Full wwPDB EM Validation Report (i)

Aug 25, 2026 – 10:33 am BST

PDB ID	:	7ODT / pdb_00007odt
EMDB ID	:	EMD-12847
Title	:	State C 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	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

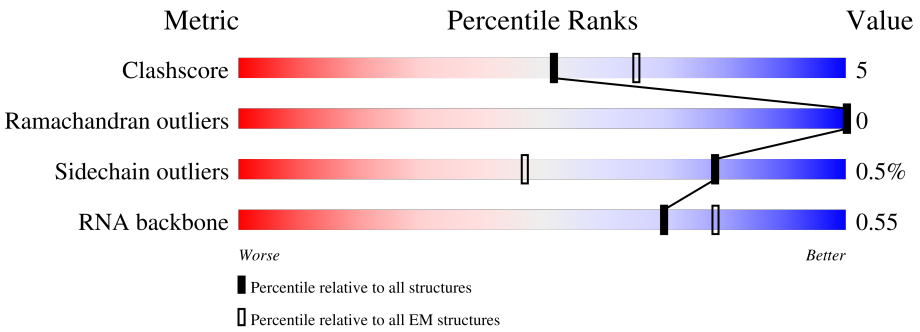
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

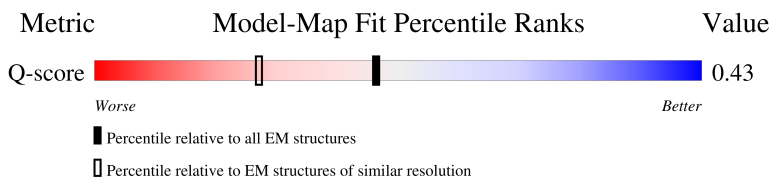
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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





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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	t	406	38% 57% 20% • 22%
2	u	234	8% 36% 10% • 53%
3	v	70	81% 73% 24% ••

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Mol	Chain	Length	Quality of chain
4	w	156	50% 42% 9% 49%
5	x	384	10% 69% 21% 10%
6	y	381	29% 49% 15% 36%
7	0	188	• 53% 5% 41%
8	1	65	5% 72% 12% 15%
9	2	92	43% 7% 50%
10	3	188	43% 7% 49%
11	4	103	31% 6% 63%
12	5	423	• 81% 12% 7%
13	6	380	9% 73% 20% 7%
14	7	338	15% 74% 13% 13%
15	8	206	38% 44% 6% 50%
16	9	137	8% 77% 13% 9%
17	A	1559	• 61% 27% 6% 7%
18	B	72	15% 62% 35% •
19	D	305	5% 65% 13% 21%
20	E	348	• 76% 12% 12%
21	F	311	• 62% 19% 19%
22	H	267	6% 29% 7% 64%
23	I	261	35% 56% 8% 36%
24	J	192	82% 82% 9% 9%
25	K	178	• 85% 15% •
26	L	145	• 65% 14% 21%
27	M	296	• 86% 12% •
28	N	251	12% 78% 10% 12%

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Mol	Chain	Length	Quality of chain
29	O	175	74% 14% 12%
30	P	180	66% 14% 20%
31	Q	292	65% 10% 24%
32	R	149	87% 7% 6%
33	S	205	68% 11% 21%
34	T	206	68% 12% 19%
35	U	153	20% 83% 16%
36	V	216	36% 80% 15% 5%
37	W	148	66% 5% 28%
38	X	256	5% 84% 11% 5%
39	Y	250	63% 10% 28%
40	Z	161	70% 6% 24%
41	a	142	11% 63% 8% 30%
42	b	215	60% 8% 31%
43	c	332	6% 77% 9% 14%
44	d	306	47% 72% 12% 15%
45	e	279	75% 67% 15% 18%
46	f	212	49% 59% 12% 29%
47	g	166	67% 14% 19%
48	h	158	26% 59% 10% 30%
49	i	128	62% 13% 24%
50	j	123	7% 68% 8% 24%
51	k	112	51% 74% 16% 10%
52	l	138	44% 52% 7% 41%
53	m	128	40% 28% 12% 60%

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Mol	Chain	Length	Quality of chain
54	o	102	78% 14% 8%
55	p	206	17% 63% 9% 29%
56	q	222	10% 58% 5% 36%
57	r	196	9% 69% 14% 17%
58	s	439	73% 15% 12%

2 Entry composition (i)

There are 65 unique types of molecules in this entry. The entry contains 110473 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 ribosome-associated GTPase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	t	316	2398	1509	440	441	8	0	0

- Molecule 2 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

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

- Molecule 3 is a protein called MIEF1 upstream open reading frame protein.

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

- Molecule 4 is a protein called Acyl carrier protein, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	x	346	2750	1753	482	498	17	0	0

- Molecule 6 is a protein called Transcription termination factor 4, mitochondrial.

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

- Molecule 7 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	0	110	898	554	176	162	6	0	0

- Molecule 8 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	1	55	455	290	87	76	2	0	0

- Molecule 9 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	2	46	377	233	83	60	1	0	0

- Molecule 10 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	3	95	832	539	162	128	3	0	0

- Molecule 11 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	4	38	342	217	72	49	4	0	0

- Molecule 12 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	5	394	3210	2073	560	566	11	0	0

- Molecule 13 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	6	354	2948	1881	525	533	9	0	0

- Molecule 14 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	7	294	2390	1529	405	438	18	0	0

- Molecule 15 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	8	102	860	543	152	163	2	0	0

- Molecule 16 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	9	124	997	644	170	181	2	0	0

- Molecule 17 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	A	1453	30850	13846	5571	9980	1453	0	0

- Molecule 18 is a RNA chain called mitochondrial tRNAVal.

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

- Molecule 19 is a protein called 39S ribosomal protein L2, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L3, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	I	168	1358	875	246	227	10	0	0

- Molecule 24 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 25 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 26 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 28 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	N	222	1786	1143	326	307	10	0	0

- Molecule 29 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 30 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 31 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 32 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 33 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L28, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L45, mitochondrial.

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

- Molecule 45 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 46 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 47 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 48 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 49 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 50 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 51 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 52 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 53 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 54 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 55 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 56 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		
56	q	141	1177	732	229	211	5	0	0

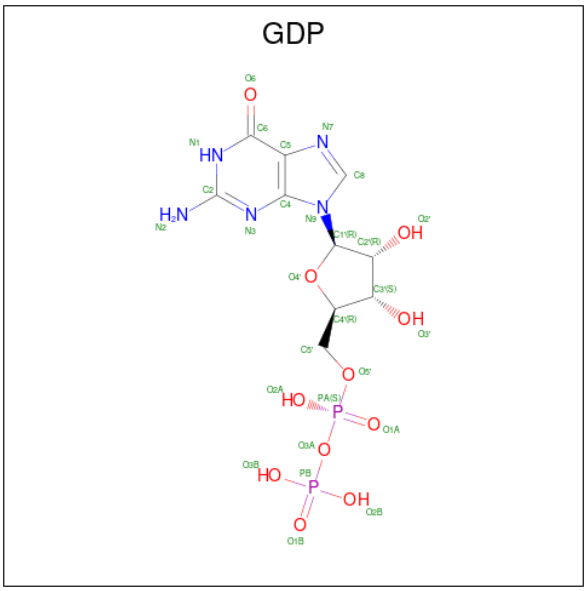
- Molecule 57 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 58 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
59	t	1	28	10	5	11	2	0

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	t	1	1	1	0

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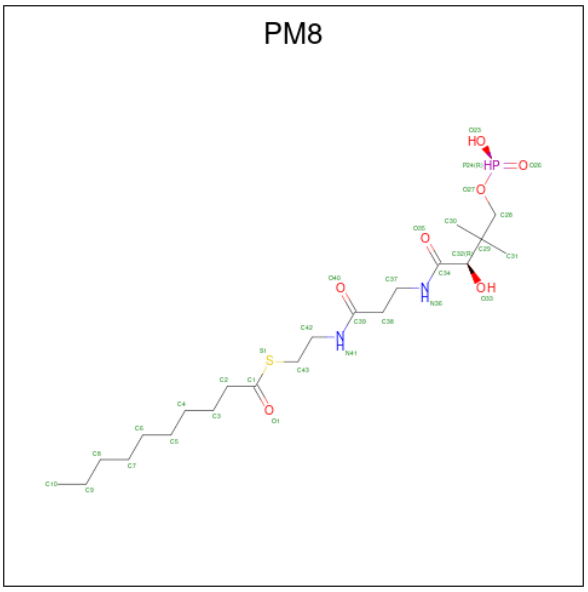
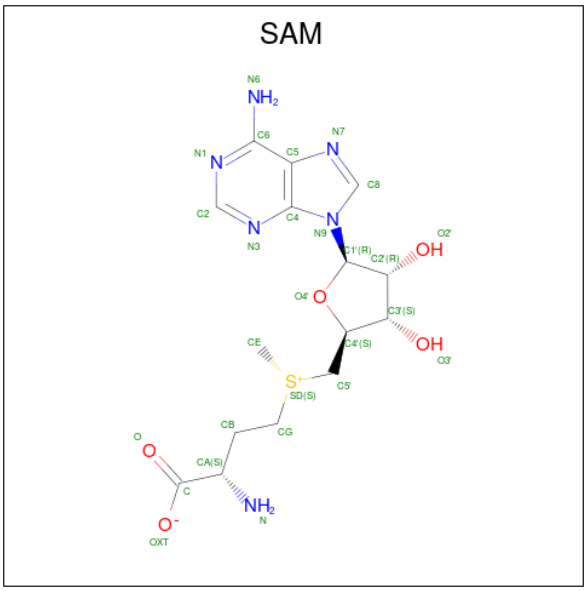
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	A	88	88	88	0
60	I	1	1	1	0
60	M	1	1	1	0
60	O	1	1	1	0
60	W	1	1	1	0
60	g	1	1	1	0
60	o	1	1	1	0

- Molecule 61 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	
61	w	1	32	21	2	7	1	1	0

- Molecule 62 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



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

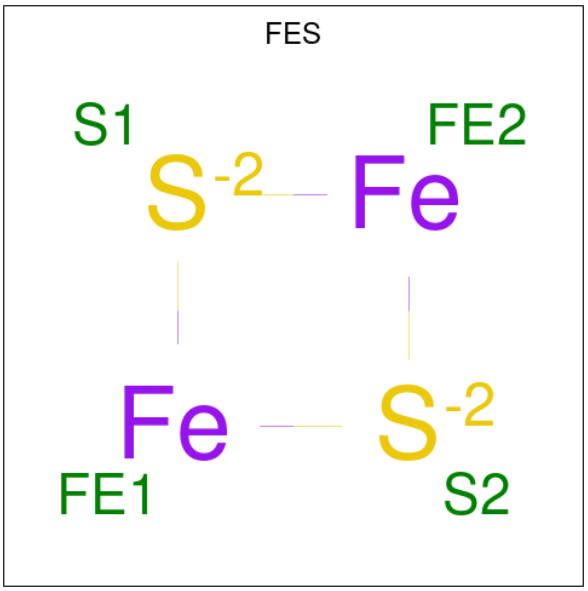
- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 64 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
64	A	10	10	10	0

- Molecule 65 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



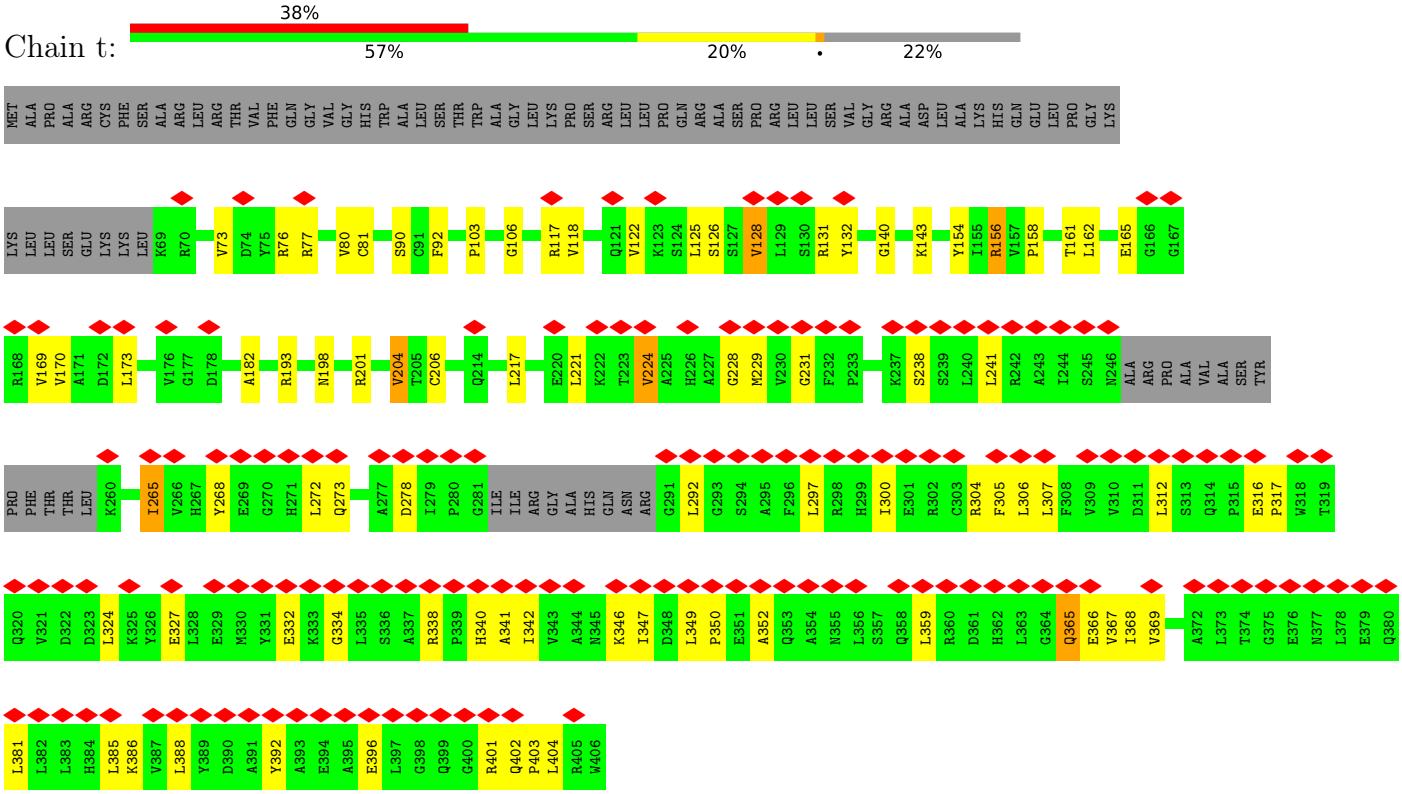
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
65	r	1	4	2	2	0

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.

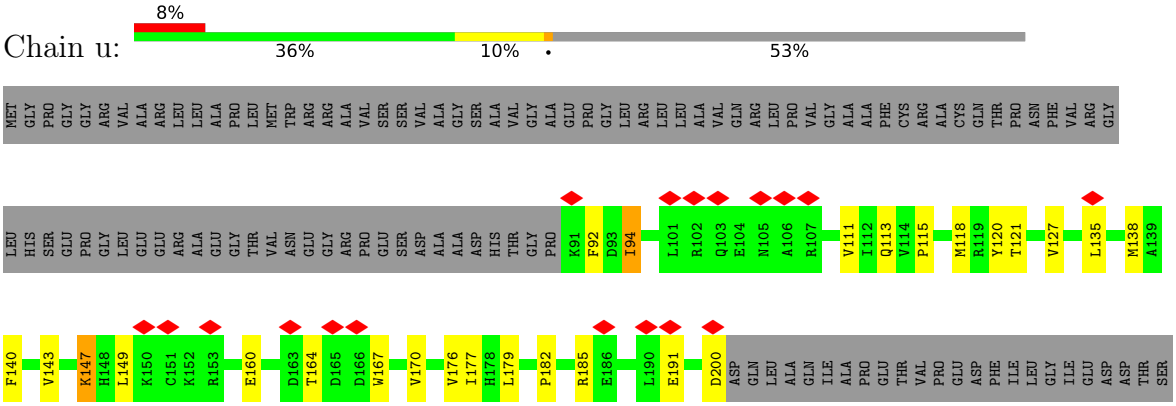
• Molecule 1: Mitochondrial ribosome-associated GTPase 2

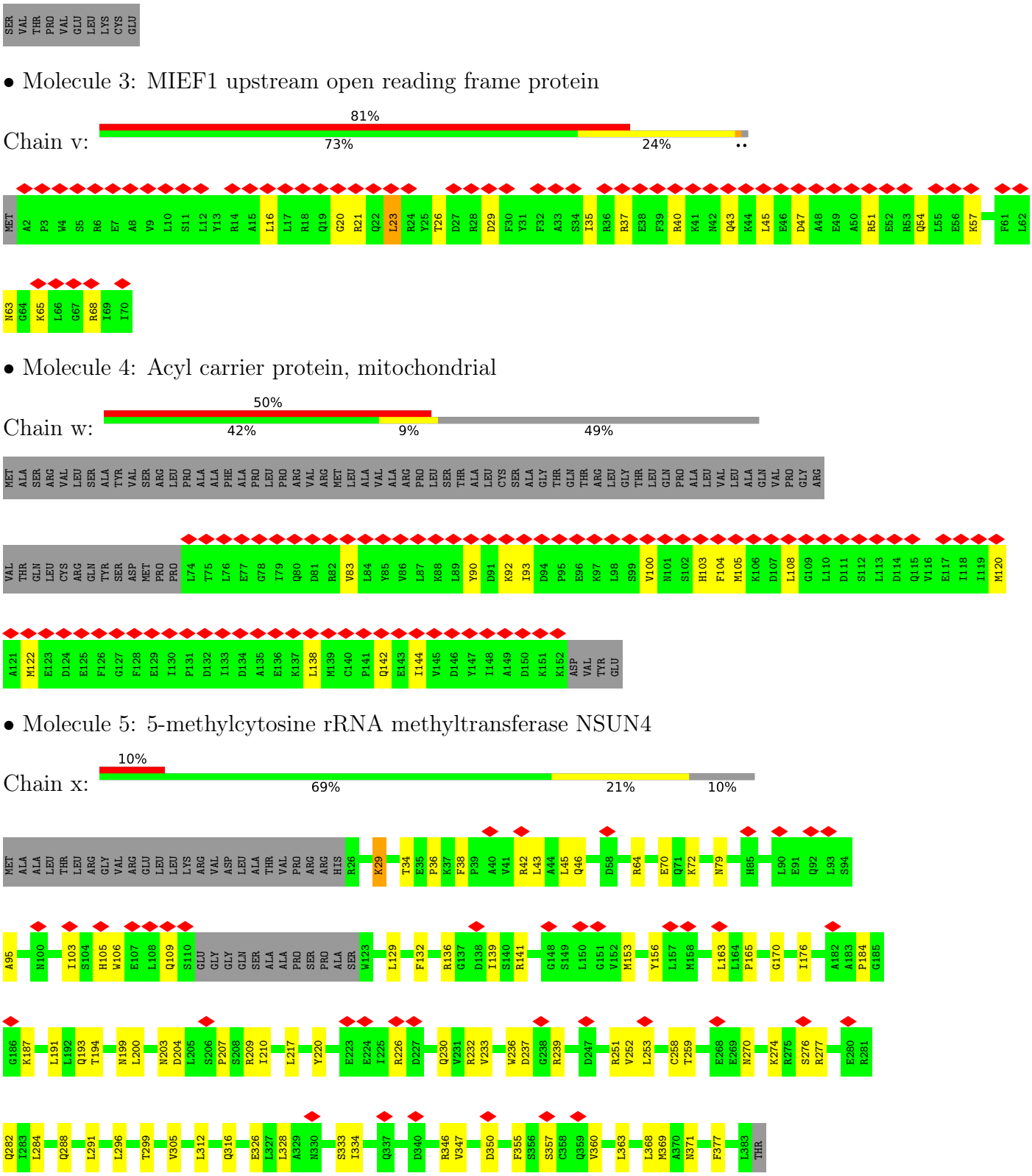
Chain t:

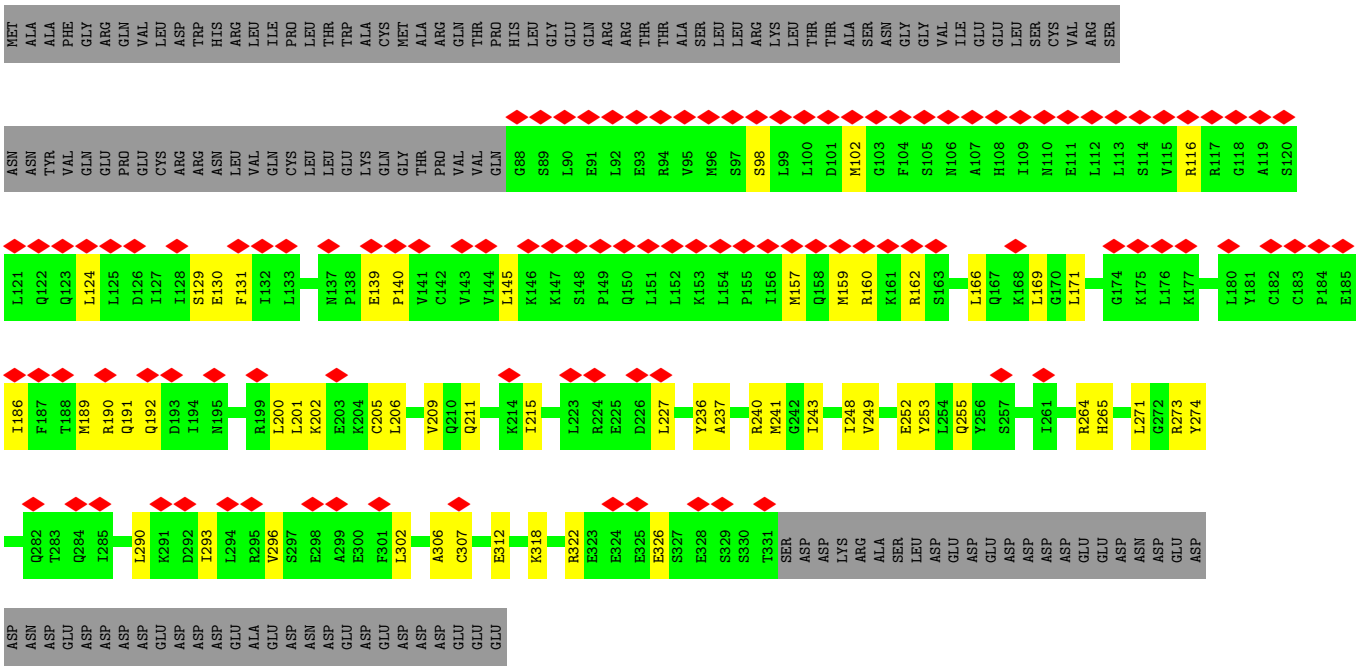


• Molecule 2: Mitochondrial assembly of ribosomal large subunit protein 1

Chain u:

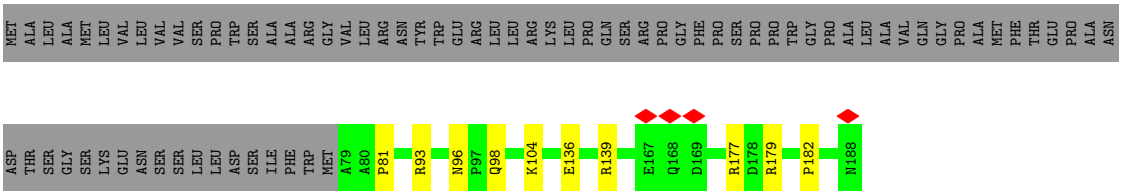



SER VAL THR PRO VAL GLU LEU LYS CYS GLU
• Molecule 3: MIEF1 upstream open reading frame protein
Chain v:
81%
73%
24%
MET A2 P3 W4 S5 R6 E7 A8 V9 L10 S11 L12 Y13 R14 A15 L16 L17 R18 Q19 G20 R21 Q22 L23 R24 Y25 T26 D27 R28 D29 F30 Y31 F32 A33 S34 I35 R36 R37 E38 F39 R40 K41 N42 Q43 K44 L45 E46 D47 A48 E49 A50 R51 E52 R53 Q54 L55 E56 K57 F61 L62
N63 G64 K65 L66 G67 R68 I69 I70
• Molecule 4: Acyl carrier protein, mitochondrial
Chain w:
50%
42%
9%
49%
MET ALA SER ARG VAL LEU SER ALA TYR VAL SER ARG LEU PRO ALA ALA PHE ALA PRO LEU PRO ARG VAL ARG MET LEU ALA VAL ALA ARG PRO LEU SER THR ALA LEU CYS SER ALA GLY THR GLN THR ARG LEU GLY THR LEU GLN PRO ALA LEU VAL LEU ALA GLN VAL PRO GLY ARG
VAL THR GLN LEU CYS ARG GLN TYR SER ASP MET PRO PRO L74 T75 L76 E77 G78 I79 Q80 D81 R82 V83 L84 Y85 V86 L87 K88 L89 Y90 D91 K92 I93 D94 P95 E96 K97 L98 S99 V100 N101 S102 H103 F104 M105 K106 D107 L108 G109 L110 D111 S112 L113 D114 Q115 V116 E117 I118 I119 M120
A121 M122 E123 D124 E125 F126 G127 F128 E129 I130 P131 D132 I133 D134 A135 E136 K137 L138 M139 C140 P141 Q142 E143 I144 V145 D146 Y147 I148 A149 D150 K151 K152 ASP VAL TYR GLU
• Molecule 5: 5-methylcytosine rRNA methyltransferase NSUN4
Chain x:
10%
69%
21%
10%
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 R26 K29 T34 E35 P36 K37 F38 P39 A40 V41 R42 L43 A44 L45 Q46 D58 R64 E70 Q71 K72 N79 H85 L90 E91 Q92 L93 S94
A95 N100 I103 S104 H105 W106 E107 L108 Q109 S110 GLU GLY GLY GLN SER ALA ALA PRO SER PRO ALA SER W123 L129 F132 R136 G137 D138 I139 S140 R141 G148 S149 L150 G151 V152 M153 Y156 L157 M158 L163 L164 P165 G170 I176 A182 A183 P184 G185
G186 K187 L191 L192 Q193 T194 N199 L200 N203 D204 L205 S206 P207 S208 R209 I210 L217 Y220 E223 E224 I225 R226 D227 Q230 V231 R232 V233 W236 D237 G238 R239 D247 R251 V252 L253 C258 T259 E268 E269 N270 K274 R275 S276 R277 E280 R281
Q282 T283 L284 Q288 L291 L296 T299 V305 L312 Q316 E326 L327 L328 A329 N330 S333 I334 Q337 D340 R346 V347 D350 F355 S356 S357 C358 Q359 V360 L363 L368 M369 A370 N371 F377 L383 THR
• Molecule 6: Transcription termination factor 4, mitochondrial
Chain y:
29%
49%
15%
36%



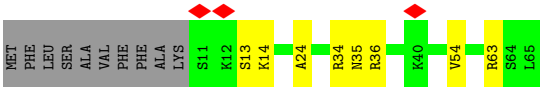
- Molecule 7: 39S ribosomal protein L32, mitochondrial

Chain 0:



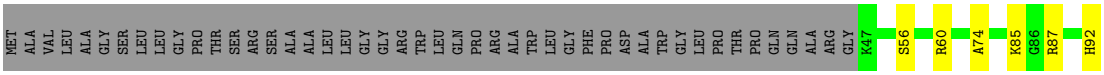
- Molecule 8: 39S ribosomal protein L33, mitochondrial

Chain 1:



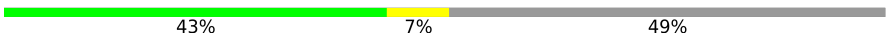
- Molecule 9: 39S ribosomal protein L34, mitochondrial

Chain 2:



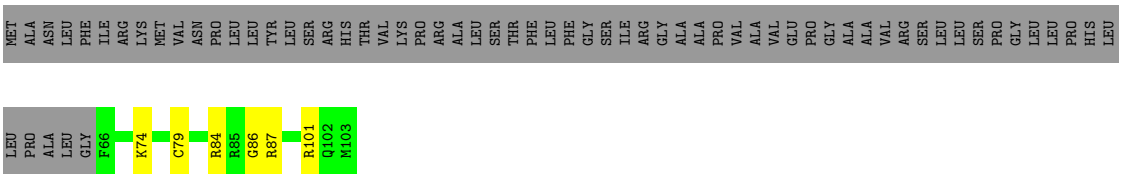
- Molecule 10: 39S ribosomal protein L35, mitochondrial

Chain 3:



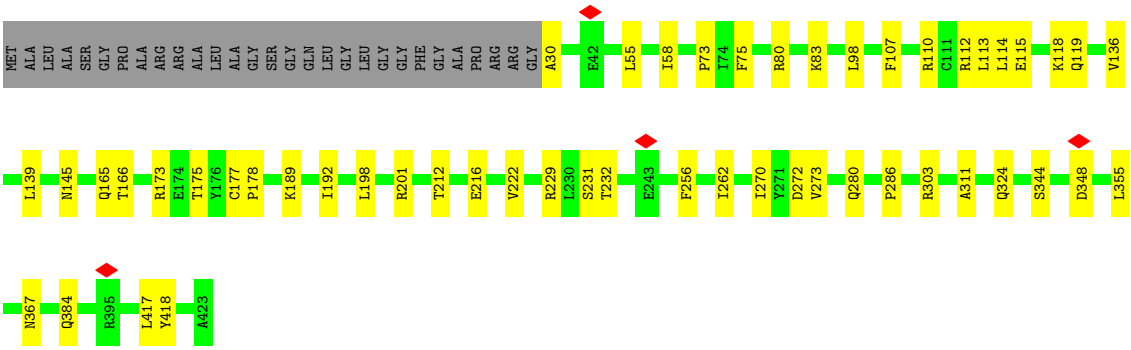
• Molecule 11: 39S ribosomal protein L36, mitochondrial

Chain 4:



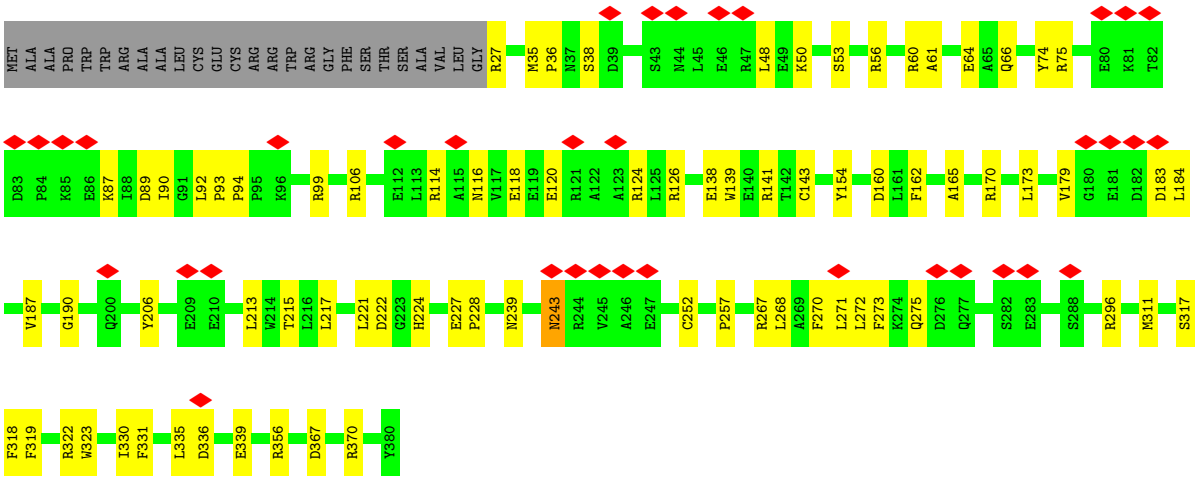
• Molecule 12: 39S ribosomal protein L37, mitochondrial

Chain 5:



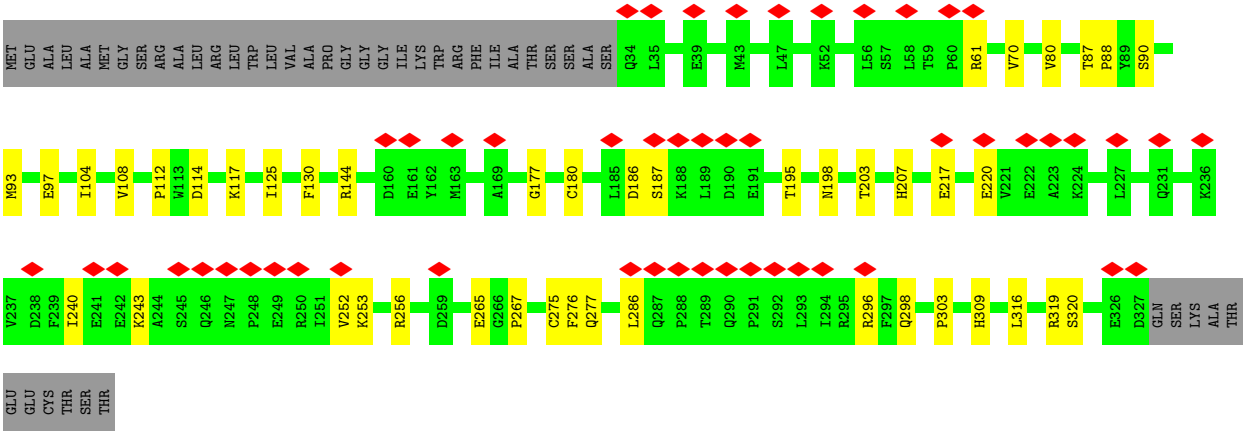
• Molecule 13: 39S ribosomal protein L38, mitochondrial

Chain 6:



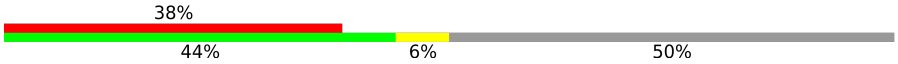
• Molecule 14: 39S ribosomal protein L39, mitochondrial

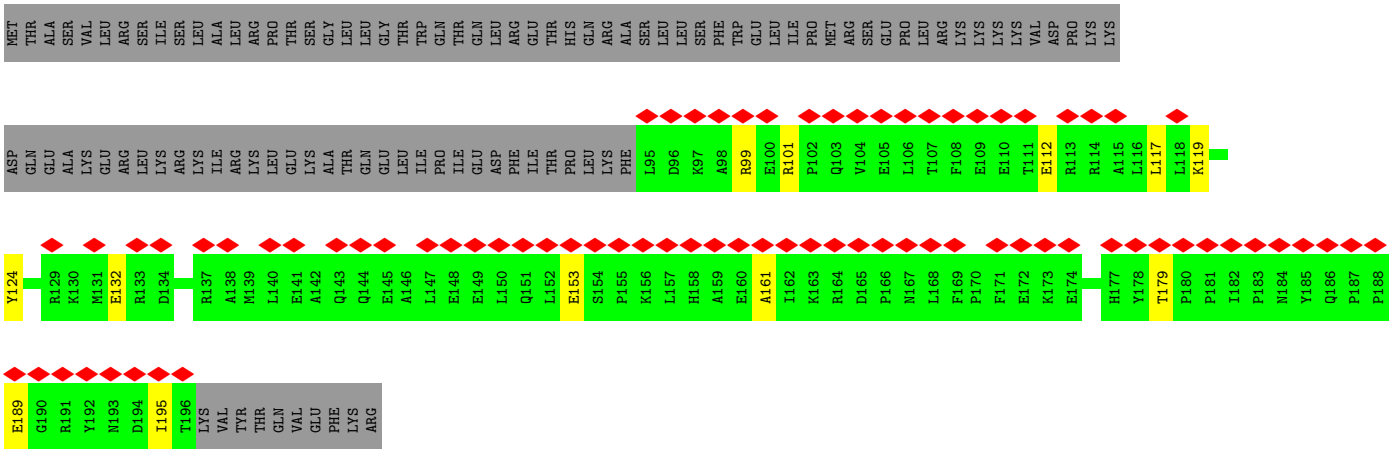
Chain 7:



• Molecule 15: 39S ribosomal protein L40, mitochondrial

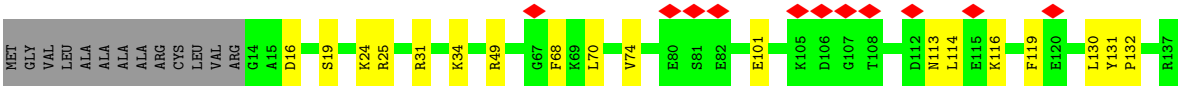
Chain 8:





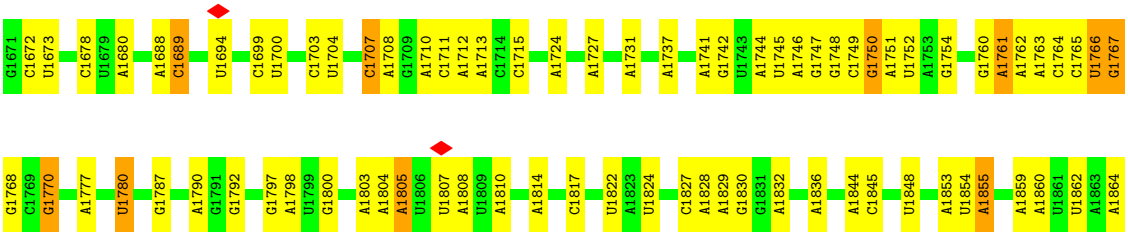
• Molecule 16: 39S ribosomal protein L41, mitochondrial

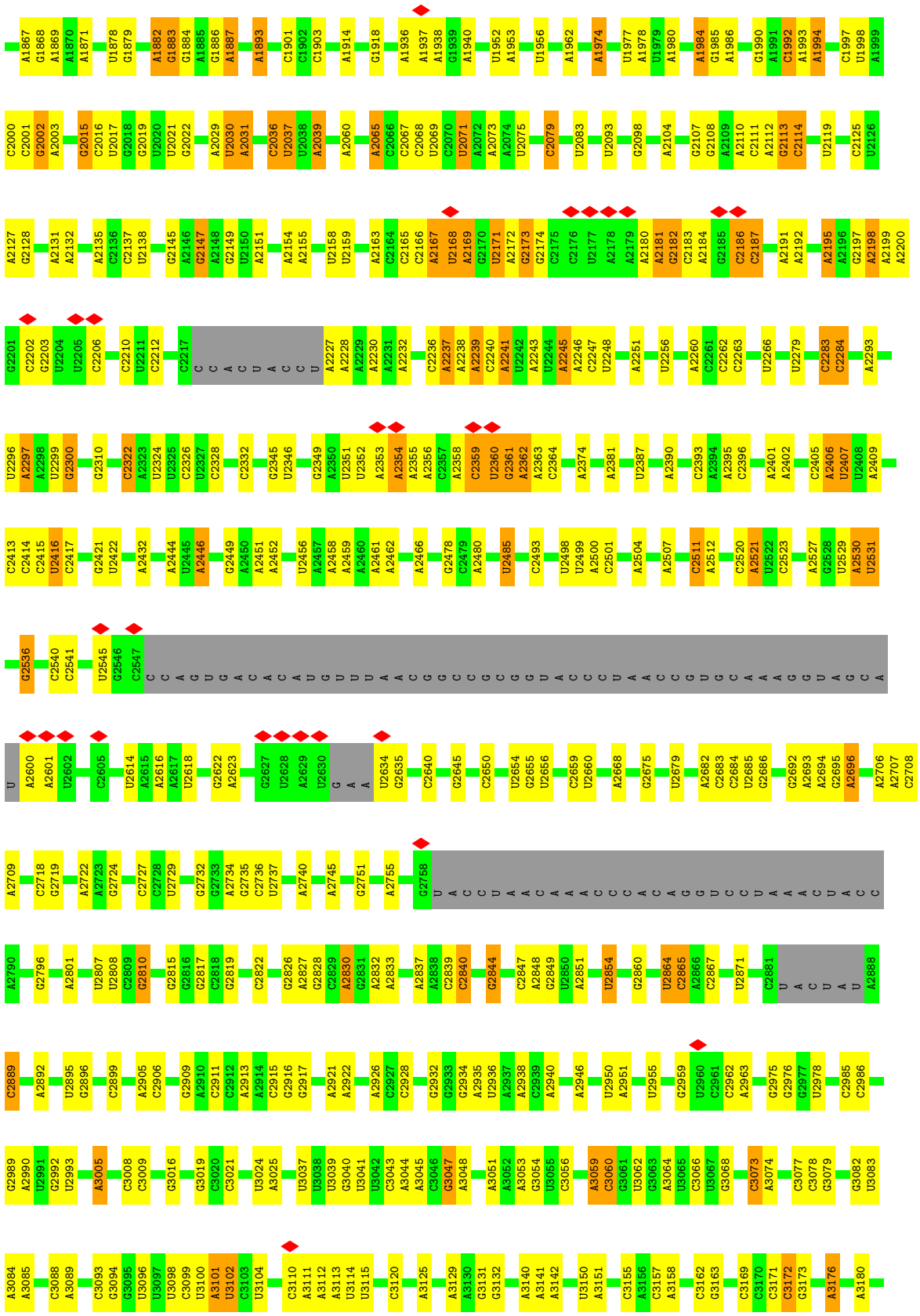
Chain 9:

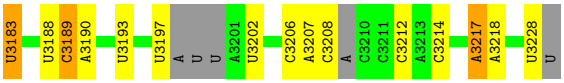


• Molecule 17: 16S mitochondrial rRNA

Chain A:

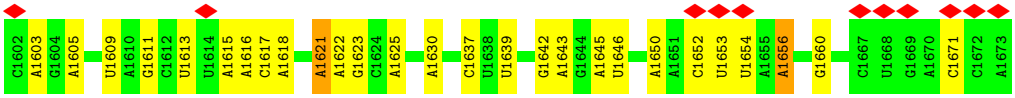



A1867 G1868 A1869 A1870 A1871 U1878 G1879 A1882 G1883 G1884 A1885 G1886 A1887 A1893 C1901 C1902 C1903 A1914 G1918 A1936 A1937 A1938 G1939 A1940 U1952 A1953 U1956 A1962 A1974 U1977 A1978 U1979 A1980 A1984 G1985 A1986 G1990 A1991 C1992 A1993 A1994 C1997 U1998 A1999
C2000 C2001 G2002 A2003 G2015 C2016 U2017 C2018 G2019 U2020 U2021 G2022 A2029 U2030 A2031 C2036 U2037 U2038 A2039 A2060 A2065 C2066 C2067 C2068 U2069 C2070 U2071 A2072 A2073 A2074 U2075 C2079 U2083 U2093 G2098 A2104 G2107 G2108 A2109 A2110 C2111 A2112 G2113 C2114 U2119 C2125 U2126
A2127 G2128 A2131 A2132 A2135 C2136 C2137 U2138 G2145 A2146 G2147 A2148 G2149 U2150 A2151 A2154 A2155 U2158 U2159 A2163 C2164 C2165 C2166 A2167 U2168 A2169 G2170 U2171 A2172 G2173 G2174 C2175 C2176 U2177 A2178 A2179 A2180 A2181 G2182 C2183 A2184 G2185 C2186 C2187 A2191 A2192 A2195 A2196 G2197 A2198 A2199 A2200
G2201 C2202 G2203 U2204 U2205 C2206 C2210 U2211 C2212 C2217 C C A C U A C C U A2227 A2228 A2229 A2230 A2231 A2232 C2236 A2237 A2238 A2239 C2240 A2241 U2242 A2243 U2244 A2245 A2246 C2247 U2248 A2251 U2256 A2260 C2261 C2262 C2263 U2266 U2279 C2283 C2284 A2293
U2296 A2297 A2298 U2299 G2300 G2310 C2322 A2323 U2324 U2325 C2326 U2327 C2328 C2332 G2345 U2346 G2349 A2350 U2351 U2352 A2353 A2354 A2355 A2356 C2357 A2358 C2359 U2360 G2361 A2362 A2363 C2364 A2374 A2381 U2387 A2390 C2393 A2394 A2395 C2396 A2401 A2402 C2405 A2406 U2407 U2408 A2409
C2413 C2414 C2415 U2416 C2417 G2421 U2422 A2432 A2444 U2445 A2446 G2449 A2450 A2451 A2452 U2456 A2457 A2458 A2459 A2460 A2461 A2462 A2466 G2478 C2479 A2480 U2485 C2493 U2498 U2499 A2500 C2501 A2504 A2507 C2511 A2512 C2520 A2521 U2522 C2523 A2527 G2528 U2529 A2530 U2531
G2536 C2540 C2541 U2545 G2546 C2547 C C A G U G A C A C A U G U U U A A C G G C C G C G G G U A C C C U A A C C G G U G C A A A G G U A G C A
U A2600 A2601 U2602 C2605 U2614 A2615 A2616 A2617 U2618 G2622 A2623 G2627 U2628 A2629 U2630 G A A U2634 G2635 C2640 G2645 C2650 U2654 G2655 U2656 C2659 U2660 A2668 G2675 U2679 A2682 C2683 C2684 U2685 G2686 G2692 A2693 A2694 G2695 A2696 A2706 A2707 C2708
A2709 C2718 G2719 A2722 A2723 G2724 C2727 C2728 U2729 G2732 G2733 A2734 G2735 C2736 U2737 A2740 A2745 G2751 A2755 G2758 U A C C U A C A A A C C C A C A G G U C C U A A A C U A C C
A2790 G2796 A2801 U2807 U2808 C2809 G2810 G2815 G2816 G2817 C2818 G2819 C2822 G2826 A2827 G2828 C2829 A2830 G2831 A2832 A2833 A2837 A2838 C2839 C2840 G2844 C2847 A2848 G2849 U2850 A2851 U2854 G2860 U2864 C2865 A2866 C2867 U2871 C2881 U A C U A U A2888
C2889 A2892 U2895 G2896 C2899 A2905 C2906 G2909 A2910 C2911 C2912 A2913 A2914 C2915 G2916 G2917 A2921 A2922 A2926 C2927 C2928 G2932 G2933 G2934 A2935 U2936 A2937 A2938 C2939 A2940 A2946 U2950 A2951 U2955 G2959 U2960 C2961 C2962 A2963 G2975 G2976 G2977 U2978 C2985 C2986
G2989 A2990 U2991 G2992 U2993 A3005 C3008 C3009 G3016 G3019 A3020 C3021 U3024 A3025 U3037 U3038 U3039 G3040 U3041 U3042 C3043 A3044 A3045 C3046 G3047 A3048 A3051 A3052 A3053 G3054 U3055 C3056 A3059 C3060 G3061 U3062 G3063 A3064 U3065 C3066 U3067 G3068 C3073 A3074 C3077 C3078 G3079 G3082 U3083
A3084 A3085 C3088 A3089 C3093 G3094 G3095 U3096 U3097 U3098 C3099 U3100 A3101 U3102 C3103 U3104 C3110 A3111 A3112 A3113 U3114 U3115 C3120 A3125 A3129 A3130 G3131 G3132 A3140 A3141 A3142 U3150 A3151 C3155 A3156 C3157 A3158 C3162 G3163 C3169 C3170 C3171 C3172 G3173 A3176 A3180



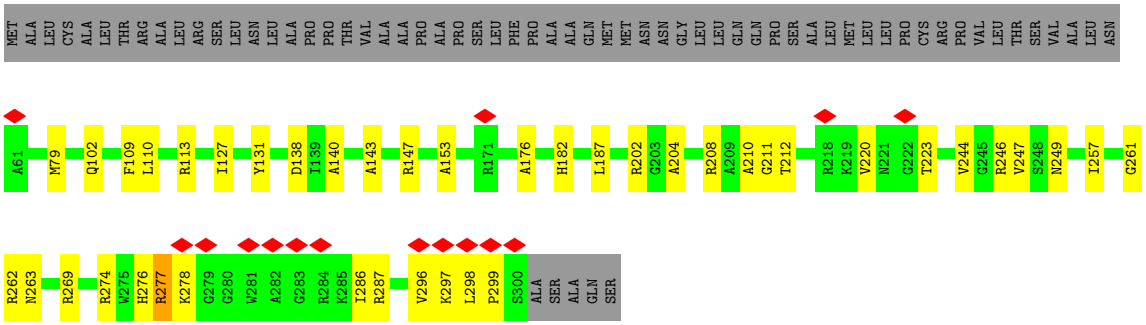
• Molecule 18: mitochondrial tRNAVal

Chain B:



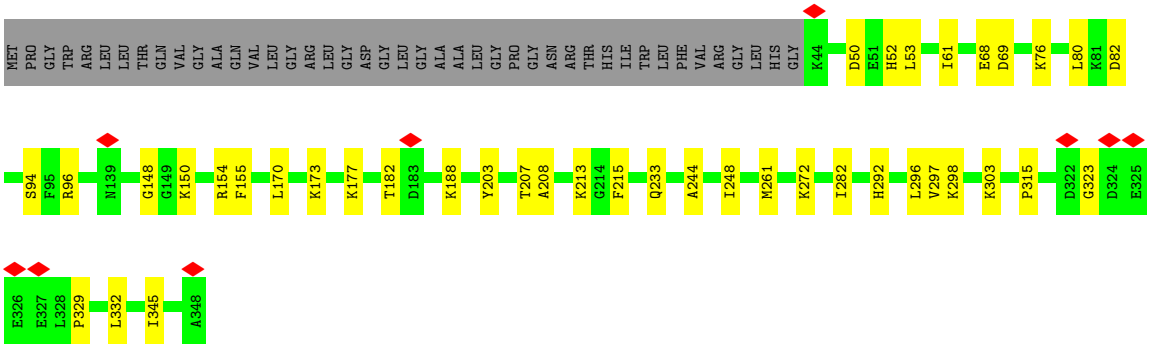
• Molecule 19: 39S ribosomal protein L2, mitochondrial

Chain D:



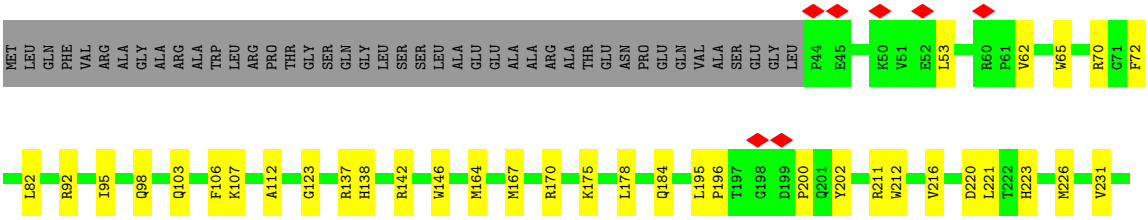
• Molecule 20: 39S ribosomal protein L3, mitochondrial

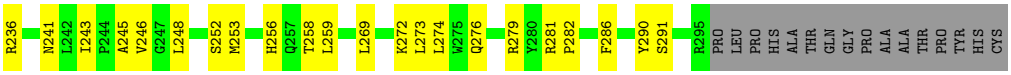
Chain E:



• Molecule 21: 39S ribosomal protein L4, mitochondrial

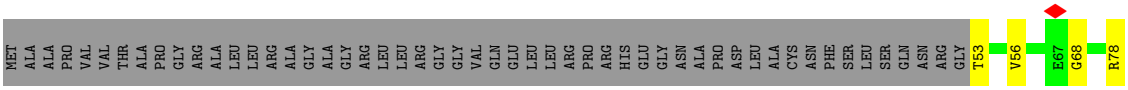
Chain F:

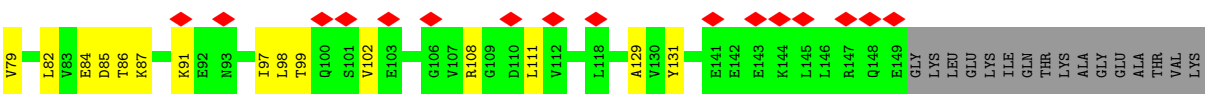




• Molecule 22: 39S ribosomal protein L9, mitochondrial

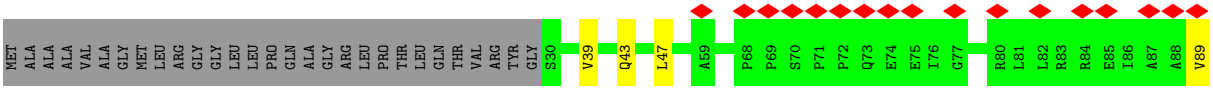
Chain H:

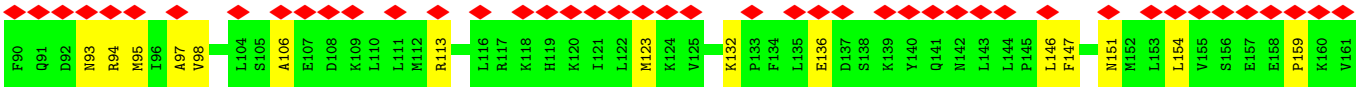


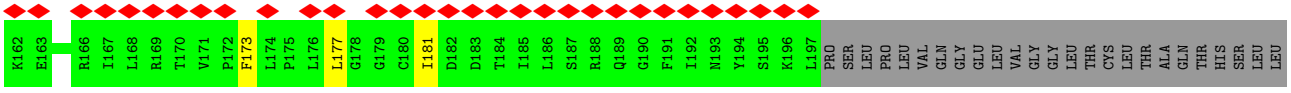


• Molecule 23: 39S ribosomal protein L10, mitochondrial

Chain I:

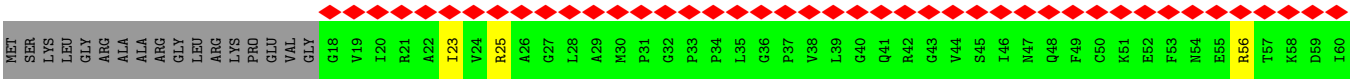


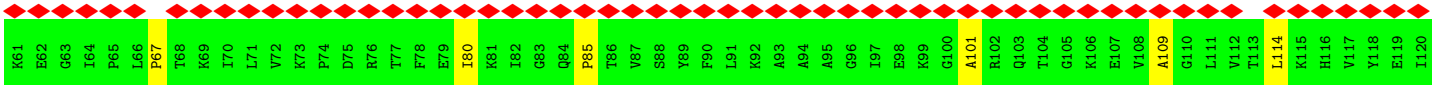


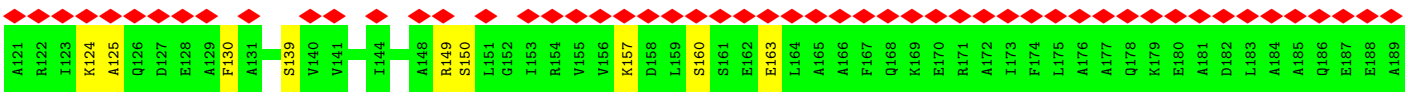


• Molecule 24: 39S ribosomal protein L11, mitochondrial

Chain J:

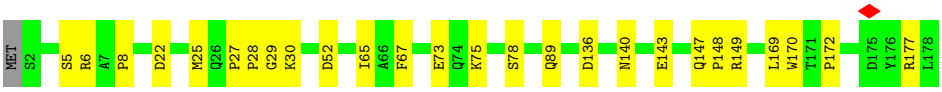






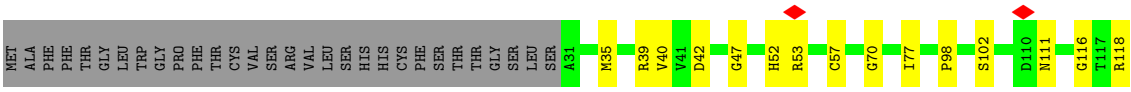
• Molecule 25: 39S ribosomal protein L13, mitochondrial

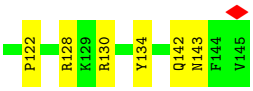
Chain K:



• Molecule 26: 39S ribosomal protein L14, mitochondrial

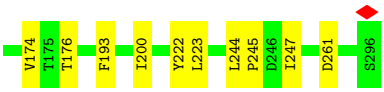
Chain L:





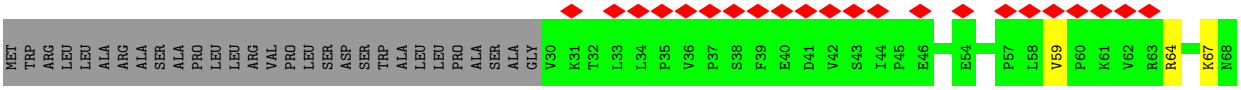
• Molecule 27: 39S ribosomal protein L15, mitochondrial

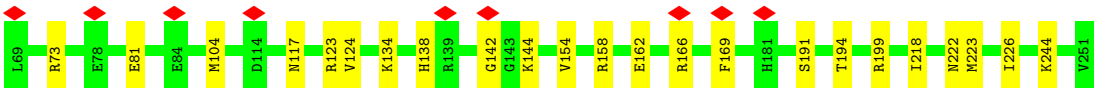
Chain M:



• Molecule 28: 39S ribosomal protein L16, mitochondrial

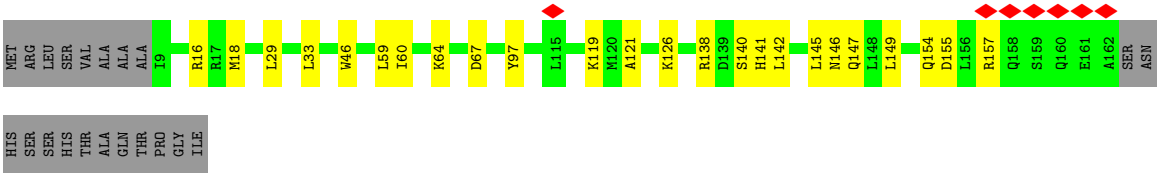
Chain N:





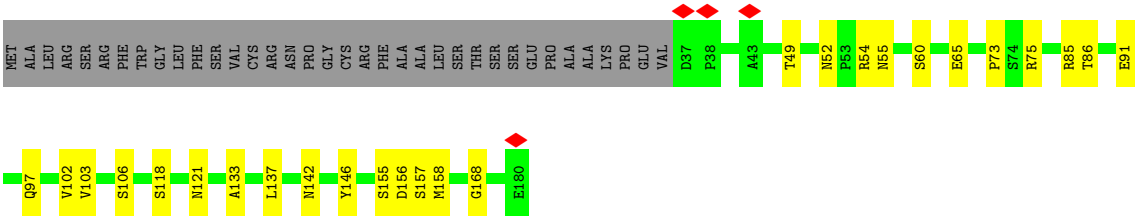
• Molecule 29: 39S ribosomal protein L17, mitochondrial

Chain O:



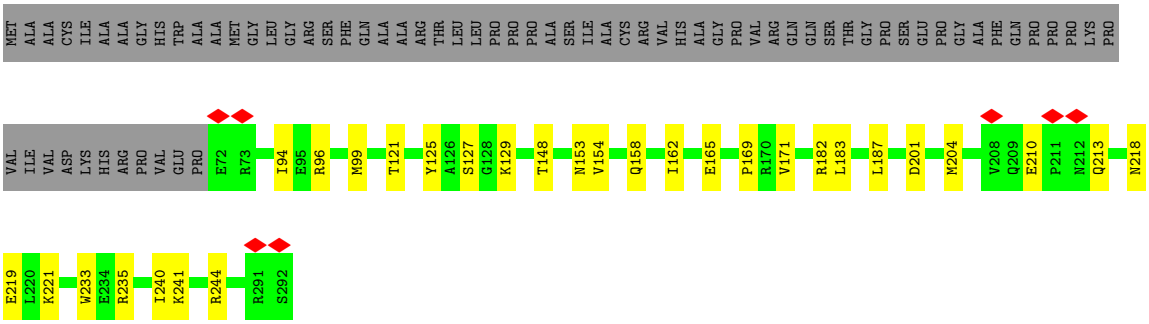
• Molecule 30: 39S ribosomal protein L18, mitochondrial

Chain P:



• Molecule 31: 39S ribosomal protein L19, mitochondrial

Chain Q:

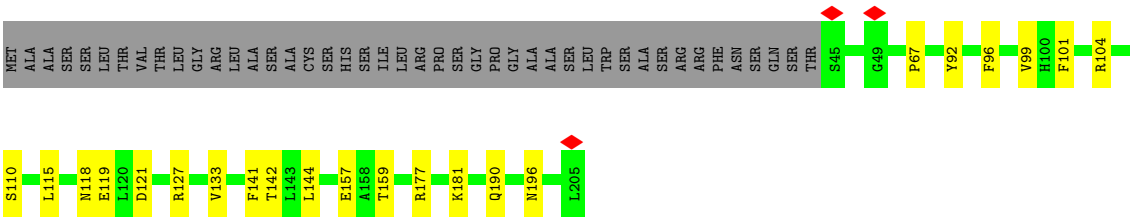


• Molecule 32: 39S ribosomal protein L20, mitochondrial

Chain R:

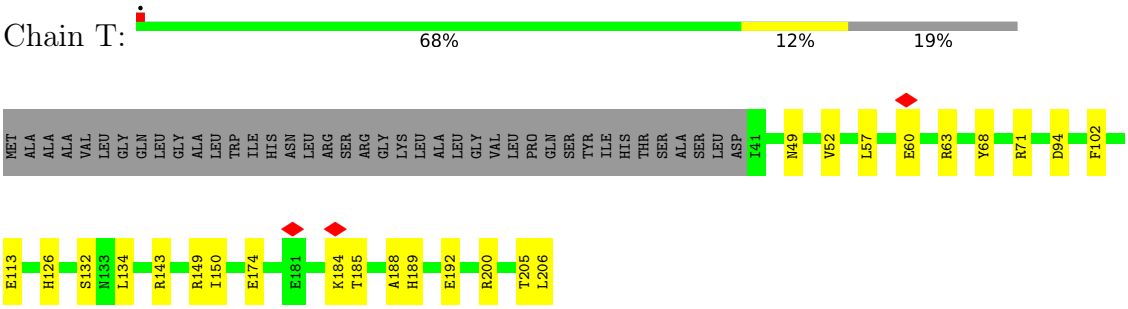
• Molecule 33: 39S ribosomal protein L21, mitochondrial

Chain S:



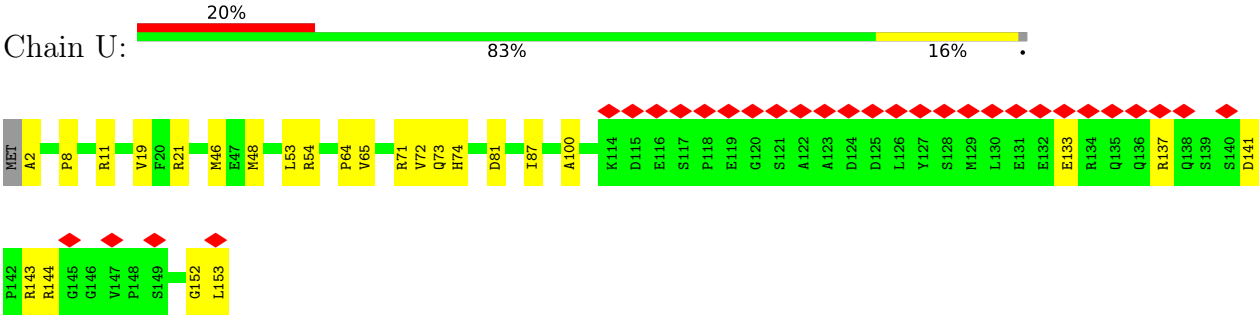
• Molecule 34: 39S ribosomal protein L22, mitochondrial

Chain T:



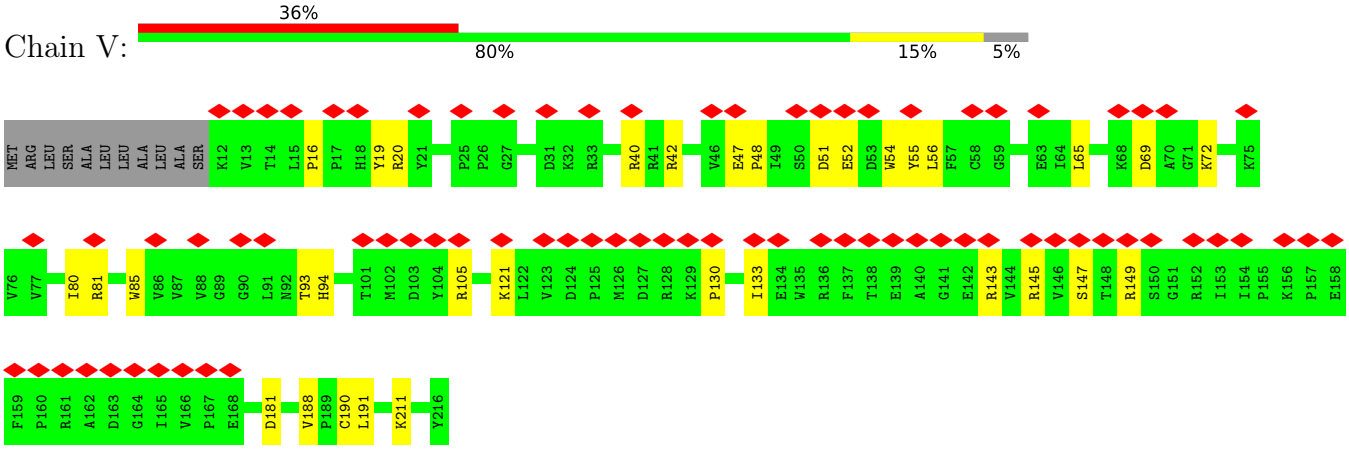
• Molecule 35: 39S ribosomal protein L23, mitochondrial

Chain U:



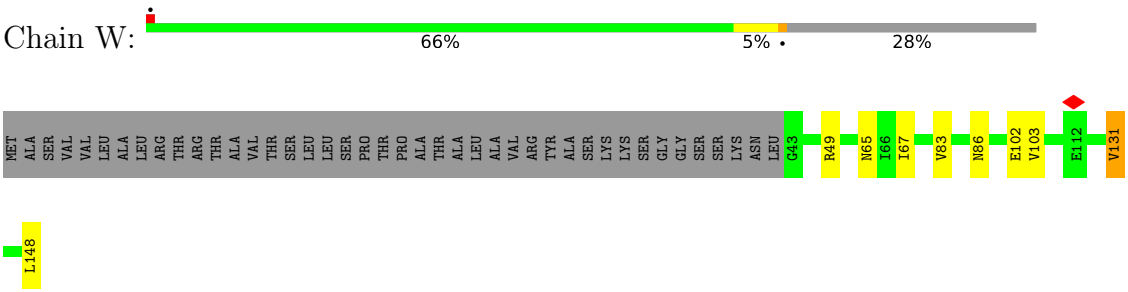
• Molecule 36: 39S ribosomal protein L24, mitochondrial

Chain V:



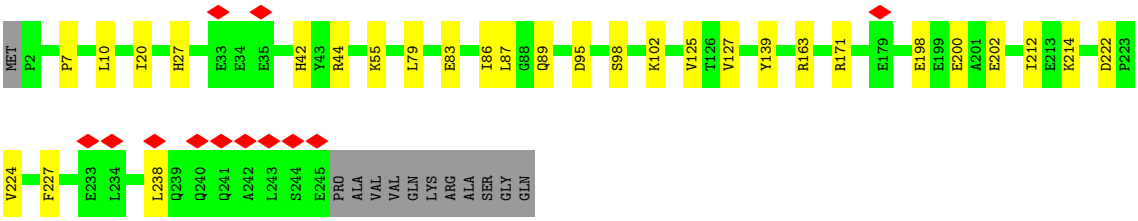
• Molecule 37: 39S ribosomal protein L27, mitochondrial

Chain W:



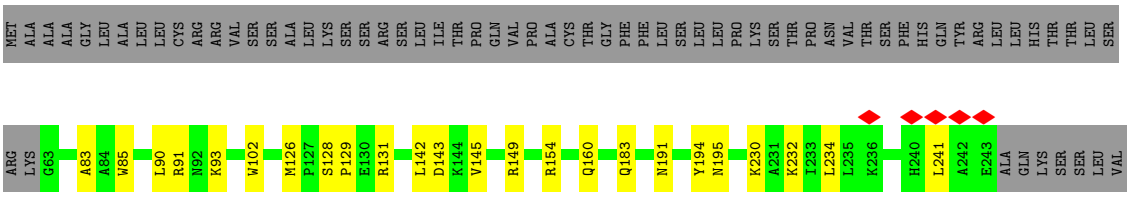
• Molecule 38: 39S ribosomal protein L28, mitochondrial

Chain X:



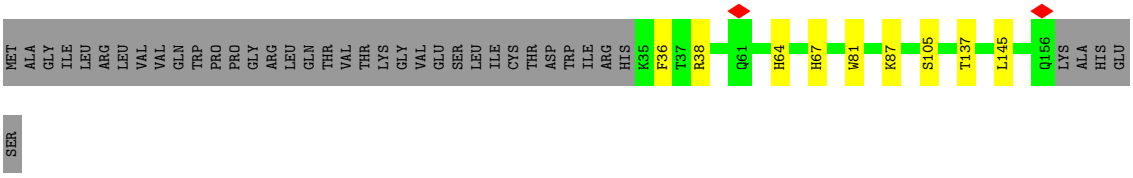
- Molecule 39: 39S ribosomal protein L47, mitochondrial

Chain Y:



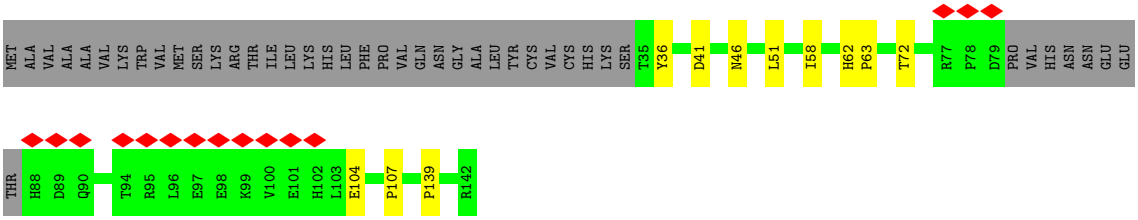
- Molecule 40: 39S ribosomal protein L30, mitochondrial

Chain Z:



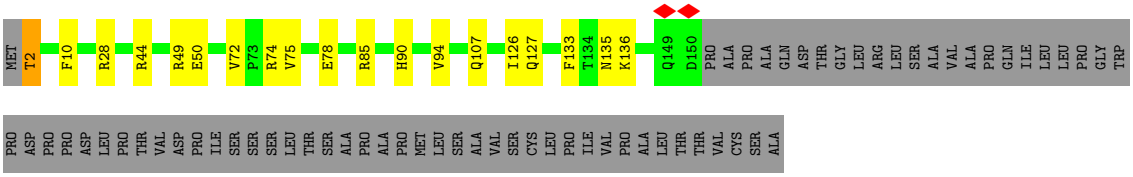
- Molecule 41: 39S ribosomal protein L42, mitochondrial

Chain a:



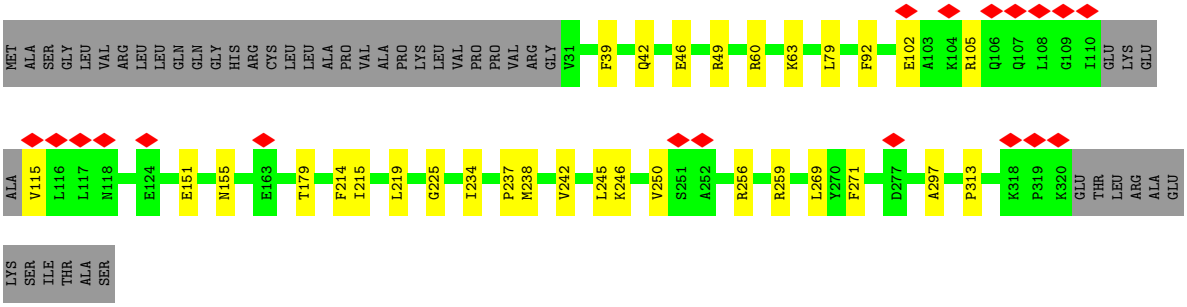
- Molecule 42: 39S ribosomal protein L43, mitochondrial

Chain b:



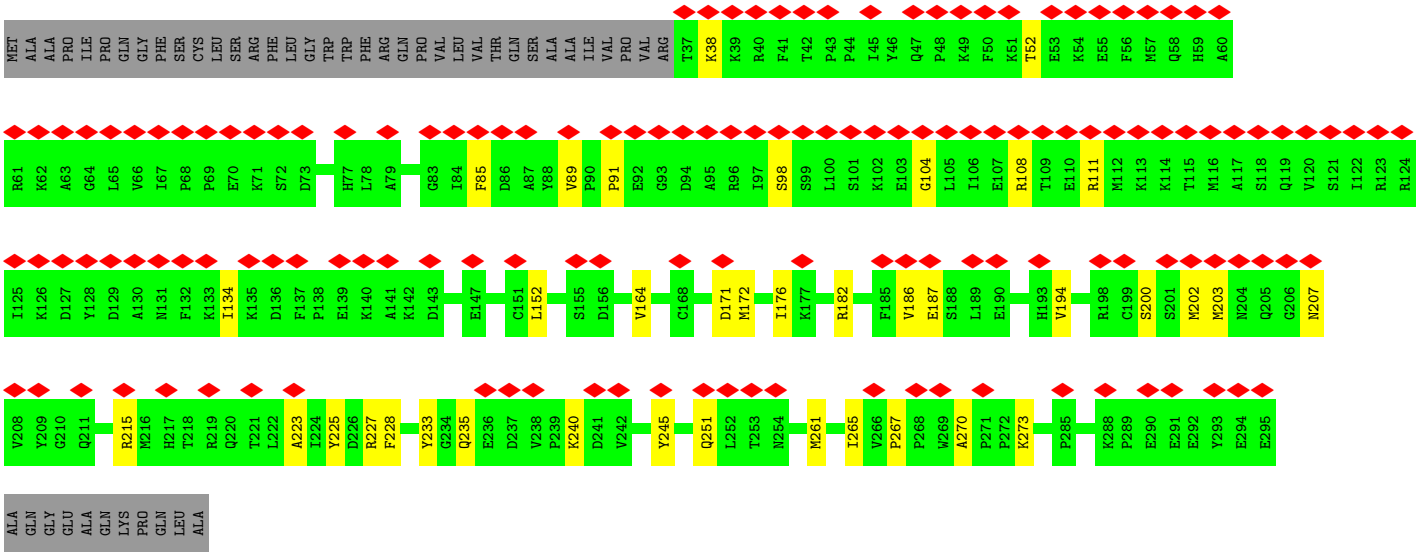
• Molecule 43: 39S ribosomal protein L44, mitochondrial

Chain c:



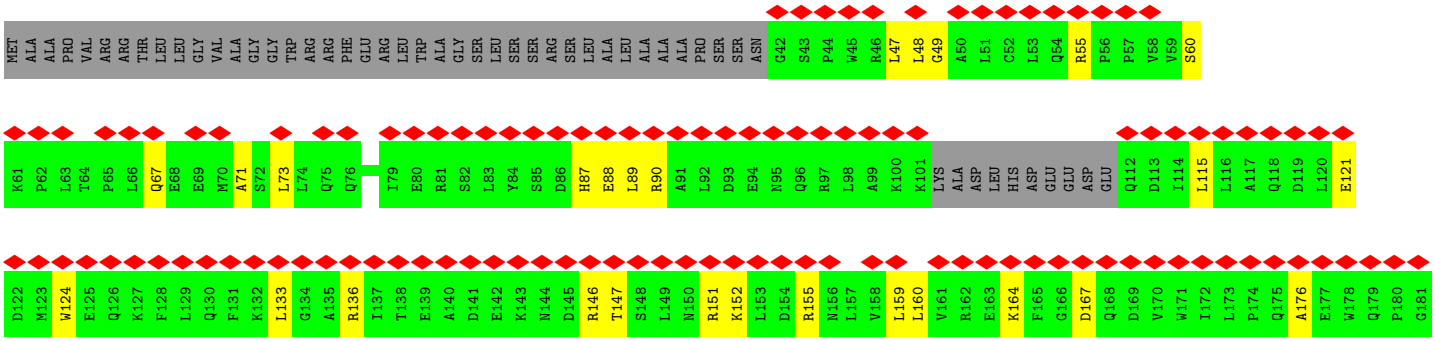
• Molecule 44: 39S ribosomal protein L45, mitochondrial

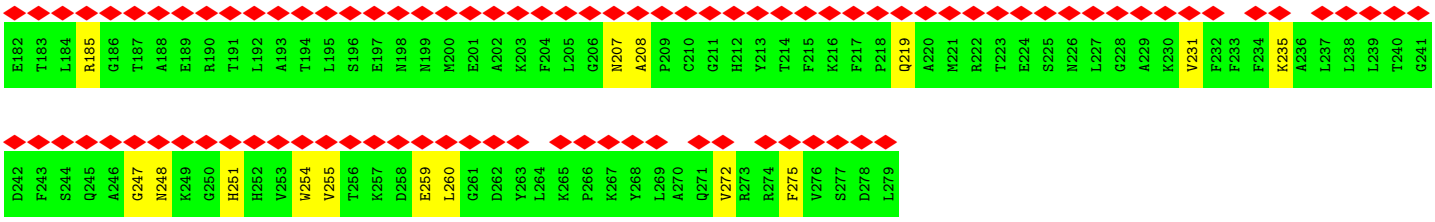
Chain d:



• Molecule 45: 39S ribosomal protein L46, mitochondrial

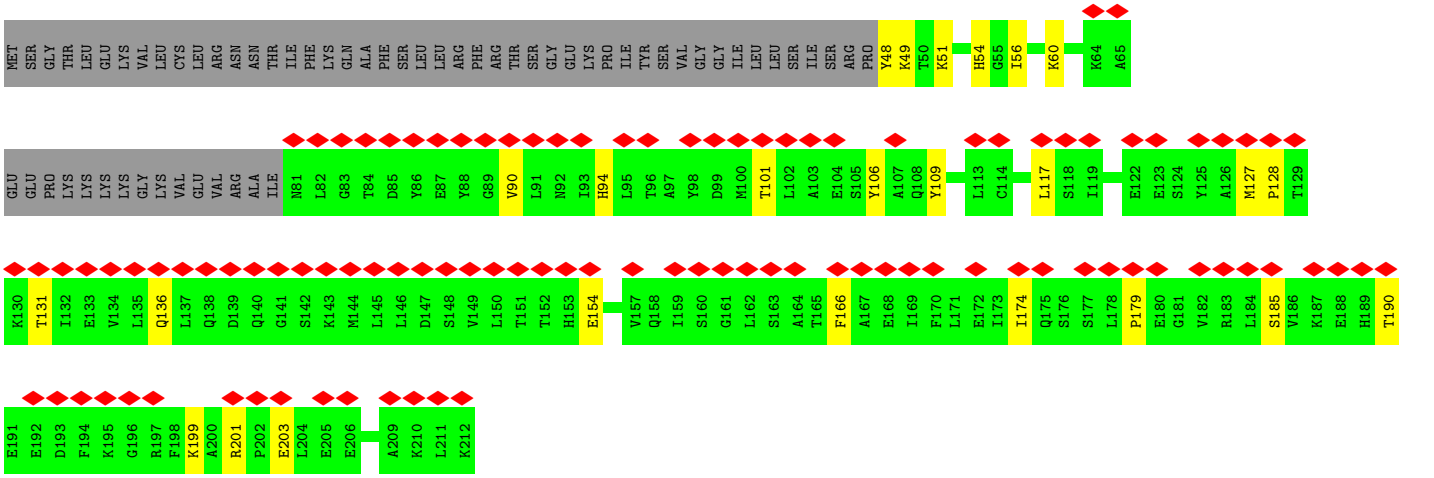
Chain e:





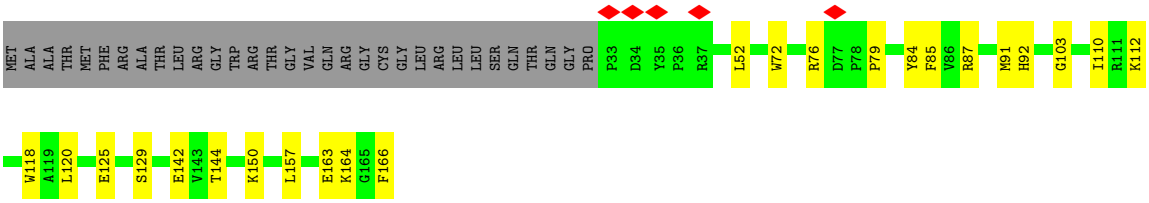
- Molecule 46: 39S ribosomal protein L48, mitochondrial

Chain f:



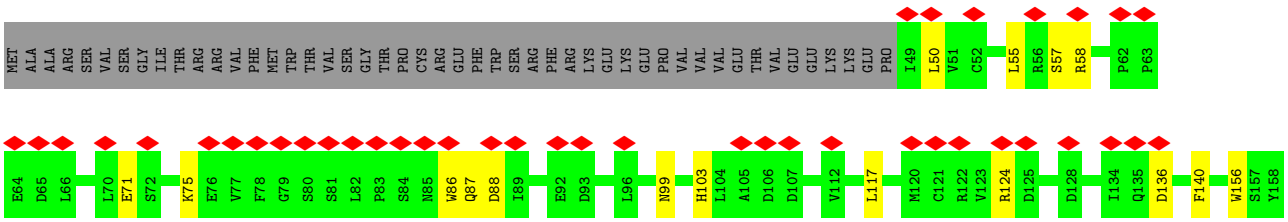
- Molecule 47: 39S ribosomal protein L49, mitochondrial

Chain g:



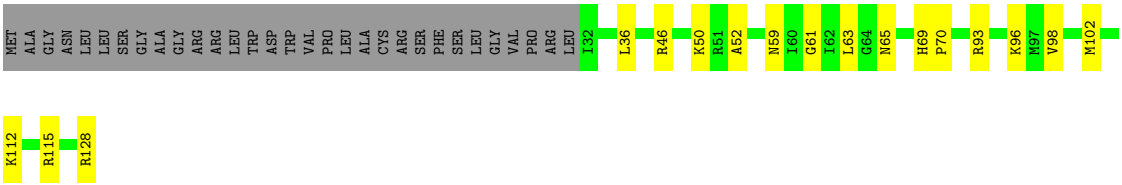
- Molecule 48: 39S ribosomal protein L50, mitochondrial

Chain h:



- Molecule 49: 39S ribosomal protein L51, mitochondrial

Chain i:

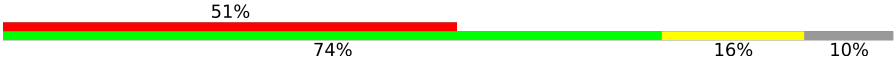


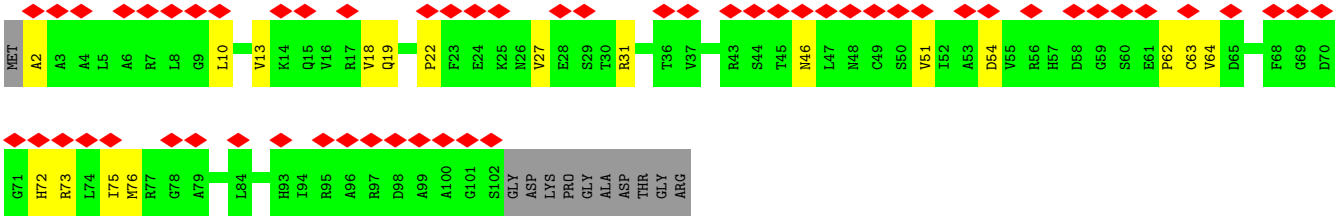
- Molecule 50: 39S ribosomal protein L52, mitochondrial

Chain j:

- Molecule 51: 39S ribosomal protein L53, mitochondrial

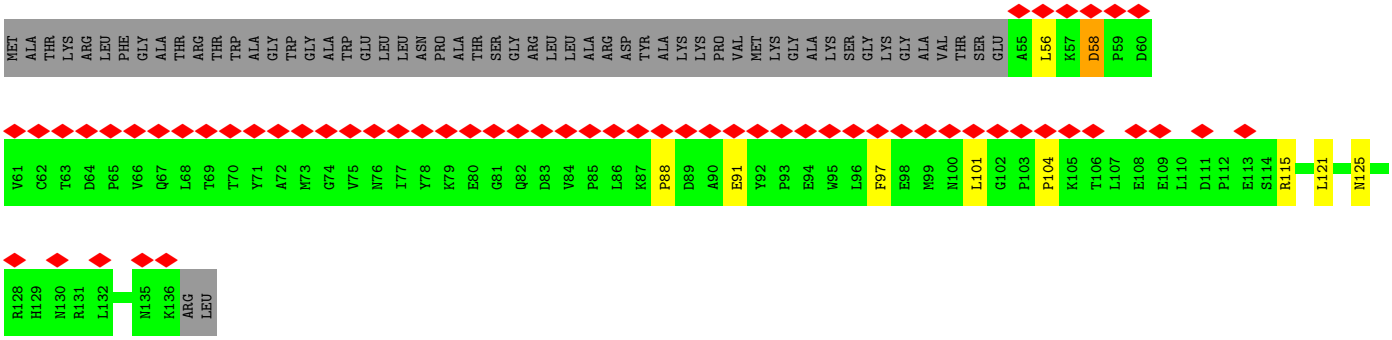
Chain k:





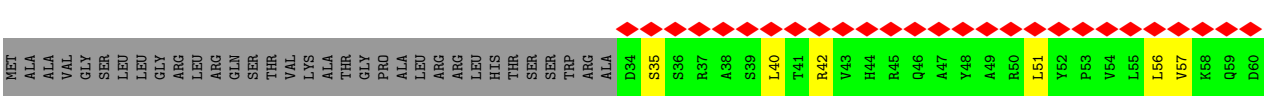
- Molecule 52: 39S ribosomal protein L54, mitochondrial

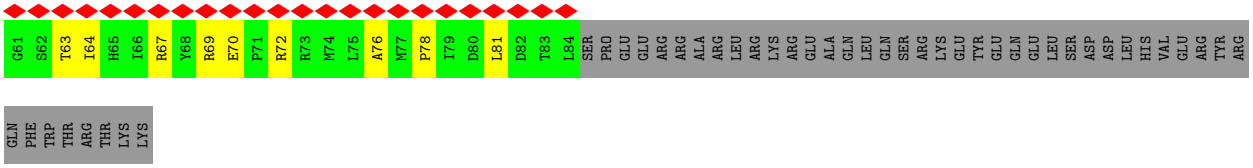
Chain l:



- Molecule 53: 39S ribosomal protein L55, mitochondrial

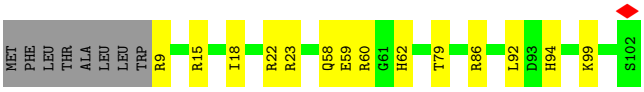
Chain m:





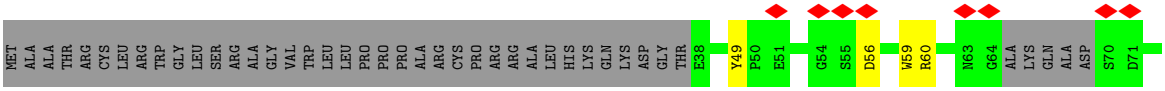
• Molecule 54: Ribosomal protein 63, mitochondrial

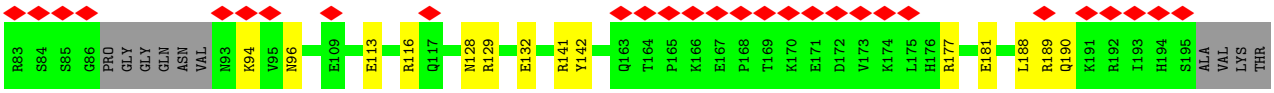
Chain o:



• Molecule 55: Peptidyl-tRNA hydrolase ICT1, mitochondrial

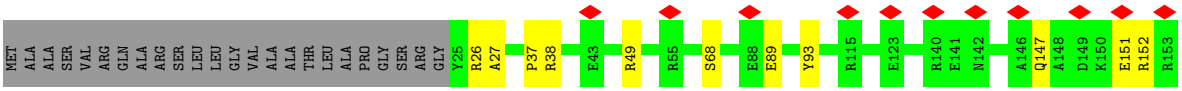
Chain p:

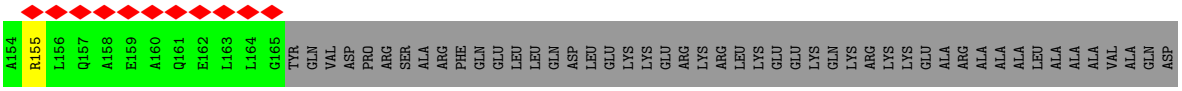




• Molecule 56: Growth arrest and DNA damage-inducible proteins-interacting protein 1

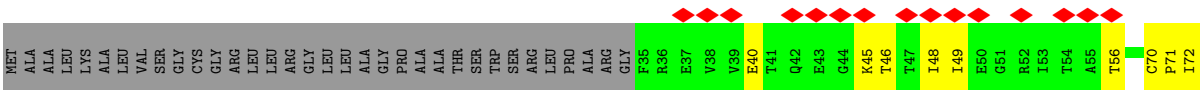
Chain q:

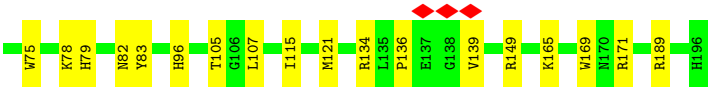




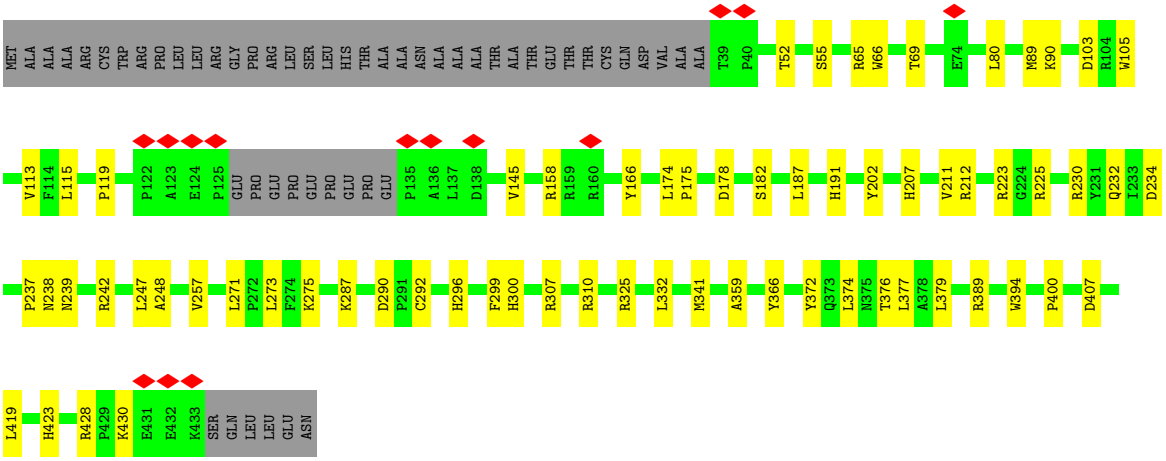
• Molecule 57: 39S ribosomal protein S18a, mitochondrial

Chain r:





• Molecule 58: 39S ribosomal protein S30, mitochondrial



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62552	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	2.962	Depositor
Minimum map value	-0.925	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.45	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: ZN, K, OMG, FES, OMU, GDP, PM8, THC, AYA, MG, SAC, SAM

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	t	0.11	0/2445	0.29	0/3301
2	u	0.10	0/941	0.28	0/1270
3	v	0.09	0/597	0.25	0/796
4	w	0.10	0/647	0.28	0/871
5	x	0.10	0/2814	0.28	0/3816
6	y	0.08	0/2011	0.23	0/2702
7	0	0.09	0/913	0.23	0/1224
8	1	0.09	0/460	0.25	0/610
9	2	0.10	0/383	0.24	0/507
10	3	0.10	0/853	0.27	0/1136
11	4	0.10	0/350	0.22	0/461
12	5	0.10	0/3305	0.26	0/4502
13	6	0.10	0/3043	0.27	0/4140
14	7	0.09	0/2447	0.25	0/3310
15	8	0.09	0/880	0.24	0/1188
16	9	0.11	0/1025	0.25	0/1379
17	A	0.09	0/34465	0.16	0/53638
18	B	0.05	0/1700	0.09	0/2641
19	D	0.10	0/1910	0.26	0/2569
20	E	0.11	0/2475	0.25	0/3355
21	F	0.11	0/2090	0.27	0/2842
22	H	0.10	0/816	0.26	0/1097
23	I	0.12	0/1388	0.29	0/1875
24	J	0.09	0/1348	0.26	0/1813
25	K	0.10	0/1490	0.26	0/2021
26	L	0.12	0/905	0.29	0/1218
27	M	0.10	0/2381	0.25	0/3212
28	N	0.09	0/1833	0.25	0/2468
29	O	0.10	0/1283	0.26	0/1727
30	P	0.10	0/1199	0.28	0/1623
31	Q	0.10	0/1884	0.26	0/2535
32	R	0.09	0/1175	0.21	0/1572

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	S	0.11	0/1320	0.29	0/1789
34	T	0.10	0/1403	0.25	0/1886
35	U	0.09	0/1274	0.25	0/1723
36	V	0.10	0/1721	0.23	0/2333
37	W	0.11	0/857	0.26	0/1155
38	X	0.09	0/2099	0.24	0/2837
39	Y	0.09	0/1593	0.24	0/2136
40	Z	0.10	0/1021	0.26	0/1378
41	a	0.11	0/866	0.25	0/1174
42	b	0.10	0/1203	0.29	0/1627
43	c	0.09	0/2347	0.27	0/3171
44	d	0.10	0/2181	0.25	0/2949
45	e	0.08	0/1885	0.26	0/2542
46	f	0.09	0/1216	0.24	0/1638
47	g	0.12	0/1151	0.28	0/1569
48	h	0.09	0/918	0.23	0/1249
49	i	0.10	0/850	0.23	0/1135
50	j	0.10	0/760	0.26	0/1023
51	k	0.09	0/777	0.24	0/1048
52	l	0.10	0/707	0.27	0/960
53	m	0.08	0/426	0.25	0/575
54	o	0.08	0/819	0.22	0/1097
55	p	0.09	0/1223	0.26	0/1641
56	q	0.08	0/1208	0.21	0/1633
57	r	0.11	0/1362	0.27	0/1846
58	s	0.10	0/3239	0.28	1/4400 (0.0%)
All	All	0.10	0/115882	0.23	1/163933 (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})
58	s	407	ASP	CB-CA-C	-5.33	110.42	116.54

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	t	2398	0	2380	51	0
2	u	919	0	917	17	0
3	v	588	0	604	13	0
4	w	638	0	636	10	0
5	x	2750	0	2733	53	0
6	y	1980	0	2066	37	0
7	0	898	0	916	9	0
8	1	455	0	498	5	0
9	2	377	0	406	5	0
10	3	832	0	883	9	0
11	4	342	0	361	4	0
12	5	3210	0	3206	35	0
13	6	2948	0	2841	58	0
14	7	2390	0	2397	28	0
15	8	860	0	852	12	0
16	9	997	0	987	17	0
17	A	30850	0	15671	266	0
18	B	1522	0	776	17	0
19	D	1872	0	1932	35	0
20	E	2406	0	2415	28	0
21	F	2031	0	2065	46	0
22	H	802	0	846	15	0
23	I	1358	0	1439	15	0
24	J	1330	0	1407	14	0
25	K	1455	0	1452	20	0
26	L	890	0	941	16	0
27	M	2327	0	2395	24	0
28	N	1786	0	1817	19	0
29	O	1259	0	1294	17	0
30	P	1173	0	1165	18	0
31	Q	1843	0	1878	19	0
32	R	1154	0	1214	11	0
33	S	1293	0	1365	17	0
34	T	1369	0	1410	20	0
35	U	1251	0	1232	16	0
36	V	1676	0	1687	23	0
37	W	835	0	858	7	0
38	X	2044	0	2060	22	0
39	Y	1556	0	1597	19	0
40	Z	996	0	1044	7	0
41	a	840	0	810	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	b	1189	0	1183	14	0
43	c	2299	0	2320	20	0
44	d	2124	0	2125	25	0
45	e	1848	0	1849	30	0
46	f	1196	0	1212	21	0
47	g	1113	0	1097	15	0
48	h	895	0	881	11	0
49	i	828	0	857	16	0
50	j	745	0	746	11	0
51	k	774	0	784	14	0
52	l	688	0	674	8	0
53	m	419	0	435	12	0
54	o	798	0	804	13	0
55	p	1205	0	1223	15	0
56	q	1177	0	1154	8	0
57	r	1322	0	1348	21	0
58	s	3155	0	3139	41	0
59	t	28	0	12	2	0
60	A	88	0	0	0	0
60	I	1	0	0	0	0
60	M	1	0	0	0	0
60	O	1	0	0	0	0
60	W	1	0	0	0	0
60	g	1	0	0	0	0
60	o	1	0	0	0	0
60	t	1	0	0	0	0
61	w	32	0	39	2	0
62	x	27	0	22	0	0
63	0	1	0	0	0	0
63	4	1	0	0	0	0
64	A	10	0	0	0	0
65	r	4	0	0	0	0
All	All	110473	0	95357	1057	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 (1057) 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)
17:A:2416:U:H3	58:s:166:TYR:HB3	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:1777:A:N6	17:A:1780:U:OP2	2.16	0.77
41:a:41:ASP:HB3	41:a:46:ASN:HD22	1.49	0.76
17:A:2499:U:OP2	17:A:2504:A:N6	2.18	0.74
14:7:80:VAL:HG21	35:U:143:ARG:HG2	1.69	0.74
35:U:11:ARG:HE	36:V:211:LYS:HB2	1.51	0.74
14:7:195:THR:H	14:7:198:ASN:HD22	1.35	0.73
17:A:2485:U:H3	17:A:2650:C:H42	1.37	0.73
17:A:2108:G:N7	28:N:67:LYS:NZ	2.36	0.72
58:s:178:ASP:HA	58:s:239:ASN:HD21	1.56	0.71
12:5:201:ARG:NH1	12:5:418:TYR:O	2.23	0.71
17:A:3172:C:O2'	17:A:3173:G:N2	2.24	0.71
19:D:113:ARG:O	19:D:147:ARG:NH2	2.24	0.70
27:M:44:ARG:HG3	27:M:45:ARG:HG3	1.75	0.69
5:x:258:CYS:SG	5:x:316:GLN:NE2	2.65	0.69
36:V:52:GLU:HB3	36:V:143:ARG:HH12	1.58	0.69
35:U:21:ARG:HH12	39:Y:143:ASP:HA	1.56	0.69
17:A:1853:A:OP2	33:S:177:ARG:NH1	2.26	0.68
21:F:200:PRO:HG3	21:F:236:ARG:HD2	1.75	0.68
24:J:101:ALA:HB2	24:J:109:ALA:HB2	1.76	0.68
56:q:37:PRO:HG2	56:q:68:SER:HA	1.75	0.68
17:A:1803:A:H4'	17:A:1804:A:H3'	1.75	0.68
22:H:53:THR:N	22:H:86:THR:HG1	1.92	0.68
12:5:229:ARG:NH1	12:5:231:SER:OG	2.28	0.67
17:A:3059:A:O2'	17:A:3062:U:OP1	2.12	0.67
45:e:48:LEU:HB2	45:e:231:VAL:HG12	1.76	0.67
14:7:286:LEU:HD21	14:7:296:ARG:HE	1.60	0.67
15:8:99:ARG:HG2	45:e:89:LEU:HD11	1.75	0.67
5:x:184:PRO:HD3	5:x:209:ARG:HH21	1.60	0.67
17:A:2167:A:N6	17:A:2212:C:OP2	2.25	0.67
58:s:271:LEU:HD23	58:s:273:LEU:HD13	1.76	0.67
1:t:117:ARG:HD3	1:t:156:ARG:HH22	1.59	0.67
17:A:2934:G:H1	17:A:2938:A:H62	1.43	0.66
5:x:170:GLY:O	5:x:251:ARG:NH1	2.28	0.66
19:D:257:ILE:O	19:D:262:ARG:NH1	2.27	0.66
17:A:2248:U:OP1	32:R:99:ARG:NH2	2.29	0.66
30:P:52:ASN:HB3	30:P:55:ASN:HB2	1.77	0.66
6:y:162:ARG:NH1	6:y:186:ILE:O	2.23	0.66
20:E:69:ASP:OD1	20:E:154:ARG:NH1	2.28	0.65
51:k:19:GLN:NE2	51:k:63:CYS:SG	2.67	0.65
1:t:304:ARG:HH22	1:t:401:ARG:HH22	1.42	0.65
17:A:1768:G:OP1	49:i:50:LYS:NZ	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:K:27:PRO:HG2	25:K:30:LYS:HB2	1.78	0.65
36:V:48:PRO:HD3	39:Y:234:LEU:HD21	1.77	0.65
5:x:368:LEU:HD12	6:y:312:GLU:HB3	1.78	0.65
25:K:28:PRO:HG3	25:K:65:ILE:HD12	1.78	0.65
36:V:130:PRO:O	36:V:149:ARG:NH2	2.30	0.65
1:t:368:ILE:HG13	1:t:381:LEU:HD13	1.79	0.65
23:I:97:ALA:HB3	23:I:154:LEU:HB2	1.78	0.65
23:I:47:LEU:HD22	28:N:226:ILE:HG12	1.80	0.64
58:s:191:HIS:O	58:s:428:ARG:NH2	2.26	0.64
21:F:70:ARG:HA	21:F:196:PRO:HD3	1.79	0.64
28:N:191:SER:H	28:N:194:THR:HG1	1.46	0.64
14:7:275:CYS:HA	14:7:303:PRO:HA	1.80	0.64
17:A:1886:G:N7	21:F:170:ARG:NH2	2.46	0.64
1:t:229:MET:HB3	1:t:278:ASP:HB3	1.78	0.63
12:5:216:GLU:OE2	12:5:367:ASN:ND2	2.31	0.63
43:c:215:ILE:HG23	43:c:219:LEU:HD12	1.80	0.63
17:A:1994:A:H61	17:A:2736:C:H4'	1.62	0.63
29:O:142:LEU:HA	29:O:147:GLN:HE21	1.64	0.63
11:4:87:ARG:HH11	11:4:101:ARG:HD3	1.62	0.63
31:Q:233:TRP:HB3	31:Q:240:ILE:HD12	1.79	0.63
13:6:367:ASP:OD1	13:6:370:ARG:NH1	2.32	0.63
17:A:2531:U:O4	19:D:246:ARG:NH2	2.32	0.63
17:A:2137:C:H4'	23:I:43:GLN:HE21	1.64	0.63
17:A:2940:A:H61	17:A:2986:C:H42	1.44	0.63
18:B:1671:C:OP1	45:e:219:GLN:NE2	2.32	0.63
20:E:213:LYS:HD2	20:E:261:MET:HE3	1.81	0.62
30:P:65:GLU:OE1	30:P:97:GLN:NE2	2.32	0.62
34:T:52:VAL:HG22	44:d:227:ARG:HG3	1.81	0.62
4:w:100:VAL:HB	4:w:142:GLN:HB2	1.81	0.62
5:x:328:LEU:HB3	5:x:334:ILE:HB	1.80	0.62
6:y:206:LEU:HD12	19:D:286:ILE:HG12	1.80	0.62
13:6:92:LEU:HB2	13:6:170:ARG:HG3	1.81	0.62
22:H:84:GLU:OE1	38:X:44:ARG:NH2	2.31	0.62
55:p:113:GLU:OE1	55:p:116:ARG:NH1	2.32	0.62
13:6:35:MET:HB2	13:6:38:SER:HB3	1.81	0.62
52:l:121:LEU:O	52:l:125:ASN:ND2	2.32	0.62
13:6:252:CYS:SG	13:6:296:ARG:NH1	2.72	0.62
17:A:1956:U:HO2'	17:A:3098:U:HO2'	1.45	0.62
5:x:36:PRO:HB2	19:D:299:PRO:HB3	1.81	0.62
6:y:190:ARG:HD2	6:y:192:GLN:H	1.64	0.62
17:A:2283:C:H4'	17:A:2284:C:H5"	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Q:201:ASP:HB3	31:Q:204:MET:HB3	1.82	0.62
50:j:45:GLU:OE2	50:j:70:ARG:NH2	2.33	0.62
51:k:10:LEU:O	51:k:46:ASN:ND2	2.33	0.62
12:5:55:LEU:HD11	38:X:163:ARG:HE	1.65	0.62
19:D:296:VAL:HG23	19:D:297:LYS:HG2	1.81	0.62
21:F:164:MET:HE1	49:i:70:PRO:HB2	1.81	0.62
47:g:76:ARG:NH2	47:g:163:GLU:O	2.32	0.62
17:A:2459:A:N6	17:A:2668:A:O2'	2.33	0.61
36:V:54:TRP:NE1	36:V:56:LEU:O	2.33	0.61
2:u:111:VAL:H	3:v:26:THR:HG22	1.63	0.61
6:y:116:ARG:HD3	6:y:124:LEU:HD22	1.83	0.61
12:5:173:ARG:NH2	17:A:2395:A:OP1	2.29	0.61
36:V:80:ILE:HB	36:V:85:TRP:HB2	1.81	0.61
2:u:135:LEU:HD22	2:u:179:LEU:HB3	1.83	0.61
5:x:72:LYS:H	5:x:371:ASN:HB3	1.65	0.61
13:6:56:ARG:NH1	18:B:1625:A:OP1	2.33	0.61
17:A:3019:G:O2'	17:A:3125:A:N1	2.33	0.61
17:A:3176:A:H61	17:A:3193:U:H3	1.47	0.61
17:A:1990:G:OP1	19:D:269:ARG:NH2	2.33	0.61
17:A:2346:U:OP1	58:s:223:ARG:NH2	2.34	0.61
17:A:3083:U:OP1	19:D:297:LYS:NZ	2.26	0.61
31:Q:183:LEU:HD21	31:Q:219:GLU:HG2	1.81	0.61
4:w:138:LEU:HD13	4:w:144:ILE:HG12	1.82	0.61
13:6:339:GLU:N	37:W:148:LEU:OXT	2.33	0.61
17:A:1673:U:O2'	34:T:143:ARG:NH1	2.32	0.61
17:A:2065:A:OP1	46:f:48:TYR:N	2.34	0.61
17:A:2959:G:H2'	17:A:2962:C:H42	1.65	0.61
5:x:270:ASN:O	5:x:277:ARG:NH2	2.34	0.61
12:5:139:LEU:O	12:5:145:ASN:ND2	2.32	0.61
1:t:368:ILE:HG21	1:t:381:LEU:HB2	1.83	0.60
17:A:2296:U:O4	33:S:181:LYS:NZ	2.34	0.60
19:D:204:ALA:O	19:D:208:ARG:NH2	2.33	0.60
1:t:161:THR:HB	1:t:173:LEU:HD12	1.81	0.60
24:J:114:LEU:HD21	52:l:101:LEU:HD21	1.83	0.60
58:s:178:ASP:OD1	58:s:238:ASN:ND2	2.33	0.60
6:y:157:MET:SD	6:y:160:ARG:NH2	2.73	0.60
33:S:127:ARG:NH1	33:S:157:GLU:OE1	2.35	0.60
35:U:153:LEU:HD11	44:d:240:LYS:HB2	1.83	0.60
3:v:20:GLY:HA2	3:v:23:LEU:HD22	1.82	0.60
6:y:264:ARG:NH1	6:y:293:ILE:O	2.35	0.60
1:t:118:VAL:HG22	1:t:173:LEU:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:V:190:CYS:SG	36:V:191:LEU:N	2.75	0.60
5:x:233:VAL:H	46:f:201:ARG:HH21	1.48	0.60
28:N:123:ARG:NH1	28:N:162:GLU:OE1	2.34	0.60
34:T:57:LEU:HB2	34:T:60:GLU:HG3	1.84	0.60
36:V:105:ARG:NH2	44:d:171:ASP:OD1	2.35	0.60
45:e:255:VAL:HB	45:e:259:GLU:HG3	1.83	0.60
8:1:63:ARG:NH1	17:A:2909:G:OP1	2.33	0.60
13:6:60:ARG:HH12	13:6:64:GLU:HB2	1.67	0.60
17:A:2830:A:N6	17:A:2837:A:OP2	2.35	0.60
24:J:25:ARG:NH1	52:l:58:ASP:OD1	2.34	0.60
31:Q:127:SER:OG	31:Q:129:LYS:NZ	2.34	0.60
5:x:288:GLN:HE22	5:x:316:GLN:HE21	1.50	0.59
5:x:95:ALA:HB1	5:x:132:PHE:HB3	1.84	0.59
17:A:2828:G:H1	17:A:2840:C:H42	1.50	0.59
33:S:119:GLU:HG2	33:S:121:ASP:H	1.67	0.59
47:g:110:ILE:HD11	47:g:157:LEU:HD13	1.84	0.59
17:A:3082:G:N2	17:A:3085:A:OP2	2.30	0.59
21:F:279:ARG:HH12	21:F:282:PRO:HD3	1.67	0.59
7:0:179:ARG:HH12	7:0:182:PRO:HG3	1.67	0.59
10:3:108:LYS:NZ	17:A:1745:U:O4	2.35	0.59
1:t:304:ARG:NH1	1:t:396:GLU:OE2	2.31	0.59
9:2:87:ARG:NH2	17:A:1792:G:N7	2.49	0.59
13:6:126:ARG:NH1	30:P:156:ASP:OD2	2.36	0.59
17:A:2149:G:OP2	32:R:65:ARG:NH2	2.35	0.59
25:K:6:ARG:NH2	43:c:225:GLY:O	2.34	0.59
28:N:218:ILE:HG23	28:N:223:MET:HB2	1.85	0.59
55:p:94:LYS:HE2	55:p:96:ASN:HB2	1.85	0.59
26:L:39:ARG:NH1	31:Q:158:GLN:OE1	2.36	0.59
4:w:103:HIS:HE1	4:w:105:MET:HE2	1.68	0.59
7:0:104:LYS:NZ	34:T:102:PHE:O	2.36	0.59
17:A:2237:A:OP1	57:r:171:ARG:NH2	2.35	0.59
6:y:131:PHE:HE2	6:y:145:LEU:HD21	1.67	0.58
14:7:112:PRO:HB2	14:7:267:PRO:HG2	1.85	0.58
14:7:240:ILE:HG23	14:7:252:VAL:HG21	1.85	0.58
1:t:228:GLY:N	1:t:305:PHE:O	2.36	0.58
14:7:108:VAL:HG22	14:7:125:ILE:HG13	1.85	0.58
17:A:1763:A:N7	56:q:38:ARG:NH1	2.51	0.58
17:A:2015:G:H22	17:A:2037:U:H5"	1.67	0.58
36:V:121:LYS:HD3	36:V:130:PRO:HB2	1.85	0.58
1:t:312:LEU:HD22	1:t:347:ILE:HG22	1.85	0.58
12:5:189:LYS:NZ	58:s:182:SER:O	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:F:248:LEU:O	49:i:59:ASN:ND2	2.37	0.58
31:Q:182:ARG:HG3	31:Q:187:LEU:HD11	1.84	0.58
42:b:28:ARG:NH1	42:b:78:GLU:OE1	2.36	0.58
46:f:94:HIS:ND1	46:f:154:GLU:OE2	2.35	0.58
16:9:34:LYS:NZ	17:A:1703:C:OP1	2.33	0.58
29:O:140:SER:O	29:O:146:ASN:ND2	2.37	0.58
30:P:60:SER:OG	55:p:177:ARG:NH1	2.36	0.58
12:5:166:THR:O	58:s:287:LYS:NZ	2.34	0.58
17:A:2240:C:H5'	25:K:29:GLY:HA3	1.85	0.58
20:E:82:ASP:O	20:E:188:LYS:NZ	2.36	0.58
15:8:153:GLU:HG2	45:e:47:LEU:HD21	1.86	0.58
17:A:1737:A:O2'	49:i:93:ARG:NH2	2.36	0.58
3:v:21:ARG:HE	4:w:120:MET:HE1	1.69	0.58
17:A:2236:C:OP1	54:o:9:ARG:NH1	2.37	0.58
20:E:244:ALA:HB1	20:E:248:ILE:HD11	1.84	0.58
12:5:384:GLN:NE2	17:A:2395:A:O2'	2.37	0.57
17:A:2069:U:H1'	17:A:2071:U:H1'	1.86	0.57
36:V:16:PRO:HD2	36:V:19:TYR:HB2	1.85	0.57
12:5:110:ARG:NH1	17:A:2406:A:O2'	2.37	0.57
28:N:117:ASN:HB3	28:N:166:ARG:HB2	1.87	0.57
13:6:215:THR:HB	13:6:273:PHE:HB2	1.86	0.57
17:A:2191:A:N6	17:A:2198:A:OP1	2.37	0.57
17:A:2511:C:O5'	19:D:263:ASN:ND2	2.37	0.57
36:V:133:ILE:HA	36:V:147:SER:HA	1.85	0.57
54:o:15:ARG:HB3	54:o:18:ILE:HG12	1.85	0.57
1:t:90:SER:HB3	1:t:206:CYS:HB3	1.85	0.57
2:u:120:TYR:O	26:L:128:ARG:NH1	2.37	0.57
5:x:232:ARG:NH1	46:f:199:LYS:O	2.38	0.57
15:8:161:ALA:HB1	45:e:208:ALA:HA	1.87	0.57
17:A:1814:A:N3	17:A:1862:U:O2'	2.36	0.57
17:A:2449:G:OP2	58:s:225:ARG:NH2	2.37	0.57
30:P:146:TYR:OH	30:P:158:MET:SD	2.62	0.57
6:y:130:GLU:HG2	6:y:159:MET:HG2	1.86	0.57
42:b:49:ARG:HG3	42:b:50:GLU:HG2	1.86	0.57
12:5:113:LEU:HD12	12:5:311:ALA:HB1	1.87	0.57
17:A:2458:A:O2'	20:E:215:PHE:O	2.19	0.57
18:B:1630:A:OP1	53:m:42:ARG:NH2	2.38	0.57
14:7:177:GLY:HA3	14:7:319:ARG:HE	1.69	0.57
45:e:185:ARG:NH1	45:e:207:ASN:OD1	2.37	0.57
46:f:199:LYS:NZ	46:f:203:GLU:OE1	2.35	0.57
57:r:72:ILE:HD11	57:r:115:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:3:94:LEU:N	17:A:1752:U:OP1	2.37	0.56
13:6:173:LEU:HD13	13:6:272:LEU:HD22	1.86	0.56
45:e:151:ARG:NH2	45:e:259:GLU:OE2	2.34	0.56
5:x:70:GLU:O	5:x:371:ASN:ND2	2.37	0.56
28:N:124:VAL:HG12	28:N:158:ARG:HE	1.70	0.56
2:u:164:THR:HG22	26:L:111:ASN:HB2	1.87	0.56
3:v:16:LEU:HD13	3:v:35:ILE:HD12	1.87	0.56
8:1:24:ALA:HB2	8:1:54:VAL:HG11	1.87	0.56
21:F:123:GLY:HA3	21:F:142:ARG:HG2	1.87	0.56
32:R:78:GLU:OE1	42:b:135:ASN:ND2	2.31	0.56
2:u:127:VAL:HG11	2:u:138:MET:HE1	1.87	0.56
13:6:224:HIS:CE1	13:6:227:GLU:H	2.23	0.56
47:g:84:TYR:OH	47:g:164:LYS:NZ	2.33	0.56
17:A:2131:A:OP1	54:o:23:ARG:NH1	2.39	0.56
17:A:3066:C:O2'	20:E:233:GLN:OE1	2.23	0.56
26:L:118:ARG:HH21	26:L:142:GLN:HE22	1.53	0.56
17:A:2002:G:OP1	44:d:38:LYS:NZ	2.37	0.56
17:A:2310:G:O2'	17:A:2675:G:O6	2.22	0.56
46:f:127:MET:HB2	46:f:154:GLU:HB3	1.88	0.56
55:p:56:ASP:O	55:p:60:ARG:NE	2.39	0.56
13:6:106:ARG:NH1	18:B:1621:A:OP2	2.36	0.56
17:A:1868:G:H2'	27:M:40:PRO:HG3	1.86	0.56
17:A:2247:C:OP1	50:j:24:GLY:N	2.39	0.56
17:A:3140:A:O2'	26:L:130:ARG:NH1	2.37	0.56
17:A:2530:A:H5"	19:D:212:THR:HG21	1.88	0.55
47:g:118:TRP:NE1	47:g:142:GLU:OE2	2.36	0.55
4:w:104:PHE:HA	4:w:108:LEU:HD13	1.88	0.55
17:A:2003:A:OP2	17:A:2734:A:O2'	2.23	0.55
17:A:2180:A:O2'	17:A:2206:C:O3'	2.23	0.55
21:F:272:LYS:NZ	49:i:65:ASN:OD1	2.33	0.55
44:d:98:SER:OG	44:d:215:ARG:NH2	2.39	0.55
57:r:71:PRO:HD2	57:r:107:LEU:HD23	1.89	0.55
13:6:206:TYR:O	13:6:243:ASN:ND2	2.40	0.55
17:A:1749:C:OP2	17:A:2899:C:O2'	2.24	0.55
20:E:68:GLU:OE1	20:E:154:ARG:NH2	2.39	0.55
58:s:182:SER:OG	58:s:202:TYR:OH	2.24	0.55
14:7:243:LYS:NZ	14:7:265:GLU:OE1	2.40	0.55
17:A:2256:U:O2'	33:S:118:ASN:ND2	2.40	0.55
18:B:1616:A:HO2'	18:B:1618:A:H62	1.54	0.55
12:5:112:ARG:HH11	17:A:2406:A:H61	1.54	0.55
15:8:101:ARG:NH2	45:e:88:GLU:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:2240:C:O2'	25:K:30:LYS:NZ	2.39	0.55
20:E:80:LEU:HD12	20:E:323:GLY:HA3	1.88	0.55
26:L:102:SER:OG	31:Q:158:GLN:NE2	2.33	0.55
46:f:90:VAL:HB	46:f:190:THR:HB	1.89	0.55
48:h:87:GLN:OE1	48:h:124:ARG:NH1	2.39	0.55
13:6:124:ARG:NH2	15:8:112:GLU:OE1	2.40	0.55
13:6:222:ASP:OD2	13:6:267:ARG:NH1	2.40	0.55
5:x:274:LYS:HE2	5:x:277:ARG:HG3	1.89	0.55
13:6:215:THR:OG1	13:6:275:GLN:OE1	2.24	0.55
17:A:2328:C:N4	58:s:52:THR:O	2.35	0.55
33:S:101:PHE:HE2	50:j:49:TRP:HB3	1.70	0.55
1:t:385:LEU:HA	1:t:388:LEU:HD12	1.88	0.54
17:A:3151:A:N1	17:A:3163:G:O2'	2.37	0.54
21:F:223:HIS:HA	21:F:226:MET:HE3	1.88	0.54
17:A:2016:C:OP2	27:M:59:ARG:NH1	2.41	0.54
31:Q:121:THR:HG22	31:Q:171:VAL:HA	1.89	0.54
9:2:85:LYS:NZ	17:A:1792:G:OP2	2.41	0.54
10:3:175:ASP:HB3	10:3:178:GLN:HB2	1.89	0.54
17:A:2147:G:OP1	33:S:104:ARG:NE	2.38	0.54
33:S:115:LEU:HD11	33:S:190:GLN:HB3	1.90	0.54
45:e:146:ARG:O	45:e:254:TRP:N	2.34	0.54
5:x:129:LEU:HD13	5:x:163:LEU:HD11	1.90	0.54
25:K:5:SER:HB2	25:K:8:PRO:HD2	1.90	0.54
26:L:42:ASP:HB2	26:L:116:GLY:HA3	1.87	0.54
17:A:1822:U:O2	17:A:2707:A:O2'	2.26	0.54
17:A:2079:C:H6	54:o:60:ARG:HH12	1.55	0.54
20:E:96:ARG:NH1	20:E:315:PRO:O	2.41	0.54
33:S:99:VAL:HG12	33:S:133:VAL:HG22	1.89	0.54
11:4:86:GLY:H	17:A:3189:C:H5"	1.73	0.54
17:A:2017:U:O2	21:F:137:ARG:NH2	2.40	0.54
17:A:2740:A:N3	17:A:2921:A:O2'	2.36	0.54
1:t:312:LEU:HG	1:t:352:ALA:HB3	1.89	0.54
7:0:96:ASN:OD1	17:A:2708:C:O2'	2.25	0.54
46:f:136:GLN:HG2	53:m:78:PRO:HG3	1.91	0.54
17:A:2299:U:H5"	17:A:2300:G:H5"	1.89	0.53
21:F:220:ASP:OD1	21:F:221:LEU:N	2.41	0.53
6:y:302:LEU:HA	6:y:306:ALA:HB3	1.90	0.53
17:A:1998:U:OP1	17:A:2001:C:N4	2.32	0.53
7:0:139:ARG:NH1	17:A:2322:C:OP1	2.42	0.53
17:A:1800:G:N1	17:A:1803:A:OP2	2.41	0.53
2:u:113:GLN:N	3:v:68:ARG:O	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:1864:A:OP1	32:R:17:ARG:NH1	2.41	0.53
40:Z:105:SER:OG	54:o:59:GLU:OE2	2.21	0.53
1:t:162:LEU:HD11	1:t:169:VAL:HG13	1.90	0.53
5:x:42:ARG:NH1	5:x:46:GLN:OE1	2.42	0.53
13:6:356:ARG:NH2	47:g:103:GLY:O	2.40	0.53
17:A:1860:A:O2'	17:A:2682:A:OP1	2.27	0.53
17:A:2892:A:O2'	37:W:49:ARG:NH2	2.40	0.53
41:a:72:THR:O	43:c:256:ARG:NH2	2.36	0.53
46:f:101:THR:OG1	53:m:67:ARG:NH1	2.41	0.53
5:x:252:VAL:HB	5:x:305:VAL:HG22	1.91	0.53
24:J:85:PRO:O	24:J:124:LYS:NZ	2.37	0.53
31:Q:221:LYS:NZ	31:Q:241:LYS:O	2.35	0.53
22:H:78:ARG:NH1	38:X:87:LEU:O	2.42	0.53
48:h:57:SER:OG	48:h:136:ASP:OD2	2.27	0.53
1:t:73:VAL:HG11	1:t:126:SER:HA	1.91	0.53
1:t:273:GLN:NE2	17:A:3129:A:O2'	2.42	0.53
5:x:258:CYS:HA	5:x:284:LEU:HD21	1.91	0.53
5:x:355:PHE:CE2	5:x:357:SER:HB2	2.44	0.53
12:5:107:PHE:HB3	12:5:222:VAL:HG22	1.89	0.53
13:6:183:ASP:HB3	55:p:189:ARG:HD3	1.90	0.53
43:c:92:PHE:HB3	43:c:179:THR:HA	1.91	0.53
50:j:63:GLN:OE1	50:j:66:ARG:NH2	2.34	0.53
17:A:2755:A:OP2	22:H:91:LYS:NZ	2.41	0.52
34:T:63:ARG:NH1	44:d:228:PHE:O	2.42	0.52
61:w:200:PM8:O40	61:w:200:PM8:N36	2.43	0.52
50:j:63:GLN:HE21	50:j:67:LYS:HE2	1.75	0.52
17:A:1787:G:N2	17:A:1790:A:OP2	2.30	0.52
20:E:52:HIS:HB2	29:O:145:LEU:HD23	1.91	0.52
21:F:243:ILE:HG22	56:q:27:ALA:HB2	1.89	0.52
23:I:95:MET:HG3	23:I:181:ILE:HG12	1.90	0.52
31:Q:148:THR:HG22	31:Q:165:GLU:HG2	1.91	0.52
44:d:267:PRO:HG2	44:d:270:ALA:HB2	1.92	0.52
45:e:164:LYS:HE2	45:e:167:ASP:HA	1.92	0.52
12:5:115:GLU:HB2	12:5:119:GLN:HB2	1.90	0.52
13:6:331:PHE:HA	13:6:335:LEU:HB2	1.92	0.52
15:8:132:GLU:OE2	46:f:109:TYR:OH	2.28	0.52
17:A:2354:A:OP2	34:T:149:ARG:NH1	2.43	0.52
27:M:31:PRO:HG2	54:o:86:ARG:HH12	1.75	0.52
30:P:102:VAL:HG12	30:P:103:VAL:HG13	1.92	0.52
2:u:147:LYS:HE2	17:A:3120:C:H5"	1.91	0.52
10:3:188:VAL:O	13:6:356:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5:303:ARG:NH1	12:5:348:ASP:OD2	2.41	0.52
13:6:90:ILE:HA	50:j:112:LYS:HB2	1.92	0.52
17:A:2173:G:N3	24:J:150:SER:OG	2.43	0.52
32:R:141:ILE:HG22	41:a:51:LEU:HD12	1.92	0.52
5:x:237:ASP:OD2	5:x:239:ARG:NE	2.41	0.52
17:A:2737:U:OP1	19:D:278:LYS:NZ	2.35	0.52
42:b:72:VAL:HG13	42:b:90:HIS:HB2	1.92	0.52
46:f:127:MET:HE3	46:f:128:PRO:HD2	1.91	0.52
17:A:2387:U:O2'	17:A:2406:A:N7	2.39	0.52
20:E:50:ASP:O	29:O:138:ARG:NH2	2.43	0.52
2:u:92:PHE:HB2	2:u:149:LEU:HD23	1.91	0.52
12:5:80:ARG:NH2	17:A:1707:C:O2	2.41	0.52
17:A:1974:A:H5'	19:D:261:GLY:HA2	1.92	0.52
44:d:164:VAL:HG12	44:d:261:MET:HB3	1.91	0.52
56:q:152:ARG:HA	56:q:155:ARG:HD2	1.92	0.52
1:t:306:LEU:HG	1:t:338:ARG:HD2	1.91	0.52
5:x:217:LEU:HB3	5:x:226:ARG:HD3	1.92	0.52
14:7:87:THR:O	14:7:90:SER:OG	2.22	0.52
43:c:151:GLU:O	43:c:155:ASN:ND2	2.43	0.52
58:s:332:LEU:HD13	58:s:372:TYR:HB2	1.92	0.52
17:A:2822:C:O2'	17:A:2915:C:OP2	2.25	0.52
42:b:49:ARG:HH21	42:b:94:VAL:HG11	1.74	0.52
53:m:57:VAL:HB	53:m:76:ALA:HA	1.92	0.52
21:F:216:VAL:HG22	21:F:258:THR:HB	1.90	0.51
27:M:68:GLU:OE1	27:M:71:GLN:NE2	2.43	0.51
12:5:136:VAL:HG11	12:5:417:LEU:HD23	1.92	0.51
17:A:1761:A:H1'	17:A:1762:A:C8	2.44	0.51
17:A:2138:U:O2'	17:A:2151:A:N3	2.42	0.51
5:x:176:ILE:HG23	5:x:199:ASN:HB2	1.92	0.51
17:A:3068:G:OP2	17:A:3068:G:N2	2.43	0.51
17:A:3125:A:H62	17:A:3132:G:H21	1.57	0.51
31:Q:182:ARG:HD2	31:Q:218:ASN:HB3	1.92	0.51
38:X:171:ARG:NE	38:X:198:GLU:OE2	2.43	0.51
43:c:238:MET:HE2	43:c:297:ALA:HB2	1.91	0.51
55:p:128:ASN:HD21	55:p:132:GLU:HB2	1.75	0.51
1:t:347:ILE:HD13	1:t:369:VAL:HG12	1.93	0.51
19:D:138:ASP:OD1	19:D:249:ASN:ND2	2.40	0.51
48:h:99:ASN:O	48:h:103:HIS:ND1	2.40	0.51
58:s:80:LEU:HD21	58:s:341:MET:HB3	1.92	0.51
17:A:2180:A:H4'	17:A:2181:A:C8	2.46	0.51
17:A:2682:A:OP1	32:R:34:ARG:NH2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:D:211:GLY:H	19:D:247:VAL:HB	1.76	0.51
38:X:202:GLU:O	38:X:214:LYS:NZ	2.44	0.51
46:f:94:HIS:HB2	46:f:185:SER:HB3	1.93	0.51
17:A:2165:C:N4	17:A:2212:C:OP1	2.43	0.51
17:A:3084:A:H4'	19:D:277:ARG:HH21	1.76	0.51
17:A:1741:A:OP2	27:M:134:ARG:NH1	2.42	0.51
31:Q:221:LYS:HB3	31:Q:244:ARG:HG3	1.92	0.51
17:A:2655:G:N2	17:A:2659:C:O2'	2.45	0.51
18:B:1613:U:O2'	18:B:1615:A:OP1	2.29	0.51
20:E:177:LYS:HG3	20:E:298:LYS:HB2	1.94	0.51
43:c:242:VAL:HG12	43:c:246:LYS:HE3	1.93	0.51
58:s:145:VAL:HG21	58:s:187:LEU:HD11	1.92	0.51
58:s:332:LEU:HD21	58:s:359:ALA:HB2	1.92	0.51
17:A:1747:G:N2	17:A:1750:G:O2'	2.43	0.50
20:E:76:LYS:HG3	20:E:170:LEU:HD21	1.92	0.50
5:x:312:LEU:HD23	5:x:363:LEU:HD11	1.93	0.50
13:6:160:ASP:OD2	13:6:267:ARG:NH2	2.44	0.50
13:6:187:VAL:HG13	13:6:319:PHE:HB3	1.92	0.50
17:A:2466:A:OP1	31:Q:235:ARG:NH1	2.42	0.50
27:M:16:LEU:HD13	54:o:92:LEU:HD22	1.94	0.50
17:A:3202:U:O2	20:E:303:LYS:NZ	2.44	0.50
45:e:247:GLY:HA3	45:e:251:HIS:CE1	2.47	0.50
1:t:272:LEU:HD12	1:t:386:LYS:HD2	1.92	0.50
26:L:35:MET:N	26:L:57:CYS:O	2.41	0.50
3:v:45:LEU:O	3:v:51:ARG:NE	2.43	0.50
6:y:248:ILE:HG23	6:y:253:TYR:HB3	1.92	0.50
17:A:2195:A:OP1	52:l:115:ARG:NH1	2.45	0.50
17:A:2529:U:H2'	19:D:208:ARG:HB2	1.92	0.50
13:6:74:TYR:N	37:W:102:GLU:OE2	2.45	0.50
25:K:52:ASP:O	34:T:200:ARG:NH1	2.45	0.50
41:a:104:GLU:HB2	41:a:107:PRO:HD2	1.93	0.50
43:c:102:GLU:OE1	43:c:105:ARG:NH2	2.38	0.50
17:A:2521:A:OP2	19:D:202:ARG:NH2	2.40	0.50
34:T:126:HIS:HD2	44:d:227:ARG:HH21	1.60	0.50
35:U:141:ASP:HB3	35:U:144:ARG:HG2	1.93	0.50
42:b:44:ARG:NH2	54:o:99:LYS:O	2.45	0.50
43:c:245:LEU:HB3	43:c:250:VAL:HB	1.94	0.50
5:x:187:LYS:HD3	5:x:253:LEU:HD21	1.93	0.50
6:y:166:LEU:HD22	6:y:171:LEU:HD12	1.93	0.50
6:y:211:GLN:HB3	6:y:249:VAL:HG21	1.93	0.50
17:A:1761:A:OP1	17:A:1887:A:N6	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:F:53:LEU:HD12	21:F:274:LEU:HD12	1.94	0.50
22:H:97:ILE:HG12	22:H:111:LEU:HG	1.93	0.50
33:S:144:LEU:HB2	41:a:58:ILE:HB	1.94	0.50
38:X:79:LEU:HB2	38:X:127:VAL:HG12	1.94	0.50
2:u:170:VAL:HB	2:u:177:ILE:HG23	1.94	0.50
17:A:2159:U:O2	17:A:2227:A:O2'	2.22	0.50
34:T:185:THR:HG23	34:T:188:ALA:H	1.77	0.50
17:A:1886:G:H1	49:i:61:GLY:HA3	1.77	0.49
17:A:2536:G:H5'	19:D:276:HIS:CD2	2.47	0.49
17:A:2745:A:O2'	38:X:102:LYS:O	2.24	0.49
24:J:149:ARG:HH12	52:l:104:PRO:HD3	1.77	0.49
29:O:33:LEU:HD21	29:O:59:LEU:HD22	1.93	0.49
32:R:71:ARG:HH12	34:T:205:THR:HB	1.76	0.49
44:d:182:ARG:HD2	44:d:225:TYR:HE2	1.77	0.49
46:f:48:TYR:HB3	46:f:51:LYS:HG2	1.94	0.49
51:k:76:MET:HG2	57:r:49:ILE:HD12	1.94	0.49
3:v:37:ARG:HA	3:v:40:ARG:HE	1.77	0.49
14:7:61:ARG:HD3	44:d:235:GLN:HE22	1.76	0.49
23:I:98:VAL:HG12	23:I:177:LEU:HD12	1.93	0.49
36:V:80:ILE:HD12	36:V:85:TRP:HE3	1.77	0.49
51:k:54:ASP:OD1	51:k:54:ASP:N	2.45	0.49
1:t:305:PHE:HB2	1:t:392:TYR:HE2	1.76	0.49
28:N:64:ARG:NH1	28:N:144:LYS:O	2.44	0.49
51:k:73:ARG:HB2	57:r:46:THR:HG23	1.94	0.49
1:t:224:VAL:HG12	1:t:404:LEU:HD13	1.93	0.49
11:4:84:ARG:NE	17:A:3188:U:OP2	2.28	0.49
16:9:113:ASN:HB3	16:9:116:LYS:HE2	1.93	0.49
25:K:143:GLU:OE1	42:b:136:LYS:NZ	2.38	0.49
51:k:18:VAL:HG13	51:k:64:VAL:HG22	1.93	0.49
16:9:70:LEU:HD22	39:Y:85:TRP:HH2	1.78	0.49
17:A:1867:A:N1	17:A:2019:G:O2'	2.43	0.49
17:A:1952:U:H2'	17:A:1953:A:C8	2.47	0.49
21:F:286:PHE:HA	21:F:290:TYR:HE2	1.77	0.49
22:H:53:THR:N	22:H:86:THR:OG1	2.44	0.49
45:e:55:ARG:NH2	45:e:155:ARG:O	2.45	0.49
45:e:60:SER:O	45:e:136:ARG:NH2	2.42	0.49
45:e:124:TRP:CD2	53:m:72:ARG:HG2	2.47	0.49
17:A:1768:G:OP2	39:Y:232:LYS:NZ	2.45	0.49
38:X:7:PRO:HD2	38:X:10:LEU:HD12	1.94	0.49
46:f:106:TYR:OH	46:f:174:ILE:O	2.28	0.49
58:s:66:TRP:O	58:s:69:THR:OG1	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:6:27:ARG:N	17:A:2073:A:OP2	2.46	0.49
14:7:203:THR:O	14:7:207:HIS:ND1	2.28	0.49
17:A:2155:A:N6	57:r:169:TRP:O	2.46	0.49
13:6:217:LEU:HB3	13:6:271:LEU:HB2	1.93	0.49
13:6:239:ASN:OD1	13:6:275:GLN:NE2	2.36	0.49
17:A:2849:G:N2	17:A:2889:C:O2	2.34	0.49
17:A:2950:U:H2'	17:A:2951:A:C8	2.48	0.49
19:D:127:ILE:HD11	19:D:143:ALA:HB2	1.94	0.49
21:F:212:TRP:O	21:F:258:THR:OG1	2.30	0.49
22:H:68:GLY:O	56:q:49:ARG:NH1	2.43	0.49
45:e:147:THR:HG21	45:e:248:ASN:HB3	1.94	0.49
5:x:136:ARG:NH1	5:x:350:ASP:O	2.45	0.49
16:9:24:LYS:NZ	17:A:2422:U:OP2	2.45	0.49
17:A:1688:A:H2'	17:A:1689:C:H4'	1.93	0.49
17:A:2361:G:H5'	17:A:2362:A:H5"	1.94	0.49
21:F:167:MET:SD	21:F:276:GLN:NE2	2.80	0.49
50:j:87:GLY:HA3	54:o:62:HIS:HB2	1.93	0.49
51:k:27:VAL:HG12	51:k:62:PRO:HG3	1.94	0.49
58:s:242:ARG:NH1	58:s:292:CYS:O	2.43	0.49
2:u:115:PRO:HG2	2:u:118:MET:HG2	1.94	0.49
5:x:105:HIS:HB2	5:x:347:VAL:HG13	1.95	0.49
8:1:14:LYS:HD3	17:A:2848:A:H5"	1.94	0.49
13:6:228:PRO:HB3	30:P:49:THR:HB	1.95	0.49
17:A:3009:C:O2'	17:A:3115:U:OP1	2.30	0.49
21:F:62:VAL:HG23	21:F:82:LEU:HB2	1.95	0.49
31:Q:153:ASN:OD1	31:Q:154:VAL:N	2.46	0.49
36:V:65:LEU:HD11	36:V:121:LYS:HB2	1.95	0.49
14:7:180:CYS:SG	14:7:296:ARG:NH1	2.86	0.48
17:A:2127:A:H4'	17:A:2251:A:C5	2.48	0.48
21:F:241:ASN:HD21	49:i:52:ALA:HB1	1.78	0.48
30:P:142:ASN:HD22	55:p:181:GLU:HG2	1.78	0.48
44:d:182:ARG:HB2	44:d:223:ALA:HB3	1.95	0.48
4:w:90:TYR:HE2	4:w:92:LYS:HB3	1.78	0.48
12:5:83:LYS:NZ	17:A:2413:C:OP1	2.35	0.48
17:A:2279:U:OP2	49:i:46:ARG:NH1	2.39	0.48
25:K:169:LEU:HD22	57:r:75:TRP:CD1	2.48	0.48
43:c:42:GLN:NE2	49:i:36:LEU:O	2.45	0.48
1:t:238:SER:OG	59:t:500:GDP:O2A	2.22	0.48
17:A:3183:U:H3	25:K:177:ARG:HB3	1.77	0.48
21:F:220:ASP:O	21:F:245:ALA:N	2.46	0.48
26:L:98:PRO:HA	31:Q:162:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:74:ALA:HB1	17:A:1914:A:H5'	1.96	0.48
17:A:2145:G:N3	33:S:104:ARG:NH2	2.60	0.48
22:H:99:THR:HA	22:H:108:ARG:HG3	1.95	0.48
34:T:150:ILE:HB	44:d:52:THR:HG21	1.95	0.48
6:y:241:MET:O	6:y:274:TYR:OH	2.26	0.48
9:2:56:SER:OG	17:A:1980:A:OP1	2.31	0.48
13:6:139:TRP:CD1	13:6:143:CYS:HG	2.31	0.48
17:A:2107:G:H5"	28:N:144:LYS:HD3	1.94	0.48
20:E:61:ILE:HD11	29:O:149:LEU:HD13	1.95	0.48
5:x:274:LYS:HE3	5:x:276:SER:HB3	1.96	0.48
6:y:237:ALA:HB2	6:y:253:TYR:CZ	2.48	0.48
17:A:1868:G:N7	27:M:51:ARG:NH1	2.61	0.48
25:K:22:ASP:HB3	25:K:147:GLN:HE21	1.78	0.48
44:d:186:VAL:HG12	44:d:187:GLU:HG3	1.96	0.48
17:A:2168:U:O2'	17:A:2169:A:O4'	2.31	0.48
43:c:259:ARG:HB2	43:c:271:PHE:HB2	1.94	0.48
12:5:165:GLN:NE2	12:5:175:THR:HG22	2.29	0.48
13:6:138:GLU:OE1	13:6:141:ARG:NH2	2.46	0.48
17:A:1672:C:O2'	34:T:143:ARG:O	2.28	0.48
17:A:1766:U:O2'	17:A:1767:G:OP2	2.26	0.48
57:r:40:GLU:HG2	57:r:49:ILE:HG12	1.94	0.48
13:6:99:ARG:NH2	18:B:1621:A:O5'	2.47	0.48
17:A:1797:G:O2'	36:V:40:ARG:O	2.30	0.48
17:A:2127:A:H2'	17:A:2128:G:H8	1.78	0.48
27:M:223:LEU:O	55:p:49:TYR:OH	2.27	0.48
35:U:46:MET:HE1	35:U:72:VAL:HG13	1.96	0.48
36:V:51:ASP:HA	36:V:81:ARG:HH22	1.79	0.48
5:x:328:LEU:O	5:x:333:SER:N	2.47	0.47
13:6:213:LEU:HB2	13:6:275:GLN:HB2	1.96	0.47
5:x:141:ARG:HH22	6:y:322:ARG:HD3	1.78	0.47
12:5:280:GLN:HG2	58:s:158:ARG:HE	1.77	0.47
16:9:19:SER:OG	16:9:25:ARG:NH1	2.46	0.47
17:A:1805:A:OP2	36:V:94:HIS:NE2	2.47	0.47
17:A:1879:G:OP1	21:F:92:ARG:NH1	2.44	0.47
21:F:164:MET:HE3	49:i:69:HIS:CE1	2.49	0.47
30:P:85:ARG:NH1	30:P:157:SER:OG	2.47	0.47
36:V:69:ASP:HB2	36:V:72:LYS:HD2	1.96	0.47
5:x:38:PHE:HB2	5:x:43:LEU:HG	1.96	0.47
21:F:291:SER:OG	47:g:52:LEU:O	2.32	0.47
29:O:154:GLN:HG2	29:O:157:ARG:HH21	1.79	0.47
44:d:152:LEU:HD21	44:d:172:MET:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:e:87:HIS:NE2	45:e:121:GLU:OE2	2.40	0.47
3:v:29:ASP:OD1	3:v:29:ASP:N	2.46	0.47
8:1:13:SER:OG	8:1:36:ARG:NH2	2.48	0.47
17:A:2932:G:OP1	21:F:137:ARG:NH1	2.41	0.47
21:F:231:VAL:HG13	56:q:26:ARG:HD2	1.97	0.47
33:S:159:THR:OG1	33:S:196:ASN:OD1	2.23	0.47
45:e:90:ARG:NH2	45:e:115:LEU:O	2.42	0.47
10:3:106:THR:HG23	10:3:162:THR:HA	1.97	0.47
16:9:49:ARG:NH1	17:A:2416:U:O2	2.46	0.47
17:A:3064:A:H2'	17:A:3101:A:N6	2.30	0.47
25:K:25:MET:O	25:K:149:ARG:NH1	2.46	0.47
26:L:52:HIS:CD2	26:L:53:ARG:HG3	2.50	0.47
44:d:202:MET:HG2	44:d:203:MET:HG2	1.96	0.47
53:m:56:LEU:HD23	53:m:64:ILE:HD11	1.97	0.47
1:t:81:CYS:N	1:t:132:TYR:O	2.39	0.47
5:x:207:PRO:HD2	17:A:2844:G:H5'	1.97	0.47
7:0:81:PRO:O	17:A:2679:U:O2'	2.28	0.47
13:6:184:LEU:N	55:p:190:GLN:O	2.45	0.47
20:E:329:PRO:HD2	20:E:332:LEU:HD21	1.95	0.47
21:F:184:GLN:HE22	27:M:22:VAL:HG23	1.78	0.47
37:W:67:ILE:HG21	37:W:131:VAL:HG21	1.96	0.47
48:h:71:GLU:HG2	48:h:75:LYS:HE3	1.97	0.47
1:t:317:PRO:HB2	1:t:359:LEU:HD21	1.96	0.47
5:x:29:LYS:H	5:x:29:LYS:HD2	1.79	0.47
6:y:190:ARG:HH22	17:A:2751:G:H5"	1.80	0.47
17:A:2093:U:O2	17:A:2266:U:O2'	2.33	0.47
17:A:2839:C:H1'	28:N:142:GLY:H	1.80	0.47
17:A:3008:C:O2'	17:A:3051:A:N3	2.45	0.47
18:B:1623:G:H5"	30:P:86:THR:HG21	1.97	0.47
20:E:282:ILE:HD12	31:Q:94:ILE:HD12	1.97	0.47
27:M:116:ILE:HB	27:M:154:ILE:HA	1.97	0.47
33:S:110:SER:HB3	43:c:313:PRO:HG2	1.96	0.47
45:e:49:GLY:N	45:e:176:ALA:O	2.33	0.47
53:m:57:VAL:HG22	53:m:63:THR:HG22	1.97	0.47
17:A:2284:C:H5'	43:c:39:PHE:CE1	2.50	0.47
51:k:10:LEU:HD22	51:k:13:VAL:HG21	1.96	0.47
17:A:2030:U:H4'	17:A:2031:A:O5'	2.14	0.47
23:I:94:ARG:HE	23:I:159:PRO:HD3	1.79	0.47
36:V:55:TYR:O	36:V:145:ARG:NH1	2.48	0.47
45:e:235:LYS:NZ	45:e:275:PHE:O	2.36	0.47
1:t:77:ARG:NH2	17:A:2959:G:OP1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5:58:ILE:HD13	38:X:214:LYS:HB2	1.97	0.47
17:A:1744:A:OP1	27:M:87:HIS:NE2	2.37	0.47
28:N:222:ASN:O	28:N:222:ASN:ND2	2.48	0.47
55:p:141:ARG:NH2	55:p:142:TYR:OH	2.48	0.47
58:s:242:ARG:NH1	58:s:290:ASP:OD2	2.45	0.47
5:x:165:PRO:HG3	5:x:377:PHE:HB3	1.97	0.46
1:t:125:LEU:HB2	1:t:221:LEU:HD22	1.96	0.46
1:t:198:ASN:HD21	17:A:3079:G:H21	1.62	0.46
13:6:61:ALA:HB1	37:W:103:VAL:HG11	1.97	0.46
1:t:346:LYS:HG2	59:t:500:GDP:C5	2.50	0.46
15:8:179:THR:HG21	45:e:133:LEU:HB3	1.98	0.46
17:A:2168:U:C2	23:I:106:ALA:HB1	2.50	0.46
1:t:76:ARG:HD3	1:t:128:VAL:HG21	1.97	0.46
1:t:365:GLN:NE2	1:t:366:GLU:O	2.48	0.46
6:y:139:GLU:HB3	6:y:140:PRO:HD3	1.97	0.46
17:A:2871:U:O2'	37:W:86:ASN:ND2	2.49	0.46
17:A:3064:A:O4'	17:A:3099:C:N4	2.48	0.46
14:7:309:HIS:CE1	20:E:155:PHE:HA	2.50	0.46
17:A:1962:A:OP2	17:A:2501:C:N4	2.46	0.46
21:F:281:ARG:NH2	27:M:128:THR:OG1	2.37	0.46
56:q:147:GLN:NE2	56:q:151:GLU:OE2	2.48	0.46
6:y:201:LEU:HA	6:y:205:CYS:HB2	1.97	0.46
6:y:243:ILE:HD13	6:y:290:LEU:HD22	1.96	0.46
14:7:144:ARG:NH2	14:7:267:PRO:O	2.48	0.46
47:g:72:TRP:NE1	47:g:92:HIS:O	2.45	0.46
58:s:239:ASN:HB2	58:s:299:PHE:HB2	1.96	0.46
2:u:164:THR:OG1	2:u:167:TRP:O	2.23	0.46
17:A:2002:G:N3	17:A:2735:G:O2'	2.42	0.46
17:A:2232:A:N6	17:A:2978:U:OP1	2.48	0.46
19:D:176:ALA:HB1	19:D:244:VAL:HG11	1.98	0.46
23:I:89:VAL:HG13	23:I:93:ASN:HD21	1.81	0.46
25:K:30:LYS:HD3	25:K:148:PRO:HB2	1.98	0.46
58:s:376:THR:HB	58:s:389:ARG:HG3	1.98	0.46
3:v:47:ASP:O	3:v:51:ARG:HG3	2.15	0.46
12:5:344:SER:HB3	12:5:355:LEU:HD23	1.96	0.46
17:A:2110:A:H2	28:N:244:LYS:HD3	1.80	0.46
17:A:2360:U:H3'	17:A:2361:G:H4'	1.96	0.46
26:L:122:PRO:HA	26:L:143:ASN:HB2	1.98	0.46
28:N:138:HIS:ND1	28:N:138:HIS:O	2.49	0.46
42:b:85:ARG:HH12	42:b:107:GLN:HE22	1.63	0.46
57:r:136:PRO:HG2	57:r:139:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:154:TYR:HB3	1:t:156:ARG:HH21	1.80	0.46
5:x:45:LEU:HD21	5:x:64:ARG:HH21	1.81	0.46
5:x:204:ASP:HB3	5:x:210:ILE:HG12	1.98	0.46
6:y:102:MET:HE1	19:D:220:VAL:HG22	1.98	0.46
14:7:298:GLN:NE2	14:7:320:SER:O	2.48	0.46
14:7:316:LEU:HD21	29:O:149:LEU:HD23	1.98	0.46
2:u:94:ILE:HD11	2:u:111:VAL:HG11	1.98	0.46
13:6:190:GLY:N	13:6:318:PHE:O	2.33	0.46
17:A:1883:G:H5'	47:g:91:MET:HG3	1.98	0.46
20:E:150:LYS:HB2	20:E:296:LEU:HD21	1.97	0.46
21:F:252:SER:O	21:F:256:HIS:ND1	2.33	0.45
30:P:91:GLU:HG3	30:P:106:SER:HB2	1.97	0.45
41:a:62:HIS:O	41:a:62:HIS:ND1	2.47	0.45
53:m:51:LEU:HB3	53:m:67:ARG:HB3	1.97	0.45
58:s:103:ASP:OD2	58:s:325:ARG:NE	2.41	0.45
5:x:191:LEU:O	5:x:194:THR:OG1	2.31	0.45
17:A:3044:A:H2'	17:A:3045:A:C8	2.51	0.45
19:D:109:PHE:HB3	19:D:204:ALA:HB3	1.98	0.45
21:F:164:MET:HE3	49:i:69:HIS:HE1	1.81	0.45
27:M:193:PHE:HE2	27:M:200:ILE:HG12	1.81	0.45
35:U:48:MET:HE2	35:U:53:LEU:HA	1.98	0.45
51:k:18:VAL:HG22	51:k:64:VAL:HG13	1.97	0.45
2:u:182:PRO:HA	2:u:185:ARG:HB2	1.98	0.45
4:w:122:MET:HE2	4:w:144:ILE:HG21	1.98	0.45
17:A:2685:U:O2'	17:A:3104:U:H5'	2.16	0.45
20:E:207:THR:HB	20:E:298:LYS:HB3	1.96	0.45
57:r:83:TYR:HB3	57:r:121:MET:HE3	1.99	0.45
58:s:105:TRP:CG	58:s:271:LEU:HD13	2.51	0.45
58:s:237:PRO:HB3	58:s:300:HIS:CE1	2.51	0.45
1:t:231:GLY:HA2	1:t:324:LEU:HD13	1.97	0.45
5:x:203:ASN:ND2	5:x:236:TRP:O	2.40	0.45
13:6:322:ARG:NH1	55:p:181:GLU:OE1	2.50	0.45
16:9:16:ASP:OD1	16:9:16:ASP:N	2.46	0.45
17:A:1746:A:OP1	38:X:55:LYS:NZ	2.34	0.45
17:A:2545:U:H1'	17:A:2601:A:C2	2.52	0.45
28:N:154:VAL:HG13	28:N:158:ARG:HD3	1.97	0.45
48:h:88:ASP:OD1	48:h:124:ARG:NH2	2.44	0.45
58:s:366:TYR:HA	58:s:400:PRO:HA	1.99	0.45
5:x:34:THR:HG22	17:A:2817:G:H22	1.81	0.45
17:A:1845:C:O2'	17:A:2297:A:N1	2.47	0.45
21:F:65:TRP:CD1	48:h:117:LEU:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:J:23:ILE:HA	24:J:67:PRO:HA	1.98	0.45
25:K:78:SER:HB3	25:K:89:GLN:HG2	1.98	0.45
34:T:71:ARG:HH22	34:T:113:GLU:HG2	1.80	0.45
43:c:79:LEU:HD13	43:c:214:PHE:HE1	1.82	0.45
44:d:245:TYR:HB2	44:d:265:ILE:HB	1.98	0.45
13:6:243:ASN:OD1	13:6:243:ASN:N	2.48	0.45
17:A:1770:G:H4'	21:F:112:ALA:HB2	1.98	0.45
17:A:1830:G:H5"	42:b:2:THC:HG21	1.97	0.45
17:A:2241:A:H61	57:r:82:ASN:CG	2.24	0.45
17:A:2456:U:OP1	29:O:16:ARG:NH1	2.50	0.45
20:E:148:GLY:HA3	20:E:173:LYS:HG3	1.98	0.45
20:E:208:ALA:HB2	20:E:297:VAL:HG12	1.99	0.45
21:F:103:GLN:O	21:F:107:LYS:NZ	2.44	0.45
33:S:142:THR:OG1	41:a:62:HIS:NE2	2.47	0.45
39:Y:128:SER:HB2	39:Y:131:ARG:NE	2.32	0.45
50:j:91:TRP:CD2	54:o:58:GLN:HG2	2.52	0.45
6:y:215:ILE:HD11	6:y:249:VAL:HG22	1.97	0.45
12:5:192:ILE:HG12	12:5:198:LEU:HB2	1.99	0.45
13:6:116:ASN:HD21	13:6:118:GLU:HB2	1.80	0.45
14:7:217:GLU:OE1	14:7:256:ARG:NE	2.45	0.45
17:A:2359:C:H5"	17:A:2361:G:H1'	1.99	0.45
17:A:2616:A:H4'	17:A:3047:G:H5"	1.97	0.45
21:F:72:PHE:HE1	48:h:50:LEU:HB3	1.81	0.45
24:J:160:SER:N	24:J:163:GLU:OE2	2.49	0.45
34:T:134:LEU:HD23	34:T:174:GLU:HA	1.97	0.45
35:U:153:LEU:O	44:d:233:TYR:OH	2.31	0.45
58:s:374:LEU:HD21	58:s:377:LEU:HD13	1.98	0.45
12:5:30:ALA:HB2	19:D:110:LEU:HD22	1.99	0.45
13:6:36:PRO:HG2	46:f:56:ILE:HG13	1.99	0.45
17:A:2166:C:N3	17:A:2167:A:N6	2.64	0.45
17:A:3141:A:H2'	17:A:3142:A:C8	2.52	0.45
26:L:40:VAL:HG11	26:L:47:GLY:HA3	1.98	0.45
51:k:72:HIS:CE1	57:r:45:LYS:HB2	2.52	0.45
12:5:212:THR:HG21	12:5:273:VAL:HG13	1.99	0.45
13:6:273:PHE:HB3	13:6:311:MET:HG2	1.99	0.45
17:A:1977:U:H2'	17:A:1978:A:C8	2.52	0.45
35:U:81:ASP:HB3	35:U:87:ILE:HD11	1.97	0.45
21:F:211:ARG:HE	48:h:55:LEU:HD11	1.81	0.44
35:U:8:PRO:HA	39:Y:183:GLN:HE22	1.82	0.44
57:r:96:HIS:CE1	57:r:134:ARG:HB2	2.52	0.44
19:D:220:VAL:O	19:D:223:THR:OG1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:H:53:THR:OG1	38:X:83:GLU:OE2	2.24	0.44
43:c:46:GLU:HA	43:c:49:ARG:HD2	1.99	0.44
17:A:2446:A:OP1	58:s:65:ARG:NH2	2.49	0.44
17:A:3024:U:H2'	17:A:3025:A:C8	2.52	0.44
21:F:95:ILE:HA	21:F:98:GLN:HE21	1.82	0.44
32:R:91:VAL:HG11	50:j:24:GLY:HA3	1.99	0.44
34:T:49:ASN:ND2	34:T:68:TYR:O	2.28	0.44
1:t:92:PHE:HZ	1:t:204:VAL:HG22	1.81	0.44
6:y:186:ILE:O	6:y:189:MET:HG2	2.18	0.44
10:3:154:GLN:NE2	17:A:2867:C:O3'	2.51	0.44
14:7:104:ILE:HG13	14:7:130:PHE:CD2	2.52	0.44
23:I:39:VAL:HG21	54:o:22:ARG:HD2	1.98	0.44
30:P:133:ALA:HB1	30:P:168:GLY:HA3	2.00	0.44
40:Z:64:HIS:HE1	40:Z:67:HIS:CE1	2.35	0.44
51:k:75:ILE:HD12	57:r:48:ILE:HG12	1.99	0.44
13:6:114:ARG:NH2	18:B:1643:A:OP1	2.51	0.44
15:8:117:LEU:HD23	45:e:73:LEU:HD22	1.99	0.44
16:9:31:ARG:HD2	17:A:2421:G:H4'	2.00	0.44
22:H:79:VAL:HG22	38:X:89:GLN:HB2	1.99	0.44
26:L:118:ARG:HE	26:L:142:GLN:NE2	2.15	0.44
28:N:81:GLU:OE2	28:N:199:ARG:NH1	2.38	0.44
28:N:134:LYS:HB3	28:N:134:LYS:HZ2	1.82	0.44
44:d:91:PRO:HG2	44:d:111:ARG:NH2	2.33	0.44
28:N:104:MET:HE3	28:N:104:MET:HB3	1.93	0.44
34:T:185:THR:O	34:T:189:HIS:ND1	2.39	0.44
57:r:70:CYS:HB2	57:r:107:LEU:HA	2.00	0.44
1:t:342:ILE:HB	1:t:367:VAL:HG12	2.00	0.44
18:B:1622:A:H2'	18:B:1623:G:C8	2.53	0.44
19:D:210:ALA:HB1	19:D:249:ASN:HB2	2.00	0.44
33:S:67:PRO:HG3	41:a:36:TYR:HB3	2.00	0.44
38:X:42:HIS:CG	38:X:86:ILE:HD11	2.53	0.44
46:f:179:PRO:HA	53:m:35:SER:HB2	1.99	0.44
6:y:237:ALA:HB1	6:y:243:ILE:HD12	2.00	0.44
12:5:201:ARG:HB3	12:5:232:THR:HG22	1.99	0.44
14:7:114:ASP:HB2	14:7:117:LYS:HB2	2.00	0.44
17:A:2512:A:O2'	17:A:2541:C:OP1	2.28	0.44
17:A:3141:A:H5'	26:L:130:ARG:HH12	1.82	0.44
35:U:133:GLU:HB3	35:U:137:ARG:NH1	2.33	0.44
36:V:47:GLU:HG3	39:Y:241:LEU:HD21	1.99	0.44
2:u:121:THR:HG21	2:u:176:VAL:HG12	1.99	0.44
6:y:169:LEU:HD11	6:y:171:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:0:96:ASN:HD22	7:0:98:GLN:H	1.66	0.44
13:6:323:TRP:NE1	13:6:339:GLU:OE2	2.48	0.44
15:8:124:TYR:OH	45:e:67:GLN:NE2	2.51	0.44
17:A:1884:G:N7	21:F:281:ARG:HD2	2.32	0.44
17:A:1984:A:N1	17:A:1997:C:O2'	2.38	0.44
22:H:56:VAL:HG12	22:H:82:LEU:HA	1.99	0.44
29:O:18:MET:HE1	29:O:29:LEU:HD21	1.99	0.44
36:V:69:ASP:OD1	36:V:69:ASP:N	2.47	0.44
44:d:152:LEU:HD22	44:d:176:ILE:HD11	2.00	0.44
1:t:103:PRO:HB2	1:t:193:ARG:HA	2.00	0.43
1:t:125:LEU:HD13	1:t:158:PRO:HD3	1.99	0.43
5:x:139:ILE:HD13	6:y:318:LYS:HB3	2.00	0.43
5:x:239:ARG:HG3	5:x:291:LEU:HD23	1.99	0.43
12:5:286:PRO:O	12:5:324:GLN:NE2	2.51	0.43
17:A:1798:A:N3	36:V:42:ARG:NH2	2.65	0.43
17:A:1952:U:H2'	17:A:1953:A:H8	1.83	0.43
17:A:2826:G:H2'	17:A:2827:A:H8	1.82	0.43
17:A:3073:C:H2'	17:A:3074:A:C8	2.53	0.43
38:X:125:VAL:HG23	38:X:127:VAL:HG13	2.00	0.43
1:t:201:ARG:NH1	17:A:3088:C:O3'	2.51	0.43
12:5:98:LEU:HD13	12:5:272:ASP:HB2	2.00	0.43
19:D:182:HIS:HB2	19:D:187:LEU:HD21	1.99	0.43
24:J:56:ARG:HH11	24:J:80:ILE:HG13	1.83	0.43
58:s:90:LYS:HD2	58:s:232:GLN:HB2	1.99	0.43
5:x:36:PRO:HG2	5:x:38:PHE:CZ	2.54	0.43
14:7:186:ASP:OD1	14:7:187:SER:N	2.51	0.43
34:T:184:LYS:NZ	34:T:192:GLU:OE1	2.41	0.43
11:4:74:LYS:HB3	11:4:79:CYS:HB2	1.99	0.43
16:9:101:GLU:HG2	38:X:238:LEU:HD11	1.98	0.43
17:A:1936:A:H1'	17:A:1938:A:C6	2.54	0.43
17:A:2245:A:C4	57:r:189:ARG:HG3	2.54	0.43
21:F:175:LYS:HE2	21:F:273:LEU:HB3	2.00	0.43
23:I:146:LEU:O	51:k:31:ARG:NH1	2.51	0.43
29:O:60:ILE:HG22	29:O:64:LYS:HE3	2.01	0.43
45:e:160:LEU:HD11	45:e:260:LEU:HD12	2.00	0.43
47:g:79:PRO:HB3	47:g:85:PHE:HE1	1.81	0.43
4:w:83:VAL:HG22	4:w:122:MET:HE1	1.99	0.43
14:7:97:GLU:N	34:T:94:ASP:OD2	2.43	0.43
17:A:1848:U:O3'	27:M:54:LYS:NZ	2.47	0.43
17:A:2039:A:N7	17:A:2729:U:O2'	2.48	0.43
17:A:2406:A:O2'	17:A:2407:U:O5'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:2692:G:N1	17:A:2696:A:OP2	2.37	0.43
49:i:93:ARG:HA	49:i:96:LYS:HE2	2.01	0.43
58:s:211:VAL:HG22	58:s:230:ARG:HG2	2.00	0.43
6:y:252:GLU:O	6:y:255:GLN:HG2	2.18	0.43
6:y:302:LEU:O	6:y:307:CYS:N	2.43	0.43
12:5:177:CYS:HB3	12:5:178:PRO:HD3	1.99	0.43
12:5:270:ILE:O	17:A:2409:A:O2'	2.36	0.43
23:I:147:PHE:HA	23:I:151:ASN:ND2	2.33	0.43
30:P:137:LEU:HB3	55:p:188:LEU:HD11	1.99	0.43
32:R:112:THR:OG1	42:b:127:GLN:NE2	2.36	0.43
13:6:162:PHE:HB3	13:6:165:ALA:HB3	2.00	0.43
17:A:3077:C:H2'	17:A:3078:C:C6	2.53	0.43
18:B:1621:A:H61	18:B:1645:A:H2'	1.84	0.43
24:J:25:ARG:HG3	52:l:56:LEU:HB3	2.00	0.43
35:U:71:ARG:NH1	35:U:73:GLN:OE1	2.52	0.43
39:Y:102:TRP:HE3	39:Y:142:LEU:HD22	1.82	0.43
45:e:272:VAL:HA	45:e:275:PHE:CE2	2.54	0.43
3:v:21:ARG:NH2	4:w:120:MET:SD	2.73	0.43
13:6:48:LEU:O	13:6:50:LYS:NZ	2.42	0.43
21:F:178:LEU:HD11	21:F:269:LEU:HD13	2.01	0.43
27:M:244:LEU:HD12	27:M:245:PRO:HD2	1.99	0.43
58:s:89:MET:HB3	58:s:275:LYS:HE2	2.01	0.43
6:y:271:LEU:HB3	6:y:273:ARG:HG2	2.00	0.43
7:0:93:ARG:HG3	17:A:2709:A:H5"	2.01	0.43
13:6:257:PRO:HB3	13:6:268:LEU:HD21	1.99	0.43
16:9:130:LEU:HD13	39:Y:154:ARG:HA	2.01	0.43
17:A:2171:U:C2	17:A:2173:G:H4'	2.54	0.43
43:c:234:ILE:HD11	43:c:237:PRO:HB3	2.01	0.43
58:s:174:LEU:HB3	58:s:175:PRO:HD3	2.01	0.43
58:s:419:LEU:O	58:s:423:HIS:ND1	2.33	0.43
5:x:38:PHE:CE1	19:D:299:PRO:HB2	2.54	0.43
5:x:136:ARG:HB3	5:x:369:MET:HE2	2.01	0.43
13:6:217:LEU:HD23	13:6:271:LEU:HD12	1.99	0.43
13:6:221:LEU:HD13	13:6:267:ARG:HG3	2.00	0.43
15:8:189:GLU:HB3	53:m:81:LEU:HD21	1.99	0.43
16:9:74:VAL:O	39:Y:83:ALA:N	2.49	0.43
17:A:1737:A:N6	17:A:1760:G:H1'	2.33	0.43
31:Q:210:GLU:HB2	31:Q:213:GLN:HG3	2.01	0.43
39:Y:191:ASN:O	39:Y:195:ASN:ND2	2.34	0.43
42:b:133:PHE:HE2	43:c:269:LEU:HD23	1.84	0.43
56:q:89:GLU:HA	56:q:93:TYR:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:6:53:SER:HB3	18:B:1637:C:H5"	2.00	0.42
17:A:2113:G:H22	17:A:2693:A:P	2.42	0.42
17:A:2180:A:H4'	17:A:2181:A:N7	2.33	0.42
17:A:2239:A:H5'	25:K:75:LYS:HZ2	1.84	0.42
20:E:50:ASP:HA	20:E:53:LEU:HG	2.01	0.42
24:J:114:LEU:HD13	52:l:97:PHE:HA	2.00	0.42
33:S:96:PHE:HD1	42:b:126:ILE:HD12	1.84	0.42
38:X:27:HIS:CE1	38:X:200:GLU:HG2	2.53	0.42
39:Y:91:ARG:HA	39:Y:149:ARG:HH21	1.82	0.42
45:e:55:ARG:NH2	45:e:152:LYS:O	2.45	0.42
1:t:307:LEU:HD23	1:t:341:ALA:HB3	2.01	0.42
21:F:253:MET:HE3	21:F:259:LEU:HD22	2.01	0.42
40:Z:137:THR:HB	40:Z:145:LEU:HD11	2.01	0.42
45:e:151:ARG:NH2	45:e:255:VAL:HA	2.34	0.42
47:g:150:LYS:NZ	54:o:79:THR:O	2.50	0.42
1:t:402:GLN:HA	1:t:403:PRO:HD3	1.85	0.42
3:v:43:GLN:CD	61:w:200:PM8:H382	2.43	0.42
16:9:114:LEU:HD22	38:X:227:PHE:HE1	1.84	0.42
17:A:1993:A:H8	17:A:2498:U:O2'	2.03	0.42
17:A:2112:A:N6	17:A:2114:C:O2	2.53	0.42
39:Y:191:ASN:HB3	39:Y:194:TYR:HB3	2.01	0.42
49:i:98:VAL:O	49:i:102:MET:HG3	2.19	0.42
1:t:297:LEU:HA	1:t:300:ILE:HG22	2.01	0.42
12:5:118:LYS:HE3	12:5:256:PHE:HB3	2.01	0.42
17:A:2075:U:OP1	40:Z:38:ARG:HD2	2.19	0.42
17:A:2402:A:OP2	19:D:131:TYR:OH	2.34	0.42
17:A:2860:G:O2'	37:W:65:ASN:OD1	2.28	0.42
27:M:111:ASP:OD1	27:M:111:ASP:N	2.45	0.42
29:O:97:TYR:OH	29:O:126:LYS:O	2.26	0.42
38:X:95:ASP:O	38:X:98:SER:OG	2.32	0.42
44:d:85:PHE:CZ	44:d:200:SER:HB3	2.54	0.42
44:d:134:ILE:HG22	44:d:194:VAL:HG21	2.00	0.42
45:e:151:ARG:HH21	45:e:255:VAL:HA	1.84	0.42
49:i:112:LYS:HG2	49:i:115:ARG:HH21	1.83	0.42
58:s:273:LEU:HD12	58:s:273:LEU:HA	1.91	0.42
1:t:143:LYS:NZ	17:A:3060:C:N3	2.49	0.42
1:t:165:GLU:HG3	1:t:170:VAL:HG21	2.02	0.42
3:v:54:GLN:O	3:v:57:LYS:HG2	2.20	0.42
10:3:152:LYS:HE3	10:3:156:LYS:HE3	2.00	0.42
17:A:1882:A:N6	17:A:1893:A:O4'	2.52	0.42
17:A:1992:C:C4	19:D:274:ARG:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:2284:C:OP2	42:b:74:ARG:NH1	2.39	0.42
17:A:3217:A:H2'	20:E:292:HIS:CD2	2.54	0.42
18:B:1617:C:OP2	18:B:1656:A:N6	2.52	0.42
20:E:345:ILE:HG12	31:Q:169:PRO:HB2	2.00	0.42
46:f:117:LEU:HD13	46:f:166:PHE:HZ	1.85	0.42
17:A:1742:G:O2'	17:A:1754:G:O6	2.36	0.42
17:A:2326:C:OP2	58:s:55:SER:OG	2.25	0.42
21:F:106:PHE:HE1	21:F:107:LYS:HZ2	1.67	0.42
30:P:73:PRO:O	30:P:75:ARG:NH1	2.51	0.42
45:e:71:ALA:HB2	53:m:40:LEU:HD22	2.01	0.42
47:g:85:PHE:HA	47:g:166:PHE:HE1	1.84	0.42
4:w:93:ILE:HG21	4:w:108:LEU:HD23	2.00	0.42
9:2:60:ARG:HH11	9:2:92:HIS:HD1	1.67	0.42
13:6:270:PHE:N	13:6:317:SER:O	2.38	0.42
17:A:1859:A:OP1	17:A:2299:U:O2'	2.30	0.42
17:A:2180:A:H1'	17:A:2206:C:H4'	2.02	0.42
18:B:1639:U:H5"	30:P:155:SER:HB3	2.01	0.42
19:D:79:MET:HE2	19:D:102:GLN:HB2	2.02	0.42
27:M:51:ARG:HB3	27:M:58:GLN:HA	2.01	0.42
27:M:98:LEU:HD12	27:M:145:ALA:HA	2.02	0.42
44:d:104:GLY:O	44:d:108:ARG:HG2	2.20	0.42
58:s:207:HIS:ND1	58:s:234:ASP:OD1	2.45	0.42
1:t:265:ILE:HG13	17:A:3129:A:H1'	2.02	0.42
5:x:153:MET:HB2	5:x:220:TYR:CE2	2.55	0.42
6:y:202:LYS:HE3	6:y:209:VAL:HG22	2.00	0.42
13:6:89:ASP:O	50:j:112:LYS:N	2.42	0.42
13:6:154:TYR:HE2	30:P:54:ARG:HD2	1.85	0.42
13:6:330:ILE:HG22	13:6:335:LEU:HG	2.01	0.42
13:6:336:ASP:OD1	55:p:129:ARG:NH2	2.41	0.42
14:7:276:PHE:CD2	14:7:277:GLN:HG3	2.55	0.42
14:7:276:PHE:HD2	14:7:277:GLN:HG3	1.83	0.42
35:U:64:PRO:HB2	35:U:100:ALA:HB3	2.02	0.42
57:r:78:LYS:HG2	57:r:79:HIS:CD2	2.55	0.42
14:7:220:GLU:HG2	14:7:253:LYS:HG2	2.02	0.42
16:9:119:PHE:HB2	38:X:227:PHE:CE1	2.55	0.42
17:A:2135:A:N3	17:A:2135:A:H2'	2.35	0.42
17:A:2238:A:OP1	57:r:165:LYS:NZ	2.53	0.42
17:A:2358:A:H2'	17:A:2361:G:H2'	2.01	0.42
17:A:2622:G:H2'	17:A:2623:A:C8	2.55	0.42
20:E:203:TYR:HA	20:E:272:LYS:HA	2.01	0.42
48:h:86:TRP:CD1	48:h:86:TRP:H	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:x:103:ILE:HA	5:x:106:TRP:HD1	1.84	0.42
5:x:139:ILE:O	6:y:322:ARG:NH2	2.38	0.42
13:6:93:PRO:HA	13:6:94:PRO:HD3	1.94	0.42
13:6:120:GLU:OE2	15:8:119:LYS:NZ	2.44	0.42
17:A:1680:A:OP1	39:Y:230:LYS:NZ	2.53	0.42
17:A:3183:U:N3	25:K:177:ARG:HB3	2.35	0.42
18:B:1642:G:H2'	18:B:1643:A:C8	2.55	0.42
29:O:46:TRP:CD1	29:O:121:ALA:HB2	2.55	0.42
36:V:181:ASP:O	39:Y:93:LYS:NZ	2.47	0.42
38:X:20:ILE:HG21	38:X:212:ILE:HG23	2.02	0.42
1:t:106:GLY:O	1:t:140:GLY:HA3	2.20	0.41
17:A:2192:A:H4'	24:J:139:SER:HB3	2.02	0.41
17:A:3047:G:H2'	17:A:3048:A:C8	2.56	0.41
18:B:1642:G:H2'	18:B:1643:A:H8	1.85	0.41
27:M:28:LYS:HD3	54:o:94:HIS:CD2	2.55	0.41
43:c:60:ARG:HD2	43:c:63:LYS:HD2	2.02	0.41
47:g:125:GLU:O	47:g:129:SER:OG	2.30	0.41
1:t:182:ALA:HB1	1:t:217:LEU:HD11	2.01	0.41
6:y:98:SER:O	6:y:102:MET:HG2	2.20	0.41
14:7:88:PRO:HB3	14:7:125:ILE:HD11	2.01	0.41
16:9:131:TYR:CD2	39:Y:160:GLN:HG3	2.54	0.41
17:A:1855:A:H2	17:A:3059:A:H61	1.68	0.41
17:A:2186:C:O2'	17:A:2187:C:OP1	2.36	0.41
17:A:3214:C:OP1	29:O:119:LYS:NZ	2.53	0.41
21:F:138:HIS:CG	21:F:146:TRP:HE1	2.39	0.41
25:K:170:TRP:CE3	57:r:105:THR:HA	2.56	0.41
28:N:169:PHE:CD1	28:N:191:SER:HB3	2.55	0.41
29:O:141:HIS:O	29:O:147:GLN:NE2	2.53	0.41
58:s:248:ALA:HB2	58:s:430:LYS:HG3	2.02	0.41
10:3:138:PRO:HG2	17:A:2854:U:H4'	2.00	0.41
27:M:156:VAL:O	27:M:176:THR:HA	2.21	0.41
43:c:105:ARG:NH1	43:c:115:VAL:O	2.53	0.41
47:g:87:ARG:HG3	47:g:112:LYS:HE2	2.01	0.41
48:h:140:PHE:HB2	48:h:156:TRP:CE3	2.56	0.41
7:0:81:PRO:HA	17:A:3102:U:C2	2.55	0.41
8:1:34:ARG:NH1	8:1:35:ASN:O	2.53	0.41
13:6:66:GLN:OE1	13:6:75:ARG:NH2	2.49	0.41
17:A:2036:C:H1'	17:A:2810:G:O2'	2.20	0.41
17:A:2634:U:H3'	17:A:2635:G:H8	1.86	0.41
19:D:140:ALA:HB2	19:D:153:ALA:HB2	2.03	0.41
25:K:136:ASP:O	25:K:140:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:l:88:PRO:HG2	52:l:91:GLU:HG3	2.02	0.41
6:y:162:ARG:HE	6:y:191:GLN:CD	2.28	0.41
14:7:93:MET:O	34:T:132:SER:OG	2.31	0.41
17:A:1710:A:H4'	17:A:1711:C:N3	2.35	0.41
17:A:2119:U:O2'	40:Z:36:PHE:O	2.27	0.41
17:A:2600:A:H2'	17:A:2601:A:C8	2.55	0.41
20:E:272:LYS:HE3	20:E:272:LYS:HB2	1.91	0.41
21:F:246:VAL:HG13	49:i:63:LEU:HB2	2.02	0.41
30:P:118:SER:HB3	30:P:121:ASN:ND2	2.36	0.41
31:Q:96:ARG:HA	31:Q:99:MET:HE2	2.03	0.41
32:R:141:ILE:HG23	32:R:144:ARG:HH12	1.85	0.41
39:Y:128:SER:HB2	39:Y:131:ARG:HE	1.86	0.41
40:Z:38:ARG:HG2	40:Z:81:TRP:CE2	2.55	0.41
55:p:128:ASN:OD1	55:p:132:GLU:N	2.53	0.41
1:t:292:LEU:N	1:t:327:GLU:OE2	2.50	0.41
17:A:2461:A:H2'	17:A:2462:A:H8	1.86	0.41
22:H:98:LEU:HD23	22:H:129:ALA:HB2	2.02	0.41
41:a:46:ASN:O	41:a:63:PRO:HD2	2.21	0.41
1:t:306:LEU:HD12	1:t:340:HIS:CE1	2.56	0.41
10:3:179:LYS:HE3	10:3:180:TYR:CZ	2.55	0.41
16:9:68:PHE:CE2	16:9:70:LEU:HB2	2.55	0.41
17:A:1878:U:H5'	47:g:144:THR:HG21	2.02	0.41
17:A:1886:G:OP1	21:F:167:MET:N	2.50	0.41
17:A:2796:G:H1'	22:H:87:LYS:HD2	2.02	0.41
17:A:2830:A:OP2	17:A:2830:A:H3'	2.20	0.41
20:E:94:SER:HA	20:E:182:THR:HG21	2.02	0.41
21:F:195:LEU:HD22	21:F:202:TYR:HE2	1.86	0.41
47:g:84:TYR:CE1	47:g:120:LEU:HD13	2.56	0.41
58:s:247:LEU:HD21	58:s:296:HIS:HD2	1.86	0.41
2:u:200:ASP:OD1	2:u:200:ASP:N	2.53	0.41
5:x:296:LEU:O	5:x:299:THR:HG22	2.21	0.41
6:y:129:SER:HB3	19:D:220:VAL:HG11	2.02	0.41
17:A:2104:A:OP1	28:N:73:ARG:NH1	2.47	0.41
17:A:2256:U:P	50:j:66:ARG:HH12	2.44	0.41
17:A:2864:U:H5'	17:A:2865:C:H4'	2.03	0.41
17:A:2976:G:O2'	17:A:3005:A:N6	2.54	0.41
18:B:1623:G:OP1	30:P:86:THR:OG1	2.30	0.41
24:J:125:ALA:HA	24:J:130:PHE:HD2	1.84	0.41
25:K:73:GLU:OE2	57:r:149:ARG:NH2	2.52	0.41
32:R:108:TYR:CE2	34:T:206:LEU:HB2	2.56	0.41
43:c:269:LEU:HD21	43:c:271:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:80:VAL:HA	1:t:132:TYR:HB2	2.03	0.41
1:t:349:LEU:HB2	1:t:350:PRO:HD3	2.03	0.41
5:x:109:GLN:NE2	5:x:346:ARG:HD2	2.36	0.41
13:6:87:LYS:HE2	13:6:87:LYS:HB3	1.90	0.41
17:A:2171:U:O2'	17:A:2173:G:OP2	2.30	0.41
17:A:3093:C:H2'	17:A:3094:G:C8	2.56	0.41
24:J:114:LEU:HD12	24:J:157:LYS:HA	2.03	0.41
25:K:172:PRO:HG2	57:r:56:THR:HG23	2.02	0.41
27:M:30:ASN:O	27:M:33:SER:OG	2.34	0.41
27:M:247:ILE:HD11	55:p:59:TRP:HB3	2.03	0.41
29:O:67:ASP:N	29:O:67:ASP:OD1	2.48	0.41
35:U:152:GLY:HA2	44:d:273:LYS:HE2	2.03	0.41
40:Z:87:LYS:HE2	40:Z:87:LYS:HB3	1.90	0.41
53:m:69:ARG:HG3	53:m:70:GLU:HG3	2.03	0.41
58:s:212:ARG:HD2	58:s:379:LEU:HB3	2.02	0.41
3:v:63:ASN:HB3	3:v:65:LYS:HG3	2.02	0.41
5:x:258:CYS:SG	5:x:259:THR:N	2.94	0.41
6:y:200:LEU:HD13	6:y:227:LEU:HD22	2.03	0.41
6:y:240:ARG:HG2	6:y:265:HIS:HE1	1.85	0.41
17:A:3043:C:H2'	17:A:3044:A:O4'	2.20	0.41
23:I:113:ARG:HD2	23:I:123:MET:HE2	2.02	0.41
27:M:62:ARG:O	49:i:128:ARG:NH2	2.42	0.41
1:t:304:ARG:HA	1:t:304:ARG:HD3	1.92	0.40
2:u:140:PHE:HA	2:u:143:VAL:HG12	2.02	0.40
2:u:160:GLU:OE2	26:L:134:TYR:N	2.54	0.40
5:x:200:LEU:N	5:x:230:GLN:O	2.49	0.40
6:y:236:TYR:CE1	6:y:240:ARG:HD3	2.55	0.40
12:5:73:PRO:HG2	12:5:75:PHE:CZ	2.56	0.40
12:5:114:LEU:HD11	19:D:127:ILE:HD13	2.03	0.40
17:A:2230:A:H62	17:A:2975:G:H1'	1.86	0.40
17:A:2896:G:C6	17:A:2915:C:H1'	2.56	0.40
21:F:282:PRO:HB3	21:F:286:PHE:CZ	2.56	0.40
39:Y:90:LEU:HB2	39:Y:145:VAL:HG21	2.03	0.40
39:Y:126:MET:HB3	39:Y:129:PRO:HG3	2.03	0.40
44:d:207:ASN:OD1	44:d:251:GLN:NE2	2.54	0.40
45:e:159:LEU:HD13	45:e:254:TRP:CE2	2.55	0.40
5:x:156:TYR:HD1	5:x:220:TYR:CZ	2.39	0.40
13:6:60:ARG:NH1	13:6:64:GLU:HB2	2.35	0.40
16:9:131:TYR:HA	16:9:132:PRO:HA	1.90	0.40
17:A:2127:A:H2'	17:A:2128:G:C8	2.56	0.40
58:s:119:PRO:HG3	58:s:394:TRP:CE3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:332:GLU:HG3	1:t:334:GLY:H	1.86	0.40
14:7:319:ARG:NH1	29:O:155:ASP:OD2	2.54	0.40
15:8:195:ILE:HB	46:f:131:THR:HB	2.02	0.40
17:A:2067:C:O3'	46:f:60:LYS:HD2	2.21	0.40
17:A:2182:G:O2'	17:A:2199:A:OP2	2.37	0.40
17:A:2796:G:O2'	22:H:85:ASP:OD2	2.27	0.40
21:F:138:HIS:CD2	21:F:146:TRP:HE1	2.39	0.40
23:I:132:LYS:O	23:I:136:GLU:HG3	2.20	0.40
26:L:70:GLY:O	26:L:134:TYR:OH	2.29	0.40
36:V:20:ARG:NH2	36:V:42:ARG:O	2.52	0.40
38:X:222:ASP:OD1	38:X:222:ASP:N	2.53	0.40
41:a:139:PRO:HB2	42:b:10:PHE:CD2	2.57	0.40
46:f:51:LYS:HA	46:f:51:LYS:HD3	1.90	0.40
48:h:58:ARG:HB2	48:h:136:ASP:HB3	2.04	0.40
58:s:115:LEU:HD11	58:s:257:VAL:HG11	2.04	0.40
5:x:79:ASN:ND2	5:x:193:GLN:O	2.45	0.40
12:5:262:ILE:H	12:5:262:ILE:HG13	1.70	0.40
17:A:1977:U:H2'	17:A:1978:A:H8	1.86	0.40
17:A:2807:U:H2'	17:A:2808:U:C6	2.56	0.40
22:H:131:TYR:HB3	38:X:139:TYR:HD1	1.87	0.40
23:I:177:LEU:HA	51:k:22:PRO:HG2	2.04	0.40
58:s:307:ARG:HG3	58:s:310:ARG:H	1.86	0.40
5:x:42:ARG:HH21	19:D:298:LEU:HB3	1.87	0.40
7:0:136:GLU:HB3	7:0:177:ARG:NH1	2.37	0.40
12:5:173:ARG:HD2	12:5:303:ARG:HD3	2.02	0.40
16:9:24:LYS:HE3	35:U:74:HIS:HB2	2.03	0.40
17:A:2349:G:H1	17:A:2364:C:H42	1.70	0.40
23:I:173:PHE:HB3	51:k:51:VAL:HB	2.04	0.40
33:S:92:TYR:HB3	33:S:141:PHE:HE1	1.86	0.40
35:U:54:ARG:NH1	35:U:65:VAL:O	2.55	0.40
46:f:49:LYS:HA	46:f:54:HIS:CG	2.57	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	t	310/406 (76%)	303 (98%)	7 (2%)	0	100	100
2	u	108/234 (46%)	105 (97%)	3 (3%)	0	100	100
3	v	67/70 (96%)	67 (100%)	0	0	100	100
4	w	77/156 (49%)	72 (94%)	5 (6%)	0	100	100
5	x	342/384 (89%)	338 (99%)	4 (1%)	0	100	100
6	y	242/381 (64%)	240 (99%)	2 (1%)	0	100	100
7	0	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
8	1	53/65 (82%)	53 (100%)	0	0	100	100
9	2	44/92 (48%)	42 (96%)	2 (4%)	0	100	100
10	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
11	4	36/103 (35%)	36 (100%)	0	0	100	100
12	5	392/423 (93%)	387 (99%)	5 (1%)	0	100	100
13	6	352/380 (93%)	342 (97%)	10 (3%)	0	100	100
14	7	292/338 (86%)	288 (99%)	4 (1%)	0	100	100
15	8	100/206 (48%)	100 (100%)	0	0	100	100
16	9	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
19	D	238/305 (78%)	233 (98%)	5 (2%)	0	100	100
20	E	303/348 (87%)	298 (98%)	5 (2%)	0	100	100
21	F	250/311 (80%)	246 (98%)	4 (2%)	0	100	100
22	H	95/267 (36%)	94 (99%)	1 (1%)	0	100	100
23	I	166/261 (64%)	165 (99%)	1 (1%)	0	100	100
24	J	173/192 (90%)	173 (100%)	0	0	100	100
25	K	175/178 (98%)	173 (99%)	2 (1%)	0	100	100
26	L	113/145 (78%)	113 (100%)	0	0	100	100
27	M	289/296 (98%)	285 (99%)	4 (1%)	0	100	100
28	N	220/251 (88%)	220 (100%)	0	0	100	100
29	O	152/175 (87%)	149 (98%)	3 (2%)	0	100	100
30	P	142/180 (79%)	138 (97%)	4 (3%)	0	100	100
31	Q	219/292 (75%)	218 (100%)	1 (0%)	0	100	100
32	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	S	159/205 (78%)	159 (100%)	0	0	100	100
34	T	164/206 (80%)	163 (99%)	1 (1%)	0	100	100
35	U	150/153 (98%)	149 (99%)	1 (1%)	0	100	100
36	V	203/216 (94%)	202 (100%)	1 (0%)	0	100	100
37	W	104/148 (70%)	101 (97%)	3 (3%)	0	100	100
38	X	242/256 (94%)	241 (100%)	1 (0%)	0	100	100
39	Y	179/250 (72%)	179 (100%)	0	0	100	100
40	Z	120/161 (74%)	117 (98%)	3 (2%)	0	100	100
41	a	96/142 (68%)	96 (100%)	0	0	100	100
42	b	147/215 (68%)	145 (99%)	2 (1%)	0	100	100
43	c	282/332 (85%)	280 (99%)	2 (1%)	0	100	100
44	d	257/306 (84%)	254 (99%)	3 (1%)	0	100	100
45	e	224/279 (80%)	222 (99%)	2 (1%)	0	100	100
46	f	146/212 (69%)	144 (99%)	2 (1%)	0	100	100
47	g	132/166 (80%)	131 (99%)	1 (1%)	0	100	100
48	h	108/158 (68%)	105 (97%)	3 (3%)	0	100	100
49	i	95/128 (74%)	95 (100%)	0	0	100	100
50	j	92/123 (75%)	89 (97%)	3 (3%)	0	100	100
51	k	99/112 (88%)	98 (99%)	1 (1%)	0	100	100
52	l	80/138 (58%)	80 (100%)	0	0	100	100
53	m	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
54	o	92/102 (90%)	92 (100%)	0	0	100	100
55	p	141/206 (68%)	138 (98%)	3 (2%)	0	100	100
56	q	139/222 (63%)	139 (100%)	0	0	100	100
57	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
58	s	382/439 (87%)	376 (98%)	6 (2%)	0	100	100
All	All	9453/12300 (77%)	9336 (99%)	117 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	t	248/320 (78%)	237 (96%)	11 (4%)	25	56
2	u	104/200 (52%)	101 (97%)	3 (3%)	37	66
3	v	59/60 (98%)	58 (98%)	1 (2%)	53	74
4	w	73/136 (54%)	73 (100%)	0	100	100
5	x	299/328 (91%)	295 (99%)	4 (1%)	61	77
6	y	226/350 (65%)	224 (99%)	2 (1%)	70	80
7	0	99/164 (60%)	99 (100%)	0	100	100
8	1	52/60 (87%)	52 (100%)	0	100	100
9	2	40/72 (56%)	40 (100%)	0	100	100
10	3	88/166 (53%)	87 (99%)	1 (1%)	65	78
11	4	37/89 (42%)	37 (100%)	0	100	100
12	5	353/368 (96%)	353 (100%)	0	100	100
13	6	313/332 (94%)	311 (99%)	2 (1%)	78	83
14	7	270/303 (89%)	269 (100%)	1 (0%)	84	86
15	8	93/190 (49%)	93 (100%)	0	100	100
16	9	104/112 (93%)	104 (100%)	0	100	100
19	D	194/245 (79%)	192 (99%)	2 (1%)	68	79
20	E	260/290 (90%)	260 (100%)	0	100	100
21	F	219/262 (84%)	219 (100%)	0	100	100
22	H	88/228 (39%)	87 (99%)	1 (1%)	65	78
23	I	155/232 (67%)	155 (100%)	0	100	100
24	J	138/150 (92%)	138 (100%)	0	100	100
25	K	154/155 (99%)	153 (99%)	1 (1%)	78	83
26	L	98/124 (79%)	97 (99%)	1 (1%)	68	79
27	M	246/249 (99%)	243 (99%)	3 (1%)	63	78
28	N	189/211 (90%)	188 (100%)	1 (0%)	81	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	O	134/150 (89%)	134 (100%)	0	100	100
30	P	126/155 (81%)	126 (100%)	0	100	100
31	Q	203/256 (79%)	202 (100%)	1 (0%)	81	85
32	R	118/126 (94%)	118 (100%)	0	100	100
33	S	146/180 (81%)	146 (100%)	0	100	100
34	T	146/176 (83%)	146 (100%)	0	100	100
35	U	134/135 (99%)	133 (99%)	1 (1%)	76	82
36	V	183/191 (96%)	181 (99%)	2 (1%)	65	78
37	W	86/119 (72%)	84 (98%)	2 (2%)	44	70
38	X	220/229 (96%)	219 (100%)	1 (0%)	81	85
39	Y	163/223 (73%)	163 (100%)	0	100	100
40	Z	113/147 (77%)	113 (100%)	0	100	100
41	a	96/133 (72%)	96 (100%)	0	100	100
42	b	130/185 (70%)	129 (99%)	1 (1%)	73	81
43	c	251/288 (87%)	251 (100%)	0	100	100
44	d	237/274 (86%)	236 (100%)	1 (0%)	84	86
45	e	198/236 (84%)	198 (100%)	0	100	100
46	f	133/188 (71%)	133 (100%)	0	100	100
47	g	124/148 (84%)	124 (100%)	0	100	100
48	h	104/148 (70%)	104 (100%)	0	100	100
49	i	86/110 (78%)	86 (100%)	0	100	100
50	j	74/97 (76%)	74 (100%)	0	100	100
51	k	83/90 (92%)	83 (100%)	0	100	100
52	l	76/116 (66%)	75 (99%)	1 (1%)	61	77
53	m	46/113 (41%)	46 (100%)	0	100	100
54	o	80/87 (92%)	80 (100%)	0	100	100
55	p	135/181 (75%)	135 (100%)	0	100	100
56	q	119/178 (67%)	119 (100%)	0	100	100
57	r	147/169 (87%)	147 (100%)	0	100	100
58	s	340/381 (89%)	339 (100%)	1 (0%)	86	87
All	All	8430/10605 (80%)	8385 (100%)	45 (0%)	78	85

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	t	122	VAL
1	t	128	VAL
1	t	131	ARG
1	t	156	ARG
1	t	204	VAL
1	t	224	VAL
1	t	241	LEU
1	t	265	ILE
1	t	268	TYR
1	t	316	GLU
1	t	365	GLN
2	u	94	ILE
2	u	147	LYS
2	u	191	GLU
3	v	23	LEU
5	x	29	LYS
5	x	282	GLN
5	x	326	GLU
5	x	360	VAL
6	y	296	VAL
6	y	326	GLU
10	3	173	VAL
13	6	179	VAL
13	6	243	ASN
14	7	70	VAL
19	D	277	ARG
19	D	287	ARG
22	H	102	VAL
25	K	67	PHE
26	L	77	ILE
27	M	174	VAL
27	M	222	TYR
27	M	261	ASP
28	N	59	VAL
31	Q	125	TYR
35	U	19	VAL
36	V	93	THR
36	V	188	VAL
37	W	83	VAL
37	W	131	VAL
38	X	224	VAL
42	b	75	VAL

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Mol	Chain	Res	Type
44	d	89	VAL
52	l	58	ASP
58	s	113	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
1	t	120	GLN
1	t	121	GLN
1	t	198	ASN
1	t	199	ASN
1	t	200	ASN
1	t	213	GLN
1	t	218	HIS
1	t	271	HIS
1	t	273	GLN
1	t	314	GLN
1	t	362	HIS
1	t	384	HIS
3	v	19	GLN
4	w	103	HIS
5	x	47	ASN
5	x	55	GLN
5	x	105	HIS
5	x	109	GLN
5	x	172	GLN
5	x	214	GLN
5	x	230	GLN
5	x	282	GLN
5	x	316	GLN
5	x	322	GLN
5	x	371	ASN
6	y	122	GLN
6	y	123	GLN
6	y	210	GLN
6	y	217	HIS
6	y	235	GLN
6	y	255	GLN
6	y	284	GLN
7	0	98	GLN
8	1	31	ASN
10	3	178	GLN

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Mol	Chain	Res	Type
11	4	100	GLN
12	5	109	HIS
12	5	165	GLN
12	5	191	GLN
12	5	214	ASN
12	5	251	HIS
12	5	324	GLN
12	5	384	GLN
12	5	385	HIS
13	6	249	GLN
13	6	295	GLN
13	6	332	HIS
14	7	45	ASN
14	7	198	ASN
14	7	232	HIS
14	7	290	GLN
15	8	158	HIS
16	9	52	GLN
19	D	276	HIS
20	E	72	GLN
20	E	117	HIS
21	F	184	GLN
21	F	223	HIS
21	F	241	ASN
21	F	251	HIS
22	H	104	ASN
23	I	43	GLN
23	I	93	ASN
23	I	101	ASN
23	I	151	ASN
24	J	84	GLN
25	K	40	GLN
25	K	56	HIS
25	K	115	ASN
26	L	52	HIS
26	L	142	GLN
27	M	84	ASN
28	N	237	HIS
29	O	141	HIS
29	O	147	GLN
29	O	154	GLN
30	P	142	ASN

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Mol	Chain	Res	Type
31	Q	139	GLN
32	R	149	HIS
33	S	118	ASN
34	T	56	GLN
34	T	73	GLN
34	T	103	ASN
34	T	126	HIS
35	U	27	GLN
35	U	77	ASN
35	U	101	HIS
37	W	80	HIS
38	X	89	GLN
39	Y	179	HIS
39	Y	207	HIS
40	Z	62	ASN
40	Z	64	HIS
40	Z	107	ASN
41	a	46	ASN
42	b	102	GLN
42	b	123	ASN
42	b	129	GLN
43	c	73	GLN
43	c	168	HIS
44	d	235	GLN
45	e	67	GLN
45	e	75	GLN
45	e	212	HIS
45	e	251	HIS
46	f	138	GLN
46	f	158	GLN
46	f	189	HIS
47	g	92	HIS
48	h	118	HIS
49	i	59	ASN
49	i	108	HIS
49	i	120	HIS
52	l	82	GLN
53	m	65	HIS
54	o	94	HIS
55	p	194	HIS
56	q	120	HIS
56	q	161	GLN

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Mol	Chain	Res	Type
57	r	79	HIS
57	r	112	HIS
57	r	131	HIS
58	s	239	ASN
58	s	343	GLN
58	s	358	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	A	1445/1559 (92%)	260 (17%)	7 (0%)
18	B	71/72 (98%)	12 (16%)	0
All	All	1516/1631 (92%)	272 (17%)	7 (0%)

All (272) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
17	A	1678	C
17	A	1689	C
17	A	1694	U
17	A	1699	C
17	A	1700	U
17	A	1704	U
17	A	1707	C
17	A	1708	A
17	A	1712	A
17	A	1713	A
17	A	1715	C
17	A	1724	A
17	A	1727	A
17	A	1731	A
17	A	1748	G
17	A	1750	G
17	A	1751	A
17	A	1761	A
17	A	1764	C
17	A	1765	C
17	A	1767	G
17	A	1770	G
17	A	1780	U
17	A	1805	A

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Mol	Chain	Res	Type
17	A	1807	U
17	A	1808	A
17	A	1810	A
17	A	1817	C
17	A	1824	U
17	A	1827	C
17	A	1828	A
17	A	1829	A
17	A	1832	A
17	A	1836	A
17	A	1844	A
17	A	1854	U
17	A	1855	A
17	A	1869	A
17	A	1871	A
17	A	1882	A
17	A	1883	G
17	A	1887	A
17	A	1893	A
17	A	1901	C
17	A	1903	C
17	A	1918	G
17	A	1937	A
17	A	1940	A
17	A	1974	A
17	A	1984	A
17	A	1985	G
17	A	1986	A
17	A	1992	C
17	A	1994	A
17	A	2000	C
17	A	2002	G
17	A	2015	G
17	A	2021	U
17	A	2022	G
17	A	2029	A
17	A	2030	U
17	A	2031	A
17	A	2036	C
17	A	2037	U
17	A	2039	A
17	A	2060	A

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Mol	Chain	Res	Type
17	A	2065	A
17	A	2068	C
17	A	2071	U
17	A	2079	C
17	A	2083	U
17	A	2098	G
17	A	2111	C
17	A	2113	G
17	A	2114	C
17	A	2125	C
17	A	2132	A
17	A	2147	G
17	A	2154	A
17	A	2158	U
17	A	2163	A
17	A	2167	A
17	A	2168	U
17	A	2169	A
17	A	2171	U
17	A	2172	A
17	A	2173	G
17	A	2174	G
17	A	2181	A
17	A	2182	G
17	A	2183	C
17	A	2184	A
17	A	2187	C
17	A	2195	A
17	A	2197	G
17	A	2198	A
17	A	2200	A
17	A	2202	C
17	A	2203	G
17	A	2210	C
17	A	2228	A
17	A	2237	A
17	A	2239	A
17	A	2241	A
17	A	2243	A
17	A	2245	A
17	A	2246	A
17	A	2260	A

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Mol	Chain	Res	Type
17	A	2262	C
17	A	2263	C
17	A	2283	C
17	A	2284	C
17	A	2293	A
17	A	2297	A
17	A	2300	G
17	A	2322	C
17	A	2324	U
17	A	2332	C
17	A	2345	G
17	A	2351	U
17	A	2352	U
17	A	2353	A
17	A	2354	A
17	A	2355	A
17	A	2356	A
17	A	2359	C
17	A	2360	U
17	A	2361	G
17	A	2362	A
17	A	2363	A
17	A	2374	A
17	A	2381	A
17	A	2390	A
17	A	2393	C
17	A	2396	C
17	A	2401	A
17	A	2405	C
17	A	2406	A
17	A	2407	U
17	A	2414	C
17	A	2415	C
17	A	2416	U
17	A	2417	C
17	A	2432	A
17	A	2444	A
17	A	2446	A
17	A	2451	A
17	A	2452	A
17	A	2478	G
17	A	2480	A

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Mol	Chain	Res	Type
17	A	2485	U
17	A	2493	C
17	A	2500	A
17	A	2507	A
17	A	2511	C
17	A	2520	C
17	A	2521	A
17	A	2523	C
17	A	2527	A
17	A	2531	U
17	A	2536	G
17	A	2540	C
17	A	2614	U
17	A	2618	U
17	A	2640	C
17	A	2645	G
17	A	2654	U
17	A	2656	U
17	A	2660	U
17	A	2683	C
17	A	2684	C
17	A	2686	G
17	A	2694	A
17	A	2695	G
17	A	2696	A
17	A	2706	A
17	A	2718	C
17	A	2719	G
17	A	2722	A
17	A	2724	G
17	A	2727	C
17	A	2732	G
17	A	2801	A
17	A	2810	G
17	A	2815	G
17	A	2819	G
17	A	2830	A
17	A	2832	A
17	A	2833	A
17	A	2840	C
17	A	2844	G
17	A	2847	C

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Mol	Chain	Res	Type
17	A	2851	A
17	A	2854	U
17	A	2864	U
17	A	2865	C
17	A	2889	C
17	A	2895	U
17	A	2906	C
17	A	2911	C
17	A	2913	A
17	A	2916	G
17	A	2917	G
17	A	2922	A
17	A	2926	A
17	A	2928	C
17	A	2935	A
17	A	2936	U
17	A	2946	A
17	A	2955	U
17	A	2963	A
17	A	2985	C
17	A	2989	G
17	A	2990	A
17	A	2992	G
17	A	2993	U
17	A	3005	A
17	A	3016	G
17	A	3021	C
17	A	3037	U
17	A	3041	U
17	A	3047	G
17	A	3053	A
17	A	3054	G
17	A	3056	C
17	A	3059	A
17	A	3060	C
17	A	3073	C
17	A	3089	A
17	A	3096	U
17	A	3100	U
17	A	3101	A
17	A	3102	U
17	A	3110	C

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Mol	Chain	Res	Type
17	A	3111	A
17	A	3112	A
17	A	3113	A
17	A	3114	U
17	A	3131	G
17	A	3150	U
17	A	3155	C
17	A	3157	C
17	A	3158	A
17	A	3162	C
17	A	3169	C
17	A	3171	C
17	A	3172	C
17	A	3176	A
17	A	3180	A
17	A	3183	U
17	A	3189	C
17	A	3190	A
17	A	3197	U
17	A	3206	C
17	A	3207	A
17	A	3208	C
17	A	3212	C
17	A	3217	A
17	A	3218	A
17	A	3228	U
18	B	1603	A
18	B	1605	A
18	B	1609	U
18	B	1611	G
18	B	1621	A
18	B	1646	U
18	B	1650	A
18	B	1652	C
18	B	1653	U
18	B	1654	U
18	B	1656	A
18	B	1660	G

All (7) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
17	A	1766	U
17	A	2030	U
17	A	2186	C
17	A	2245	A
17	A	2530	A
17	A	2905	A
17	A	2992	G

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

6 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	$\#\|Z\| > 2$
17	OMG	A	3040	17	23,26,27	1.43	4 (17%)	33,38,41	1.81	5 (15%)
35	AYA	U	2	35	6,7,8	1.30	1 (16%)	5,8,10	1.24	1 (20%)
25	SAC	K	2	25	7,8,9	1.00	0	8,9,11	0.81	0
17	OMU	A	3039	17	19,22,23	1.39	3 (15%)	26,31,34	1.90	8 (30%)
51	AYA	k	2	51	6,7,8	1.21	1 (16%)	5,8,10	1.26	1 (20%)
42	THC	b	2	42	8,9,10	1.04	1 (12%)	9,11,13	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	OMG	A	3040	17	-	0/9/27/28	0/3/3/3
35	AYA	U	2	35	-	1/4/6/8	-
25	SAC	K	2	25	-	2/7/8/10	-
17	OMU	A	3039	17	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	AYA	k	2	51	-	0/4/6/8	-
42	THC	b	2	42	-	0/8/10/12	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	3040	OMG	C6-N1	-3.18	1.32	1.38
17	A	3039	OMU	C4-N3	-3.14	1.32	1.38
17	A	3039	OMU	C2-N3	-2.93	1.32	1.38
17	A	3040	OMG	C5-N7	-2.88	1.33	1.39
17	A	3040	OMG	C5-C4	2.76	1.46	1.38
35	U	2	AYA	CA-N	-2.57	1.43	1.46
17	A	3039	OMU	C5-C4	-2.39	1.38	1.43
17	A	3040	OMG	C4-N9	-2.35	1.32	1.38
51	k	2	AYA	CA-N	-2.23	1.44	1.46
42	b	2	THC	CA-N1	-2.07	1.43	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	3040	OMG	C5-C4-N3	-5.72	119.18	128.46
17	A	3040	OMG	N9-C4-N3	4.65	135.27	125.94
17	A	3039	OMU	C4-N3-C2	-4.36	120.83	126.58
17	A	3039	OMU	N3-C2-N1	4.13	120.38	114.89
17	A	3040	OMG	C2-N3-C4	4.05	119.51	112.30
17	A	3039	OMU	C5-C4-N3	3.69	120.36	114.84
17	A	3039	OMU	O2'-C2'-C1'	-2.88	103.46	109.08
17	A	3039	OMU	O4-C4-C5	-2.78	120.27	125.16
17	A	3039	OMU	C2'-C3'-C4'	-2.73	96.07	101.99
35	U	2	AYA	CB-CA-N	2.65	112.55	109.61
51	k	2	AYA	CB-CA-N	2.60	112.50	109.61
17	A	3040	OMG	C6-C5-N7	2.59	135.06	130.25
17	A	3040	OMG	O6-C6-C5	-2.36	120.35	126.60
17	A	3039	OMU	O4'-C4'-C3'	-2.28	100.59	105.11
17	A	3039	OMU	O4'-C1'-C2'	-2.04	102.98	106.57

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
25	K	2	SAC	C-CA-CB-OG
35	U	2	AYA	C-CA-N-CT

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 111 ligands modelled in this entry, 107 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
65	FES	r	201	57,23	0,4,4	-	-	-		
59	GDP	t	500	60	28,30,30	1.14	3 (10%)	44,47,47	1.84	8 (18%)
62	SAM	x	401	-	27,29,29	1.08	4 (14%)	36,42,42	2.02	9 (25%)
61	PM8	w	200	4	25,31,31	0.20	0	30,38,38	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	FES	r	201	57,23	-	-	0/1/1/1
59	GDP	t	500	60	-	1/16/32/32	0/3/3/3
62	SAM	x	401	-	-	6/16/33/33	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PM8	w	200	4	-	10/36/38/38	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	t	500	GDP	C5-C4	3.15	1.47	1.38
62	x	401	SAM	C2-N3	2.49	1.38	1.33
59	t	500	GDP	C6-N1	-2.45	1.34	1.38
62	x	401	SAM	C2-N1	2.43	1.38	1.33
62	x	401	SAM	C8-N7	2.17	1.35	1.31
62	x	401	SAM	OXT-C	-2.14	1.23	1.30
59	t	500	GDP	C5-N7	-2.08	1.35	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	t	500	GDP	C5-C4-N3	-6.07	118.61	128.46
62	x	401	SAM	N3-C2-N1	-5.40	120.15	128.60
62	x	401	SAM	C5-C4-N3	-4.87	120.39	126.75
59	t	500	GDP	C2-N3-C4	4.83	120.91	112.30
59	t	500	GDP	N9-C4-N3	4.58	135.13	125.94
62	x	401	SAM	N9-C8-N7	-3.99	108.46	113.91
62	x	401	SAM	C5-N7-C8	3.67	108.73	103.51
59	t	500	GDP	PA-O3A-PB	-3.63	120.37	132.83
62	x	401	SAM	C2-N3-C4	3.61	120.28	111.75
62	x	401	SAM	N3-C4-N9	3.27	132.47	127.08
59	t	500	GDP	C6-C5-N7	3.14	136.08	130.25
62	x	401	SAM	OXT-C-O	-2.78	117.77	124.09
59	t	500	GDP	C4-C5-N7	-2.58	106.63	110.72
59	t	500	GDP	C3'-C2'-C1'	2.33	105.85	101.43
62	x	401	SAM	OXT-C-CA	2.19	120.83	113.38
62	x	401	SAM	C4-C5-N7	-2.15	108.00	110.62
59	t	500	GDP	O6-C6-C5	-2.12	120.99	126.60

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	w	200	PM8	O33-C32-C34-O35
61	w	200	PM8	C32-C34-N36-C37
61	w	200	PM8	O1-C1-S1-C43

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Mol	Chain	Res	Type	Atoms
61	w	200	PM8	C2-C1-S1-C43
62	x	401	SAM	N-CA-CB-CG
62	x	401	SAM	C-CA-CB-CG
62	x	401	SAM	CB-CG-SD-C5'
61	w	200	PM8	O35-C34-N36-C37
61	w	200	PM8	C38-C39-N41-C42
61	w	200	PM8	O40-C39-N41-C42
62	x	401	SAM	CB-CG-SD-CE
61	w	200	PM8	N36-C37-C38-C39
62	x	401	SAM	C2'-C1'-N9-C8
61	w	200	PM8	C42-C43-S1-C1
61	w	200	PM8	O33-C32-C34-N36
59	t	500	GDP	C5'-O5'-PA-O1A
62	x	401	SAM	O4'-C1'-N9-C8

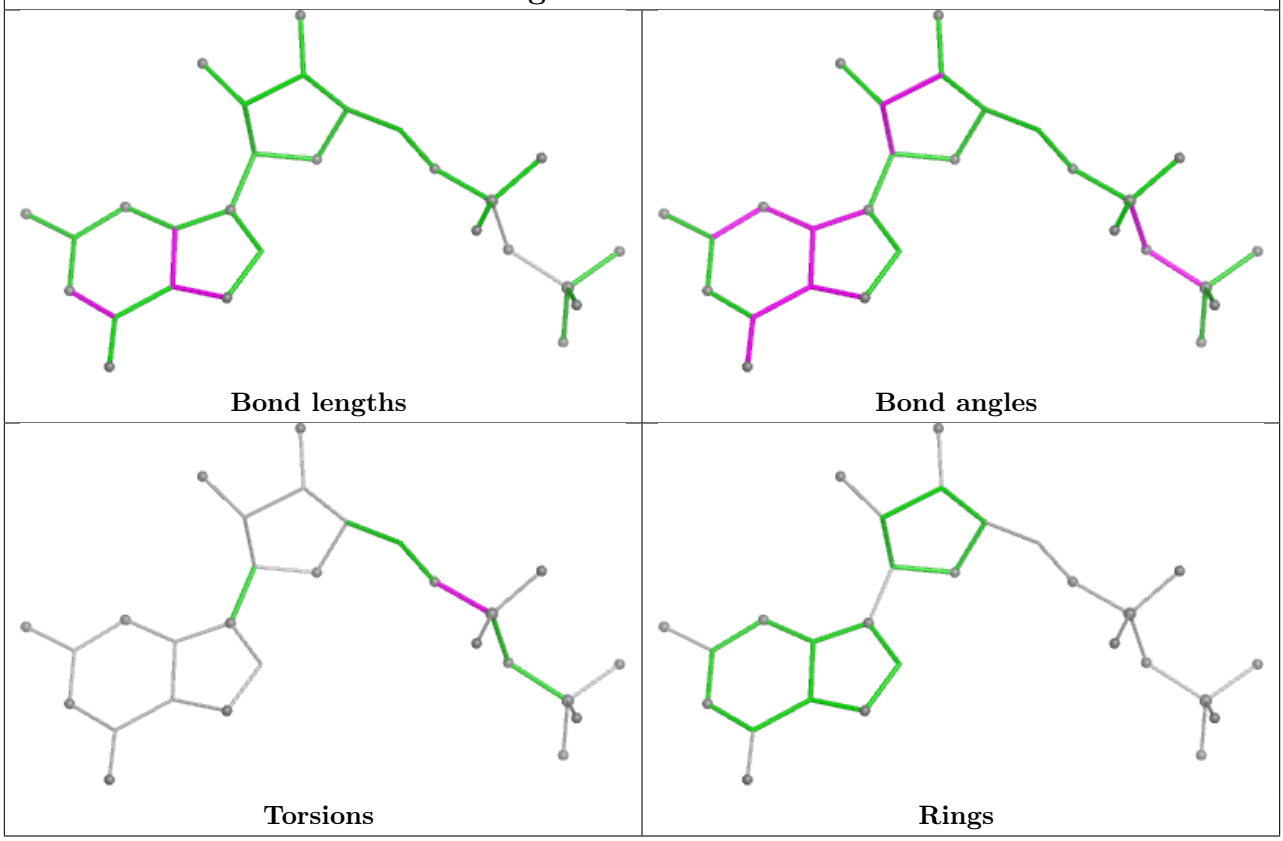
There are no ring outliers.

2 monomers are involved in 4 short contacts:

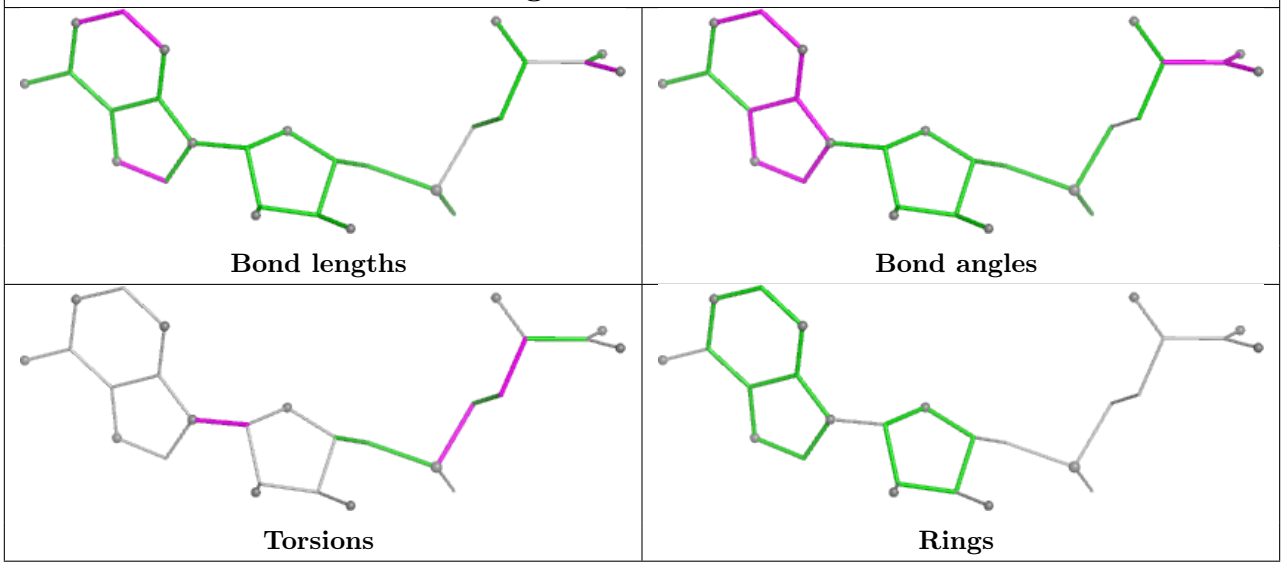
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	t	500	GDP	2	0
61	w	200	PM8	2	0

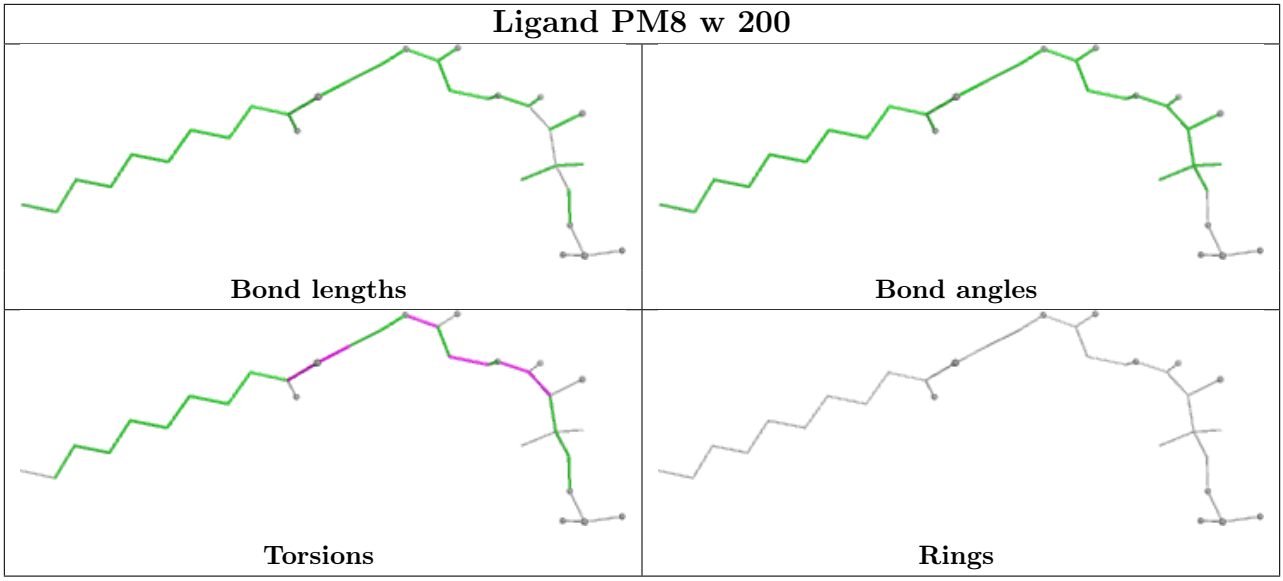
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 GDP t 500



Ligand SAM x 401





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

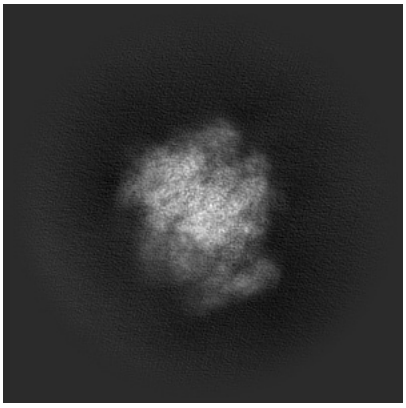
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12847. These allow visual inspection of the internal detail of the map and identification of artifacts.

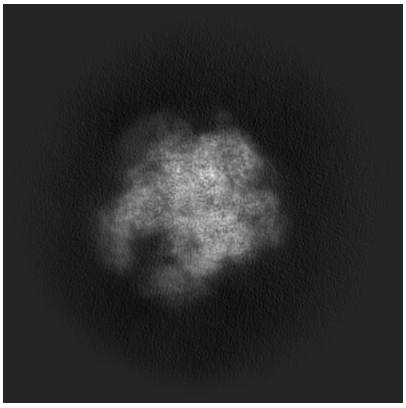
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

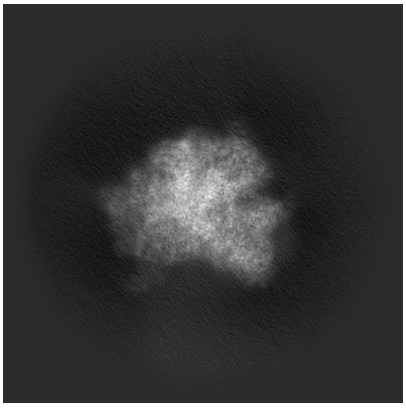
6.1.1 Primary map



X



Y

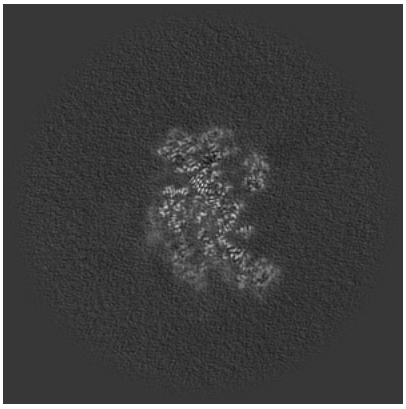


Z

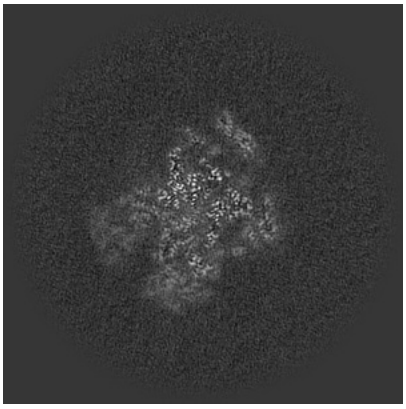
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

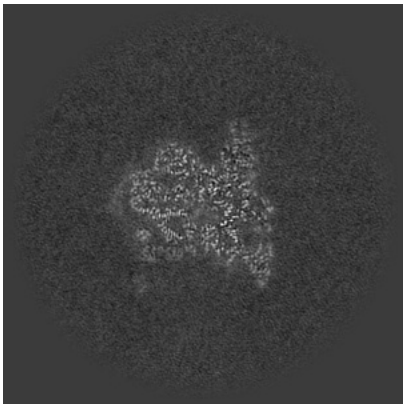
6.2.1 Primary map



X Index: 224



Y Index: 224

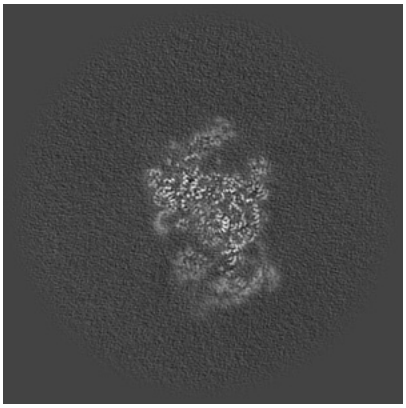


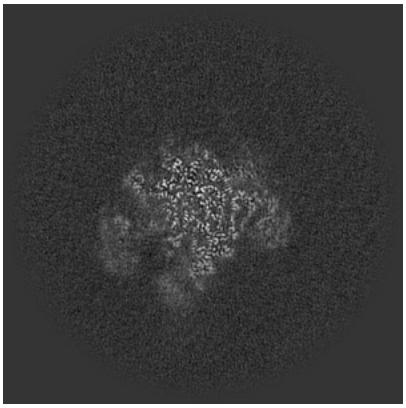
Z Index: 224

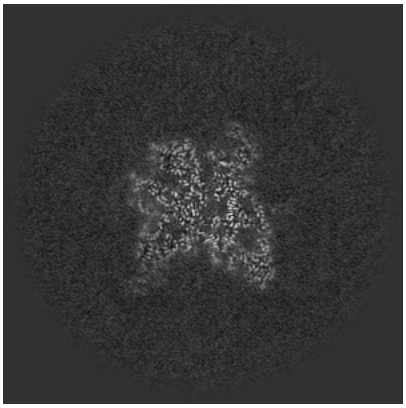
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 206

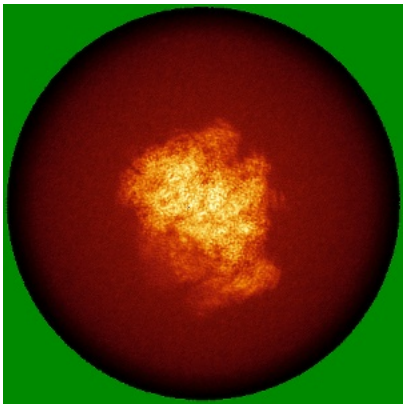

Y Index: 241

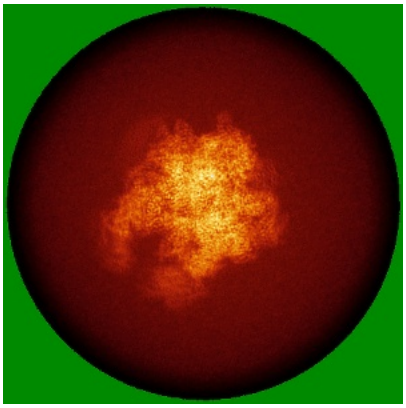

Z Index: 234

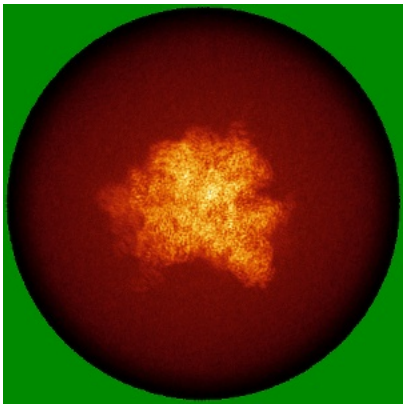
The images above show the largest variance slices of the map in three orthogonal directions.

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

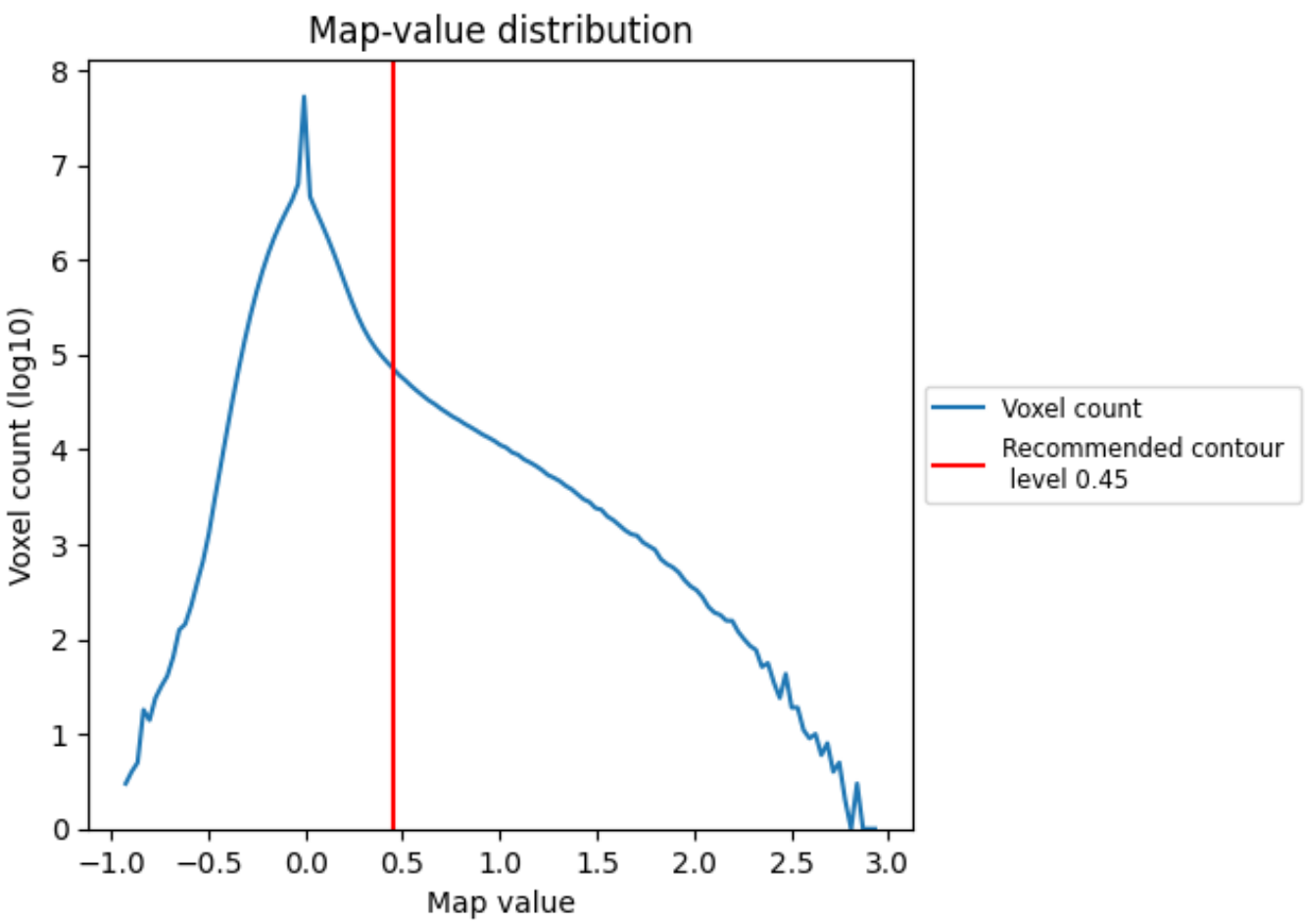
6.6 Mask visualisation (i)

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

7 Map analysis (i)

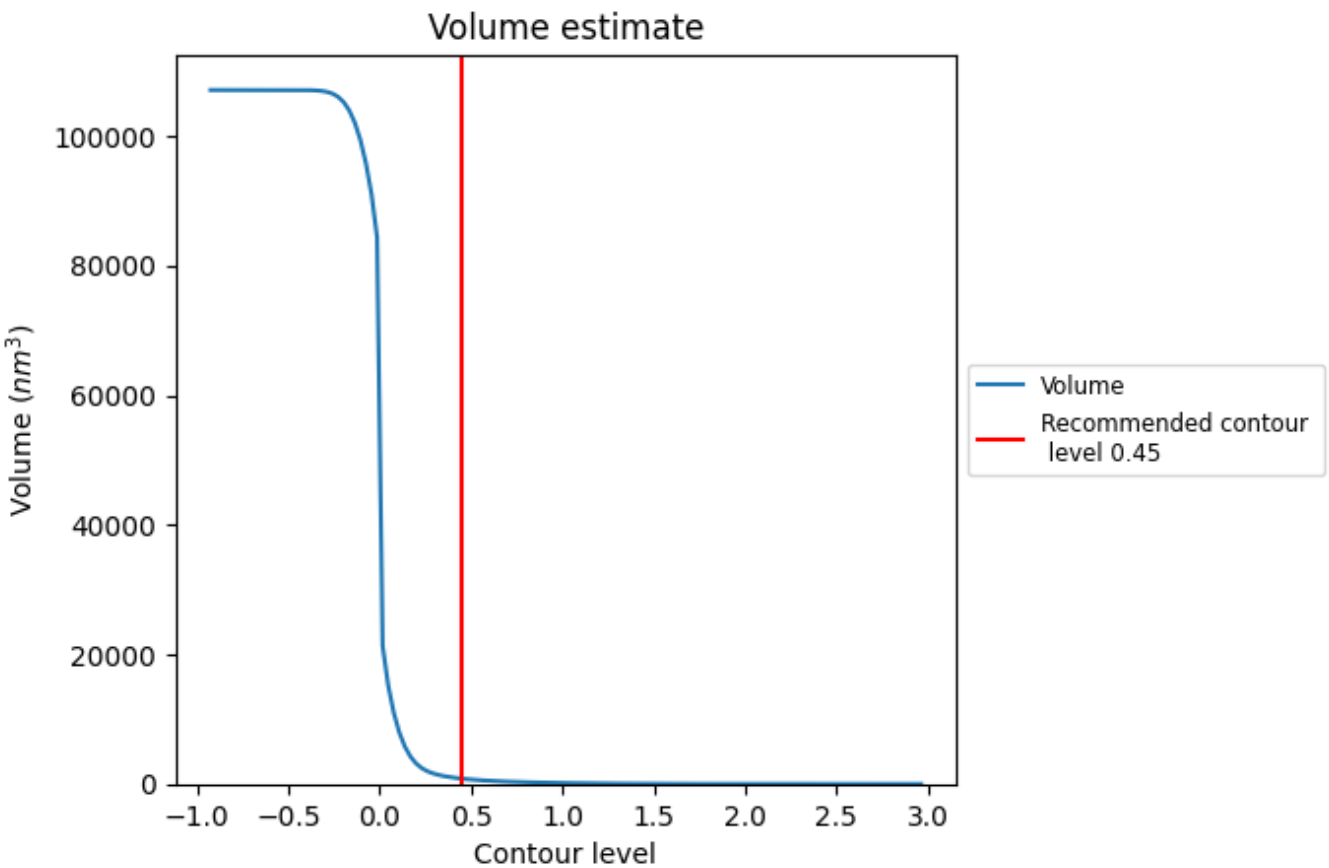
This section contains the results of statistical analysis of the map.

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.

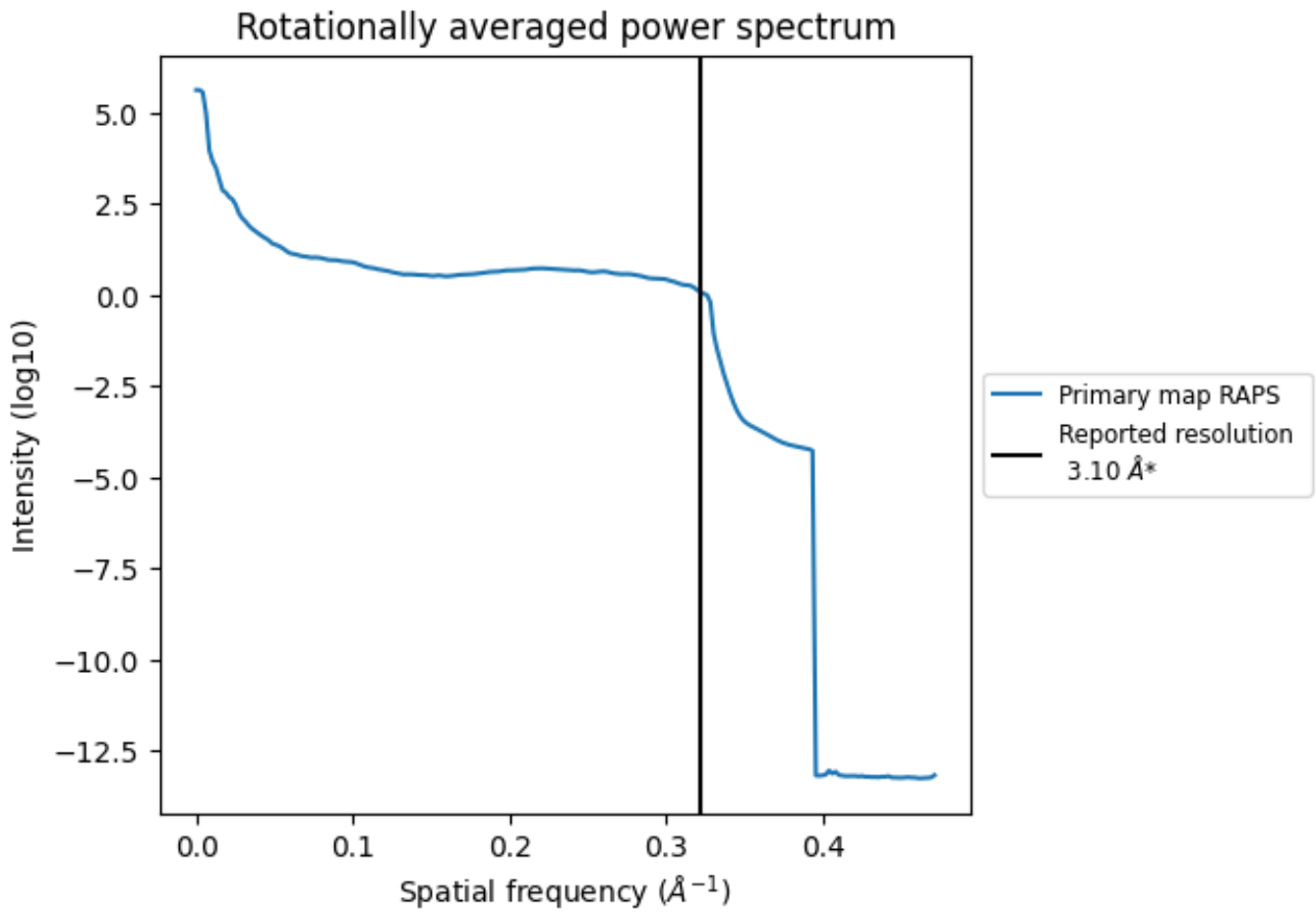
7.2 Volume estimate (i)



The volume at the recommended contour level is 820 nm^3; this corresponds to an approximate mass of 740 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 0.323 Å^{-1}

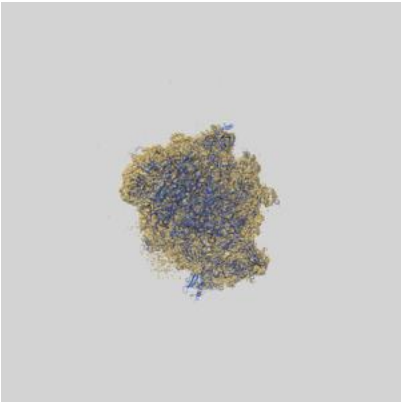
8 Fourier-Shell correlation (i)

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

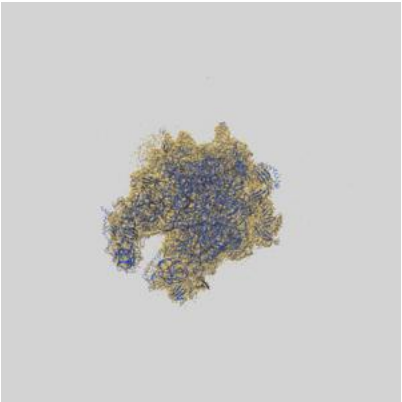
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12847 and PDB model 7ODT. Per-residue inclusion information can be found in section 3 on page 18.

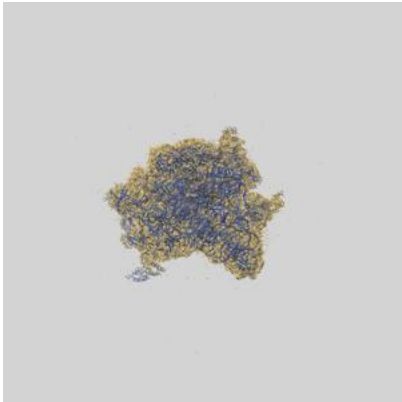
9.1 Map-model overlay (i)



X



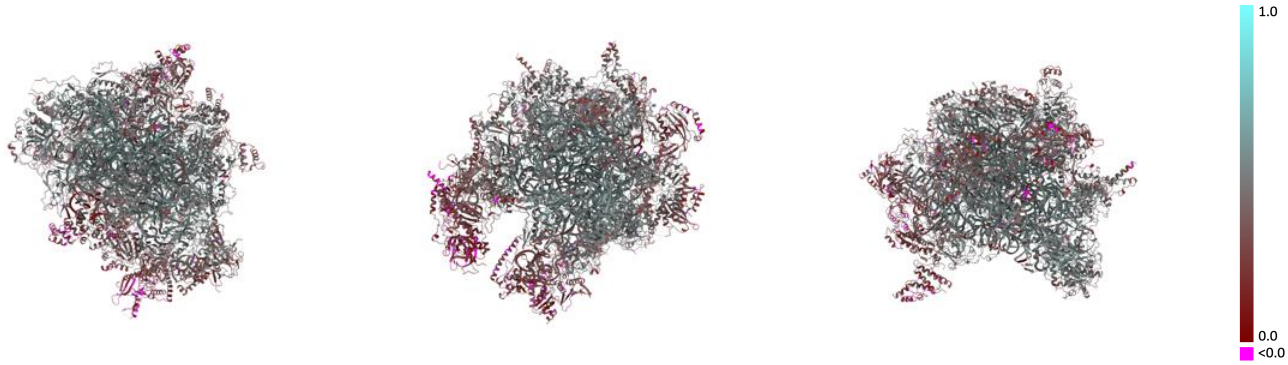
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 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.

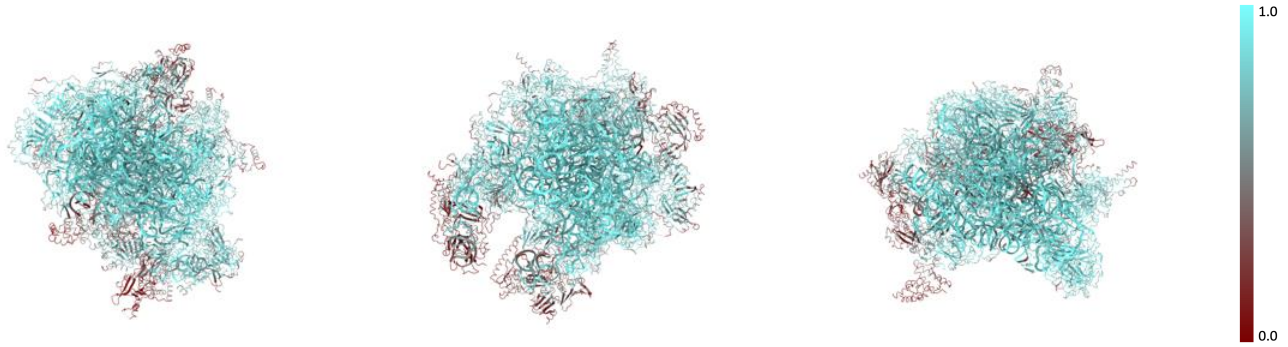
9.2 Q-score mapped to coordinate model (i)



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.

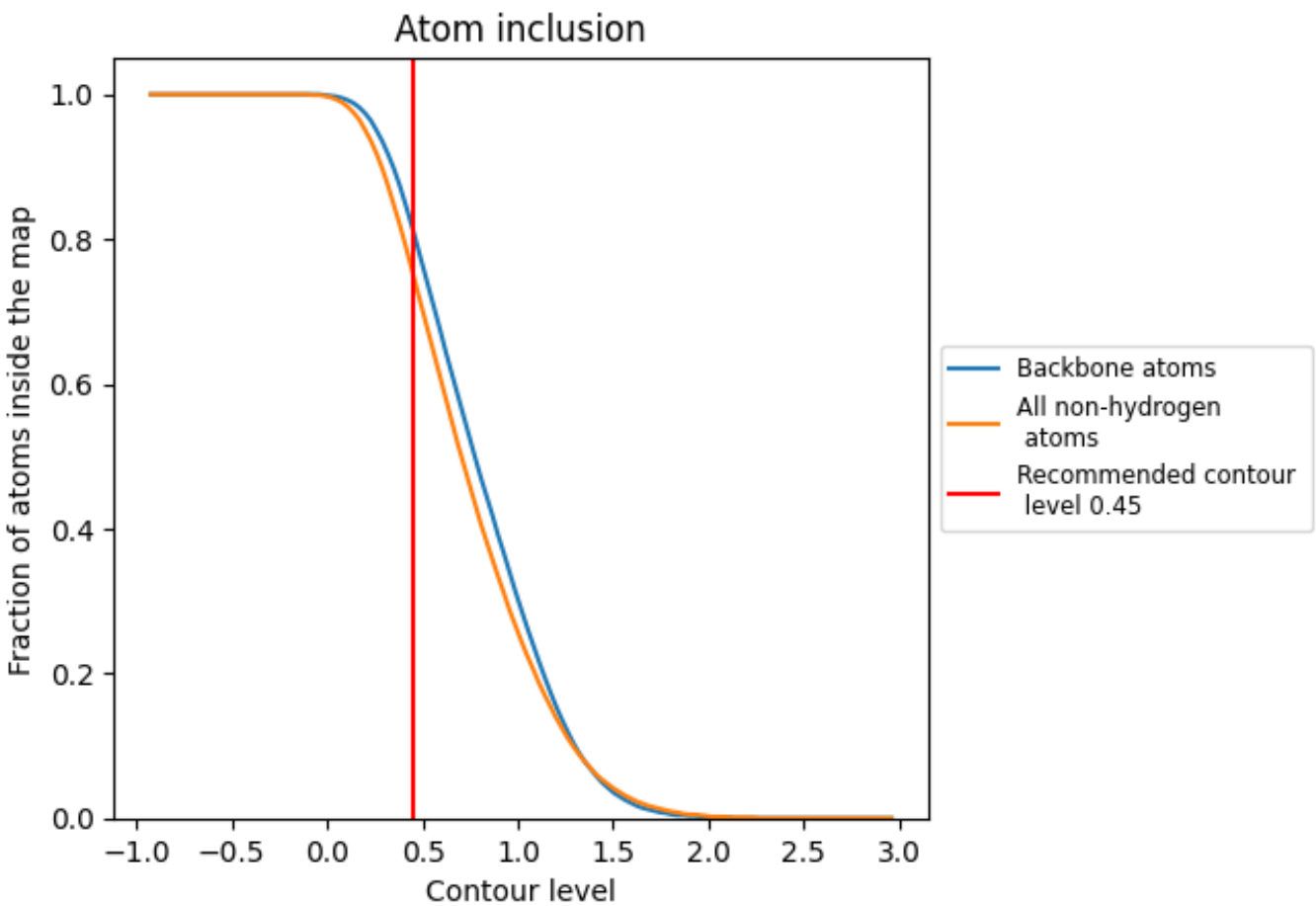
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.45).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 75% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7520	0.4300
0	0.7910	0.4660
1	0.7330	0.4480
2	0.9390	0.5690
3	0.9310	0.5550
4	0.8900	0.4830
5	0.8360	0.4690
6	0.7470	0.3900
7	0.6580	0.3460
8	0.2210	0.2000
9	0.7930	0.4550
A	0.9260	0.5010
B	0.7310	0.2760
D	0.7930	0.4700
E	0.8500	0.4740
F	0.8340	0.4820
H	0.6730	0.4070
I	0.4180	0.2610
J	0.1440	0.1740
K	0.8990	0.5050
L	0.7990	0.4520
M	0.8380	0.4880
N	0.7090	0.4340
O	0.8550	0.4850
P	0.8240	0.4480
Q	0.8190	0.4530
R	0.8990	0.5190
S	0.8660	0.4970
T	0.8380	0.4940
U	0.7390	0.4460
V	0.5050	0.3510
W	0.8760	0.5270
X	0.7790	0.4700
Y	0.8240	0.4740
Z	0.8630	0.5160

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Chain	Atom inclusion	Q-score
a	0.7390	0.4340
b	0.8550	0.4820
c	0.7630	0.4230
d	0.3600	0.2940
e	0.1350	0.1570
f	0.3010	0.2490
g	0.8350	0.4620
h	0.5110	0.3310
i	0.9020	0.5230
j	0.8070	0.4420
k	0.3980	0.2640
l	0.2440	0.2240
m	0.0700	0.1180
o	0.8550	0.5000
p	0.5840	0.3660
q	0.6740	0.3770
r	0.7920	0.4460
s	0.8490	0.4960
t	0.4460	0.2800
u	0.6260	0.3700
v	0.2410	0.2620
w	0.0420	0.1530
x	0.6580	0.3550
y	0.4390	0.2830