILE:HD12	13:O:120:MET:HB3	1.99	0.44
15:Q:112:TYR:HE2	15:Q:215:VAL:HG21	1.83	0.44
40:f:166:PHE:O	40:f:170:PHE:HB3	2.18	0.44
52:s:237:PRO:HG3	52:s:298:GLN:HE21	1.83	0.44
55:v:6:ARG:NH1	59:v:101:PNS:O23	2.51	0.44
17:S:76:HIS:ND1	35:a:50:ALA:HA	2.33	0.44
17:S:160:VAL:HA	17:S:193:LEU:CD2	2.45	0.44
48:o:65:VAL:HG22	48:o:68:ARG:HH12	1.82	0.44
52:s:87:GLN:O	52:s:277:GLN:NE2	2.50	0.44
1:A:1882:A:N1	1:A:1891:A:O2'	2.43	0.44
1:A:2348:A:H1'	38:d:63:ALA:HA	2.00	0.44
17:S:96:PHE:HB3	36:b:126:ILE:HD12	1.98	0.44
39:e:146:ARG:HB3	39:e:253:VAL:HG13	2.00	0.44
5:F:230:ILE:HG23	5:F:242:LEU:HD11	1.99	0.44
7:I:47:LEU:HD21	12:N:215:PHE:CE2	2.53	0.44
7:I:98:VAL:HG11	7:I:146:LEU:HD11	1.99	0.44
9:K:5:SER:HB2	9:K:8:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:59:ILE:HB	9:K:127:LEU:HD23	2.00	0.44
11:M:295:THR:HG22	49:p:39:PHE:HE1	1.82	0.44
21:W:100:THR:OG1	21:W:132:HIS:NE2	2.46	0.44
36:b:27:GLN:HE21	36:b:80:LEU:HA	1.82	0.44
36:b:64:TYR:OH	37:c:67:ASP:N	2.51	0.44
39:e:124:TRP:CD1	47:m:72:ARG:HA	2.53	0.44
39:e:165:PHE:HB2	39:e:168:GLN:HB2	1.99	0.44
54:u:167:TRP:HB2	54:u:184:THR:HG21	2.00	0.44
1:A:1783:U:H5''	27:2:88:LYS:HE3	2.00	0.44
1:A:2106:A:N7	7:I:31:LYS:NZ	2.66	0.44
5:F:103:GLN:HE22	5:F:249:ASN:HB2	1.82	0.44
13:O:97:TYR:OH	13:O:126:LYS:O	2.26	0.44
33:8:168:LEU:HD21	39:e:205:LEU:HA	2.00	0.44
39:e:74:LEU:HA	39:e:77:ILE:HG22	2.00	0.44
44:j:49:TRP:CE3	44:j:49:TRP:O	2.70	0.44
1:A:2310:G:O2'	1:A:2675:G:O6	2.25	0.43
1:A:3048:A:HO2'	10:L:59:HIS:HD1	1.64	0.43
7:I:160:LYS:HG2	7:I:163:GLU:HB3	1.98	0.43
20:V:54:TRP:NE1	20:V:56:LEU:O	2.49	0.43
37:c:41:PHE:HE2	43:i:36:LEU:HD13	1.82	0.43
39:e:124:TRP:CH2	47:m:70:GLU:HB3	2.52	0.43
52:s:62:ARG:HA	52:s:65:ARG:HG2	2.00	0.43
15:Q:154:VAL:HG12	15:Q:159:GLY:HA2	2.00	0.43
51:r:72:ILE:HD11	51:r:115:ILE:HD11	1.99	0.43
52:s:152:GLN:HA	52:s:156:TYR:HB2	2.01	0.43
1:A:1881:A:H62	41:g:111:ARG:HD3	1.82	0.43
1:A:2387:U:O2'	1:A:2406:A:N6	2.46	0.43
1:A:2553:G:H2'	1:A:2554:A:C8	2.53	0.43
1:A:2745:A:O2'	22:X:102:LYS:O	2.30	0.43
4:E:65:VAL:HG22	32:7:315:LYS:HE2	2.00	0.43
4:E:331:ASP:OD1	4:E:331:ASP:N	2.49	0.43
5:F:241:ASN:OD1	5:F:256:HIS:NE2	2.37	0.43
14:P:64:LYS:HA	14:P:97:GLN:HE22	1.83	0.43
14:P:72:PHE:HB2	21:W:107:HIS:HA	2.00	0.43
32:7:77:THR:HG22	38:d:284:GLY:H	1.83	0.43
1:A:2830:A:N6	1:A:2837:A:OP2	2.44	0.43
4:E:116:LYS:HD2	15:Q:165:GLU:OE2	2.18	0.43
9:K:46:VAL:HG13	18:T:208:ILE:HG23	2.00	0.43
31:6:224:HIS:HA	31:6:232:TYR:CE2	2.53	0.43
52:s:184:LEU:O	52:s:188:LEU:HB2	2.17	0.43
1:A:2265:A:OP1	11:M:47:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2691:U:H4'	48:o:16:GLN:HE21	1.83	0.43
1:A:3216:C:O3'	15:Q:86:ARG:NH2	2.49	0.43
3:D:138:ASP:OD1	3:D:138:ASP:N	2.46	0.43
5:F:113:LYS:HD2	5:F:157:GLY:HA2	2.01	0.43
15:Q:123:ASP:OD2	15:Q:125:TYR:HB2	2.19	0.43
18:T:72:GLU:HG2	18:T:179:VAL:HG22	2.00	0.43
36:b:35:ARG:HD3	42:h:156:TRP:HZ3	1.81	0.43
54:u:167:TRP:CD1	54:u:180:MET:HB3	2.53	0.43
55:v:23:LEU:HD23	55:v:28:ARG:HG2	2.00	0.43
1:A:2093:U:O2	1:A:2266:U:O2'	2.37	0.43
3:D:225:ILE:HA	3:D:234:MET:O	2.17	0.43
7:I:97:ALA:HB3	7:I:154:LEU:HB2	2.01	0.43
11:M:94:LYS:HG3	11:M:129:ILE:HG22	2.01	0.43
32:7:143:TRP:NE1	32:7:172:VAL:O	2.52	0.43
52:s:165:ARG:HE	52:s:307:ARG:HH12	1.67	0.43
56:w:123:GLU:OE2	56:w:130:ILE:HB	2.19	0.43
5:F:217:LEU:HA	5:F:217:LEU:HD12	1.79	0.43
32:7:103:SER:HB2	32:7:127:PHE:HB3	2.00	0.43
37:c:74:ALA:O	37:c:78:ARG:HB2	2.19	0.43
40:f:163:SER:H	40:f:166:PHE:HB3	1.84	0.43
19:U:128:SER:O	19:U:132:GLU:HB2	2.19	0.43
30:5:133:PRO:HD3	30:5:375:TRP:CG	2.54	0.43
31:6:235:TRP:HE3	31:6:237:LEU:HD13	1.84	0.43
33:8:139:MET:HG2	39:e:275:PHE:HA	2.01	0.43
37:c:223:MET:HE3	37:c:231:MET:HE1	2.01	0.43
1:A:1868:G:OP2	11:M:41:ARG:NH1	2.45	0.43
1:A:1992:C:C4	3:D:274:ARG:HB2	2.54	0.43
1:A:2515:U:O2'	3:D:283:GLY:O	2.29	0.43
2:B:1628:C:H5'	33:8:125:LYS:HG2	2.01	0.43
12:N:103:GLU:O	12:N:107:LEU:HB3	2.19	0.43
37:c:170:ALA:HB3	37:c:191:LEU:HD21	2.01	0.43
37:c:228:LEU:HB2	37:c:307:PHE:CD1	2.53	0.43
1:A:2695:G:OP1	1:A:2941:G:O2'	2.31	0.43
3:D:113:ARG:HG3	3:D:147:ARG:HH12	1.83	0.43
9:K:73:GLU:HG2	51:r:149:ARG:HH22	1.84	0.43
13:O:46:TRP:HD1	13:O:121:ALA:HB2	1.84	0.43
15:Q:131:SER:HB3	54:u:119:ARG:HD3	1.99	0.43
20:V:109:ILE:HD13	38:d:76:ILE:HD13	2.01	0.43
22:X:150:LYS:CG	22:X:159:MET:HE1	2.28	0.43
23:Y:186:ILE:HD12	23:Y:190:LEU:HD12	2.01	0.43
7:I:168:LEU:HD11	7:I:174:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:90:PHE:HE2	8:J:120:ILE:HD13	1.84	0.42
11:M:104:LEU:HD11	11:M:126:GLY:HA3	2.01	0.42
12:N:94:GLY:CA	12:N:154:VAL:O	2.67	0.42
17:S:87:ILE:HG22	17:S:202:PRO:HG3	2.01	0.42
20:V:123:VAL:HG13	20:V:128:ARG:HA	2.01	0.42
20:V:126:MET:SD	20:V:126:MET:N	2.91	0.42
36:b:27:GLN:HE21	36:b:80:LEU:HD23	1.83	0.42
12:N:233:TYR:HB3	12:N:237:HIS:CD2	2.53	0.42
16:R:126:GLU:O	16:R:130:ALA:HB2	2.20	0.42
30:5:295:ASP:HB3	30:5:303:ARG:HG2	2.01	0.42
39:e:125:GLU:HG2	47:m:73:ARG:NH1	2.34	0.42
39:e:171:TRP:CD1	39:e:263:TYR:HB3	2.55	0.42
39:e:198:ASN:HD21	39:e:200:MET:HE2	1.84	0.42
39:e:199:ASN:HB2	39:e:242:ASP:HB2	2.00	0.42
39:e:203:LYS:N	39:e:237:LEU:O	2.51	0.42
39:e:259:GLU:HA	39:e:262:ASP:HB2	2.01	0.42
39:e:264:LEU:HB3	39:e:269:LEU:HB3	2.01	0.42
1:A:2511:C:OP1	3:D:263:ASN:ND2	2.52	0.42
1:A:2857:U:H5''	28:3:142:LYS:HE2	2.01	0.42
7:I:192:ILE:O	7:I:196:LYS:CB	2.67	0.42
11:M:83:PHE:HB3	28:3:115:LEU:HD13	2.00	0.42
11:M:212:PRO:HD3	50:q:103:LEU:HD13	2.00	0.42
17:S:133:VAL:HG23	17:S:149:LEU:HD12	2.01	0.42
17:S:168:PRO:HA	17:S:187:THR:HG22	2.01	0.42
23:Y:160:GLN:HG3	34:9:131:TYR:CG	2.54	0.42
27:2:82:ARG:HA	27:2:82:ARG:HD2	1.86	0.42
30:5:230:LEU:O	30:5:289:HIS:HB3	2.19	0.42
31:6:235:TRP:CE3	31:6:237:LEU:HD13	2.55	0.42
32:7:143:TRP:HE1	32:7:172:VAL:HB	1.82	0.42
36:b:77:ALA:HB2	36:b:104:LEU:HD13	2.02	0.42
1:A:1775:A:O2'	16:R:10:LEU:N	2.52	0.42
1:A:2101:C:H2'	1:A:2102:A:H8	1.84	0.42
1:A:2348:A:H5'	38:d:62:LYS:HB3	2.01	0.42
1:A:3011:A:O2'	1:A:3173:G:N2	2.52	0.42
1:A:3219:G:H2'	1:A:3220:A:H5''	2.02	0.42
3:D:192:LEU:O	3:D:245:GLY:N	2.52	0.42
9:K:11:TRP:CD1	37:c:269:LEU:HD23	2.54	0.42
17:S:97:ALA:HA	17:S:135:LEU:O	2.19	0.42
38:d:183:TRP:CH2	38:d:185:PHE:HB2	2.54	0.42
45:k:68:PHE:HB2	45:k:72:HIS:HB2	2.01	0.42
51:r:72:ILE:HD12	51:r:111:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2318:A:H2'	1:A:2319:A:C8	2.54	0.42
2:B:1627:C:H5''	33:8:129:ARG:HD2	2.02	0.42
4:E:76:LYS:HG3	4:E:170:LEU:HD21	2.00	0.42
8:J:22:ALA:HB1	8:J:24:VAL:HG23	2.01	0.42
11:M:140:LEU:HG	11:M:156:VAL:HG11	2.01	0.42
11:M:277:MET:HE1	41:g:52:LEU:HD21	2.01	0.42
14:P:109:GLU:OE2	14:P:135:ARG:NH2	2.51	0.42
18:T:157:ARG:HB2	18:T:167:MET:HE3	2.02	0.42
29:4:81:LEU:HA	29:4:89:TYR:O	2.20	0.42
32:7:99:TYR:O	32:7:103:SER:OG	2.24	0.42
39:e:47:LEU:HB3	39:e:178:TRP:CE2	2.55	0.42
52:s:228:ASP:OD1	52:s:228:ASP:N	2.52	0.42
1:A:1719:G:H2'	1:A:1720:C:H6	1.84	0.42
1:A:2094:G:O2'	1:A:2265:A:N3	2.49	0.42
1:A:2693:A:OP1	48:o:15:ARG:NH2	2.48	0.42
1:A:3224:G:H2'	1:A:3225:G:H8	1.84	0.42
5:F:203:LEU:HD22	5:F:240:PHE:CD2	2.54	0.42
1:A:2052:A:H5''	41:g:150:LYS:HE3	2.02	0.42
1:A:2594:U:H2'	1:A:2595:A:H8	1.85	0.42
1:A:2625:C:O2'	1:A:2627:G:OP1	2.37	0.42
17:S:116:ILE:HD11	17:S:193:LEU:HD12	2.02	0.42
22:X:64:ASP:OD1	22:X:64:ASP:N	2.52	0.42
24:Z:100:HIS:HB3	24:Z:106:VAL:HG11	2.02	0.42
24:Z:118:ARG:HD3	24:Z:120:LYS:HE3	2.02	0.42
44:j:48:ASP:OD1	44:j:48:ASP:N	2.51	0.42
56:w:81:ASP:HA	56:w:84:LEU:HB3	2.01	0.42
1:A:1749:C:OP2	1:A:2899:C:O2'	2.34	0.42
1:A:2217:C:H5''	7:I:128:ASN:HD22	1.84	0.42
11:M:96:LEU:HD12	11:M:127:VAL:HG21	2.01	0.42
16:R:112:THR:HG23	17:S:142:THR:HG21	2.02	0.42
22:X:38:PRO:HB2	22:X:152:ASP:OD1	2.19	0.42
23:Y:169:ARG:HH22	30:5:64:MET:HB2	1.85	0.42
32:7:166:LEU:HD22	32:7:181:TYR:HE2	1.85	0.42
44:j:49:TRP:HH2	44:j:58:PRO:HD2	1.85	0.42
5:F:249:ASN:OD1	5:F:249:ASN:N	2.52	0.42
9:K:16:ARG:HH22	9:K:124:ARG:NH2	2.17	0.42
12:N:104:MET:HE3	12:N:108:THR:HG21	2.01	0.42
14:P:152:GLU:HG3	14:P:158:MET:HG3	2.02	0.42
17:S:99:VAL:HA	17:S:133:VAL:HA	2.02	0.42
31:6:221:LEU:HD12	31:6:267:ARG:HG3	2.02	0.42
31:6:224:HIS:CE1	31:6:227:GLU:H	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:b:76:VAL:HG22	36:b:86:GLU:HG3	2.02	0.42
39:e:44:PRO:HG2	39:e:227:LEU:HA	2.02	0.42
1:A:1962:A:OP2	1:A:2501:C:N4	2.52	0.42
9:K:27:PRO:HG2	9:K:30:LYS:HB3	2.02	0.42
13:O:41:ARG:NH2	13:O:124:GLU:OE1	2.47	0.42
13:O:145:LEU:H	32:7:306:LEU:HD23	1.85	0.42
17:S:164:THR:HG22	36:b:107:GLN:HB2	2.02	0.42
19:U:65:VAL:HG13	19:U:97:VAL:HG13	2.02	0.42
19:U:71:ARG:NH2	19:U:96:TYR:OH	2.53	0.42
20:V:183:LEU:HD11	34:9:79:PRO:HD2	2.02	0.42
30:5:358:GLN:HB2	30:5:375:TRP:HZ3	1.84	0.42
39:e:187:THR:O	39:e:191:THR:OG1	2.29	0.42
50:q:140:ARG:HA	50:q:143:TRP:HD1	1.85	0.42
54:u:143:VAL:O	54:u:147:LYS:HB2	2.20	0.42
1:A:2363:A:H5''	1:A:2364:C:H5	1.85	0.41
1:A:2430:A:N6	18:T:161:ARG:O	2.53	0.41
4:E:179:PHE:CE1	4:E:298:LYS:HE3	2.55	0.41
6:H:107:VAL:HG12	6:H:108:ARG:H	1.85	0.41
9:K:171:THR:HG22	51:r:58:LYS:HA	2.01	0.41
12:N:224:LEU:HD11	48:o:38:ARG:HB3	2.02	0.41
14:P:154:ALA:HA	14:P:159:LYS:HE3	2.01	0.41
30:5:310:ARG:HA	30:5:313:MET:HE2	2.02	0.41
56:w:148:ILE:HG22	56:w:152:LYS:HE2	2.01	0.41
16:R:30:HIS:O	35:a:133:ARG:NH2	2.51	0.41
17:S:201:ALA:HA	17:S:202:PRO:HD3	1.84	0.41
26:1:20:MET:HE2	26:1:43:LEU:HD12	2.02	0.41
28:3:115:LEU:HB3	28:3:123:VAL:HB	2.02	0.41
31:6:46:GLU:HG3	40:f:64:LYS:HD2	2.01	0.41
33:8:97:LYS:HB2	39:e:84:TYR:CE2	2.55	0.41
1:A:1782:G:O2'	1:A:1793:G:O6	2.34	0.41
2:B:1604:G:H2'	2:B:1605:A:H8	1.85	0.41
3:D:193:ILE:HD11	3:D:226:ILE:HG23	2.02	0.41
5:F:70:ARG:O	5:F:202:TYR:OH	2.29	0.41
11:M:292:LYS:O	11:M:296:SER:OG	2.39	0.41
35:a:69:TYR:OH	37:c:256:ARG:NH2	2.53	0.41
1:A:2243:A:H5''	51:r:188:SER:HB3	2.01	0.41
3:D:199:GLU:HB2	3:D:202:ARG:HB2	2.02	0.41
5:F:97:HIS:HD2	11:M:27:LEU:HB3	1.86	0.41
11:M:220:ARG:HH21	11:M:233:ARG:HG2	1.84	0.41
12:N:118:MET:HA	12:N:164:GLY:O	2.20	0.41
14:P:126:GLU:OE2	14:P:130:ARG:NE	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:116:ILE:HD13	15:Q:178:LYS:HD3	2.03	0.41
15:Q:124:PRO:HD3	15:Q:170:ARG:NH1	2.36	0.41
30:5:163:LEU:HB2	30:5:386:PHE:CE2	2.55	0.41
36:b:62:VAL:HA	42:h:151:ASN:HB2	2.03	0.41
40:f:127:MET:HB2	40:f:154:GLU:HB2	2.01	0.41
42:h:62:PRO:HA	42:h:63:PRO:HD3	1.97	0.41
42:h:98:PHE:O	42:h:102:ALA:CB	2.68	0.41
43:i:32:ILE:HG22	43:i:34:ILE:HG22	2.01	0.41
1:A:2245:A:C4	51:r:189:ARG:HG3	2.55	0.41
1:A:2425:A:OP1	52:s:221:HIS:ND1	2.43	0.41
4:E:106:MET:HG2	4:E:120:THR:HG22	2.03	0.41
5:F:165:LEU:HB2	5:F:170:ARG:HD3	2.03	0.41
11:M:264:GLN:NE2	11:M:269:LEU:O	2.46	0.41
12:N:55:ARG:HG2	12:N:99:TRP:CG	2.55	0.41
13:O:106:ARG:O	13:O:123:ILE:HA	2.21	0.41
21:W:72:HIS:O	21:W:74:ARG:N	2.54	0.41
22:X:7:PRO:HA	43:i:101:ARG:HB3	2.03	0.41
33:8:128:GLU:HB3	47:m:37:ARG:NH1	2.35	0.41
39:e:125:GLU:HG2	47:m:73:ARG:CZ	2.50	0.41
52:s:366:TYR:HA	52:s:400:PRO:HA	2.02	0.41
1:A:2661:U:H2'	1:A:2662:A:C8	2.56	0.41
1:A:2807:U:O2'	1:A:2921:A:N7	2.50	0.41
4:E:179:PHE:HE1	4:E:298:LYS:HE3	1.85	0.41
4:E:348:ALA:HB2	15:Q:128:GLY:HA3	2.03	0.41
6:H:103:GLU:HG2	6:H:104:ASN:H	1.85	0.41
17:S:131:GLU:HG2	17:S:151:LYS:HE2	2.03	0.41
19:U:37:GLU:HB3	19:U:104:THR:HG23	2.01	0.41
23:Y:69:ASP:OD1	23:Y:69:ASP:N	2.53	0.41
26:1:33:LYS:HE3	26:1:65:LEU:HD11	2.01	0.41
37:c:121:SER:OG	37:c:122:ASN:N	2.53	0.41
1:A:2085:A:H2'	1:A:2086:A:C8	2.56	0.41
1:A:2094:G:H2'	1:A:2095:U:H6	1.85	0.41
3:D:193:ILE:HD11	3:D:226:ILE:HD12	2.02	0.41
4:E:78:CYS:HB3	4:E:81:LYS:HB2	2.03	0.41
4:E:208:ALA:O	4:E:265:TYR:HA	2.21	0.41
5:F:255:LYS:HE2	43:i:52:ALA:HA	2.02	0.41
7:I:93:ASN:HD22	7:I:155:VAL:HG12	1.86	0.41
12:N:218:ILE:HG23	12:N:223:MET:HB2	2.03	0.41
15:Q:119:VAL:O	15:Q:132:GLN:HA	2.21	0.41
18:T:73:ILE:HD11	18:T:134:VAL:HG21	2.02	0.41
19:U:112:PRO:HD2	23:Y:75:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:5:350:ARG:HE	30:5:351:VAL:HG23	1.84	0.41
31:6:57:TYR:O	31:6:61:ALA:CB	2.69	0.41
32:7:87:THR:O	32:7:90:SER:OG	2.31	0.41
56:w:79:ILE:HG12	56:w:126:PHE:HZ	1.86	0.41
1:A:2408:U:H2'	1:A:2409:A:C8	2.55	0.41
3:D:95:GLY:HA2	3:D:269:ARG:HB2	2.02	0.41
4:E:218:VAL:HG21	4:E:240:PRO:HB3	2.03	0.41
9:K:21:LEU:HD12	9:K:145:LEU:HD12	2.02	0.41
22:X:36:ARG:CG	22:X:151:GLU:OE1	2.68	0.41
22:X:39:THR:H	22:X:152:ASP:CG	2.29	0.41
22:X:150:LYS:HA	22:X:159:MET:SD	2.61	0.41
54:u:143:VAL:HG11	54:u:159:ILE:HD11	2.02	0.41
1:A:1737:A:N6	1:A:1760:G:H1'	2.36	0.41
1:A:2054:U:C5	48:o:75:LYS:HG3	2.56	0.41
1:A:2114:C:OP1	1:A:2115:U:OP2	2.39	0.41
1:A:2374:A:N6	52:s:272:PRO:O	2.38	0.41
1:A:2682:A:H5''	16:R:34:ARG:HH12	1.86	0.41
7:I:140:TYR:HB3	7:I:143:LEU:HD13	2.02	0.41
13:O:113:ARG:HG2	13:O:115:LEU:H	1.85	0.41
20:V:44:VAL:HG21	20:V:83:ARG:HH12	1.84	0.41
22:X:2:PRO:HB2	22:X:3:LEU:H	1.65	0.41
22:X:52:ILE:HA	22:X:59:ARG:HA	2.03	0.41
26:1:42:THR:HG22	26:1:57:VAL:HG22	2.03	0.41
27:2:69:ARG:HA	27:2:69:ARG:HD3	1.91	0.41
29:4:82:VAL:HG11	29:4:84:ARG:HE	1.85	0.41
38:d:210:GLY:O	38:d:249:GLU:HA	2.21	0.41
45:k:18:VAL:HG23	45:k:64:VAL:HG22	2.02	0.41
1:A:2256:U:C4'	17:S:102:ALA:HB1	2.51	0.41
1:A:2897:A:O2'	11:M:77:ARG:O	2.38	0.41
4:E:87:ILE:HG23	4:E:317:PRO:HG2	2.03	0.41
9:K:16:ARG:HB2	9:K:55:ASP:HA	2.02	0.41
9:K:174:GLU:HA	51:r:56:THR:HG21	2.03	0.41
22:X:148:THR:OG1	22:X:153:LEU:HB2	2.20	0.41
31:6:237:LEU:HD11	31:6:250:VAL:HG22	2.02	0.41
40:f:94:HIS:HA	40:f:155:ARG:O	2.20	0.41
44:j:53:ASP:OD2	44:j:55:ARG:NH2	2.49	0.41
44:j:91:TRP:CD2	48:o:58:GLN:HG2	2.56	0.41
3:D:262:ARG:HG2	3:D:265:TRP:CZ3	2.56	0.40
5:F:223:HIS:CE1	50:q:26:ARG:HH21	2.39	0.40
5:F:279:ARG:HH12	5:F:282:PRO:HD3	1.85	0.40
11:M:141:VAL:HG12	11:M:143:GLU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:3:ARG:H	19:U:23:ASN:HB3	1.85	0.40
41:g:87:ARG:HB2	41:g:112:LYS:HB3	2.02	0.40
1:A:2086:A:H2'	1:A:2087:U:C6	2.56	0.40
1:A:2286:A:H2'	1:A:2287:U:C6	2.56	0.40
1:A:2695:G:N2	1:A:3059:A:OP2	2.55	0.40
1:A:3157:C:H2'	15:Q:85:GLY:HA2	2.03	0.40
9:K:67:PHE:HB3	9:K:71:LYS:HB2	2.03	0.40
16:R:97:LEU:HD22	16:R:101:VAL:HG11	2.03	0.40
20:V:25:PRO:HA	20:V:26:PRO:HD3	1.92	0.40
20:V:139:GLU:N	20:V:139:GLU:CD	2.73	0.40
52:s:105:TRP:HZ3	52:s:268:PRO:HA	1.87	0.40
1:A:1829:A:H5'	16:R:31:PHE:CD1	2.56	0.40
1:A:2157:U:OP1	51:r:182:ARG:NH1	2.53	0.40
4:E:275:ARG:HE	4:E:331:ASP:HB2	1.84	0.40
8:J:24:VAL:HG21	8:J:35:LEU:HD21	2.02	0.40
8:J:115:LYS:HA	8:J:118:TYR:HD2	1.85	0.40
11:M:39:ARG:HA	11:M:40:PRO:HD3	1.88	0.40
13:O:123:ILE:HD13	13:O:123:ILE:HG21	1.86	0.40
15:Q:201:ASP:HB3	15:Q:204:MET:HB3	2.04	0.40
31:6:60:ARG:NH2	31:6:64:GLU:OE2	2.48	0.40
48:o:12:ILE:CD1	48:o:16:GLN:HG2	2.51	0.40
56:w:81:ASP:O	56:w:85:TYR:CB	2.66	0.40
1:A:3108:U:O4'	4:E:221:ARG:NH2	2.55	0.40
1:A:3205:C:OP2	4:E:298:LYS:NZ	2.54	0.40
3:D:126:VAL:HG22	3:D:142:VAL:HG22	2.03	0.40
3:D:248:SER:OG	3:D:249:ASN:N	2.53	0.40
5:F:175:LYS:O	5:F:179:THR:HG23	2.21	0.40
7:I:150:HIS:N	45:k:35:GLN:HE22	2.18	0.40
10:L:74:LEU:HD23	10:L:74:LEU:HA	1.90	0.40
18:T:76:CYS:HA	18:T:174:TYR:O	2.22	0.40
20:V:136:ARG:HB2	20:V:146:VAL:HG21	2.04	0.40
30:5:122:TRP:O	30:5:215:ARG:NH1	2.52	0.40
30:5:216:GLU:OE2	30:5:367:ASN:HB2	2.21	0.40
32:7:106:ALA:HA	32:7:126:LYS:O	2.21	0.40
32:7:167:VAL:HG23	32:7:235:TYR:HB3	2.02	0.40
52:s:212:ARG:HD3	52:s:379:LEU:HD12	2.02	0.40
3:D:220:VAL:HG12	3:D:221:ASN:H	1.86	0.40
5:F:110:SER:O	5:F:110:SER:OG	2.39	0.40
8:J:32:GLY:HA3	8:J:33:PRO:HD3	1.90	0.40
11:M:98:LEU:HD21	11:M:167:ILE:HD11	2.04	0.40
11:M:247:ILE:HG22	11:M:253:PHE:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:291:LEU:O	11:M:295:THR:OG1	2.34	0.40
30:5:304:LEU:HD12	30:5:308:GLN:HB3	2.02	0.40
39:e:64:THR:HG22	39:e:66:LEU:H	1.86	0.40
39:e:201:GLU:OE1	39:e:240:THR:OG1	2.39	0.40
55:v:9:VAL:HG22	55:v:55:LEU:HD11	2.02	0.40
55:v:51:ARG:HA	59:v:101:PNS:H422	2.03	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	
3	D	234/305 (77%)	223 (95%)	11 (5%)	0	100	100
4	E	302/348 (87%)	287 (95%)	15 (5%)	0	100	100
5	F	248/311 (80%)	233 (94%)	15 (6%)	0	100	100
6	H	93/267 (35%)	87 (94%)	6 (6%)	0	100	100
7	I	154/261 (59%)	142 (92%)	12 (8%)	0	100	100
8	J	138/192 (72%)	125 (91%)	13 (9%)	0	100	100
9	K	175/178 (98%)	169 (97%)	6 (3%)	0	100	100
10	L	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
11	M	285/296 (96%)	270 (95%)	15 (5%)	0	100	100
12	N	203/251 (81%)	193 (95%)	10 (5%)	0	100	100
13	O	150/175 (86%)	146 (97%)	4 (3%)	0	100	100
14	P	139/180 (77%)	130 (94%)	9 (6%)	0	100	100
15	Q	215/292 (74%)	201 (94%)	14 (6%)	0	100	100
16	R	138/149 (93%)	134 (97%)	4 (3%)	0	100	100
17	S	154/205 (75%)	148 (96%)	5 (3%)	1 (1%)	21	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	T	164/206 (80%)	161 (98%)	3 (2%)	0	100	100
19	U	135/153 (88%)	125 (93%)	10 (7%)	0	100	100
20	V	188/216 (87%)	179 (95%)	8 (4%)	1 (0%)	24	52
21	W	107/148 (72%)	104 (97%)	3 (3%)	0	100	100
22	X	241/256 (94%)	235 (98%)	6 (2%)	0	100	100
23	Y	174/250 (70%)	169 (97%)	5 (3%)	0	100	100
24	Z	118/161 (73%)	112 (95%)	6 (5%)	0	100	100
25	0	106/188 (56%)	103 (97%)	3 (3%)	0	100	100
26	1	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
27	2	43/92 (47%)	41 (95%)	1 (2%)	1 (2%)	5	19
28	3	93/188 (50%)	89 (96%)	4 (4%)	0	100	100
29	4	35/103 (34%)	35 (100%)	0	0	100	100
30	5	383/423 (90%)	368 (96%)	15 (4%)	0	100	100
31	6	316/380 (83%)	304 (96%)	12 (4%)	0	100	100
32	7	285/338 (84%)	265 (93%)	20 (7%)	0	100	100
33	8	97/206 (47%)	91 (94%)	6 (6%)	0	100	100
34	9	113/137 (82%)	106 (94%)	7 (6%)	0	100	100
35	a	78/142 (55%)	75 (96%)	3 (4%)	0	100	100
36	b	146/215 (68%)	133 (91%)	13 (9%)	0	100	100
37	c	271/332 (82%)	263 (97%)	8 (3%)	0	100	100
38	d	203/306 (66%)	193 (95%)	10 (5%)	0	100	100
39	e	211/279 (76%)	184 (87%)	27 (13%)	0	100	100
40	f	110/212 (52%)	101 (92%)	8 (7%)	1 (1%)	14	39
41	g	127/166 (76%)	119 (94%)	8 (6%)	0	100	100
42	h	96/158 (61%)	92 (96%)	4 (4%)	0	100	100
43	i	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
44	j	83/123 (68%)	83 (100%)	0	0	100	100
45	k	76/112 (68%)	70 (92%)	6 (8%)	0	100	100
46	l	21/138 (15%)	20 (95%)	1 (5%)	0	100	100
47	m	43/128 (34%)	34 (79%)	8 (19%)	1 (2%)	5	19
48	o	89/102 (87%)	86 (97%)	2 (2%)	1 (1%)	11	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	p	119/206 (58%)	113 (95%)	6 (5%)	0	100	100
50	q	126/222 (57%)	125 (99%)	1 (1%)	0	100	100
51	r	140/196 (71%)	135 (96%)	5 (4%)	0	100	100
52	s	366/439 (83%)	351 (96%)	15 (4%)	0	100	100
54	u	109/234 (47%)	103 (94%)	6 (6%)	0	100	100
55	v	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
56	w	77/156 (49%)	70 (91%)	7 (9%)	0	100	100
All	All	8042/11129 (72%)	7635 (95%)	401 (5%)	6 (0%)	49	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	S	102	ALA
27	2	52	GLU
47	m	71	PRO
48	o	15	ARG
20	V	144	VAL
40	f	179	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	
3	D	190/245 (78%)	188 (99%)	2 (1%)	65	76
4	E	259/290 (89%)	257 (99%)	2 (1%)	73	79
5	F	217/262 (83%)	216 (100%)	1 (0%)	81	82
6	H	86/228 (38%)	85 (99%)	1 (1%)	63	75
7	I	145/232 (62%)	144 (99%)	1 (1%)	76	80
8	J	113/150 (75%)	113 (100%)	0	100	100
9	K	155/156 (99%)	153 (99%)	2 (1%)	61	74
10	L	98/124 (79%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	M	245/249 (98%)	243 (99%)	2 (1%)	73	79
12	N	172/211 (82%)	171 (99%)	1 (1%)	78	81
13	O	133/150 (89%)	132 (99%)	1 (1%)	73	79
14	P	123/155 (79%)	123 (100%)	0	100	100
15	Q	199/256 (78%)	198 (100%)	1 (0%)	81	82
16	R	118/126 (94%)	118 (100%)	0	100	100
17	S	141/180 (78%)	138 (98%)	3 (2%)	47	68
18	T	146/176 (83%)	145 (99%)	1 (1%)	76	80
19	U	124/135 (92%)	123 (99%)	1 (1%)	73	79
20	V	172/191 (90%)	172 (100%)	0	100	100
21	W	89/119 (75%)	89 (100%)	0	100	100
22	X	219/229 (96%)	219 (100%)	0	100	100
23	Y	159/223 (71%)	159 (100%)	0	100	100
24	Z	111/147 (76%)	111 (100%)	0	100	100
25	0	97/164 (59%)	97 (100%)	0	100	100
26	1	49/60 (82%)	49 (100%)	0	100	100
27	2	39/72 (54%)	38 (97%)	1 (3%)	40	65
28	3	88/166 (53%)	87 (99%)	1 (1%)	65	76
29	4	36/89 (40%)	36 (100%)	0	100	100
30	5	348/368 (95%)	344 (99%)	4 (1%)	65	76
31	6	265/332 (80%)	265 (100%)	0	100	100
32	7	263/303 (87%)	261 (99%)	2 (1%)	73	79
33	8	91/190 (48%)	91 (100%)	0	100	100
34	9	99/112 (88%)	98 (99%)	1 (1%)	68	77
35	a	78/133 (59%)	78 (100%)	0	100	100
36	b	130/186 (70%)	128 (98%)	2 (2%)	57	73
37	c	241/288 (84%)	240 (100%)	1 (0%)	84	84
38	d	193/274 (70%)	192 (100%)	1 (0%)	81	82
39	e	188/236 (80%)	188 (100%)	0	100	100
40	f	101/188 (54%)	101 (100%)	0	100	100
41	g	119/148 (80%)	118 (99%)	1 (1%)	73	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	h	95/148 (64%)	95 (100%)	0	100	100
43	i	86/110 (78%)	85 (99%)	1 (1%)	63	75
44	j	68/97 (70%)	67 (98%)	1 (2%)	57	73
45	k	71/90 (79%)	70 (99%)	1 (1%)	59	73
46	l	23/116 (20%)	23 (100%)	0	100	100
47	m	40/113 (35%)	40 (100%)	0	100	100
48	o	78/87 (90%)	78 (100%)	0	100	100
49	p	117/181 (65%)	117 (100%)	0	100	100
50	q	110/178 (62%)	110 (100%)	0	100	100
51	r	133/169 (79%)	132 (99%)	1 (1%)	73	79
52	s	326/381 (86%)	324 (99%)	2 (1%)	78	81
54	u	105/200 (52%)	105 (100%)	0	100	100
55	v	59/60 (98%)	59 (100%)	0	100	100
56	w	73/136 (54%)	73 (100%)	0	100	100
All	All	7223/9609 (75%)	7184 (100%)	39 (0%)	78	82

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	220	VAL
3	D	236	VAL
4	E	218	VAL
4	E	345	ILE
5	F	125	ARG
6	H	107	VAL
7	I	47	LEU
9	K	16	ARG
9	K	125	LEU
11	M	39	ARG
11	M	57	ARG
12	N	151	VAL
13	O	89	LEU
15	Q	76	LEU
17	S	104	ARG
17	S	133	VAL
17	S	144	LEU
18	T	176	VAL

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Mol	Chain	Res	Type
19	U	6	VAL
27	2	52	GLU
28	3	168	ARG
30	5	98	LEU
30	5	140	VAL
30	5	155	LEU
30	5	218	LEU
32	7	67	VAL
32	7	167	VAL
34	9	91	LEU
36	b	11	LEU
36	b	26	LEU
37	c	202	LEU
38	d	164	VAL
41	g	68	THR
43	i	80	LEU
44	j	48	ASP
45	k	16	VAL
51	r	86	VAL
52	s	360	VAL
52	s	361	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	195	ASN
4	E	57	ASN
4	E	128	HIS
4	E	227	GLN
4	E	231	HIS
4	E	280	HIS
5	F	103	GLN
5	F	223	HIS
7	I	93	ASN
7	I	189	GLN
8	J	84	GLN
10	L	142	GLN
11	M	53	HIS
12	N	98	HIS
12	N	222	ASN
13	O	69	ASN
14	P	134	GLN

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Mol	Chain	Res	Type
17	S	118	ASN
17	S	140	ASN
18	T	62	GLN
18	T	125	GLN
18	T	210	HIS
19	U	4	ASN
19	U	35	GLN
19	U	55	ASN
19	U	73	GLN
19	U	82	HIS
19	U	101	HIS
20	V	119	GLN
21	W	72	HIS
21	W	76	HIS
22	X	237	GLN
22	X	240	GLN
23	Y	195	ASN
24	Z	67	HIS
24	Z	100	HIS
24	Z	107	ASN
25	0	144	GLN
25	0	170	GLN
30	5	102	GLN
30	5	119	GLN
30	5	150	GLN
30	5	160	HIS
30	5	165	GLN
30	5	269	ASN
30	5	289	HIS
30	5	385	HIS
31	6	200	GLN
31	6	277	GLN
31	6	354	GLN
32	7	45	ASN
32	7	232	HIS
32	7	247	ASN
32	7	284	HIS
33	8	143	GLN
36	b	24	GLN
36	b	27	GLN
36	b	102	GLN
37	c	123	GLN

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Mol	Chain	Res	Type
37	c	155	ASN
38	d	167	HIS
38	d	251	GLN
38	d	274	GLN
39	e	54	GLN
39	e	67	GLN
39	e	156	ASN
39	e	212	HIS
39	e	248	ASN
39	e	251	HIS
42	h	99	ASN
43	i	65	ASN
43	i	108	HIS
43	i	120	HIS
45	k	15	GLN
48	o	21	HIS
49	p	163	GLN
50	q	142	ASN
51	r	112	HIS
51	r	131	HIS
51	r	148	ASN
52	s	298	GLN
52	s	315	ASN
52	s	343	GLN
52	s	373	GLN
52	s	375	ASN
55	v	42	ASN
55	v	63	ASN
56	w	103	HIS
56	w	115	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1425/1559 (91%)	378 (26%)	17 (1%)
2	B	51/69 (73%)	15 (29%)	1 (1%)
All	All	1476/1628 (90%)	393 (26%)	18 (1%)

All (393) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1674	A
1	A	1676	A
1	A	1677	C
1	A	1678	C
1	A	1679	U
1	A	1681	G
1	A	1689	C
1	A	1699	C
1	A	1700	U
1	A	1704	U
1	A	1707	C
1	A	1708	A
1	A	1713	A
1	A	1714	C
1	A	1715	C
1	A	1724	A
1	A	1727	A
1	A	1728	U
1	A	1731	A
1	A	1741	A
1	A	1748	G
1	A	1750	G
1	A	1751	A
1	A	1760	G
1	A	1770	G
1	A	1773	A
1	A	1777	A
1	A	1780	U
1	A	1791	G
1	A	1794	A
1	A	1803	A
1	A	1804	A
1	A	1805	A
1	A	1812	C
1	A	1813	C
1	A	1817	C
1	A	1820	A
1	A	1821	A
1	A	1823	A
1	A	1824	U
1	A	1827	C
1	A	1828	A
1	A	1829	A

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Mol	Chain	Res	Type
1	A	1832	A
1	A	1836	A
1	A	1839	C
1	A	1844	A
1	A	1849	C
1	A	1853	A
1	A	1854	U
1	A	1856	A
1	A	1867	A
1	A	1869	A
1	A	1871	A
1	A	1872	U
1	A	1878	U
1	A	1882	A
1	A	1883	G
1	A	1887	A
1	A	1888	G
1	A	1890	C
1	A	1892	A
1	A	1893	A
1	A	1901	C
1	A	1903	C
1	A	1918	G
1	A	1927	G
1	A	1939	G
1	A	1940	A
1	A	1944	C
1	A	1946	C
1	A	1968	G
1	A	1972	A
1	A	1974	A
1	A	1985	G
1	A	1987	G
1	A	1992	C
1	A	1993	A
1	A	1994	A
1	A	1995	A
1	A	1998	U
1	A	2000	C
1	A	2001	C
1	A	2015	G
1	A	2021	U

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Mol	Chain	Res	Type
1	A	2022	G
1	A	2023	U
1	A	2029	A
1	A	2030	U
1	A	2031	A
1	A	2032	G
1	A	2036	C
1	A	2037	U
1	A	2039	A
1	A	2040	G
1	A	2053	U
1	A	2060	A
1	A	2065	A
1	A	2074	A
1	A	2079	C
1	A	2083	U
1	A	2085	A
1	A	2096	U
1	A	2097	A
1	A	2098	G
1	A	2109	A
1	A	2113	G
1	A	2124	A
1	A	2125	C
1	A	2126	U
1	A	2129	G
1	A	2131	A
1	A	2132	A
1	A	2134	A
1	A	2136	C
1	A	2141	U
1	A	2142	A
1	A	2147	G
1	A	2154	A
1	A	2157	U
1	A	2159	U
1	A	2163	A
1	A	2168	U
1	A	2171	U
1	A	2172	A
1	A	2173	G
1	A	2181	A

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Mol	Chain	Res	Type
1	A	2182	G
1	A	2183	C
1	A	2187	C
1	A	2193	U
1	A	2194	U
1	A	2195	A
1	A	2197	G
1	A	2198	A
1	A	2199	A
1	A	2200	A
1	A	2201	G
1	A	2204	U
1	A	2210	C
1	A	2211	U
1	A	2215	C
1	A	2229	A
1	A	2230	A
1	A	2233	U
1	A	2237	A
1	A	2239	A
1	A	2241	A
1	A	2242	U
1	A	2243	A
1	A	2244	U
1	A	2245	A
1	A	2246	A
1	A	2259	C
1	A	2262	C
1	A	2263	C
1	A	2264	A
1	A	2283	C
1	A	2284	C
1	A	2285	U
1	A	2290	A
1	A	2296	U
1	A	2297	A
1	A	2299	U
1	A	2300	G
1	A	2315	A
1	A	2316	U
1	A	2322	C
1	A	2324	U

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Mol	Chain	Res	Type
1	A	2332	C
1	A	2345	G
1	A	2371	U
1	A	2372	U
1	A	2374	A
1	A	2381	A
1	A	2386	C
1	A	2387	U
1	A	2390	A
1	A	2393	C
1	A	2397	C
1	A	2401	A
1	A	2404	U
1	A	2405	C
1	A	2406	A
1	A	2407	U
1	A	2414	C
1	A	2415	C
1	A	2416	U
1	A	2426	C
1	A	2427	C
1	A	2434	A
1	A	2435	G
1	A	2443	C
1	A	2444	A
1	A	2446	A
1	A	2449	G
1	A	2451	A
1	A	2454	G
1	A	2457	A
1	A	2458	A
1	A	2468	A
1	A	2478	G
1	A	2484	C
1	A	2493	C
1	A	2500	A
1	A	2502	C
1	A	2507	A
1	A	2508	C
1	A	2511	C
1	A	2512	A
1	A	2520	C

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Mol	Chain	Res	Type
1	A	2521	A
1	A	2522	U
1	A	2523	C
1	A	2524	A
1	A	2527	A
1	A	2531	U
1	A	2539	A
1	A	2540	C
1	A	2556	A
1	A	2557	C
1	A	2558	A
1	A	2559	U
1	A	2560	G
1	A	2563	U
1	A	2564	A
1	A	2570	C
1	A	2592	G
1	A	2593	G
1	A	2594	U
1	A	2601	A
1	A	2603	C
1	A	2607	U
1	A	2618	U
1	A	2623	A
1	A	2626	U
1	A	2627	G
1	A	2628	U
1	A	2629	A
1	A	2630	U
1	A	2632	A
1	A	2633	A
1	A	2634	U
1	A	2635	G
1	A	2645	G
1	A	2654	U
1	A	2655	G
1	A	2656	U
1	A	2660	U
1	A	2683	C
1	A	2684	C
1	A	2686	G
1	A	2693	A

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Mol	Chain	Res	Type
1	A	2694	A
1	A	2695	G
1	A	2696	A
1	A	2697	G
1	A	2698	G
1	A	2706	A
1	A	2708	C
1	A	2709	A
1	A	2718	C
1	A	2719	G
1	A	2722	A
1	A	2723	A
1	A	2724	G
1	A	2732	G
1	A	2739	U
1	A	2740	A
1	A	2743	U
1	A	2744	U
1	A	2748	A
1	A	2750	U
1	A	2755	A
1	A	2756	C
1	A	2804	A
1	A	2810	G
1	A	2814	G
1	A	2831	G
1	A	2832	A
1	A	2833	A
1	A	2842	C
1	A	2844	G
1	A	2847	C
1	A	2852	C
1	A	2854	U
1	A	2859	A
1	A	2861	A
1	A	2864	U
1	A	2865	C
1	A	2871	U
1	A	2880	A
1	A	2895	U
1	A	2896	G
1	A	2899	C

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Mol	Chain	Res	Type
1	A	2901	A
1	A	2902	A
1	A	2906	C
1	A	2910	A
1	A	2912	C
1	A	2913	A
1	A	2915	C
1	A	2917	G
1	A	2918	A
1	A	2919	A
1	A	2922	A
1	A	2926	A
1	A	2928	C
1	A	2932	G
1	A	2935	A
1	A	2952	U
1	A	2954	C
1	A	2955	U
1	A	2956	A
1	A	2962	C
1	A	2963	A
1	A	2971	A
1	A	2989	G
1	A	2990	A
1	A	2991	U
1	A	2992	G
1	A	2993	U
1	A	3000	A
1	A	3005	A
1	A	3007	C
1	A	3012	U
1	A	3016	G
1	A	3022	G
1	A	3030	A
1	A	3041	U
1	A	3042	U
1	A	3043	C
1	A	3051	A
1	A	3053	A
1	A	3054	G
1	A	3056	C
1	A	3060	C

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Mol	Chain	Res	Type
1	A	3063	G
1	A	3065	U
1	A	3067	U
1	A	3069	A
1	A	3070	G
1	A	3072	U
1	A	3073	C
1	A	3077	C
1	A	3086	U
1	A	3093	C
1	A	3098	U
1	A	3100	U
1	A	3102	U
1	A	3114	U
1	A	3122	U
1	A	3123	G
1	A	3131	G
1	A	3141	A
1	A	3150	U
1	A	3152	C
1	A	3155	C
1	A	3157	C
1	A	3158	A
1	A	3160	A
1	A	3162	C
1	A	3168	C
1	A	3169	C
1	A	3170	C
1	A	3172	C
1	A	3176	A
1	A	3180	A
1	A	3184	C
1	A	3188	U
1	A	3189	C
1	A	3190	A
1	A	3202	U
1	A	3206	C
1	A	3207	A
1	A	3217	A
1	A	3218	A
1	A	3228	U
2	B	1607	U

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Mol	Chain	Res	Type
2	B	1608	G
2	B	1611	G
2	B	1614	U
2	B	1615	A
2	B	1625	A
2	B	1631	C
2	B	1632	U
2	B	1634	A
2	B	1641	G
2	B	1644	G
2	B	1645	A
2	B	1649	C
2	B	1651	A
2	B	1669	G

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1703	C
1	A	1713	A
1	A	1811	A
1	A	1823	A
1	A	1871	A
1	A	2030	U
1	A	2186	C
1	A	2243	A
1	A	2245	A
1	A	2457	A
1	A	2507	A
1	A	2530	A
1	A	2559	U
1	A	2653	C
1	A	2905	A
1	A	3041	U
1	A	3092	U
2	B	1607	U

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 96 ligands modelled in this entry, 95 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	$\# Z > 2$
59	PNS	v	101	-	14,20,21	2.12	4 (28%)	18,26,29	1.32	2 (11%)

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
59	PNS	v	101	-	-	12/24/26/27	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	v	101	PNS	C39-N41	5.02	1.45	1.33
59	v	101	PNS	C34-N36	4.81	1.44	1.33
59	v	101	PNS	O40-C39	-2.32	1.18	1.23
59	v	101	PNS	O35-C34	-2.30	1.19	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	v	101	PNS	C38-C37-N36	-2.26	107.20	112.00
59	v	101	PNS	C37-C38-C39	-2.09	108.92	112.39

There are no chirality outliers.

All (12) torsion outliers are listed below:

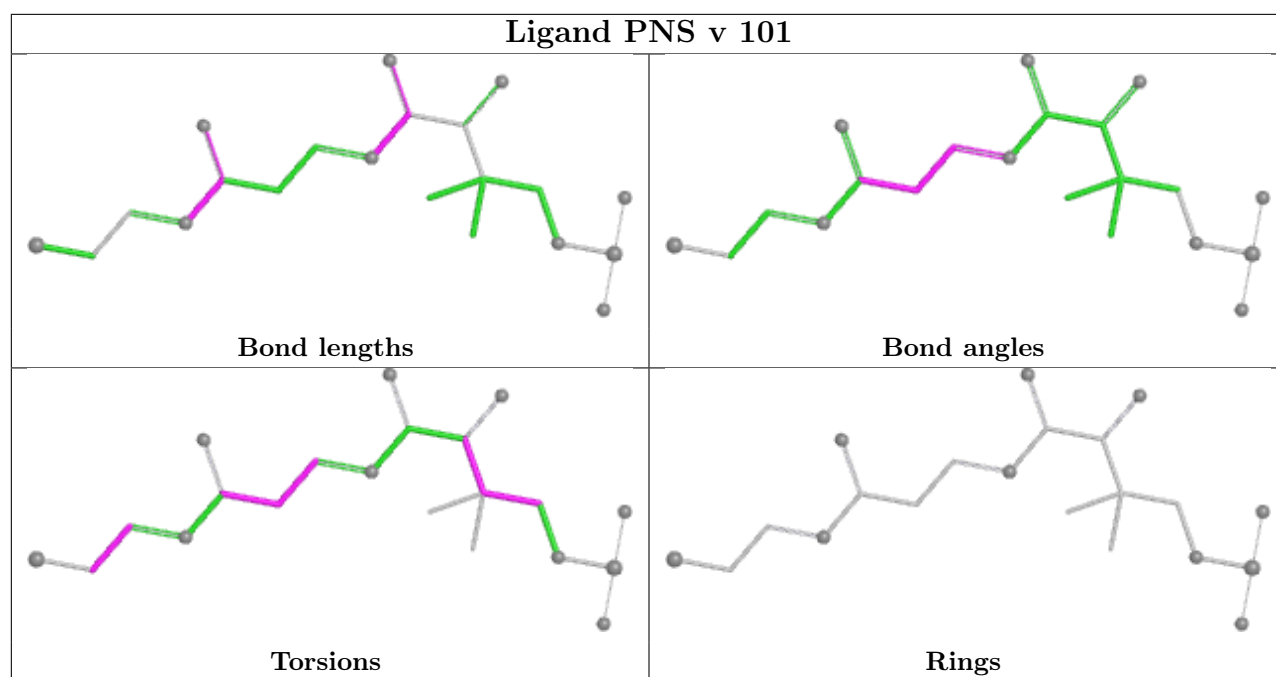
Mol	Chain	Res	Type	Atoms
59	v	101	PNS	O27-C28-C29-C30
59	v	101	PNS	O27-C28-C29-C31
59	v	101	PNS	C28-C29-C32-O33
59	v	101	PNS	C28-C29-C32-C34
59	v	101	PNS	C31-C29-C32-O33
59	v	101	PNS	C31-C29-C32-C34
59	v	101	PNS	N36-C37-C38-C39
59	v	101	PNS	N41-C42-C43-S44
59	v	101	PNS	C30-C29-C32-O33
59	v	101	PNS	C30-C29-C32-C34
59	v	101	PNS	C37-C38-C39-O40
59	v	101	PNS	C37-C38-C39-N41

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	v	101	PNS	2	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.

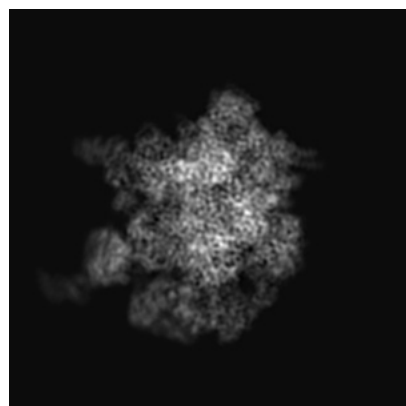
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3842. These allow visual inspection of the internal detail of the map and identification of artifacts.

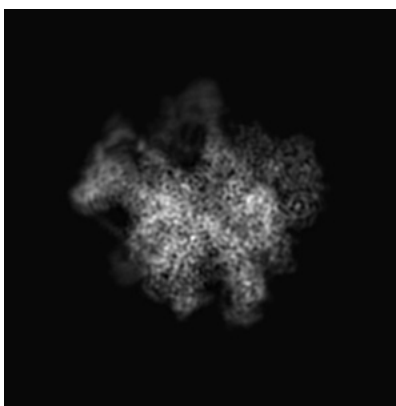
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

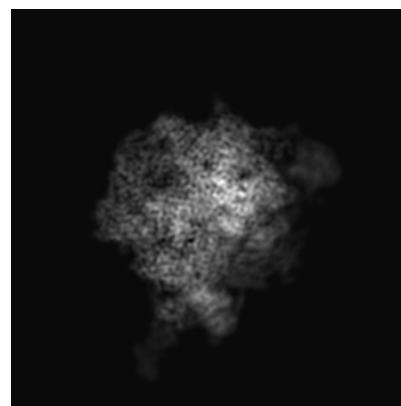
6.1.1 Primary map



X

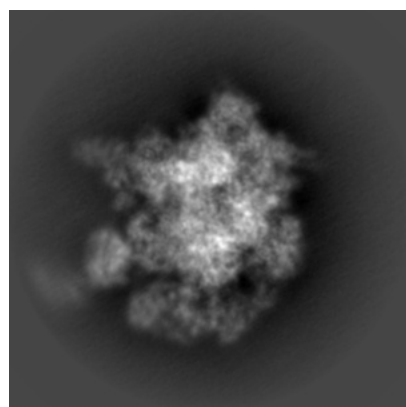


Y

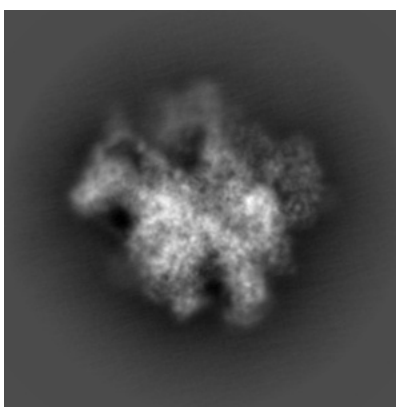


Z

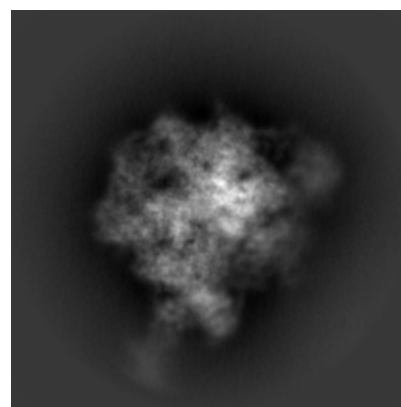
6.1.2 Raw map



X



Y

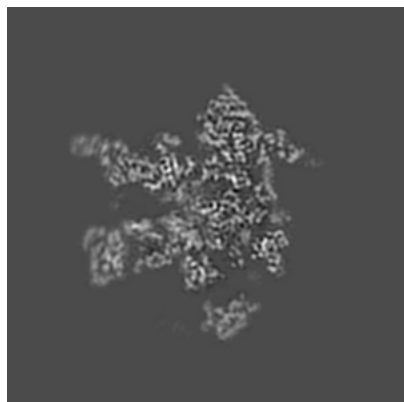


Z

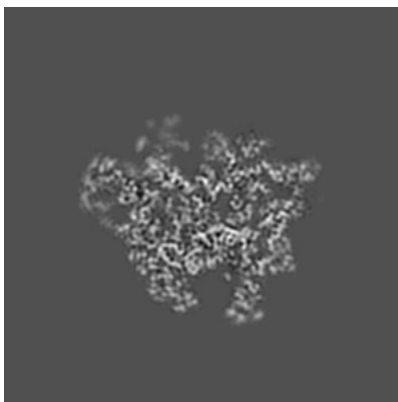
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

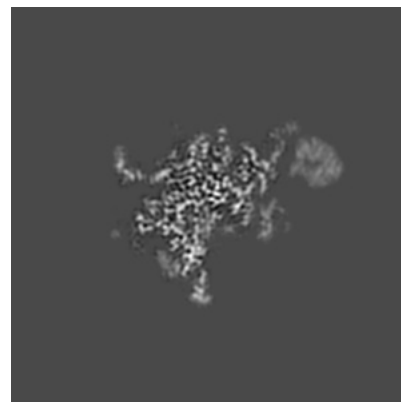
6.2.1 Primary map



X Index: 176

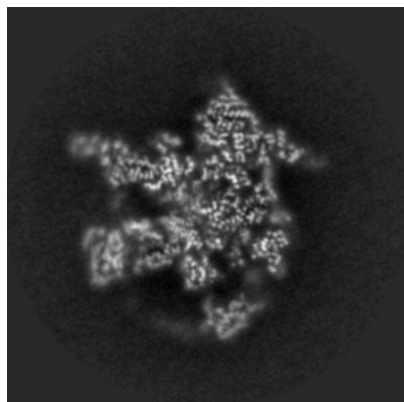


Y Index: 176

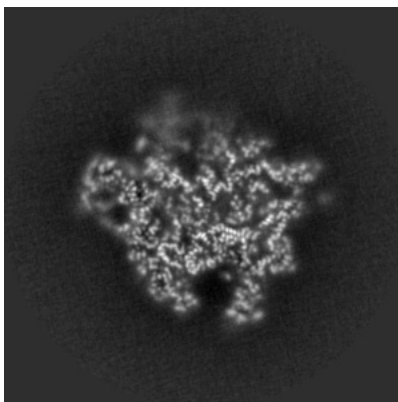


Z Index: 176

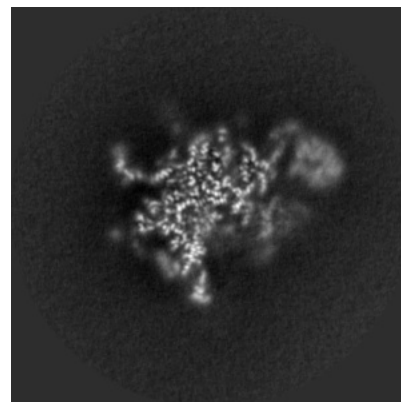
6.2.2 Raw map



X Index: 176



Y Index: 176

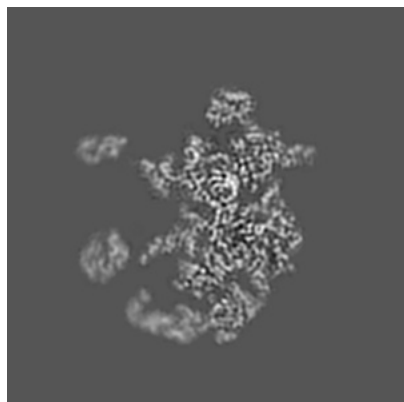


Z Index: 176

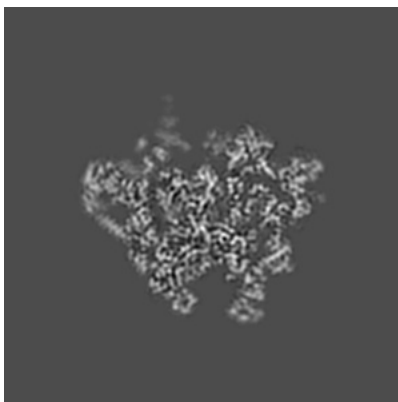
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

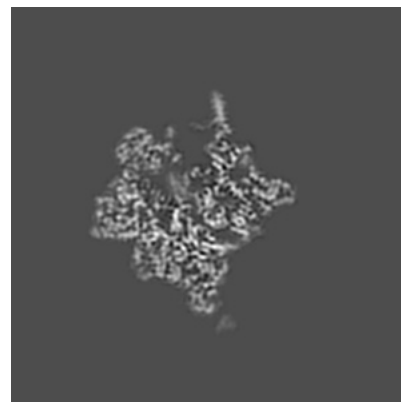
6.3.1 Primary map



X Index: 188

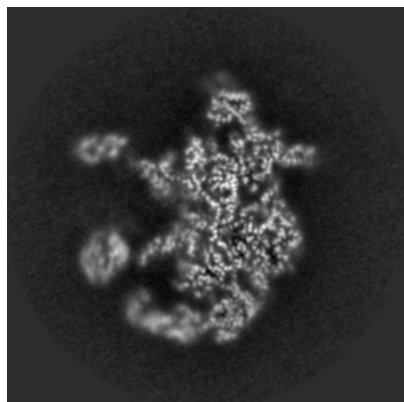


Y Index: 179

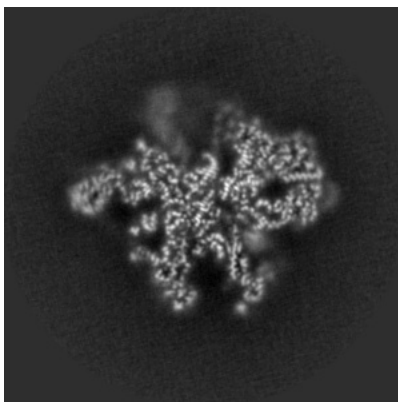


Z Index: 214

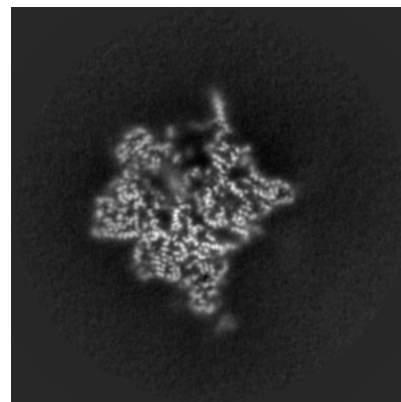
6.3.2 Raw map



X Index: 187



Y Index: 189

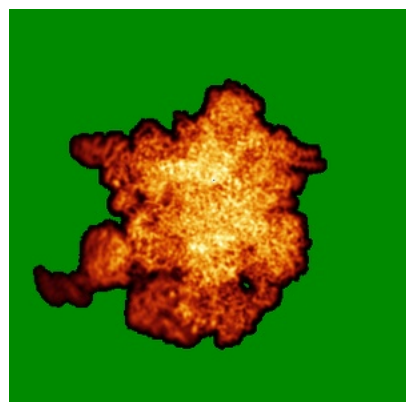


Z Index: 214

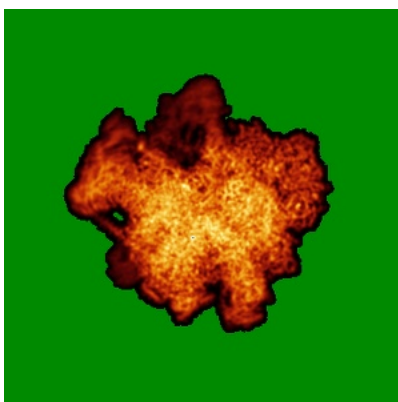
The images above show the largest variance slices of the map in three orthogonal directions.

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

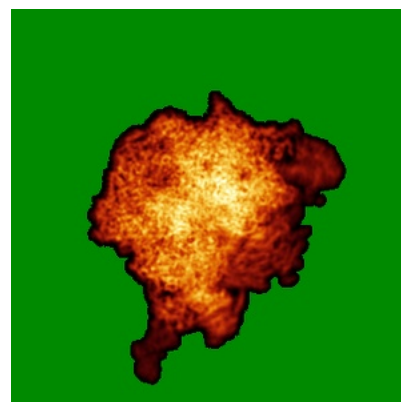
6.4.1 Primary map



X

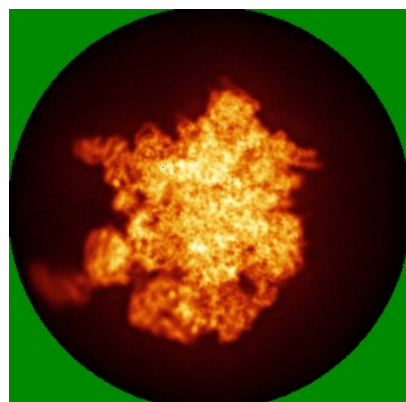


Y

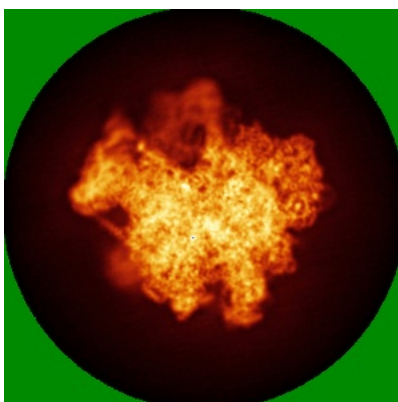


Z

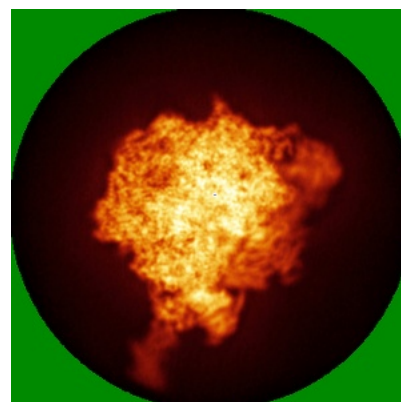
6.4.2 Raw map



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 0.0853. 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.

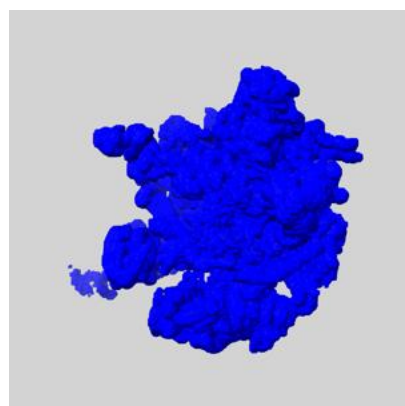
6.6 Mask visualisation [i](#)

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

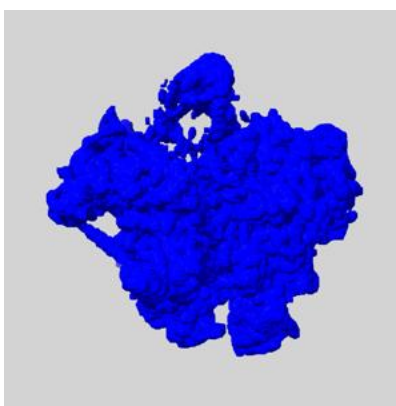
A mask typically either:

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

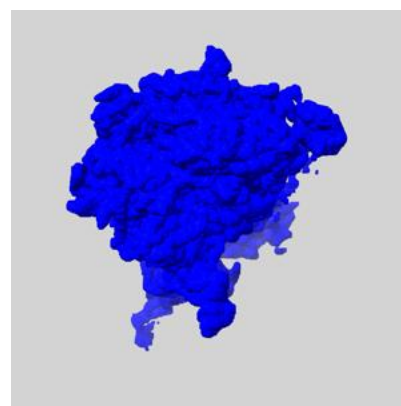
6.6.1 emd_3842_msk_1.map [i](#)



X



Y

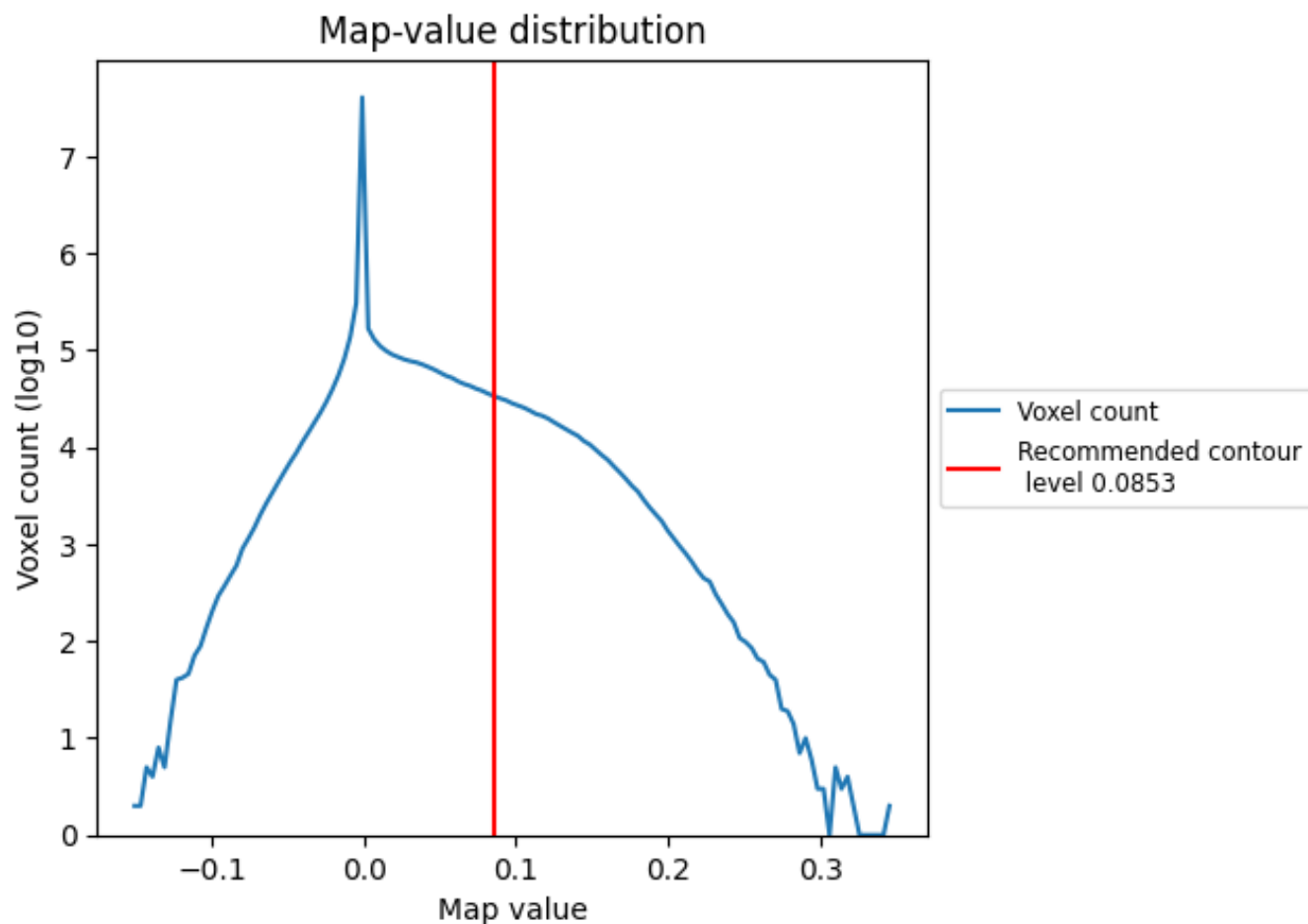


Z

7 Map analysis [i](#)

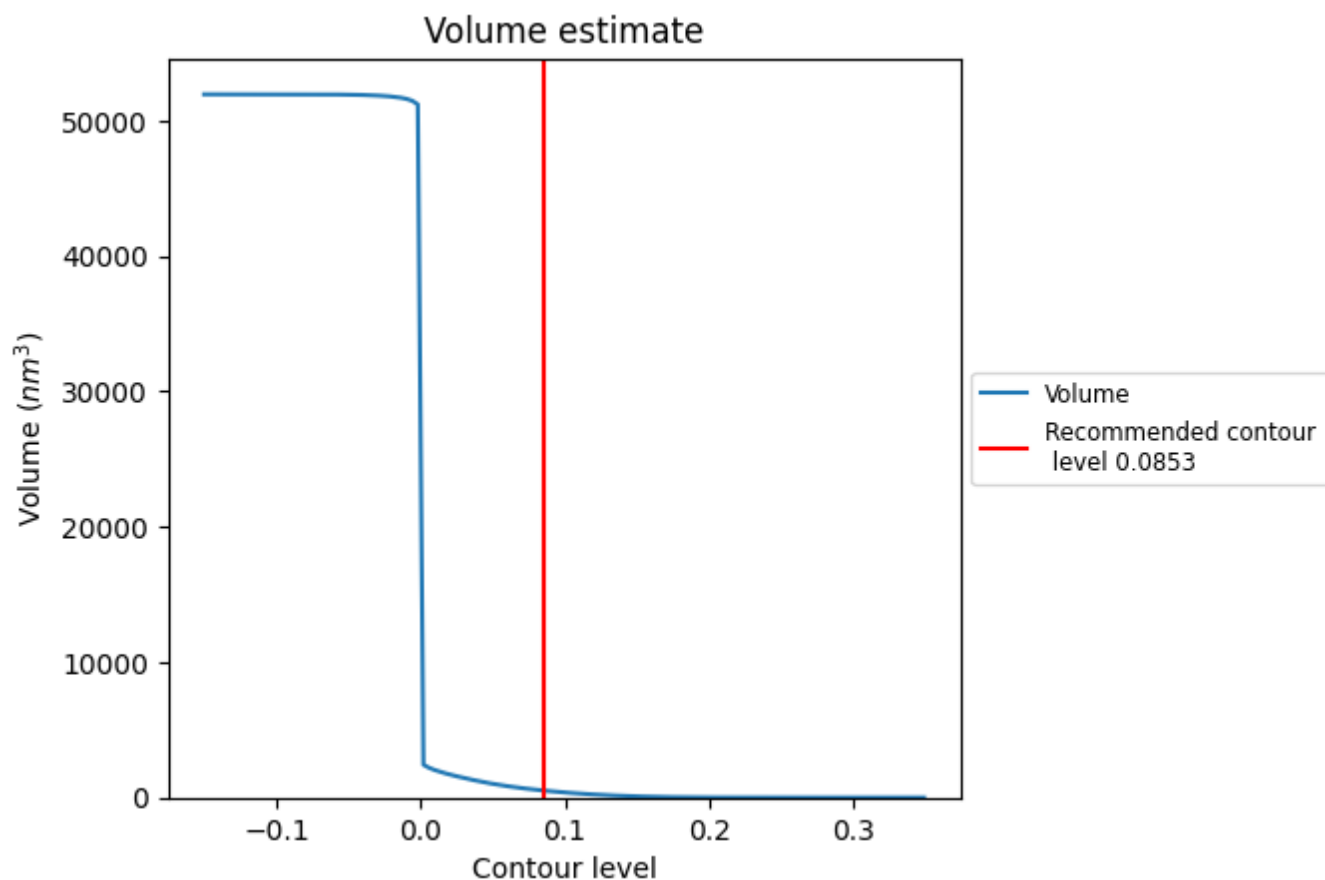
This section contains the results of statistical analysis of the map.

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.

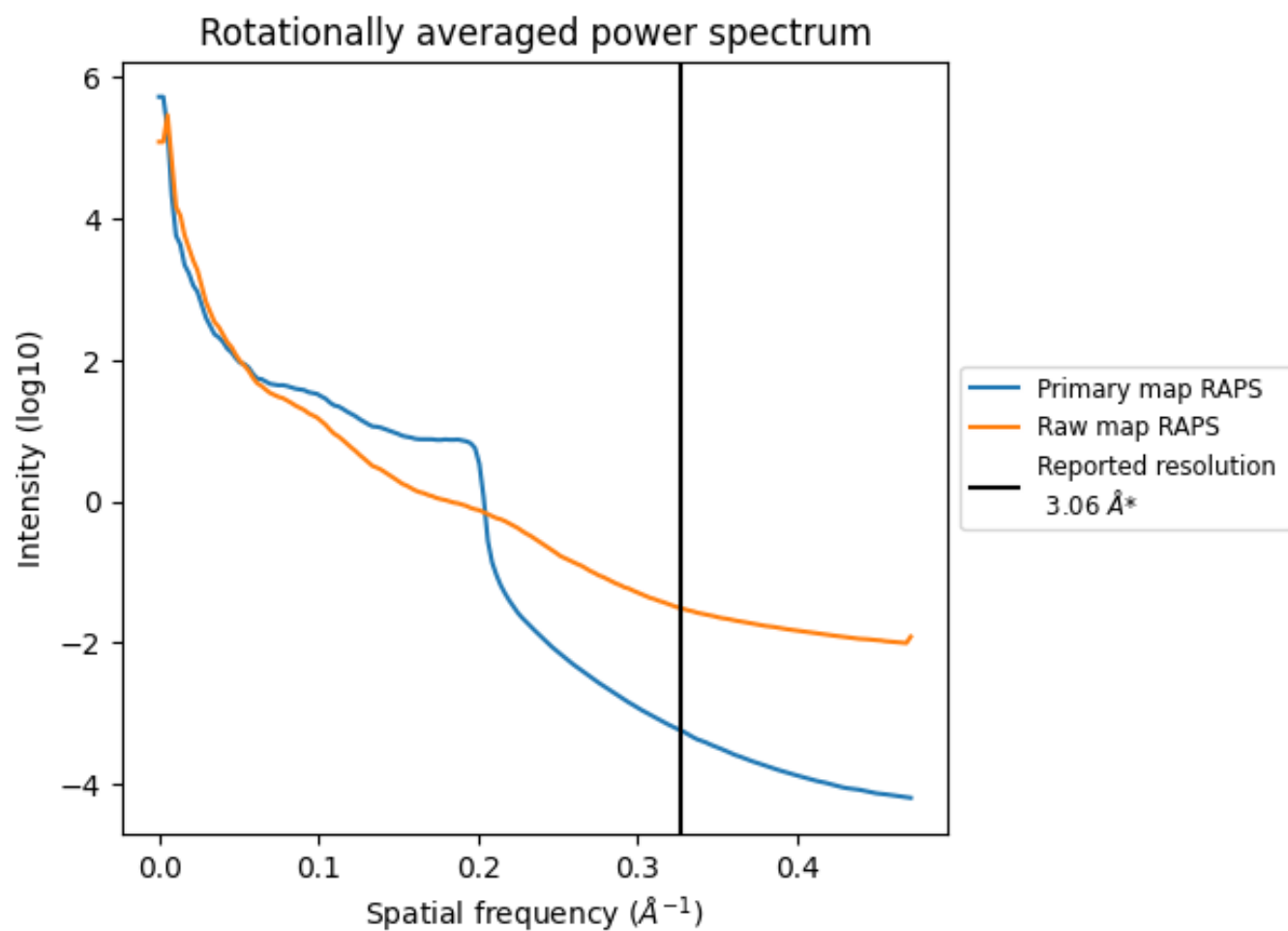
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 517 nm³; this corresponds to an approximate mass of 467 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 ⓘ

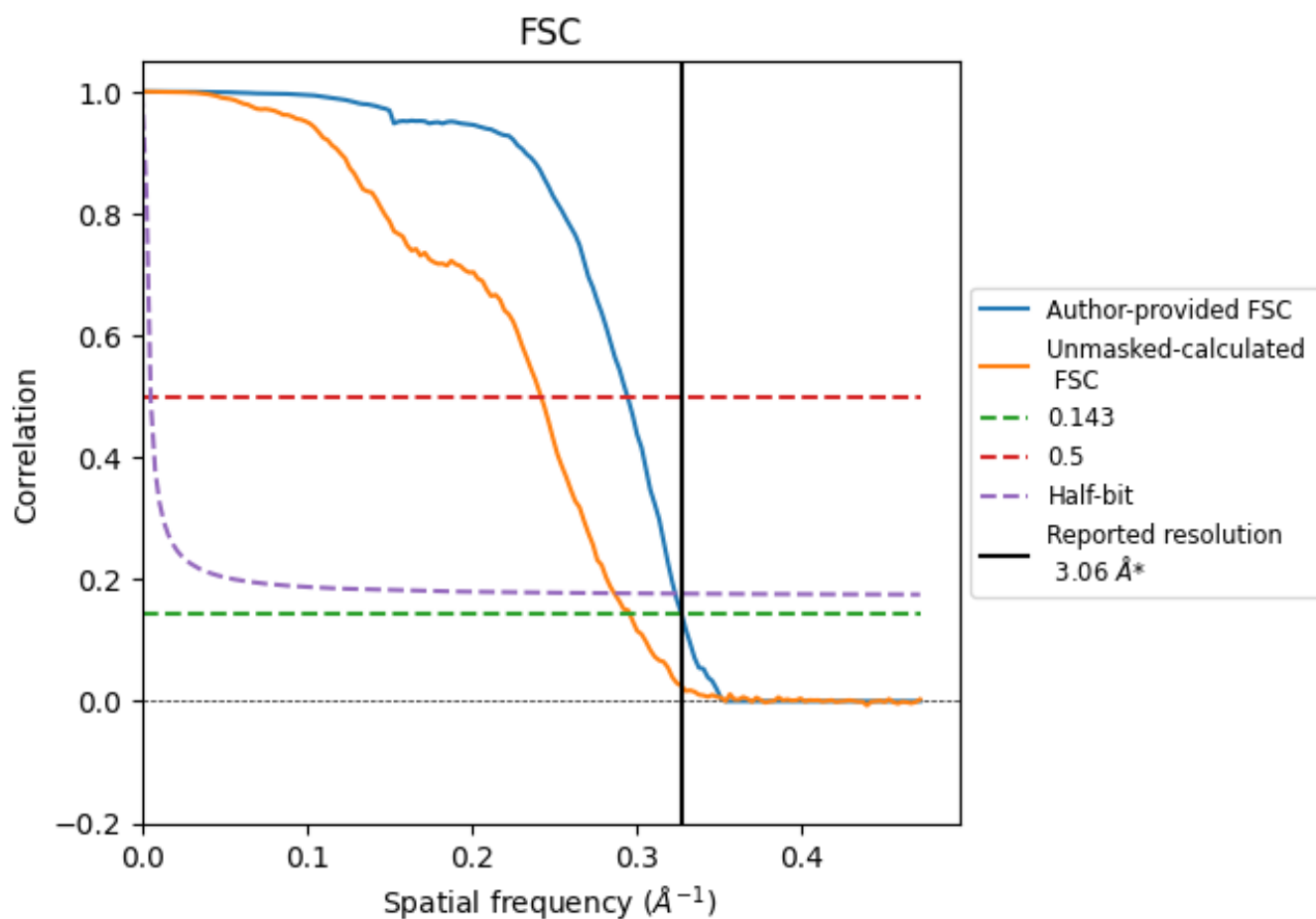


*Reported resolution corresponds to spatial frequency of $0.327 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.327 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

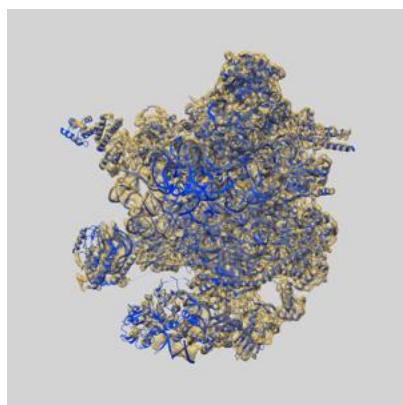
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.06	3.40	3.09
Unmasked-calculated*	3.38	4.13	3.49

*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 3.38 differs from the reported value 3.06 by more than 10 %

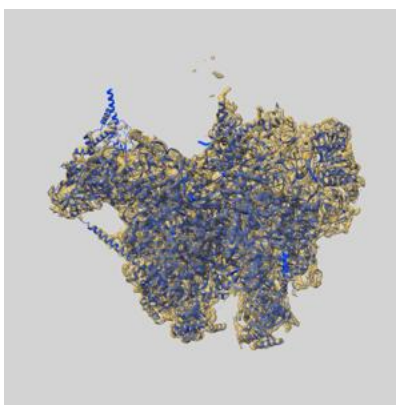
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3842 and PDB model 5OOL. Per-residue inclusion information can be found in section 3 on page 16.

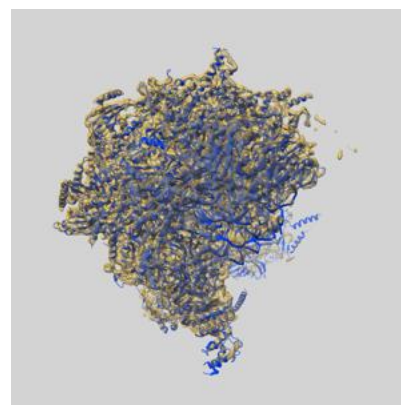
9.1 Map-model overlay [i](#)



X



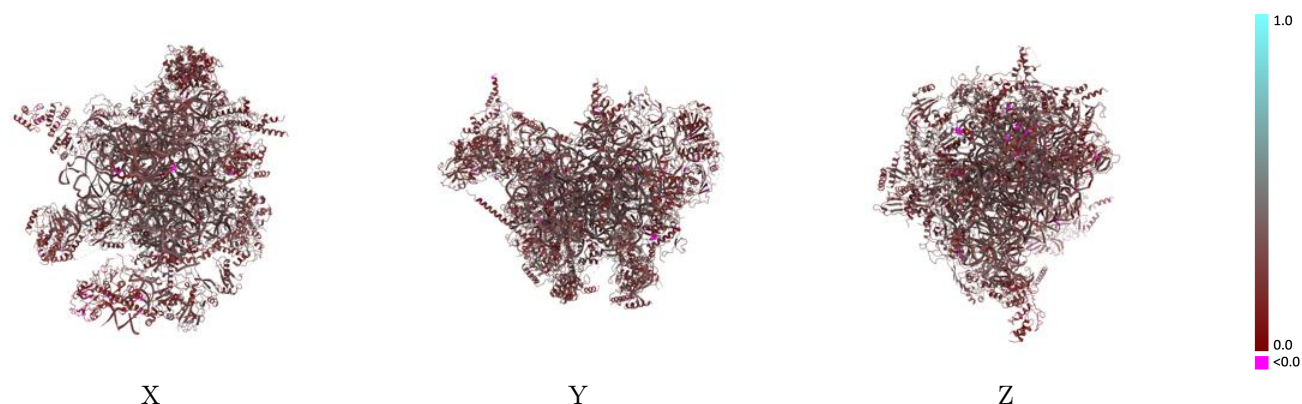
Y



Z

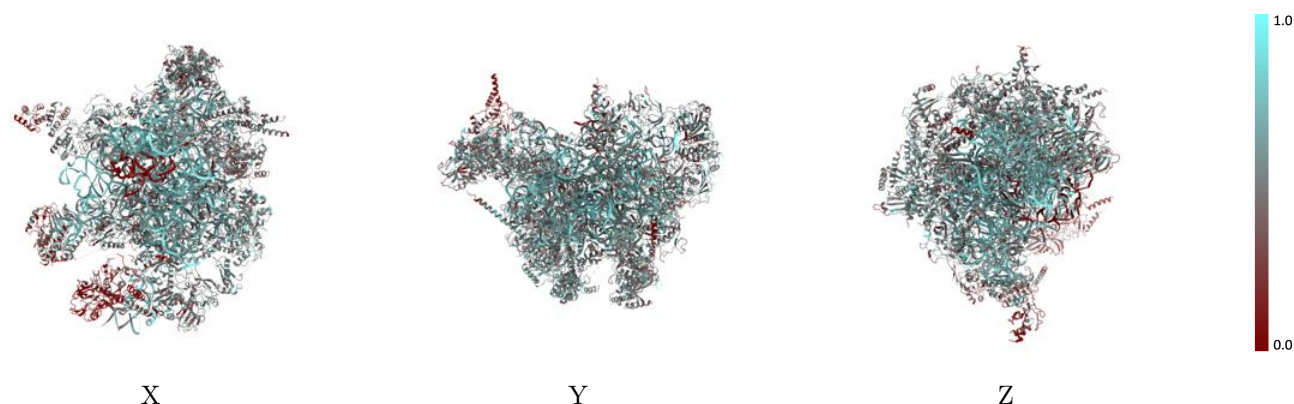
The images above show the 3D surface view of the map at the recommended contour level 0.0853 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



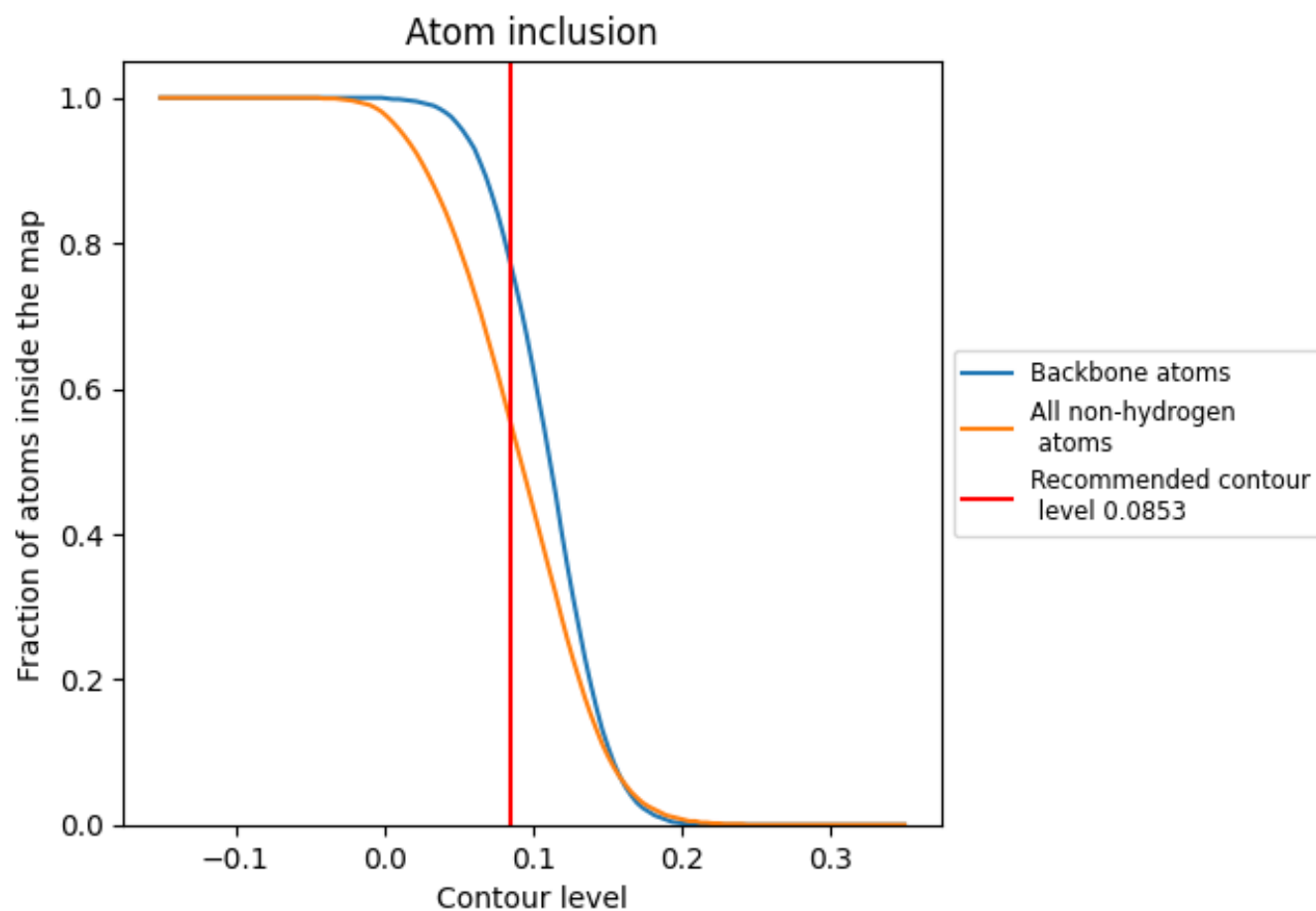
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0853).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 55% 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 (0.0853) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5490	 0.2930
0	 0.4980	 0.2790
1	 0.5050	 0.2890
2	 0.5210	 0.2830
3	 0.4840	 0.2980
4	 0.5190	 0.2620
5	 0.5030	 0.2590
6	 0.4980	 0.2950
7	 0.5120	 0.2840
8	 0.1850	 0.1970
9	 0.4860	 0.2820
A	 0.7090	 0.3340
B	 0.6520	 0.2880
D	 0.4700	 0.2720
E	 0.5200	 0.3030
F	 0.5400	 0.3000
H	 0.4370	 0.2750
I	 0.3280	 0.2460
J	 0.1890	 0.2150
K	 0.5360	 0.2930
L	 0.4770	 0.2860
M	 0.5230	 0.2900
N	 0.4460	 0.2830
O	 0.5210	 0.2840
P	 0.5020	 0.2790
Q	 0.5060	 0.2850
R	 0.4840	 0.2690
S	 0.5420	 0.3150
T	 0.5010	 0.2900
U	 0.5020	 0.2800
V	 0.4830	 0.2940
W	 0.4800	 0.2800
X	 0.4930	 0.2710
Y	 0.5200	 0.2600
Z	 0.5220	 0.3030



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	 0.5250	 0.3100
b	 0.5550	 0.3060
c	 0.5390	 0.2880
d	 0.4280	 0.2770
e	 0.1030	 0.1660
f	 0.2300	 0.2170
g	 0.5820	 0.3180
h	 0.5080	 0.2870
i	 0.5090	 0.2790
j	 0.5630	 0.2900
k	 0.3930	 0.2390
l	 0.5150	 0.2170
m	 0.0790	 0.2160
o	 0.5220	 0.2920
p	 0.4740	 0.2840
q	 0.5220	 0.2720
r	 0.5400	 0.3120
s	 0.5250	 0.2630
t	 0.3000	 0.2630
u	 0.4960	 0.2590
v	 0.4030	 0.2170
w	 0.1220	 0.1620