Full wwPDB EM Validation Report (i)

Aug 23, 2026 – 10:09 am BST

PDB ID	:	7ODR / pdb_00007odr
EMDB ID	:	EMD-12845
Title	:	State A of the human mitoribosomal large subunit assembly intermediate
Authors	:	Lenarcic, T.; Jaskolowski, M.; Leibundgut, M.; Scaiola, A.; Schoenhut, T.; Saurer, M.; Lee, R.G.; Rackham, O.; Filipovska, A.; Ban, N.
Deposited on	:	2021-04-30
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

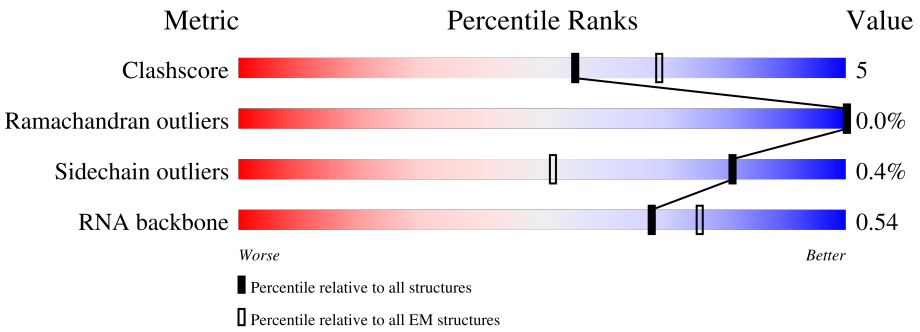
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

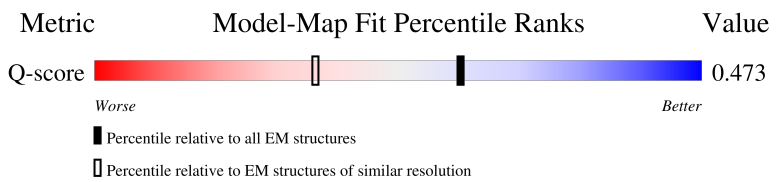
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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 <=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	u	234	6% 38% 9% 53%
2	v	70	74% 76% 23% •
3	w	156	50% 42% 9% 49%

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Mol	Chain	Length	Quality of chain
4	x	384	69% 19% 12%
5	y	381	50% 14% 36%
6	0	188	53% 5% 41%
7	1	65	74% 9% 15%
8	2	92	48% 50%
9	3	188	44% 6% 49%
10	4	103	31% 6% 63%
11	5	423	82% 11% 7%
12	6	380	74% 19% 7%
13	7	338	7% 70% 17% 13%
14	8	206	26% 43% 7% 50%
15	9	137	80% 10% 9%
16	A	1590	61% 26% 9%
17	B	72	10% 62% 32% 6%
18	D	305	64% 14% 21%
19	E	348	76% 11% 12%
20	F	311	63% 18% 19%
21	H	267	30% 7% 64%
22	I	261	19% 53% 10% 38%
23	J	192	68% 86% 5% 9%
24	K	178	87% 12%
25	L	145	64% 15% 21%
26	M	296	88% 10%
27	N	251	75% 9% 16%
28	O	175	74% 14% 12%

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Mol	Chain	Length	Quality of chain
29	P	180	64% 16% 20%
30	Q	292	62% 13% 24%
31	R	149	85% 9% 6%
32	S	205	69% 9% 21%
33	T	206	70% 10% 19%
34	U	153	16% 85% 14%
35	V	216	23% 81% 13% 5%
36	W	148	65% 7% 28%
37	X	256	87% 9% 5%
38	Y	250	64% 8% 28%
39	Z	161	69% 7% 24%
40	a	142	8% 61% 9% 30%
41	b	215	57% 12% 31%
42	c	332	77% 9% 14%
43	d	306	29% 75% 9% 15%
44	e	279	56% 62% 20% 18%
45	f	212	28% 60% 10% 29%
46	g	166	68% 13% 19%
47	h	158	13% 64% 6% 30%
48	i	128	64% 12% 24%
49	j	123	64% 12% 24%
50	k	112	28% 76% 14% 10%
51	l	138	38% 49% 10% 41%
52	m	128	32% 29% 10% 60%
53	o	102	76% 16% 8%

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Mol	Chain	Length	Quality of chain
54	p	206	11% 65% 6% 29%
55	q	222	5% 59% 5% 36%
56	r	196	5% 70% 12% 17%
57	s	439	75% 13% 12%

2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 107464 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	u	110	919	591	154	164	10	0	0

- Molecule 2 is a protein called MIEF1 upstream open reading frame protein.

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

- Molecule 3 is a protein called Acyl carrier protein, mitochondrial.

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

- Molecule 4 is a protein called 5-methylcytosine rRNA methyltransferase NSUN4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	x	336	2660	1694	465	484	17	0	0

- Molecule 5 is a protein called Transcription termination factor 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	y	244	1980	1264	342	362	12	0	0

- Molecule 6 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	0	110	898	554	176	162	6	0	0

- Molecule 7 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	1	55	455	290	87	76	2	0	0

- Molecule 8 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	2	46	377	233	83	60	1	0	0

- Molecule 9 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	3	95	832	539	162	128	3	0	0

- Molecule 10 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	4	38	342	217	72	49	4	0	0

- Molecule 11 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	5	394	3210	2073	560	566	11	0	0

- Molecule 12 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	6	354	2948	1881	525	533	9	0	0

- Molecule 13 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	7	294	2390	1529	405	438	18	0	0

- Molecule 14 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	8	102	860	543	152	163	2	0	0

- Molecule 15 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	9	124	997	644	170	181	2	0	0

- Molecule 16 is a RNA chain called 16S mitochondrial rRNA, DNA (31-MER),16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	A	1448	30460	13658	5442	9912	1448	0	0

- Molecule 17 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	B	72	1522	683	269	498	72	0	0

- Molecule 18 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	D	240	1872	1165	378	320	9	0	0

- Molecule 19 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	E	305	2406	1545	418	432	11	0	0

- Molecule 20 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	F	252	2031	1305	370	350	6	0	0

- Molecule 21 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	H	97	802	508	155	139	0	0

- Molecule 22 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	I	163	1324	854	240	220	10	0	0

- Molecule 23 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	J	175	1330	847	237	244	2	0	0

- Molecule 24 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	K	177	1455	936	259	253	7	0	0

- Molecule 25 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	L	115	890	559	171	155	5	0	0

- Molecule 26 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	M	291	2327	1483	430	408	6	0	0

- Molecule 27 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	N	212	1723	1107	310	297	9	0	0

- Molecule 28 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	O	154	1259	792	241	219	7	0	0

- Molecule 29 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	P	144	1173	733	224	211	5	0	0

- Molecule 30 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Q	221	1843	1179	327	328	9	0	0

- Molecule 31 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	R	140	1154	732	231	187	4	0	0

- Molecule 32 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	S	161	1293	835	227	227	4	0	0

- Molecule 33 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	T	166	1369	875	254	233	7	0	0

- Molecule 34 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	U	152	1251	788	234	226	3	0	0

- Molecule 35 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	V	205	1676	1068	298	302	8	0	0

- Molecule 36 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	W	106	835	536	157	139	3	0	0

- Molecule 37 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	X	244	2044	1322	352	365	5	0	0

- Molecule 38 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Y	181	1556	995	298	259	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Z	122	996	636	186	171	3	0	0

- Molecule 40 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	a	100	840	529	152	154	5	0	0

- Molecule 41 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	b	149	1189	739	230	217	3	0	0

- Molecule 42 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	c	286	2299	1470	397	423	9	0	0

- Molecule 43 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	d	259	2124	1357	369	384	14	0	0

- Molecule 44 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	e	228	1848	1174	326	342	6	0	0

- Molecule 45 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	f	150	1196	764	197	231	4	0	0

- Molecule 46 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	g	134	1113	719	193	199	2	0	0

- Molecule 47 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	h	110	895	568	156	168	3	0	0

- Molecule 48 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	i	97	828	532	165	127	4	0	0

- Molecule 49 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	j	94	745	463	144	136	2	0	0

- Molecule 50 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	k	101	774	479	148	142	5	0	0

- Molecule 51 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	l	82	688	437	120	128	3	0	0

- Molecule 52 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	m	51	419	262	82	73	2	0	0

- Molecule 53 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	o	94	798	501	165	129	3	0	0

- Molecule 54 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	p	147	1205	748	228	225	4	0	0

- Molecule 55 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	q	141	1177	732	229	211	5	0	0

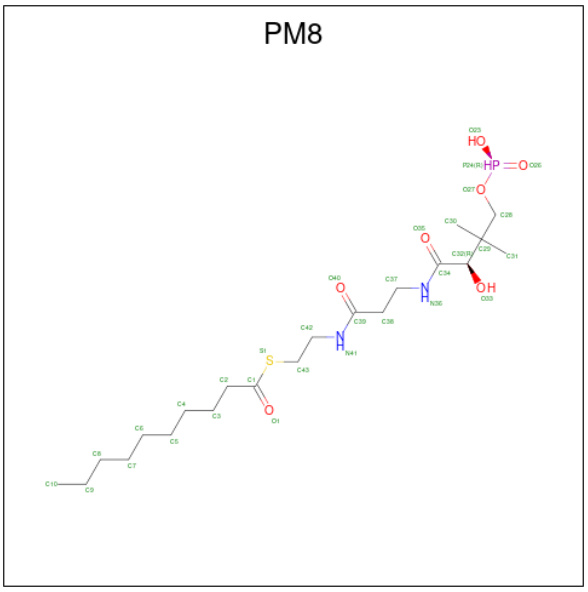
- Molecule 56 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	r	162	1322	839	252	223	8	0	0

- Molecule 57 is a protein called 39S ribosomal protein S30, mitochondrial.

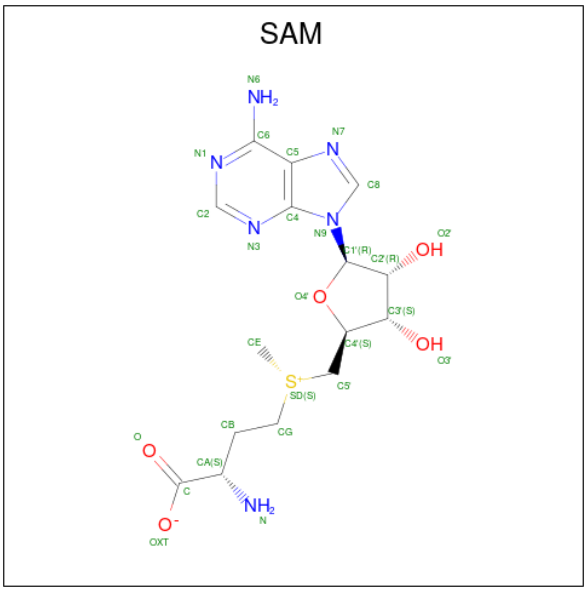
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	s	386	3155	2023	559	559	14	0	0

- Molecule 58 is S-(2-{[N-(2-HYDROXY-4-{[HYDROXY(OXIDO)PHOSPHINO]OXY}-3,3-DIMETHYLBUTANOYL)-BETA-ALANYL]AMINO}ETHYL) DECANETHIOATE (CCD ID: PM8) (formula: $C_{21}H_{41}N_2O_7PS$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
58	w	1	32	21	2	7	1	1	0

- Molecule 59 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
59	x	1	27	15	6	5	1	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
60	0	1	1	1	0
60	4	1	1	1	0

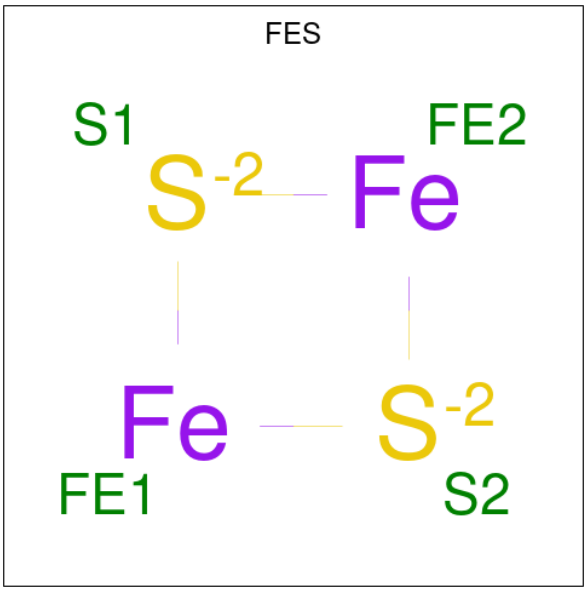
- Molecule 61 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
61	9	1	1	1	0
61	A	92	92	92	0
61	D	1	1	1	0
61	M	1	1	1	0
61	O	1	1	1	0
61	g	1	1	1	0

- Molecule 62 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
62	A	2	2	2	0

- Molecule 63 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



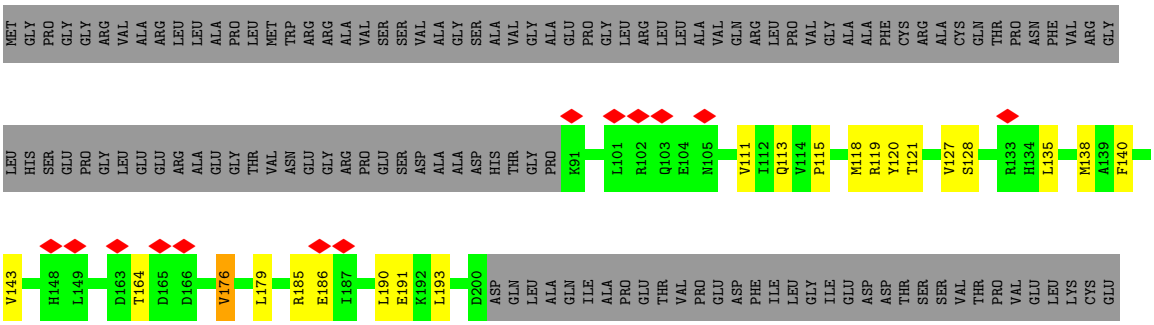
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
63	r	1	4	2	2	0

3 Residue-property plots (i)

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

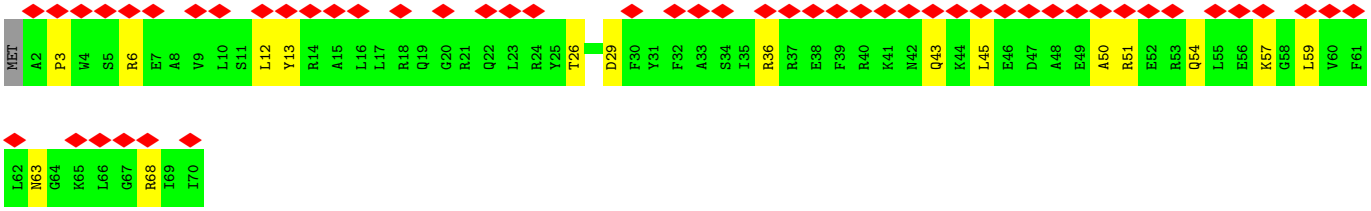
- Molecule 1: Mitochondrial assembly of ribosomal large subunit protein 1

Chain u:



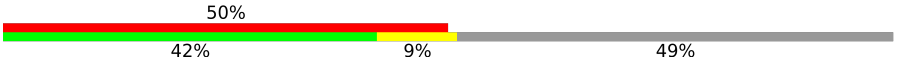
- Molecule 2: MIEF1 upstream open reading frame protein

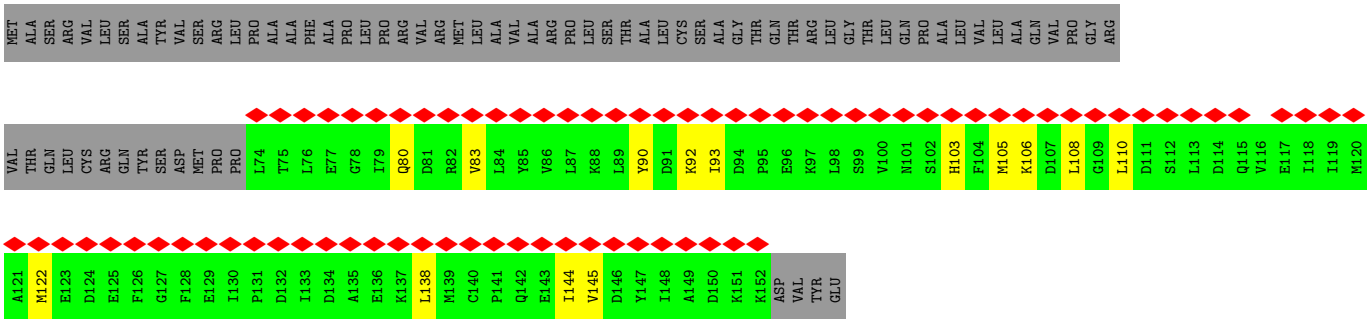
Chain v:



- Molecule 3: Acyl carrier protein, mitochondrial

Chain w:





• Molecule 4: 5-methylcytosine rRNA methyltransferase NSUN4

Chain x: 69% 19% 12%

MET ALA ALA LEU THR LEU ARG GLY VAL ARG GLU LEU LEU LYS ARG VAL ASP LEU ALA THR VAL PRO ARG ARG HIS ARG TYR LYS LYS LYS TRP ALA ALA THR GLU P36 R42 L45 Q46 D58 P61 R64 V65 S66 S69 E70 Q71 K72 A82 H85 V86

H105 W106 E107 S110 GLU GLU GLY GLN SER ALA ALA PRO SER PRO ALA SER W123 L129 D135 R136 R141 E154 Y155 L163 G170 L171 I176 V177 L180 G186 K187 L191 L192 L200 I210 V221 P222 E223 E224 D227 Q230 Y249 D250

R251 V252 L253 V254 C258 R262 N270 N271 I272 F273 K274 R275 S276 R277 Q282 I283 L284 Q288 L296 T299 V305 L312 Q316 E326 L327 L328 S333 I334 D340 L341 T342 R345 R346 V347 D350 F354 F355 S356 S357 V360 L363

L368 N371 R382 L383 THR

• Molecule 5: Transcription termination factor 4, mitochondrial

Chain y: 50% 14% 36%

MET ALA ALA ALA PHE GLY ARG GLN VAL LEU ASP TRP HIS ARG LEU ILE PRO LEU THR TRP ALA CYS MET ALA ARG GLN THR PRO HIS LEU GLU GLY GLU GLN ARG ARG THR THR ALA SER LEU LEU ARG LYS LEU THR THR ALA SER ASN GLY GLY VAL ILE GLU GLU LEU SER CYS VAL ARG SER

ASN ASN TYR VAL GLN GLU PRO GLU CYS ARG ARG ASN LEU VAL GLN CYS LEU LEU GLU LYS GLN GLY THR PRO VAL VAL GLN G88 S89 L90 S98 L99 L100 D101 M102 G103 F104 I109 L112 R116 R117 G118 Q122 Q123 L124 I127 I128 S129 E130 F131 I132 G135

E139 P140 L145 L152 M157 Q158 M159 R160 K161 R162 E173 R178 Y181 I186 M189 T197 Q211 K214 I215 L223 Q235 Y236 A237 R240 I243 V249 E252 Y253 L254 Q255 Y256 H265 L290 R295 E300 F301 L302 A303 R304

T305 A306 C307 V310 E311 E312 F313 Q314 R322 E326 S327 E328 S329 S330 T331 SER ASP ASP LYS ARG ALA ALA SER LEU ASP GLU ASP GLU ASP ASP ASP ASP GLU GLU ASP ASN ASP GLU ASP ASP ASN ASP GLU ASP ASP ASP ASP GLU ALA GLU ASP ASN ASP GLU

ASP GLU ASP ASP ASP GLU GLU GLU

• Molecule 6: 39S ribosomal protein L32, mitochondrial

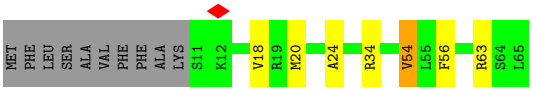
Chain 0: 53% 5% 41%

MET ALA LEU ALA MET LEU VAL LEU VAL VAL SER PRO TRP SER ALA ALA ARG GLY VAL LEU ARG ASN TYR TRP GLU ARG LEU LEU ARG LYS LEU PRO GLN SER ARG PRO GLY PHE PRO SER PRO PRO TRP GLY PRO ALA LEU ALA VAL GLN GLY PRO ALA MET PHE THR GLU PRO ALA ASN

ASP THR SER GLY SER LYS GLU ASN SER SER LEU LEU ASP SER ILE PHE TRP MET A79 K82 N83 R84 N96 P97 Q98 R138 R139 S166 E167 Q168 D169 R179 P182 Q187 N188

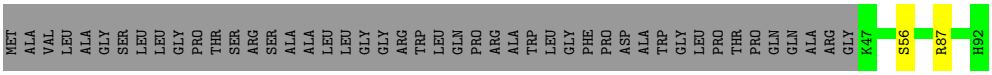
• Molecule 7: 39S ribosomal protein L33, mitochondrial

Chain 1: 74% 9% • 15%



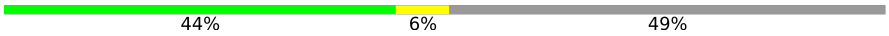
• Molecule 8: 39S ribosomal protein L34, mitochondrial

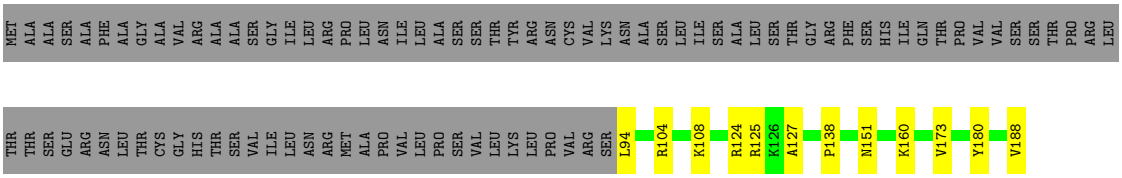
Chain 2:



• Molecule 9: 39S ribosomal protein L35, mitochondrial

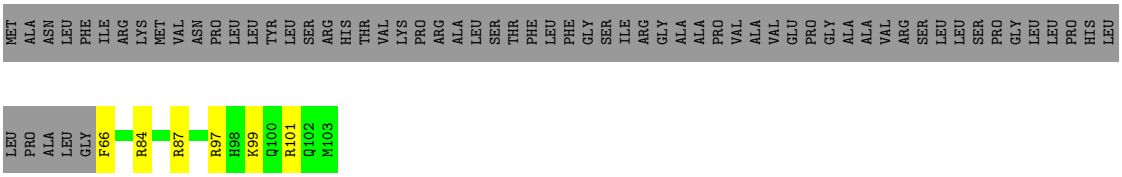
Chain 3:





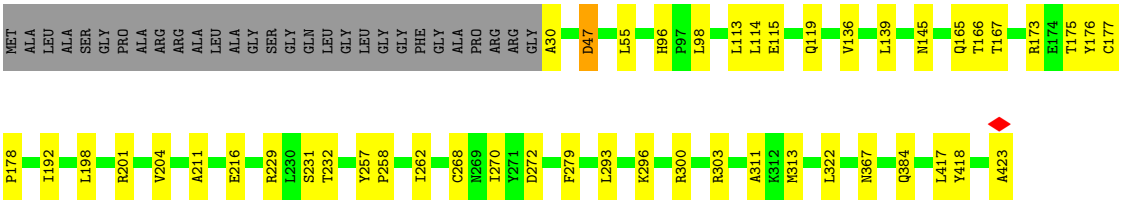
• Molecule 10: 39S ribosomal protein L36, mitochondrial

Chain 4:



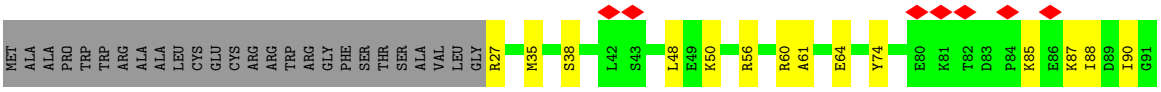
• Molecule 11: 39S ribosomal protein L37, mitochondrial

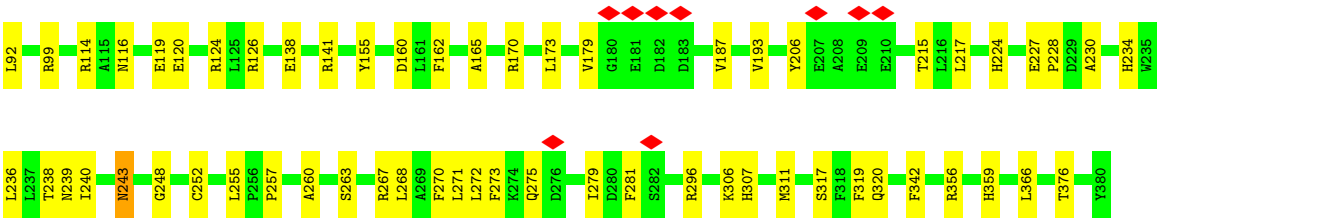
Chain 5:



• Molecule 12: 39S ribosomal protein L38, mitochondrial

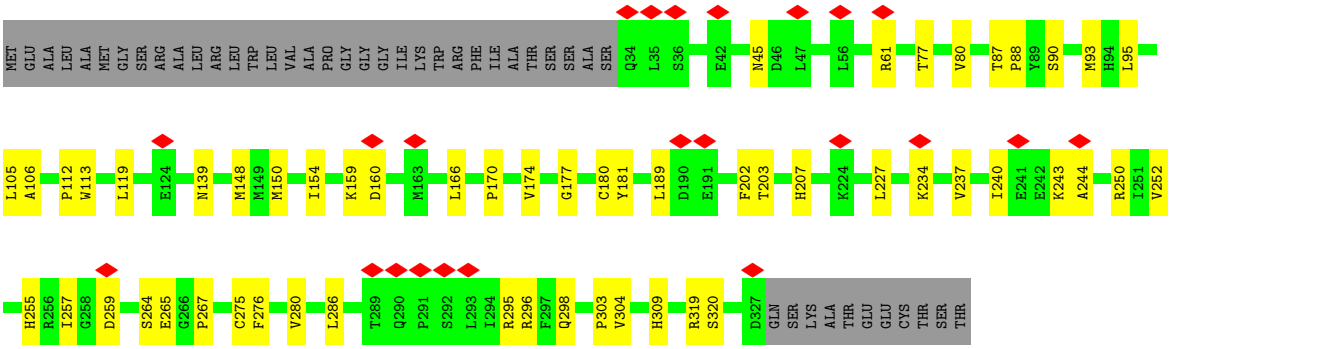
Chain 6:





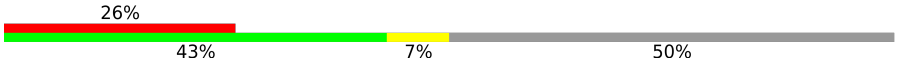
• Molecule 13: 39S ribosomal protein L39, mitochondrial

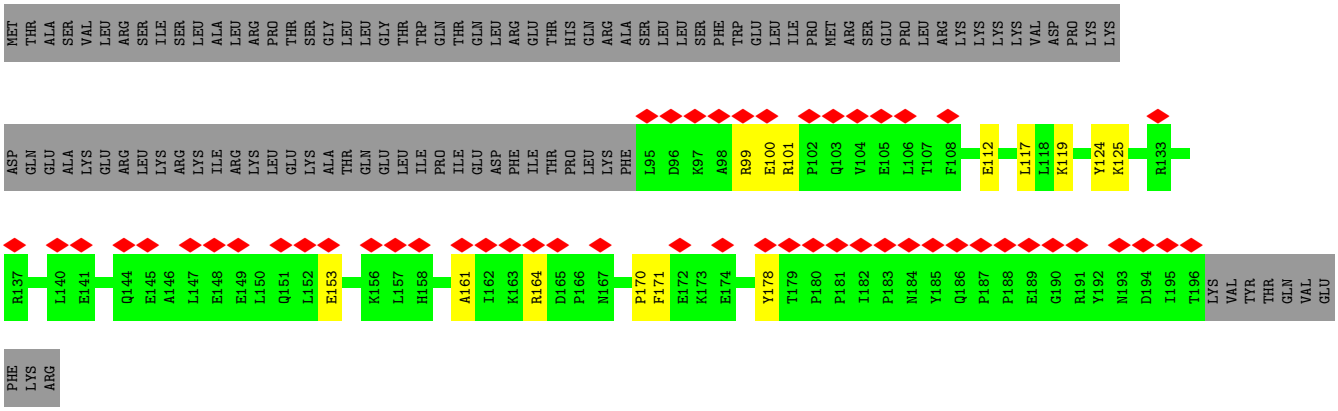
Chain 7:



• Molecule 14: 39S ribosomal protein L40, mitochondrial

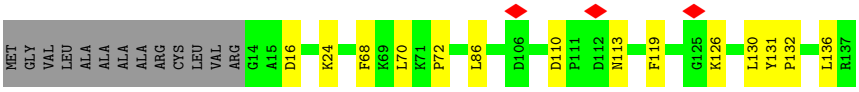
Chain 8:





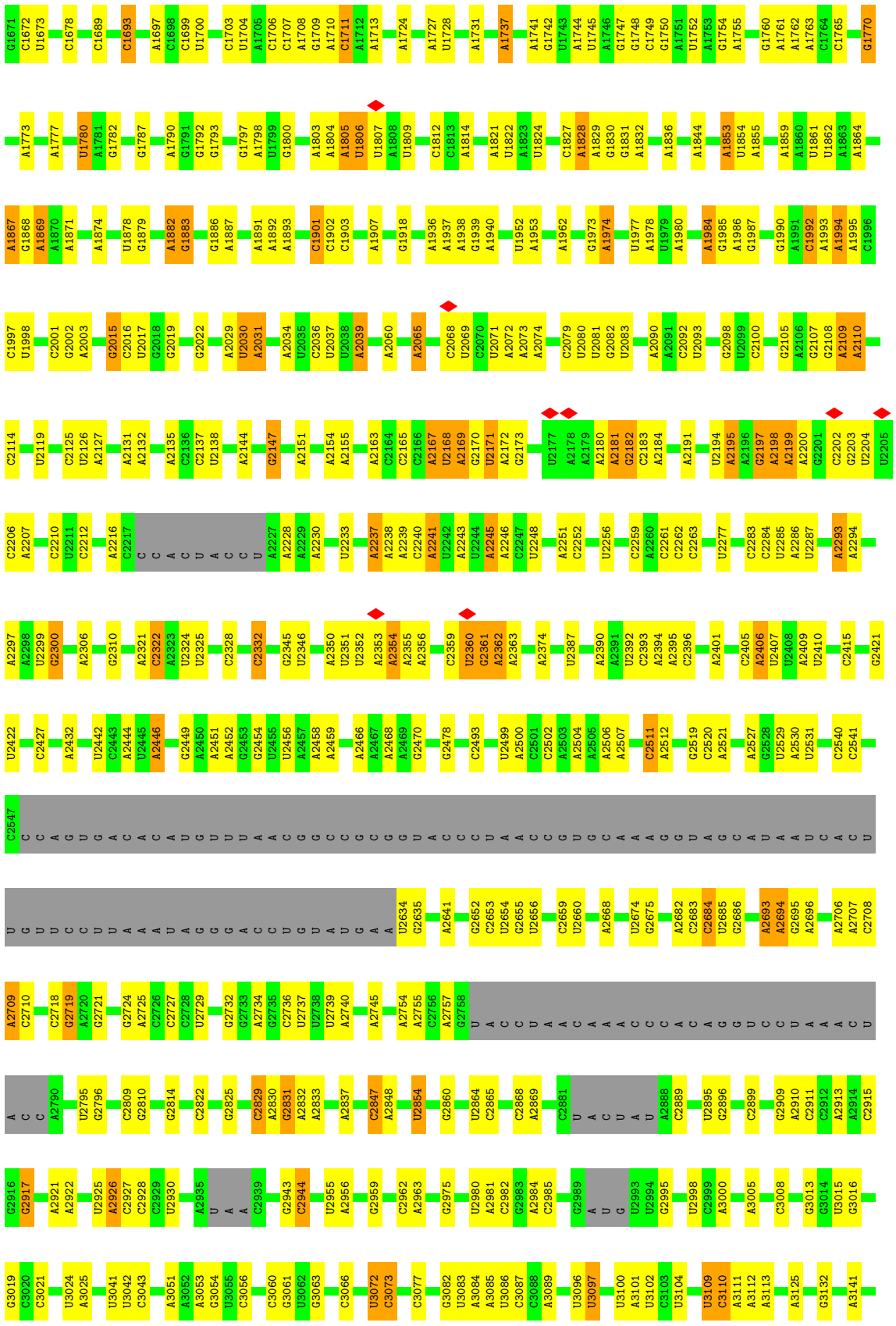
• Molecule 15: 39S ribosomal protein L41, mitochondrial

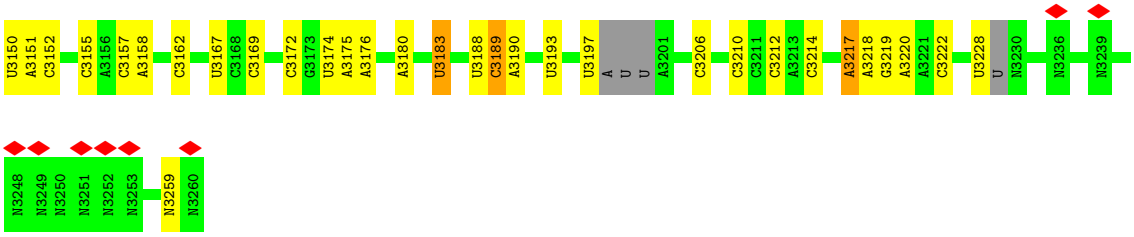
Chain 9:



• Molecule 16: 16S mitochondrial rRNA, DNA (31-MER),16S mitochondrial rRNA

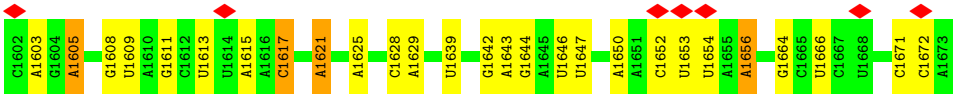
Chain A:


G1671 C1672 U1673 C1678 C1689 C1693 A1697 C1698 C1699 U1700 C1703 U1704 A1705 C1706 C1707 A1708 G1709 A1710 C1711 A1712 A1713 A1724 A1727 U1728 A1731 A1737 A1741 G1742 U1743 A1744 U1745 A1746 G1747 G1748 C1749 G1750 A1751 U1752 A1753 G1754 A1755 G1760 A1761 A1762 A1763 C1764 C1765 G1770
A1773 A1777 U1780 A1781 G1782 G1787 A1790 G1791 G1792 G1793 G1797 A1798 U1799 G1800 A1803 A1804 A1805 U1806 U1807 A1808 U1809 C1812 C1813 A1814 A1821 U1822 A1823 U1824 C1827 A1828 A1829 G1830 G1831 A1832 A1836 A1844 A1853 U1854 A1855 A1859 A1860 U1861 U1862 A1863 A1864
A1867 G1868 A1869 A1870 A1871 A1874 U1878 G1879 A1882 G1883 G1886 A1887 A1891 A1892 A1893 C1901 A1902 C1903 A1907 G1918 A1936 A1937 A1938 G1939 A1940 U1952 A1953 A1962 G1973 A1974 U1977 A1978 U1979 A1980 A1984 G1985 A1986 G1987 G1990 A1991 C1992 A1993 A1994 A1995 C1996
C1997 U1998 C2001 G2002 A2003 G2015 C2016 U2017 G2018 G2019 G2022 A2029 U2030 A2031 A2034 U2035 C2036 U2037 U2038 A2039 A2060 A2065 C2068 U2069 C2070 U2071 A2072 A2073 A2074 C2079 U2080 U2081 G2082 U2083 A2090 A2091 C2092 U2093 G2098 U2099 C2100 G2105 A2106 G2107 G2108 A2109 A2110
C2114 U2119 C2125 U2126 A2127 A2131 A2132 A2135 C2136 C2137 U2138 A2144 G2147 A2151 A2154 A2155 A2163 C2164 C2165 C2166 A2167 U2168 A2169 G2170 U2171 A2172 G2173 U2177 A2178 A2179 A2180 A2181 G2182 C2183 A2184 A2191 U2194 A2195 A2196 G2197 A2198 A2199 A2200 G2201 C2202 G2203 U2204 U2205
C2206 A2207 C2210 U2211 C2212 A2216 C2217 C C A C U A C C U A2227 A2228 A2229 A2230 U2233 A2237 A2238 A2239 C2240 A2241 U2242 A2243 U2244 A2245 A2246 C2247 U2248 A2251 C2252 U2256 C2259 A2260 C2261 C2262 C2263 U2277 C2283 C2284 U2285 A2286 U2287 A2293 A2294
A2297 A2298 U2299 G2300 A2306 G2310 A2321 C2322 A2323 U2324 U2325 C2328 C2332 G2345 U2346 A2350 U2351 U2352 A2353 A2354 A2355 A2356 C2359 U2360 G2361 A2362 A2363 A2374 U2387 A2390 A2391 U2392 C2393 A2394 A2395 C2396 A2401 C2405 A2406 U2407 U2408 A2409 U2410 C2415 G2421
U2422 C2427 A2432 U2442 C2443 A2444 U2445 A2446 G2449 A2450 A2451 A2452 G2453 G2454 U2455 U2456 A2457 A2458 A2459 A2466 A2467 A2468 A2469 G2470 G2478 C2493 U2499 A2500 C2501 C2502 A2503 A2504 A2505 A2506 A2507 C2511 A2512 G2519 C2520 A2521 A2527 G2528 U2529 A2530 U2531 C2540 C2541
C2547 C C A G U G A C A C A U A U U U A A C C G G C C G G U A C C C U A A C C G U G C A A A G G G U A G G C A U U A A C C U
U G U U C C U U A A A U A U G A A U A A U U A C C U G G G A U U A A A C C C A A A C C C C A A A A A A C C U
U2634 G2635 A2641 C2652 C2653 U2654 G2655 U2656 C2659 U2660 A2668 U2674 G2675 A2682 C2683 C2684 U2685 G2686 A2693 A2694 G2695 A2696 A2706 A2707 C2708
A2709 C2710 C2718 G2719 A2720 G2721 G2724 A2725 C2726 C2727 C2728 U2729 G2732 G2733 A2734 G2735 C2736 U2737 U2738 U2739 A2740 A2745 A2754 A2755 C2756 A2757 G2758 U A A C C U A A C A A A C C U A C C A C A C A A G G G U C C C U A A A C C U
A C C A2790 U2795 G2796 C2809 G2810 G2814 C2822 G2825 C2829 A2830 G2831 A2832 A2833 A2837 C2847 A2848 U2854 G2860 U2864 C2865 C2868 A2869 C2881 U A C U A U A2888 C2889 U2895 G2896 C2899 G2909 A2910 C2911 C2912 A2913 A2914 C2915
G2916 G2917 A2921 A2922 U2925 A2926 C2927 C2928 C2929 U2930 A2935 U A A C2939 G2943 C2944 U2955 A2956 G2959 C2962 A2963 G2975 U2980 A2981 C2982 G2983 A2984 C2985 G2989 A U G U2993 U2994 G2995 U2998 C2999 A3000 A3005 C3008 G3013 G3014 U3015 G3016
G3019 C3020 C3021 U3024 A3025 U3041 U3042 C3043 A3051 A3052 A3053 G3054 U3055 C3056 C3060 G3061 U3062 G3063 C3066 U3072 C3073 C3077 G3082 U3083 A3084 A3085 U3086 C3087 C3088 A3089 U3096 U3097 U3100 A3101 U3102 C3103 U3104 U3109 C3110 A3111 A3112 A3113 A3125 G3132 A3141



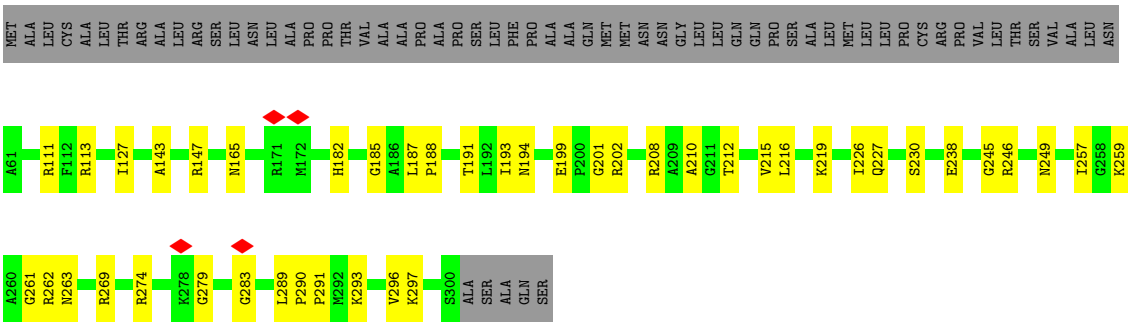
• Molecule 17: mitochondrial tRNAVal

Chain B:



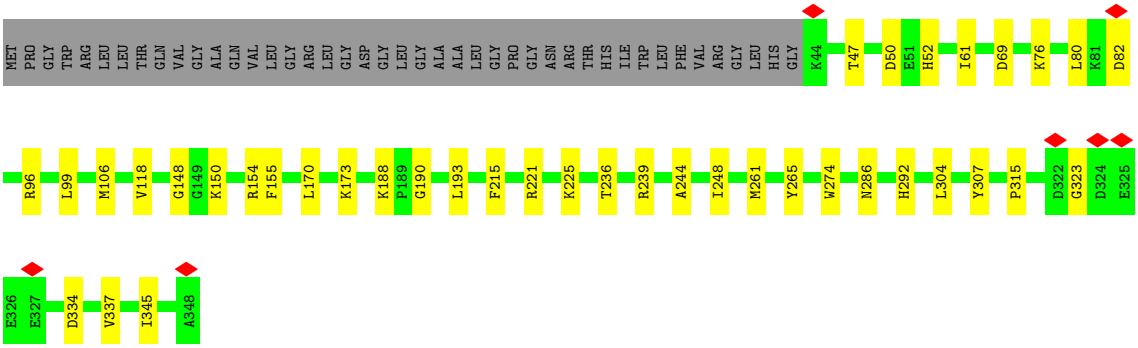
• Molecule 18: 39S ribosomal protein L2, mitochondrial

Chain D:



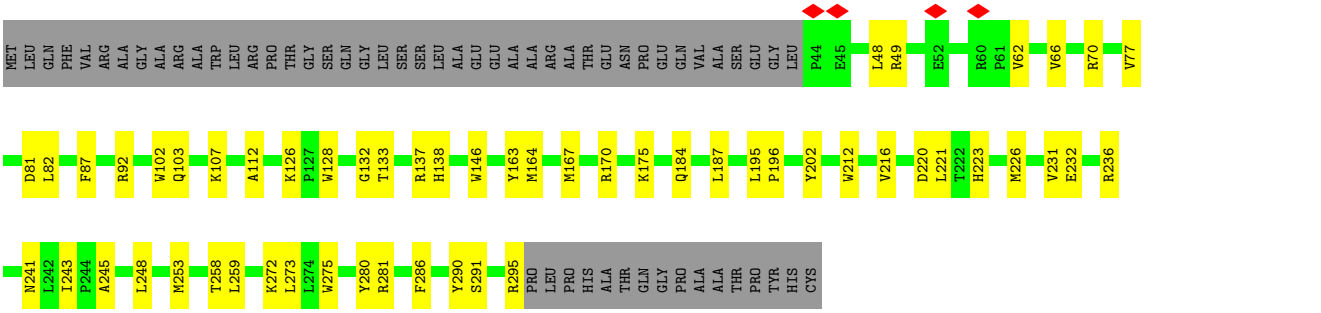
• Molecule 19: 39S ribosomal protein L3, mitochondrial

Chain E:



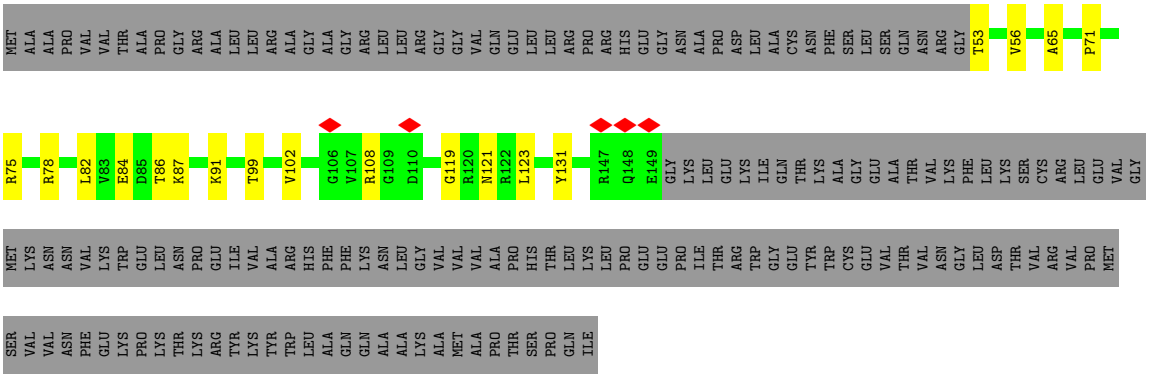
• Molecule 20: 39S ribosomal protein L4, mitochondrial

Chain F:



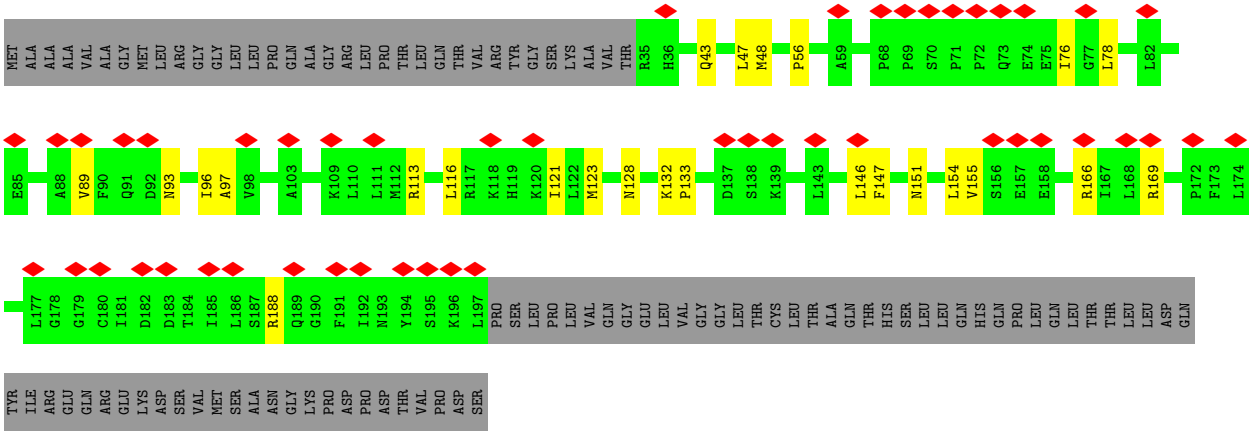
- Molecule 21: 39S ribosomal protein L9, mitochondrial

Chain H:



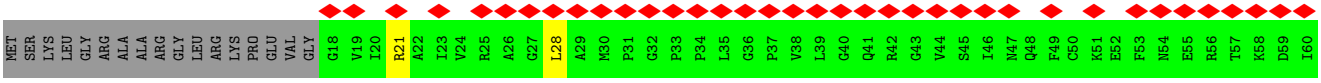
- Molecule 22: 39S ribosomal protein L10, mitochondrial

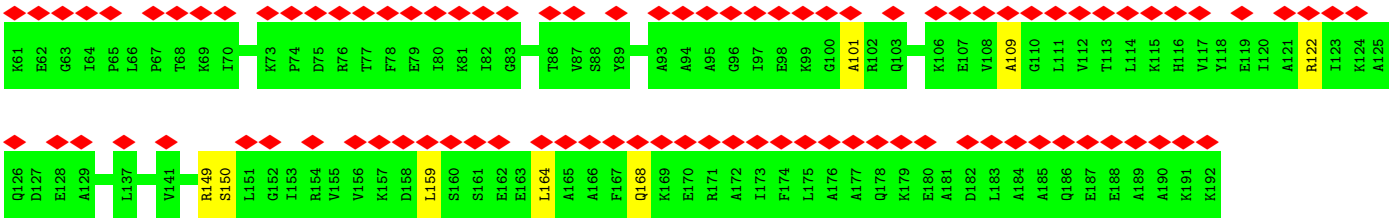
Chain I:



- Molecule 23: 39S ribosomal protein L11, mitochondrial

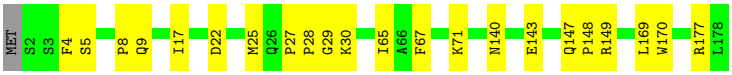
Chain J:





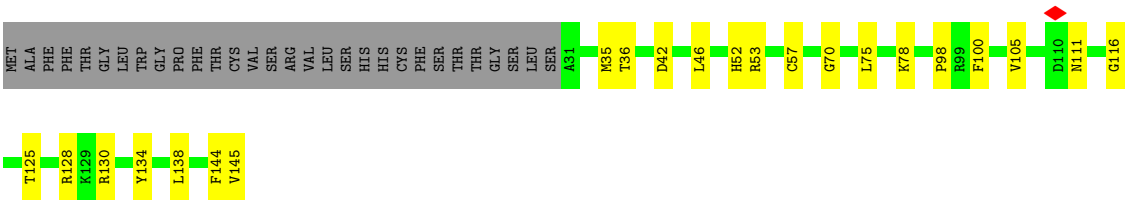
• Molecule 24: 39S ribosomal protein L13, mitochondrial

Chain K:



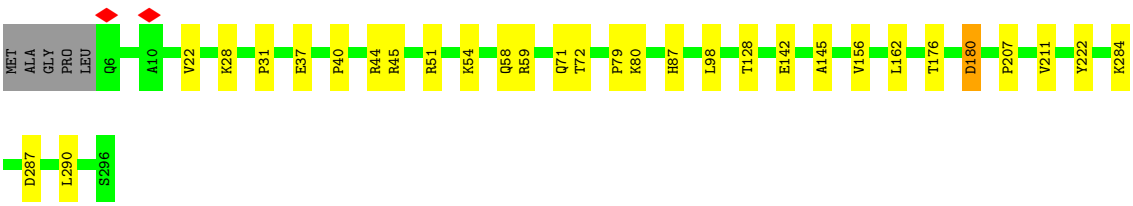
• Molecule 25: 39S ribosomal protein L14, mitochondrial

Chain L:



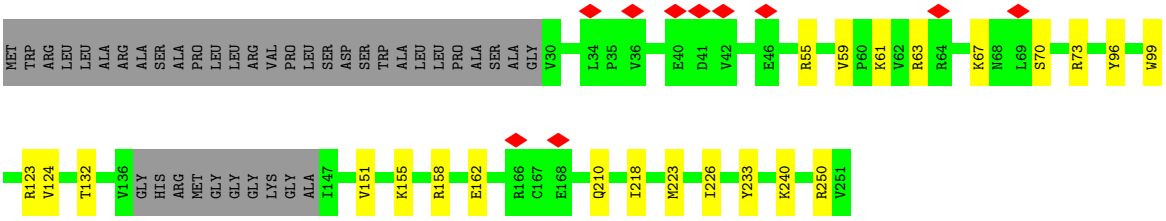
• Molecule 26: 39S ribosomal protein L15, mitochondrial

Chain M:



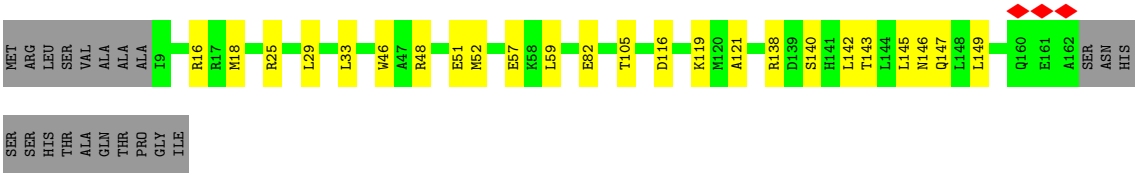
• Molecule 27: 39S ribosomal protein L16, mitochondrial

Chain N:



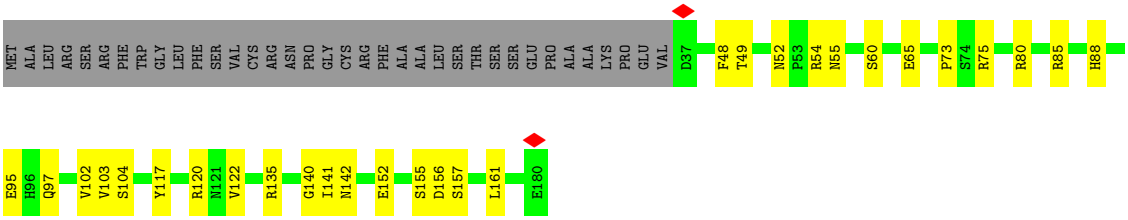
• Molecule 28: 39S ribosomal protein L17, mitochondrial

Chain O:



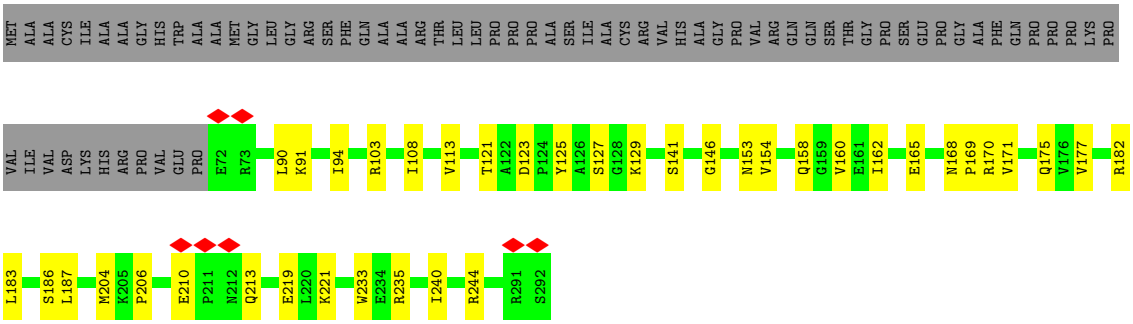
• Molecule 29: 39S ribosomal protein L18, mitochondrial

Chain P:



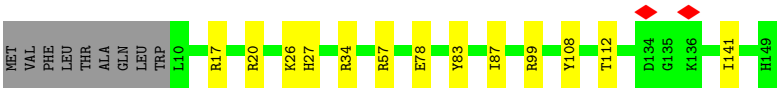
• Molecule 30: 39S ribosomal protein L19, mitochondrial

Chain Q:



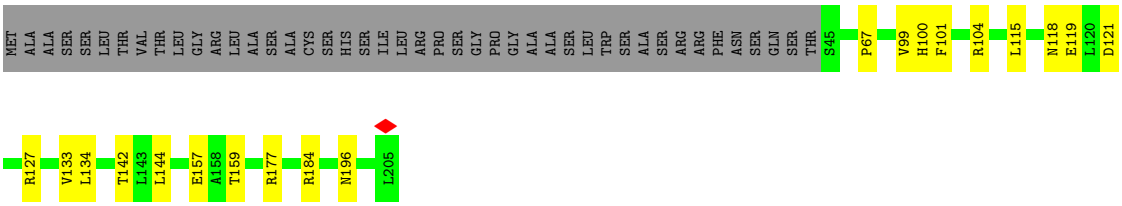
• Molecule 31: 39S ribosomal protein L20, mitochondrial

Chain R:



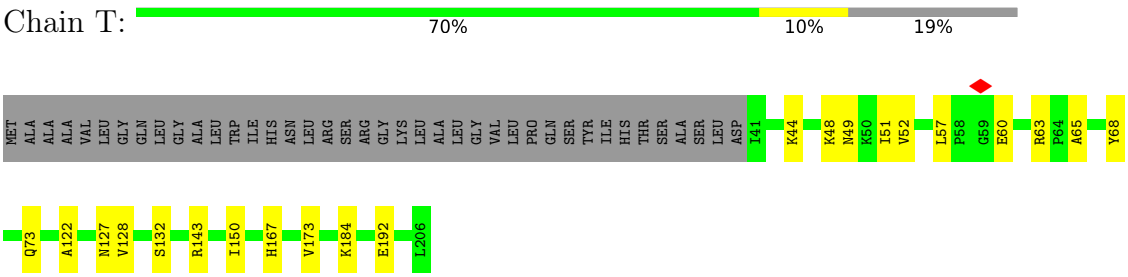
• Molecule 32: 39S ribosomal protein L21, mitochondrial

Chain S:



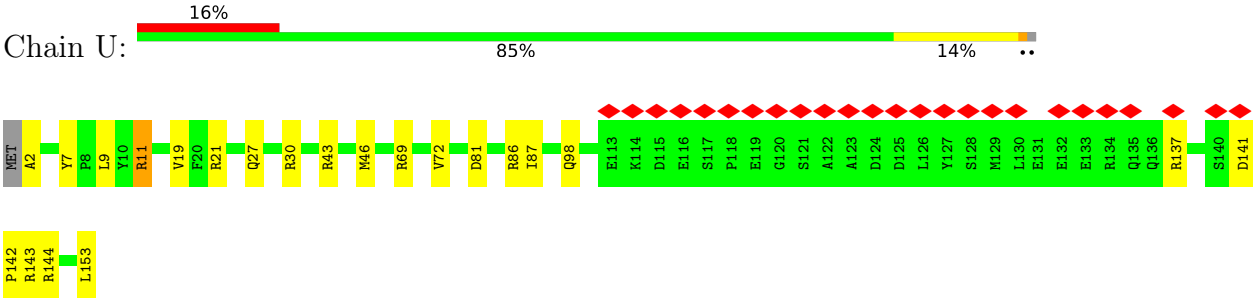
• Molecule 33: 39S ribosomal protein L22, mitochondrial

Chain T:



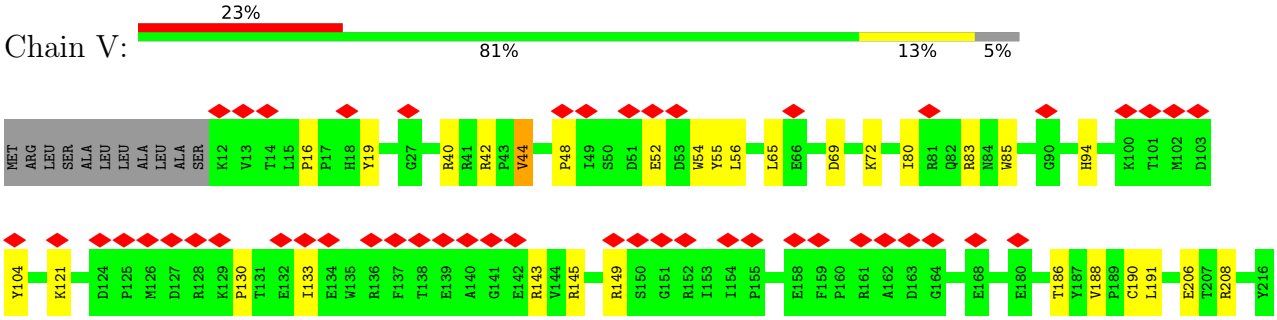
• Molecule 34: 39S ribosomal protein L23, mitochondrial

Chain U:



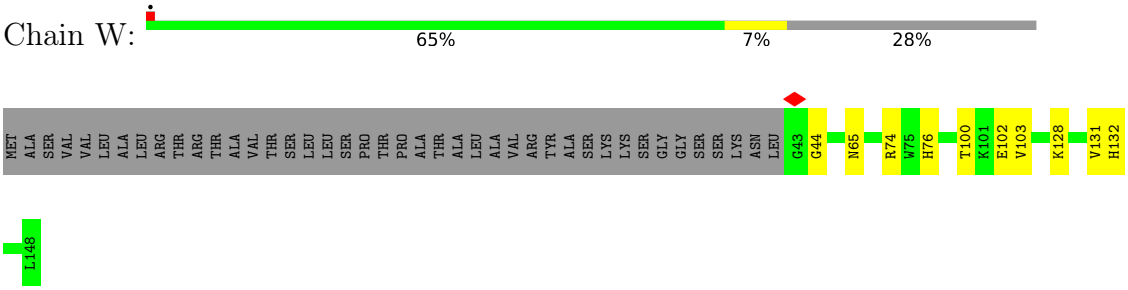
• Molecule 35: 39S ribosomal protein L24, mitochondrial

Chain V:



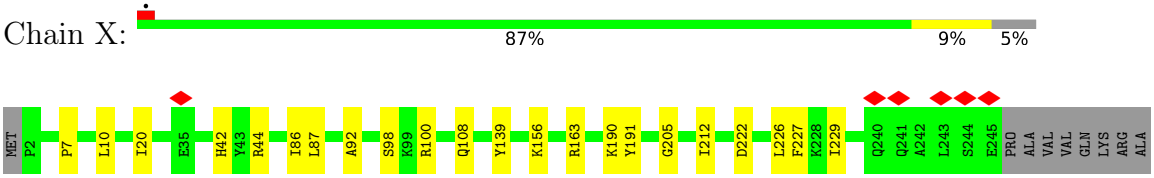
• Molecule 36: 39S ribosomal protein L27, mitochondrial

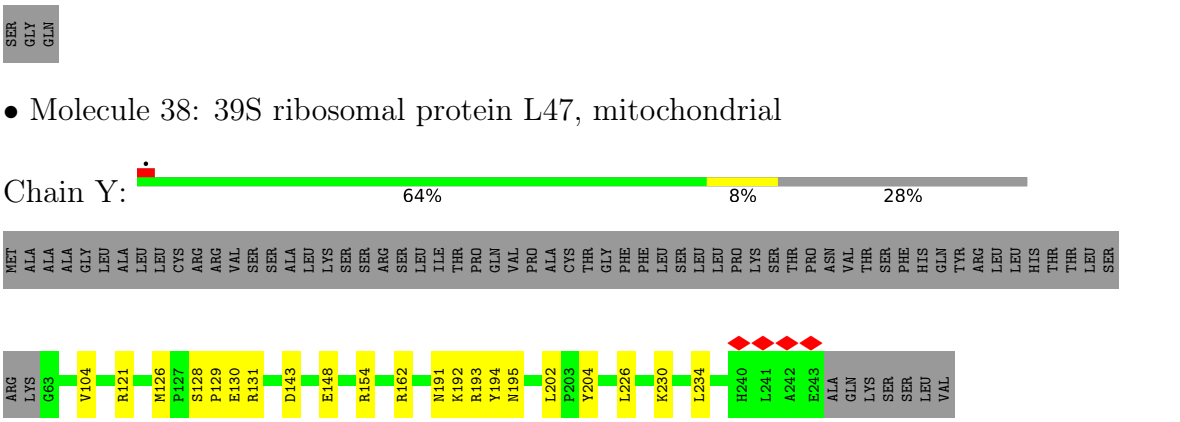
Chain W:

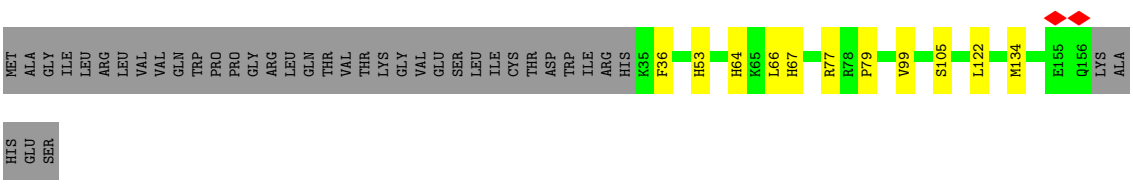


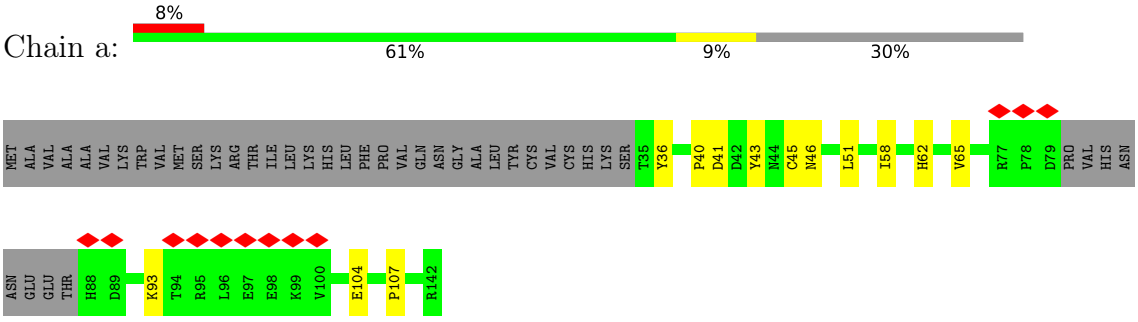
• Molecule 37: 39S ribosomal protein L28, mitochondrial

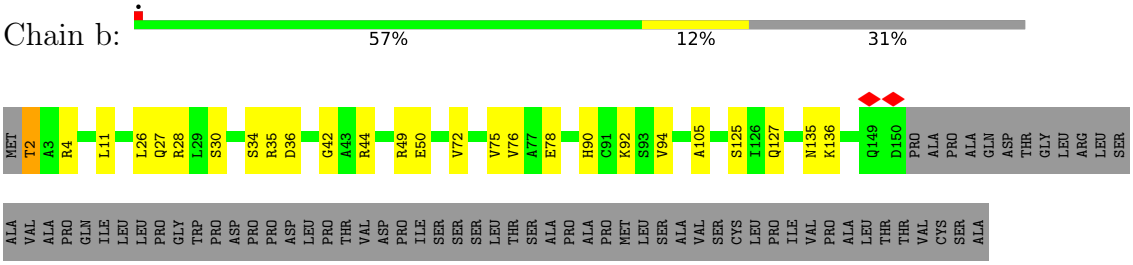
Chain X:

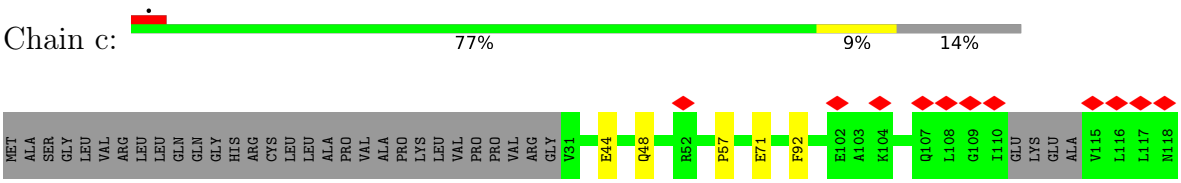


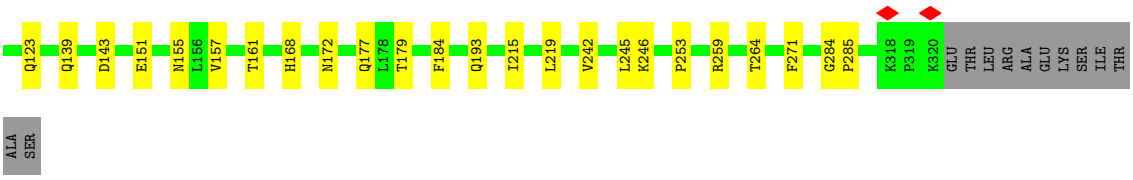

SER GLY GLN
• Molecule 38: 39S ribosomal protein L47, mitochondrial
Chain Y:
64%
8%
28%
MET ALA ALA ALA GLY LEU ALA LEU LEU CYS ARG ARG VAL SER SER ALA LEU LYS SER SER ARG SER LEU ILE THR PRO GLN VAL PRO ALA CYS THR GLY PHE PHE LEU SER LEU LEU PRO LYS SER THR PRO ASN VAL THR SER PHE HIS GLN TYR ARG LEU LEU HIS THR THR LEU SER
ARG LYS G63 V104 R121 M126 P127 S128 P129 E130 R131 D143 E148 R154 R162 N191 K192 R193 Y194 N195 L202 P203 Y204 L226 K230 L234 H240 L241 A242 E243 ALA GLN LYS SER SER LEU VAL


• Molecule 39: 39S ribosomal protein L30, mitochondrial
Chain Z:
69%
7%
24%
MET ALA GLY ILE LEU ARG LEU VAL VAL GLN TRP PRO PRO GLY ARG LEU GLN THR VAL THR LYS GLY VAL GLU SER LEU LEU ILE CYS THR ASP TRP ILE ARG HIS K35 F36 H53 H64 K65 L66 H67 R77 R78 P79 V99 S105 L122 M134 E155 Q156 LYS ALA
HIS GLU SER


• Molecule 40: 39S ribosomal protein L42, mitochondrial
Chain a:
8%
61%
9%
30%
MET ALA VAL ALA ALA VAL LYS TRP VAL MET SER LYS ARG THR ILE LEU LYS HIS LEU PHE PRO VAL GLN ASN GLY ALA LEU TYR CYS VAL CYS HIS LYS SER T35 Y36 P40 D41 D42 Y43 N44 C45 N46 L51 I58 H62 V65 R77 P78 D79 PRO VAL HIS ASN
ASN GLU GLU THR H88 D89 K93 T94 R95 L96 E97 E98 K99 V100 E104 P107 R142

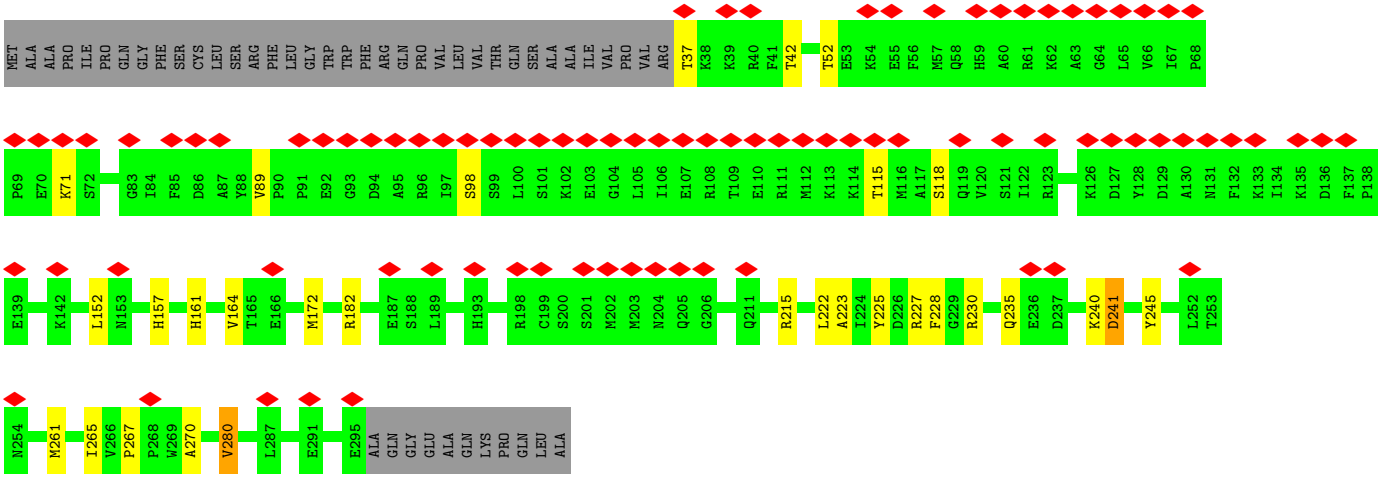

• Molecule 41: 39S ribosomal protein L43, mitochondrial
Chain b:
57%
12%
31%
MET T2 A3 R4 L11 L26 Q27 R28 L29 S30 S34 R35 D36 G42 A43 R44 R49 E50 V72 V75 V76 A77 E78 H90 C91 K92 S93 V94 A105 S125 I126 Q127 N135 K136 Q149 D150 PRO ALA PRO ALA GLN ASP THR GLY LEU ARG LEU SER
ALA VAL ALA PRO GLN ILE LEU LEU PRO GLY TRP PRO ASP PRO PRO ASP LEU PRO THR VAL ASP PRO ILE SER SER SER LEU THR SER ALA PRO ALA PRO MET LEU SER ALA VAL SER CYS LEU PRO ILE VAL PRO ALA LEU THR THR VAL CYS SER ALA


• Molecule 42: 39S ribosomal protein L44, mitochondrial
Chain c:
77%
9%
14%
MET ALA SER GLY LEU VAL ARG LEU LEU GLN GLN GLY HIS ARG CYS LEU LEU ALA PRO VAL ALA PRO LYS LEU VAL PRO PRO VAL ARG GLY V31 E44 Q48 R52 P57 E71 F92 E102 A103 K104 Q107 L108 G109 I110 GLU LYS GLU ALA V115 L116 L117 N118



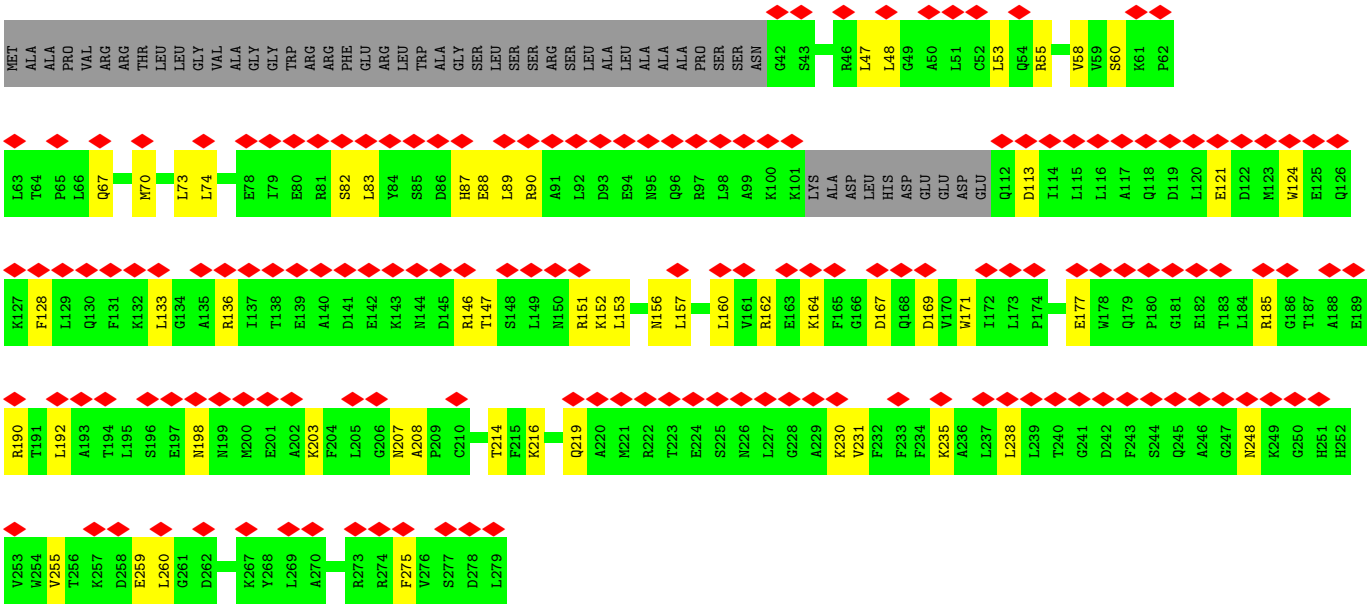
• Molecule 43: 39S ribosomal protein L45, mitochondrial

Chain d:



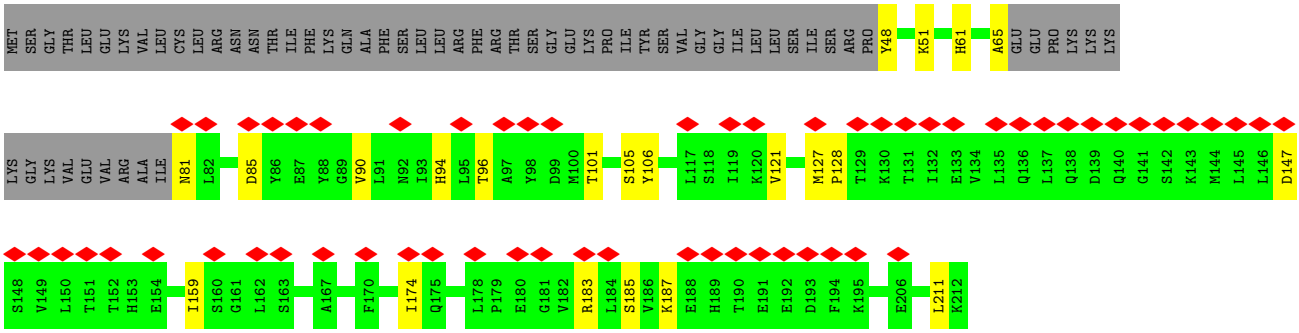
• Molecule 44: 39S ribosomal protein L46, mitochondrial

Chain e:



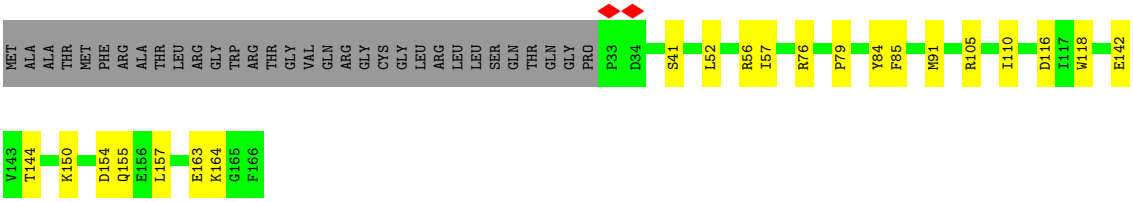
• Molecule 45: 39S ribosomal protein L48, mitochondrial

Chain f:



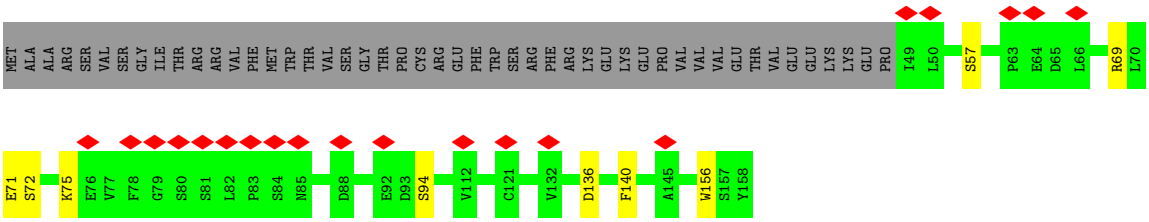
• Molecule 46: 39S ribosomal protein L49, mitochondrial

Chain g:



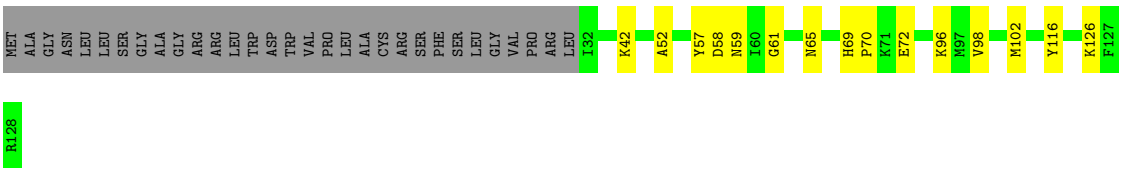
• Molecule 47: 39S ribosomal protein L50, mitochondrial

Chain h:



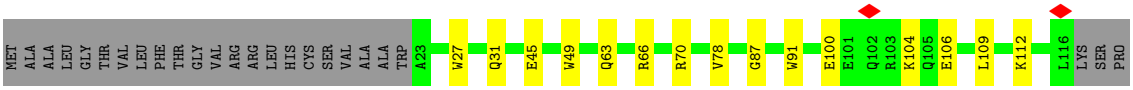
• Molecule 48: 39S ribosomal protein L51, mitochondrial

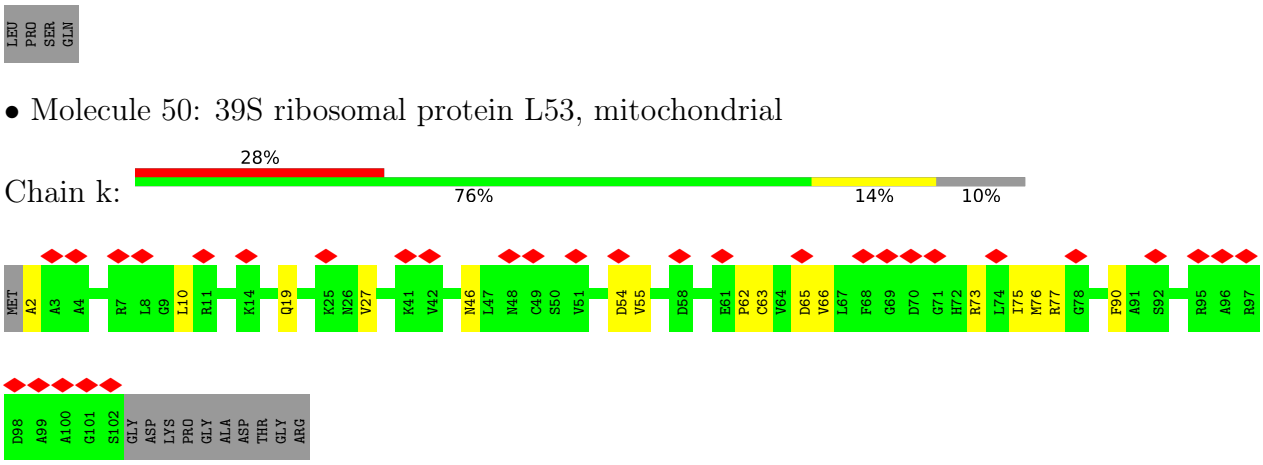
Chain i:



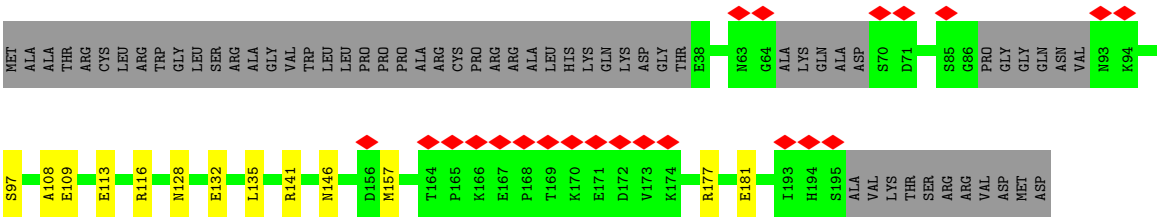
• Molecule 49: 39S ribosomal protein L52, mitochondrial

Chain j:



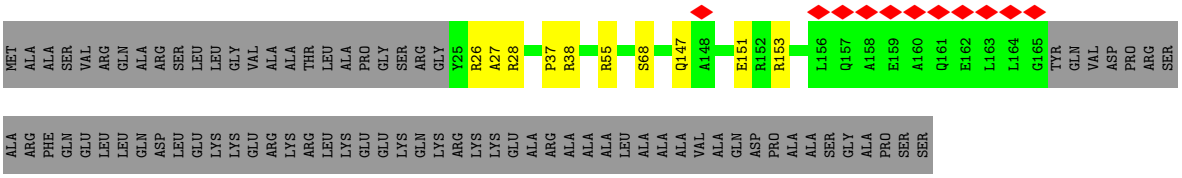

LEU PRO SER GLN
• Molecule 50: 39S ribosomal protein L53, mitochondrial
Chain k:
28%
76%
14%
10%
MET A2 A3 A4 R7 L8 G9 L10 R11 K14 Q19 K25 N26 V27 K41 V42 N46 L47 N48 C49 S50 V51 D54 V55 D58 E61 P62 C63 V64 D65 V66 L67 F68 G69 D70 G71 H72 R73 L74 I75 M76 R77 G78 F90 A91 S92 R95 A96 R97
D98 A99 A100 G101 S102 GLY ASP LYS PRO GLY ALA ASP THR GLY ARG
• Molecule 51: 39S ribosomal protein L54, mitochondrial
Chain l:
38%
49%
10%
41%
MET ALA THR LYS ARG LEU PHE GLY ALA THR ARG THR TRP ALA GLY TRP GLY ALA TRP GLU LEU LEU ASN PRO ALA THR SER GLY ARG LEU LEU ALA ARG ASP TYR ALA LYS LYS PRO VAL MET LYS GLY ALA LYS SER GLY LYS GLY ALA VAL THR SER GLU A55 L56 K57 D58 P59 D60
V61 C62 T63 D64 P65 V66 Q67 L68 T69 T70 Y71 A72 M73 G74 V75 N76 I77 Y78 K79 E80 G81 Q82 D83 V84 P85 L86 K87 P88 D89 A90 E91 Y92 P93 E94 W95 L96 F97 E98 N99 N100 L101 G102 P103 P104 K105 T106 L107 E108 D111 R115 E116 L121 R122 K123 Q124 N125 I126
W127 N135 K136 ARG LEU
• Molecule 52: 39S ribosomal protein L55, mitochondrial
Chain m:
32%
29%
10%
60%
MET ALA ALA ALA VAL GLY SER LEU LEU GLY ARG LEU ARG GLN SER THR VAL LYS ALA THR GLY PRO ALA LEU ARG ARG LEU HIS THR SER SER TRP ARG ALA D34 S35 S36 R37 A38 S39 L40 T41 R42 V43 H44 R45 Q46 A47 Y48 A49 R50 L51 V54 L55 L56 V57 K58 Q59 D60 G61
S62 T63 I64 H65 I66 R67 Y68 R69 E70 P71 R72 R73 M74 L75 A76 M77 P78 I79 D80 L81 D82 T83 L84 SER PRO GLU GLU ARG ARG ALA ARG LEU ARG LYS ARG GLU ALA GLN LEU GLN SER ARG LYS GLU TYR GLU GLN GLU LEU SER ASP ASP LEU HIS VAL GLU ARG TYR ARG GLN
PHE TRP THR ARG THR LYS LYS
• Molecule 53: Ribosomal protein 63, mitochondrial
Chain o:
76%
16%
8%
MET PHE LEU THR ALA LEU LEU TRP R9 G10 R11 R15 Q16 W17 I18 G19 K20 R23 P24 R25 Y47 Q58 E59 R60 G61 H62 T79 P83 R86 H94 W101 S102
• Molecule 54: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:



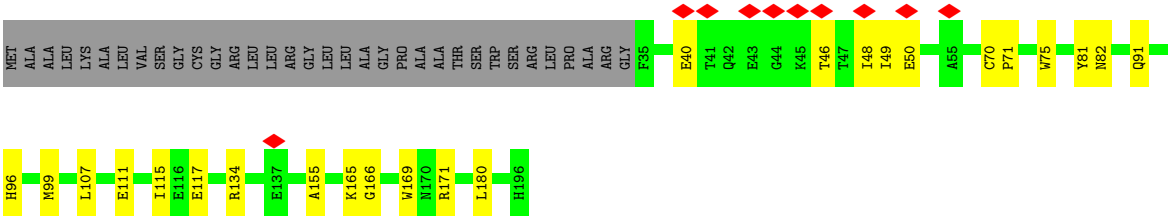
- Molecule 55: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:



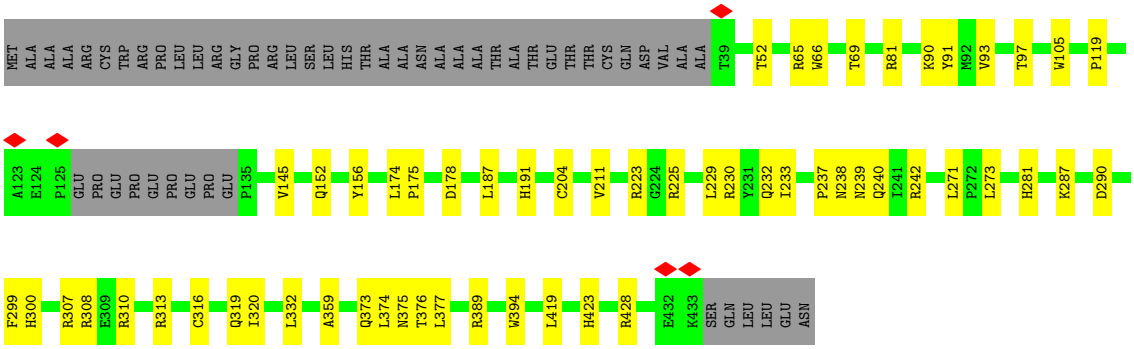
- Molecule 56: 39S ribosomal protein S18a, mitochondrial

Chain r:



- Molecule 57: 39S ribosomal protein S30, mitochondrial

Chain s:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123267	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.222	Depositor
Minimum map value	-1.532	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.118	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	474.87997, 474.87997, 474.87997	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: THC, SAC, K, MG, SAM, PM8, ZN, FES, AYA

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	u	0.10	0/941	0.28	0/1270
2	v	0.09	0/597	0.24	0/796
3	w	0.09	0/647	0.28	0/871
4	x	0.10	0/2721	0.28	0/3691
5	y	0.08	0/2011	0.22	0/2702
6	0	0.09	0/913	0.24	0/1224
7	1	0.08	0/460	0.23	0/610
8	2	0.11	0/383	0.24	0/507
9	3	0.11	0/853	0.25	0/1136
10	4	0.10	0/350	0.24	0/461
11	5	0.11	0/3305	0.27	0/4502
12	6	0.11	0/3043	0.27	0/4140
13	7	0.10	0/2447	0.25	0/3310
14	8	0.10	0/880	0.24	0/1188
15	9	0.12	0/1025	0.26	0/1379
16	A	0.09	0/33664	0.16	0/52392
17	B	0.05	0/1700	0.09	0/2641
18	D	0.11	0/1910	0.27	0/2569
19	E	0.11	0/2475	0.26	0/3355
20	F	0.11	0/2090	0.28	0/2842
21	H	0.11	0/816	0.27	0/1097
22	I	0.11	0/1354	0.30	0/1829
23	J	0.09	0/1348	0.28	0/1813
24	K	0.11	0/1490	0.28	0/2021
25	L	0.11	0/905	0.30	0/1218
26	M	0.11	0/2381	0.28	1/3212 (0.0%)
27	N	0.09	0/1768	0.24	0/2383
28	O	0.11	0/1283	0.27	0/1727
29	P	0.10	0/1199	0.27	0/1623
30	Q	0.10	0/1884	0.26	0/2535
31	R	0.10	0/1175	0.24	0/1572
32	S	0.12	0/1320	0.30	0/1789

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	T	0.11	0/1403	0.27	0/1886
34	U	0.11	0/1274	0.27	0/1723
35	V	0.10	0/1721	0.23	0/2333
36	W	0.12	0/857	0.27	0/1155
37	X	0.09	0/2099	0.24	0/2837
38	Y	0.09	0/1593	0.24	0/2136
39	Z	0.11	0/1021	0.27	0/1378
40	a	0.10	0/866	0.25	0/1174
41	b	0.12	0/1203	0.29	0/1627
42	c	0.09	0/2347	0.25	0/3171
43	d	0.10	0/2181	0.26	0/2949
44	e	0.08	0/1885	0.26	0/2542
45	f	0.09	0/1216	0.27	0/1638
46	g	0.12	0/1151	0.29	0/1569
47	h	0.09	0/918	0.23	0/1249
48	i	0.11	0/850	0.25	0/1135
49	j	0.10	0/760	0.24	0/1023
50	k	0.09	0/777	0.23	0/1048
51	l	0.10	0/707	0.27	0/960
52	m	0.08	0/426	0.24	0/575
53	o	0.08	0/819	0.22	0/1097
54	p	0.09	0/1223	0.23	0/1641
55	q	0.08	0/1208	0.20	0/1633
56	r	0.10	0/1362	0.26	0/1846
57	s	0.11	0/3239	0.27	0/4400
All	All	0.10	0/112444	0.23	1/159130 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	M	54	LYS	CB-CA-C	-5.03	109.80	115.79

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	u	919	0	917	13	0
2	v	588	0	604	13	0
3	w	638	0	636	8	0
4	x	2660	0	2640	43	0
5	y	1980	0	2066	33	0
6	0	898	0	916	9	0
7	1	455	0	498	4	0
8	2	377	0	406	2	0
9	3	832	0	883	10	0
10	4	342	0	361	6	0
11	5	3210	0	3206	34	0
12	6	2948	0	2841	56	0
13	7	2390	0	2397	32	0
14	8	860	0	852	15	0
15	9	997	0	987	13	0
16	A	30460	0	15537	256	0
17	B	1522	0	776	13	0
18	D	1872	0	1932	30	0
19	E	2406	0	2415	26	0
20	F	2031	0	2065	44	0
21	H	802	0	846	14	0
22	I	1324	0	1400	16	0
23	J	1330	0	1407	8	0
24	K	1455	0	1452	15	0
25	L	890	0	941	16	0
26	M	2327	0	2395	23	0
27	N	1723	0	1754	15	0
28	O	1259	0	1294	17	0
29	P	1173	0	1165	21	0
30	Q	1843	0	1878	25	0
31	R	1154	0	1214	12	0
32	S	1293	0	1365	15	0
33	T	1369	0	1410	15	0
34	U	1251	0	1232	15	0
35	V	1676	0	1687	20	0
36	W	835	0	858	7	0
37	X	2044	0	2060	15	0
38	Y	1556	0	1597	17	0
39	Z	996	0	1044	8	0
40	a	840	0	810	11	0
41	b	1189	0	1183	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	c	2299	0	2320	17	0
43	d	2124	0	2125	22	0
44	e	1848	0	1849	39	0
45	f	1196	0	1212	13	0
46	g	1113	0	1097	15	0
47	h	895	0	881	5	0
48	i	828	0	857	15	0
49	j	745	0	746	13	0
50	k	774	0	784	12	0
51	l	688	0	674	9	0
52	m	419	0	435	16	0
53	o	798	0	804	18	0
54	p	1205	0	1223	9	0
55	q	1177	0	1154	8	0
56	r	1322	0	1348	20	0
57	s	3155	0	3139	34	0
58	w	32	0	39	5	0
59	x	27	0	22	0	0
60	0	1	0	0	0	0
60	4	1	0	0	0	0
61	9	1	0	0	0	0
61	A	92	0	0	0	0
61	D	1	0	0	0	0
61	M	1	0	0	0	0
61	O	1	0	0	0	0
61	g	1	0	0	0	0
62	A	2	0	0	0	0
63	r	4	0	0	0	0
All	All	107464	0	92636	961	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 5.

All (961) 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)
16:A:2499:U:OP2	16:A:2504:A:N6	2.18	0.76
40:a:41:ASP:HB3	40:a:46:ASN:HD22	1.51	0.75
5:y:162:ARG:NH1	5:y:186:ILE:O	2.19	0.74
4:x:258:CYS:SG	4:x:316:GLN:NE2	2.62	0.73
2:v:45:LEU:HD23	2:v:50:ALA:HB1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:2725:A:H4'	16:A:3072:U:H3	1.52	0.72
4:x:328:LEU:HB3	4:x:334:ILE:HB	1.72	0.72
16:A:2259:C:O2'	16:A:2261:C:OP2	2.08	0.72
16:A:1990:G:OP1	18:D:269:ARG:NH2	2.22	0.71
22:I:97:ALA:HB3	22:I:154:LEU:HB2	1.72	0.71
16:A:1777:A:N6	16:A:1780:U:OP2	2.22	0.71
34:U:21:ARG:HH12	38:Y:143:ASP:HA	1.53	0.71
16:A:2354:A:H61	16:A:2361:G:H1	1.37	0.71
16:A:2248:U:OP1	31:R:99:ARG:NH2	2.24	0.71
21:H:53:THR:N	21:H:86:THR:HG1	1.88	0.70
13:7:80:VAL:HG21	34:U:143:ARG:HG2	1.74	0.70
1:u:135:LEU:HD22	1:u:179:LEU:HB3	1.74	0.70
11:5:115:GLU:HB2	11:5:119:GLN:HB2	1.73	0.70
32:S:144:LEU:HB2	40:a:58:ILE:HB	1.75	0.69
16:A:2165:C:N4	16:A:2212:C:OP1	2.27	0.68
23:J:28:LEU:HB3	51:l:56:LEU:HD22	1.75	0.68
53:o:15:ARG:HB3	53:o:18:ILE:HG12	1.75	0.68
11:5:229:ARG:NH1	11:5:231:SER:OG	2.27	0.68
16:A:2360:U:H3'	16:A:2361:G:H4'	1.76	0.68
20:F:132:GLY:HA3	43:d:42:THR:HG21	1.75	0.67
28:O:142:LEU:HA	28:O:147:GLN:HE21	1.59	0.67
17:B:1605:A:H61	17:B:1666:U:H3	1.41	0.67
7:1:24:ALA:HB2	7:1:54:VAL:HG11	1.77	0.67
13:7:170:PRO:HG2	13:7:296:ARG:HH12	1.58	0.67
16:A:2442:U:OP1	57:s:81:ARG:NH2	2.25	0.67
44:e:255:VAL:HB	44:e:259:GLU:HG3	1.76	0.67
4:x:170:GLY:O	4:x:251:ARG:NH1	2.27	0.67
4:x:274:LYS:HE3	4:x:276:SER:HB3	1.77	0.67
14:8:153:GLU:HG2	44:e:47:LEU:HD21	1.77	0.66
22:I:128:ASN:HB3	22:I:132:LYS:HE3	1.78	0.66
13:7:112:PRO:HB2	13:7:267:PRO:HG2	1.78	0.66
57:s:191:HIS:O	57:s:428:ARG:NH2	2.28	0.66
12:6:88:ILE:HD13	49:j:109:LEU:HB3	1.78	0.66
13:7:180:CYS:SG	13:7:296:ARG:NH1	2.69	0.66
43:d:182:ARG:HB2	43:d:223:ALA:HB3	1.78	0.66
16:A:1853:A:OP2	32:S:177:ARG:NH1	2.29	0.65
4:x:42:ARG:NH1	4:x:46:GLN:OE1	2.29	0.65
24:K:27:PRO:HG2	24:K:30:LYS:HB2	1.77	0.65
12:6:90:ILE:HA	49:j:112:LYS:HB2	1.77	0.65
18:D:113:ARG:O	18:D:147:ARG:NH2	2.30	0.65
16:A:2167:A:N6	16:A:2212:C:OP2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:257:ILE:O	18:D:262:ARG:NH1	2.25	0.65
42:c:259:ARG:HB2	42:c:271:PHE:HB2	1.79	0.65
50:k:19:GLN:NE2	50:k:63:CYS:SG	2.71	0.64
50:k:73:ARG:HB2	56:r:46:THR:HG23	1.79	0.64
16:A:2110:A:N1	16:A:2980:U:O2'	2.28	0.64
19:E:82:ASP:O	19:E:188:LYS:NZ	2.30	0.63
20:F:164:MET:HE1	48:i:70:PRO:HB2	1.80	0.63
29:P:142:ASN:HD22	54:p:181:GLU:HG2	1.62	0.63
46:g:84:TYR:OH	46:g:164:LYS:NZ	2.28	0.63
6:0:139:ARG:NH1	16:A:2322:C:OP1	2.31	0.63
11:5:113:LEU:HD12	11:5:311:ALA:HB1	1.80	0.63
16:A:2191:A:N6	16:A:2198:A:OP1	2.31	0.63
29:P:104:SER:O	29:P:135:ARG:NH1	2.31	0.63
52:m:57:VAL:N	52:m:75:LEU:O	2.30	0.63
16:A:2531:U:O4	18:D:246:ARG:NH2	2.31	0.63
18:D:194:ASN:ND2	18:D:245:GLY:O	2.30	0.63
33:T:184:LYS:NZ	33:T:192:GLU:OE1	2.29	0.63
20:F:272:LYS:NZ	48:i:65:ASN:OD1	2.31	0.63
18:D:296:VAL:HG23	18:D:297:LYS:HG2	1.81	0.62
19:E:244:ALA:HB1	19:E:248:ILE:HD11	1.81	0.62
35:V:54:TRP:NE1	35:V:56:LEU:O	2.32	0.62
46:g:110:ILE:HD11	46:g:157:LEU:HD13	1.80	0.62
13:7:61:ARG:HD3	43:d:235:GLN:HE22	1.64	0.62
1:u:111:VAL:H	2:v:26:THR:HG22	1.62	0.62
19:E:69:ASP:OD1	19:E:154:ARG:NH1	2.32	0.62
30:Q:182:ARG:HG3	30:Q:187:LEU:HD11	1.81	0.62
12:6:60:ARG:HH12	12:6:64:GLU:HB2	1.64	0.62
13:7:244:ALA:HB1	13:7:250:ARG:HE	1.65	0.62
4:x:288:GLN:HE22	4:x:316:GLN:HE21	1.48	0.62
12:6:187:VAL:HG13	12:6:319:PHE:HB3	1.82	0.62
16:A:2137:C:H4'	22:I:43:GLN:HE21	1.65	0.62
33:T:63:ARG:NH1	43:d:228:PHE:O	2.33	0.62
16:A:1737:A:H5'	48:i:96:LYS:HE3	1.82	0.62
44:e:55:ARG:NH2	44:e:152:LYS:O	2.30	0.61
29:P:60:SER:OG	54:p:177:ARG:NH1	2.34	0.61
30:Q:183:LEU:HD21	30:Q:219:GLU:HG2	1.82	0.61
5:y:135:GLY:HA3	5:y:173:GLU:HB3	1.82	0.61
16:A:3082:G:N2	16:A:3085:A:OP2	2.28	0.61
34:U:9:LEU:O	34:U:11:ARG:NH1	2.33	0.61
45:f:94:HIS:HB2	45:f:185:SER:HB3	1.83	0.61
12:6:124:ARG:NH2	14:8:112:GLU:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:4:66:PHE:N	16:A:3013:G:HO2'	1.98	0.61
16:A:2277:U:OP2	48:i:42:LYS:NZ	2.34	0.61
30:Q:121:THR:HG22	30:Q:171:VAL:HA	1.83	0.61
30:Q:127:SER:OG	30:Q:129:LYS:NZ	2.33	0.61
44:e:235:LYS:NZ	44:e:275:PHE:O	2.32	0.61
5:y:157:MET:SD	5:y:160:ARG:NH2	2.72	0.61
22:I:47:LEU:HD22	27:N:226:ILE:HG12	1.83	0.61
24:K:140:ASN:ND2	42:c:264:THR:OG1	2.33	0.61
3:w:138:LEU:HD13	3:w:144:ILE:HG12	1.83	0.60
5:y:116:ARG:HD3	5:y:124:LEU:HD22	1.83	0.60
41:b:28:ARG:NH1	41:b:78:GLU:OE1	2.33	0.60
45:f:61:HIS:HA	45:f:65:ALA:HB3	1.82	0.60
9:3:94:LEU:N	16:A:1752:U:OP1	2.34	0.60
51:l:121:LEU:O	51:l:125:ASN:ND2	2.34	0.60
16:A:2039:A:N7	16:A:2729:U:O2'	2.33	0.60
16:A:2119:U:O2'	39:Z:36:PHE:O	2.18	0.60
44:e:48:LEU:HB2	44:e:231:VAL:HG12	1.81	0.60
16:A:1994:A:H61	16:A:2736:C:H4'	1.67	0.60
16:A:3113:A:OP1	16:A:3167:U:O2'	2.18	0.60
29:P:52:ASN:HB3	29:P:55:ASN:HB2	1.82	0.60
12:6:252:CYS:SG	12:6:296:ARG:NH1	2.75	0.60
16:A:2795:U:O2	21:H:87:LYS:NZ	2.33	0.60
32:S:99:VAL:HG12	32:S:133:VAL:HG22	1.84	0.60
13:7:276:PHE:HB2	13:7:304:VAL:HG22	1.84	0.60
16:A:2003:A:OP2	16:A:2734:A:O2'	2.18	0.60
16:A:2015:G:H22	16:A:2037:U:H5"	1.65	0.60
17:B:1671:C:OP1	44:e:219:GLN:NE2	2.34	0.60
54:p:113:GLU:OE1	54:p:116:ARG:NH1	2.33	0.60
57:s:271:LEU:HD23	57:s:273:LEU:HD13	1.82	0.60
42:c:215:ILE:HG23	42:c:219:LEU:HD12	1.84	0.60
16:A:2740:A:N3	16:A:2921:A:O2'	2.29	0.60
57:s:178:ASP:OD1	57:s:238:ASN:ND2	2.35	0.60
26:M:44:ARG:HG3	26:M:45:ARG:HG3	1.84	0.59
28:O:140:SER:O	28:O:146:ASN:ND2	2.35	0.59
11:5:216:GLU:OE2	11:5:367:ASN:ND2	2.33	0.59
13:7:189:LEU:O	13:7:295:ARG:NH2	2.34	0.59
16:A:1749:C:OP2	16:A:2899:C:O2'	2.20	0.59
16:A:2195:A:OP1	51:l:115:ARG:NH1	2.34	0.59
16:A:3189:C:O2'	56:r:155:ALA:N	2.31	0.59
32:S:101:PHE:HE1	49:j:49:TRP:HB3	1.66	0.59
19:E:96:ARG:NH1	19:E:315:PRO:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:218:ILE:HG23	27:N:223:MET:HB2	1.84	0.59
31:R:78:GLU:OE1	41:b:135:ASN:ND2	2.35	0.59
43:d:98:SER:OG	43:d:215:ARG:NH2	2.35	0.59
12:6:138:GLU:OE1	12:6:141:ARG:NH2	2.36	0.59
14:8:170:PRO:HB3	45:f:187:LYS:HG2	1.84	0.59
11:5:178:PRO:HG3	11:5:296:LYS:HD3	1.85	0.59
16:A:2346:U:OP1	57:s:223:ARG:NH2	2.36	0.59
45:f:96:THR:HB	45:f:183:ARG:HB3	1.84	0.59
42:c:151:GLU:O	42:c:155:ASN:ND2	2.34	0.59
46:g:118:TRP:NE1	46:g:142:GLU:OE2	2.33	0.59
57:s:178:ASP:HA	57:s:239:ASN:HD21	1.67	0.59
13:7:286:LEU:HD21	13:7:296:ARG:HE	1.68	0.59
16:A:2456:U:OP1	28:O:16:ARG:NH1	2.35	0.58
16:A:3019:G:O2'	16:A:3125:A:N1	2.35	0.58
19:E:80:LEU:HD12	19:E:323:GLY:HA3	1.85	0.58
25:L:100:PHE:HB3	30:Q:158:GLN:HE21	1.69	0.58
44:e:185:ARG:NH1	44:e:207:ASN:OD1	2.31	0.58
6:0:98:GLN:NE2	16:A:2709:A:N3	2.52	0.58
30:Q:165:GLU:HB2	30:Q:168:ASN:HB2	1.85	0.58
56:r:71:PRO:HD2	56:r:107:LEU:HD23	1.84	0.58
1:u:128:SER:HB2	1:u:185:ARG:HE	1.68	0.58
16:A:2016:C:OP2	26:M:59:ARG:NH1	2.36	0.58
30:Q:233:TRP:HB3	30:Q:240:ILE:HD12	1.84	0.58
16:A:1747:G:OP2	16:A:1749:C:N4	2.37	0.58
16:A:3219:G:O2'	16:A:3222:C:N4	2.34	0.58
4:x:86:VAL:HG21	4:x:154:GLU:HB2	1.85	0.58
11:5:98:LEU:HD13	11:5:272:ASP:HB2	1.85	0.58
16:A:1706:C:OP1	38:Y:193:ARG:NH2	2.35	0.58
35:V:130:PRO:O	35:V:149:ARG:NH2	2.37	0.58
36:W:100:THR:HG1	36:W:132:HIS:HE2	1.52	0.58
12:6:215:THR:HB	12:6:273:PHE:HB2	1.86	0.58
20:F:253:MET:HE3	20:F:259:LEU:HD22	1.85	0.58
24:K:28:PRO:HG3	24:K:65:ILE:HD12	1.86	0.58
6:0:96:ASN:OD1	16:A:2708:C:O2'	2.18	0.58
16:A:1883:G:H5'	46:g:91:MET:HG3	1.86	0.58
20:F:281:ARG:NH2	26:M:128:THR:OG1	2.36	0.58
20:F:232:GLU:O	20:F:236:ARG:NH1	2.37	0.57
24:K:25:MET:O	24:K:149:ARG:NH1	2.37	0.57
56:r:81:TYR:OH	56:r:111:GLU:OE1	2.21	0.57
13:7:275:CYS:HA	13:7:303:PRO:HA	1.85	0.57
28:O:143:THR:OG1	28:O:146:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:5:30:ALA:N	18:D:201:GLY:O	2.37	0.57
14:8:161:ALA:HB1	44:e:208:ALA:HA	1.87	0.57
16:A:1805:A:OP2	35:V:94:HIS:NE2	2.34	0.57
16:A:2180:A:O2'	16:A:2206:C:O3'	2.21	0.57
39:Z:105:SER:OG	53:o:59:GLU:OE2	2.20	0.57
9:3:104:ARG:NH2	16:A:1871:A:N3	2.52	0.57
20:F:70:ARG:HA	20:F:196:PRO:HD3	1.85	0.57
21:H:131:TYR:HB3	37:X:139:TYR:HD1	1.70	0.57
12:6:35:MET:HB2	12:6:38:SER:HB3	1.87	0.57
12:6:126:ARG:NH1	29:P:156:ASP:OD2	2.38	0.57
2:v:43:GLN:HG2	58:w:200:PM8:H431	1.87	0.57
16:A:2237:A:OP1	56:r:171:ARG:NH2	2.38	0.57
3:w:83:VAL:HG22	3:w:122:MET:HE1	1.88	0.56
13:7:243:LYS:NZ	13:7:265:GLU:OE1	2.38	0.56
16:A:1814:A:N3	16:A:1862:U:O2'	2.36	0.56
56:r:70:CYS:HB2	56:r:107:LEU:HA	1.86	0.56
1:u:120:TYR:O	25:L:128:ARG:NH1	2.39	0.56
16:A:1693:C:O2	38:Y:162:ARG:NH1	2.38	0.56
12:6:270:PHE:N	12:6:317:SER:O	2.34	0.56
35:V:55:TYR:HB2	35:V:133:ILE:HD11	1.87	0.56
16:A:2721:G:H1	16:A:3097:U:H3	1.51	0.56
41:b:72:VAL:HG13	41:b:90:HIS:HB2	1.88	0.56
4:x:272:ILE:HA	4:x:277:ARG:HE	1.69	0.56
9:3:188:VAL:O	12:6:356:ARG:NH2	2.39	0.56
11:5:201:ARG:NH1	11:5:418:TYR:O	2.35	0.56
16:A:2109:A:N6	27:N:61:LYS:O	2.38	0.56
16:A:2238:A:OP1	56:r:165:LYS:NZ	2.39	0.56
16:A:2310:G:O2'	16:A:2675:G:O6	2.22	0.56
16:A:1822:U:O2	16:A:2707:A:O2'	2.22	0.56
16:A:2943:G:H5"	53:o:20:LYS:HD2	1.88	0.56
31:R:112:THR:OG1	41:b:127:GLN:NE2	2.34	0.56
35:V:121:LYS:HD3	35:V:130:PRO:HB2	1.87	0.56
57:s:374:LEU:HD21	57:s:377:LEU:HD13	1.87	0.56
11:5:300:ARG:NH2	16:A:2394:A:O2'	2.39	0.56
33:T:52:VAL:HG22	43:d:227:ARG:HG3	1.87	0.56
35:V:48:PRO:HD3	38:Y:234:LEU:HD21	1.89	0.56
16:A:2107:G:H2'	16:A:2981:A:C8	2.42	0.55
35:V:16:PRO:HD2	35:V:19:TYR:HB2	1.87	0.55
35:V:80:ILE:HB	35:V:85:TRP:HB2	1.89	0.55
16:A:1763:A:N7	55:q:38:ARG:NH1	2.50	0.55
54:p:109:GLU:HA	54:p:116:ARG:HH21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:6:240:ILE:HG12	12:6:248:GLY:HA3	1.88	0.55
16:A:2822:C:O2'	16:A:2915:C:OP2	2.23	0.55
20:F:241:ASN:HD21	48:i:52:ALA:HB1	1.70	0.55
5:y:130:GLU:HG2	5:y:159:MET:HG2	1.87	0.55
20:F:248:LEU:O	48:i:59:ASN:ND2	2.38	0.55
42:c:245:LEU:HD12	42:c:253:PRO:HD3	1.88	0.55
50:k:10:LEU:O	50:k:46:ASN:ND2	2.31	0.55
16:A:2299:U:H5"	16:A:2300:G:H5"	1.87	0.55
44:e:214:THR:HG22	44:e:230:LYS:HG2	1.89	0.55
20:F:220:ASP:OD1	20:F:221:LEU:N	2.40	0.55
4:x:180:LEU:HD13	4:x:254:VAL:HG22	1.87	0.55
16:A:1742:G:O2'	16:A:1754:G:O6	2.24	0.55
16:A:2354:A:N6	16:A:2361:G:H1	2.04	0.55
32:S:100:HIS:HB2	32:S:134:LEU:HD11	1.89	0.55
33:T:57:LEU:HB2	33:T:60:GLU:HG3	1.89	0.54
34:U:81:ASP:HB3	34:U:87:ILE:HD11	1.88	0.54
16:A:1709:G:H4'	38:Y:192:LYS:HG3	1.89	0.54
16:A:2182:G:O2'	16:A:2199:A:OP2	2.25	0.54
16:A:2830:A:H5"	16:A:2831:G:H5"	1.89	0.54
20:F:62:VAL:HG23	20:F:82:LEU:HB2	1.89	0.54
57:s:204:CYS:SG	57:s:240:GLN:NE2	2.80	0.54
8:2:87:ARG:NH2	16:A:1792:G:N7	2.50	0.54
16:A:2332:C:H42	16:A:2442:U:H3	1.54	0.54
20:F:49:ARG:NH1	20:F:81:ASP:O	2.35	0.54
27:N:63:ARG:HH22	27:N:67:LYS:HG2	1.72	0.54
45:f:147:ASP:O	52:m:72:ARG:NH1	2.41	0.54
9:3:108:LYS:NZ	16:A:1745:U:O4	2.41	0.54
18:D:127:ILE:HD11	18:D:143:ALA:HB2	1.90	0.54
5:y:302:LEU:HA	5:y:306:ALA:HB3	1.89	0.54
16:A:1803:A:H4'	16:A:1804:A:H3'	1.89	0.54
41:b:49:ARG:HG3	41:b:50:GLU:HG2	1.88	0.54
25:L:98:PRO:HA	30:Q:162:ILE:HG12	1.90	0.54
11:5:166:THR:O	57:s:287:LYS:NZ	2.38	0.54
16:A:2138:U:O2'	16:A:2151:A:N3	2.41	0.54
15:9:130:LEU:HD13	38:Y:154:ARG:HA	1.90	0.54
16:A:2392:U:H2'	16:A:2394:A:H62	1.73	0.54
16:A:2458:A:O2'	19:E:215:PHE:O	2.25	0.54
16:A:2459:A:N6	16:A:2668:A:O2'	2.40	0.54
19:E:274:TRP:HE1	19:E:286:ASN:HB2	1.73	0.54
20:F:164:MET:HE3	48:i:69:HIS:HE1	1.73	0.54
45:f:48:TYR:HB3	45:f:51:LYS:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:5:270:ILE:O	16:A:2409:A:O2'	2.26	0.54
12:6:217:LEU:HD13	12:6:236:LEU:HD13	1.90	0.54
5:y:300:GLU:OE2	5:y:304:ARG:NH2	2.41	0.54
33:T:49:ASN:ND2	33:T:68:TYR:O	2.41	0.54
12:6:114:ARG:NH1	29:P:117:TYR:O	2.41	0.53
13:7:139:ASN:HB3	13:7:174:VAL:HG21	1.90	0.53
16:A:2093:U:H4'	48:i:126:LYS:HE2	1.89	0.53
16:A:2261:C:O2'	32:S:184:ARG:NH1	2.40	0.53
16:A:1760:G:N7	55:q:55:ARG:NH2	2.56	0.53
37:X:7:PRO:HD2	37:X:10:LEU:HD12	1.88	0.53
57:s:152:GLN:HA	57:s:156:TYR:HB2	1.90	0.53
16:A:1749:C:O2'	26:M:80:LYS:NZ	2.39	0.53
22:I:116:LEU:HB3	22:I:121:ILE:HB	1.91	0.53
22:I:188:ARG:HD3	50:k:55:VAL:HB	1.91	0.53
24:K:5:SER:HB2	24:K:8:PRO:HD2	1.90	0.53
32:S:142:THR:OG1	40:a:62:HIS:NE2	2.35	0.53
16:A:1787:G:N2	16:A:1790:A:OP2	2.29	0.53
15:9:24:LYS:NZ	16:A:2422:U:OP2	2.40	0.53
35:V:80:ILE:HD12	35:V:85:TRP:HE3	1.73	0.53
11:5:55:LEU:HD11	37:X:163:ARG:HE	1.72	0.53
14:8:101:ARG:NE	44:e:82:SER:O	2.36	0.53
17:B:1672:C:O2'	44:e:216:LYS:O	2.23	0.53
52:m:57:VAL:HG22	52:m:63:THR:HG22	1.90	0.53
5:y:178:ARG:HA	5:y:181:TYR:CZ	2.44	0.53
11:5:173:ARG:NH2	16:A:2395:A:OP1	2.26	0.53
13:7:177:GLY:HA3	13:7:319:ARG:HE	1.74	0.53
16:A:2107:G:H2'	16:A:2981:A:H8	1.72	0.53
42:c:139:GLN:NE2	42:c:143:ASP:OD2	2.42	0.53
16:A:1867:A:N1	16:A:2019:G:O2'	2.38	0.53
11:5:139:LEU:O	11:5:145:ASN:ND2	2.35	0.53
16:A:2519:G:N7	18:D:230:SER:OG	2.40	0.53
12:6:173:LEU:HD13	12:6:272:LEU:HD22	1.90	0.52
13:7:93:MET:O	33:T:132:SER:OG	2.26	0.52
27:N:123:ARG:NH1	27:N:162:GLU:OE1	2.42	0.52
57:s:373:GLN:NE2	57:s:375:ASN:OD1	2.39	0.52
20:F:223:HIS:HA	20:F:226:MET:HE3	1.91	0.52
32:S:119:GLU:HG2	32:S:121:ASP:H	1.74	0.52
39:Z:64:HIS:HE1	39:Z:67:HIS:CE1	2.26	0.52
4:x:252:VAL:HB	4:x:305:VAL:HG22	1.91	0.52
12:6:162:PHE:HB3	12:6:165:ALA:HB3	1.91	0.52
16:A:2071:U:H2'	16:A:2831:G:N2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:q:37:PRO:HG2	55:q:68:SER:HA	1.89	0.52
15:9:16:ASP:OD2	34:U:86:ARG:NH1	2.42	0.52
16:A:1831:G:O6	41:b:4:ARG:NH2	2.38	0.52
16:A:1859:A:OP1	16:A:2299:U:O2'	2.23	0.52
34:U:153:LEU:HD11	43:d:240:LYS:HB2	1.90	0.52
9:3:104:ARG:NH1	9:3:160:LYS:O	2.42	0.52
29:P:85:ARG:NH1	29:P:157:SER:OG	2.42	0.52
44:e:60:SER:O	44:e:136:ARG:NH2	2.41	0.52
33:T:51:ILE:O	43:d:227:ARG:NH1	2.43	0.52
10:4:84:ARG:NE	16:A:3188:U:OP2	2.40	0.52
13:7:202:PHE:HB2	13:7:280:VAL:HG21	1.92	0.52
16:A:2240:C:H5'	24:K:29:GLY:HA3	1.91	0.52
33:T:127:ASN:O	43:d:230:ARG:NH2	2.42	0.52
41:b:49:ARG:HH21	41:b:94:VAL:HG11	1.75	0.52
44:e:177:GLU:O	44:e:190:ARG:NH2	2.43	0.52
16:A:1737:A:H61	16:A:1760:G:H1'	1.75	0.52
42:c:57:PRO:HB2	42:c:184:PHE:HE2	1.74	0.52
44:e:162:ARG:HD2	44:e:169:ASP:HB3	1.92	0.52
5:y:131:PHE:HE2	5:y:145:LEU:HD21	1.73	0.52
5:y:215:ILE:HD11	5:y:249:VAL:HG22	1.92	0.52
12:6:217:LEU:HB3	12:6:271:LEU:HB2	1.92	0.52
14:8:124:TYR:OH	44:e:67:GLN:NE2	2.43	0.52
34:U:69:ARG:NH1	34:U:98:GLN:OE1	2.37	0.52
42:c:157:VAL:O	42:c:161:THR:OG1	2.22	0.52
45:f:127:MET:HE3	45:f:128:PRO:HD2	1.92	0.52
10:4:87:ARG:HH11	10:4:101:ARG:HD3	1.75	0.52
45:f:101:THR:OG1	52:m:67:ARG:NH1	2.42	0.52
12:6:56:ARG:NH1	17:B:1625:A:OP1	2.40	0.51
20:F:216:VAL:HG22	20:F:258:THR:HB	1.92	0.51
38:Y:126:MET:HB3	38:Y:129:PRO:HG3	1.92	0.51
44:e:128:PHE:HD1	52:m:74:MET:HB3	1.75	0.51
4:x:299:THR:O	4:x:382:ARG:NH1	2.43	0.51
57:s:419:LEU:O	57:s:423:HIS:ND1	2.41	0.51
9:3:138:PRO:HG2	16:A:2854:U:H4'	1.91	0.51
16:A:1868:G:H2'	26:M:40:PRO:HG3	1.91	0.51
48:i:57:TYR:OH	55:q:28:ARG:O	2.28	0.51
20:F:103:GLN:O	20:F:107:LYS:NZ	2.43	0.51
26:M:31:PRO:HG2	53:o:86:ARG:HH12	1.76	0.51
16:A:2710:C:O2'	16:A:3220:A:N1	2.39	0.51
32:S:127:ARG:NH1	32:S:157:GLU:OE1	2.43	0.51
39:Z:134:MET:HE1	49:j:78:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:x:82:ALA:HA	55:q:153:ARG:HE	1.76	0.51
11:5:268:CYS:SG	16:A:2409:A:O2'	2.62	0.51
16:A:3125:A:H62	16:A:3132:G:H21	1.58	0.51
23:J:149:ARG:HH12	51:l:104:PRO:HD3	1.75	0.51
25:L:70:GLY:O	25:L:134:TYR:OH	2.27	0.51
26:M:156:VAL:O	26:M:176:THR:HA	2.10	0.51
43:d:245:TYR:HB2	43:d:265:ILE:HB	1.91	0.51
11:5:384:GLN:NE2	16:A:2395:A:O2'	2.44	0.51
40:a:62:HIS:O	40:a:62:HIS:ND1	2.44	0.51
56:r:166:GLY:O	56:r:171:ARG:NH1	2.44	0.51
2:v:45:LEU:O	2:v:51:ARG:NE	2.34	0.51
20:F:128:TRP:HB2	20:F:133:THR:HG21	1.92	0.50
49:j:63:GLN:OE1	49:j:66:ARG:NH2	2.39	0.50
16:A:3109:U:H3'	16:A:3110:C:H4'	1.93	0.50
44:e:90:ARG:NH2	44:e:113:ASP:OD2	2.45	0.50
44:e:147:THR:HG21	44:e:248:ASN:HB3	1.92	0.50
5:y:236:TYR:CE1	5:y:240:ARG:HD3	2.46	0.50
11:5:47:ASP:OD1	11:5:47:ASP:N	2.44	0.50
16:A:1879:G:OP1	20:F:92:ARG:NH1	2.39	0.50
16:A:3152:C:OP1	30:Q:141:SER:OG	2.21	0.50
16:A:2998:U:H5"	19:E:225:LYS:HB2	1.93	0.50
57:s:239:ASN:HB2	57:s:299:PHE:HB2	1.92	0.50
13:7:77:THR:HG21	13:7:95:LEU:HD21	1.94	0.50
16:A:2470:G:HO2'	25:L:36:THR:HG1	1.58	0.50
44:e:70:MET:HE3	44:e:74:LEU:HD21	1.93	0.50
47:h:71:GLU:HG2	47:h:75:LYS:HE3	1.94	0.50
5:y:211:GLN:HB3	5:y:249:VAL:HG21	1.93	0.50
16:A:2943:G:O3'	53:o:20:LYS:NZ	2.38	0.50
17:B:1613:U:O2'	17:B:1615:A:OP1	2.29	0.50
47:h:69:ARG:O	47:h:72:SER:OG	2.25	0.50
11:5:211:ALA:HB1	11:5:322:LEU:HD23	1.94	0.50
16:A:1828:A:O2'	16:A:2684:C:N3	2.38	0.50
16:A:2245:A:H1'	16:A:2246:A:C8	2.46	0.50
4:x:72:LYS:H	4:x:371:ASN:HB3	1.76	0.50
16:A:3176:A:H61	16:A:3193:U:H3	1.60	0.50
28:O:18:MET:HE1	28:O:29:LEU:HD21	1.92	0.50
35:V:69:ASP:HB2	35:V:72:LYS:HD2	1.93	0.50
48:i:69:HIS:HB3	48:i:72:GLU:HG3	1.94	0.50
16:A:2917:G:N7	26:M:72:THR:OG1	2.45	0.50
19:E:221:ARG:HG3	19:E:261:MET:HB3	1.92	0.50
43:d:164:VAL:HG12	43:d:261:MET:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:j:91:TRP:CD2	53:o:58:GLN:HG2	2.47	0.50
12:6:74:TYR:N	36:W:102:GLU:OE2	2.45	0.49
13:7:159:LYS:HZ3	40:a:93:LYS:HA	1.78	0.49
16:A:1830:G:H5"	41:b:2:THC:HG21	1.94	0.49
17:B:1608:G:O2'	17:B:1647:U:OP2	2.27	0.49
20:F:102:TRP:NE1	20:F:163:TYR:O	2.43	0.49
35:V:52:GLU:HB3	35:V:143:ARG:HH12	1.77	0.49
35:V:65:LEU:HD11	35:V:121:LYS:HB2	1.93	0.49
45:f:81:ASN:HD22	45:f:90:VAL:HG23	1.77	0.49
38:Y:191:ASN:O	38:Y:195:ASN:ND2	2.32	0.49
12:6:27:ARG:N	16:A:2073:A:OP2	2.46	0.49
57:s:376:THR:HB	57:s:389:ARG:HG3	1.94	0.49
12:6:243:ASN:OD1	12:6:243:ASN:N	2.44	0.49
16:A:2127:A:H4'	16:A:2251:A:C5	2.47	0.49
20:F:175:LYS:HE2	20:F:273:LEU:HB3	1.94	0.49
27:N:124:VAL:HG12	27:N:158:ARG:HE	1.77	0.49
4:x:129:LEU:HD13	4:x:163:LEU:HD11	1.93	0.49
12:6:206:TYR:O	12:6:243:ASN:ND2	2.45	0.49
16:A:1878:U:H5'	46:g:144:THR:HG21	1.95	0.49
16:A:1886:G:N7	20:F:170:ARG:NH2	2.47	0.49
29:P:80:ARG:NH2	29:P:95:GLU:OE2	2.45	0.49
45:f:105:SER:HB2	52:m:41:THR:HG21	1.94	0.49
49:j:87:GLY:HA3	53:o:62:HIS:HB2	1.94	0.49
57:s:66:TRP:O	57:s:69:THR:OG1	2.25	0.49
12:6:306:LYS:HG3	12:6:307:HIS:ND1	2.27	0.49
16:A:1882:A:N1	16:A:1891:A:O2'	2.46	0.49
16:A:2860:G:O2'	36:W:65:ASN:OD1	2.22	0.49
16:A:3073:C:C2	43:d:37:THR:HG21	2.48	0.49
21:H:78:ARG:NH1	37:X:87:LEU:O	2.43	0.49
54:p:108:ALA:O	54:p:116:ARG:NE	2.43	0.49
56:r:40:GLU:HG2	56:r:49:ILE:HG12	1.94	0.49
1:u:115:PRO:HG2	1:u:118:MET:HG2	1.95	0.49
1:u:190:LEU:HD23	1:u:193:LEU:HD12	1.95	0.49
5:y:99:LEU:HD12	5:y:109:ILE:HG23	1.94	0.49
12:6:311:MET:O	49:j:112:LYS:NZ	2.46	0.49
23:J:101:ALA:HB2	23:J:109:ALA:HB2	1.93	0.49
16:A:2755:A:OP2	21:H:91:LYS:NZ	2.40	0.49
57:s:316:CYS:HB3	57:s:319:GLN:HB2	1.94	0.49
12:6:155:TYR:HE2	12:6:320:GLN:HE21	1.61	0.49
16:A:2328:C:N4	57:s:52:THR:O	2.41	0.49
21:H:53:THR:N	21:H:86:THR:OG1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:L:75:LEU:HD11	25:L:105:VAL:HG21	1.95	0.49
43:d:182:ARG:HD2	43:d:225:TYR:HE2	1.78	0.49
11:5:96:HIS:HD1	16:A:2410:U:HO2'	1.56	0.48
13:7:166:LEU:HB3	13:7:181:TYR:HE1	1.78	0.48
45:f:106:TYR:OH	45:f:174:ILE:O	2.28	0.48
52:m:56:LEU:HB3	52:m:64:ILE:HG13	1.93	0.48
4:x:66:SER:O	4:x:262:ARG:NH1	2.40	0.48
11:5:167:THR:HG21	57:s:281:HIS:CD2	2.48	0.48
12:6:85:LYS:HZ1	49:j:106:GLU:HG2	1.79	0.48
12:6:224:HIS:CE1	12:6:227:GLU:H	2.31	0.48
16:A:2204:U:N3	16:A:2207:A:OP2	2.46	0.48
16:A:2830:A:O4'	16:A:2837:A:N6	2.46	0.48
42:c:242:VAL:HG12	42:c:246:LYS:HE3	1.93	0.48
57:s:332:LEU:HD21	57:s:359:ALA:HB2	1.95	0.48
16:A:1886:G:H1	48:i:61:GLY:HA3	1.77	0.48
16:A:2737:U:O2'	16:A:3084:A:N3	2.43	0.48
22:I:146:LEU:O	22:I:151:ASN:ND2	2.46	0.48
6:0:82:LYS:NZ	16:A:2719:G:O3'	2.47	0.48
6:0:179:ARG:HH12	6:0:182:PRO:HG3	1.78	0.48
20:F:243:ILE:HG22	55:q:27:ALA:HB2	1.95	0.48
25:L:42:ASP:HB2	25:L:116:GLY:HA3	1.95	0.48
42:c:168:HIS:O	42:c:172:ASN:ND2	2.45	0.48
50:k:65:ASP:OD2	50:k:73:ARG:NH2	2.47	0.48
4:x:105:HIS:HB2	4:x:347:VAL:HG13	1.95	0.48
16:A:1672:C:O2'	33:T:143:ARG:O	2.24	0.48
16:A:1977:U:H2'	16:A:1978:A:C8	2.48	0.48
16:A:3008:C:O2'	16:A:3051:A:N3	2.43	0.48
20:F:66:VAL:O	20:F:77:VAL:N	2.46	0.48
20:F:164:MET:HE3	48:i:69:HIS:CE1	2.48	0.48
29:P:102:VAL:HG11	29:P:141:ILE:HG13	1.94	0.48
16:A:2361:G:H5'	16:A:2362:A:H5"	1.94	0.48
22:I:166:ARG:HA	22:I:169:ARG:HE	1.79	0.48
2:v:29:ASP:OD1	2:v:29:ASP:N	2.47	0.48
3:w:103:HIS:HE1	3:w:105:MET:HE2	1.78	0.48
3:w:108:LEU:HB3	3:w:110:LEU:HG	1.95	0.48
12:6:260:ALA:O	12:6:263:SER:OG	2.32	0.48
16:A:2256:U:O2'	32:S:118:ASN:ND2	2.46	0.48
25:L:145:VAL:HG11	30:Q:160:VAL:HG11	1.95	0.48
30:Q:103:ARG:HG2	30:Q:108:ILE:HD12	1.95	0.48
44:e:164:LYS:HE2	44:e:167:ASP:HA	1.96	0.48
2:v:12:LEU:HD21	2:v:59:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:8:100:GLU:HA	44:e:83:LEU:HD22	1.96	0.48
15:9:110:ASP:OD1	15:9:110:ASP:N	2.45	0.48
16:A:2137:C:OP2	39:Z:77:ARG:NH1	2.46	0.48
16:A:3151:A:H4'	30:Q:146:GLY:O	2.14	0.48
18:D:185:GLY:N	18:D:238:GLU:O	2.46	0.48
24:K:22:ASP:HB3	24:K:147:GLN:HE21	1.79	0.48
35:V:190:CYS:SG	35:V:191:LEU:N	2.85	0.48
44:e:87:HIS:NE2	44:e:121:GLU:OE2	2.43	0.48
13:7:87:THR:O	13:7:90:SER:OG	2.24	0.48
16:A:2147:G:OP1	32:S:104:ARG:NE	2.43	0.48
19:E:52:HIS:HB2	28:O:145:LEU:HD23	1.96	0.48
19:E:334:ASP:HB3	19:E:337:VAL:HG23	1.94	0.48
22:I:56:PRO:HB3	27:N:210:GLN:HE21	1.79	0.48
31:R:141:ILE:HG22	40:a:51:LEU:HD12	1.96	0.48
40:a:40:PRO:HG2	40:a:43:TYR:HE1	1.79	0.48
4:x:258:CYS:HA	4:x:284:LEU:HD21	1.95	0.48
11:5:201:ARG:HB3	11:5:232:THR:HG22	1.96	0.48
12:6:85:LYS:HZ3	49:j:109:LEU:HD12	1.79	0.48
44:e:88:GLU:OE2	52:m:50:ARG:NH1	2.42	0.48
11:5:173:ARG:HD2	11:5:303:ARG:HD3	1.96	0.47
30:Q:168:ASN:HD21	30:Q:170:ARG:HD3	1.79	0.47
41:b:26:LEU:HD22	41:b:105:ALA:HA	1.96	0.47
41:b:34:SER:O	41:b:44:ARG:NH1	2.40	0.47
40:a:104:GLU:HB2	40:a:107:PRO:HD2	1.96	0.47
11:5:192:ILE:HG12	11:5:198:LEU:HB2	1.95	0.47
13:7:255:HIS:CD2	13:7:264:SER:HB2	2.49	0.47
16:A:1871:A:N7	16:A:1902:C:N4	2.61	0.47
18:D:215:VAL:HB	18:D:227:GLN:HB3	1.95	0.47
18:D:216:LEU:HD21	18:D:219:LYS:HD3	1.97	0.47
20:F:286:PHE:HA	20:F:290:TYR:HE2	1.79	0.47
30:Q:153:ASN:OD1	30:Q:154:VAL:N	2.47	0.47
4:x:312:LEU:HD23	4:x:363:LEU:HD11	1.96	0.47
16:A:1874:A:HO2'	16:A:2090:A:HO2'	1.63	0.47
16:A:2198:A:N6	23:J:150:SER:HB2	2.29	0.47
20:F:275:TRP:HD1	20:F:295:ARG:HH21	1.62	0.47
26:M:287:ASP:HB3	26:M:290:LEU:HB2	1.95	0.47
29:P:122:VAL:HG13	29:P:157:SER:HA	1.94	0.47
12:6:376:THR:HG22	54:p:141:ARG:HH12	1.80	0.47
16:A:1869:A:N6	48:i:116:TYR:OH	2.46	0.47
16:A:1936:A:H1'	16:A:1938:A:C6	2.50	0.47
16:A:2107:G:H1	16:A:2114:C:H42	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:E:76:LYS:HG3	19:E:170:LEU:HD21	1.96	0.47
57:s:242:ARG:NH1	57:s:290:ASP:OD2	2.47	0.47
7:1:18:VAL:HG11	7:1:34:ARG:HE	1.79	0.47
13:7:298:GLN:NE2	13:7:320:SER:O	2.48	0.47
2:v:6:ARG:NH2	58:w:200:PM8:O23	2.47	0.47
12:6:61:ALA:HB1	36:W:103:VAL:HG11	1.97	0.47
12:6:92:LEU:HB2	12:6:170:ARG:HG3	1.95	0.47
16:A:2110:A:O2'	16:A:2981:A:N6	2.47	0.47
16:A:3083:U:OP1	18:D:297:LYS:NZ	2.33	0.47
41:b:27:GLN:NE2	42:c:177:GLN:OE1	2.36	0.47
42:c:92:PHE:HB3	42:c:179:THR:HA	1.96	0.47
54:p:128:ASN:HD21	54:p:132:GLU:HB2	1.79	0.47
5:y:214:LYS:HE3	5:y:249:VAL:HG11	1.96	0.47
14:8:117:LEU:HD23	44:e:73:LEU:HD22	1.97	0.47
50:k:54:ASP:OD1	50:k:54:ASP:N	2.47	0.47
7:1:63:ARG:NH1	16:A:2909:G:OP1	2.39	0.47
12:6:215:THR:HG23	12:6:238:THR:HG22	1.96	0.47
16:A:2682:A:OP1	31:R:34:ARG:NH2	2.42	0.47
26:M:28:LYS:HD3	53:o:94:HIS:CD2	2.49	0.47
50:k:75:ILE:HD12	56:r:48:ILE:HG12	1.97	0.47
2:v:43:GLN:HB3	58:w:200:PM8:H36	1.80	0.47
4:x:192:LEU:HD13	4:x:221:VAL:HG21	1.97	0.47
13:7:106:ALA:O	13:7:113:TRP:N	2.48	0.47
16:A:2072:A:H62	16:A:2831:G:H2'	1.80	0.47
39:Z:66:LEU:HD12	39:Z:122:LEU:HD23	1.97	0.47
50:k:27:VAL:HG12	50:k:62:PRO:HG3	1.97	0.47
2:v:3:PRO:HB3	58:w:200:PM8:H371	1.96	0.46
11:5:204:VAL:HG11	11:5:279:PHE:HZ	1.80	0.46
14:8:178:TYR:O	44:e:136:ARG:NH1	2.48	0.46
47:h:57:SER:OG	47:h:136:ASP:OD2	2.32	0.46
4:x:342:THR:HG22	4:x:346:ARG:HE	1.80	0.46
5:y:104:PHE:HE2	5:y:132:ILE:HD11	1.80	0.46
5:y:243:ILE:HD13	5:y:290:LEU:HD22	1.98	0.46
16:A:1800:G:N1	16:A:1803:A:OP2	2.49	0.46
20:F:291:SER:OG	46:g:52:LEU:O	2.33	0.46
56:r:96:HIS:CE1	56:r:134:ARG:HB2	2.50	0.46
5:y:237:ALA:HB2	5:y:253:TYR:CZ	2.50	0.46
16:A:1974:A:H5'	18:D:261:GLY:HA2	1.98	0.46
16:A:2693:A:H4'	16:A:2694:A:H8	1.80	0.46
23:J:159:LEU:HD21	23:J:164:LEU:HD13	1.96	0.46
28:O:33:LEU:HD21	28:O:59:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:y:186:ILE:O	5:y:189:MET:HG2	2.16	0.46
12:6:239:ASN:OD1	12:6:275:GLN:NE2	2.44	0.46
20:F:184:GLN:HE22	26:M:22:VAL:HG23	1.81	0.46
22:I:76:ILE:HG22	22:I:78:LEU:H	1.81	0.46
50:k:76:MET:HG2	56:r:49:ILE:HD12	1.97	0.46
52:m:55:LEU:O	52:m:75:LEU:N	2.47	0.46
16:A:1812:C:O2'	42:c:48:GLN:OE1	2.32	0.46
17:B:1617:C:OP2	17:B:1656:A:N6	2.34	0.46
27:N:70:SER:O	27:N:155:LYS:NZ	2.49	0.46
29:P:65:GLU:OE1	29:P:97:GLN:NE2	2.49	0.46
4:x:45:LEU:HD21	4:x:64:ARG:HH21	1.81	0.46
17:B:1644:G:O6	29:P:88:HIS:NE2	2.47	0.46
42:c:44:GLU:OE2	42:c:48:GLN:NE2	2.49	0.46
16:A:2034:A:O2'	26:M:71:GLN:OE1	2.24	0.46
16:A:2795:U:H2'	16:A:2796:G:H8	1.81	0.46
26:M:51:ARG:HB3	26:M:58:GLN:HA	1.98	0.46
57:s:145:VAL:HG21	57:s:187:LEU:HD11	1.96	0.46
11:5:165:GLN:NE2	11:5:175:THR:HG22	2.30	0.46
13:7:148:MET:HE2	13:7:257:ILE:HG13	1.98	0.46
13:7:150:MET:O	13:7:154:ILE:HG12	2.16	0.46
16:A:2071:U:H2'	16:A:2831:G:H22	1.81	0.46
16:A:2529:U:H2'	18:D:208:ARG:HB2	1.98	0.46
16:A:3024:U:H2'	16:A:3025:A:C8	2.50	0.46
44:e:146:ARG:HD3	44:e:255:VAL:HG12	1.97	0.46
1:u:119:ARG:HD2	25:L:125:THR:HG21	1.98	0.46
1:u:164:THR:HG22	25:L:111:ASN:HB2	1.98	0.46
4:x:177:VAL:HG11	4:x:191:LEU:HD13	1.98	0.46
4:x:368:LEU:HD12	5:y:312:GLU:HB3	1.97	0.46
12:6:215:THR:OG1	12:6:275:GLN:OE1	2.34	0.46
16:A:1995:A:H4'	16:A:2499:U:H4'	1.98	0.46
16:A:2030:U:H4'	16:A:2031:A:O5'	2.16	0.46
44:e:156:ASN:OD1	44:e:157:LEU:N	2.48	0.46
5:y:112:LEU:HD13	5:y:128:ILE:HD13	1.99	0.45
16:A:2468:A:H61	16:A:2659:C:H42	1.63	0.45
29:P:54:ARG:HH12	29:P:140:GLY:C	2.24	0.45
4:x:187:LYS:HD3	4:x:253:LEU:HD21	1.97	0.45
12:6:99:ARG:NH2	17:B:1621:A:O5'	2.49	0.45
16:A:1798:A:N3	35:V:42:ARG:NH2	2.64	0.45
16:A:1992:C:C4	18:D:274:ARG:HB2	2.52	0.45
16:A:2131:A:OP1	53:o:23:ARG:NH1	2.49	0.45
16:A:2293:A:N6	26:M:37:GLU:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Q:91:LYS:HA	30:Q:94:ILE:HD12	1.98	0.45
30:Q:210:GLU:HB2	30:Q:213:GLN:HG3	1.97	0.45
37:X:156:LYS:NZ	37:X:205:GLY:O	2.48	0.45
53:o:17:TRP:HZ3	53:o:25:ARG:HB2	1.81	0.45
57:s:211:VAL:HG22	57:s:230:ARG:HG2	1.97	0.45
1:u:127:VAL:HG11	1:u:138:MET:HE1	1.99	0.45
5:y:181:TYR:CE1	16:A:3259:N:H4'	2.51	0.45
16:A:2230:A:H62	16:A:2975:G:H1'	1.82	0.45
16:A:2959:G:H2'	16:A:2962:C:H42	1.81	0.45
17:B:1642:G:H2'	17:B:1643:A:C8	2.51	0.45
1:u:113:GLN:N	2:v:68:ARG:O	2.41	0.45
5:y:252:GLU:O	5:y:255:GLN:HG2	2.16	0.45
19:E:99:LEU:HD22	19:E:193:LEU:HB3	1.99	0.45
21:H:75:ARG:NH2	37:X:100:ARG:HH22	2.15	0.45
24:K:67:PHE:HB3	24:K:71:LYS:HB2	1.97	0.45
29:P:102:VAL:HG12	29:P:103:VAL:HG13	1.98	0.45
31:R:26:LYS:HE3	31:R:27:HIS:CE1	2.52	0.45
44:e:151:ARG:NH2	44:e:259:GLU:OE2	2.47	0.45
7:1:20:MET:HB3	7:1:56:PHE:HB3	1.98	0.45
12:6:217:LEU:HD23	12:6:271:LEU:HD12	1.99	0.45
16:A:1761:A:H2'	16:A:1762:A:C8	2.51	0.45
31:R:83:TYR:CZ	31:R:87:ILE:HG13	2.52	0.45
35:V:69:ASP:OD1	35:V:69:ASP:N	2.49	0.45
3:w:90:TYR:HE1	3:w:92:LYS:HB3	1.80	0.45
4:x:200:LEU:N	4:x:230:GLN:O	2.43	0.45
15:9:136:LEU:HD21	34:U:7:TYR:HA	1.97	0.45
16:A:3063:G:N2	16:A:3063:G:OP1	2.50	0.45
19:E:50:ASP:O	28:O:138:ARG:NH2	2.50	0.45
24:K:169:LEU:HD22	56:r:75:TRP:CD1	2.52	0.45
36:W:76:HIS:NE2	36:W:128:LYS:HD3	2.32	0.45
41:b:30:SER:HB2	41:b:76:VAL:HB	1.99	0.45
4:x:65:VAL:HG12	4:x:368:LEU:HD21	1.99	0.45
6:0:96:ASN:HD22	6:0:98:GLN:HB3	1.81	0.45
16:A:2634:U:H2'	16:A:2635:G:H8	1.82	0.45
17:B:1628:C:H2'	17:B:1629:A:H8	1.82	0.45
45:f:121:VAL:HG22	45:f:159:ILE:HG22	1.97	0.45
3:w:90:TYR:HB3	3:w:93:ILE:HG12	1.99	0.45
5:y:302:LEU:O	5:y:307:CYS:N	2.42	0.45
11:5:136:VAL:HG11	11:5:417:LEU:HD23	1.98	0.45
14:8:178:TYR:N	52:m:63:THR:O	2.44	0.45
20:F:295:ARG:HH22	46:g:56:ARG:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:240:LYS:NZ	27:N:250:ARG:O	2.50	0.45
14:8:99:ARG:HG2	44:e:89:LEU:HD11	1.98	0.45
15:9:86:LEU:N	38:Y:148:GLU:OE2	2.49	0.45
16:A:2944:C:C6	53:o:20:LYS:HE3	2.52	0.45
22:I:48:MET:O	27:N:250:ARG:NH1	2.47	0.45
46:g:105:ARG:NH2	53:o:83:PRO:HD3	2.31	0.45
16:A:1697:A:N3	16:A:1703:C:O2'	2.50	0.45
43:d:267:PRO:HG2	43:d:270:ALA:HB2	1.99	0.45
4:x:288:GLN:NE2	4:x:316:GLN:HE21	2.13	0.44
15:9:68:PHE:CE2	15:9:70:LEU:HB2	2.52	0.44
16:A:2240:C:O2'	24:K:30:LYS:NZ	2.49	0.44
16:A:2795:U:H2'	16:A:2796:G:C8	2.52	0.44
16:A:2926:A:O2'	16:A:3087:C:OP1	2.23	0.44
18:D:111:ARG:NH2	18:D:165:ASN:OD1	2.42	0.44
50:k:77:ARG:HD2	56:r:50:GLU:HG2	1.98	0.44
54:p:97:SER:O	54:p:146:ASN:ND2	2.50	0.44
13:7:227:LEU:HD22	13:7:237:VAL:HG13	1.98	0.44
16:A:1744:A:OP1	26:M:87:HIS:NE2	2.39	0.44
16:A:2168:U:O2'	16:A:2169:A:O4'	2.33	0.44
16:A:2847:C:H2'	16:A:2848:A:O4'	2.17	0.44
20:F:220:ASP:O	20:F:245:ALA:N	2.51	0.44
55:q:147:GLN:NE2	55:q:151:GLU:OE2	2.49	0.44
5:y:98:SER:O	5:y:102:MET:HG2	2.17	0.44
12:6:48:LEU:O	12:6:50:LYS:NZ	2.44	0.44
12:6:257:PRO:HB3	12:6:268:LEU:HD21	1.97	0.44
16:A:1984:A:N1	16:A:1997:C:O2'	2.38	0.44
16:A:2361:G:H5"	16:A:2362:A:H8	1.81	0.44
20:F:231:VAL:HG13	55:q:26:ARG:HD2	1.99	0.44
24:K:4:PHE:HB2	24:K:9:GLN:HB2	1.99	0.44
33:T:122:ALA:HB1	33:T:128:VAL:HG21	1.99	0.44
51:l:64:ASP:HB3	51:l:67:GLN:HB3	1.99	0.44
4:x:141:ARG:HH22	5:y:322:ARG:HD3	1.81	0.44
16:A:1886:G:OP1	20:F:167:MET:N	2.48	0.44
16:A:1907:A:N3	16:A:2930:U:O2'	2.47	0.44
22:I:132:LYS:HB2	22:I:133:PRO:HD3	1.99	0.44
42:c:123:GLN:OE1	42:c:193:GLN:NE2	2.50	0.44
44:e:160:LEU:HD11	44:e:260:LEU:HD12	1.98	0.44
11:5:139:LEU:HD22	11:5:423:ALA:HB3	2.00	0.44
16:A:1770:G:H4'	20:F:112:ALA:HB2	1.99	0.44
16:A:1939:G:C5	18:D:259:LYS:HB2	2.53	0.44
28:O:46:TRP:HD1	28:O:121:ALA:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Y:128:SER:HB2	38:Y:131:ARG:NE	2.33	0.44
56:r:117:GLU:HG3	56:r:180:LEU:HD12	1.99	0.44
1:u:140:PHE:HA	1:u:143:VAL:HG12	2.00	0.44
12:6:228:PRO:HB3	29:P:49:THR:HB	2.00	0.44
16:A:2449:G:OP2	57:s:225:ARG:NH2	2.48	0.44
27:N:55:ARG:HG2	27:N:99:TRP:CD1	2.53	0.44
50:k:75:ILE:HB	56:r:48:ILE:HA	2.00	0.44
3:w:103:HIS:ND1	3:w:106:LYS:HG2	2.32	0.44
14:8:125:LYS:NZ	52:m:37:ARG:O	2.51	0.44
16:A:2754:A:N3	37:X:108:GLN:NE2	2.65	0.44
18:D:199:GLU:HG2	18:D:202:ARG:HB2	2.00	0.44
21:H:119:GLY:HA2	21:H:123:LEU:HB2	2.00	0.44
31:R:112:THR:HG23	32:S:142:THR:HG21	1.99	0.44
35:V:44:VAL:HG21	35:V:83:ARG:HH21	1.82	0.44
1:u:121:THR:HG21	1:u:176:VAL:HG12	2.00	0.44
3:w:80:GLN:HG2	3:w:145:VAL:HG11	1.98	0.44
16:A:1998:U:OP1	16:A:2001:C:N4	2.35	0.44
16:A:2454:G:OP1	28:O:48:ARG:NH2	2.48	0.44
16:A:3214:C:OP1	28:O:119:LYS:NZ	2.48	0.44
26:M:180:ASP:OD1	26:M:180:ASP:N	2.40	0.44
32:S:67:PRO:HG3	40:a:36:TYR:HB3	2.00	0.44
34:U:141:ASP:HB3	34:U:144:ARG:HG2	1.98	0.44
12:6:234:HIS:ND1	12:6:255:LEU:O	2.50	0.44
13:7:45:ASN:HD21	13:7:259:ASP:HA	1.83	0.44
15:9:24:LYS:HG2	16:A:2421:G:H5"	1.99	0.44
16:A:1861:U:H2'	16:A:1862:U:C6	2.52	0.44
16:A:2065:A:H5'	36:W:74:ARG:HE	1.83	0.44
16:A:3141:A:H4'	25:L:130:ARG:HH22	1.82	0.44
21:H:84:GLU:OE1	37:X:44:ARG:NH2	2.50	0.44
13:7:203:THR:O	13:7:207:HIS:ND1	2.34	0.43
16:A:2724:G:H2'	16:A:2725:A:H8	1.83	0.43
34:U:142:PRO:O	43:d:280:VAL:HG11	2.18	0.43
44:e:53:LEU:HD21	44:e:238:LEU:HD13	1.99	0.43
52:m:51:LEU:HB3	52:m:67:ARG:HB3	1.99	0.43
57:s:91:TYR:HE1	57:s:229:LEU:HD22	1.82	0.43
4:x:136:ARG:NH1	4:x:350:ASP:O	2.46	0.43
20:F:138:HIS:CD2	20:F:146:TRP:HE1	2.36	0.43
25:L:46:LEU:HD12	25:L:78:LYS:HD3	2.00	0.43
27:N:73:ARG:O	27:N:155:LYS:NZ	2.51	0.43
43:d:241:ASP:OD1	43:d:241:ASP:N	2.52	0.43
57:s:105:TRP:CG	57:s:271:LEU:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:1741:A:N1	16:A:1755:A:H5"	2.34	0.43
16:A:2512:A:O2'	16:A:2541:C:OP1	2.29	0.43
18:D:188:PRO:HG2	18:D:191:THR:OG1	2.18	0.43
28:O:116:ASP:OD1	28:O:116:ASP:N	2.50	0.43
43:d:152:LEU:HD21	43:d:172:MET:HE2	1.99	0.43
47:h:140:PHE:HB2	47:h:156:TRP:CE3	2.54	0.43
57:s:237:PRO:HB3	57:s:300:HIS:CE1	2.53	0.43
12:6:279:ILE:HG21	12:6:307:HIS:HD2	1.82	0.43
16:A:2017:U:O2	20:F:137:ARG:NH2	2.52	0.43
16:A:2180:A:H4'	16:A:2181:A:C8	2.54	0.43
16:A:2685:U:O2'	16:A:3104:U:H5'	2.19	0.43
4:x:154:GLU:HG3	4:x:155:TYR:CD2	2.54	0.43
4:x:355:PHE:CE2	4:x:357:SER:HB2	2.53	0.43
5:y:139:GLU:HB3	5:y:140:PRO:HD3	2.01	0.43
9:3:127:ALA:HA	26:M:79:PRO:HD3	2.00	0.43
16:A:2100:C:H1'	16:A:2135:A:C8	2.53	0.43
16:A:2724:G:H2'	16:A:2725:A:C8	2.53	0.43
19:E:106:MET:HE2	19:E:118:VAL:HG22	1.99	0.43
27:N:96:TYR:HB3	27:N:151:VAL:HB	2.01	0.43
5:y:102:MET:HG3	5:y:132:ILE:HD13	2.00	0.43
5:y:235:GLN:HE22	18:D:289:LEU:H	1.65	0.43
12:6:120:GLU:OE2	14:8:119:LYS:NZ	2.37	0.43
30:Q:113:VAL:HG11	30:Q:186:SER:HA	1.99	0.43
33:T:73:GLN:H	33:T:167:HIS:CE1	2.36	0.43
54:p:135:LEU:HD21	54:p:157:MET:HE1	2.00	0.43
57:s:174:LEU:HB3	57:s:175:PRO:HD3	2.00	0.43
6:0:84:ARG:NH2	16:A:2306:A:O2'	2.43	0.43
16:A:2072:A:N6	16:A:2831:G:H2'	2.34	0.43
16:A:2294:A:H1'	31:R:20:ARG:HH12	1.84	0.43
17:B:1643:A:H62	29:P:120:ARG:HH12	1.65	0.43
18:D:193:ILE:HD11	18:D:226:ILE:HG23	2.01	0.43
21:H:56:VAL:HG12	21:H:82:LEU:HA	2.00	0.43
31:R:108:TYR:HD1	41:b:125:SER:HB2	1.84	0.43
33:T:44:LYS:O	33:T:48:LYS:HG3	2.19	0.43
35:V:206:GLU:OE2	35:V:208:ARG:NE	2.40	0.43
11:5:177:CYS:HB3	11:5:178:PRO:HD3	2.01	0.43
15:9:131:TYR:HA	15:9:132:PRO:HA	1.90	0.43
16:A:2197:G:O2'	16:A:2199:A:H5'	2.19	0.43
18:D:210:ALA:HB1	18:D:249:ASN:HB2	2.00	0.43
23:J:122:ARG:HH12	51:l:87:LYS:NZ	2.16	0.43
10:4:97:ARG:HH21	16:A:3015:U:H5"	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:2757:A:OP2	21:H:121:ASN:ND2	2.46	0.43
44:e:162:ARG:HB2	44:e:171:TRP:CD2	2.53	0.43
4:x:135:ASP:OD1	4:x:136:ARG:N	2.48	0.43
16:A:2925:U:O2'	16:A:2927:C:OP1	2.29	0.43
18:D:182:HIS:HB2	18:D:187:LEU:HD21	2.01	0.43
34:U:153:LEU:HD23	43:d:222:LEU:HB3	2.01	0.43
43:d:157:HIS:O	43:d:161:HIS:ND1	2.50	0.43
46:g:84:TYR:HB3	46:g:116:ASP:O	2.19	0.43
5:y:310:VAL:O	5:y:314:GLN:HG2	2.19	0.42
11:5:262:ILE:H	11:5:262:ILE:HG13	1.68	0.42
12:6:74:TYR:OH	29:P:65:GLU:OE1	2.35	0.42
16:A:2332:C:N4	16:A:2442:U:H3	2.15	0.42
16:A:2693:A:H4'	16:A:2694:A:C8	2.54	0.42
19:E:304:LEU:HD12	19:E:307:TYR:HE2	1.84	0.42
23:J:168:GLN:HE22	51:l:63:THR:HB	1.84	0.42
26:M:142:GLU:HB2	26:M:162:LEU:HD23	2.01	0.42
38:Y:202:LEU:HB2	38:Y:204:TYR:CE2	2.54	0.42
4:x:82:ALA:HB1	4:x:85:HIS:HD2	1.84	0.42
13:7:160:ASP:OD1	13:7:160:ASP:N	2.52	0.42
16:A:1977:U:H2'	16:A:1978:A:H8	1.83	0.42
19:E:236:THR:HG23	19:E:239:ARG:HD3	2.02	0.42
20:F:187:LEU:HD13	20:F:259:LEU:HD23	2.01	0.42
4:x:328:LEU:O	4:x:333:SER:N	2.52	0.42
16:A:1710:A:H5"	16:A:1711:C:H5'	2.00	0.42
16:A:1901:C:OP1	26:M:37:GLU:HG3	2.19	0.42
16:A:2105:G:OP1	27:N:233:TYR:OH	2.30	0.42
19:E:148:GLY:HA3	19:E:173:LYS:HG3	2.01	0.42
24:K:143:GLU:OE1	41:b:136:LYS:NZ	2.43	0.42
32:S:159:THR:OG1	32:S:196:ASN:OD1	2.30	0.42
35:V:133:ILE:HD12	35:V:145:ARG:HB2	2.01	0.42
37:X:20:ILE:HG21	37:X:212:ILE:HG23	2.01	0.42
44:e:58:VAL:HB	44:e:153:LEU:HB3	2.00	0.42
57:s:307:ARG:HG3	57:s:310:ARG:H	1.84	0.42
4:x:296:LEU:O	4:x:299:THR:HG22	2.20	0.42
15:9:126:LYS:HE2	15:9:126:LYS:HB3	1.83	0.42
16:A:1782:G:O2'	16:A:1793:G:O6	2.31	0.42
48:i:98:VAL:O	48:i:102:MET:HG3	2.20	0.42
53:o:17:TRP:CZ3	53:o:25:ARG:HB2	2.54	0.42
4:x:345:ARG:HG3	4:x:354:PHE:CG	2.55	0.42
11:5:257:TYR:CG	11:5:258:PRO:HA	2.54	0.42
16:A:1762:A:H2'	16:A:1763:A:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:1803:A:H2	16:A:1806:U:H5'	1.85	0.42
16:A:2135:A:N3	16:A:2135:A:H2'	2.33	0.42
16:A:2155:A:N6	56:r:169:TRP:O	2.52	0.42
16:A:2466:A:OP1	30:Q:235:ARG:NH1	2.49	0.42
16:A:2511:C:O5'	18:D:263:ASN:ND2	2.52	0.42
16:A:2655:G:N2	16:A:2659:C:O2'	2.53	0.42
16:A:3063:G:O2'	16:A:3066:C:OP2	2.36	0.42
25:L:35:MET:N	25:L:57:CYS:O	2.47	0.42
38:Y:226:LEU:O	38:Y:230:LYS:HG2	2.19	0.42
16:A:1939:G:O2'	16:A:1973:G:H4'	2.19	0.42
16:A:3072:U:H1'	16:A:3073:C:O4'	2.19	0.42
37:X:190:LYS:HE3	37:X:191:TYR:CZ	2.55	0.42
42:c:284:GLY:HA2	42:c:285:PRO:HD3	1.93	0.42
14:8:171:PHE:HD1	44:e:203:LYS:HE2	1.84	0.42
16:A:1678:C:N4	16:A:1773:A:OP2	2.35	0.42
16:A:2144:A:OP1	31:R:57:ARG:NH1	2.53	0.42
20:F:195:LEU:HD22	20:F:202:TYR:HE2	1.85	0.42
22:I:147:PHE:HA	22:I:151:ASN:ND2	2.35	0.42
29:P:73:PRO:O	29:P:75:ARG:NH1	2.53	0.42
38:Y:191:ASN:HB3	38:Y:194:TYR:HB3	2.01	0.42
5:y:240:ARG:HG2	5:y:265:HIS:HE1	1.84	0.42
10:4:99:LYS:NZ	16:A:3175:A:OP1	2.48	0.42
11:5:257:TYR:CD1	11:5:258:PRO:HA	2.55	0.42
13:7:240:ILE:HG23	13:7:252:VAL:HG21	2.00	0.42
16:A:2171:U:C2	16:A:2173:G:H4'	2.55	0.42
16:A:3183:U:H3	24:K:177:ARG:HB3	1.84	0.42
27:N:218:ILE:HG22	27:N:226:ILE:HG21	2.02	0.42
34:U:27:GLN:HG3	34:U:43:ARG:HB2	2.00	0.42
39:Z:36:PHE:HE2	39:Z:79:PRO:HG3	1.85	0.42
49:j:100:GLU:HG2	49:j:104:LYS:HE3	2.01	0.42
17:B:1639:U:H5"	29:P:155:SER:HB3	2.02	0.42
22:I:96:ILE:HG12	22:I:155:VAL:HG12	2.01	0.42
24:K:30:LYS:HD3	24:K:148:PRO:HB2	2.01	0.42
33:T:150:ILE:HB	43:d:52:THR:HG21	2.01	0.42
37:X:226:LEU:HD23	37:X:229:ILE:HD12	2.00	0.42
44:e:124:TRP:CD2	52:m:72:ARG:HG2	2.55	0.42
50:k:66:VAL:HG11	50:k:90:PHE:HE1	1.85	0.42
10:4:66:PHE:CE2	16:A:3174:U:H5'	2.55	0.42
11:5:114:LEU:HD11	18:D:127:ILE:HD13	2.02	0.42
13:7:88:PRO:HG3	13:7:119:LEU:HD21	2.01	0.42
16:A:3217:A:H2'	19:E:292:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:F:82:LEU:HB3	20:F:87:PHE:CD2	2.55	0.42
21:H:99:THR:HA	21:H:108:ARG:HG3	2.01	0.42
37:X:222:ASP:OD1	37:X:222:ASP:N	2.53	0.42
11:5:293:LEU:HD12	11:5:313:MET:HG2	2.02	0.41
13:7:309:HIS:CE1	19:E:155:PHE:HA	2.55	0.41
16:A:2182:G:H1'	16:A:2199:A:C8	2.55	0.41
44:e:192:LEU:O	44:e:198:ASN:ND2	2.53	0.41
2:v:54:GLN:O	2:v:57:LYS:HG2	2.19	0.41
4:x:69:SER:O	4:x:262:ARG:NH1	2.53	0.41
16:A:2829:C:OP2	16:A:2829:C:H3'	2.20	0.41
20:F:212:TRP:O	20:F:258:THR:OG1	2.38	0.41
26:M:98:LEU:HD12	26:M:145:ALA:HA	2.02	0.41
26:M:284:LYS:NZ	46:g:41:SER:HB3	2.35	0.41
30:Q:175:GLN:NE2	30:Q:206:PRO:HG3	2.35	0.41
39:Z:53:HIS:ND1	53:o:47:TYR:OH	2.35	0.41
56:r:99:MET:HE1	56:r:115:ILE:HG22	2.00	0.41
57:s:90:LYS:HD2	57:s:232:GLN:HB2	2.02	0.41
57:s:93:VAL:HB	57:s:233:ILE:HG12	2.01	0.41
1:u:119:ARG:HD3	30:Q:123:ASP:OD2	2.19	0.41
2:v:63:ASN:O	2:v:68:ARG:NH2	2.51	0.41
12:6:342:PHE:CE1	29:P:48:PHE:HB2	2.55	0.41
40:a:45:CYS:HA	40:a:65:VAL:HG13	2.02	0.41
51:l:88:PRO:HG2	51:l:91:GLU:HG3	2.03	0.41
4:x:58:ASP:O	4:x:61:PRO:HD2	2.20	0.41
4:x:223:GLU:O	4:x:227:ASP:N	2.53	0.41
16:A:1673:U:O2'	33:T:143:ARG:NH1	2.53	0.41
16:A:2530:A:H5"	18:D:212:THR:HG21	2.02	0.41
20:F:280:TYR:CD1	46:g:57:ILE:HG12	2.55	0.41
25:L:138:LEU:HD22	25:L:144:PHE:HE1	1.85	0.41
26:M:207:PRO:O	26:M:211:VAL:HG23	2.20	0.41
34:U:46:MET:HE1	34:U:72:VAL:HG13	2.01	0.41
51:l:123:LYS:HE2	51:l:127:TRP:CZ2	2.55	0.41
57:s:119:PRO:HG3	57:s:394:TRP:CE3	2.55	0.41
16:A:1952:U:H2'	16:A:1953:A:C8	2.56	0.41
29:P:152:GLU:O	29:P:155:SER:OG	2.34	0.41
32:S:115:LEU:HB2	41:b:11:LEU:HD22	2.01	0.41
37:X:92:ALA:O	37:X:98:SER:OG	2.39	0.41
44:e:133:LEU:HD22	52:m:63:THR:HG21	2.02	0.41
46:g:150:LYS:NZ	53:o:79:THR:O	2.51	0.41
57:s:308:ARG:HG3	57:s:320:ILE:HD13	2.02	0.41
9:3:180:TYR:HD1	12:6:366:LEU:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:6:160:ASP:OD2	12:6:267:ARG:NH2	2.54	0.41
14:8:164:ARG:N	45:f:85:ASP:O	2.50	0.41
16:A:1868:G:N7	26:M:51:ARG:NH1	2.66	0.41
16:A:2446:A:OP1	57:s:65:ARG:NH2	2.51	0.41
16:A:2796:G:H1'	21:H:87:LYS:HD2	2.02	0.41
43:d:115:THR:HG22	43:d:118:SER:H	1.86	0.41
5:y:123:GLN:O	5:y:127:ILE:HG12	2.21	0.41
5:y:256:TYR:OH	5:y:295:ARG:HG2	2.20	0.41
6:0:166:SER:H	6:0:169:ASP:HB2	1.85	0.41
12:6:173:LEU:HD22	12:6:272:LEU:HB2	2.03	0.41
12:6:234:HIS:CE1	12:6:257:PRO:HA	2.55	0.41
16:A:2081:U:H2'	16:A:2082:G:C8	2.55	0.41
16:A:2182:G:N3	16:A:2199:A:O2'	2.38	0.41
16:A:2387:U:O2'	16:A:2406:A:N7	2.48	0.41
18:D:279:GLY:H	18:D:283:GLY:H	1.68	0.41
28:O:25:ARG:NH2	28:O:51:GLU:OE2	2.35	0.41
30:Q:177:VAL:HG11	30:Q:204:MET:HG3	2.02	0.41
41:b:35:ARG:HG3	53:o:101:TRP:HB2	2.03	0.41
8:2:56:SER:OG	16:A:1980:A:OP1	2.33	0.41
12:6:87:LYS:HE2	12:6:87:LYS:HB3	1.87	0.41
16:A:2325:U:O2'	28:O:82:GLU:OE2	2.39	0.41
16:A:2739:U:H1'	18:D:293:LYS:NZ	2.35	0.41
19:E:170:LEU:HD11	19:E:190:GLY:HA2	2.03	0.41
19:E:274:TRP:NE1	19:E:286:ASN:HB2	2.34	0.41
38:Y:128:SER:HB2	38:Y:131:ARG:HE	1.86	0.41
4:x:70:GLU:O	4:x:371:ASN:ND2	2.54	0.41
4:x:176:ILE:HG22	4:x:249:TYR:HD2	1.85	0.41
4:x:210:ILE:HD13	4:x:210:ILE:HA	1.92	0.41
9:3:124:ARG:NH1	9:3:125:ARG:O	2.54	0.41
9:3:151:ASN:HB3	12:6:359:HIS:CD2	2.56	0.41
12:6:116:ASN:HD22	12:6:119:GLU:HG2	1.86	0.41
13:7:105:LEU:HD11	13:7:267:PRO:HB2	2.02	0.41
16:A:2030:U:H1'	16:A:2031:A:OP2	2.20	0.41
16:A:2080:U:O2'	53:o:60:ARG:HA	2.21	0.41
16:A:2286:A:H2'	16:A:2287:U:C6	2.56	0.41
16:A:2674:U:H2'	16:A:2675:G:O4'	2.21	0.41
16:A:2825:G:O6	36:W:44:GLY:HA3	2.20	0.41
19:E:61:ILE:HD11	28:O:149:LEU:HD13	2.02	0.41
22:I:89:VAL:O	22:I:93:ASN:ND2	2.54	0.41
22:I:113:ARG:HD2	22:I:123:MET:HE2	2.02	0.41
25:L:52:HIS:HD2	25:L:53:ARG:HG3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:O:52:MET:HE3	28:O:52:MET:HB3	1.94	0.41
30:Q:221:LYS:HB3	30:Q:244:ARG:HG3	2.02	0.41
40:a:51:LEU:HD21	40:a:58:ILE:HG12	2.02	0.41
44:e:128:PHE:CD1	52:m:74:MET:HB3	2.55	0.41
44:e:235:LYS:HD2	44:e:275:PHE:HD1	1.86	0.41
49:j:45:GLU:OE2	49:j:70:ARG:NH2	2.54	0.41
4:x:171:LEU:HD12	4:x:171:LEU:HA	1.91	0.41
12:6:227:GLU:HB2	12:6:230:ALA:HB3	2.02	0.41
12:6:279:ILE:HB	12:6:281:PHE:CE1	2.56	0.41
16:A:2169:A:OP2	23:J:21:ARG:NH1	2.54	0.41
16:A:3210:C:O2'	19:E:47:THR:O	2.34	0.41
18:D:290:PRO:N	18:D:291:PRO:HD2	2.36	0.41
19:E:345:ILE:HG12	30:Q:169:PRO:HB2	2.02	0.41
20:F:107:LYS:NZ	48:i:58:ASP:OD2	2.42	0.41
24:K:170:TRP:NE1	56:r:91:GLN:O	2.54	0.41
30:Q:90:LEU:HG	30:Q:94:ILE:HD11	2.03	0.41
41:b:28:ARG:HH21	42:c:71:GLU:CD	2.29	0.41
6:0:138:ARG:NH1	16:A:2321:A:OP1	2.49	0.40
11:5:173:ARG:HA	11:5:176:TYR:CE2	2.56	0.40
15:9:72:PRO:HG3	38:Y:104:VAL:HG12	2.02	0.40
16:A:2868:C:H2'	16:A:2869:A:O4'	2.21	0.40
20:F:48:LEU:HD22	47:h:94:SER:HB3	2.03	0.40
28:O:57:GLU:OE2	28:O:105:THR:OG1	2.30	0.40
37:X:42:HIS:CG	37:X:86:ILE:HD11	2.56	0.40
53:o:17:TRP:CH2	53:o:25:ARG:HD3	2.55	0.40
58:w:200:PM8:O40	58:w:200:PM8:N36	2.54	0.40
16:A:2241:A:H61	56:r:82:ASN:CG	2.28	0.40
34:U:30:ARG:O	38:Y:121:ARG:NH1	2.49	0.40
38:Y:130:GLU:OE1	43:d:71:LYS:NZ	2.41	0.40
46:g:79:PRO:HB3	46:g:85:PHE:HE1	1.87	0.40
52:m:60:ASP:OD1	52:m:60:ASP:N	2.52	0.40
15:9:119:PHE:HB2	37:X:227:PHE:CE1	2.56	0.40
16:A:1864:A:OP1	31:R:17:ARG:NH1	2.52	0.40
41:b:42:GLY:HA3	41:b:92:LYS:O	2.21	0.40
2:v:13:TYR:OH	2:v:36:ARG:HG2	2.21	0.40
5:y:197:THR:HG21	5:y:223:LEU:HD23	2.03	0.40
15:9:110:ASP:OD1	15:9:113:ASN:ND2	2.55	0.40
16:A:1797:G:O2'	35:V:40:ARG:O	2.38	0.40
16:A:1907:A:OP1	20:F:126:LYS:NZ	2.53	0.40
16:A:2652:G:H2'	16:A:2653:C:O4'	2.21	0.40
20:F:138:HIS:CG	20:F:146:TRP:HE1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:H:65:ALA:HB2	21:H:71:PRO:HA	2.04	0.40
34:U:137:ARG:NH1	35:V:104:TYR:OH	2.52	0.40
49:j:27:TRP:O	49:j:31:GLN:HG2	2.22	0.40
12:6:193:VAL:HB	12:6:319:PHE:CD2	2.57	0.40
16:A:2502:C:H1'	16:A:3096:U:H5'	2.04	0.40
16:A:2896:G:C6	16:A:2915:C:H1'	2.57	0.40
16:A:3110:C:H42	19:E:265:TYR:HB2	1.86	0.40
25:L:100:PHE:HB3	30:Q:158:GLN:NE2	2.35	0.40
33:T:65:ALA:O	33:T:173:VAL:HA	2.21	0.40
41:b:34:SER:OG	41:b:36:ASP:O	2.39	0.40
46:g:76:ARG:NH2	46:g:163:GLU:O	2.54	0.40
46:g:154:ASP:OD2	46:g:155:GLN:NE2	2.54	0.40
57:s:310:ARG:HG3	57:s:313:ARG:HH21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	u	108/234 (46%)	104 (96%)	4 (4%)	0	100	100
2	v	67/70 (96%)	67 (100%)	0	0	100	100
3	w	77/156 (49%)	73 (95%)	4 (5%)	0	100	100
4	x	332/384 (86%)	328 (99%)	4 (1%)	0	100	100
5	y	242/381 (64%)	240 (99%)	2 (1%)	0	100	100
6	0	108/188 (57%)	108 (100%)	0	0	100	100
7	1	53/65 (82%)	52 (98%)	1 (2%)	0	100	100
8	2	44/92 (48%)	42 (96%)	2 (4%)	0	100	100
9	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
10	4	36/103 (35%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	5	392/423 (93%)	389 (99%)	3 (1%)	0	100	100
12	6	352/380 (93%)	346 (98%)	6 (2%)	0	100	100
13	7	292/338 (86%)	287 (98%)	5 (2%)	0	100	100
14	8	100/206 (48%)	100 (100%)	0	0	100	100
15	9	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
18	D	238/305 (78%)	234 (98%)	4 (2%)	0	100	100
19	E	303/348 (87%)	298 (98%)	4 (1%)	1 (0%)	36	65
20	F	250/311 (80%)	248 (99%)	2 (1%)	0	100	100
21	H	95/267 (36%)	94 (99%)	1 (1%)	0	100	100
22	I	161/261 (62%)	159 (99%)	2 (1%)	0	100	100
23	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
24	K	175/178 (98%)	174 (99%)	1 (1%)	0	100	100
25	L	113/145 (78%)	113 (100%)	0	0	100	100
26	M	289/296 (98%)	287 (99%)	2 (1%)	0	100	100
27	N	208/251 (83%)	206 (99%)	2 (1%)	0	100	100
28	O	152/175 (87%)	150 (99%)	2 (1%)	0	100	100
29	P	142/180 (79%)	138 (97%)	4 (3%)	0	100	100
30	Q	219/292 (75%)	219 (100%)	0	0	100	100
31	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
32	S	159/205 (78%)	159 (100%)	0	0	100	100
33	T	164/206 (80%)	164 (100%)	0	0	100	100
34	U	150/153 (98%)	148 (99%)	2 (1%)	0	100	100
35	V	203/216 (94%)	202 (100%)	1 (0%)	0	100	100
36	W	104/148 (70%)	102 (98%)	2 (2%)	0	100	100
37	X	242/256 (94%)	241 (100%)	1 (0%)	0	100	100
38	Y	179/250 (72%)	178 (99%)	1 (1%)	0	100	100
39	Z	120/161 (74%)	118 (98%)	2 (2%)	0	100	100
40	a	96/142 (68%)	95 (99%)	1 (1%)	0	100	100
41	b	147/215 (68%)	145 (99%)	2 (1%)	0	100	100
42	c	282/332 (85%)	280 (99%)	2 (1%)	0	100	100
43	d	257/306 (84%)	255 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	e	224/279 (80%)	219 (98%)	5 (2%)	0	100	100
45	f	146/212 (69%)	143 (98%)	3 (2%)	0	100	100
46	g	132/166 (80%)	131 (99%)	1 (1%)	0	100	100
47	h	108/158 (68%)	106 (98%)	2 (2%)	0	100	100
48	i	95/128 (74%)	95 (100%)	0	0	100	100
49	j	92/123 (75%)	92 (100%)	0	0	100	100
50	k	99/112 (88%)	97 (98%)	2 (2%)	0	100	100
51	l	80/138 (58%)	80 (100%)	0	0	100	100
52	m	49/128 (38%)	49 (100%)	0	0	100	100
53	o	92/102 (90%)	92 (100%)	0	0	100	100
54	p	141/206 (68%)	139 (99%)	2 (1%)	0	100	100
55	q	139/222 (63%)	139 (100%)	0	0	100	100
56	r	160/196 (82%)	158 (99%)	2 (1%)	0	100	100
57	s	382/439 (87%)	374 (98%)	8 (2%)	0	100	100
All	All	9116/11894 (77%)	9015 (99%)	100 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	E	150	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	u	104/200 (52%)	101 (97%)	3 (3%)	37	71
2	v	59/60 (98%)	59 (100%)	0	100	100
3	w	73/136 (54%)	73 (100%)	0	100	100
4	x	291/328 (89%)	288 (99%)	3 (1%)	68	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	y	226/350 (65%)	225 (100%)	1 (0%)	84	94
6	0	99/164 (60%)	99 (100%)	0	100	100
7	1	52/60 (87%)	51 (98%)	1 (2%)	50	79
8	2	40/72 (56%)	40 (100%)	0	100	100
9	3	88/166 (53%)	87 (99%)	1 (1%)	65	88
10	4	37/89 (42%)	37 (100%)	0	100	100
11	5	353/368 (96%)	352 (100%)	1 (0%)	86	96
12	6	313/332 (94%)	311 (99%)	2 (1%)	78	93
13	7	270/303 (89%)	269 (100%)	1 (0%)	84	94
14	8	93/190 (49%)	93 (100%)	0	100	100
15	9	104/112 (93%)	104 (100%)	0	100	100
18	D	194/245 (79%)	194 (100%)	0	100	100
19	E	260/290 (90%)	260 (100%)	0	100	100
20	F	219/262 (84%)	219 (100%)	0	100	100
21	H	88/228 (39%)	87 (99%)	1 (1%)	65	88
22	I	151/232 (65%)	151 (100%)	0	100	100
23	J	138/150 (92%)	138 (100%)	0	100	100
24	K	154/155 (99%)	153 (99%)	1 (1%)	78	93
25	L	98/124 (79%)	98 (100%)	0	100	100
26	M	246/249 (99%)	244 (99%)	2 (1%)	73	90
27	N	185/211 (88%)	183 (99%)	2 (1%)	65	88
28	O	134/150 (89%)	134 (100%)	0	100	100
29	P	126/155 (81%)	125 (99%)	1 (1%)	73	90
30	Q	203/256 (79%)	202 (100%)	1 (0%)	81	93
31	R	118/126 (94%)	118 (100%)	0	100	100
32	S	146/180 (81%)	146 (100%)	0	100	100
33	T	146/176 (83%)	146 (100%)	0	100	100
34	U	134/135 (99%)	132 (98%)	2 (2%)	57	84
35	V	183/191 (96%)	180 (98%)	3 (2%)	55	83
36	W	86/119 (72%)	85 (99%)	1 (1%)	63	86
37	X	220/229 (96%)	220 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	Y	163/223 (73%)	163 (100%)	0	100	100
39	Z	113/147 (77%)	112 (99%)	1 (1%)	70	90
40	a	96/133 (72%)	96 (100%)	0	100	100
41	b	130/185 (70%)	129 (99%)	1 (1%)	73	90
42	c	251/288 (87%)	251 (100%)	0	100	100
43	d	237/274 (86%)	234 (99%)	3 (1%)	61	86
44	e	198/236 (84%)	198 (100%)	0	100	100
45	f	133/188 (71%)	132 (99%)	1 (1%)	73	90
46	g	124/148 (84%)	124 (100%)	0	100	100
47	h	104/148 (70%)	104 (100%)	0	100	100
48	i	86/110 (78%)	86 (100%)	0	100	100
49	j	74/97 (76%)	74 (100%)	0	100	100
50	k	83/90 (92%)	83 (100%)	0	100	100
51	l	76/116 (66%)	75 (99%)	1 (1%)	61	86
52	m	46/113 (41%)	45 (98%)	1 (2%)	45	77
53	o	80/87 (92%)	80 (100%)	0	100	100
54	p	135/181 (75%)	135 (100%)	0	100	100
55	q	119/178 (67%)	119 (100%)	0	100	100
56	r	147/169 (87%)	147 (100%)	0	100	100
57	s	340/381 (89%)	339 (100%)	1 (0%)	86	96
All	All	8166/10285 (79%)	8130 (100%)	36 (0%)	81	94

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	u	176	VAL
1	u	186	GLU
1	u	191	GLU
4	x	282	GLN
4	x	326	GLU
4	x	360	VAL
5	y	326	GLU
7	1	54	VAL
9	3	173	VAL
11	5	47	ASP

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Mol	Chain	Res	Type
12	6	179	VAL
12	6	243	ASN
13	7	234	LYS
21	H	102	VAL
24	K	17	ILE
26	M	180	ASP
26	M	222	TYR
27	N	59	VAL
27	N	132	THR
29	P	161	LEU
30	Q	125	TYR
34	U	11	ARG
34	U	19	VAL
35	V	44	VAL
35	V	186	THR
35	V	188	VAL
36	W	131	VAL
39	Z	99	VAL
41	b	75	VAL
43	d	89	VAL
43	d	241	ASP
43	d	280	VAL
45	f	211	LEU
51	l	58	ASP
52	m	41	THR
57	s	97	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	u	136	HIS
2	v	19	GLN
2	v	63	ASN
3	w	103	HIS
4	x	47	ASN
4	x	85	HIS
4	x	172	GLN
4	x	214	GLN
4	x	230	GLN
4	x	316	GLN
4	x	322	GLN
4	x	371	ASN

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Mol	Chain	Res	Type
5	y	122	GLN
5	y	123	GLN
5	y	192	GLN
5	y	195	ASN
5	y	210	GLN
5	y	235	GLN
5	y	255	GLN
5	y	284	GLN
6	0	115	HIS
7	1	31	ASN
7	1	52	GLN
11	5	160	HIS
11	5	165	GLN
11	5	191	GLN
11	5	214	ASN
11	5	266	HIS
11	5	384	GLN
12	6	174	HIS
12	6	320	GLN
12	6	359	HIS
13	7	45	ASN
13	7	255	HIS
13	7	290	GLN
18	D	195	ASN
20	F	223	HIS
20	F	241	ASN
22	I	43	GLN
22	I	114	HIS
23	J	168	GLN
24	K	94	GLN
25	L	52	HIS
27	N	202	GLN
27	N	210	GLN
27	N	237	HIS
28	O	146	ASN
28	O	147	GLN
29	P	79	HIS
29	P	134	GLN
29	P	142	ASN
30	Q	107	HIS
31	R	27	HIS
31	R	77	GLN

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Mol	Chain	Res	Type
32	S	75	HIS
32	S	84	ASN
32	S	118	ASN
35	V	73	GLN
36	W	80	HIS
37	X	89	GLN
37	X	93	ASN
38	Y	99	HIS
38	Y	179	HIS
38	Y	189	HIS
39	Z	64	HIS
40	a	46	ASN
40	a	102	HIS
40	a	126	HIS
41	b	25	GLN
42	c	139	GLN
43	d	153	ASN
43	d	157	HIS
43	d	235	GLN
44	e	54	GLN
44	e	67	GLN
44	e	75	GLN
44	e	212	HIS
44	e	251	HIS
45	f	138	GLN
46	g	93	ASN
46	g	155	GLN
48	i	111	ASN
48	i	120	HIS
48	i	124	HIS
51	l	82	GLN
52	m	65	HIS
53	o	94	HIS
54	p	194	HIS
55	q	51	GLN
56	r	96	HIS
56	r	112	HIS
56	r	130	ASN
57	s	107	GLN
57	s	239	ASN
57	s	240	GLN
57	s	343	GLN

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Mol	Chain	Res	Type
57	s	358	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	A	1409/1590 (88%)	246 (17%)	1 (0%)
17	B	71/72 (98%)	13 (18%)	0
All	All	1480/1662 (89%)	259 (17%)	1 (0%)

All (259) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	A	1689	C
16	A	1693	C
16	A	1699	C
16	A	1700	U
16	A	1704	U
16	A	1707	C
16	A	1708	A
16	A	1711	C
16	A	1713	A
16	A	1724	A
16	A	1727	A
16	A	1728	U
16	A	1731	A
16	A	1737	A
16	A	1748	G
16	A	1750	G
16	A	1765	C
16	A	1770	G
16	A	1780	U
16	A	1805	A
16	A	1806	U
16	A	1807	U
16	A	1809	U
16	A	1821	A
16	A	1824	U
16	A	1827	C
16	A	1828	A
16	A	1829	A
16	A	1832	A

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Mol	Chain	Res	Type
16	A	1836	A
16	A	1844	A
16	A	1853	A
16	A	1854	U
16	A	1855	A
16	A	1867	A
16	A	1869	A
16	A	1882	A
16	A	1883	G
16	A	1887	A
16	A	1892	A
16	A	1893	A
16	A	1901	C
16	A	1903	C
16	A	1918	G
16	A	1937	A
16	A	1940	A
16	A	1962	A
16	A	1974	A
16	A	1984	A
16	A	1985	G
16	A	1986	A
16	A	1987	G
16	A	1992	C
16	A	1993	A
16	A	1994	A
16	A	2002	G
16	A	2015	G
16	A	2022	G
16	A	2029	A
16	A	2030	U
16	A	2031	A
16	A	2036	C
16	A	2039	A
16	A	2060	A
16	A	2065	A
16	A	2068	C
16	A	2069	U
16	A	2074	A
16	A	2079	C
16	A	2083	U
16	A	2092	C

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Mol	Chain	Res	Type
16	A	2098	G
16	A	2108	G
16	A	2109	A
16	A	2110	A
16	A	2125	C
16	A	2126	U
16	A	2132	A
16	A	2147	G
16	A	2154	A
16	A	2163	A
16	A	2167	A
16	A	2168	U
16	A	2169	A
16	A	2170	G
16	A	2171	U
16	A	2172	A
16	A	2181	A
16	A	2182	G
16	A	2183	C
16	A	2184	A
16	A	2194	U
16	A	2195	A
16	A	2197	G
16	A	2198	A
16	A	2199	A
16	A	2200	A
16	A	2202	C
16	A	2203	G
16	A	2210	C
16	A	2216	A
16	A	2228	A
16	A	2233	U
16	A	2237	A
16	A	2239	A
16	A	2241	A
16	A	2243	A
16	A	2245	A
16	A	2252	C
16	A	2262	C
16	A	2263	C
16	A	2283	C
16	A	2284	C

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Mol	Chain	Res	Type
16	A	2285	U
16	A	2293	A
16	A	2297	A
16	A	2300	G
16	A	2322	C
16	A	2324	U
16	A	2332	C
16	A	2345	G
16	A	2350	A
16	A	2351	U
16	A	2352	U
16	A	2353	A
16	A	2354	A
16	A	2355	A
16	A	2356	A
16	A	2359	C
16	A	2360	U
16	A	2361	G
16	A	2362	A
16	A	2363	A
16	A	2374	A
16	A	2390	A
16	A	2393	C
16	A	2396	C
16	A	2401	A
16	A	2405	C
16	A	2406	A
16	A	2407	U
16	A	2415	C
16	A	2427	C
16	A	2432	A
16	A	2444	A
16	A	2446	A
16	A	2451	A
16	A	2452	A
16	A	2478	G
16	A	2493	C
16	A	2500	A
16	A	2506	A
16	A	2507	A
16	A	2511	C
16	A	2520	C

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Mol	Chain	Res	Type
16	A	2521	A
16	A	2527	A
16	A	2540	C
16	A	2641	A
16	A	2654	U
16	A	2656	U
16	A	2660	U
16	A	2683	C
16	A	2684	C
16	A	2686	G
16	A	2693	A
16	A	2694	A
16	A	2695	G
16	A	2696	A
16	A	2706	A
16	A	2709	A
16	A	2718	C
16	A	2719	G
16	A	2727	C
16	A	2732	G
16	A	2745	A
16	A	2809	C
16	A	2810	G
16	A	2814	G
16	A	2829	C
16	A	2831	G
16	A	2832	A
16	A	2833	A
16	A	2847	C
16	A	2854	U
16	A	2864	U
16	A	2865	C
16	A	2889	C
16	A	2895	U
16	A	2910	A
16	A	2911	C
16	A	2913	A
16	A	2917	G
16	A	2922	A
16	A	2926	A
16	A	2928	C
16	A	2944	C

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Mol	Chain	Res	Type
16	A	2955	U
16	A	2956	A
16	A	2963	A
16	A	2982	C
16	A	2984	A
16	A	2985	C
16	A	2995	G
16	A	3000	A
16	A	3005	A
16	A	3016	G
16	A	3021	C
16	A	3041	U
16	A	3042	U
16	A	3043	C
16	A	3053	A
16	A	3054	G
16	A	3056	C
16	A	3060	C
16	A	3061	G
16	A	3072	U
16	A	3073	C
16	A	3077	C
16	A	3086	U
16	A	3089	A
16	A	3097	U
16	A	3100	U
16	A	3101	A
16	A	3102	U
16	A	3109	U
16	A	3110	C
16	A	3111	A
16	A	3112	A
16	A	3150	U
16	A	3155	C
16	A	3157	C
16	A	3158	A
16	A	3162	C
16	A	3169	C
16	A	3172	C
16	A	3180	A
16	A	3183	U
16	A	3189	C

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Mol	Chain	Res	Type
16	A	3190	A
16	A	3197	U
16	A	3206	C
16	A	3212	C
16	A	3217	A
16	A	3218	A
16	A	3228	U
17	B	1603	A
17	B	1605	A
17	B	1609	U
17	B	1611	G
17	B	1617	C
17	B	1621	A
17	B	1646	U
17	B	1650	A
17	B	1652	C
17	B	1653	U
17	B	1654	U
17	B	1656	A
17	B	1664	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	A	2030	U

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	SAC	K	2	24	7,8,9	1.02	0	8,9,11	0.81	0
34	AYA	U	2	34	6,7,8	1.30	1 (16%)	5,8,10	1.22	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
41	THC	b	2	41	8,9,10	1.06	1 (12%)	9,11,13	0.71	0
50	AYA	k	2	50	6,7,8	1.24	1 (16%)	5,8,10	1.32	1 (20%)

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
24	SAC	K	2	24	-	2/7/8/10	-
34	AYA	U	2	34	-	0/4/6/8	-
41	THC	b	2	41	-	0/8/10/12	-
50	AYA	k	2	50	-	0/4/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	U	2	AYA	CA-N	-2.57	1.43	1.46
50	k	2	AYA	CA-N	-2.27	1.44	1.46
41	b	2	THC	CA-N1	-2.15	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	k	2	AYA	CB-CA-N	2.71	112.63	109.61
34	U	2	AYA	CB-CA-N	2.58	112.48	109.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	K	2	SAC	N-CA-CB-OG
24	K	2	SAC	C-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	b	2	THC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 104 ligands modelled in this entry, 101 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	SAM	x	401	-	27,29,29	1.08	4 (14%)	36,42,42	2.03	9 (25%)
58	PM8	w	200	3	25,31,31	0.22	0	30,38,38	0.43	0
63	FES	r	201	56,22	0,4,4	-	-	-		

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	SAM	x	401	-	-	8/16/33/33	0/3/3/3
58	PM8	w	200	3	-	14/36/38/38	-
63	FES	r	201	56,22	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	x	401	SAM	C2-N3	2.50	1.38	1.33
59	x	401	SAM	C2-N1	2.46	1.38	1.33
59	x	401	SAM	C8-N7	2.18	1.35	1.31
59	x	401	SAM	OXT-C	-2.17	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	x	401	SAM	N3-C2-N1	-5.40	120.16	128.60
59	x	401	SAM	C5-C4-N3	-4.97	120.27	126.75
59	x	401	SAM	N9-C8-N7	-3.95	108.51	113.91
59	x	401	SAM	C5-N7-C8	3.69	108.76	103.51
59	x	401	SAM	C2-N3-C4	3.63	120.34	111.75
59	x	401	SAM	N3-C4-N9	3.29	132.50	127.08
59	x	401	SAM	OXT-C-O	-2.84	117.63	124.09
59	x	401	SAM	OXT-C-CA	2.21	120.91	113.38
59	x	401	SAM	C4-C5-N7	-2.20	107.94	110.62

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	w	200	PM8	O27-C28-C29-C32
58	w	200	PM8	C32-C34-N36-C37
58	w	200	PM8	O1-C1-S1-C43
58	w	200	PM8	C2-C1-S1-C43
59	x	401	SAM	N-CA-CB-CG
59	x	401	SAM	C-CA-CB-CG
59	x	401	SAM	CB-CG-SD-C5'
58	w	200	PM8	C38-C39-N41-C42
58	w	200	PM8	O35-C34-N36-C37
58	w	200	PM8	O40-C39-N41-C42
58	w	200	PM8	O27-C28-C29-C30
58	w	200	PM8	O27-C28-C29-C31
58	w	200	PM8	O33-C32-C34-O35
59	x	401	SAM	CB-CG-SD-CE
58	w	200	PM8	O33-C32-C34-N36
59	x	401	SAM	C2'-C1'-N9-C8
58	w	200	PM8	C42-C43-S1-C1
59	x	401	SAM	O4'-C1'-N9-C8
58	w	200	PM8	C31-C29-C32-C34
59	x	401	SAM	OXT-C-CA-N
58	w	200	PM8	C28-C29-C32-C34
59	x	401	SAM	C2'-C1'-N9-C4

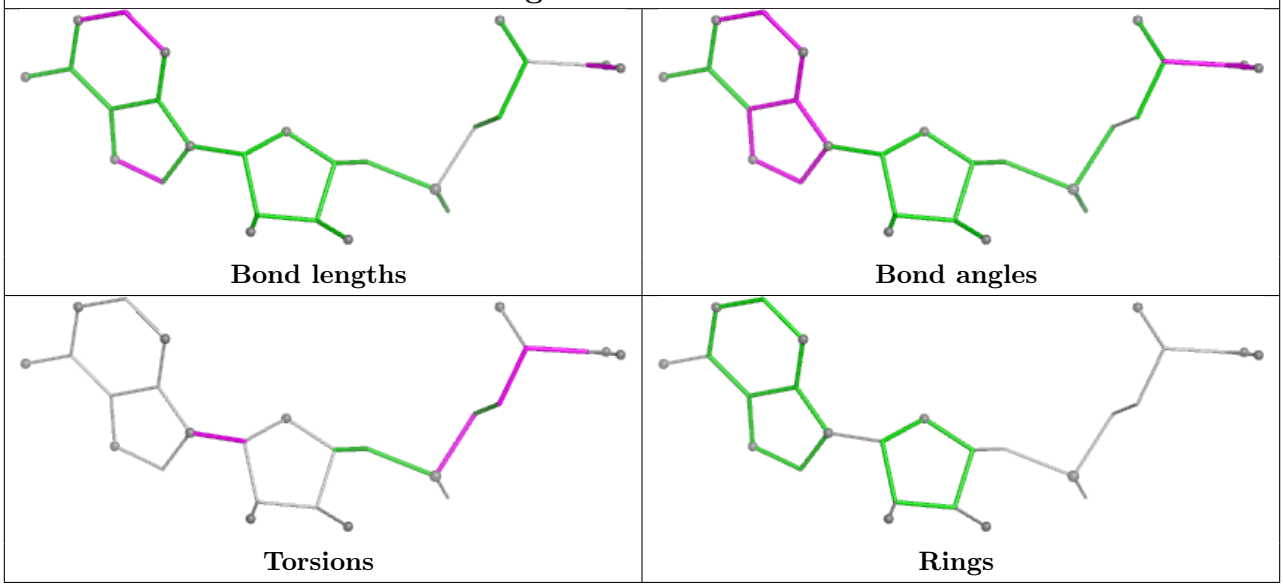
There are no ring outliers.

1 monomer is involved in 5 short contacts:

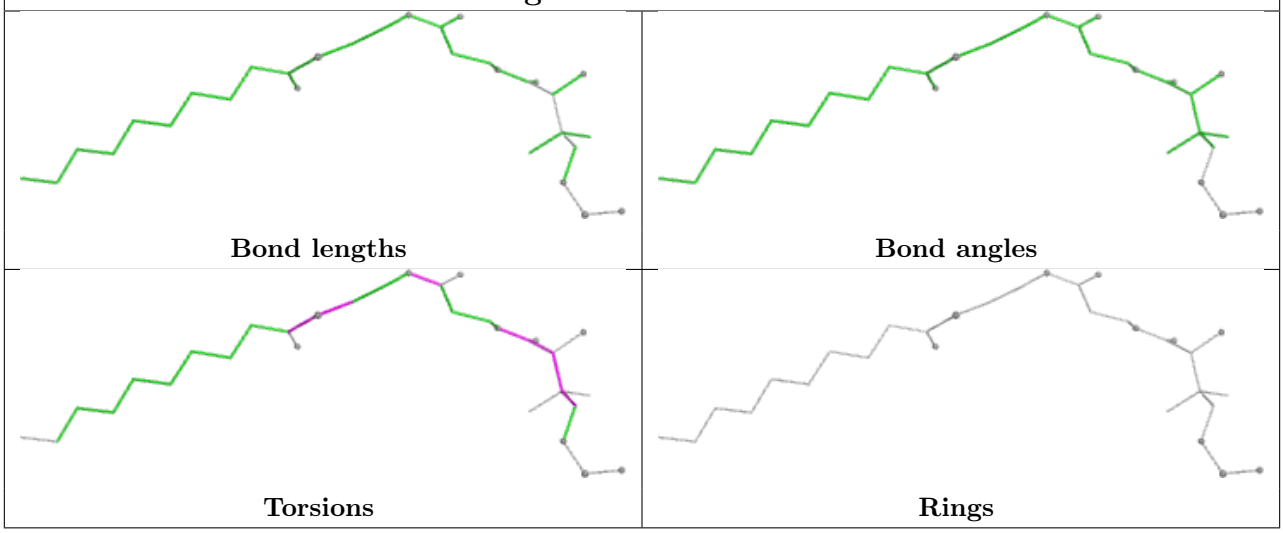
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	w	200	PM8	5	0

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 then 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.

Ligand SAM x 401



Ligand PM8 w 200



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3251:N	O3'	3252:N	P	17.10
1	A	3236:N	O3'	3237:N	P	13.81

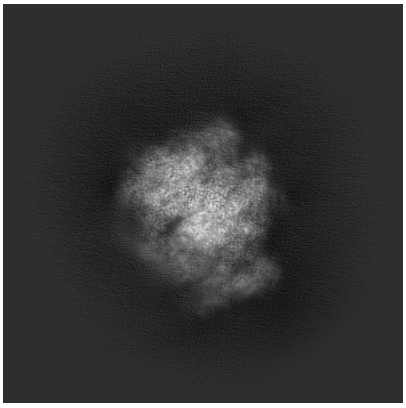
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12845. These allow visual inspection of the internal detail of the map and identification of artifacts.

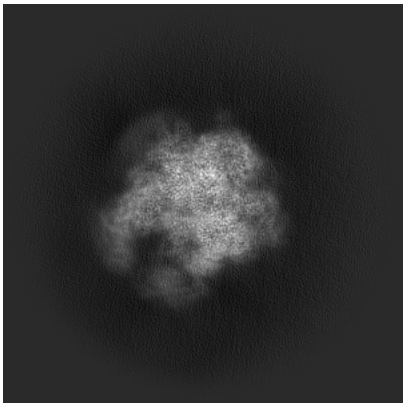
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

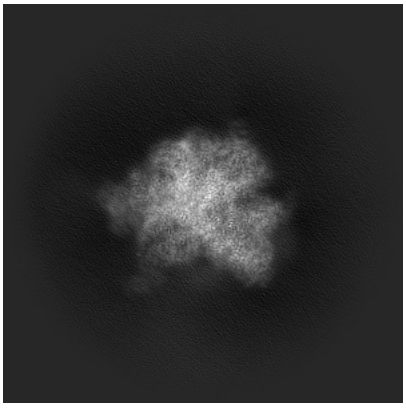
6.1.1 Primary map



X



Y

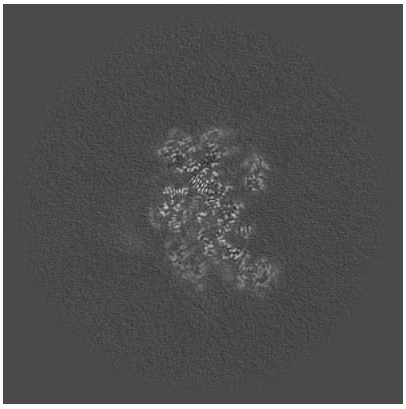


Z

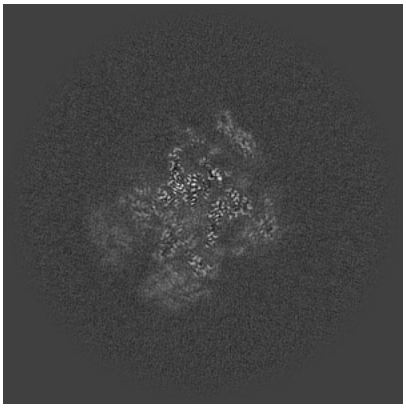
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

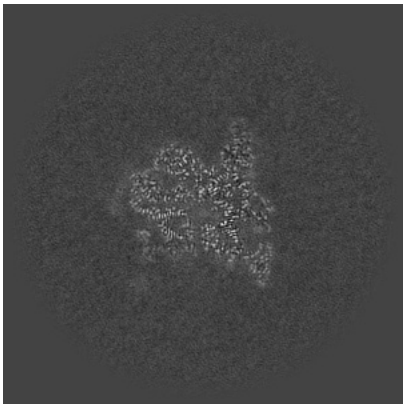
6.2.1 Primary map



X Index: 224



Y Index: 224

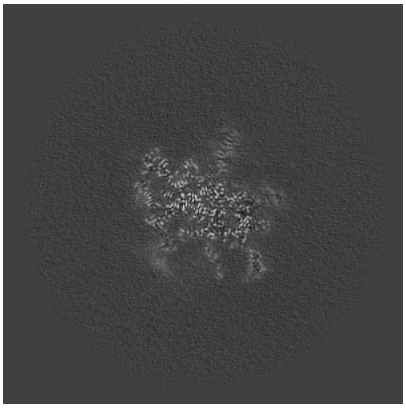


Z Index: 224

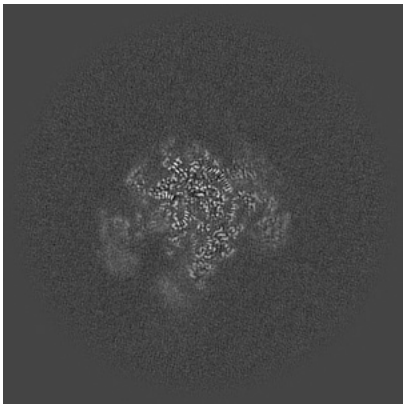
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

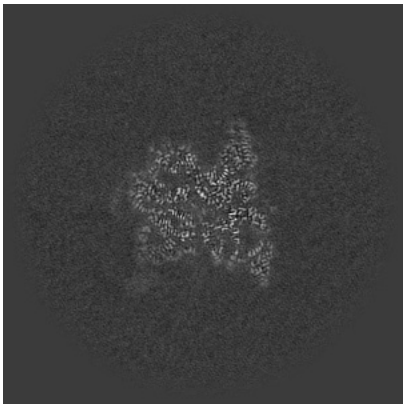
6.3.1 Primary map



X Index: 256



Y Index: 242

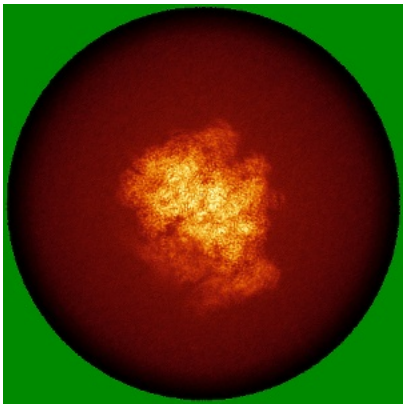


Z Index: 227

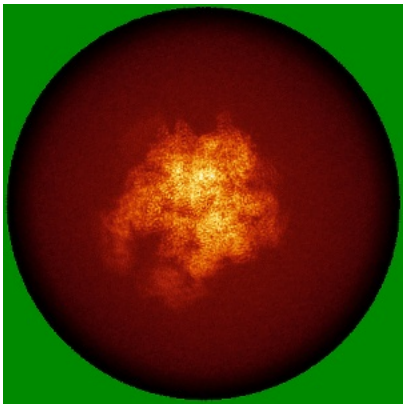
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

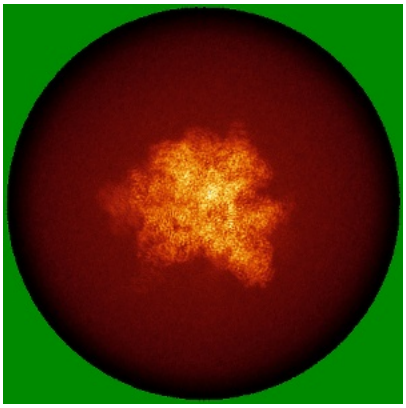
6.4.1 Primary map



X



Y

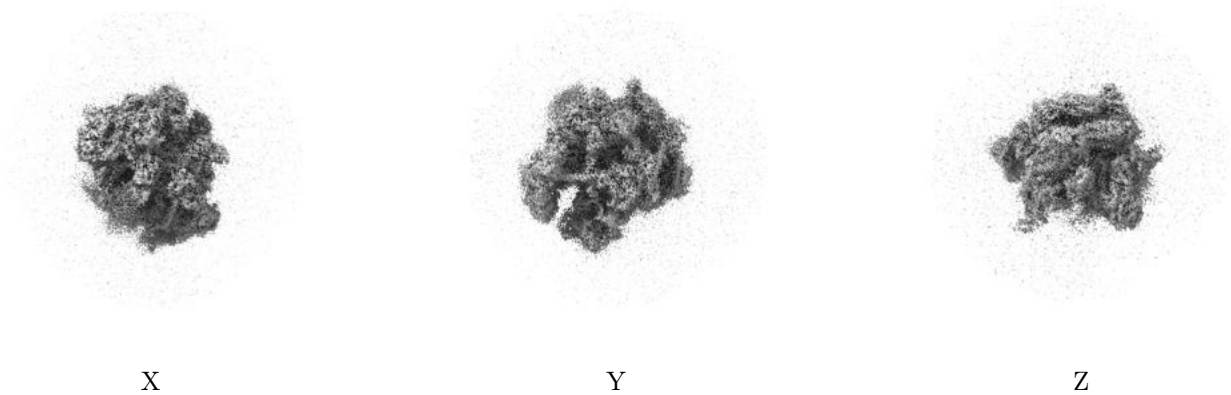


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

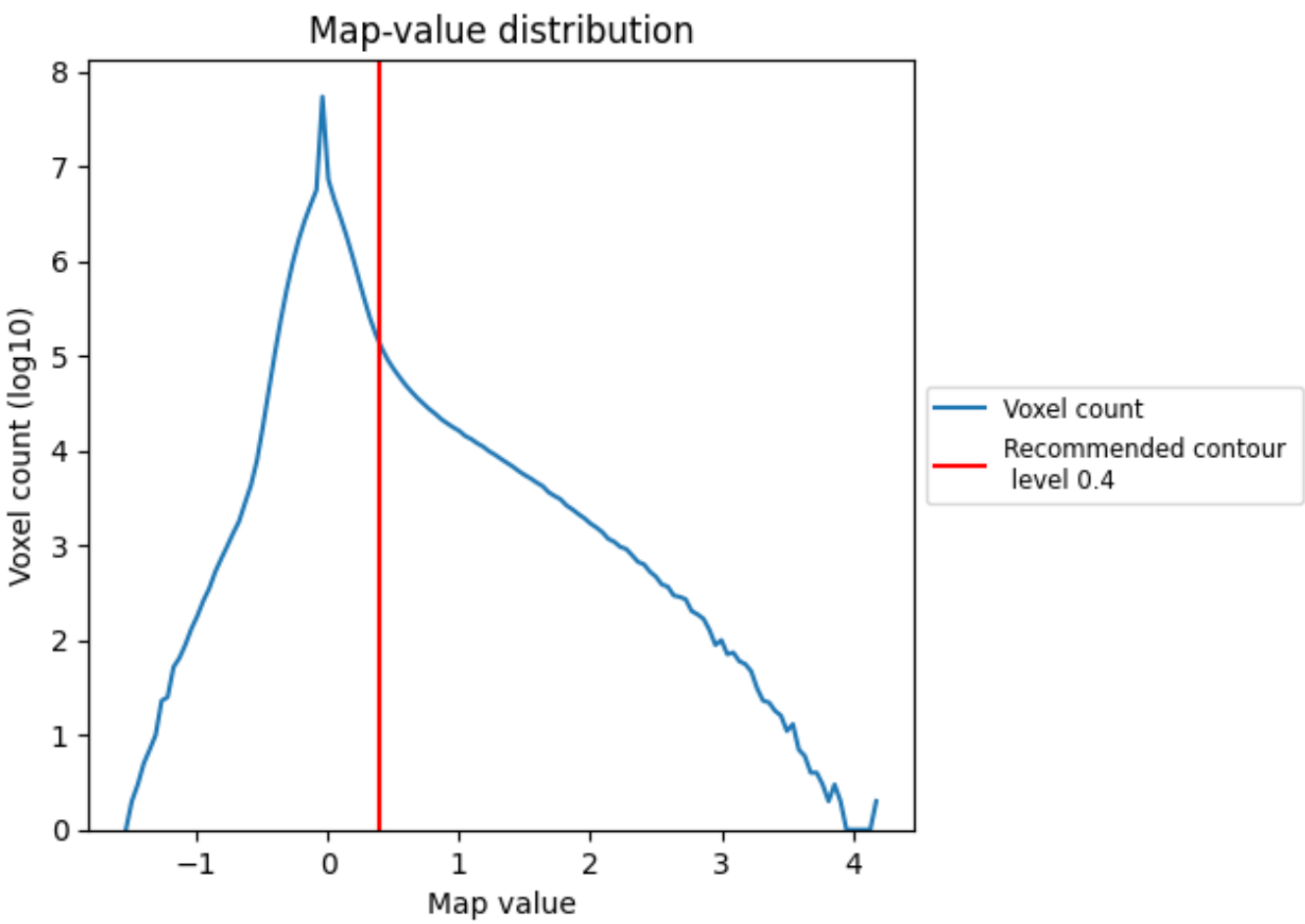
6.6 Mask visualisation (i)

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

7 Map analysis (i)

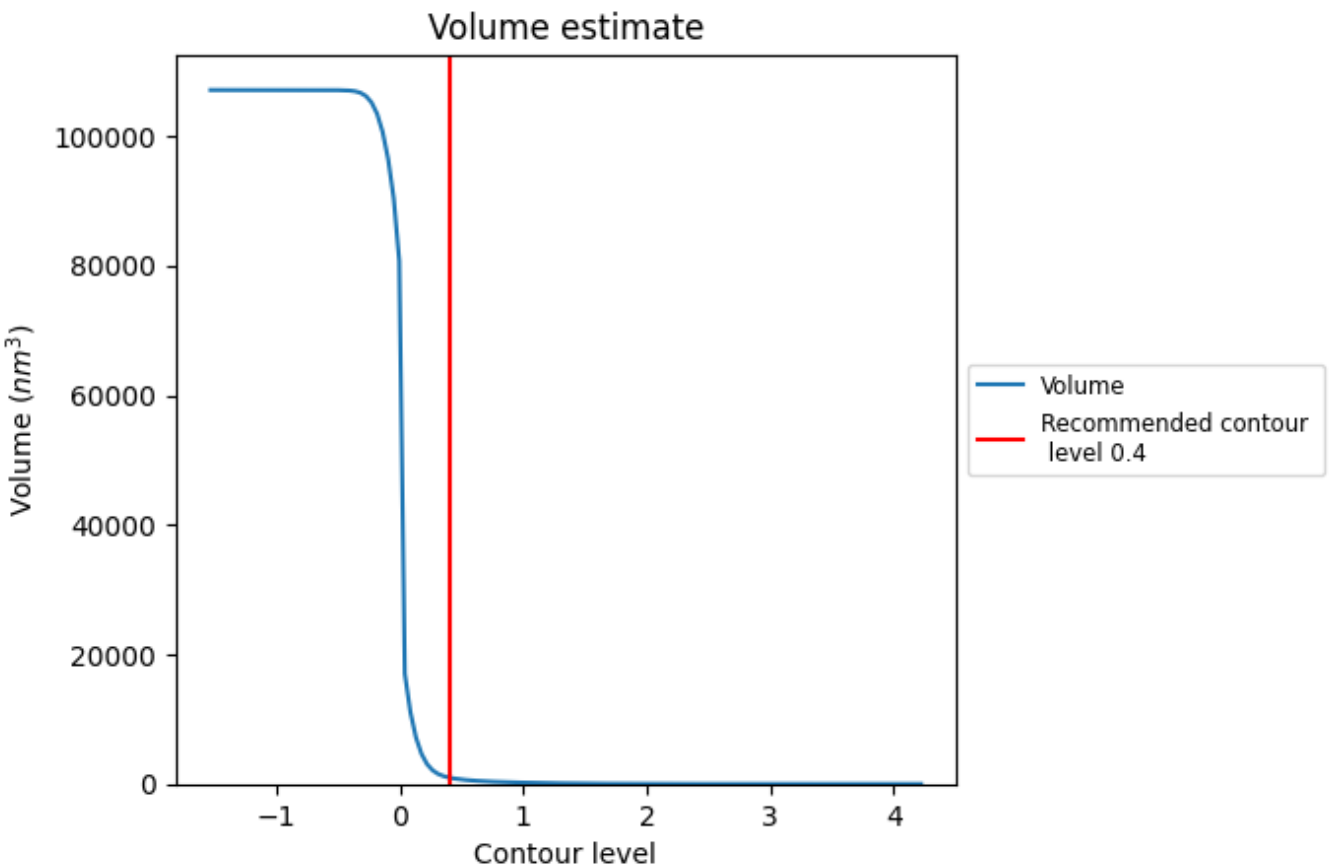
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

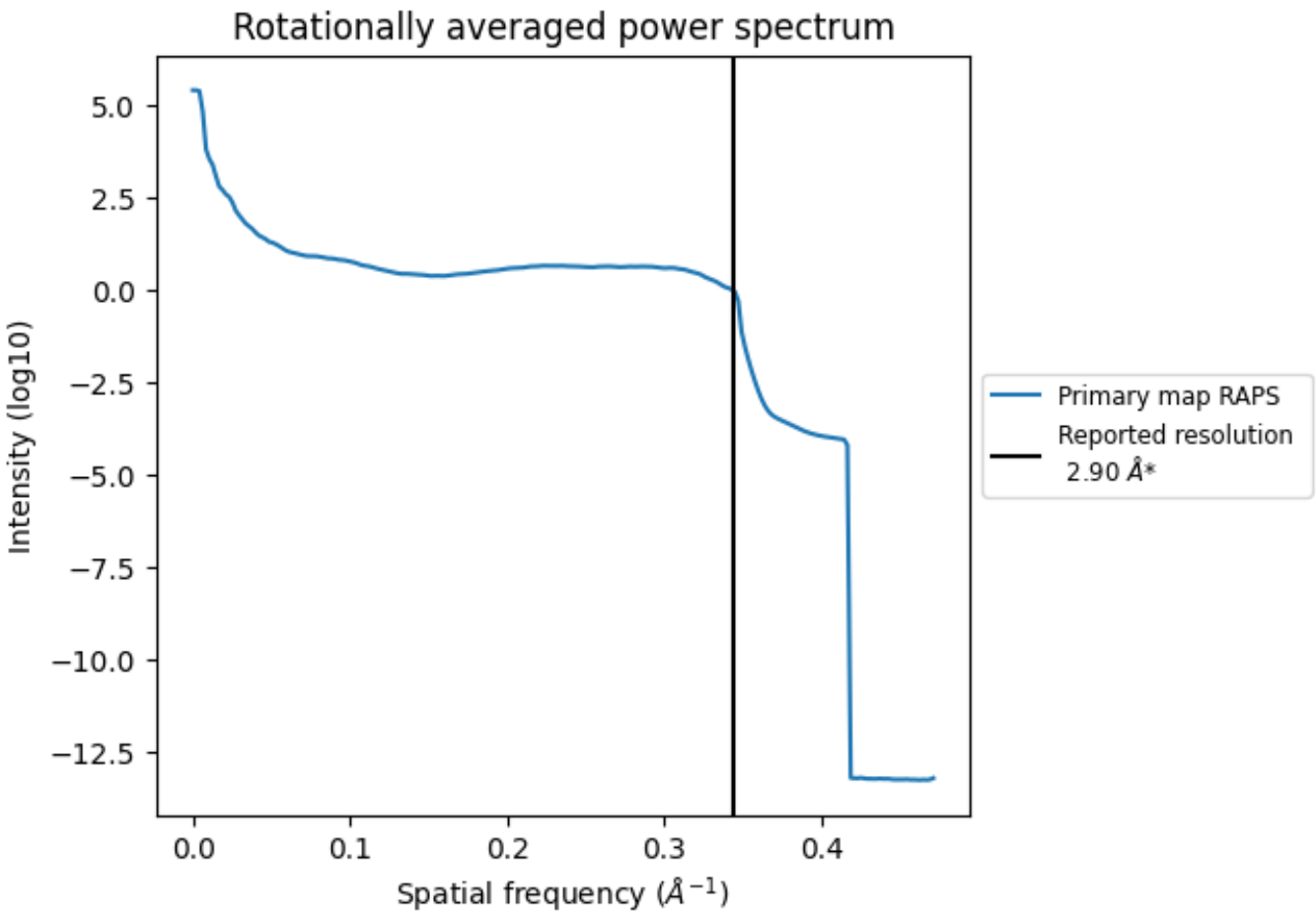
7.2 Volume estimate (i)



The volume at the recommended contour level is 985 nm^3; this corresponds to an approximate mass of 890 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

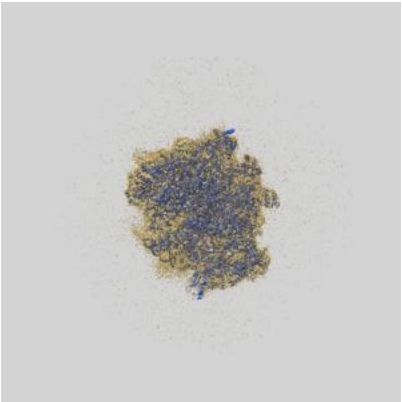
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

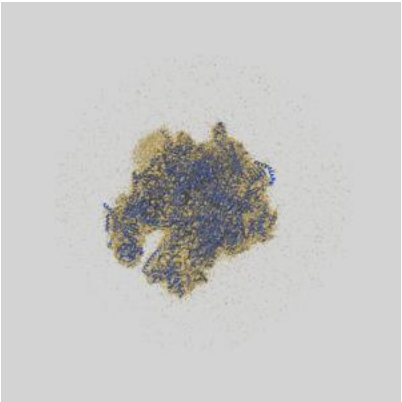
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12845 and PDB model 7ODR. Per-residue inclusion information can be found in section 3 on page 17.

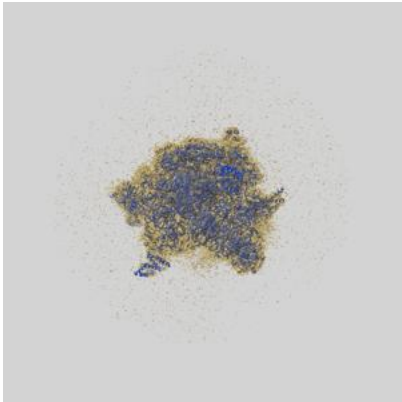
9.1 Map-model overlay (i)



X



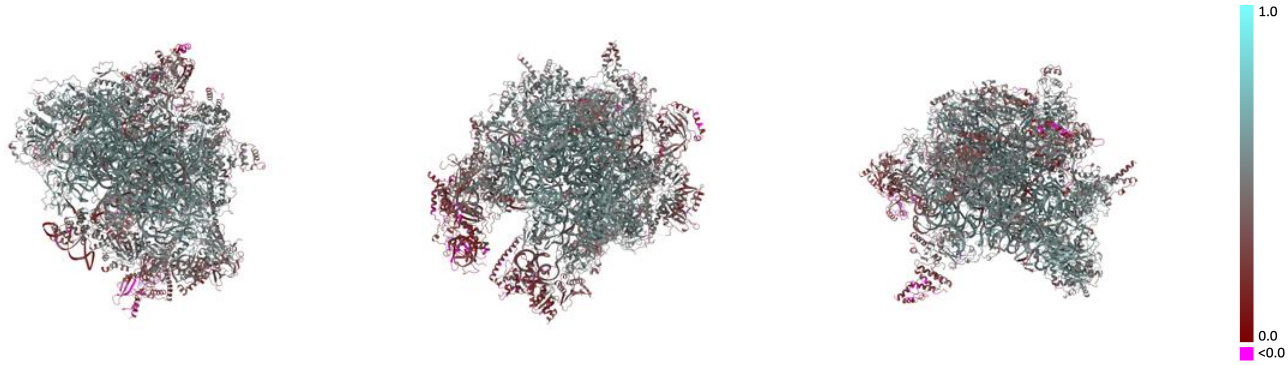
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

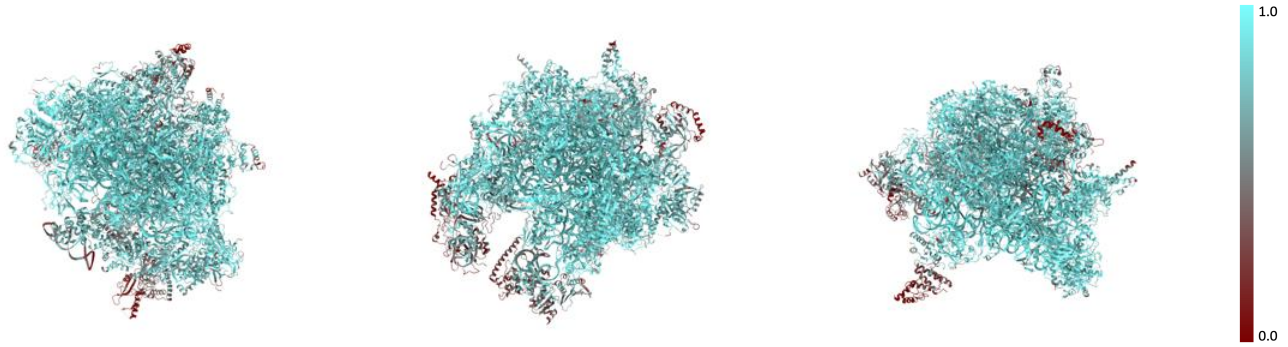
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

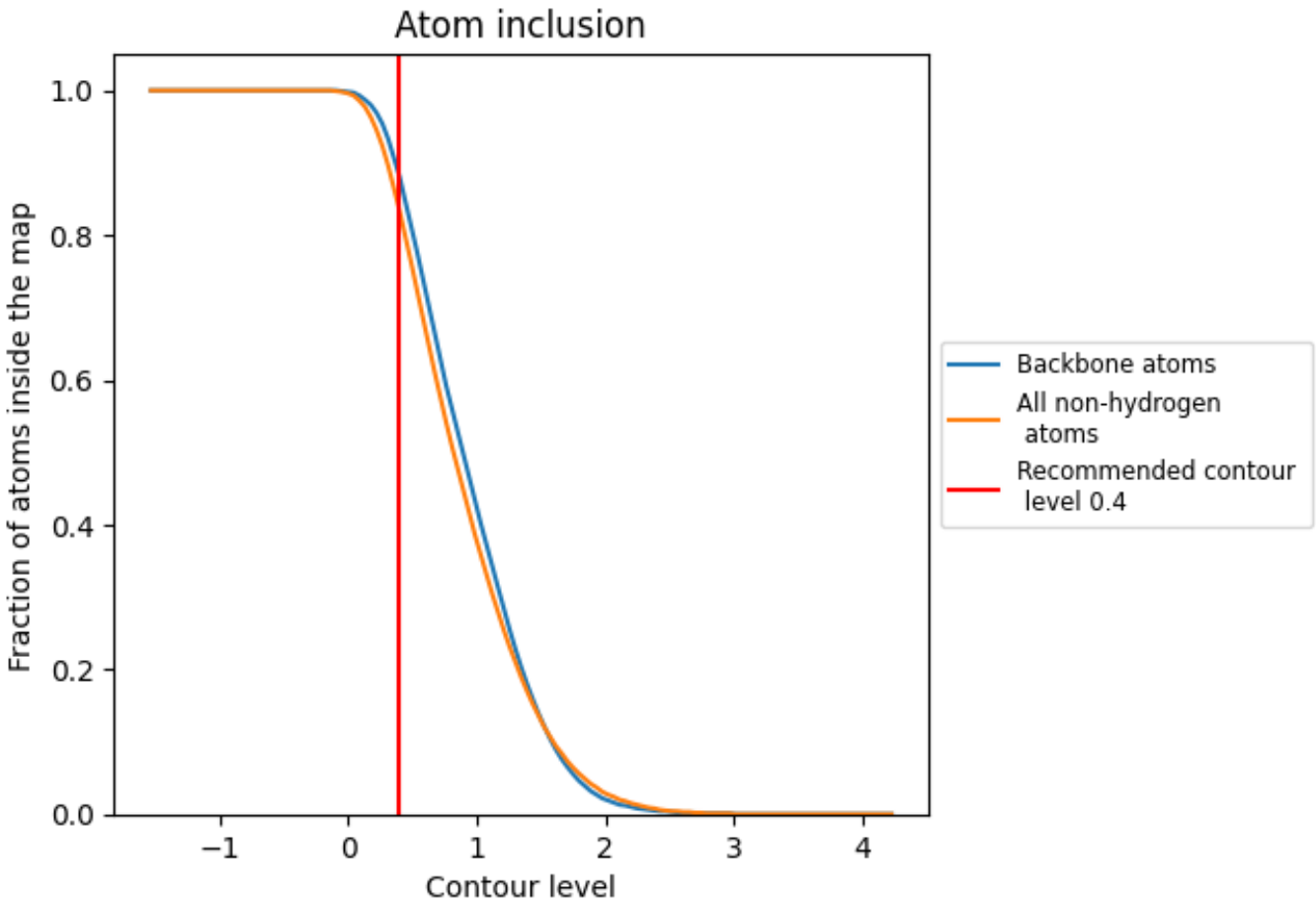
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8330	0.4730
0	0.8600	0.5060
1	0.8620	0.5230
2	0.9780	0.6110
3	0.9700	0.5930
4	0.9330	0.5280
5	0.8930	0.5110
6	0.8300	0.4200
7	0.7720	0.3860
8	0.4000	0.2120
9	0.8600	0.4840
A	0.9540	0.5400
B	0.7920	0.2830
D	0.8960	0.5290
E	0.9100	0.5170
F	0.8970	0.5250
H	0.8210	0.4780
I	0.5630	0.2770
J	0.2810	0.1600
K	0.9310	0.5430
L	0.8760	0.4930
M	0.9180	0.5410
N	0.8220	0.4720
O	0.9140	0.5310
P	0.8920	0.4850
Q	0.8820	0.4920
R	0.9320	0.5610
S	0.9160	0.5270
T	0.9100	0.5450
U	0.8100	0.4800
V	0.6370	0.3980
W	0.9300	0.5690
X	0.8610	0.5120
Y	0.8860	0.5180
Z	0.9070	0.5550

Continued on next page...

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Chain	Atom inclusion	Q-score
a	0.8070	0.4750
b	0.9100	0.5330
c	0.8340	0.4610
d	0.5190	0.3270
e	0.2960	0.1340
f	0.4860	0.2730
g	0.8990	0.5160
h	0.6780	0.3880
i	0.9490	0.5720
j	0.8660	0.4880
k	0.5290	0.2690
l	0.3600	0.1960
m	0.2680	0.1890
o	0.8910	0.5140
p	0.7180	0.4100
q	0.7890	0.4370
r	0.8510	0.4860
s	0.9060	0.5320
u	0.6770	0.3790
v	0.2930	0.2360
w	0.0680	0.1330
x	0.8160	0.4410
y	0.7570	0.4190