



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:01 PM UTC

PDB ID : 7PD3 / pdb_00007pd3
EMDB ID : EMD-13329
Title : Structure of the human mitoribosomal large subunit in complex with NSUN4.MTERF4.GTPBP7 and MALSU1.L0R8F8.mt-ACP
Authors : Chandrasekaran, V.; Desai, N.; Burton, N.O.; Yang, H.; Price, J.; Miska, E.A.; Ramakrishnan, V.
Deposited on : 2021-08-04
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

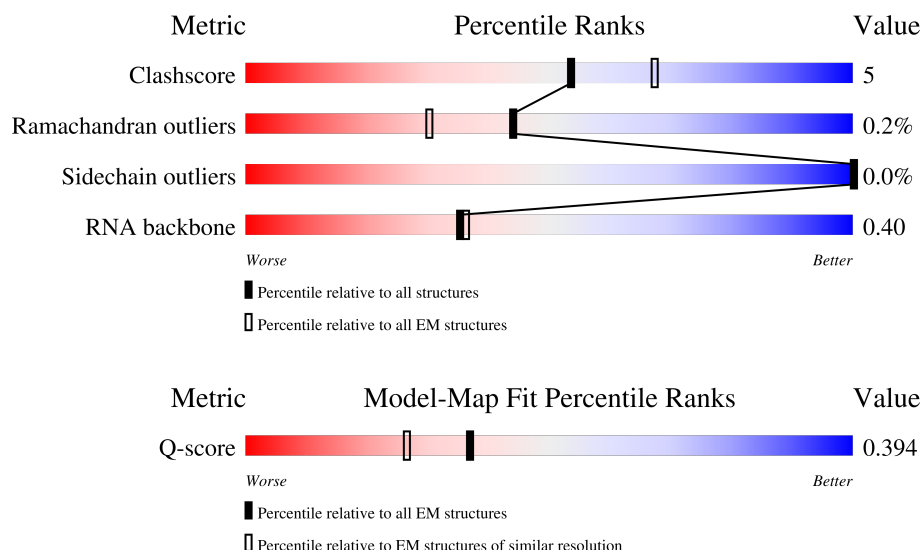
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	0	188	23% 46% 11% 43%
2	1	65	35% 65% 15% 20%
3	2	92	45% 51%

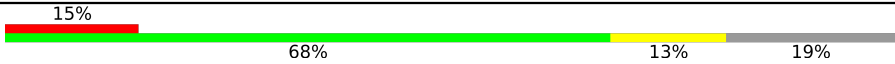
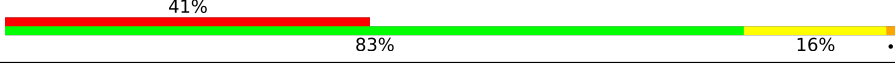
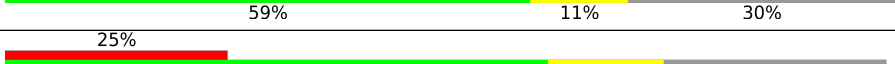
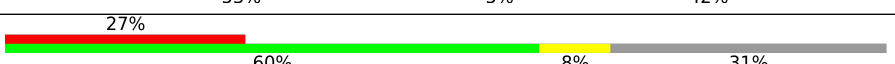
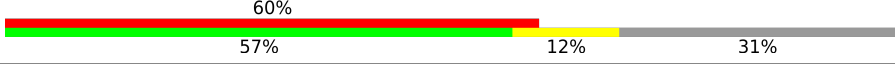
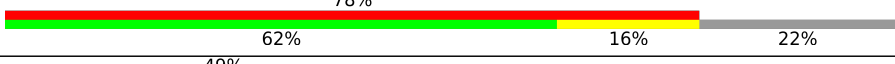
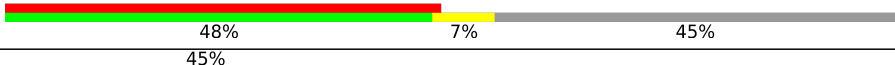
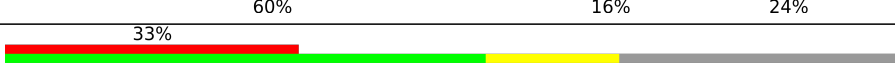
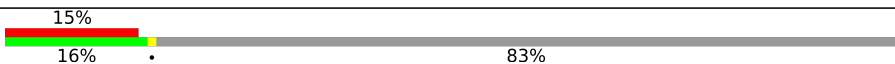
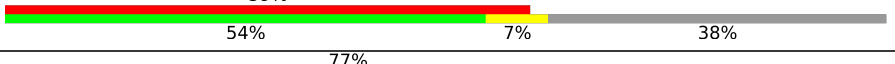
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Mol	Chain	Length	Quality of chain
4	3	188	
5	4	103	
6	5	423	
7	6	380	
8	7	338	
9	8	206	
10	9	137	
11	A	1737	
12	B	69	
13	C	267	
13	H	267	
14	D	305	
15	E	348	
16	F	311	
17	G	261	
18	J	192	
19	K	178	
20	L	145	
21	M	296	
22	N	251	
23	O	175	
24	P	180	
25	Q	292	
26	R	149	
27	S	205	

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Mol	Chain	Length	Quality of chain
28	T	206	
29	U	153	
30	V	216	
31	W	148	
32	X	256	
33	Y	250	
34	Z	161	
35	a	142	
36	b	215	
37	c	332	
38	d	306	
39	e	279	
40	f	212	
41	g	166	
42	h	158	
43	i	128	
44	j	123	
45	k	112	
46	l	138	
47	m	128	
48	o	102	
49	p	206	
50	q	222	
51	r	196	
52	s	439	

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Mol	Chain	Length	Quality of chain
53	t	28	
54	u	234	
55	v	70	
56	w	156	
57	y	381	
58	x	384	
59	z	334	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	OMG	A	2815	X	-	-	-
11	OMG	A	3040	X	-	-	-
63	SAM	x	401	X	-	X	-
64	GCP	z	401	X	-	-	-
64	GCP	z	402	X	-	-	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 108075 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 39S ribosomal protein L32, mitochondrial.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	45	Total	C	N	O	S	0	0
			367	227	81	58	1		

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

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

- Molecule 5 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			333	212	71	47	3		

- Molecule 6 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	392	Total	C	N	O	S	0	0
			3199	2067	558	563	11		

- Molecule 7 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	324	Total	C	N	O	S	0	0
			2640	1694	470	468	8		

- Molecule 8 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	287	Total	C	N	O	S	0	0
			2334	1495	397	425	17		

- Molecule 9 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	94	Total	C	N	O	S	0	0
			759	477	137	143	2		

- Molecule 10 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	117	Total	C	N	O	S	0	0
			947	614	163	168	2		

- Molecule 11 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1458	Total	C	N	O	P	0	0
			30973	13897	5598	10020	1458		

- Molecule 12 is a RNA chain called mt-tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	64	Total	C	N	O	P	0	0
			1348	607	237	441	63		

- Molecule 13 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	80	Total	C	N	O	S	0	0
			648	421	111	112	4		
13	H	95	Total	C	N	O		0	0
			784	498	152	134			

- Molecule 14 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	217	Total	C	N	O	S	0	0
			1692	1046	344	294	8		

- Molecule 15 is a protein called 39S ribosomal protein L3, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 17 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	165	Total	C	N	O	S	0	0
			1338	863	242	223	10		

- Molecule 18 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 19 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	200	Total	C	N	O	S	0	0
			1617	1035	298	275	9		

- Molecule 23 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 25 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 26 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 28 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 29 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	152	Total	C	N	O	S	0	0
			1218	772	233	210	3		

- Molecule 30 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	202	Total	C	N	O	S	0	0
			1624	1032	291	293	8		

- Molecule 31 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 32 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 33 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L30, mitochondrial.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	198	Total	C	N	O	S	0	0
			1625	1006	317	297	5		

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

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

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

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

- Molecule 53 is a protein called mL65.

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

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

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

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

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

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

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

- Molecule 57 is a protein called Transcription termination factor 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	245	Total	C	N	O	S	0	0
			1989	1269	344	364	12		

- Molecule 58 is a protein called 5-methylcytosine rRNA methyltransferase NSUN4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	x	366	Total	C	N	O	S	0	0
			2889	1834	511	527	17		

- Molecule 59 is a protein called Mitochondrial ribosome-associated GTPase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	z	311	Total	C	N	O	S	0	0
			2443	1549	445	433	16		

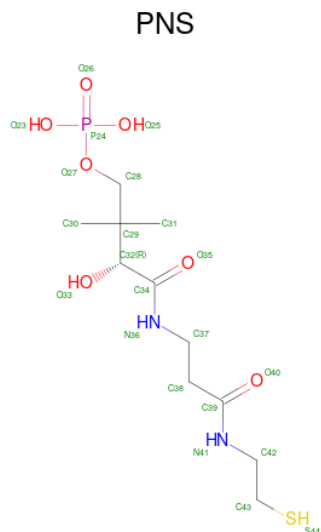
- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

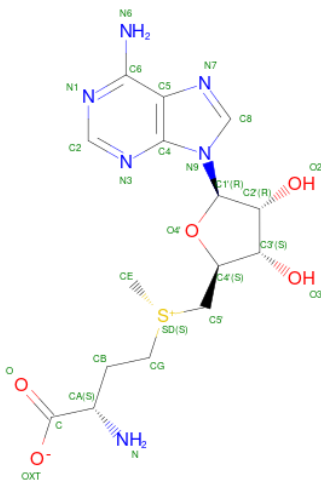
Mol	Chain	Residues	Atoms		AltConf
61	A	89	Total	Mg	0
			89	89	
61	E	1	Total	Mg	0
			1	1	
61	o	1	Total	Mg	0
			1	1	

- Molecule 62 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C₁₁H₂₃N₂O₇PS).



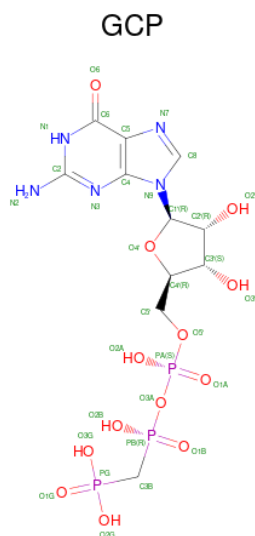
Mol	Chain	Residues	Atoms					AltConf	
62	v	1	Total 21	C 11	N 2	O 6	P 1	S 1	0

- Molecule 63 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).

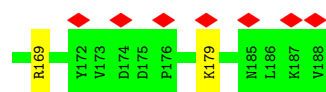


Mol	Chain	Residues	Atoms					AltConf
63	x	1	Total 27	C 15	N 6	O 5	S 1	0

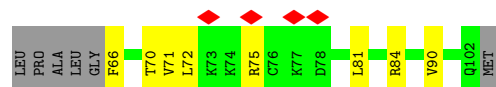
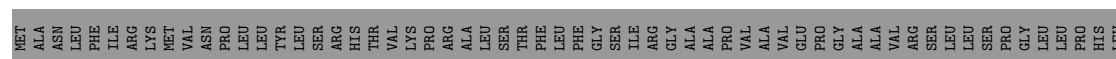
- Molecule 64 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



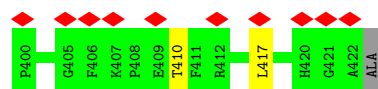
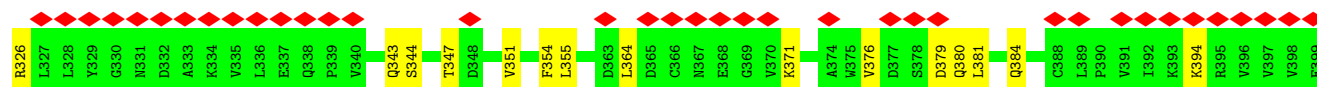
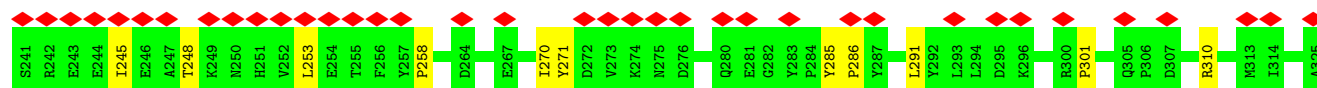
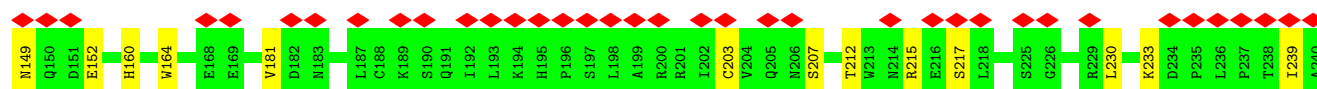
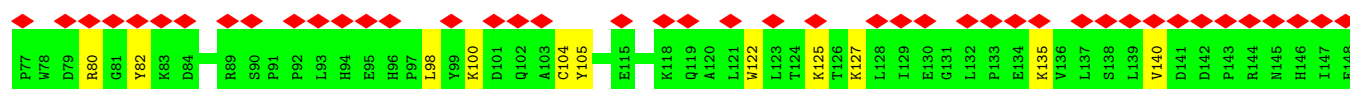
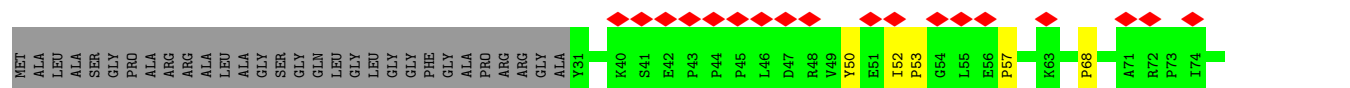
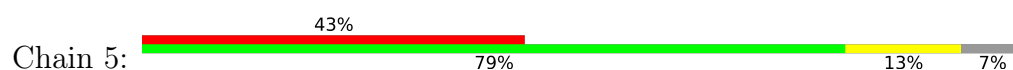
Mol	Chain	Residues	Atoms					AltConf
64	z	1	Total 32	C 11	N 5	O 13	P 3	0
64	z	1	Total 32	C 11	N 5	O 13	P 3	0



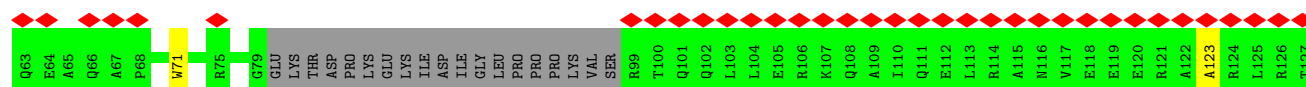
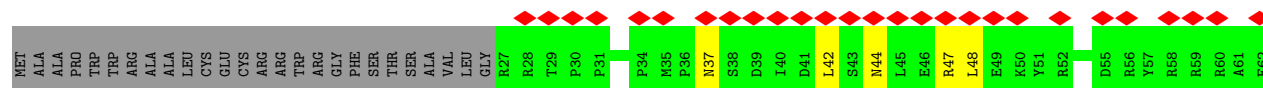
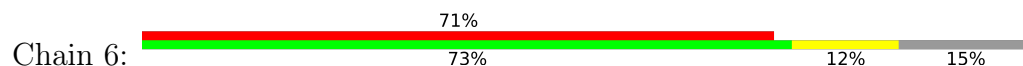
- Molecule 5: 39S ribosomal protein L36, mitochondrial

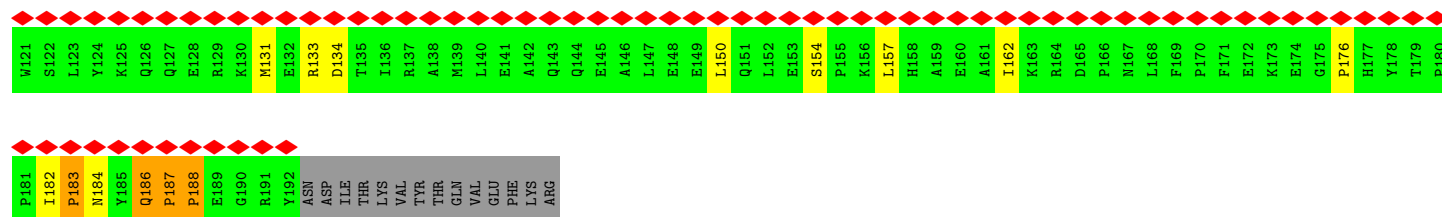


- Molecule 6: 39S ribosomal protein L37, mitochondrial

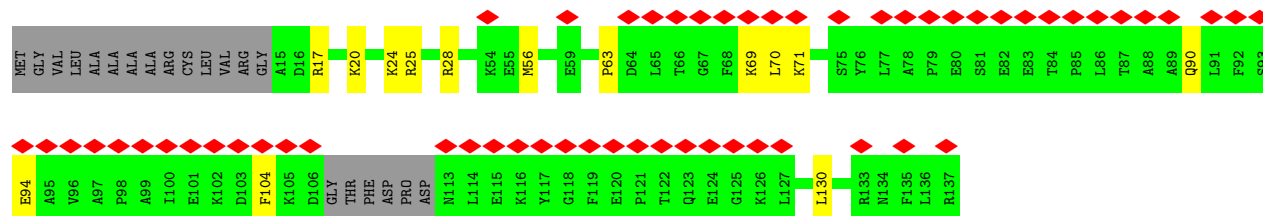
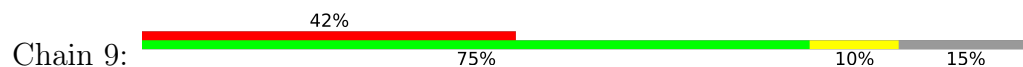


- Molecule 7: 39S ribosomal protein L38, mitochondrial

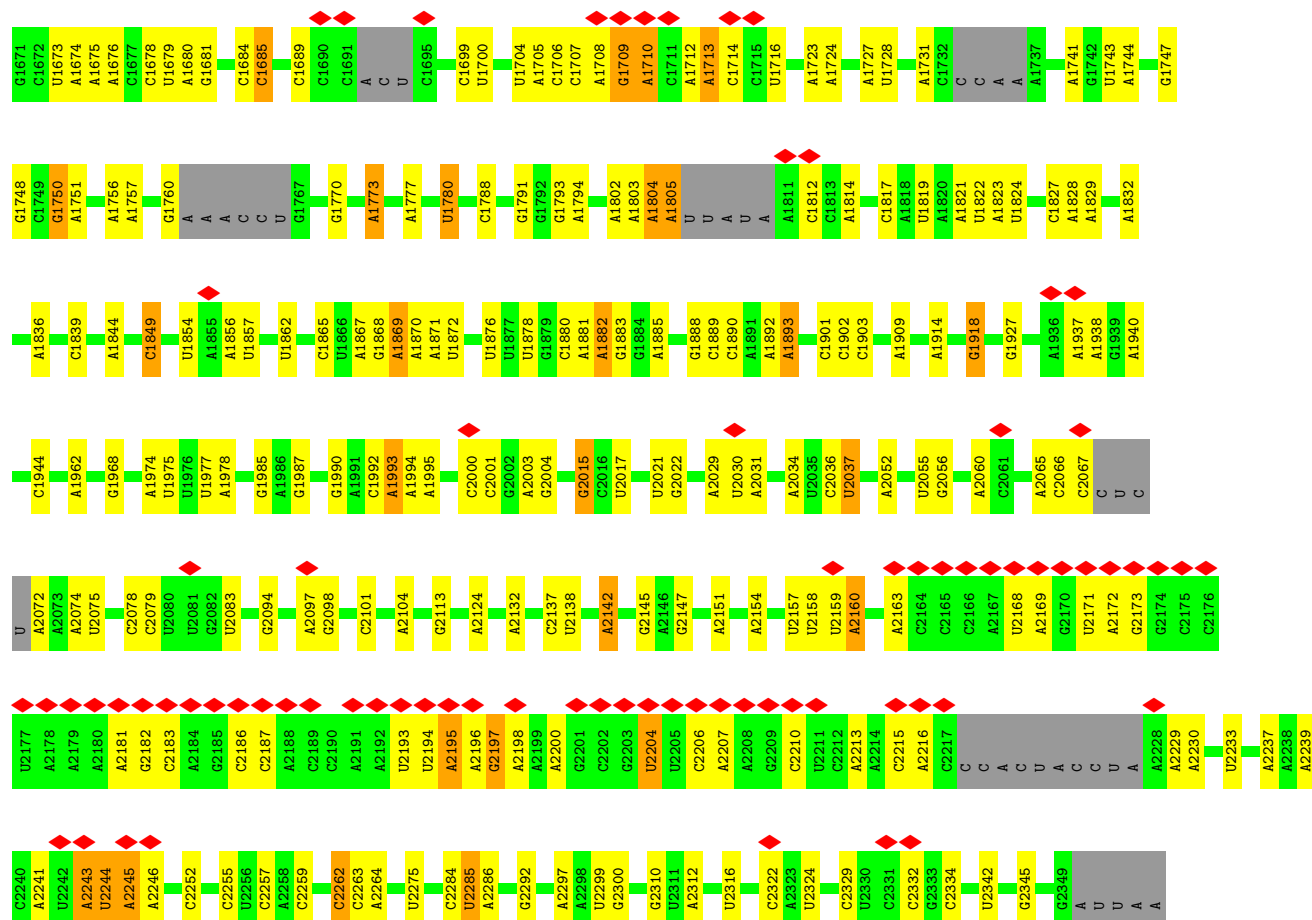




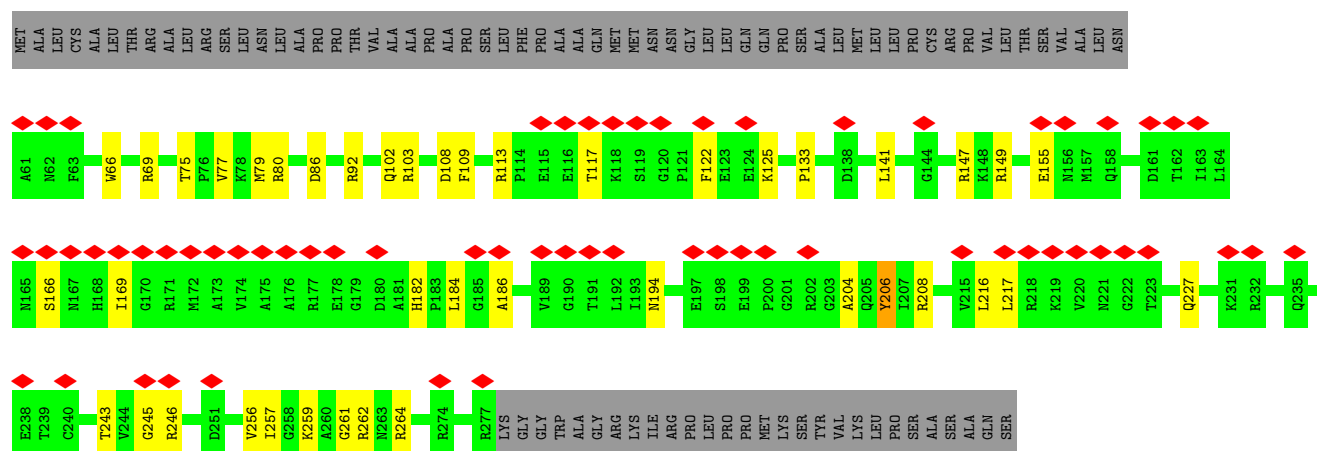
- Molecule 10: 39S ribosomal protein L41, mitochondrial



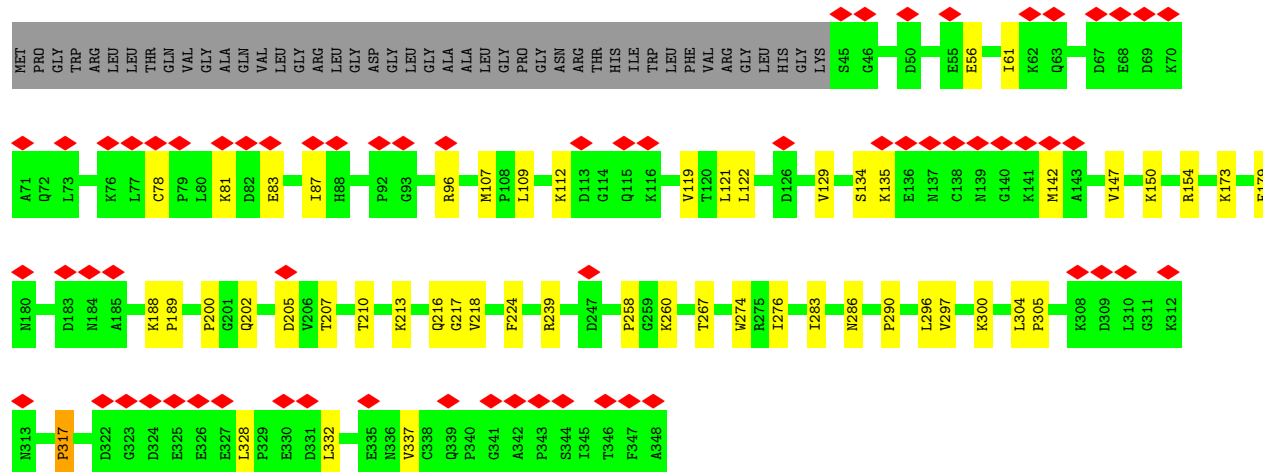
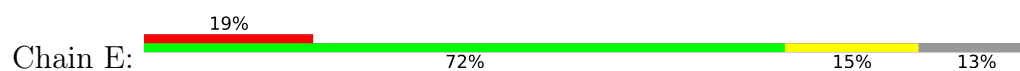
- Molecule 11: 16S rRNA



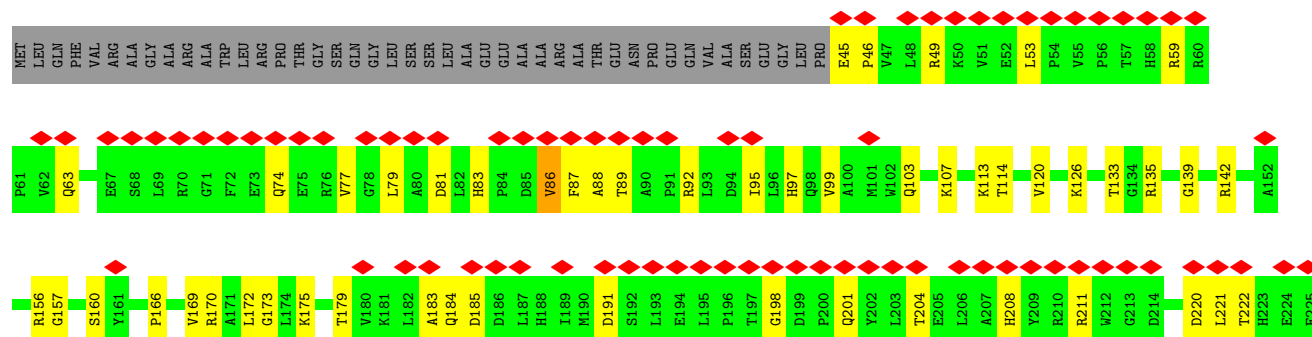


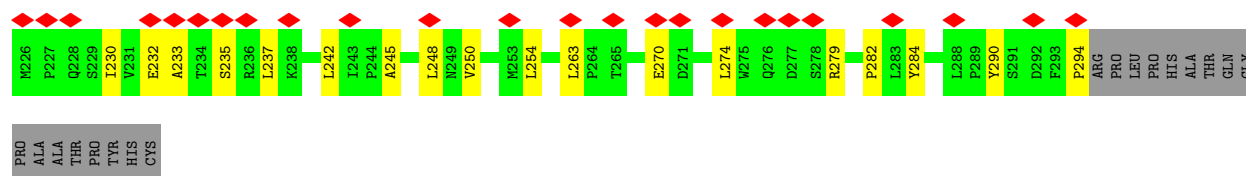


• Molecule 15: 39S ribosomal protein L3, mitochondrial

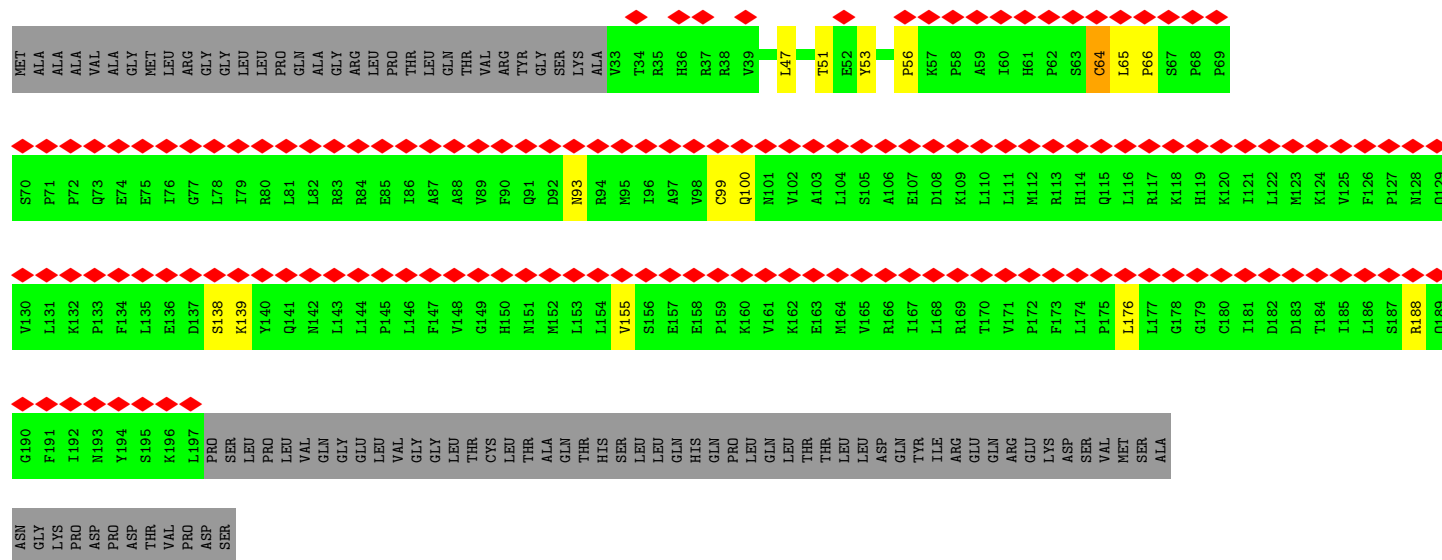


• Molecule 16: 39S ribosomal protein L4, mitochondrial

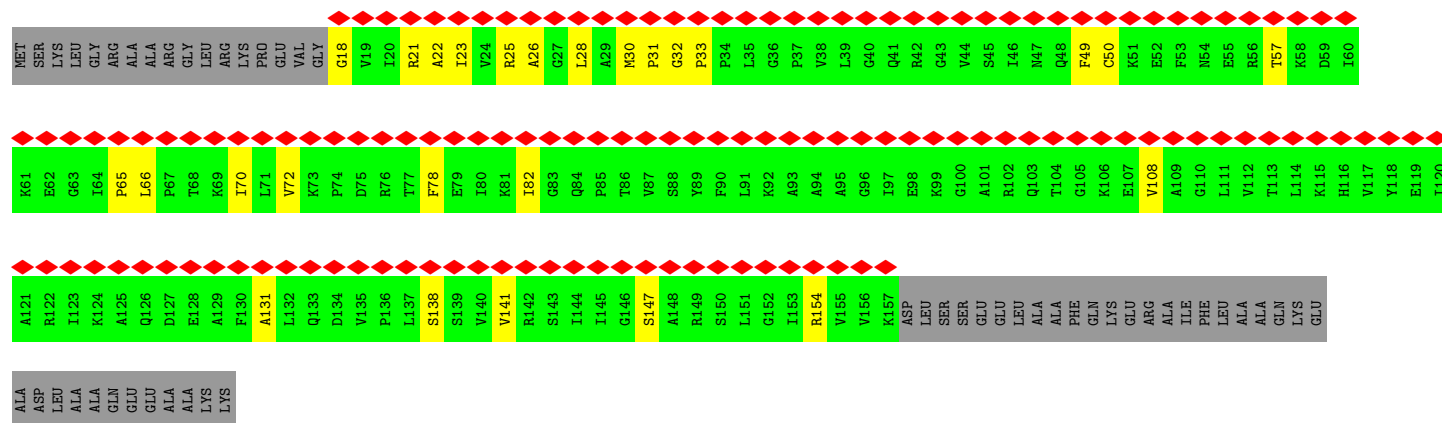
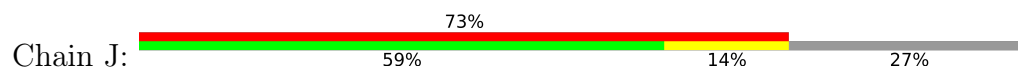




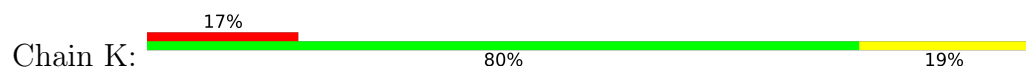
- Molecule 17: 39S ribosomal protein L10, mitochondrial

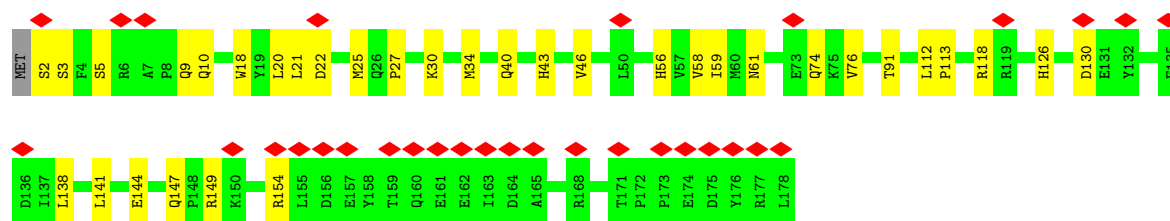


- Molecule 18: 39S ribosomal protein L11, mitochondrial

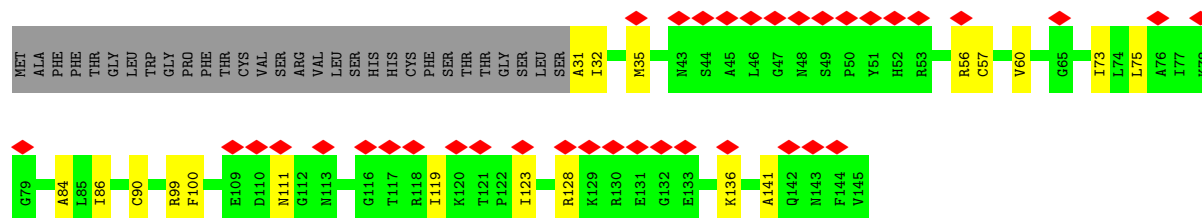


- Molecule 19: 39S ribosomal protein L13, mitochondrial

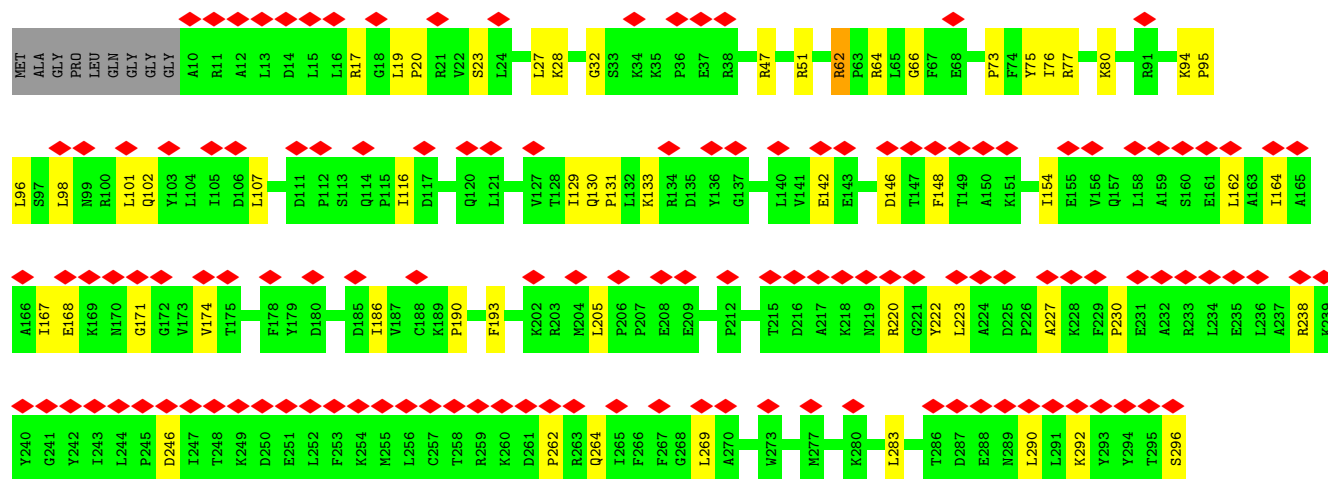
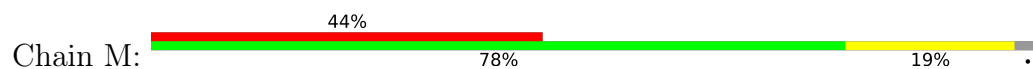




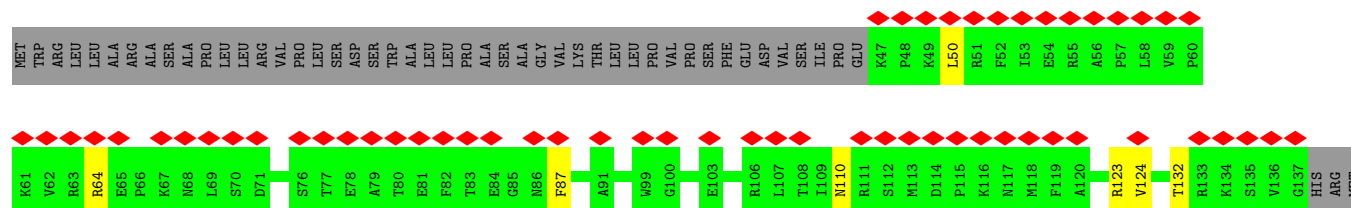
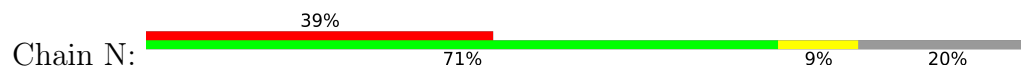
- Molecule 20: 39S ribosomal protein L14, mitochondrial

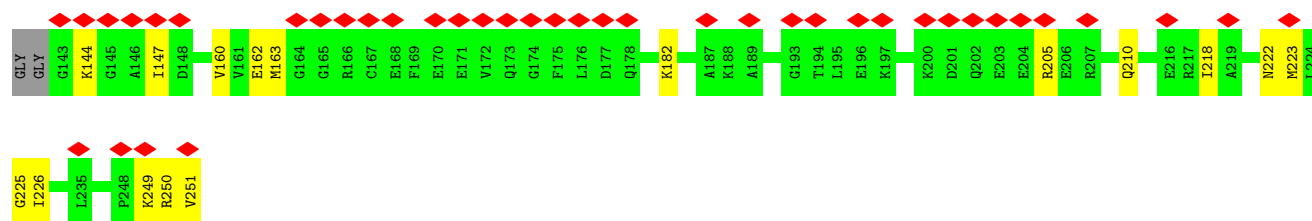


- Molecule 21: 39S ribosomal protein L15, mitochondrial

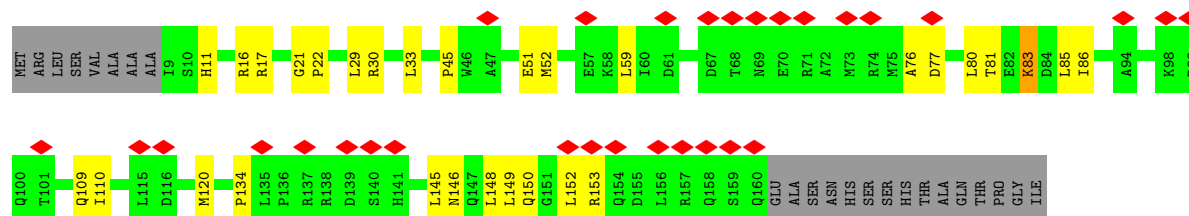


- Molecule 22: 39S ribosomal protein L16, mitochondrial

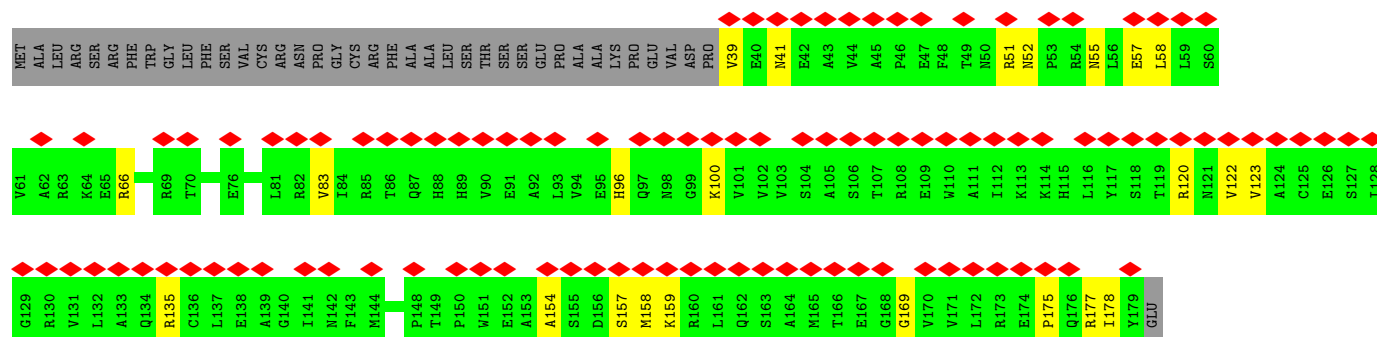




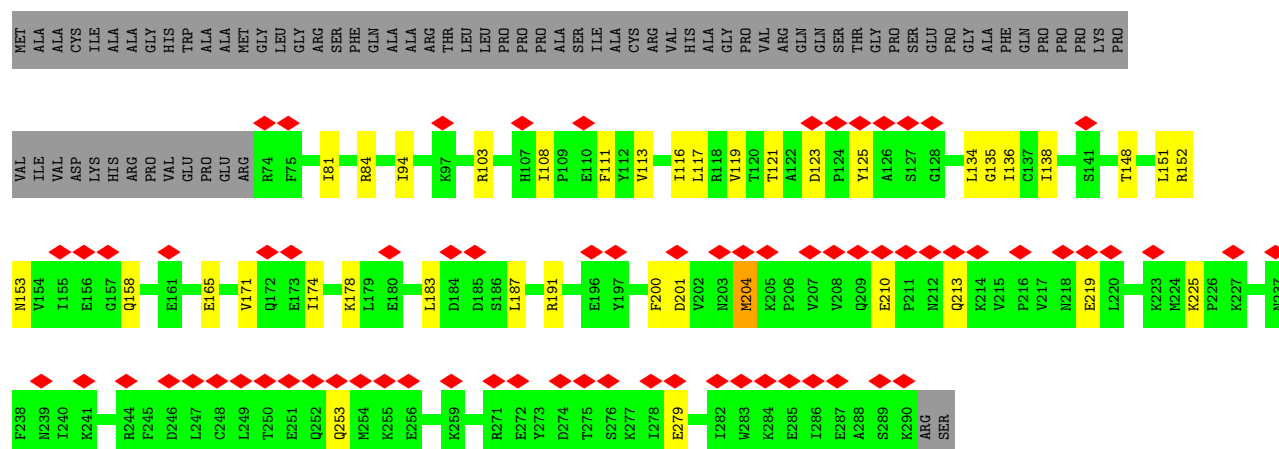
- Molecule 23: 39S ribosomal protein L17, mitochondrial



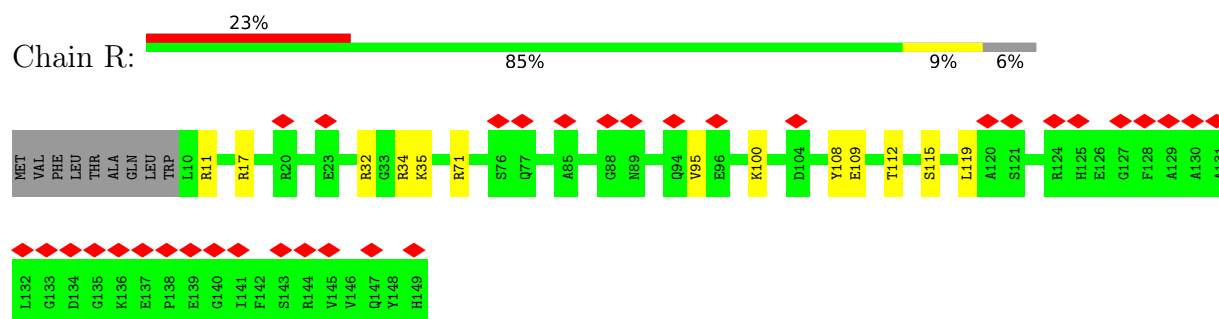
- Molecule 24: 39S ribosomal protein L18, mitochondrial



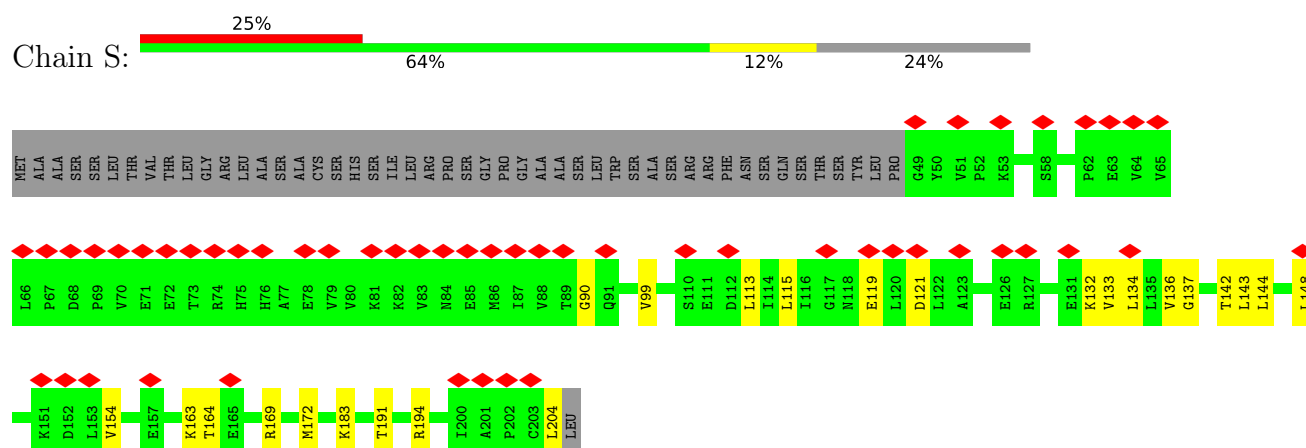
- Molecule 25: 39S ribosomal protein L19, mitochondrial



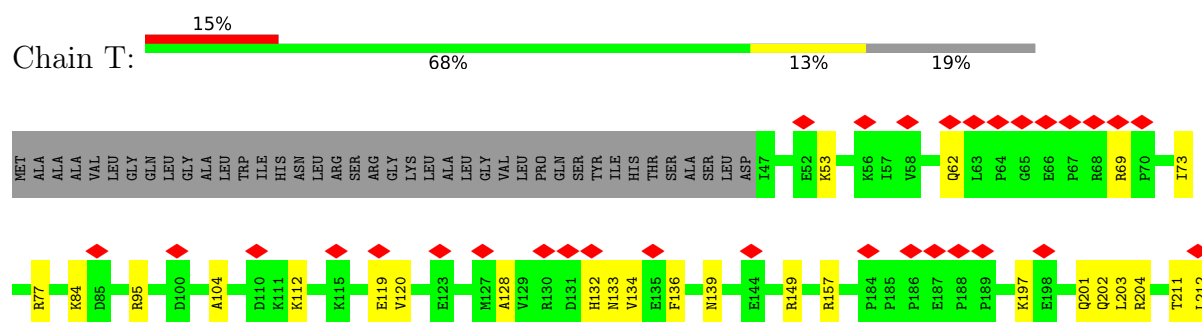
- Molecule 26: 39S ribosomal protein L20, mitochondrial



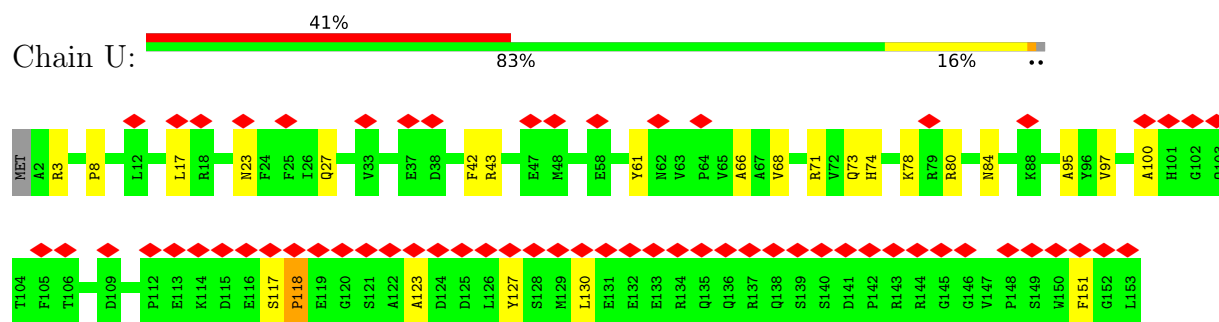
- Molecule 27: 39S ribosomal protein L21, mitochondrial



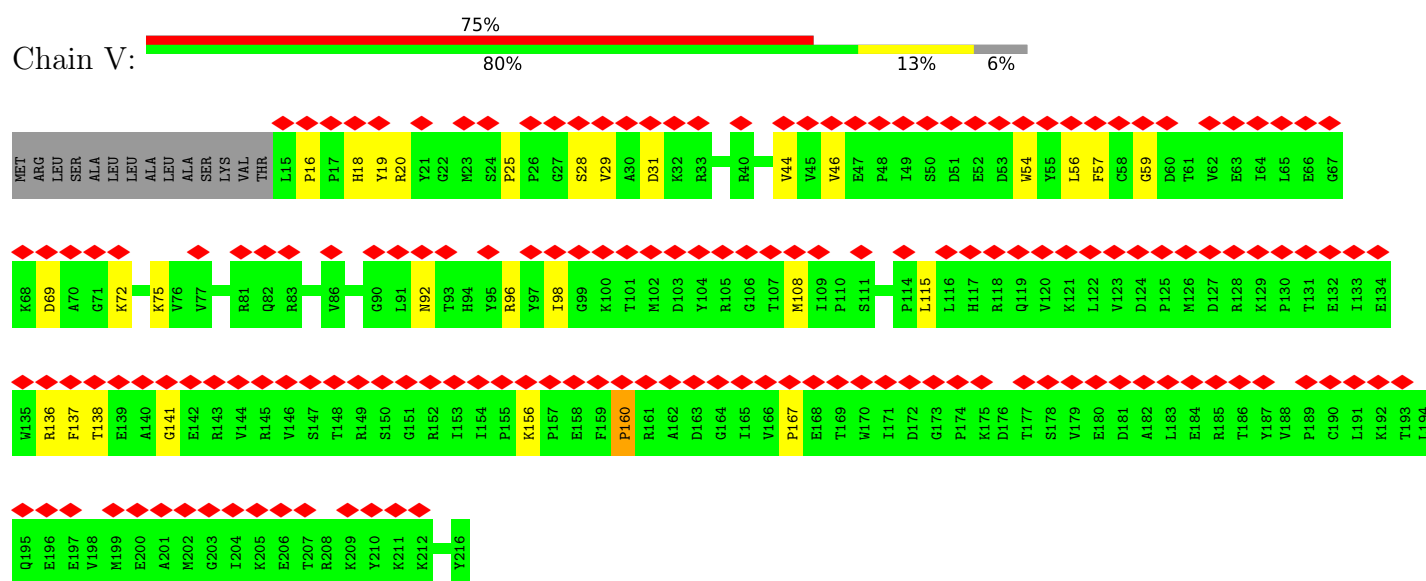
- Molecule 28: 39S ribosomal protein L22, mitochondrial



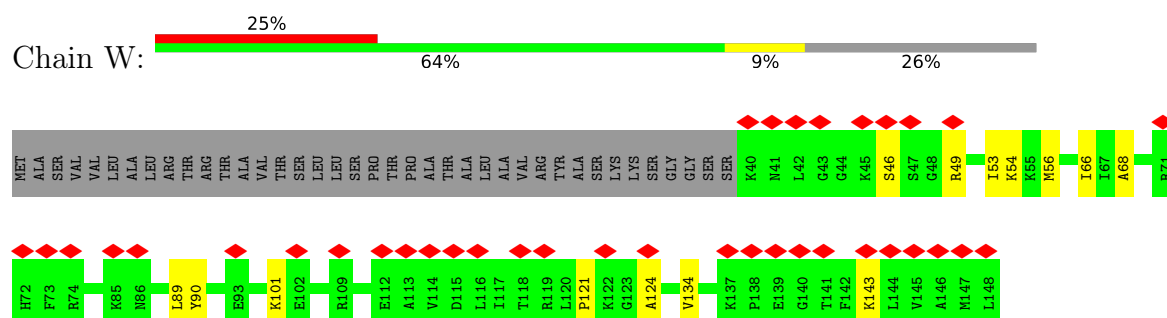
- Molecule 29: 39S ribosomal protein L23, mitochondrial



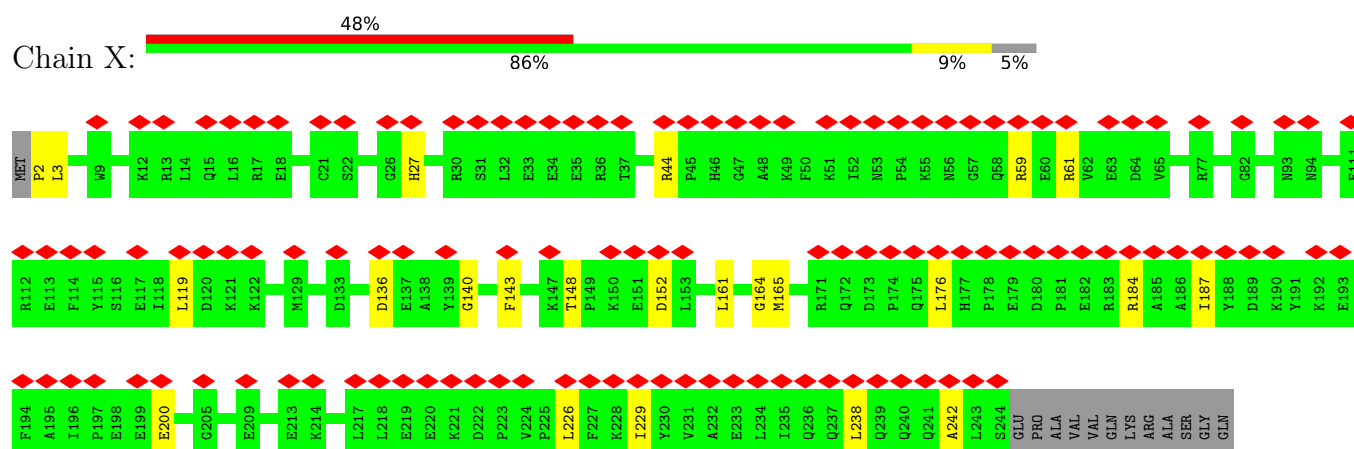
- Molecule 30: 39S ribosomal protein L24, mitochondrial



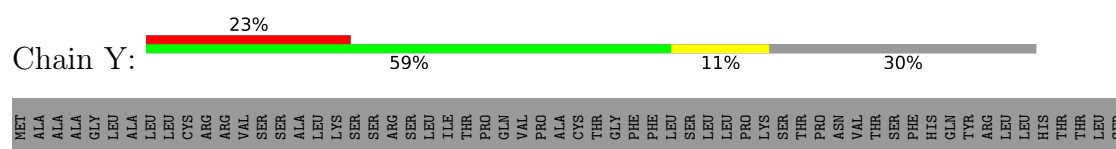
- Molecule 31: 39S ribosomal protein L27, mitochondrial

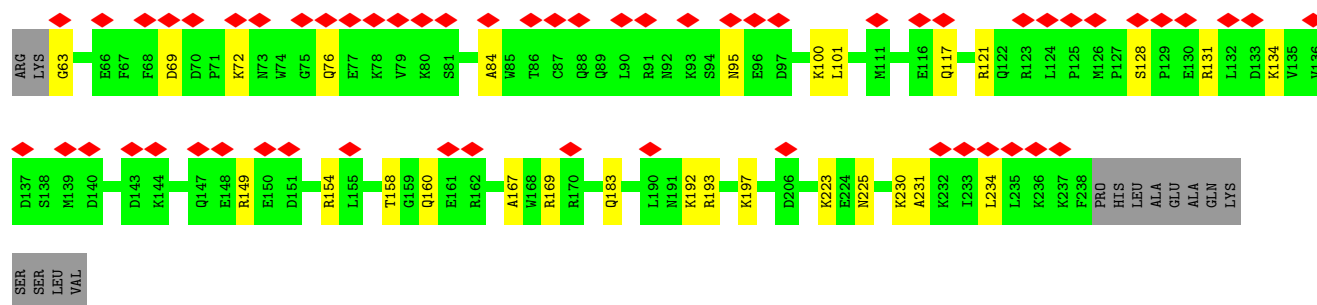


- Molecule 32: 39S ribosomal protein L28, mitochondrial

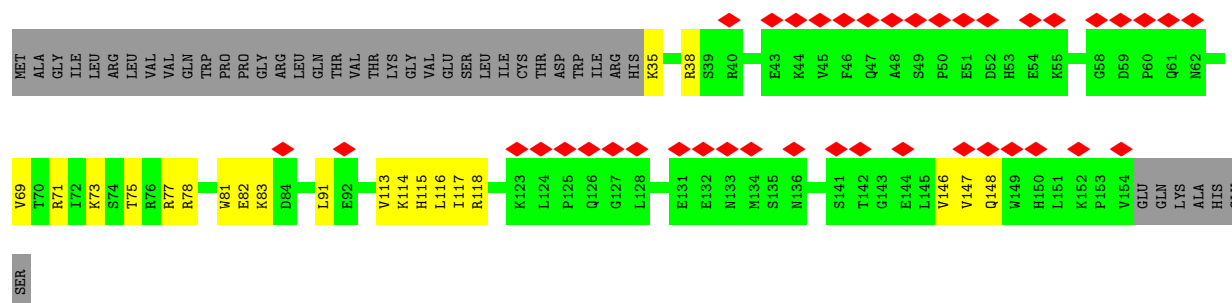


- Molecule 33: 39S ribosomal protein L47, mitochondrial

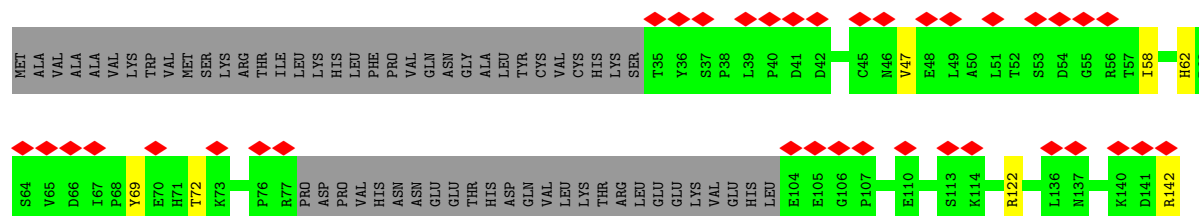




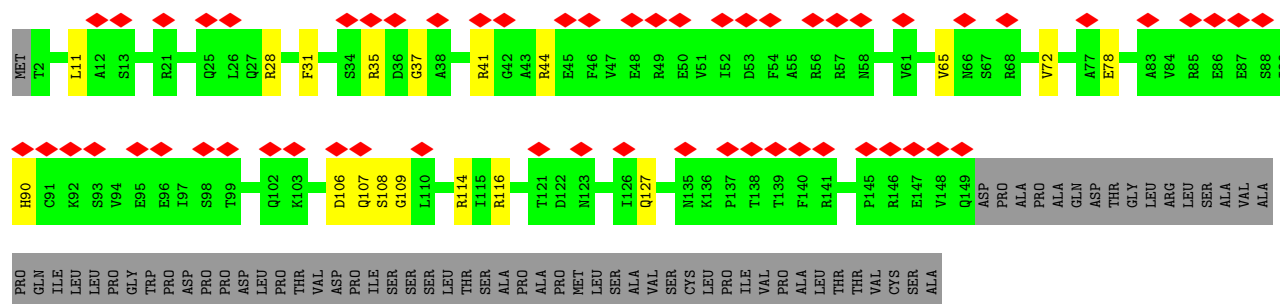
- Molecule 34: 39S ribosomal protein L30, mitochondrial



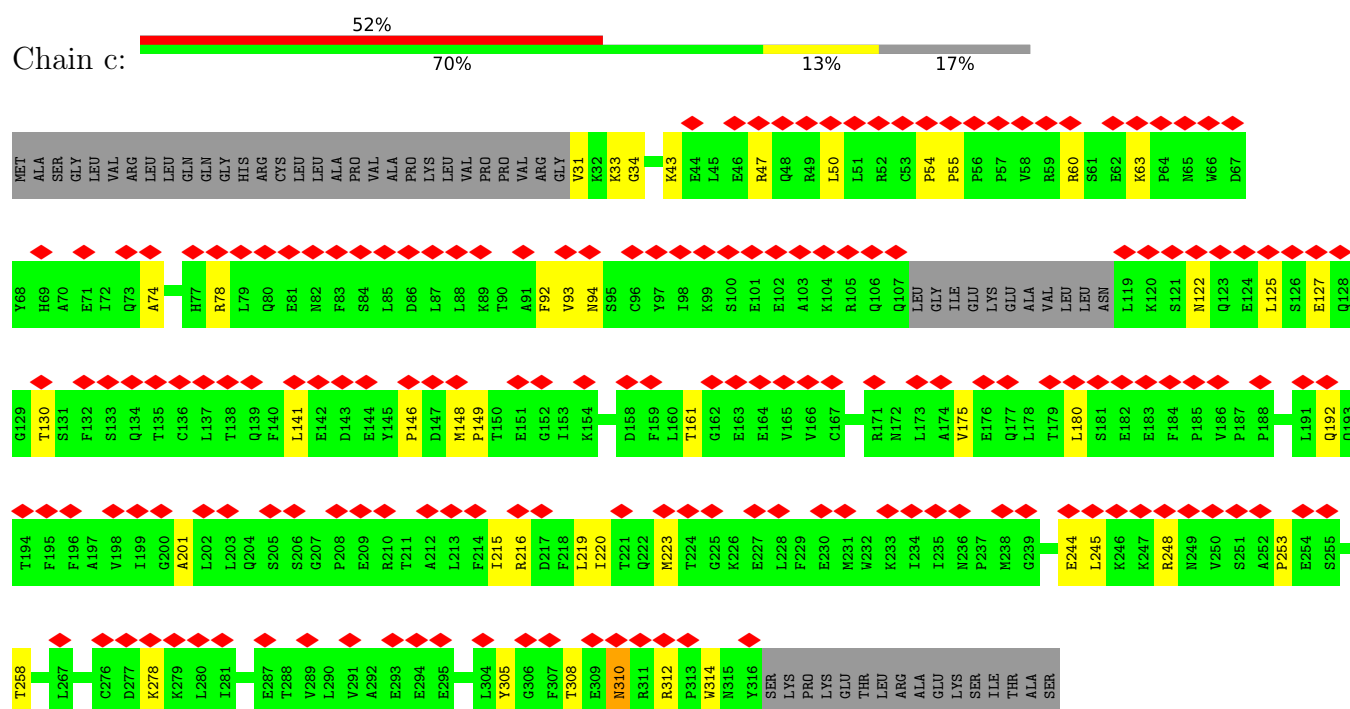
- Molecule 35: 39S ribosomal protein L42, mitochondrial



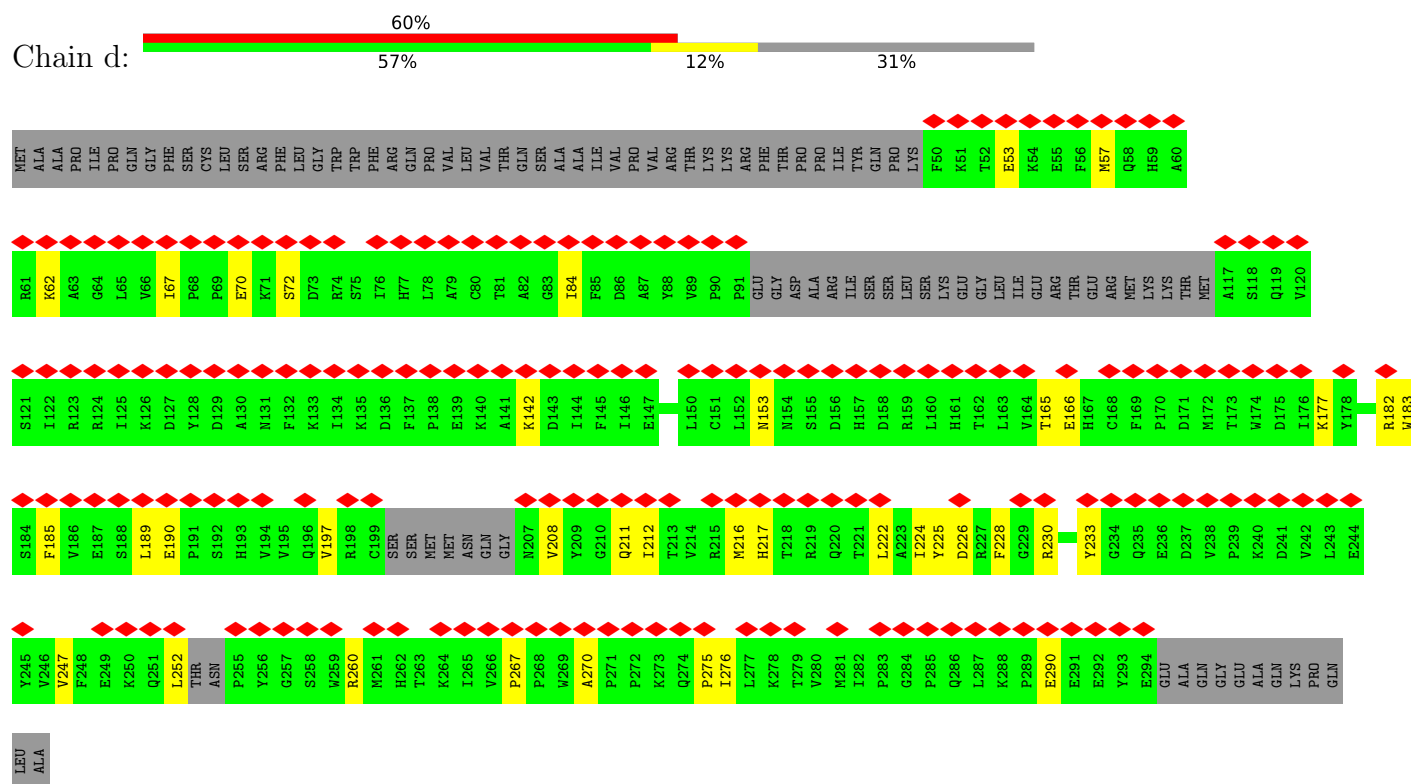
- Molecule 36: 39S ribosomal protein L43, mitochondrial



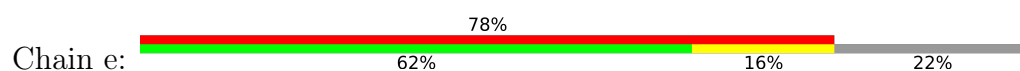
- Molecule 37: 39S ribosomal protein L44, mitochondrial

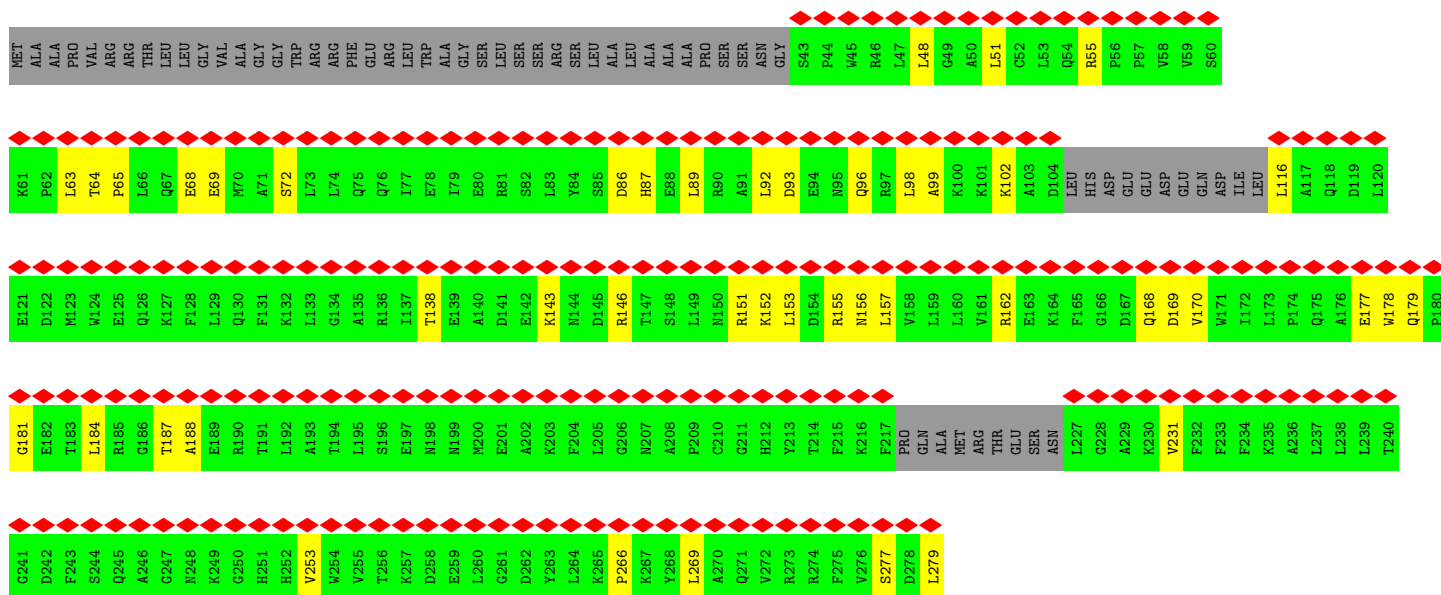


• Molecule 38: 39S ribosomal protein L45, mitochondrial



• Molecule 39: 39S ribosomal protein L46, mitochondrial

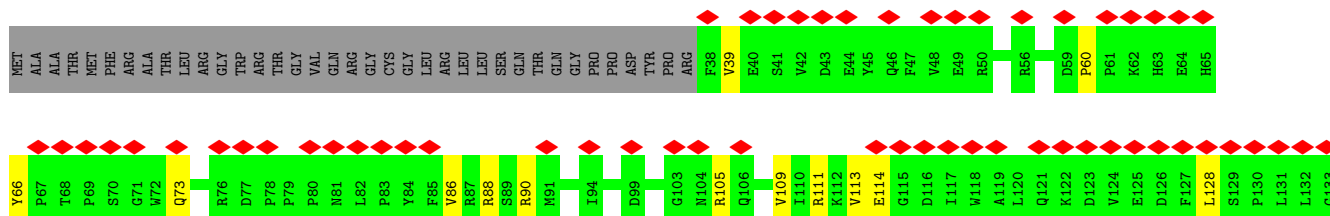
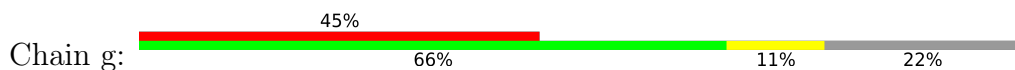




- Molecule 40: 39S ribosomal protein L48, mitochondrial

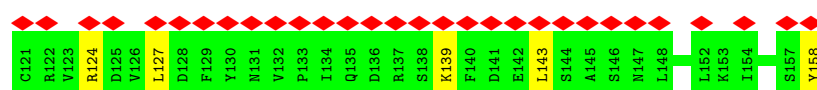
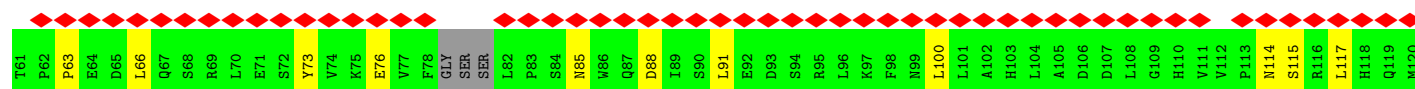
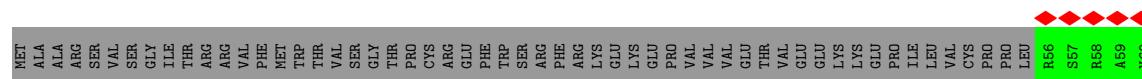


- Molecule 41: 39S ribosomal protein L49, mitochondrial

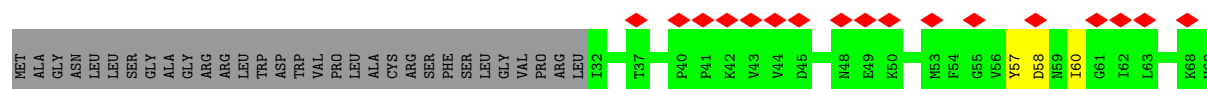




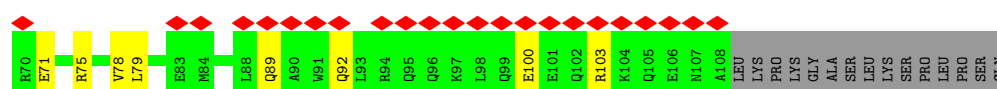
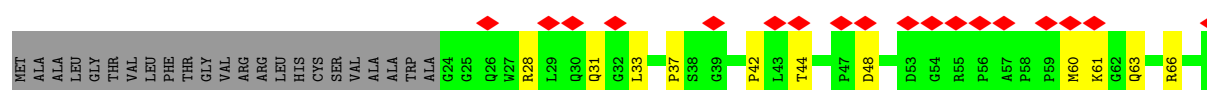
- Molecule 42: 39S ribosomal protein L50, mitochondrial



- Molecule 43: 39S ribosomal protein L51, mitochondrial

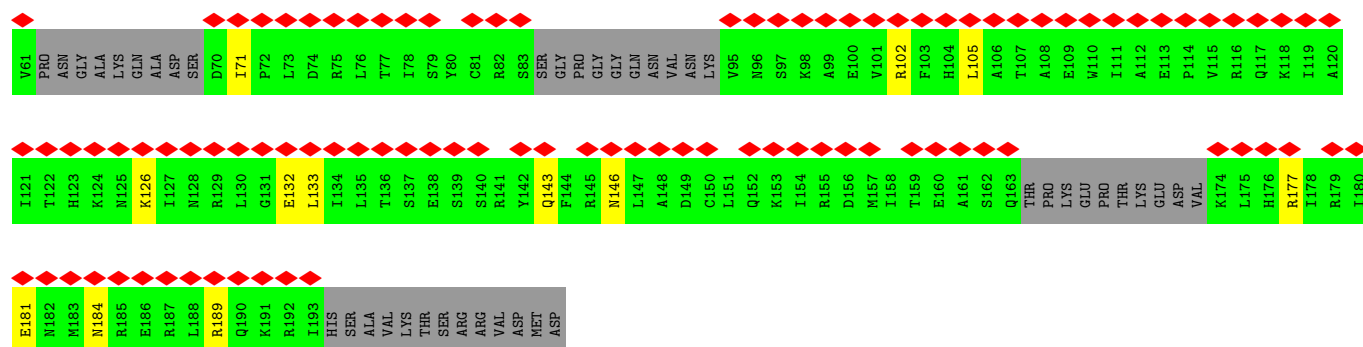


- Molecule 44: 39S ribosomal protein L52, mitochondrial

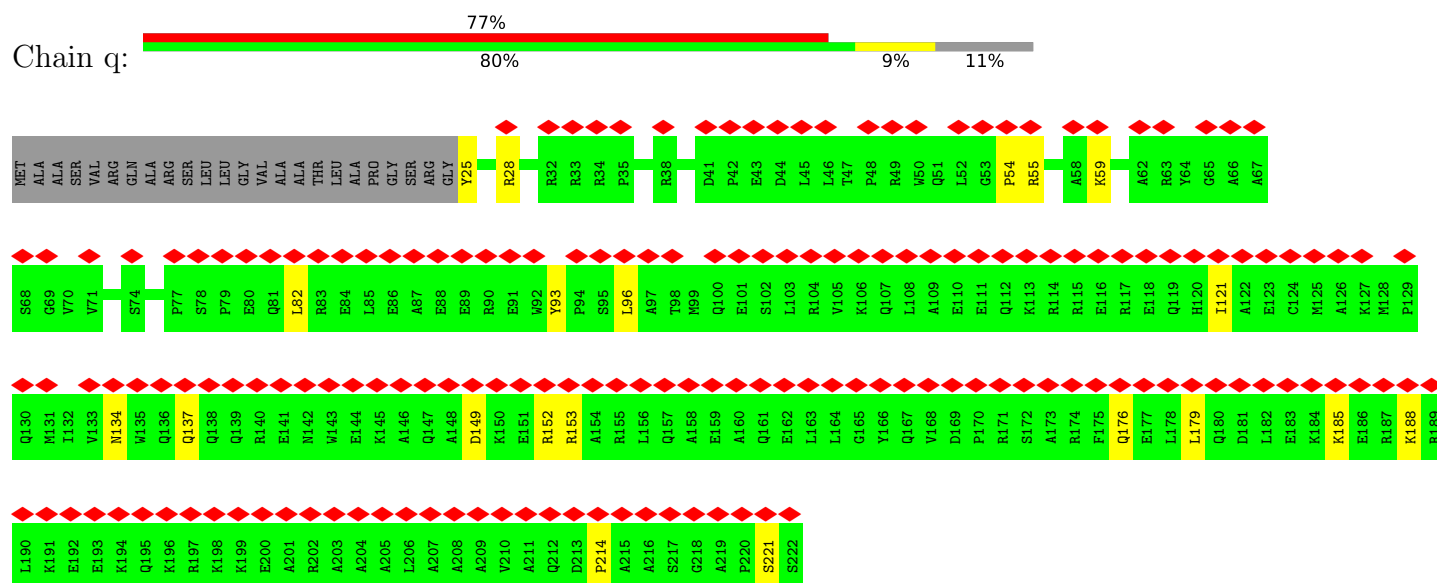


- Molecule 45: 39S ribosomal protein L53, mitochondrial

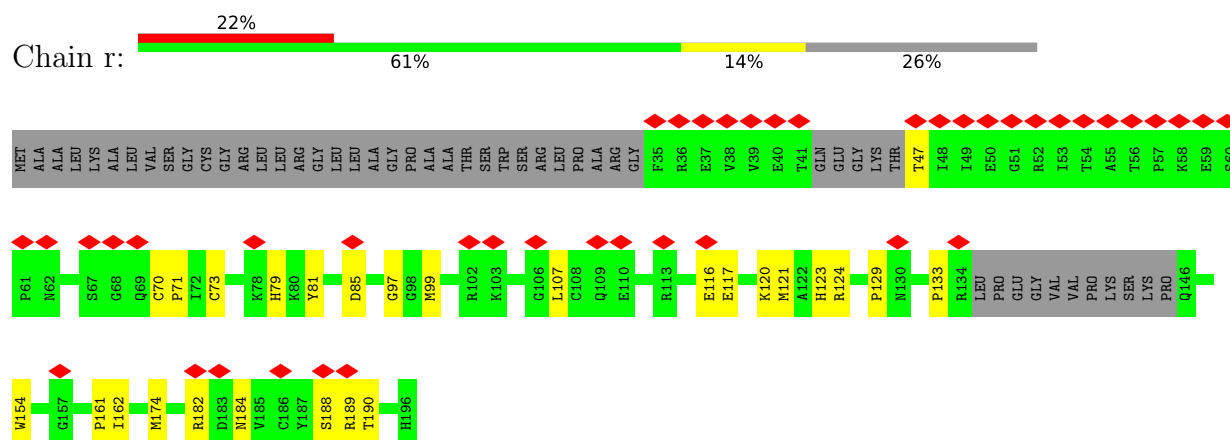




- Molecule 50: Growth arrest and DNA damage-inducible proteins-interacting protein 1



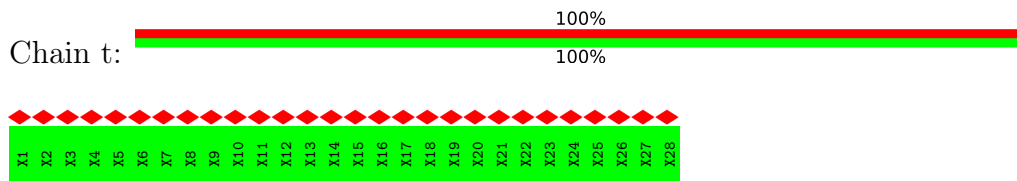
- Molecule 51: 39S ribosomal protein S18a, mitochondrial



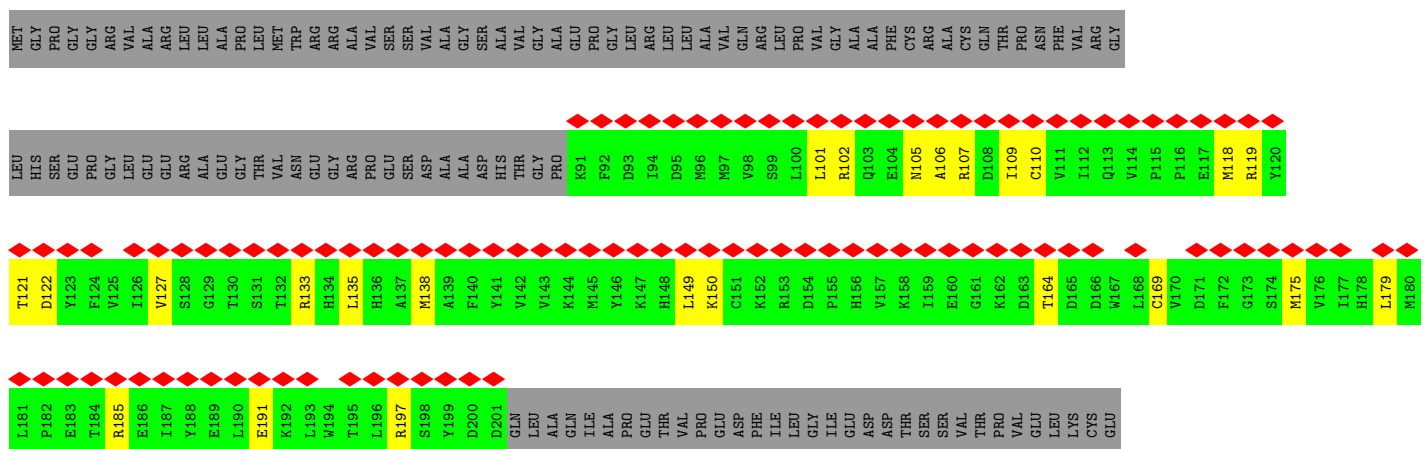
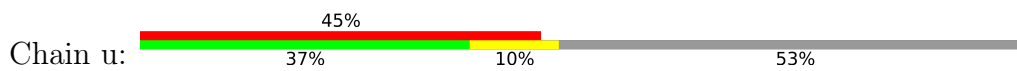
- Molecule 52: 39S ribosomal protein S30, mitochondrial



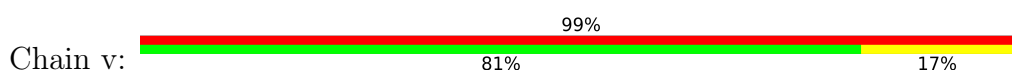
- Molecule 53: mL65

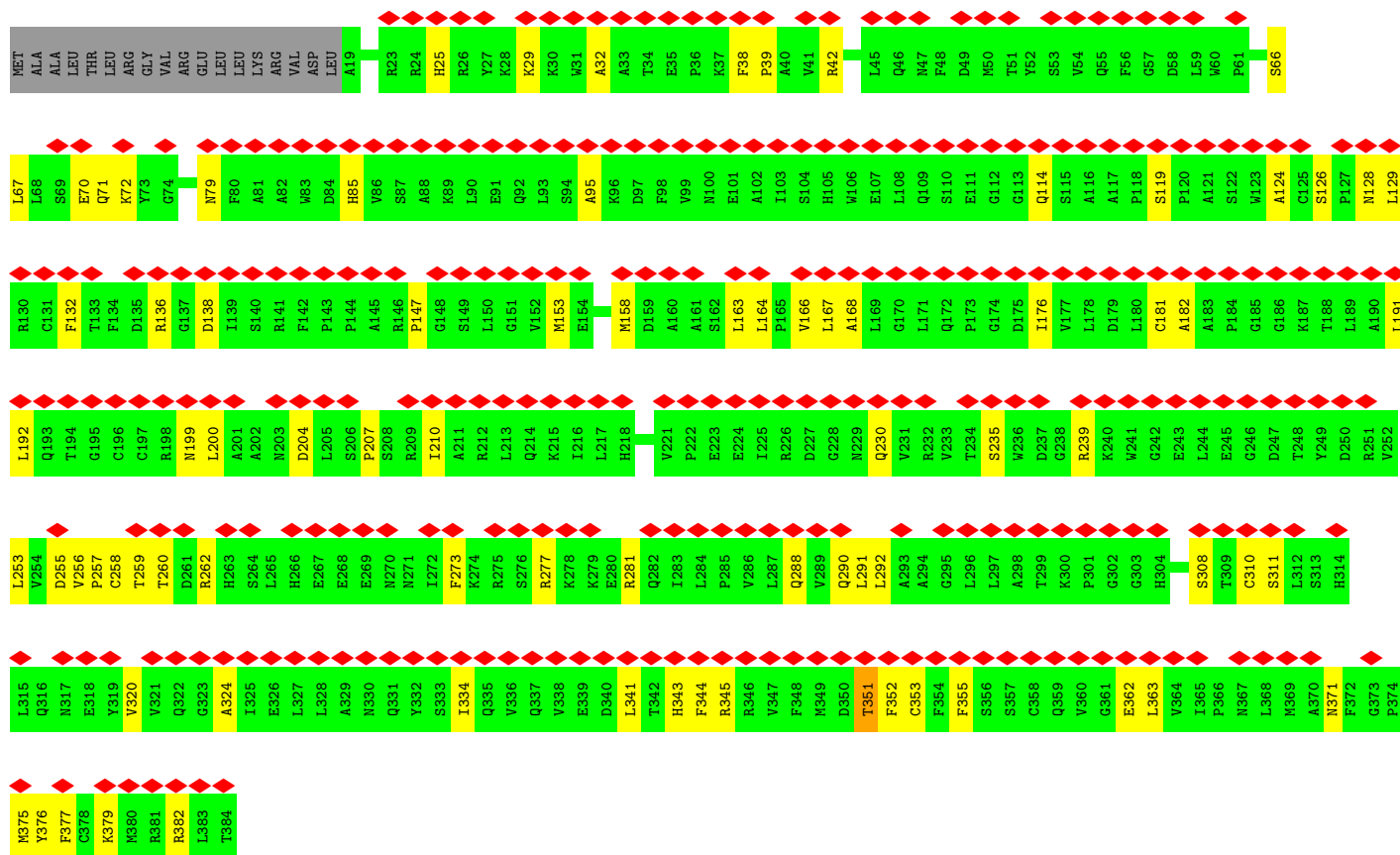


- Molecule 54: Mitochondrial assembly of ribosomal large subunit protein 1



- Molecule 55: MIEF1 upstream open reading frame protein.





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66340	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.723	Depositor
Minimum map value	-0.325	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.32	0/895	0.70	0/1201
2	1	0.21	0/438	0.55	0/583
3	2	0.25	0/373	0.65	0/496
4	3	0.29	0/852	0.60	0/1136
5	4	0.29	0/341	0.62	0/451
6	5	0.32	1/3294 (0.0%)	0.68	3/4488 (0.1%)
7	6	0.27	0/2726	0.60	0/3715
8	7	0.27	0/2391	0.64	0/3234
9	8	0.27	0/774	0.77	5/1043 (0.5%)
10	9	0.27	0/972	0.62	0/1306
11	A	0.19	0/34547	0.35	1/53754 (0.0%)
12	B	3.02	7/1504 (0.5%)	0.48	1/2333 (0.0%)
13	C	0.23	0/665	0.64	0/905
13	H	0.24	0/798	0.65	0/1073
14	D	0.38	0/1723	0.84	1/2317 (0.0%)
15	E	0.30	0/2465	0.65	0/3344
16	F	0.34	0/2071	0.70	4/2817 (0.1%)
17	G	0.27	0/1368	0.65	1/1849 (0.1%)
18	J	0.28	0/1077	0.72	2/1452 (0.1%)
19	K	0.35	1/1495 (0.1%)	0.85	3/2029 (0.1%)
20	L	0.33	0/904	0.80	2/1218 (0.2%)
21	M	0.31	0/2359	0.83	6/3185 (0.2%)
22	N	0.30	0/1658	0.67	0/2229
23	O	0.48	1/1269 (0.1%)	0.88	6/1708 (0.4%)
24	P	0.35	0/1173	0.76	1/1588 (0.1%)
25	Q	0.30	0/1846	0.72	2/2487 (0.1%)
26	R	0.25	0/1174	0.61	0/1572
27	S	0.32	0/1276	0.66	0/1729
28	T	0.30	0/1402	0.65	2/1886 (0.1%)
29	U	0.27	0/1248	0.68	1/1692 (0.1%)
30	V	0.27	0/1666	0.68	2/2260 (0.1%)
31	W	0.31	0/881	0.69	1/1188 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	X	0.31	0/2090	0.70	0/2825
33	Y	0.27	0/1552	0.63	0/2079
34	Z	0.29	0/1003	0.63	0/1354
35	a	0.28	0/709	0.72	0/963
36	b	0.34	0/1202	0.68	0/1626
37	c	0.31	0/2264	0.72	3/3059 (0.1%)
38	d	0.29	0/1790	0.65	0/2423
39	e	0.23	0/1797	0.58	0/2422
40	f	0.26	0/931	0.61	0/1259
41	g	0.30	0/1102	0.70	0/1503
42	h	0.28	0/847	0.58	0/1150
43	i	0.33	0/849	0.68	0/1135
44	j	0.28	0/698	0.62	0/940
45	k	0.22	0/635	0.74	1/855 (0.1%)
46	l	0.13	0/226	0.45	0/299
47	m	0.38	0/379	0.88	1/510 (0.2%)
48	o	0.27	0/792	0.70	0/1064
49	p	0.20	0/1071	0.53	1/1433 (0.1%)
50	q	0.18	0/1661	0.50	0/2236
51	r	0.37	0/1238	0.81	2/1676 (0.1%)
52	s	0.30	0/3114	0.66	1/4225 (0.0%)
54	u	0.23	0/949	0.68	2/1281 (0.2%)
55	v	0.17	0/597	0.49	0/796
56	w	0.21	0/647	0.61	2/871 (0.2%)
57	y	0.29	0/2020	0.65	1/2714 (0.0%)
58	x	0.32	0/2958	0.76	4/4014 (0.1%)
59	z	0.30	0/2484	0.74	0/3349
All	All	0.44	10/113230 (0.0%)	0.59	62/160329 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	A	5	0
14	D	0	3
17	G	0	1
21	M	0	1
25	Q	0	1
41	g	0	1
51	r	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
58	x	0	1
59	z	0	1
All	All	5	10

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1625	A	P-OP2	71.52	2.92	1.49
12	B	1635	C	C2-N3	39.98	2.15	1.35
12	B	1635	C	N1-C2	39.83	2.19	1.40
12	B	1635	C	N3-C4	38.92	2.11	1.33
12	B	1635	C	N1-C6	37.71	2.12	1.37
12	B	1635	C	C4-C5	35.82	2.14	1.43
12	B	1635	C	C5-C6	33.95	2.02	1.34
23	O	22	PRO	CG-CD	-11.01	1.13	1.50
6	5	285	TYR	C-O	7.74	1.27	1.23
19	K	43	HIS	C-N	-5.78	1.24	1.33

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	22	PRO	N-CD-CG	-14.56	81.36	103.20
19	K	43	HIS	CA-C-N	13.57	140.48	121.61
19	K	43	HIS	C-N-CA	13.57	140.48	121.61
12	B	1624	C	OP1-P-O3'	-9.53	79.41	108.00
9	8	187	PRO	N-CA-CB	8.45	111.28	103.08
45	k	27	VAL	N-CA-C	-7.95	105.44	113.47
21	M	95	PRO	CA-N-CD	-7.72	101.20	112.00
37	c	146	PRO	CA-N-CD	-7.53	101.46	112.00
54	u	149	LEU	CA-C-N	7.29	135.47	121.54
54	u	149	LEU	C-N-CA	7.29	135.47	121.54
9	8	188	PRO	N-CA-CB	7.28	110.89	103.25
23	O	22	PRO	CA-CB-CG	-7.27	90.69	104.50
29	U	118	PRO	N-CA-CB	7.25	110.86	103.25
9	8	183	PRO	N-CA-CB	7.14	110.75	103.25
18	J	22	ALA	CA-C-N	7.12	134.79	121.97
18	J	22	ALA	C-N-CA	7.12	134.79	121.97
51	r	73	CYS	CA-CB-SG	7.00	130.49	114.40
49	p	126	LYS	CA-CB-CG	6.99	128.08	114.10
30	V	167	PRO	N-CA-CB	6.63	109.88	103.51
6	5	258	PRO	N-CD-CG	-6.52	95.98	103.80
28	T	62	GLN	CA-C-N	6.47	144.49	121.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	T	62	GLN	C-N-CA	6.47	144.49	121.59
30	V	160	PRO	N-CA-CB	6.26	109.82	103.25
23	O	22	PRO	CA-N-CD	-6.23	103.28	112.00
6	5	258	PRO	CA-N-CD	-6.14	102.91	111.50
52	s	315	ASN	CA-C-O	6.06	126.76	119.43
21	M	95	PRO	N-CD-CG	-5.96	94.27	103.20
24	P	175	PRO	CA-N-CD	-5.88	103.76	112.00
37	c	310	ASN	CA-C-N	5.87	129.45	120.82
37	c	310	ASN	C-N-CA	5.87	129.45	120.82
47	m	74	MET	CA-CB-CG	5.71	125.52	114.10
14	D	264	ARG	N-CA-C	-5.69	105.99	114.64
51	r	70	CYS	CA-CB-SG	5.64	127.37	114.40
21	M	190	PRO	CA-C-N	5.58	124.80	120.33
21	M	190	PRO	C-N-CA	5.58	124.80	120.33
21	M	227	ALA	N-CA-C	-5.55	107.76	114.75
11	A	1709	G	P-O3'-C3'	5.46	128.40	120.20
20	L	90	CYS	CA-C-N	5.38	131.17	120.94
20	L	90	CYS	C-N-CA	5.38	131.17	120.94
58	x	351	THR	CA-C-N	5.38	131.82	121.54
58	x	351	THR	C-N-CA	5.38	131.82	121.54
6	5	140	VAL	N-CA-C	-5.35	107.60	113.43
58	x	182	ALA	CA-C-N	-5.28	116.53	123.34
58	x	182	ALA	C-N-CA	-5.28	116.53	123.34
21	M	47	ARG	N-CA-C	-5.25	106.82	113.43
56	w	127	GLY	CA-C-N	5.21	131.96	123.93
56	w	127	GLY	C-N-CA	5.21	131.96	123.93
16	F	294	PRO	CA-N-CD	-5.21	104.71	112.00
16	F	198	GLY	CA-C-N	5.19	127.61	120.39
16	F	198	GLY	C-N-CA	5.19	127.61	120.39
23	O	85	LEU	CA-C-N	5.12	123.47	120.24
23	O	85	LEU	C-N-CA	5.12	123.47	120.24
25	Q	204	MET	CA-C-N	5.11	128.44	120.68
25	Q	204	MET	C-N-CA	5.11	128.44	120.68
9	8	186	GLN	CA-C-N	5.10	125.63	120.38
9	8	186	GLN	C-N-CA	5.10	125.63	120.38
23	O	83	LYS	CB-CG-CD	5.08	122.99	111.30
19	K	46	VAL	CA-CB-CG1	5.07	119.01	110.40
57	y	155	PRO	CA-N-CD	-5.04	104.94	112.00
31	W	134	VAL	CB-CA-C	5.02	115.61	110.94
17	G	64	CYS	CA-CB-SG	5.01	125.92	114.40
16	F	86	VAL	N-CA-C	-5.01	108.62	113.53

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	2815	OMG	C4',C3'
11	A	3040	OMG	C1',C2',C4'

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	D	122	PHE	Peptide
14	D	206	TYR	Peptide
14	D	208	ARG	Sidechain
17	G	64	CYS	Peptide
21	M	62	ARG	Sidechain
25	Q	253	GLN	Peptide
41	g	66	TYR	Peptide
51	r	124	ARG	Sidechain
58	x	38	PHE	Peptide
59	z	195	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	880	0	904	15	0
2	1	433	0	475	9	0
3	2	367	0	393	3	0
4	3	831	0	883	11	0
5	4	333	0	352	8	0
6	5	3199	0	3196	37	0
7	6	2640	0	2464	32	0
8	7	2334	0	2343	30	0
9	8	759	0	725	7	0
10	9	947	0	949	13	0
11	A	30973	0	15733	169	0
12	B	1348	0	691	23	0
13	C	648	0	657	3	0
13	H	784	0	832	10	0
14	D	1692	0	1732	24	0
15	E	2396	0	2402	33	0
16	F	2013	0	2044	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	G	1338	0	1416	11	0
18	J	1061	0	1141	14	0
19	K	1451	0	1447	20	0
20	L	889	0	941	14	0
21	M	2305	0	2378	41	0
22	N	1617	0	1645	17	0
23	O	1245	0	1283	21	0
24	P	1148	0	1148	17	0
25	Q	1805	0	1841	23	0
26	R	1153	0	1214	13	0
27	S	1251	0	1322	18	0
28	T	1368	0	1410	21	0
29	U	1218	0	1187	17	0
30	V	1624	0	1606	18	0
31	W	859	0	888	9	0
32	X	2035	0	2054	18	0
33	Y	1517	0	1561	23	0
34	Z	978	0	1030	16	0
35	a	686	0	658	7	0
36	b	1178	0	1180	16	0
37	c	2217	0	2220	26	0
38	d	1741	0	1727	28	0
39	e	1762	0	1767	28	0
40	f	915	0	917	13	0
41	g	1067	0	1056	15	0
42	h	827	0	806	11	0
43	i	827	0	857	18	0
44	j	684	0	673	11	0
45	k	627	0	636	10	0
46	l	221	0	227	1	0
47	m	372	0	387	6	0
48	o	771	0	775	10	0
49	p	1058	0	1083	12	0
50	q	1625	0	1619	17	0
51	r	1203	0	1219	20	0
52	s	3036	0	3022	30	0
53	t	140	0	30	0	0
54	u	927	0	921	16	0
55	v	588	0	604	11	0
56	w	638	0	637	9	0
57	y	1989	0	2074	20	0
58	x	2889	0	2862	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	z	2443	0	2547	26	0
60	0	1	0	0	0	0
60	4	1	0	0	0	0
61	A	89	0	0	0	0
61	E	1	0	0	0	0
61	o	1	0	0	0	0
62	v	21	0	21	1	0
63	x	27	0	16	34	0
64	z	64	0	26	7	0
All	All	108075	0	92854	1000	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 (1000) 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)
58:x:257:PRO:HG3	63:x:401:SAM:C8	1.04	1.52
58:x:257:PRO:CG	63:x:401:SAM:H8	1.34	1.50
12:B:1635:C:C6	12:B:1635:C:C5	2.02	1.47
58:x:257:PRO:CG	63:x:401:SAM:C8	1.87	1.44
58:x:255:ASP:OD2	63:x:401:SAM:CB	1.71	1.38
12:B:1635:C:C5	12:B:1635:C:C4	2.14	1.35
12:B:1635:C:C4	12:B:1635:C:N3	2.11	1.16
12:B:1635:C:C6	12:B:1635:C:N1	2.12	1.15
12:B:1635:C:N3	12:B:1635:C:C2	2.15	1.13
12:B:1635:C:N1	12:B:1635:C:C2	2.19	1.10
58:x:255:ASP:OD2	63:x:401:SAM:HB2	1.39	1.09
58:x:255:ASP:CG	63:x:401:SAM:HB2	1.78	1.09
58:x:255:ASP:OD2	63:x:401:SAM:CG	2.02	1.07
58:x:255:ASP:HB3	63:x:401:SAM:HG1	1.33	1.06
58:x:255:ASP:OD2	63:x:401:SAM:CE	2.12	0.97
11:A:2469:A:HO2'	20:L:31:ALA:N	1.62	0.96
58:x:257:PRO:CD	63:x:401:SAM:C8	2.45	0.94
58:x:204:ASP:OD1	63:x:401:SAM:H1'	1.70	0.92
58:x:181:CYS:HB3	63:x:401:SAM:O4'	1.73	0.88
58:x:255:ASP:OD2	63:x:401:SAM:HB1	1.71	0.88
58:x:255:ASP:OD2	63:x:401:SAM:HE3	1.76	0.85
58:x:255:ASP:CB	63:x:401:SAM:HG1	2.07	0.84
58:x:257:PRO:HD3	63:x:401:SAM:C1'	2.08	0.83
12:B:1625:A:OP2	12:B:1635:C:C2	2.31	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:x:257:PRO:HD3	63:x:401:SAM:O4'	1.79	0.82
5:4:66:PHE:N	11:A:3013:G:HO2'	1.80	0.80
12:B:1625:A:OP2	12:B:1635:C:C4	2.37	0.77
58:x:257:PRO:HG3	63:x:401:SAM:N7	1.94	0.76
12:B:1625:A:P	12:B:1635:C:C2	2.82	0.73
44:j:28:ARG:HH22	44:j:37:PRO:HG3	1.53	0.72
12:B:1625:A:OP2	12:B:1635:C:N3	2.23	0.72
14:D:166:SER:HG	14:D:182:HIS:HD1	1.37	0.71
7:6:320:GLN:HE22	24:P:52:ASN:HD21	1.38	0.69
12:B:1625:A:OP2	12:B:1635:C:N1	2.26	0.69
20:L:99:ARG:HH22	25:Q:191:ARG:HE	1.40	0.69
24:P:52:ASN:HB3	24:P:55:ASN:HB2	1.75	0.69
59:z:156:LYS:NZ	64:z:401:GCP:O1B	2.26	0.69
58:x:257:PRO:CB	63:x:401:SAM:H8	2.22	0.68
58:x:363:LEU:HD12	58:x:376:TYR:HB2	1.76	0.68
12:B:1625:A:OP2	12:B:1635:C:C6	2.46	0.68
12:B:1625:A:P	12:B:1635:C:C4	2.87	0.67
58:x:176:ILE:HG23	58:x:199:ASN:HB3	1.77	0.67
14:D:109:PHE:HB3	14:D:204:ALA:HB3	1.77	0.67
19:K:20:LEU:HD11	19:K:141:LEU:HD13	1.77	0.66
58:x:147:PRO:HA	58:x:153:MET:HA	1.77	0.65
12:B:1625:A:OP2	12:B:1635:C:C5	2.49	0.65
6:5:384:GLN:NE2	11:A:2395:A:O2'	2.30	0.65
21:M:230:PRO:HD3	49:p:58:ALA:HA	1.78	0.65
30:V:136:ARG:NH1	30:V:137:PHE:O	2.30	0.65
34:Z:71:ARG:HA	34:Z:117:ILE:HA	1.77	0.65
14:D:102:GLN:HG2	14:D:133:PRO:HB2	1.78	0.64
58:x:257:PRO:HB3	63:x:401:SAM:H2'	1.78	0.64
21:M:107:LEU:HD12	41:g:60:PRO:HB3	1.80	0.64
58:x:70:GLU:O	58:x:371:ASN:ND2	2.30	0.64
55:v:40:ARG:HH12	56:w:113:LEU:HB2	1.63	0.64
15:E:213:LYS:O	15:E:216:GLN:NE2	2.30	0.64
6:5:380:GLN:HE21	6:5:410:THR:HG22	1.62	0.63
11:A:2812:U:H3	11:A:2820:A:H61	1.47	0.63
16:F:254:LEU:HB3	21:M:23:SER:HA	1.80	0.63
58:x:257:PRO:CG	63:x:401:SAM:N7	2.58	0.63
8:7:89:TYR:HB2	8:7:115:MET:HB3	1.80	0.63
15:E:78:CYS:HB2	15:E:81:LYS:HD2	1.81	0.63
30:V:29:VAL:HG21	38:d:67:ILE:HG23	1.81	0.62
30:V:59:GLY:HA2	30:V:75:LYS:HE2	1.81	0.62
20:L:35:MET:HB3	20:L:56:ARG:HH21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:49:ALA:HB3	52:s:61:ARG:HG3	1.82	0.62
24:P:57:GLU:O	49:p:177:ARG:NH2	2.32	0.62
8:7:120:THR:HG23	8:7:121:LYS:HG3	1.80	0.62
11:A:1869:A:N6	43:i:116:TYR:OH	2.33	0.62
11:A:2629:A:N6	57:y:173:GLU:O	2.33	0.62
11:A:2665:U:OP2	23:O:17:ARG:NH1	2.29	0.62
19:K:112:LEU:HD23	19:K:118:ARG:HG3	1.81	0.62
11:A:1889:C:OP1	21:M:133:LYS:NZ	2.27	0.62
37:c:93:VAL:HG22	37:c:180:LEU:HD22	1.82	0.62
11:A:2158:U:OP2	51:r:182:ARG:NH2	2.33	0.61
52:s:307:ARG:HD2	52:s:309:GLU:HB2	1.82	0.61
35:a:47:VAL:HG22	35:a:62:HIS:HB3	1.83	0.61
33:Y:225:ASN:C	33:Y:225:ASN:HD22	2.07	0.61
21:M:62:ARG:HG3	43:i:128:ARG:HD2	1.81	0.61
21:M:168:GLU:OE2	21:M:220:ARG:NH1	2.34	0.61
58:x:136:ARG:NH2	58:x:353:CYS:SG	2.73	0.61
59:z:177:GLY:N	64:z:402:GCP:O2A	2.33	0.61
1:0:119:LYS:O	1:0:120:HIS:ND1	2.34	0.60
6:5:53:PRO:HD2	32:X:119:LEU:HD22	1.82	0.60
11:A:2874:A:O2'	24:P:66:ARG:NH1	2.34	0.60
11:A:1747:G:N2	11:A:1750:G:O2'	2.34	0.60
11:A:1885:A:N6	16:F:282:PRO:O	2.34	0.60
28:T:77:ARG:HG3	28:T:120:VAL:HG22	1.83	0.60
1:0:123:CYS:HB2	1:0:126:CYS:HB2	1.83	0.60
1:0:132:LYS:HE3	38:d:290:GLU:HB2	1.84	0.60
8:7:41:THR:O	8:7:45:ASN:ND2	2.35	0.60
16:F:114:THR:O	16:F:156:ARG:NH1	2.33	0.60
16:F:133:THR:HG23	16:F:135:ARG:H	1.67	0.60
50:q:54:PRO:HD2	50:q:55:ARG:HH21	1.66	0.60
11:A:2312:A:N1	28:T:157:ARG:NH1	2.49	0.60
12:B:1625:A:P	12:B:1635:C:N3	2.75	0.60
57:y:130:GLU:HB3	57:y:159:MET:HE2	1.83	0.60
6:5:301:PRO:HB3	11:A:2389:C:H5"	1.84	0.59
12:B:1625:A:P	12:B:1635:C:C6	2.95	0.59
11:A:2137:C:OP2	34:Z:77:ARG:NH1	2.35	0.59
38:d:189:LEU:HD23	38:d:190:GLU:HB2	1.83	0.59
58:x:255:ASP:OD2	63:x:401:SAM:SD	2.60	0.59
6:5:212:THR:O	6:5:326:ARG:NH1	2.35	0.59
16:F:59:ARG:NH2	16:F:88:ALA:O	2.35	0.59
33:Y:167:ALA:HB3	33:Y:169:ARG:HH21	1.68	0.59
34:Z:118:ARG:HA	48:o:45:ASN:HD21	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:c:94:ASN:HA	37:c:122:ASN:HB2	1.85	0.59
37:c:141:LEU:HD21	37:c:223:MET:HE1	1.85	0.59
6:5:343:GLN:NE2	6:5:417:LEU:O	2.35	0.59
22:N:50:LEU:HB2	22:N:110:ASN:HD21	1.68	0.59
30:V:25:PRO:HG2	30:V:28:SER:HB3	1.85	0.58
11:A:2917:G:O6	21:M:77:ARG:NH1	2.36	0.58
7:6:44:ASN:HB3	7:6:47:ARG:HB2	1.86	0.58
18:J:108:VAL:HG21	18:J:154:ARG:HB2	1.85	0.58
58:x:255:ASP:OD2	63:x:401:SAM:HG1	2.00	0.58
11:A:2456:U:OP1	23:O:16:ARG:NH1	2.37	0.58
11:A:2665:U:H5'	23:O:21:GLY:HA2	1.84	0.58
10:9:63:PRO:HB2	33:Y:100:LYS:HE2	1.86	0.58
52:s:371:CYS:HB3	52:s:394:TRP:HB2	1.86	0.58
44:j:89:GLN:HA	44:j:92:GLN:HB2	1.86	0.58
11:A:2499:U:OP2	11:A:2504:A:N6	2.34	0.57
12:B:1625:A:P	12:B:1635:C:N1	2.77	0.57
10:9:24:LYS:HG2	11:A:2421:G:H5''	1.86	0.57
17:G:53:TYR:HB2	22:N:251:VAL:HB	1.86	0.57
30:V:16:PRO:HG2	30:V:19:TYR:HB2	1.85	0.57
38:d:53:GLU:HG2	38:d:57:MET:HE3	1.84	0.57
57:y:135:GLY:HA3	57:y:173:GLU:HA	1.86	0.57
59:z:156:LYS:N	64:z:401:GCP:O1A	2.38	0.57
2:1:19:ARG:NH1	11:A:2906:C:O2	2.36	0.57
29:U:68:VAL:HG22	29:U:97:VAL:HG12	1.86	0.57
52:s:51:MET:HE2	52:s:65:ARG:HD3	1.86	0.57
57:y:91:GLU:HA	57:y:94:ARG:HE	1.69	0.57
58:x:192:LEU:HB3	58:x:200:LEU:HD13	1.84	0.57
58:x:258:CYS:SG	58:x:259:THR:N	2.76	0.57
16:F:160:SER:HB2	43:i:80:LEU:HD13	1.86	0.57
20:L:32:ILE:HD13	20:L:86:ILE:HD13	1.85	0.57
2:1:63:ARG:NH2	11:A:2909:G:OP1	2.37	0.57
19:K:27:PRO:HG2	19:K:30:LYS:HB3	1.86	0.57
35:a:72:THR:HG22	37:c:258:THR:HA	1.87	0.57
18:J:21:ARG:NH2	18:J:70:ILE:O	2.38	0.57
19:K:154:ARG:HD3	51:r:129:PRO:HG3	1.87	0.57
39:e:48:LEU:HA	39:e:177:GLU:HA	1.87	0.57
58:x:257:PRO:HD3	63:x:401:SAM:N9	2.17	0.57
7:6:322:ARG:NH2	49:p:181:GLU:OE2	2.38	0.57
25:Q:134:LEU:O	25:Q:153:ASN:ND2	2.38	0.57
25:Q:183:LEU:HD11	25:Q:219:GLU:HA	1.87	0.57
15:E:328:LEU:HD22	15:E:332:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:G:51:THR:OG1	22:N:250:ARG:NH2	2.38	0.57
27:S:143:LEU:HD21	27:S:204:LEU:HD11	1.86	0.57
55:v:9:VAL:HG12	56:w:113:LEU:HD21	1.87	0.57
18:J:28:LEU:HB3	18:J:31:PRO:HG3	1.87	0.56
26:R:108:TYR:OH	35:a:142:ARG:NH1	2.38	0.56
45:k:66:VAL:HB	45:k:74:LEU:HB3	1.87	0.56
6:5:122:TRP:O	6:5:215:ARG:NH1	2.37	0.56
6:5:160:HIS:HA	6:5:164:TRP:HB2	1.86	0.56
7:6:143:CYS:HA	7:6:146:TYR:HD2	1.70	0.56
34:Z:82:GLU:OE2	34:Z:115:HIS:NE2	2.38	0.56
51:r:162:ILE:HD11	51:r:174:MET:HE2	1.86	0.56
59:z:65:ARG:HH21	59:z:80:LEU:HD13	1.71	0.56
4:3:107:VAL:HG21	4:3:161:MET:HE2	1.86	0.56
36:b:31:PHE:HB2	36:b:65:VAL:HG12	1.88	0.56
16:F:184:GLN:NE2	21:M:19:LEU:O	2.39	0.56
21:M:238:ARG:NH1	49:p:71:ILE:O	2.39	0.56
58:x:255:ASP:CG	63:x:401:SAM:CG	2.77	0.56
58:x:334:ILE:HD12	58:x:382:ARG:HE	1.70	0.56
8:7:79:PHE:HB3	8:7:81:MET:HE3	1.86	0.56
8:7:203:THR:HG22	8:7:280:VAL:H	1.71	0.56
17:G:99:CYS:SG	17:G:100:GLN:N	2.78	0.56
11:A:1710:A:N1	33:Y:192:LYS:NZ	2.52	0.56
58:x:362:GLU:HB2	58:x:377:PHE:HB2	1.86	0.56
11:A:2292:G:C8	26:R:11:ARG:HB2	2.40	0.55
17:G:188:ARG:HH12	45:k:54:ASP:HA	1.72	0.55
27:S:121:ASP:OD2	44:j:61:LYS:NZ	2.38	0.55
39:e:138:THR:HG22	39:e:153:LEU:HD22	1.88	0.55
58:x:257:PRO:CD	63:x:401:SAM:N9	2.69	0.55
6:5:104:CYS:SG	6:5:105:TYR:N	2.79	0.55
4:3:179:LYS:O	7:6:370:ARG:NH2	2.37	0.55
12:B:1625:A:P	12:B:1635:C:C5	2.99	0.55
8:7:103:SER:HA	8:7:129:THR:HG22	1.88	0.55
12:B:1608:G:N2	12:B:1664:G:N3	2.54	0.55
31:W:68:ALA:HB3	31:W:89:LEU:HD23	1.89	0.55
58:x:255:ASP:CG	63:x:401:SAM:HG1	2.31	0.55
8:7:286:LEU:HD21	8:7:296:ARG:HH21	1.72	0.55
11:A:2899:C:H5"	21:M:80:LYS:HD3	1.89	0.55
15:E:134:SER:OG	15:E:135:LYS:N	2.39	0.55
38:d:197:VAL:HG12	38:d:212:ILE:HG12	1.88	0.55
2:1:25:GLY:HA2	50:q:121:ILE:HG12	1.88	0.55
15:E:96:ARG:NH2	15:E:202:GLN:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:K:20:LEU:HB2	19:K:144:GLU:HA	1.89	0.55
28:T:69:ARG:HD2	38:d:228:PHE:HB3	1.88	0.55
57:y:258:LEU:HA	57:y:261:ILE:HG22	1.88	0.55
11:A:1990:G:O2'	11:A:1993:A:N6	2.40	0.55
51:r:117:GLU:HA	51:r:120:LYS:HG2	1.88	0.55
15:E:218:VAL:HG13	15:E:224:PHE:HD2	1.72	0.55
30:V:54:TRP:NE1	30:V:56:LEU:O	2.40	0.55
10:9:28:ARG:O	11:A:2377:G:O2'	2.25	0.54
11:A:2169:A:H4'	18:J:131:ALA:HB2	1.89	0.54
29:U:66:ALA:HB2	29:U:100:ALA:HB2	1.88	0.54
58:x:210:ILE:HD13	58:x:235:SER:HB3	1.89	0.54
23:O:80:LEU:HD12	23:O:86:ILE:HD13	1.89	0.54
39:e:178:TRP:HB3	39:e:187:THR:HG21	1.90	0.54
58:x:95:ALA:HB1	58:x:132:PHE:HB3	1.89	0.54
58:x:239:ARG:NH1	58:x:290:GLN:OE1	2.40	0.54
7:6:173:LEU:HD12	7:6:272:LEU:HD22	1.89	0.54
7:6:185:MET:HB3	49:p:189:ARG:HG2	1.89	0.54
11:A:1881:A:OP2	41:g:111:ARG:NH1	2.40	0.54
11:A:2285:U:H2'	11:A:2286:A:H8	1.71	0.54
18:J:26:ALA:HB1	18:J:57:THR:HG23	1.88	0.54
14:D:169:ILE:HA	14:D:186:ALA:HB2	1.90	0.54
16:F:237:LEU:O	50:q:25:TYR:N	2.41	0.54
28:T:77:ARG:HH12	28:T:119:GLU:HG2	1.73	0.54
42:h:114:ASN:HA	42:h:117:LEU:HD23	1.89	0.54
58:x:351:THR:HG22	58:x:352:PHE:H	1.72	0.54
11:A:1760:G:OP2	50:q:59:LYS:NZ	2.39	0.54
12:B:1608:G:O6	12:B:1662:C:N4	2.41	0.54
21:M:283:LEU:HD11	41:g:39:VAL:HB	1.90	0.54
37:c:244:GLU:OE1	37:c:248:ARG:NH1	2.41	0.54
44:j:63:GLN:OE1	44:j:66:ARG:NH1	2.41	0.54
13:C:185:ASN:H	13:C:188:ILE:HD12	1.73	0.54
16:F:230:ILE:HD12	16:F:233:ALA:HB3	1.90	0.54
43:i:92:ILE:HD13	43:i:95:ARG:HH21	1.71	0.54
43:i:103:PHE:O	43:i:107:LEU:N	2.37	0.54
7:6:123:ALA:HA	24:P:123:VAL:HG21	1.90	0.54
11:A:3344:C:O2'	25:Q:84:ARG:O	2.23	0.54
13:H:58:ARG:NH1	13:H:77:HIS:O	2.40	0.54
23:O:29:LEU:HD22	23:O:52:MET:HB2	1.89	0.54
59:z:113:CYS:SG	59:z:162:SER:OG	2.66	0.54
8:7:189:LEU:O	8:7:295:ARG:NH2	2.41	0.53
11:A:2374:A:N6	52:s:272:PRO:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:1644:G:N7	24:P:120:ARG:NH2	2.53	0.53
14:D:217:LEU:HD11	14:D:227:GLN:HB2	1.90	0.53
27:S:164:THR:HG22	36:b:107:GLN:HB2	1.90	0.53
37:c:161:THR:O	37:c:192:GLN:NE2	2.40	0.53
58:x:260:THR:HG22	58:x:310:CYS:HB2	1.91	0.53
23:O:30:ARG:HH21	23:O:81:THR:HG22	1.72	0.53
29:U:123:ALA:HB3	29:U:127:TYR:HB2	1.89	0.53
58:x:345:ARG:NH1	58:x:355:PHE:O	2.40	0.53
55:v:10:LEU:HD23	56:w:113:LEU:HD23	1.89	0.53
7:6:37:ASN:HB3	40:f:62:LEU:HD21	1.90	0.53
11:A:2157:U:OP1	51:r:182:ARG:NH1	2.41	0.53
27:S:136:VAL:HG21	27:S:154:VAL:HG11	1.90	0.53
11:A:2643:G:O2'	11:A:2645:G:OP2	2.25	0.53
20:L:100:PHE:HB3	25:Q:158:GLN:HE22	1.72	0.53
54:u:135:LEU:HD22	54:u:179:LEU:HB3	1.91	0.53
56:w:126:PHE:HZ	56:w:152:LYS:HD3	1.73	0.53
6:5:98:LEU:HD12	6:5:270:ILE:HG13	1.91	0.53
6:5:125:LYS:HA	6:5:253:LEU:HD21	1.90	0.53
7:6:224:HIS:CE1	7:6:226:LEU:HB2	2.43	0.53
19:K:58:VAL:HG12	19:K:126:HIS:HB2	1.90	0.53
40:f:93:ILE:H	40:f:156:VAL:HG13	1.74	0.53
50:q:134:ASN:ND2	50:q:137:GLN:OE1	2.42	0.53
11:A:2072:A:H62	11:A:2831:G:H2'	1.74	0.53
29:U:27:GLN:HG3	29:U:43:ARG:HB2	1.91	0.53
51:r:71:PRO:HD2	51:r:107:LEU:HD23	1.90	0.53
11:A:1804:A:N6	38:d:72:SER:OG	2.42	0.53
11:A:1878:U:O3'	16:F:92:ARG:NH2	2.42	0.53
11:A:2749:A:O2'	57:y:199:ARG:NH2	2.42	0.53
31:W:121:PRO:HG2	31:W:124:ALA:HB2	1.90	0.53
36:b:37:GLY:O	36:b:44:ARG:NH2	2.42	0.53
58:x:291:LEU:HD11	63:x:401:SAM:C6	2.39	0.53
11:A:1882:A:N6	11:A:1893:A:O4'	2.42	0.53
28:T:133:ASN:O	38:d:230:ARG:NH2	2.42	0.53
52:s:228:ASP:OD1	52:s:228:ASP:N	2.42	0.53
56:w:111:ASP:H	56:w:114:ASP:HB2	1.74	0.53
58:x:32:ALA:O	58:x:42:ARG:NH2	2.41	0.53
6:5:125:LYS:HG3	6:5:253:LEU:HD11	1.92	0.52
19:K:25:MET:O	19:K:149:ARG:NH2	2.36	0.52
38:d:267:PRO:HG2	38:d:270:ALA:HB2	1.89	0.52
58:x:260:THR:H	58:x:311:SER:HB2	1.74	0.52
11:A:1673:U:O2'	28:T:149:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2015:G:H22	11:A:2037:U:H5''	1.73	0.52
23:O:149:LEU:HA	23:O:152:LEU:HD23	1.91	0.52
25:Q:123:ASP:OD2	54:u:119:ARG:NH2	2.43	0.52
39:e:51:LEU:HD12	39:e:188:ALA:HB1	1.91	0.52
45:k:63:CYS:HA	45:k:77:ARG:HA	1.91	0.52
58:x:119:SER:HB2	58:x:124:ALA:HB2	1.91	0.52
59:z:32:PRO:HD2	59:z:35:MET:HE3	1.90	0.52
47:m:55:LEU:HD22	47:m:63:THR:HB	1.92	0.52
57:y:91:GLU:HG2	57:y:121:LEU:HD23	1.92	0.52
1:O:94:ARG:NH2	11:A:2310:G:OP2	2.38	0.52
10:9:20:LYS:O	10:9:25:ARG:NH1	2.42	0.52
20:L:111:ASN:HB2	54:u:164:THR:HB	1.90	0.52
21:M:264:GLN:NE2	21:M:269:LEU:O	2.43	0.52
33:Y:128:SER:OG	33:Y:131:ARG:NE	2.41	0.52
52:s:84:THR:HB	52:s:280:ASN:HB2	1.90	0.52
59:z:112:ASN:OD1	64:z:401:GCP:O6	2.28	0.52
4:3:104:ARG:NH2	4:3:160:LYS:O	2.38	0.52
13:H:120:ARG:NH2	32:X:136:ASP:OD2	2.42	0.52
19:K:56:HIS:HD2	19:K:126:HIS:HE1	1.58	0.52
58:x:257:PRO:CB	63:x:401:SAM:H2'	2.40	0.52
2:1:38:ARG:HB3	58:x:147:PRO:HG2	1.92	0.52
6:5:233:LYS:HA	6:5:286:PRO:HD2	1.91	0.52
11:A:2197:G:H5'	46:l:123:LYS:HG2	1.91	0.52
16:F:63:GLN:HG3	16:F:81:ASP:HB3	1.90	0.52
16:F:220:ASP:O	16:F:245:ALA:N	2.42	0.52
24:P:39:VAL:HG12	24:P:41:ASN:H	1.75	0.52
29:U:71:ARG:NH1	29:U:73:GLN:OE1	2.36	0.52
8:7:185:LEU:HB2	8:7:295:ARG:HH12	1.75	0.52
39:e:155:ARG:NH1	39:e:279:LEU:O	2.43	0.52
14:D:194:ASN:ND2	14:D:245:GLY:O	2.30	0.52
15:E:109:LEU:HD21	15:E:337:VAL:HG12	1.92	0.52
16:F:183:ALA:HA	42:h:115:SER:HB3	1.92	0.52
27:S:137:GLY:HA2	27:S:142:THR:HA	1.92	0.52
52:s:159:ARG:HH21	52:s:171:VAL:HG12	1.75	0.52
11:A:2067:C:H5'	40:f:60:LYS:HB2	1.92	0.51
16:F:113:LYS:HG3	16:F:157:GLY:H	1.75	0.51
27:S:134:LEU:HB3	27:S:148:LEU:HD23	1.91	0.51
29:U:8:PRO:HA	33:Y:183:GLN:HE22	1.75	0.51
41:g:154:ASP:OD1	41:g:154:ASP:N	2.41	0.51
52:s:152:GLN:HA	52:s:156:TYR:HB2	1.92	0.51
8:7:316:LEU:HD11	23:O:148:LEU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2949:C:H42	11:A:2975:G:H1	1.58	0.51
16:F:208:HIS:O	16:F:211:ARG:NH1	2.43	0.51
16:F:221:LEU:HD23	16:F:222:THR:HG23	1.91	0.51
58:x:67:LEU:HA	58:x:262:ARG:HH21	1.75	0.51
11:A:3067:PSU:OP2	11:A:3258:G:N2	2.43	0.51
21:M:205:LEU:HD13	50:q:96:LEU:HG	1.92	0.51
39:e:146:ARG:HB3	39:e:253:VAL:HG13	1.93	0.51
57:y:327:SER:O	57:y:331:THR:OG1	2.27	0.51
16:F:107:LYS:HG2	43:i:74:ILE:HG22	1.91	0.51
40:f:183:ARG:HE	40:f:184:LEU:H	1.59	0.51
16:F:86:VAL:HG23	16:F:175:LYS:HG2	1.93	0.51
36:b:35:ARG:NH1	42:h:158:TYR:O	2.43	0.51
6:5:80:ARG:NH1	6:5:82:TYR:OH	2.43	0.51
6:5:125:LYS:HE2	6:5:364:LEU:HD23	1.91	0.51
11:A:2052:A:OP1	41:g:150:LYS:NZ	2.44	0.51
16:F:63:GLN:HB3	16:F:79:LEU:HD11	1.92	0.51
19:K:10:GLN:NE2	28:T:203:LEU:O	2.43	0.51
32:X:148:THR:HB	32:X:152:ASP:HB2	1.92	0.51
33:Y:84:ALA:HB2	33:Y:134:LYS:HB2	1.92	0.51
43:i:60:ILE:HG22	43:i:70:PRO:HG3	1.93	0.51
50:q:176:GLN:HA	50:q:179:LEU:HD12	1.92	0.51
11:A:1777:A:N6	11:A:1780:U:OP2	2.35	0.51
11:A:2483:U:O2	11:A:2652:G:N2	2.43	0.51
37:c:125:LEU:HD13	37:c:201:ALA:HB2	1.91	0.51
39:e:55:ARG:HD3	39:e:157:LEU:HD22	1.93	0.51
45:k:73:ARG:O	51:r:47:THR:N	2.44	0.51
58:x:341:LEU:HB3	58:x:344:PHE:HB3	1.93	0.51
26:R:109:GLU:HA	36:b:127:GLN:HB2	1.93	0.51
6:5:248:THR:O	6:5:371:LYS:NZ	2.43	0.51
25:Q:111:PHE:HB2	25:Q:117:LEU:HD11	1.93	0.51
39:e:156:ASN:ND2	39:e:277:SER:O	2.44	0.51
49:p:102:ARG:NH1	49:p:132:GLU:OE1	2.44	0.51
49:p:143:GLN:HA	49:p:146:ASN:HB2	1.92	0.51
58:x:255:ASP:OD2	63:x:401:SAM:HE2	2.08	0.51
58:x:257:PRO:HD3	63:x:401:SAM:C2'	2.40	0.51
11:A:1876:U:O2'	21:M:32:GLY:O	2.28	0.50
11:A:2196:A:O2'	11:A:2213:A:N1	2.41	0.50
20:L:136:LYS:NZ	54:u:169:CYS:SG	2.71	0.50
22:N:225:GLY:O	34:Z:78:ARG:NH1	2.44	0.50
59:z:77:PRO:HB2	59:z:129:LEU:HD21	1.93	0.50
13:C:179:ASN:HB3	13:C:182:TRP:HD1	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:V:138:THR:OG1	30:V:141:GLY:O	2.28	0.50
41:g:86:VAL:HG22	41:g:113:VAL:HG22	1.92	0.50
7:6:235:TRP:HB3	7:6:254:TYR:HD1	1.75	0.50
11:A:1678:C:N4	11:A:1773:A:OP2	2.37	0.50
36:b:108:SER:OG	36:b:109:GLY:N	2.43	0.50
54:u:102:ARG:NH2	55:v:27:ASP:OD1	2.44	0.50
9:8:162:ILE:HG22	40:f:86:TYR:HB2	1.94	0.50
10:9:90:GLN:NE2	10:9:94:GLU:OE2	2.43	0.50
25:Q:103:ARG:HG2	25:Q:108:ILE:HD12	1.93	0.50
10:9:130:LEU:HD12	33:Y:154:ARG:HG3	1.94	0.50
11:A:2682:A:OP1	26:R:34:ARG:NH2	2.42	0.50
14:D:257:ILE:O	14:D:262:ARG:NH1	2.43	0.50
24:P:177:ARG:NH1	24:P:178:ILE:O	2.44	0.50
38:d:182:ARG:NH2	38:d:225:TYR:OH	2.44	0.50
17:G:176:LEU:HB3	17:G:188:ARG:HG3	1.93	0.50
21:M:66:GLY:HA3	21:M:75:TYR:HE2	1.77	0.50
54:u:175:MET:SD	54:u:175:MET:N	2.85	0.50
58:x:256:VAL:HG21	58:x:288:GLN:HG3	1.92	0.50
18:J:30:MET:HB2	18:J:50:CYS:HB3	1.94	0.50
21:M:223:LEU:HA	49:p:45:LEU:HD21	1.93	0.50
32:X:161:LEU:HD22	32:X:165:MET:HE3	1.94	0.50
33:Y:95:ASN:OD1	33:Y:149:ARG:NH1	2.35	0.50
1:0:117:LYS:NZ	1:0:118:GLN:O	2.36	0.50
16:F:170:ARG:HH22	43:i:70:PRO:HG2	1.77	0.50
25:Q:210:GLU:HG3	25:Q:213:GLN:HB2	1.93	0.50
45:k:18:VAL:HG11	45:k:34:LEU:HD21	1.94	0.50
58:x:158:MET:HE1	58:x:163:LEU:HB2	1.93	0.50
7:6:195:PRO:HA	7:6:198:ALA:HB3	1.94	0.50
11:A:2055:U:H2'	11:A:2056:G:H8	1.76	0.50
20:L:73:ILE:HG13	20:L:84:ALA:HB3	1.93	0.50
7:6:42:LEU:HD22	7:6:48:LEU:HD21	1.94	0.49
11:A:1685:C:H5'	43:i:79:TRP:HH2	1.77	0.49
11:A:2459:A:N6	11:A:2668:A:O2'	2.45	0.49
36:b:114:ARG:HH12	36:b:116:ARG:HA	1.75	0.49
9:8:131:MET:HA	9:8:134:ASP:HB2	1.94	0.49
11:A:2244:U:O2'	51:r:189:ARG:NH1	2.45	0.49
31:W:66:ILE:HA	31:W:90:TYR:HA	1.94	0.49
40:f:179:PRO:HB3	47:m:38:ALA:HB3	1.94	0.49
10:9:56:MET:HA	29:U:17:LEU:HD13	1.93	0.49
14:D:147:ARG:HH21	14:D:149:ARG:HH11	1.60	0.49
27:S:119:GLU:HG2	27:S:121:ASP:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:e:64:THR:O	39:e:68:GLU:N	2.42	0.49
6:5:207:SER:HB3	52:s:157:LEU:HD22	1.95	0.49
9:8:133:ARG:HD2	12:B:1611:G:H22	1.78	0.49
11:A:2342:U:H5''	29:U:78:LYS:HB2	1.94	0.49
15:E:129:VAL:HG13	15:E:189:PRO:HA	1.94	0.49
18:J:18:GLY:N	18:J:72:VAL:O	2.46	0.49
49:p:43:TYR:HB3	50:q:96:LEU:HD12	1.94	0.49
52:s:91:TYR:HE2	52:s:229:LEU:HD12	1.77	0.49
22:N:205:ARG:NH2	22:N:249:LYS:O	2.46	0.49
54:u:110:CYS:HA	55:v:26:THR:HG23	1.95	0.49
22:N:123:ARG:NH1	22:N:162:GLU:OE2	2.46	0.49
38:d:211:GLN:HE21	38:d:247:VAL:HG11	1.77	0.49
8:7:144:ARG:NH2	8:7:171:GLU:OE1	2.38	0.49
11:A:1819:U:OP1	28:T:95:ARG:NH2	2.39	0.49
15:E:112:LYS:NZ	15:E:337:VAL:O	2.44	0.49
16:F:279:ARG:O	41:g:90:ARG:NH1	2.45	0.49
58:x:126:SER:OG	58:x:166:VAL:O	2.27	0.49
58:x:292:LEU:HD12	58:x:320:VAL:HG12	1.95	0.49
8:7:64:LYS:NZ	38:d:276:ILE:O	2.39	0.49
9:8:176:PRO:HD2	40:f:181:GLY:H	1.77	0.49
11:A:1865:C:OP2	26:R:17:ARG:NH1	2.41	0.49
52:s:92:MET:HE2	52:s:276:ARG:HH11	1.77	0.49
9:8:176:PRO:HG2	40:f:180:GLU:HA	1.94	0.49
16:F:59:ARG:NH1	41:g:114:GLU:OE2	2.46	0.49
32:X:140:GLY:HA3	32:X:143:PHE:HD2	1.78	0.49
37:c:308:THR:HG23	37:c:310:ASN:H	1.77	0.49
57:y:237:ALA:HB2	57:y:253:TYR:CZ	2.48	0.49
11:A:2694:A:N3	11:A:2942:C:O2'	2.39	0.48
15:E:107:MET:HE3	15:E:121:LEU:HD21	1.95	0.48
34:Z:75:THR:HA	34:Z:116:LEU:HD11	1.95	0.48
45:k:15:GLN:HB3	45:k:67:LEU:HD12	1.95	0.48
15:E:205:ASP:N	15:E:300:LYS:O	2.44	0.48
29:U:3:ARG:O	29:U:23:ASN:ND2	2.38	0.48
43:i:57:TYR:OH	50:q:28:ARG:O	2.30	0.48
4:3:113:ARG:NH2	11:A:2898:U:O2'	2.41	0.48
6:5:351:VAL:HG12	6:5:381:LEU:HB3	1.95	0.48
19:K:138:LEU:HD12	19:K:141:LEU:HD12	1.95	0.48
27:S:99:VAL:HG12	27:S:133:VAL:HG12	1.95	0.48
52:s:90:LYS:HG2	52:s:230:ARG:HB2	1.95	0.48
59:z:321:LEU:HA	59:z:324:LEU:HB2	1.95	0.48
11:A:1822:U:O2	11:A:2707:A:O2'	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:f:114:CYS:HA	40:f:119:ILE:HD12	1.96	0.48
59:z:113:CYS:HG	59:z:162:SER:HG	1.54	0.48
8:7:81:MET:HE1	8:7:91:CYS:HA	1.95	0.48
28:T:128:ALA:HA	28:T:132:HIS:HB2	1.95	0.48
43:i:57:TYR:HB3	43:i:60:ILE:HD12	1.95	0.48
11:A:3309:U:H1'	11:A:3310:G:H4'	1.94	0.48
11:A:3317:A:OP1	54:u:133:ARG:NH2	2.47	0.48
17:G:56:PRO:HB3	22:N:210:GLN:HE22	1.77	0.48
21:M:142:GLU:HB2	21:M:162:LEU:HD22	1.95	0.48
21:M:246:ASP:OD1	21:M:246:ASP:N	2.44	0.48
33:Y:72:LYS:O	33:Y:76:GLN:NE2	2.46	0.48
39:e:162:ARG:NH1	39:e:169:ASP:OD1	2.47	0.48
54:u:197:ARG:HG2	55:v:66:LEU:HB3	1.96	0.48
58:x:66:SER:O	58:x:262:ARG:NH2	2.46	0.48
8:7:64:LYS:HE2	38:d:275:PRO:HB2	1.94	0.48
11:A:2145:G:OP1	27:S:169:ARG:NH1	2.47	0.48
15:E:150:LYS:HB3	15:E:296:LEU:HD21	1.95	0.48
22:N:87:PHE:HB2	22:N:163:MET:HB2	1.96	0.48
26:R:11:ARG:O	37:c:33:LYS:NZ	2.35	0.48
33:Y:158:THR:OG1	33:Y:160:GLN:NE2	2.46	0.48
19:K:74:GLN:HA	51:r:161:PRO:HA	1.96	0.48
26:R:32:ARG:O	26:R:35:LYS:NZ	2.46	0.48
37:c:47:ARG:HH21	37:c:50:LEU:HD22	1.79	0.48
10:9:70:LEU:HB3	33:Y:101:LEU:HD13	1.96	0.48
11:A:1699:C:H2'	33:Y:197:LYS:HG2	1.95	0.48
11:A:2903:U:O2'	11:A:2905:A:N7	2.39	0.48
25:Q:148:THR:HG22	25:Q:165:GLU:HG2	1.96	0.48
15:E:274:TRP:HE1	15:E:286:ASN:HB2	1.78	0.48
8:7:281:SER:H	8:7:299:GLY:HA2	1.79	0.47
17:G:93:ASN:HD22	17:G:155:VAL:HG12	1.79	0.47
41:g:109:VAL:HG22	41:g:148:ARG:HG2	1.95	0.47
11:A:1914:A:N6	11:A:2004:G:O6	2.47	0.47
13:H:53:THR:N	13:H:86:THR:HG1	2.12	0.47
21:M:222:TYR:HE2	21:M:262:PRO:HB3	1.78	0.47
59:z:251:GLY:O	59:z:254:GLN:NE2	2.44	0.47
6:5:127:LYS:HB2	6:5:371:LYS:HD2	1.95	0.47
14:D:108:ASP:OD2	14:D:149:ARG:NH1	2.46	0.47
14:D:184:LEU:HD22	14:D:216:LEU:HD21	1.95	0.47
25:Q:136:ILE:HB	25:Q:200:PHE:HE2	1.78	0.47
40:f:166:PHE:HA	40:f:169:ILE:HD12	1.96	0.47
57:y:198:VAL:HG23	57:y:212:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:z:148:VAL:HG22	59:z:156:LYS:HD2	1.95	0.47
27:S:163:LYS:HB2	36:b:106:ASP:HB3	1.95	0.47
35:a:69:TYR:CG	37:c:278:LYS:HG2	2.50	0.47
7:6:327:VAL:HA	7:6:330:ILE:HD12	1.96	0.47
11:A:1962:A:OP2	11:A:2501:C:N4	2.43	0.47
14:D:69:ARG:HD2	14:D:77:VAL:HG21	1.96	0.47
8:7:70:VAL:HG23	8:7:126:LYS:HB3	1.95	0.47
11:A:3009:C:O2'	11:A:3302:U:OP1	2.29	0.47
15:E:217:GLY:HA2	15:E:258:PRO:HB3	1.96	0.47
39:e:146:ARG:HA	39:e:151:ARG:HD2	1.95	0.47
3:2:85:LYS:NZ	11:A:1793:G:O6	2.46	0.47
7:6:71:TRP:CD1	31:W:101:LYS:HB2	2.50	0.47
7:6:224:HIS:HE1	7:6:226:LEU:HB2	1.79	0.47
7:6:234:HIS:ND1	7:6:255:LEU:O	2.41	0.47
7:6:335:LEU:HB3	7:6:337:MET:HG2	1.96	0.47
11:A:1814:A:N3	11:A:1862:U:O2'	2.46	0.47
11:A:1868:G:N7	21:M:51:ARG:NH1	2.56	0.47
11:A:2392:U:H2'	11:A:2394:A:H62	1.79	0.47
11:A:2410:U:OP2	52:s:160:ARG:NH2	2.48	0.47
14:D:125:LYS:HE3	14:D:125:LYS:HB2	1.80	0.47
16:F:230:ILE:HG23	16:F:242:LEU:HD11	1.95	0.47
20:L:128:ARG:NH1	25:Q:125:TYR:O	2.47	0.47
27:S:163:LYS:HG2	27:S:191:THR:HG22	1.95	0.47
28:T:136:PHE:HB2	28:T:139:ASN:HB2	1.97	0.47
33:Y:72:LYS:HA	33:Y:72:LYS:HD3	1.72	0.47
38:d:208:VAL:HB	38:d:252:LEU:HB2	1.97	0.47
39:e:48:LEU:HD22	39:e:231:VAL:HG22	1.97	0.47
59:z:155:GLY:N	64:z:401:GCP:O5'	2.48	0.47
2:1:30:PHE:HZ	2:1:43:LEU:HD11	1.79	0.47
6:5:135:LYS:HZ1	6:5:239:ILE:HG12	1.79	0.47
11:A:1706:C:OP1	33:Y:193:ARG:NH2	2.40	0.47
11:A:2003:A:OP2	11:A:2734:A:O2'	2.30	0.47
11:A:2138:U:O2'	11:A:2151:A:N3	2.47	0.47
11:A:2157:U:H5'	51:r:182:ARG:HH22	1.79	0.47
21:M:28:LYS:HG3	48:o:94:HIS:CD2	2.50	0.47
21:M:96:LEU:HD13	21:M:101:LEU:HD21	1.96	0.47
23:O:33:LEU:HD21	23:O:59:LEU:HD22	1.96	0.47
38:d:189:LEU:HD22	38:d:217:HIS:HD2	1.79	0.47
11:A:2017:U:O2'	11:A:2723:A:N1	2.48	0.47
16:F:95:ILE:HD13	16:F:172:LEU:HD22	1.96	0.47
16:F:113:LYS:HE2	16:F:157:GLY:HA2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:H:57:GLU:O	13:H:81:LYS:N	2.44	0.47
13:H:84:GLU:HB3	32:X:44:ARG:HH22	1.80	0.47
21:M:116:ILE:HB	21:M:154:ILE:HG13	1.97	0.47
29:U:61:TYR:O	33:Y:63:GLY:N	2.48	0.47
58:x:207:PRO:HA	58:x:210:ILE:HG12	1.96	0.47
11:A:2469:A:O2'	20:L:31:ALA:N	2.39	0.47
11:A:2954:C:O2'	22:N:182:LYS:NZ	2.48	0.47
16:F:49:ARG:NH2	16:F:270:GLU:OE2	2.46	0.47
19:K:18:TRP:HB3	19:K:141:LEU:HD23	1.97	0.47
2:1:16:ILE:HA	2:1:64:SER:HA	1.97	0.46
6:5:122:TRP:HA	6:5:253:LEU:HD23	1.96	0.46
11:A:2739:U:O4	58:x:29:LYS:NZ	2.47	0.46
11:A:3345:A:O2'	23:O:11:HIS:O	2.28	0.46
15:E:210:THR:HG22	15:E:290:PRO:HB3	1.97	0.46
16:F:53:LEU:HG	16:F:274:LEU:HD11	1.97	0.46
21:M:20:PRO:HG3	48:o:99:LYS:HA	1.95	0.46
42:h:91:LEU:HD21	42:h:100:LEU:HD13	1.96	0.46
55:v:40:ARG:NH2	56:w:111:ASP:OD2	2.48	0.46
59:z:83:ASN:HD22	59:z:155:GLY:HA3	1.80	0.46
1:0:107:ILE:HD13	28:T:104:ALA:HB1	1.96	0.46
17:G:65:LEU:HD12	17:G:66:PRO:HD2	1.97	0.46
41:g:73:GLN:O	41:g:88:ARG:NH2	2.48	0.46
51:r:85:ASP:OD1	51:r:85:ASP:N	2.44	0.46
52:s:251:VAL:O	52:s:373:GLN:NE2	2.44	0.46
57:y:277:PRO:HA	57:y:282:GLN:H	1.79	0.46
16:F:103:GLN:HE21	43:i:58:ASP:HB2	1.79	0.46
13:H:53:THR:N	13:H:86:THR:OG1	2.48	0.46
18:J:66:LEU:HB3	18:J:82:ILE:HD11	1.98	0.46
24:P:154:ALA:HA	24:P:159:LYS:HE3	1.98	0.46
27:S:90:GLY:O	37:c:312:ARG:NH2	2.48	0.46
52:s:376:THR:OG1	52:s:391:ASN:ND2	2.47	0.46
7:6:153:GLU:HG3	7:6:158:TYR:HD2	1.80	0.46
21:M:292:LYS:O	21:M:296:SER:OG	2.34	0.46
39:e:151:ARG:HG2	39:e:152:LYS:HG2	1.96	0.46
1:0:130:VAL:HG21	23:O:134:PRO:HD3	1.98	0.46
11:A:1849:C:OP1	11:A:2935:A:N6	2.48	0.46
11:A:2935:A:H3'	11:A:2936:U:H2'	1.96	0.46
16:F:74:GLN:HE21	16:F:77:VAL:HG21	1.79	0.46
30:V:92:ASN:HD22	30:V:115:LEU:HD21	1.81	0.46
34:Z:146:VAL:HG22	34:Z:148:GLN:H	1.80	0.46
34:Z:147:VAL:HG23	34:Z:148:GLN:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2075:U:O2'	11:A:2833:A:N7	2.42	0.46
19:K:22:ASP:HB2	19:K:147:GLN:HE22	1.81	0.46
33:Y:69:ASP:OD1	33:Y:69:ASP:N	2.38	0.46
36:b:35:ARG:HG3	48:o:101:TRP:HE3	1.80	0.46
37:c:74:ALA:O	37:c:78:ARG:NE	2.42	0.46
32:X:2:PRO:HB2	32:X:3:LEU:H	1.62	0.46
36:b:28:ARG:HB2	36:b:78:GLU:HB3	1.97	0.46
40:f:183:ARG:HE	40:f:184:LEU:N	2.14	0.46
50:q:185:LYS:HA	50:q:188:LYS:HD2	1.98	0.46
56:w:74:LEU:HD13	56:w:152:LYS:HD2	1.97	0.46
11:A:1902:C:O2	43:i:126:LYS:N	2.48	0.46
16:F:191:ASP:OD1	16:F:191:ASP:N	2.45	0.46
1:0:95:ARG:NH2	11:A:1819:U:OP2	2.48	0.46
16:F:83:HIS:HB3	16:F:86:VAL:HG12	1.97	0.46
16:F:99:VAL:HG21	16:F:173:GLY:HA3	1.97	0.46
30:V:57:PHE:HD2	30:V:156:LYS:HE2	1.81	0.46
31:W:53:ILE:HG21	31:W:56:MET:HG3	1.98	0.46
33:Y:231:ALA:HA	33:Y:234:LEU:HD12	1.98	0.46
38:d:216:MET:SD	38:d:216:MET:N	2.89	0.46
54:u:185:ARG:NH2	54:u:191:GLU:OE2	2.49	0.46
11:A:2104:A:H1'	34:Z:35:LYS:HD2	1.97	0.46
11:A:2987:U:O2'	11:A:2991:U:OP1	2.33	0.46
45:k:18:VAL:HG23	45:k:64:VAL:HG12	1.97	0.46
54:u:118:MET:HG3	54:u:197:ARG:HE	1.81	0.46
6:5:68:PRO:O	11:A:1713:A:N6	2.49	0.45
8:7:254:LEU:HD13	8:7:261:ILE:HD11	1.98	0.45
14:D:194:ASN:HD22	14:D:243:THR:HG22	1.80	0.45
16:F:86:VAL:HG13	16:F:87:PHE:HD2	1.81	0.45
16:F:120:VAL:HG13	16:F:142:ARG:HG3	1.97	0.45
18:J:28:LEU:HD23	18:J:31:PRO:HB3	1.98	0.45
23:O:45:PRO:HA	23:O:120:MET:HA	1.98	0.45
37:c:60:ARG:HA	37:c:63:LYS:HG2	1.98	0.45
54:u:105:ASN:O	54:u:107:ARG:NH1	2.49	0.45
11:A:2617:A:O2'	11:A:2619:A:N7	2.49	0.45
16:F:284:TYR:O	16:F:290:TYR:OH	2.32	0.45
43:i:102:MET:HE1	43:i:110:LEU:HD22	1.97	0.45
52:s:60:LEU:HD23	52:s:63:ILE:HD12	1.98	0.45
4:3:133:LEU:HD22	4:3:141:LYS:HG2	1.97	0.45
11:A:1681:G:OP1	30:V:18:HIS:NE2	2.50	0.45
4:3:142:LYS:HE2	11:A:2857:U:H5''	1.97	0.45
5:4:71:VAL:HA	11:A:2160:A:H61	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:259:LYS:HB3	14:D:261:GLY:H	1.82	0.45
18:J:49:PHE:HD1	18:J:78:PHE:HE2	1.64	0.45
22:N:218:ILE:HG23	22:N:223:MET:HB3	1.98	0.45
25:Q:116:ILE:HD13	25:Q:178:LYS:HB3	1.99	0.45
32:X:59:ARG:NH2	50:q:93:TYR:OH	2.45	0.45
44:j:71:GLU:O	44:j:75:ARG:N	2.49	0.45
57:y:189:MET:HE2	57:y:194:ILE:HG13	1.97	0.45
58:x:320:VAL:O	58:x:324:ALA:N	2.49	0.45
6:5:248:THR:HB	6:5:371:LYS:HG2	1.99	0.45
11:A:2171:U:O4	18:J:147:SER:OG	2.33	0.45
11:A:3398:G:O2'	11:A:3401:C:N4	2.47	0.45
19:K:21:LEU:HB2	19:K:59:ILE:HG12	1.97	0.45
36:b:41:ARG:HA	36:b:44:ARG:HH21	1.82	0.45
42:h:85:ASN:HB3	42:h:88:ASP:HB3	1.99	0.45
11:A:2055:U:H2'	11:A:2056:G:C8	2.52	0.45
15:E:56:GLU:O	23:O:153:ARG:NH1	2.49	0.45
25:Q:138:ILE:HD13	25:Q:152:ARG:HD2	1.99	0.45
34:Z:82:GLU:HG2	34:Z:113:VAL:HG23	1.99	0.45
44:j:48:ASP:HB2	44:j:60:MET:HE3	1.98	0.45
11:A:3399:A:OP1	15:E:260:LYS:NZ	2.50	0.45
27:S:172:MET:HG2	27:S:183:LYS:HA	1.98	0.45
29:U:3:ARG:H	29:U:23:ASN:HB3	1.80	0.45
57:y:274:TYR:HD1	57:y:288:PRO:HD2	1.81	0.45
59:z:55:VAL:HB	59:z:156:LYS:HG2	1.98	0.45
1:0:121:VAL:HG12	23:O:109:GLN:HG2	1.98	0.45
8:7:155:GLU:HG2	8:7:164:VAL:HG21	1.98	0.45
11:A:2142:A:O2'	11:A:2262:C:OP1	2.34	0.45
13:H:108:ARG:NH2	13:H:143:GLU:OE1	2.50	0.45
19:K:2:SER:OG	19:K:3:SER:N	2.49	0.45
21:M:290:LEU:HD23	50:q:82:LEU:HD21	1.99	0.45
28:T:84:LYS:HD3	28:T:149:ARG:HB3	1.97	0.45
33:Y:154:ARG:O	33:Y:158:THR:OG1	2.33	0.45
57:y:239:PHE:HD2	58:x:25:HIS:HE1	1.65	0.45
58:x:79:ASN:ND2	58:x:128:ASN:O	2.50	0.45
58:x:114:GLN:HB3	58:x:343:HIS:CE1	2.51	0.45
11:A:2388:A:H5''	14:D:75:THR:HA	1.99	0.45
15:E:107:MET:HE1	25:Q:94:ILE:HG22	1.99	0.45
22:N:222:ASN:O	34:Z:114:LYS:NZ	2.50	0.45
43:i:71:LYS:HB2	43:i:82:GLY:HA3	1.98	0.45
6:5:100:LYS:HD2	6:5:271:TYR:CZ	2.52	0.45
11:A:1684:C:H4'	16:F:113:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:212:PRO:HA	13:C:213:ILE:HA	1.64	0.45
15:E:122:LEU:HD11	15:E:297:VAL:HG21	1.98	0.45
16:F:185:ASP:OD1	42:h:114:ASN:ND2	2.50	0.45
39:e:55:ARG:HB3	39:e:157:LEU:HB2	1.99	0.45
42:h:63:PRO:HD2	42:h:66:LEU:HD13	1.98	0.45
11:A:3065:U:OP2	15:E:239:ARG:NH2	2.50	0.44
14:D:155:GLU:N	14:D:246:ARG:O	2.50	0.44
16:F:89:THR:HG22	16:F:179:THR:HG21	1.98	0.44
25:Q:121:THR:HG22	25:Q:171:VAL:HG12	1.98	0.44
57:y:237:ALA:HA	57:y:241:MET:HB2	1.98	0.44
7:6:162:PHE:HB3	7:6:165:ALA:HB3	1.99	0.44
9:8:150:LEU:O	9:8:154:SER:OG	2.32	0.44
11:A:1773:A:OP1	37:c:31:VAL:N	2.50	0.44
14:D:66:TRP:CE2	14:D:79:MET:HG3	2.52	0.44
23:O:77:ASP:O	23:O:83:LYS:NZ	2.50	0.44
11:A:1756:A:H2'	11:A:1757:A:H8	1.82	0.44
15:E:147:VAL:HB	15:E:179:PHE:HE2	1.82	0.44
37:c:216:ARG:HA	37:c:220:ILE:HD13	1.98	0.44
54:u:101:LEU:HD23	54:u:138:MET:HE2	1.99	0.44
58:x:79:ASN:HD21	58:x:129:LEU:HA	1.82	0.44
6:5:351:VAL:HA	6:5:381:LEU:HA	1.99	0.44
11:A:2695:G:OP1	11:A:2941:G:O2'	2.28	0.44
11:A:2813:U:O4'	11:A:2839:C:N4	2.48	0.44
20:L:123:ILE:HD12	20:L:141:ALA:HB2	1.98	0.44
27:S:137:GLY:HA3	27:S:142:THR:HG22	1.99	0.44
36:b:72:VAL:HG13	36:b:90:HIS:HB2	1.98	0.44
52:s:91:TYR:CE2	52:s:268:PRO:HG2	2.52	0.44
52:s:241:ILE:HG12	52:s:297:THR:HB	1.99	0.44
5:4:75:ARG:HD3	11:A:2964:U:C4	2.53	0.44
17:G:47:LEU:HD13	22:N:226:ILE:HD13	1.99	0.44
19:K:5:SER:O	19:K:9:GLN:N	2.43	0.44
38:d:183:TRP:CH2	38:d:185:PHE:HB2	2.52	0.44
41:g:128:LEU:HD22	41:g:136:PRO:HB3	1.99	0.44
50:q:214:PRO:HG2	50:q:221:SER:HA	1.98	0.44
55:v:9:VAL:HG22	55:v:55:LEU:HD11	1.99	0.44
15:E:200:PRO:HD3	15:E:276:ILE:HD12	2.00	0.44
17:G:47:LEU:HD11	22:N:218:ILE:HG21	2.00	0.44
32:X:226:LEU:HD23	32:X:229:ILE:HD12	1.99	0.44
37:c:220:ILE:HG21	37:c:314:TRP:CE2	2.52	0.44
37:c:245:LEU:HD12	37:c:253:PRO:HD3	1.99	0.44
51:r:81:TYR:O	51:r:184:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:185:VAL:HG13	52:s:195:LEU:HD23	2.00	0.44
54:u:106:ALA:HB2	54:u:138:MET:HE1	2.00	0.44
1:0:107:ILE:HD11	1:0:116:LEU:HD13	1.99	0.44
6:5:291:LEU:H	6:5:344:SER:HA	1.82	0.44
11:A:2405:C:OP1	14:D:103:ARG:NH1	2.50	0.44
32:X:27:HIS:CG	32:X:200:GLU:HG3	2.52	0.44
38:d:153:ASN:ND2	38:d:183:TRP:O	2.44	0.44
49:p:105:LEU:HG	49:p:133:LEU:HB2	1.98	0.44
58:x:168:ALA:O	58:x:379:LYS:NZ	2.38	0.44
1:0:158:VAL:HG23	1:0:175:ILE:HG13	1.99	0.44
6:5:245:ILE:O	6:5:248:THR:OG1	2.35	0.44
8:7:112:PRO:HB2	8:7:267:PRO:HG2	1.99	0.44
11:A:2369:A:H5'	33:Y:121:ARG:HD3	2.00	0.44
11:A:2650:C:OP1	59:z:229:HIS:NE2	2.51	0.44
11:A:2828:G:N2	11:A:2840:C:O2	2.39	0.44
19:K:34:MET:HE3	19:K:34:MET:HB2	1.85	0.44
21:M:98:LEU:HD23	21:M:101:LEU:HD12	2.00	0.44
25:Q:135:GLY:HA3	25:Q:151:LEU:HB3	2.00	0.44
30:V:19:TYR:OH	30:V:31:ASP:OD2	2.35	0.44
57:y:154:LEU:HD13	57:y:188:THR:HG22	1.98	0.44
4:3:169:ARG:H	4:3:169:ARG:HG2	1.60	0.44
5:4:72:LEU:HD23	5:4:90:VAL:HG23	1.99	0.44
7:6:320:GLN:HE22	24:P:52:ASN:ND2	2.11	0.44
14:D:108:ASP:OD1	14:D:113:ARG:NH2	2.51	0.44
21:M:94:LYS:HG3	21:M:129:ILE:HG22	2.00	0.44
52:s:91:TYR:CE2	52:s:229:LEU:HD12	2.53	0.44
59:z:100:LEU:HD13	59:z:108:VAL:HG21	1.99	0.44
8:7:243:LYS:HA	8:7:243:LYS:HD3	1.76	0.43
11:A:1802:A:OP1	30:V:20:ARG:NH1	2.42	0.43
15:E:142:MET:SD	15:E:142:MET:N	2.91	0.43
20:L:57:CYS:HA	20:L:75:LEU:HA	1.99	0.43
24:P:58:LEU:HA	49:p:177:ARG:HH21	1.83	0.43
37:c:148:MET:HE3	37:c:148:MET:HB3	1.81	0.43
50:q:149:ASP:HA	50:q:152:ARG:HG2	1.99	0.43
55:v:68:ARG:HH21	55:v:70:ILE:HD11	1.83	0.43
4:3:97:PHE:HB3	43:i:88:LEU:HD22	2.00	0.43
7:6:139:TRP:CD1	24:P:135:ARG:HH22	2.36	0.43
11:A:2181:A:N7	11:A:2206:C:O2'	2.48	0.43
21:M:130:GLN:HA	21:M:131:PRO:HD3	1.90	0.43
47:m:53:PRO:HB2	47:m:65:HIS:HD2	1.83	0.43
7:6:345:VAL:HG21	31:W:143:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:157:LEU:HD22	39:e:184:LEU:HD11	2.00	0.43
11:A:1805:A:H4'	30:V:96:ARG:HB3	1.99	0.43
15:E:61:ILE:HD11	23:O:149:LEU:HD23	2.00	0.43
13:H:67:GLU:HG2	32:X:61:ARG:HH12	1.83	0.43
30:V:108:MET:HG3	38:d:166:GLU:HB3	2.00	0.43
37:c:92:PHE:HE1	37:c:175:VAL:HG13	1.82	0.43
44:j:31:GLN:HE22	44:j:33:LEU:HD12	1.83	0.43
44:j:100:GLU:HG2	44:j:103:ARG:HH21	1.83	0.43
51:r:79:HIS:HB2	51:r:184:ASN:HA	2.00	0.43
5:4:84:ARG:NE	11:A:3375:U:OP2	2.50	0.43
7:6:355:LYS:HE3	7:6:355:LYS:HB2	1.85	0.43
11:A:2471:G:O2'	11:A:2654:U:O4	2.32	0.43
11:A:2651:A:O2'	59:z:281:LYS:O	2.35	0.43
16:F:97:HIS:HA	21:M:27:LEU:HD13	1.99	0.43
39:e:87:HIS:HB2	47:m:69:ARG:HB2	1.99	0.43
57:y:107:ALA:O	57:y:111:GLU:N	2.51	0.43
6:5:310:ARG:HH21	6:5:379:ASP:H	1.65	0.43
6:5:355:LEU:HD12	6:5:376:VAL:HG12	2.01	0.43
10:9:24:LYS:NZ	11:A:2422:U:OP2	2.48	0.43
16:F:170:ARG:NH2	43:i:58:ASP:O	2.49	0.43
28:T:133:ASN:ND2	38:d:226:ASP:OD1	2.51	0.43
51:r:97:GLY:O	51:r:123:HIS:NE2	2.51	0.43
51:r:121:MET:HE3	51:r:121:MET:HB2	1.85	0.43
26:R:112:THR:N	36:b:127:GLN:OE1	2.48	0.43
3:2:69:ARG:HA	3:2:69:ARG:HD3	1.85	0.43
6:5:394:LYS:HA	6:5:394:LYS:HD2	1.74	0.43
7:6:267:ARG:HH22	24:P:51:ARG:HG3	1.84	0.43
8:7:311:THR:HG23	15:E:154:ARG:HE	1.82	0.43
11:A:2693:A:OP1	48:o:15:ARG:NH2	2.51	0.43
11:A:2809:C:O2'	11:A:2923:G:OP2	2.34	0.43
11:A:2863:U:OP1	31:W:54:LYS:NZ	2.45	0.43
15:E:122:LEU:HB3	15:E:283:ILE:HB	2.00	0.43
27:S:113:LEU:HD23	27:S:194:ARG:HB3	2.01	0.43
34:Z:73:LYS:HB3	34:Z:116:LEU:HG	2.00	0.43
1:0:97:PRO:HA	1:0:100:LEU:HB3	2.01	0.43
11:A:2243:A:H5''	51:r:188:SER:HB3	2.01	0.43
11:A:2275:U:H5''	37:c:34:GLY:HA3	2.01	0.43
11:A:2512:A:H5''	14:D:256:VAL:HG22	2.00	0.43
11:A:3008:C:O2'	11:A:3051:A:N3	2.44	0.43
22:N:218:ILE:HA	22:N:223:MET:HB2	2.00	0.43
28:T:202:GLN:OE1	35:a:122:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:x:39:PRO:HG2	58:x:42:ARG:HE	1.83	0.43
6:5:149:ASN:HB3	6:5:152:GLU:HB3	2.01	0.43
7:6:307:HIS:HB3	7:6:311:MET:HE2	2.01	0.43
15:E:207:THR:HB	15:E:267:THR:HG23	2.01	0.43
19:K:76:VAL:HA	19:K:91:THR:HA	2.00	0.43
58:x:72:LYS:NZ	58:x:138:ASP:O	2.45	0.43
11:A:2853:A:N1	11:A:2878:G:O2'	2.40	0.43
11:A:3344:C:H1'	25:Q:84:ARG:HG2	2.01	0.43
19:K:61:ASN:ND2	19:K:130:ASP:O	2.51	0.43
26:R:95:VAL:HG11	27:S:144:LEU:HD23	2.01	0.43
27:S:132:LYS:NZ	44:j:42:PRO:O	2.52	0.43
29:U:151:PHE:CG	38:d:222:LEU:HD21	2.53	0.43
30:V:44:VAL:HG12	30:V:46:VAL:HG13	2.00	0.43
36:b:35:ARG:O	36:b:44:ARG:NH1	2.52	0.43
44:j:78:VAL:HG23	44:j:79:LEU:HD12	2.01	0.43
7:6:351:HIS:ND1	11:A:2860:G:OP1	2.43	0.42
11:A:2612:C:O2	11:A:2621:G:N2	2.52	0.42
11:A:2673:G:H5''	28:T:112:LYS:HB2	2.01	0.42
27:S:115:LEU:HB2	36:b:11:LEU:HD11	2.01	0.42
55:v:51:ARG:HG2	62:v:101:PNS:H432	2.01	0.42
58:x:277:ARG:O	58:x:281:ARG:N	2.47	0.42
5:4:70:THR:O	11:A:2160:A:N6	2.52	0.42
11:A:2101:C:H5'	48:o:18:ILE:HG22	2.00	0.42
29:U:42:PHE:HB2	29:U:95:ALA:HB3	2.00	0.42
38:d:165:THR:HA	38:d:260:ARG:HH21	1.84	0.42
39:e:92:LEU:O	39:e:96:GLN:N	2.47	0.42
39:e:99:ALA:HA	39:e:102:LYS:HB2	2.00	0.42
39:e:143:LYS:HE2	39:e:143:LYS:HB3	1.80	0.42
39:e:266:PRO:HD2	39:e:269:LEU:HB2	2.01	0.42
8:7:275:CYS:HA	8:7:303:PRO:HA	2.01	0.42
11:A:1681:G:OP2	33:Y:230:LYS:NZ	2.52	0.42
11:A:2848:A:H2'	11:A:2849:G:C8	2.53	0.42
15:E:87:ILE:HG23	15:E:317:PRO:HG2	2.01	0.42
16:F:232:GLU:O	16:F:235:SER:OG	2.36	0.42
19:K:40:GLN:NE2	19:K:113:PRO:HD3	2.34	0.42
21:M:222:TYR:CE2	21:M:262:PRO:HB3	2.55	0.42
31:W:46:SER:OG	31:W:49:ARG:NH2	2.52	0.42
32:X:176:LEU:HB3	32:X:184:ARG:HG2	2.00	0.42
38:d:177:LYS:HD2	38:d:177:LYS:HA	1.84	0.42
51:r:99:MET:HG3	51:r:116:GLU:HG2	2.01	0.42
6:5:203:CYS:HA	6:5:230:LEU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2520:C:H2'	14:D:206:TYR:HE1	1.84	0.42
20:L:60:VAL:HA	20:L:73:ILE:HG22	2.00	0.42
21:M:186:ILE:HD12	21:M:193:PHE:CG	2.55	0.42
28:T:53:LYS:HA	28:T:53:LYS:HD3	1.89	0.42
28:T:197:LYS:HA	28:T:197:LYS:HD3	1.76	0.42
42:h:73:TYR:HA	42:h:76:GLU:HG2	2.01	0.42
52:s:236:LYS:HB3	52:s:236:LYS:HE3	1.82	0.42
59:z:153:ASN:H	64:z:401:GCP:H3B1	1.84	0.42
4:3:154:GLN:NE2	11:A:2867:C:O3'	2.50	0.42
7:6:177:TYR:CD1	7:6:202:PRO:HB3	2.54	0.42
11:A:1743:U:H2'	11:A:1744:A:H8	1.85	0.42
11:A:2204:U:N3	11:A:2207:A:OP2	2.51	0.42
21:M:146:ASP:OD1	21:M:146:ASP:N	2.53	0.42
23:O:146:ASN:O	23:O:150:GLN:N	2.49	0.42
25:Q:113:VAL:HG12	25:Q:187:LEU:HG	2.02	0.42
29:U:130:LEU:HD21	30:V:98:ILE:HG23	2.02	0.42
34:Z:71:ARG:HH21	34:Z:75:THR:HG23	1.85	0.42
52:s:366:TYR:HB3	52:s:398:SER:HB2	2.01	0.42
58:x:71:GLN:HG3	58:x:262:ARG:NH1	2.35	0.42
58:x:257:PRO:HG3	63:x:401:SAM:H8	0.42	0.42
58:x:257:PRO:CG	63:x:401:SAM:H2'	2.49	0.42
11:A:2366:G:N2	38:d:62:LYS:O	2.53	0.42
15:E:328:LEU:HB3	15:E:332:LEU:HD11	2.01	0.42
36:b:44:ARG:NH1	48:o:99:LYS:O	2.53	0.42
37:c:215:ILE:HG23	37:c:219:LEU:HD12	2.02	0.42
39:e:168:GLN:HB3	39:e:170:VAL:HG23	2.01	0.42
47:m:53:PRO:HB2	47:m:65:HIS:CD2	2.54	0.42
50:q:153:ARG:HH22	58:x:85:HIS:HB2	1.85	0.42
52:s:101:ASN:HA	52:s:322:VAL:HG11	2.02	0.42
57:y:195:ASN:HA	57:y:198:VAL:HG12	2.01	0.42
4:3:129:TYR:HA	4:3:144:LEU:HD13	2.02	0.42
11:A:2655:G:N2	11:A:2659:C:O2'	2.53	0.42
16:F:86:VAL:HA	16:F:175:LYS:HD3	2.02	0.42
21:M:17:ARG:NH2	42:h:115:SER:OG	2.40	0.42
21:M:102:GLN:HB2	21:M:148:PHE:HD1	1.84	0.42
23:O:16:ARG:N	23:O:51:GLU:OE2	2.52	0.42
24:P:122:VAL:HG22	24:P:157:SER:HB3	2.01	0.42
25:Q:81:ILE:HD11	25:Q:279:GLU:HG3	2.02	0.42
42:h:139:LYS:HG3	42:h:143:LEU:HG	2.00	0.42
52:s:249:GLU:HA	52:s:356:VAL:HG21	2.01	0.42
7:6:360:ARG:NH1	11:A:2869:A:OP2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2625:C:H2'	11:A:2626:U:H5''	2.02	0.42
30:V:28:SER:HA	38:d:70:GLU:HG3	2.02	0.42
57:y:241:MET:HE2	57:y:241:MET:HB3	1.91	0.42
58:x:164:LEU:HD23	58:x:167:LEU:HD12	2.00	0.42
8:7:40:LEU:HD11	8:7:232:HIS:HB2	2.02	0.42
18:J:32:GLY:HA3	18:J:33:PRO:HD3	1.93	0.42
29:U:80:ARG:NH1	29:U:84:ASN:O	2.53	0.42
1:0:156:THR:HG22	1:0:173:ARG:HB3	2.02	0.42
2:1:17:LEU:HD12	2:1:65:LEU:HD11	2.00	0.42
5:4:81:LEU:HD12	5:4:90:VAL:HG22	2.01	0.42
11:A:2556:A:O2'	11:A:2600:A:OP1	2.31	0.42
14:D:66:TRP:HB3	14:D:80:ARG:HB2	2.02	0.42
16:F:126:LYS:HD2	16:F:139:GLY:HA2	2.01	0.42
20:L:119:ILE:HG21	20:L:123:ILE:HD11	2.00	0.42
22:N:124:VAL:HG23	22:N:160:VAL:HA	2.02	0.42
26:R:115:SER:HA	35:a:47:VAL:HG11	2.02	0.42
37:c:54:PRO:HA	37:c:55:PRO:HD2	1.94	0.42
58:x:191:LEU:HD11	58:x:253:LEU:HD13	2.01	0.42
18:J:138:SER:HA	18:J:141:VAL:HG12	2.01	0.41
26:R:100:LYS:HE2	28:T:212:LEU:HD11	2.02	0.41
39:e:63:LEU:HB2	39:e:68:GLU:HG2	2.02	0.41
2:1:65:LEU:HD23	2:1:65:LEU:HA	1.87	0.41
6:5:50:TYR:HE1	6:5:57:PRO:HG3	1.85	0.41
7:6:366:LEU:HD23	7:6:366:LEU:HA	1.89	0.41
10:9:69:LYS:HD3	10:9:71:LYS:HE2	2.01	0.41
28:T:201:GLN:HA	28:T:204:ARG:HB2	2.01	0.41
37:c:43:LYS:HD3	37:c:43:LYS:HA	1.75	0.41
38:d:224:ILE:HB	38:d:233:TYR:HB3	2.02	0.41
39:e:65:PRO:HA	39:e:68:GLU:HB2	2.02	0.41
39:e:93:ASP:HA	39:e:96:GLN:HB2	2.02	0.41
39:e:179:GLN:HG2	39:e:181:GLY:H	1.84	0.41
41:g:139:GLN:HB3	41:g:148:ARG:HB2	2.00	0.41
52:s:177:LEU:HD21	52:s:299:PHE:HB3	2.01	0.41
56:w:132:ASP:OD1	56:w:132:ASP:N	2.48	0.41
14:D:86:ASP:OD2	14:D:92:ARG:NE	2.51	0.41
23:O:76:ALA:HB1	23:O:86:ILE:HD12	2.01	0.41
37:c:127:GLU:HA	37:c:130:THR:HG22	2.01	0.41
41:g:154:ASP:O	41:g:158:LYS:N	2.53	0.41
56:w:76:LEU:HD12	56:w:79:ILE:HD12	2.02	0.41
59:z:198:MET:HE2	59:z:198:MET:HB3	1.85	0.41
2:1:17:LEU:N	2:1:63:ARG:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2511:C:H3'	11:A:2512:A:H8	1.86	0.41
11:A:2825:G:H5''	31:W:49:ARG:HH21	1.84	0.41
16:F:184:GLN:HE22	21:M:20:PRO:C	2.29	0.41
23:O:110:ILE:HB	23:O:120:MET:HG3	2.02	0.41
52:s:66:TRP:O	52:s:69:THR:OG1	2.36	0.41
11:A:2255:C:H4'	44:j:44:THR:HG21	2.02	0.41
16:F:45:GLU:HA	16:F:46:PRO:HD3	1.90	0.41
16:F:156:ARG:HD2	16:F:156:ARG:HA	1.86	0.41
24:P:169:GLY:O	49:p:184:ASN:ND2	2.47	0.41
25:Q:119:VAL:HG13	25:Q:174:ILE:HG22	2.03	0.41
41:g:105:ARG:HH22	48:o:83:PRO:HD2	1.86	0.41
50:q:153:ARG:HH12	58:x:85:HIS:H	1.69	0.41
52:s:164:HIS:H	52:s:167:GLU:HG2	1.85	0.41
10:9:24:LYS:HE3	29:U:74:HIS:HB2	2.03	0.41
12:B:1603:A:N6	12:B:1668:U:O2	2.53	0.41
16:F:201:GLN:O	16:F:204:THR:OG1	2.35	0.41
18:J:25:ARG:HG2	18:J:65:PRO:HB3	2.02	0.41
26:R:71:ARG:HH12	28:T:211:THR:HB	1.85	0.41
34:Z:38:ARG:HE	34:Z:81:TRP:CG	2.39	0.41
43:i:77:PRO:HD2	43:i:80:LEU:HD11	2.02	0.41
48:o:15:ARG:HA	48:o:15:ARG:HD3	1.84	0.41
57:y:96:MET:HG3	57:y:109:ILE:HD13	2.02	0.41
1:0:81:PRO:HA	11:A:3292:U:C2	2.56	0.41
3:2:92:HIS:CE1	10:9:17:ARG:HG2	2.56	0.41
5:4:66:PHE:N	11:A:3013:G:O2'	2.50	0.41
10:9:104:PHE:HZ	32:X:242:ALA:HB2	1.85	0.41
11:A:2686:G:H5'	11:A:3294:U:H4'	2.01	0.41
11:A:3378:A:C4	51:r:133:PRO:HG3	2.56	0.41
45:k:54:ASP:N	45:k:54:ASP:OD1	2.54	0.41
52:s:114:PHE:CE2	52:s:325:ARG:HD3	2.56	0.41
58:x:292:LEU:HD23	58:x:292:LEU:HA	1.91	0.41
64:z:401:GCP:H5'2	64:z:402:GCP:O3A	2.19	0.41
1:0:86:THR:HG21	11:A:2683:C:H5'	2.02	0.41
11:A:1857:U:H4'	11:A:2989:G:C8	2.55	0.41
11:A:2194:U:O2'	11:A:2195:A:O4'	2.39	0.41
17:G:138:SER:OG	17:G:139:LYS:N	2.53	0.41
22:N:64:ARG:HD2	22:N:144:LYS:HG2	2.03	0.41
28:T:73:ILE:HD11	28:T:134:VAL:HG21	2.02	0.41
30:V:69:ASP:HB3	30:V:72:LYS:HD3	2.03	0.41
37:c:149:PRO:HD3	37:c:305:TYR:CE1	2.55	0.41
48:o:12:ILE:HD12	48:o:16:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:q:134:ASN:HA	50:q:137:GLN:HB2	2.02	0.41
54:u:109:ILE:HA	54:u:127:VAL:HG12	2.03	0.41
8:7:67:VAL:HG12	8:7:123:CYS:H	1.86	0.41
11:A:2245:A:H61	51:r:190:THR:HG23	1.86	0.41
11:A:2334:C:OP1	52:s:221:HIS:NE2	2.45	0.41
11:A:3067:PSU:H3'	11:A:3258:G:H5'	2.03	0.41
11:A:3376:C:H1'	51:r:154:TRP:HB3	2.03	0.41
15:E:304:LEU:HA	15:E:305:PRO:HD2	1.96	0.41
16:F:263:LEU:HD23	16:F:263:LEU:HA	1.90	0.41
13:H:55:ILE:HG21	32:X:44:ARG:HG2	2.03	0.41
22:N:132:THR:HG22	22:N:147:ILE:HD13	2.03	0.41
38:d:142:LYS:HD3	38:d:142:LYS:HA	1.93	0.41
39:e:69:GLU:O	39:e:72:SER:OG	2.32	0.41
39:e:86:ASP:HA	39:e:89:LEU:HD12	2.03	0.41
45:k:40:GLU:HA	45:k:43:ARG:HB2	2.03	0.41
58:x:308:SER:HB2	58:x:375:MET:HE3	2.01	0.41
59:z:163:LEU:HD23	59:z:163:LEU:HA	1.91	0.41
4:3:114:PHE:CE1	4:3:124:ARG:HB3	2.55	0.41
7:6:161:LEU:HD11	7:6:219:THR:HG21	2.02	0.41
15:E:83:GLU:O	15:E:188:LYS:NZ	2.38	0.41
21:M:164:ILE:HG12	21:M:174:VAL:HG11	2.03	0.41
33:Y:223:LYS:HB3	33:Y:223:LYS:HE2	1.80	0.41
40:f:60:LYS:HE3	40:f:60:LYS:HB3	1.90	0.41
47:m:51:LEU:HB3	47:m:67:ARG:HB2	2.01	0.41
54:u:121:THR:OG1	54:u:122:ASP:N	2.54	0.41
59:z:52:ILE:HD13	59:z:52:ILE:HA	1.94	0.41
6:5:354:PHE:HB3	6:5:417:LEU:HD11	2.03	0.40
15:E:173:LYS:HZ2	15:E:173:LYS:HG3	1.61	0.40
13:H:56:VAL:HB	13:H:80:TYR:HB3	2.03	0.40
25:Q:225:LYS:HD3	59:z:291:VAL:HG12	2.03	0.40
45:k:49:CYS:SG	45:k:50:SER:N	2.95	0.40
59:z:123:ILE:HG13	59:z:167:HIS:NE2	2.35	0.40
6:5:181:VAL:HG11	6:5:347:THR:HG21	2.03	0.40
8:7:67:VAL:O	8:7:79:PHE:N	2.45	0.40
8:7:67:VAL:HG11	8:7:119:LEU:HD21	2.02	0.40
8:7:306:LEU:HD23	23:O:145:LEU:HB2	2.04	0.40
11:A:3312:A:H62	11:A:3319:G:H21	1.69	0.40
15:E:109:LEU:HD13	15:E:119:VAL:HG21	2.03	0.40
39:e:98:LEU:HD11	39:e:116:LEU:HA	2.03	0.40
59:z:37:LYS:HB3	59:z:37:LYS:HE3	1.95	0.40
59:z:240:LEU:HD21	59:z:309:PHE:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:104:ILE:HD12	8:7:129:THR:HA	2.04	0.40
8:7:210:ILE:HA	8:7:272:THR:HG22	2.04	0.40
16:F:99:VAL:HG11	16:F:250:VAL:HG21	2.03	0.40
21:M:73:PRO:HG2	21:M:76:ILE:HD12	2.03	0.40
24:P:96:HIS:HB3	24:P:100:LYS:HB2	2.03	0.40
34:Z:75:THR:HB	34:Z:83:LYS:HG3	2.03	0.40
40:f:130:LYS:HA	40:f:130:LYS:HD2	1.87	0.40
58:x:259:THR:HG23	58:x:273:PHE:HE1	1.86	0.40
6:5:52:ILE:HG21	32:X:164:GLY:HA3	2.03	0.40
8:7:230:PHE:HD2	8:7:240:ILE:HD11	1.86	0.40
11:A:1977:U:H2'	11:A:1978:A:H8	1.87	0.40
11:A:2094:G:P	21:M:62:ARG:HH22	2.44	0.40
16:F:166:PRO:HB2	16:F:169:VAL:HG23	2.04	0.40
16:F:248:LEU:HD12	16:F:248:LEU:HA	1.84	0.40
32:X:176:LEU:HD21	32:X:187:ILE:HG13	2.03	0.40
32:X:176:LEU:HD22	32:X:184:ARG:HA	2.04	0.40
34:Z:69:VAL:HG13	34:Z:91:LEU:HD21	2.03	0.40
38:d:84:ILE:HG23	38:d:211:GLN:HE22	1.86	0.40
42:h:124:ARG:HA	42:h:127:LEU:HD12	2.04	0.40
55:v:63:ASN:HB3	55:v:65:LYS:HG3	2.03	0.40
58:x:239:ARG:HH21	63:x:401:SAM:HN61	1.67	0.40
6:5:301:PRO:HD3	11:A:2390:A:H4'	2.03	0.40
7:6:310:THR:OG1	7:6:311:MET:SD	2.64	0.40
11:A:1723:A:O3'	21:M:64:ARG:NH1	2.54	0.40
11:A:1788:C:O2	11:A:1918:G:N2	2.54	0.40
11:A:1880:C:OP2	41:g:111:ARG:NH2	2.54	0.40
11:A:2388:A:H1'	14:D:141:LEU:HD11	2.03	0.40
21:M:167:ILE:O	21:M:171:GLY:N	2.53	0.40
24:P:83:VAL:HB	24:P:158:MET:HE1	2.03	0.40
25:Q:201:ASP:HB2	25:Q:204:MET:HB2	2.03	0.40
26:R:119:LEU:HD21	35:a:58:ILE:HG21	2.04	0.40
29:U:27:GLN:HB2	33:Y:117:GLN:HE22	1.86	0.40
32:X:238:LEU:O	32:X:242:ALA:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	106/188 (56%)	101 (95%)	5 (5%)	0	100	100
2	1	50/65 (77%)	50 (100%)	0	0	100	100
3	2	43/92 (47%)	42 (98%)	0	1 (2%)	5	23
4	3	93/188 (50%)	93 (100%)	0	0	100	100
5	4	35/103 (34%)	35 (100%)	0	0	100	100
6	5	390/423 (92%)	367 (94%)	22 (6%)	1 (0%)	36	65
7	6	316/380 (83%)	305 (96%)	11 (4%)	0	100	100
8	7	285/338 (84%)	262 (92%)	23 (8%)	0	100	100
9	8	92/206 (45%)	77 (84%)	9 (10%)	6 (6%)	1	6
10	9	113/137 (82%)	104 (92%)	9 (8%)	0	100	100
13	C	78/267 (29%)	68 (87%)	8 (10%)	2 (3%)	4	21
13	H	93/267 (35%)	90 (97%)	3 (3%)	0	100	100
14	D	215/305 (70%)	186 (86%)	28 (13%)	1 (0%)	24	54
15	E	302/348 (87%)	286 (95%)	15 (5%)	1 (0%)	36	65
16	F	248/311 (80%)	234 (94%)	14 (6%)	0	100	100
17	G	163/261 (62%)	155 (95%)	8 (5%)	0	100	100
18	J	138/192 (72%)	120 (87%)	17 (12%)	1 (1%)	18	47
19	K	175/178 (98%)	167 (95%)	8 (5%)	0	100	100
20	L	113/145 (78%)	104 (92%)	9 (8%)	0	100	100
21	M	285/296 (96%)	270 (95%)	15 (5%)	0	100	100
22	N	196/251 (78%)	189 (96%)	7 (4%)	0	100	100
23	O	150/175 (86%)	144 (96%)	6 (4%)	0	100	100
24	P	139/180 (77%)	133 (96%)	6 (4%)	0	100	100
25	Q	215/292 (74%)	200 (93%)	15 (7%)	0	100	100
26	R	138/149 (93%)	136 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	S	154/205 (75%)	146 (95%)	8 (5%)	0	100	100
28	T	164/206 (80%)	158 (96%)	6 (4%)	0	100	100
29	U	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	9	33
30	V	200/216 (93%)	192 (96%)	7 (4%)	1 (0%)	24	54
31	W	107/148 (72%)	107 (100%)	0	0	100	100
32	X	241/256 (94%)	228 (95%)	13 (5%)	0	100	100
33	Y	174/250 (70%)	170 (98%)	4 (2%)	0	100	100
34	Z	118/161 (73%)	113 (96%)	5 (4%)	0	100	100
35	a	78/142 (55%)	74 (95%)	4 (5%)	0	100	100
36	b	146/215 (68%)	134 (92%)	12 (8%)	0	100	100
37	c	271/332 (82%)	264 (97%)	7 (3%)	0	100	100
38	d	203/306 (66%)	194 (96%)	9 (4%)	0	100	100
39	e	211/279 (76%)	196 (93%)	15 (7%)	0	100	100
40	f	110/212 (52%)	97 (88%)	13 (12%)	0	100	100
41	g	127/166 (76%)	118 (93%)	9 (7%)	0	100	100
42	h	96/158 (61%)	92 (96%)	4 (4%)	0	100	100
43	i	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
44	j	83/123 (68%)	80 (96%)	3 (4%)	0	100	100
45	k	76/112 (68%)	73 (96%)	3 (4%)	0	100	100
46	l	21/138 (15%)	21 (100%)	0	0	100	100
47	m	43/128 (34%)	35 (81%)	8 (19%)	0	100	100
48	o	89/102 (87%)	82 (92%)	7 (8%)	0	100	100
49	p	119/206 (58%)	117 (98%)	2 (2%)	0	100	100
50	q	196/222 (88%)	195 (100%)	1 (0%)	0	100	100
51	r	140/196 (71%)	134 (96%)	6 (4%)	0	100	100
52	s	366/439 (83%)	354 (97%)	12 (3%)	0	100	100
54	u	109/234 (47%)	102 (94%)	6 (6%)	1 (1%)	14	42
55	v	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
56	w	77/156 (49%)	69 (90%)	8 (10%)	0	100	100
57	y	243/381 (64%)	228 (94%)	14 (6%)	1 (0%)	30	59
58	x	364/384 (95%)	326 (90%)	37 (10%)	1 (0%)	36	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	z	309/334 (92%)	275 (89%)	33 (11%)	1 (0%)	36	65
All	All	9118/12495 (73%)	8586 (94%)	512 (6%)	20 (0%)	44	71

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	52	GLU
6	5	217	SER
9	8	182	ILE
9	8	184	ASN
9	8	186	GLN
9	8	187	PRO
9	8	188	PRO
18	J	23	ILE
29	U	117	SER
29	U	118	PRO
54	u	150	LYS
13	C	205	THR
58	x	230	GLN
9	8	183	PRO
13	C	204	HIS
14	D	117	THR
30	V	160	PRO
59	z	212	GLU
57	y	282	GLN
15	E	317	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	97/164 (59%)	97 (100%)	0	100	100
2	1	49/60 (82%)	49 (100%)	0	100	100
3	2	39/72 (54%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	36/89 (40%)	36 (100%)	0	100	100
6	5	353/368 (96%)	353 (100%)	0	100	100
7	6	265/332 (80%)	265 (100%)	0	100	100
8	7	263/303 (87%)	263 (100%)	0	100	100
9	8	76/190 (40%)	76 (100%)	0	100	100
10	9	99/112 (88%)	99 (100%)	0	100	100
13	C	73/228 (32%)	73 (100%)	0	100	100
13	H	86/228 (38%)	86 (100%)	0	100	100
14	D	175/245 (71%)	175 (100%)	0	100	100
15	E	259/290 (89%)	259 (100%)	0	100	100
16	F	217/262 (83%)	217 (100%)	0	100	100
17	G	153/232 (66%)	153 (100%)	0	100	100
18	J	113/150 (75%)	113 (100%)	0	100	100
19	K	155/156 (99%)	155 (100%)	0	100	100
20	L	98/124 (79%)	98 (100%)	0	100	100
21	M	245/249 (98%)	245 (100%)	0	100	100
22	N	169/211 (80%)	169 (100%)	0	100	100
23	O	133/150 (89%)	133 (100%)	0	100	100
24	P	123/155 (79%)	123 (100%)	0	100	100
25	Q	199/256 (78%)	199 (100%)	0	100	100
26	R	118/126 (94%)	118 (100%)	0	100	100
27	S	141/180 (78%)	141 (100%)	0	100	100
28	T	146/176 (83%)	146 (100%)	0	100	100
29	U	124/135 (92%)	124 (100%)	0	100	100
30	V	172/191 (90%)	172 (100%)	0	100	100
31	W	89/119 (75%)	89 (100%)	0	100	100
32	X	219/229 (96%)	219 (100%)	0	100	100
33	Y	159/223 (71%)	159 (100%)	0	100	100
34	Z	111/147 (76%)	111 (100%)	0	100	100
35	a	78/133 (59%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	b	130/186 (70%)	130 (100%)	0	100	100
37	c	241/288 (84%)	241 (100%)	0	100	100
38	d	193/274 (70%)	193 (100%)	0	100	100
39	e	188/236 (80%)	188 (100%)	0	100	100
40	f	101/188 (54%)	101 (100%)	0	100	100
41	g	119/148 (80%)	119 (100%)	0	100	100
42	h	95/148 (64%)	95 (100%)	0	100	100
43	i	86/110 (78%)	86 (100%)	0	100	100
44	j	68/97 (70%)	68 (100%)	0	100	100
45	k	71/90 (79%)	71 (100%)	0	100	100
46	l	23/116 (20%)	23 (100%)	0	100	100
47	m	40/113 (35%)	40 (100%)	0	100	100
48	o	78/87 (90%)	78 (100%)	0	100	100
49	p	117/181 (65%)	117 (100%)	0	100	100
50	q	163/178 (92%)	163 (100%)	0	100	100
51	r	133/169 (79%)	133 (100%)	0	100	100
52	s	326/381 (86%)	326 (100%)	0	100	100
54	u	105/200 (52%)	105 (100%)	0	100	100
55	v	59/60 (98%)	59 (100%)	0	100	100
56	w	73/136 (54%)	73 (100%)	0	100	100
57	y	227/350 (65%)	226 (100%)	1 (0%)	84	83
58	x	313/328 (95%)	313 (100%)	0	100	100
59	z	270/287 (94%)	270 (100%)	0	100	100
All	All	8139/10802 (75%)	8138 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	y	195	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	178	GLN
4	3	181	HIS
6	5	94	HIS
6	5	186	GLN
6	5	251	HIS
6	5	269	ASN
6	5	289	HIS
6	5	353	HIS
6	5	380	GLN
6	5	420	HIS
7	6	163	HIS
7	6	239	ASN
7	6	373	HIS
8	7	247	ASN
10	9	90	GLN
10	9	123	GLN
10	9	134	ASN
14	D	87	HIS
15	E	277	ASN
15	E	281	ASN
16	F	58	HIS
16	F	83	HIS
16	F	184	GLN
16	F	228	GLN
16	F	276	GLN
17	G	43	GLN
19	K	26	GLN
19	K	61	ASN
19	K	64	HIS
19	K	126	HIS
19	K	147	GLN
20	L	48	ASN
22	N	178	GLN
22	N	210	GLN
23	O	91	GLN
24	P	52	ASN
24	P	89	HIS
26	R	77	GLN
26	R	89	ASN
27	S	84	ASN
29	U	62	ASN
31	W	59	HIS
31	W	76	HIS

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Mol	Chain	Res	Type
32	X	177	HIS
33	Y	117	GLN
33	Y	195	ASN
33	Y	225	ASN
34	Z	98	GLN
34	Z	102	ASN
34	Z	107	ASN
35	a	126	HIS
36	b	102	GLN
37	c	65	ASN
37	c	177	GLN
37	c	260	GLN
38	d	211	GLN
40	f	54	HIS
40	f	112	ASN
42	h	99	ASN
44	j	105	GLN
45	k	93	HIS
46	l	130	ASN
48	o	58	GLN
49	p	104	HIS
50	q	134	ASN
50	q	176	GLN
51	r	131	HIS
51	r	184	ASN
52	s	107	GLN
52	s	327	ASN
52	s	343	GLN
52	s	387	ASN
52	s	420	GLN
54	u	136	HIS
55	v	42	ASN
57	y	195	ASN
58	x	79	ASN
58	x	230	GLN
58	x	263	HIS
58	x	314	HIS
58	x	335	GLN
59	z	121	GLN
59	z	166	GLN
59	z	191	GLN
59	z	245	ASN

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Mol	Chain	Res	Type
59	z	292	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1443/1737 (83%)	376 (26%)	22 (1%)
12	B	61/69 (88%)	31 (50%)	2 (3%)
All	All	1504/1806 (83%)	407 (27%)	24 (1%)

All (407) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1674	A
11	A	1675	A
11	A	1676	A
11	A	1679	U
11	A	1680	A
11	A	1685	C
11	A	1689	C
11	A	1700	U
11	A	1704	U
11	A	1705	A
11	A	1707	C
11	A	1708	A
11	A	1709	G
11	A	1710	A
11	A	1712	A
11	A	1713	A
11	A	1714	C
11	A	1716	U
11	A	1724	A
11	A	1727	A
11	A	1728	U
11	A	1731	A
11	A	1741	A
11	A	1748	G
11	A	1750	G
11	A	1751	A
11	A	1770	G
11	A	1773	A
11	A	1780	U

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Mol	Chain	Res	Type
11	A	1791	G
11	A	1794	A
11	A	1803	A
11	A	1804	A
11	A	1805	A
11	A	1812	C
11	A	1817	C
11	A	1821	A
11	A	1824	U
11	A	1827	C
11	A	1828	A
11	A	1829	A
11	A	1832	A
11	A	1836	A
11	A	1839	C
11	A	1844	A
11	A	1849	C
11	A	1854	U
11	A	1856	A
11	A	1867	A
11	A	1869	A
11	A	1870	A
11	A	1872	U
11	A	1882	A
11	A	1883	G
11	A	1888	G
11	A	1890	C
11	A	1892	A
11	A	1893	A
11	A	1901	C
11	A	1903	C
11	A	1909	A
11	A	1918	G
11	A	1927	G
11	A	1937	A
11	A	1938	A
11	A	1940	A
11	A	1944	C
11	A	1968	G
11	A	1974	A
11	A	1975	U
11	A	1985	G

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Mol	Chain	Res	Type
11	A	1987	G
11	A	1992	C
11	A	1993	A
11	A	1994	A
11	A	1995	A
11	A	2000	C
11	A	2001	C
11	A	2015	G
11	A	2021	U
11	A	2022	G
11	A	2029	A
11	A	2030	U
11	A	2031	A
11	A	2034	A
11	A	2036	C
11	A	2037	U
11	A	2060	A
11	A	2065	A
11	A	2066	C
11	A	2074	A
11	A	2078	C
11	A	2079	C
11	A	2083	U
11	A	2097	A
11	A	2098	G
11	A	2113	G
11	A	2124	A
11	A	2132	A
11	A	2142	A
11	A	2147	G
11	A	2154	A
11	A	2159	U
11	A	2160	A
11	A	2163	A
11	A	2168	U
11	A	2172	A
11	A	2173	G
11	A	2182	G
11	A	2183	C
11	A	2187	C
11	A	2193	U
11	A	2195	A

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Mol	Chain	Res	Type
11	A	2197	G
11	A	2198	A
11	A	2200	A
11	A	2204	U
11	A	2210	C
11	A	2215	C
11	A	2216	A
11	A	2229	A
11	A	2230	A
11	A	2233	U
11	A	2237	A
11	A	2239	A
11	A	2241	A
11	A	2243	A
11	A	2244	U
11	A	2245	A
11	A	2246	A
11	A	2252	C
11	A	2257	C
11	A	2259	C
11	A	2262	C
11	A	2263	C
11	A	2264	A
11	A	2284	C
11	A	2285	U
11	A	2297	A
11	A	2299	U
11	A	2300	G
11	A	2316	U
11	A	2322	C
11	A	2324	U
11	A	2329	C
11	A	2332	C
11	A	2345	G
11	A	2371	U
11	A	2374	A
11	A	2381	A
11	A	2386	C
11	A	2387	U
11	A	2388	A
11	A	2390	A
11	A	2393	C

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Mol	Chain	Res	Type
11	A	2394	A
11	A	2401	A
11	A	2404	U
11	A	2405	C
11	A	2406	A
11	A	2407	U
11	A	2414	C
11	A	2415	C
11	A	2416	U
11	A	2418	A
11	A	2426	C
11	A	2443	C
11	A	2444	A
11	A	2446	A
11	A	2449	G
11	A	2451	A
11	A	2452	A
11	A	2458	A
11	A	2468	A
11	A	2478	G
11	A	2484	C
11	A	2489	C
11	A	2493	C
11	A	2500	A
11	A	2502	C
11	A	2507	A
11	A	2508	C
11	A	2511	C
11	A	2520	C
11	A	2521	A
11	A	2523	C
11	A	2524	A
11	A	2527	A
11	A	2531	U
11	A	2539	A
11	A	2540	C
11	A	2545	U
11	A	2546	G
11	A	2547	C
11	A	2548	C
11	A	2549	C
11	A	2551	G

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Mol	Chain	Res	Type
11	A	2554	A
11	A	2556	A
11	A	2558	A
11	A	2559	U
11	A	2563	U
11	A	2564	A
11	A	2565	A
11	A	2568	G
11	A	2569	C
11	A	2575	U
11	A	2581	A
11	A	2586	U
11	A	2593	G
11	A	2594	U
11	A	2595	A
11	A	2596	G
11	A	2598	A
11	A	2599	U
11	A	2600	A
11	A	2601	A
11	A	2602	U
11	A	2604	A
11	A	2605	C
11	A	2606	U
11	A	2607	U
11	A	2608	G
11	A	2615	A
11	A	2616	A
11	A	2617	A
11	A	2618	U
11	A	2619	A
11	A	2622	G
11	A	2624	C
11	A	2626	U
11	A	2627	G
11	A	2628	U
11	A	2630	U
11	A	2631	G
11	A	2632	A
11	A	2633	A
11	A	2635	G
11	A	2639	C

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Mol	Chain	Res	Type
11	A	2640	C
11	A	2645	G
11	A	2654	U
11	A	2655	G
11	A	2656	U
11	A	2660	U
11	A	2683	C
11	A	2684	C
11	A	2686	G
11	A	2694	A
11	A	2695	G
11	A	2696	A
11	A	2697	G
11	A	2698	G
11	A	2706	A
11	A	2708	C
11	A	2709	A
11	A	2718	C
11	A	2719	G
11	A	2723	A
11	A	2724	G
11	A	2732	G
11	A	2739	U
11	A	2740	A
11	A	2744	U
11	A	2750	U
11	A	2797	C
11	A	2804	A
11	A	2810	G
11	A	2814	G
11	A	2815	OMG
11	A	2816	G
11	A	2817	G
11	A	2819	G
11	A	2820	A
11	A	2822	C
11	A	2823	U
11	A	2826	G
11	A	2831	G
11	A	2832	A
11	A	2833	A
11	A	2842	C

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Mol	Chain	Res	Type
11	A	2844	G
11	A	2847	C
11	A	2851	A
11	A	2853	A
11	A	2854	U
11	A	2859	A
11	A	2861	A
11	A	2864	U
11	A	2865	C
11	A	2869	A
11	A	2871	U
11	A	2895	U
11	A	2896	G
11	A	2901	A
11	A	2906	C
11	A	2910	A
11	A	2913	A
11	A	2915	C
11	A	2916	G
11	A	2917	G
11	A	2918	A
11	A	2919	A
11	A	2922	A
11	A	2926	A
11	A	2928	C
11	A	2932	G
11	A	2935	A
11	A	2946	A
11	A	2955	U
11	A	2956	A
11	A	2963	A
11	A	2971	A
11	A	2985	C
11	A	2989	G
11	A	2990	A
11	A	2991	U
11	A	2993	U
11	A	3000	A
11	A	3005	A
11	A	3016	G
11	A	3022	G
11	A	3040	OMG

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Mol	Chain	Res	Type
11	A	3041	U
11	A	3042	U
11	A	3045	A
11	A	3051	A
11	A	3053	A
11	A	3054	G
11	A	3056	C
11	A	3060	C
11	A	3063	G
11	A	3067	PSU
11	A	3259	A
11	A	3260	G
11	A	3262	U
11	A	3263	C
11	A	3267	C
11	A	3276	U
11	A	3279	A
11	A	3280	G
11	A	3283	C
11	A	3287	U
11	A	3288	U
11	A	3290	U
11	A	3292	U
11	A	3298	U
11	A	3299	U
11	A	3301	U
11	A	3309	U
11	A	3310	G
11	A	3318	G
11	A	3328	A
11	A	3337	U
11	A	3342	C
11	A	3344	C
11	A	3345	A
11	A	3347	A
11	A	3348	G
11	A	3349	C
11	A	3355	C
11	A	3356	C
11	A	3359	C
11	A	3360	G
11	A	3367	A

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Mol	Chain	Res	Type
11	A	3371	C
11	A	3376	C
11	A	3377	A
11	A	3383	G
11	A	3385	U
11	A	3389	C
11	A	3390	A
11	A	3396	A
11	A	3397	A
11	A	3399	A
11	A	3407	U
12	B	1606	G
12	B	1608	G
12	B	1609	U
12	B	1610	A
12	B	1611	G
12	B	1612	C
12	B	1614	U
12	B	1618	A
12	B	1619	C
12	B	1620	A
12	B	1621	A
12	B	1622	A
12	B	1623	G
12	B	1624	C
12	B	1626	C
12	B	1633	U
12	B	1635	C
12	B	1636	A
12	B	1646	U
12	B	1647	U
12	B	1648	U
12	B	1649	C
12	B	1650	A
12	B	1651	A
12	B	1653	U
12	B	1654	U
12	B	1655	A
12	B	1656	A
12	B	1657	C
12	B	1659	U
12	B	1667	C

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	1709	G
11	A	1713	A
11	A	1823	A
11	A	1871	A
11	A	2030	U
11	A	2186	C
11	A	2243	A
11	A	2245	A
11	A	2457	A
11	A	2507	A
11	A	2530	A
11	A	2544	C
11	A	2574	G
11	A	2617	A
11	A	2631	G
11	A	2653	C
11	A	2815	OMG
11	A	2816	G
11	A	2818	C
11	A	2905	A
11	A	3040	OMG
11	A	3282	U
12	B	1607	U
12	B	1635	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	OMG	A	2815	11	23,26,27	2.40	6 (26%)	32,38,41	2.99	16 (50%)
11	PSU	A	3067	11	18,21,22	2.05	8 (44%)	21,30,33	2.02	4 (19%)
11	OMG	A	3040	11	23,26,27	2.39	5 (21%)	32,38,41	3.22	15 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	OMU	A	3039	11	19,22,23	2.57	6 (31%)	25,31,34	2.01	6 (24%)

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
11	OMG	A	2815	11	2/2/5/5	1/9/27/28	0/3/3/3
11	PSU	A	3067	11	-	1/7/25/26	0/2/2/2
11	OMG	A	3040	11	3/3/5/5	4/9/27/28	0/3/3/3
11	OMU	A	3039	11	-	6/9/27/28	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	3039	OMU	O4-C4	9.20	1.42	1.24
11	A	2815	OMG	O6-C6	8.97	1.40	1.23
11	A	3040	OMG	O6-C6	8.95	1.40	1.23
11	A	3040	OMG	C2-N2	4.92	1.45	1.34
11	A	2815	OMG	C2-N2	4.88	1.45	1.34
11	A	3067	PSU	C4-N3	-3.68	1.32	1.38
11	A	3067	PSU	C2-N3	-3.54	1.31	1.37
11	A	3067	PSU	C2-N1	-3.53	1.32	1.36
11	A	3067	PSU	C6-C5	3.31	1.39	1.35
11	A	2815	OMG	C6-N1	-3.25	1.32	1.38
11	A	3040	OMG	C6-N1	-3.17	1.32	1.38
11	A	3039	OMU	C2-N1	-3.01	1.33	1.38
11	A	3039	OMU	C2-N3	-2.89	1.32	1.38
11	A	3067	PSU	O4-C4	-2.69	1.18	1.23
11	A	3039	OMU	O2-C2	-2.50	1.18	1.23
11	A	3067	PSU	C6-N1	-2.41	1.32	1.36
11	A	3067	PSU	O2-C2	-2.40	1.18	1.23
11	A	3039	OMU	C4-N3	-2.37	1.34	1.38
11	A	3039	OMU	C5-C4	-2.34	1.38	1.43
11	A	3040	OMG	C5-N7	-2.26	1.34	1.39
11	A	2815	OMG	C5-N7	-2.21	1.34	1.39
11	A	3040	OMG	C8-N9	-2.21	1.32	1.37
11	A	3067	PSU	C4-C5	-2.20	1.38	1.44
11	A	2815	OMG	C8-N9	-2.19	1.32	1.37
11	A	2815	OMG	C2-N1	-2.00	1.32	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	3040	OMG	O2'-C2'-C1'	7.65	123.52	108.99
11	A	3040	OMG	C2'-C1'-N9	7.00	127.53	114.24
11	A	2815	OMG	O2'-C2'-C1'	6.58	121.48	108.99
11	A	2815	OMG	C2'-C1'-N9	6.36	126.30	114.24
11	A	3067	PSU	N1-C2-N3	6.23	121.74	115.17
11	A	2815	OMG	C5-C4-N3	-6.09	118.69	128.39
11	A	3040	OMG	C5-C4-N3	-6.09	118.69	128.39
11	A	3040	OMG	C2-N3-C4	5.43	121.66	112.30
11	A	3039	OMU	N3-C2-N1	5.40	121.92	114.89
11	A	2815	OMG	C2-N3-C4	5.32	121.47	112.30
11	A	3040	OMG	O3'-C3'-C2'	5.07	125.37	111.19
11	A	3040	OMG	O4'-C1'-N9	4.96	119.61	108.36
11	A	2815	OMG	O4'-C1'-N9	4.84	119.33	108.36
11	A	3039	OMU	C4-N3-C2	-4.68	120.80	126.61
11	A	3067	PSU	C4-N3-C2	-4.08	120.74	126.37
11	A	3040	OMG	O3'-C3'-C4'	4.05	122.73	111.08
11	A	2815	OMG	N9-C4-N3	4.03	134.01	125.95
11	A	3039	OMU	C5-C4-N3	3.88	120.23	114.80
11	A	3040	OMG	N9-C4-N3	3.86	133.68	125.95
11	A	3040	OMG	O4'-C4'-C5'	3.82	121.57	109.33
11	A	2815	OMG	O3'-C3'-C2'	3.77	121.73	111.19
11	A	3039	OMU	O4-C4-C5	-3.72	118.74	125.16
11	A	2815	OMG	O3'-C3'-C4'	3.63	121.51	111.08
11	A	3040	OMG	C5'-C4'-C3'	3.60	128.16	115.21
11	A	2815	OMG	O4'-C4'-C5'	3.46	120.41	109.33
11	A	2815	OMG	C5'-C4'-C3'	3.35	127.28	115.21
11	A	3067	PSU	O2-C2-N1	-2.99	119.70	122.79
11	A	3040	OMG	C6-C5-N7	2.56	134.94	130.29
11	A	2815	OMG	C6-C5-N7	2.56	134.94	130.29
11	A	2815	OMG	C4-C5-N7	-2.40	106.86	110.67
11	A	3040	OMG	C4-C5-N7	-2.40	106.86	110.67
11	A	2815	OMG	C5-C6-N1	2.40	119.36	113.25
11	A	3040	OMG	C5-C6-N1	2.38	119.31	113.25
11	A	3067	PSU	C6-N1-C2	-2.35	120.51	122.69
11	A	2815	OMG	O6-C6-C5	-2.34	120.35	126.53
11	A	3040	OMG	O6-C6-C5	-2.34	120.35	126.53
11	A	2815	OMG	C2-N1-C6	-2.29	120.95	125.11
11	A	3040	OMG	C2-N1-C6	-2.28	120.98	125.11
11	A	3039	OMU	C6-C5-C4	-2.12	116.83	119.53
11	A	2815	OMG	C8-N7-C5	2.10	108.00	104.26
11	A	3039	OMU	O2-C2-N1	-2.06	120.12	122.80

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	2815	OMG	C4'
11	A	2815	OMG	C3'
11	A	3040	OMG	C1'
11	A	3040	OMG	C2'
11	A	3040	OMG	C4'

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2815	OMG	C4'-C5'-O5'-P
11	A	3039	OMU	C2'-C1'-N1-C2
11	A	3039	OMU	C2'-C1'-N1-C6
11	A	3040	OMG	C1'-C2'-O2'-CM2
11	A	3040	OMG	C3'-C4'-C5'-O5'
11	A	3067	PSU	C3'-C4'-C5'-O5'
11	A	3039	OMU	O4'-C4'-C5'-O5'
11	A	3040	OMG	O4'-C4'-C5'-O5'
11	A	3039	OMU	O4'-C1'-N1-C6
11	A	3039	OMU	C4'-C5'-O5'-P
11	A	3039	OMU	O4'-C1'-N1-C2
11	A	3040	OMG	C2'-C1'-N9-C8

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	3067	PSU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 97 ligands modelled in this entry, 93 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
64	GCP	z	402	-	32,34,34	3.55	13 (40%)	49,54,54	1.79	9 (18%)
64	GCP	z	401	-	32,34,34	3.43	14 (43%)	49,54,54	2.08	15 (30%)
62	PNS	v	101	-	14,20,21	2.17	4 (28%)	18,26,29	1.25	1 (5%)
63	SAM	x	401	-	27,29,29	0.48	0	34,42,42	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
64	GCP	z	402	-	2/2/7/7	5/19/38/38	0/3/3/3
62	PNS	v	101	-	-	8/24/26/27	-
64	GCP	z	401	-	1/1/7/7	7/19/38/38	0/3/3/3
63	SAM	x	401	-	1/1/7/7	9/17/33/33	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	z	402	GCP	O6-C6	8.81	1.40	1.23
64	z	401	GCP	O6-C6	8.72	1.40	1.23
64	z	402	GCP	C3'-C4'	-8.52	1.31	1.53
64	z	401	GCP	C3'-C4'	-8.32	1.31	1.53
64	z	402	GCP	O4'-C4'	7.71	1.62	1.45
64	z	401	GCP	O4'-C4'	7.57	1.61	1.45
64	z	402	GCP	PB-O3A	7.06	1.66	1.58
64	z	402	GCP	PA-O3A	6.07	1.66	1.59
64	z	401	GCP	PB-O3A	5.94	1.65	1.58
62	v	101	PNS	C34-N36	5.09	1.45	1.33
62	v	101	PNS	C39-N41	5.09	1.45	1.33
64	z	401	GCP	O4'-C1'	-4.97	1.30	1.42
64	z	402	GCP	C2-N2	4.89	1.45	1.34
64	z	401	GCP	C2-N2	4.88	1.45	1.34
64	z	401	GCP	PA-O3A	4.75	1.64	1.59
64	z	402	GCP	O4'-C1'	-4.64	1.31	1.42
64	z	401	GCP	C6-N1	-3.43	1.32	1.38
64	z	402	GCP	C6-N1	-3.37	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	z	401	GCP	O3'-C3'	2.84	1.50	1.43
64	z	402	GCP	O3'-C3'	2.83	1.50	1.43
64	z	401	GCP	O2'-C2'	-2.81	1.36	1.43
64	z	402	GCP	PB-O2B	-2.64	1.49	1.56
64	z	402	GCP	O2'-C2'	-2.63	1.36	1.43
64	z	401	GCP	C5-N7	-2.62	1.33	1.39
64	z	401	GCP	C8-N9	-2.61	1.31	1.37
62	v	101	PNS	O35-C34	-2.28	1.19	1.23
62	v	101	PNS	O40-C39	-2.21	1.18	1.23
64	z	402	GCP	C5-N7	-2.18	1.34	1.39
64	z	401	GCP	PB-O2B	-2.10	1.51	1.56
64	z	402	GCP	C2-N1	-2.01	1.32	1.37
64	z	401	GCP	C2-N1	-2.01	1.32	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	z	402	GCP	C5-C4-N3	-6.26	118.42	128.39
64	z	401	GCP	C5-C4-N3	-6.03	118.80	128.39
64	z	402	GCP	C2-N3-C4	5.63	122.00	112.30
64	z	401	GCP	C2-N3-C4	5.49	121.76	112.30
64	z	401	GCP	N9-C4-N3	4.45	134.86	125.95
64	z	402	GCP	N9-C4-N3	4.40	134.74	125.95
64	z	401	GCP	C8-N7-C5	3.72	110.88	104.26
64	z	401	GCP	N9-C8-N7	-3.58	106.76	113.40
64	z	401	GCP	PB-O3A-PA	-3.13	122.16	132.37
64	z	401	GCP	C4-C5-N7	-3.11	105.73	110.67
64	z	401	GCP	C6-C5-N7	2.93	135.63	130.29
64	z	402	GCP	C6-C5-N7	2.71	135.23	130.29
64	z	402	GCP	C8-N7-C5	2.68	109.04	104.26
64	z	402	GCP	C4-C5-N7	-2.58	106.58	110.67
62	v	101	PNS	C37-N36-C34	-2.49	118.08	122.55
64	z	401	GCP	O6-C6-C5	-2.47	120.00	126.53
64	z	402	GCP	C5-C6-N1	2.33	119.19	113.25
64	z	402	GCP	N9-C8-N7	-2.33	109.08	113.40
64	z	401	GCP	C8-N9-C4	2.27	110.28	106.03
64	z	401	GCP	C4'-O4'-C1'	-2.23	104.54	109.47
64	z	401	GCP	O3G-PG-O1G	-2.17	106.78	112.39
64	z	401	GCP	C5-C6-N1	2.17	118.77	113.25
64	z	401	GCP	O2G-PG-O1G	-2.14	106.85	112.39
64	z	401	GCP	O2A-PA-O1A	-2.04	102.95	112.44
64	z	402	GCP	O6-C6-C5	-2.02	121.21	126.53

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
63	x	401	SAM	CA
64	z	401	GCP	C2'
64	z	402	GCP	C2'
64	z	402	GCP	C4'

All (29) torsion outliers are listed below:

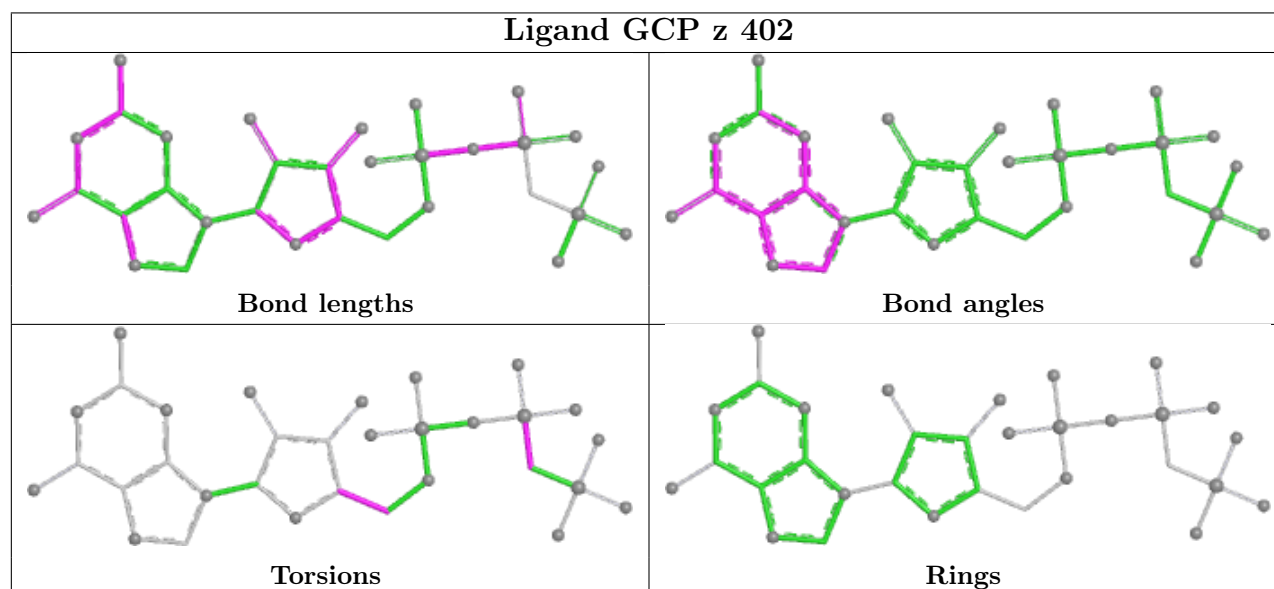
Mol	Chain	Res	Type	Atoms
62	v	101	PNS	C28-C29-C32-O33
62	v	101	PNS	C28-C29-C32-C34
62	v	101	PNS	C31-C29-C32-O33
62	v	101	PNS	C31-C29-C32-C34
63	x	401	SAM	C4'-C5'-SD-CE
64	z	401	GCP	PB-C3B-PG-O1G
64	z	401	GCP	PB-C3B-PG-O2G
64	z	401	GCP	PB-C3B-PG-O3G
64	z	401	GCP	C5'-O5'-PA-O3A
64	z	401	GCP	C5'-O5'-PA-O1A
64	z	402	GCP	PG-C3B-PB-O1B
64	z	402	GCP	PG-C3B-PB-O2B
64	z	402	GCP	PG-C3B-PB-O3A
64	z	401	GCP	C3'-C4'-C5'-O5'
64	z	402	GCP	C3'-C4'-C5'-O5'
63	x	401	SAM	C2'-C1'-N9-C8
62	v	101	PNS	C30-C29-C32-O33
64	z	401	GCP	O4'-C4'-C5'-O5'
63	x	401	SAM	OXT-C-CA-N
62	v	101	PNS	C30-C29-C32-C34
63	x	401	SAM	CA-CB-CG-SD
63	x	401	SAM	C2'-C1'-N9-C4
64	z	402	GCP	O4'-C4'-C5'-O5'
62	v	101	PNS	C37-C38-C39-O40
62	v	101	PNS	C37-C38-C39-N41
63	x	401	SAM	O-C-CA-CB
63	x	401	SAM	O4'-C1'-N9-C8
63	x	401	SAM	OXT-C-CA-CB
63	x	401	SAM	CB-CG-SD-C5'

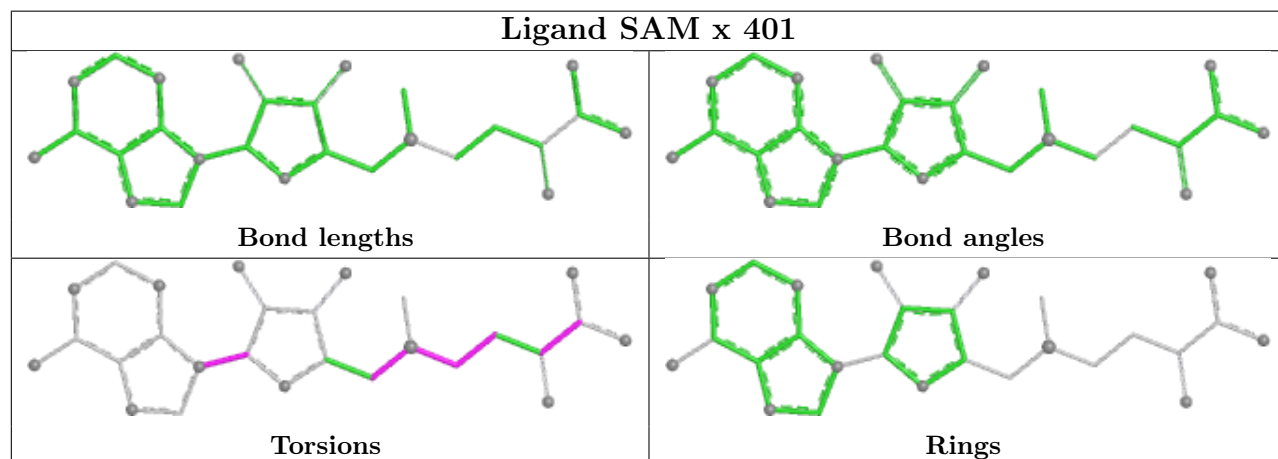
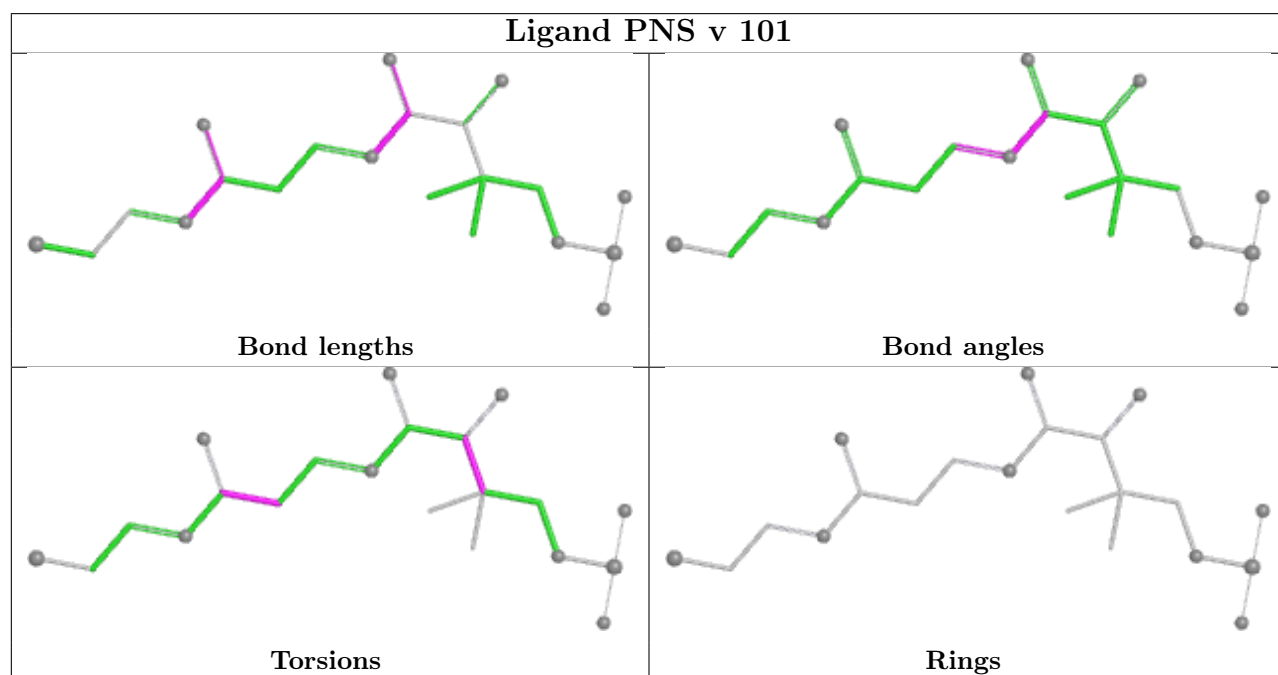
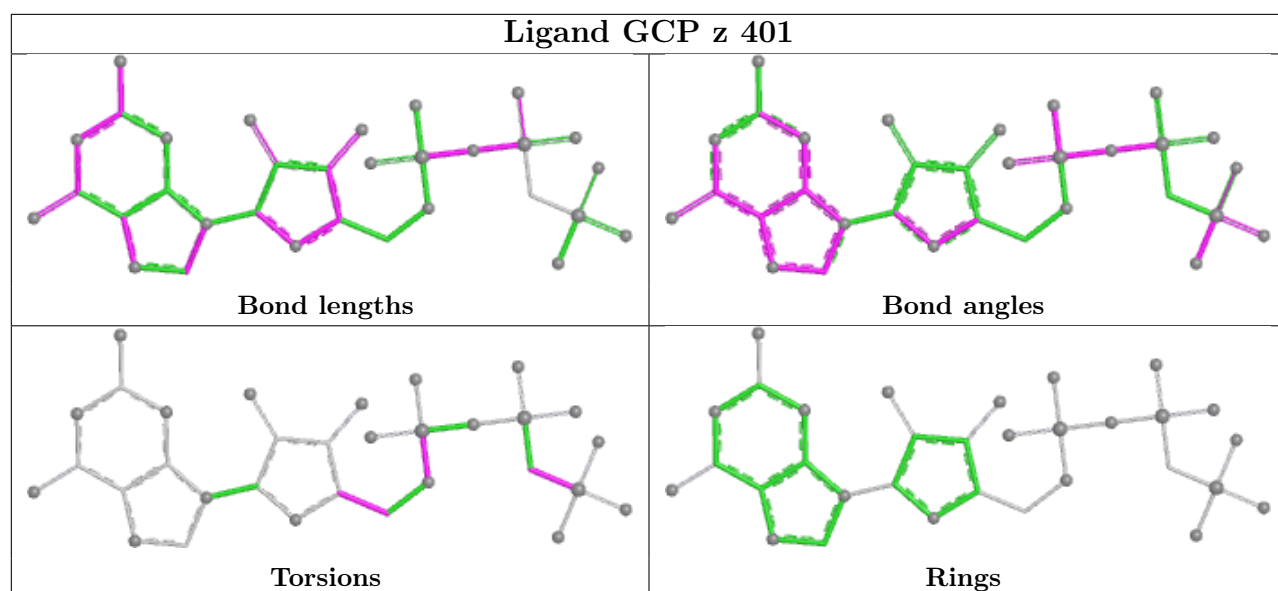
There are no ring outliers.

4 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	z	402	GCP	2	0
64	z	401	GCP	6	0
62	v	101	PNS	1	0
63	x	401	SAM	34	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3390:A	O3'	3391:C	P	21.25
1	A	3383:G	O3'	3384:A	P	15.46
1	A	3299:U	O3'	3300:A	P	11.65

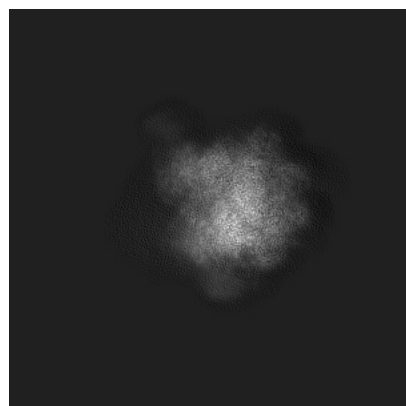
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13329. These allow visual inspection of the internal detail of the map and identification of artifacts.

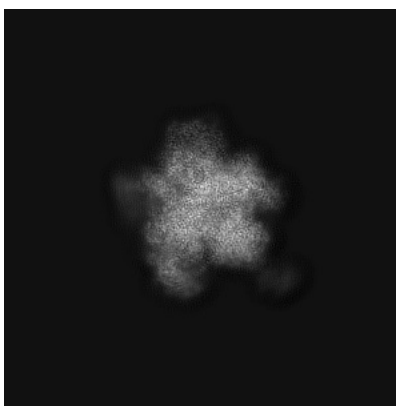
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

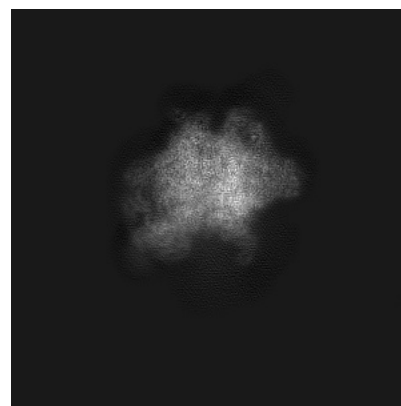
6.1.1 Primary map



X

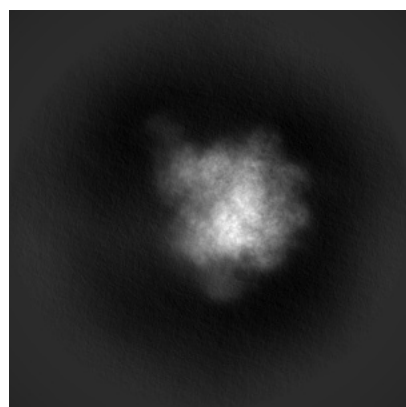


Y

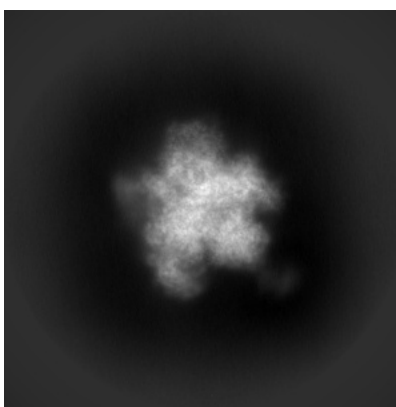


Z

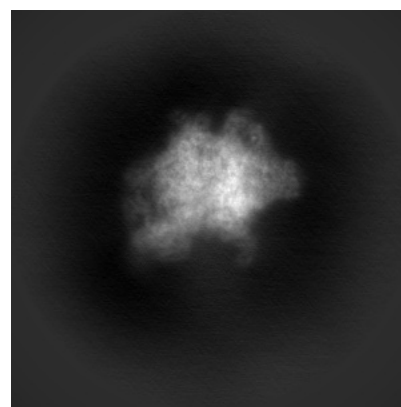
6.1.2 Raw map



X



Y

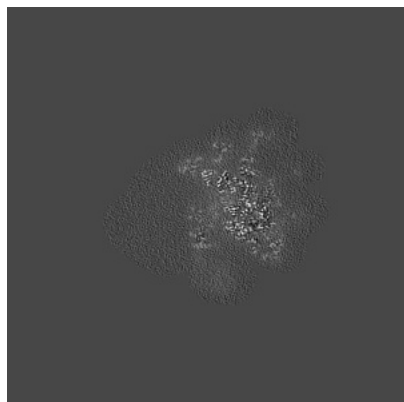


Z

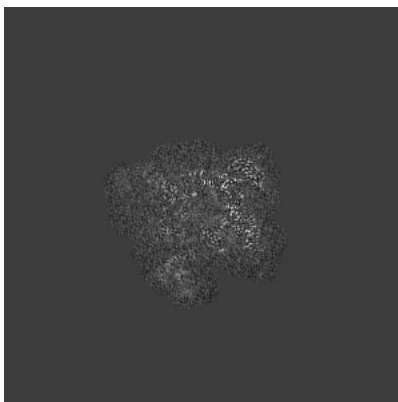
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

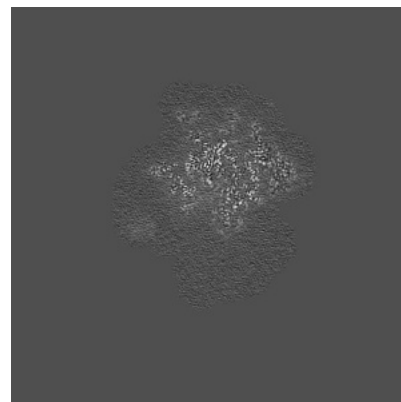
6.2.1 Primary map



X Index: 256

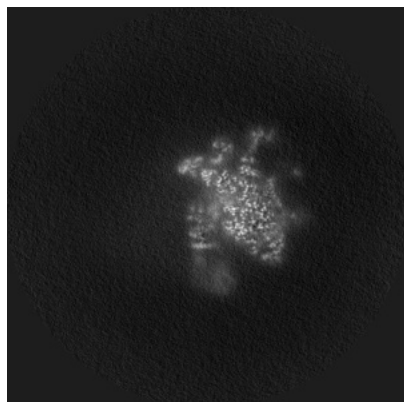


Y Index: 256

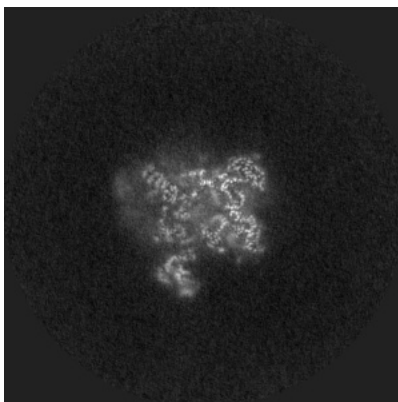


Z Index: 256

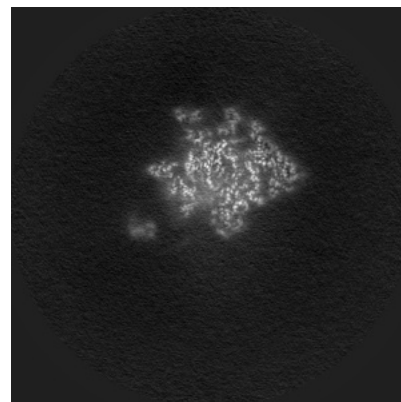
6.2.2 Raw map



X Index: 256



Y Index: 256

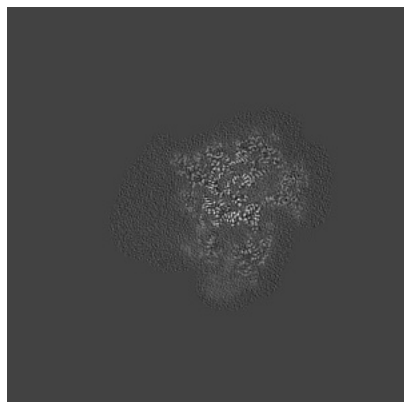


Z Index: 256

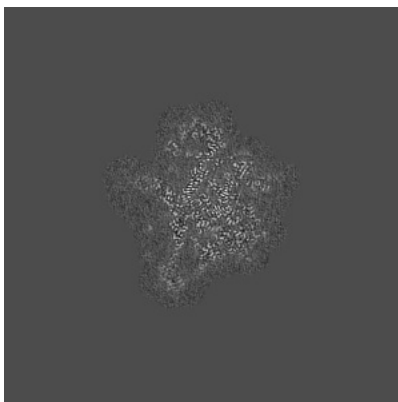
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

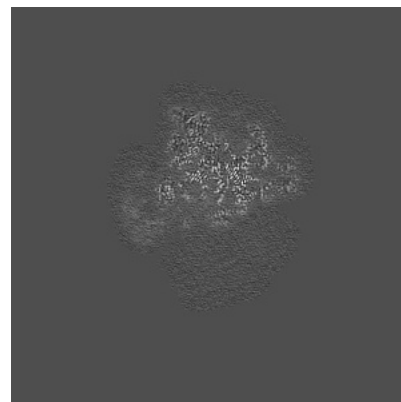
6.3.1 Primary map



X Index: 286

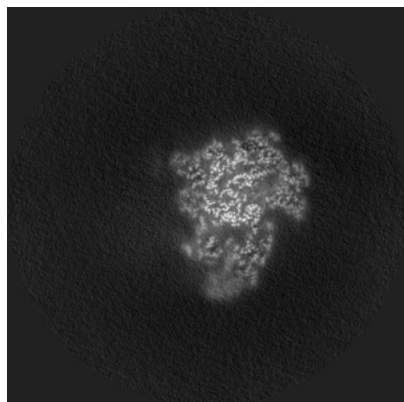


Y Index: 304

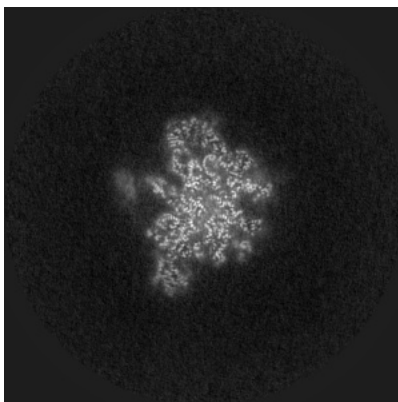


Z Index: 240

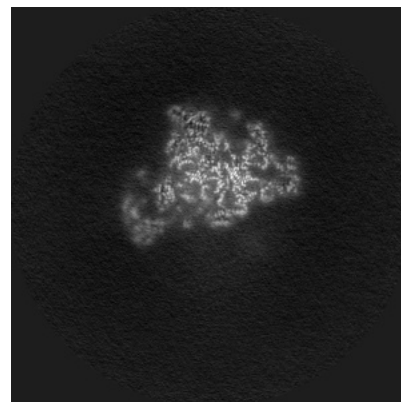
6.3.2 Raw map



X Index: 285



Y Index: 291

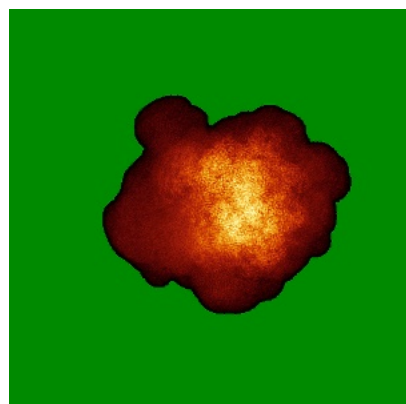


Z Index: 240

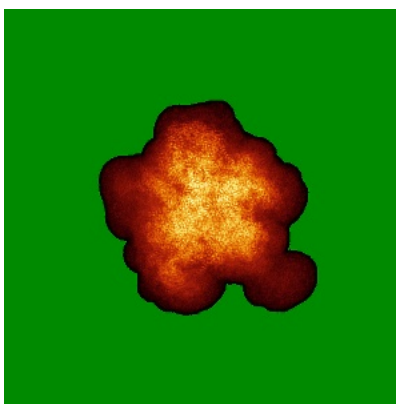
The images above show the largest variance slices of the map in three orthogonal directions.

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

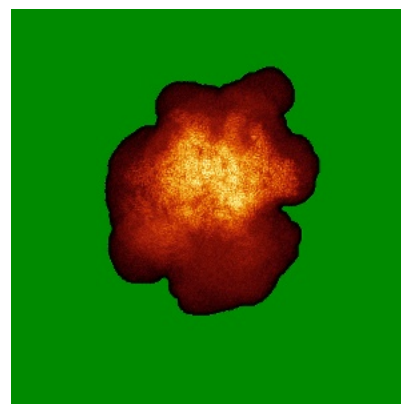
6.4.1 Primary map



X

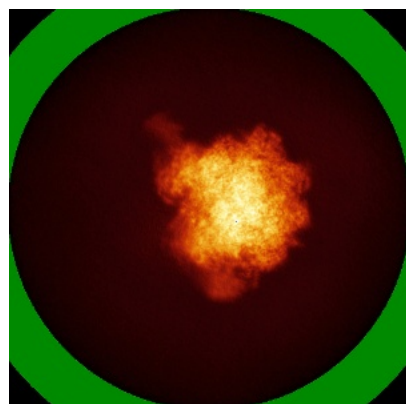


Y

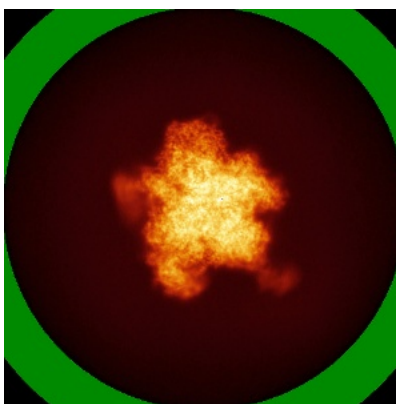


Z

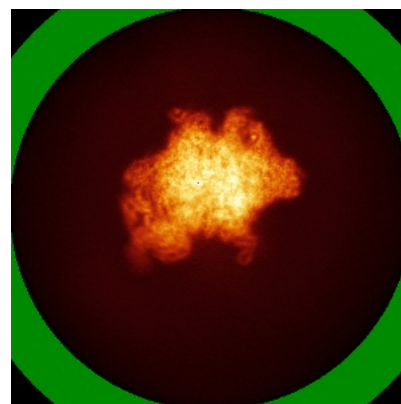
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

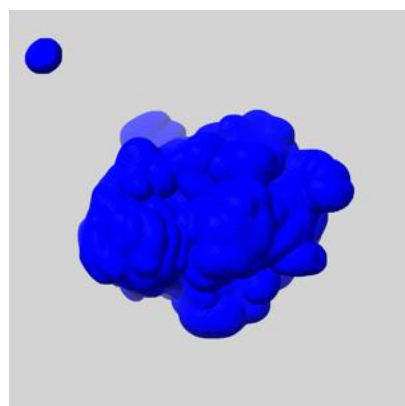
6.6 Mask visualisation [i](#)

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

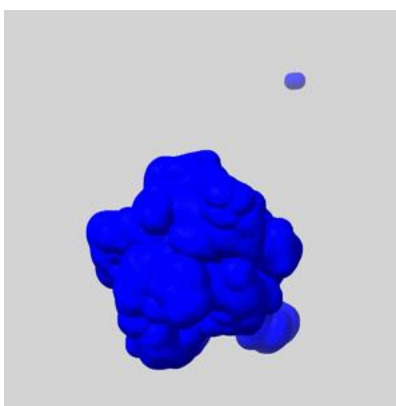
A mask typically either:

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

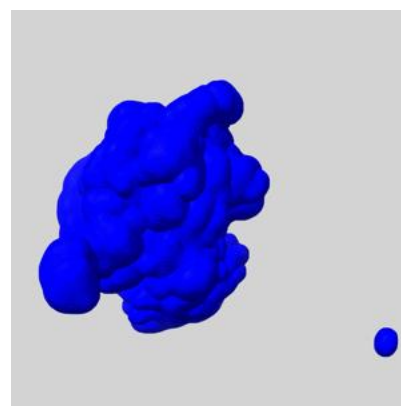
6.6.1 emd_13329_msk_1.map [i](#)



X



Y

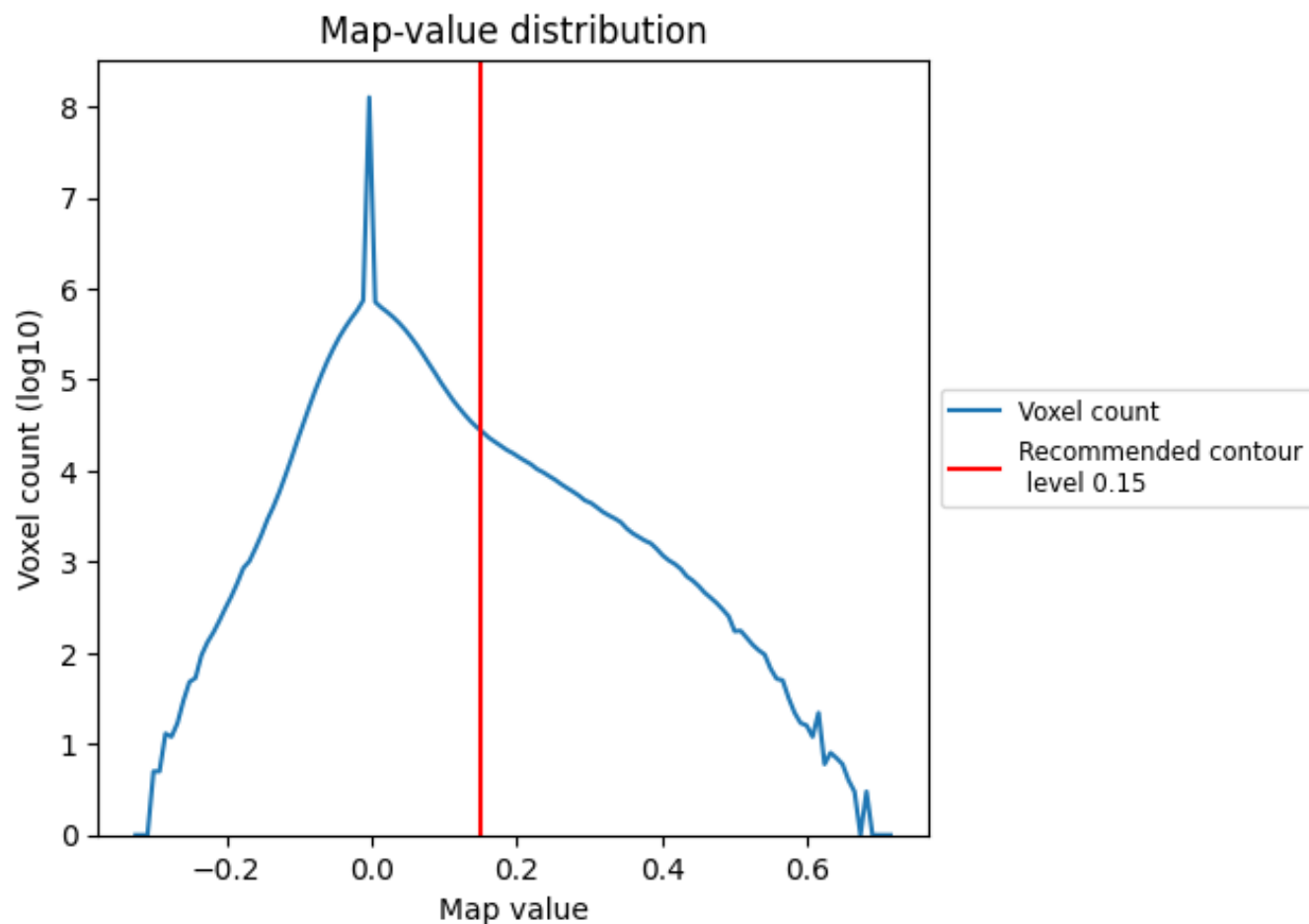


Z

7 Map analysis [i](#)

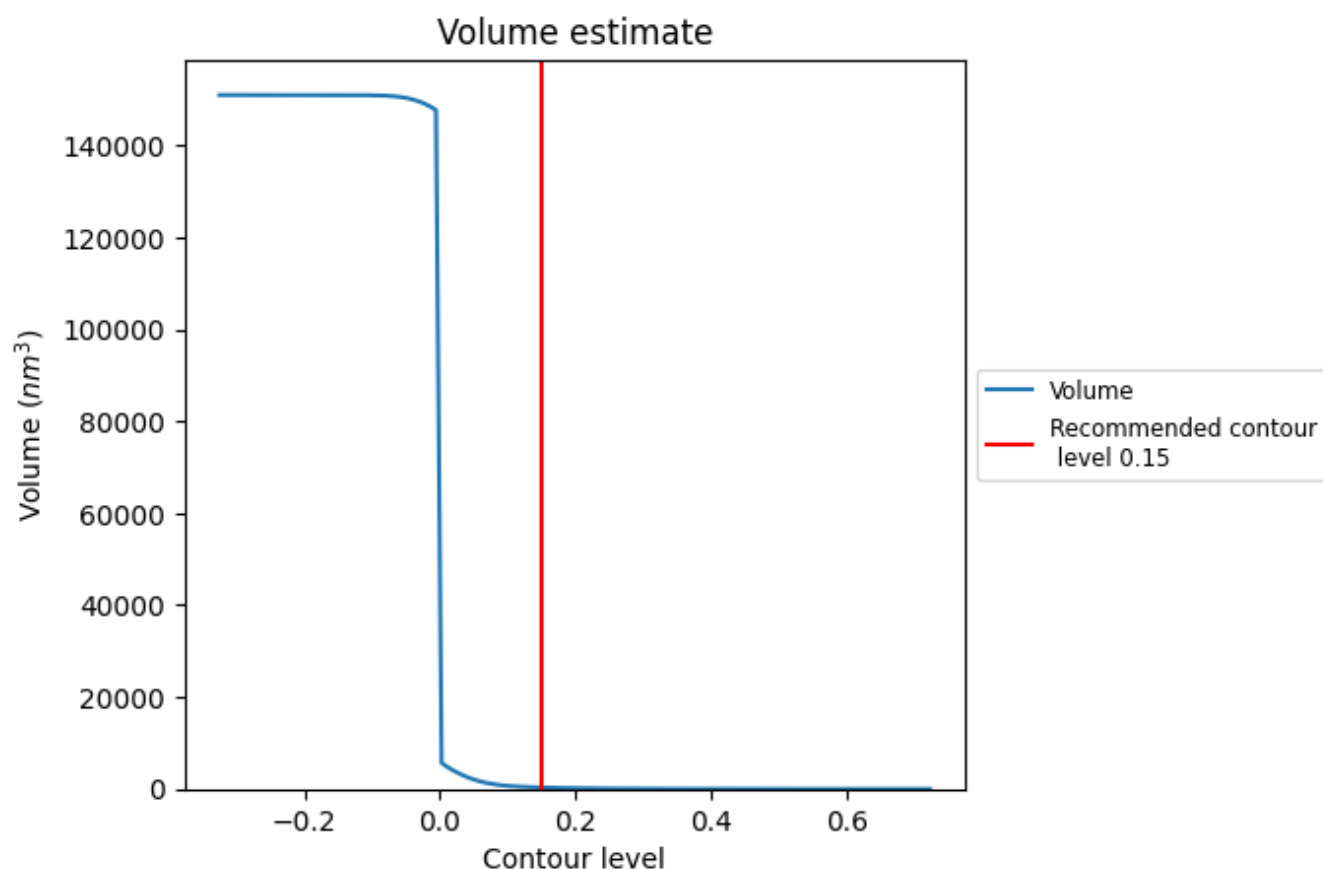
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

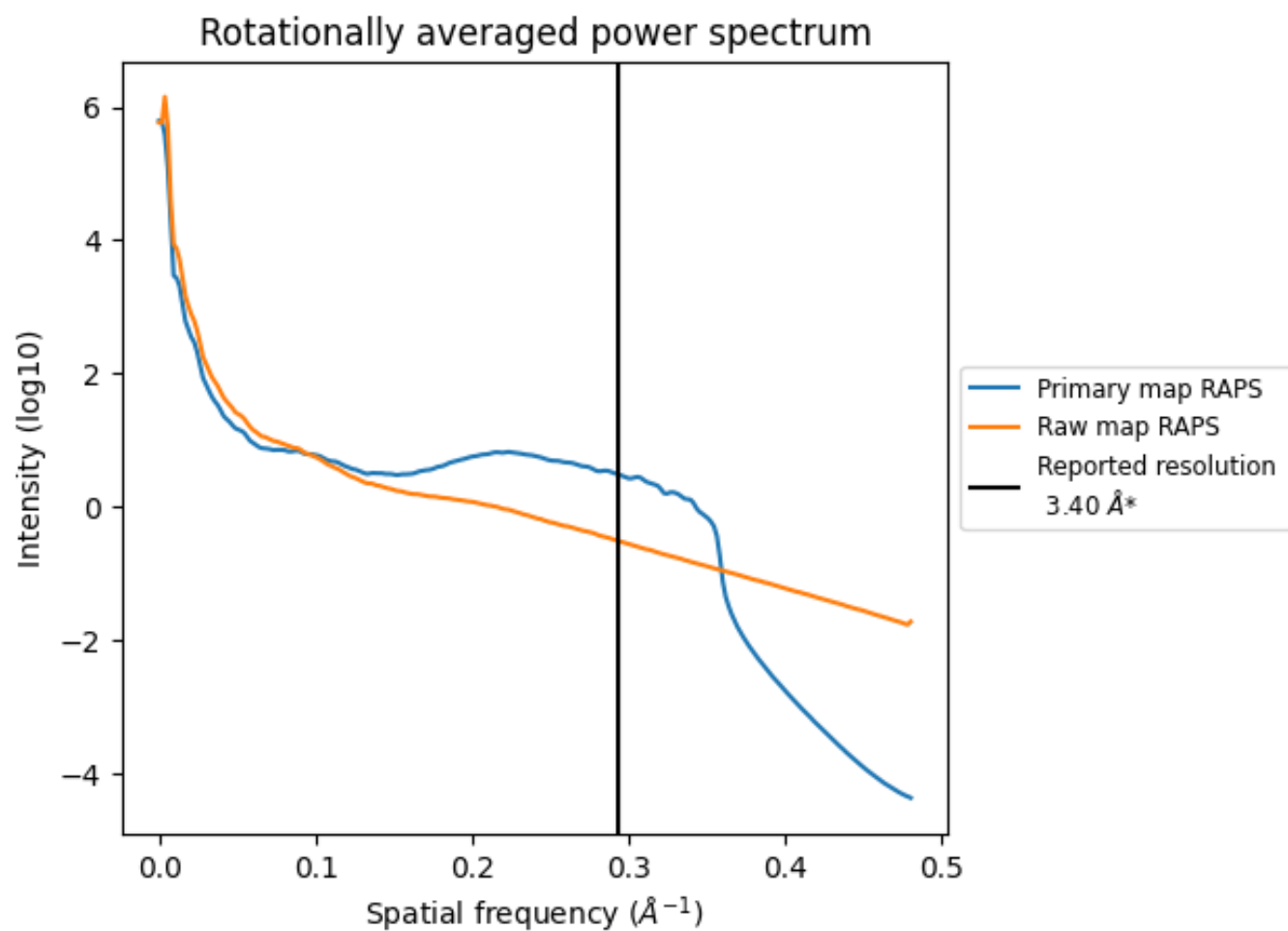
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 315 nm³; this corresponds to an approximate mass of 284 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

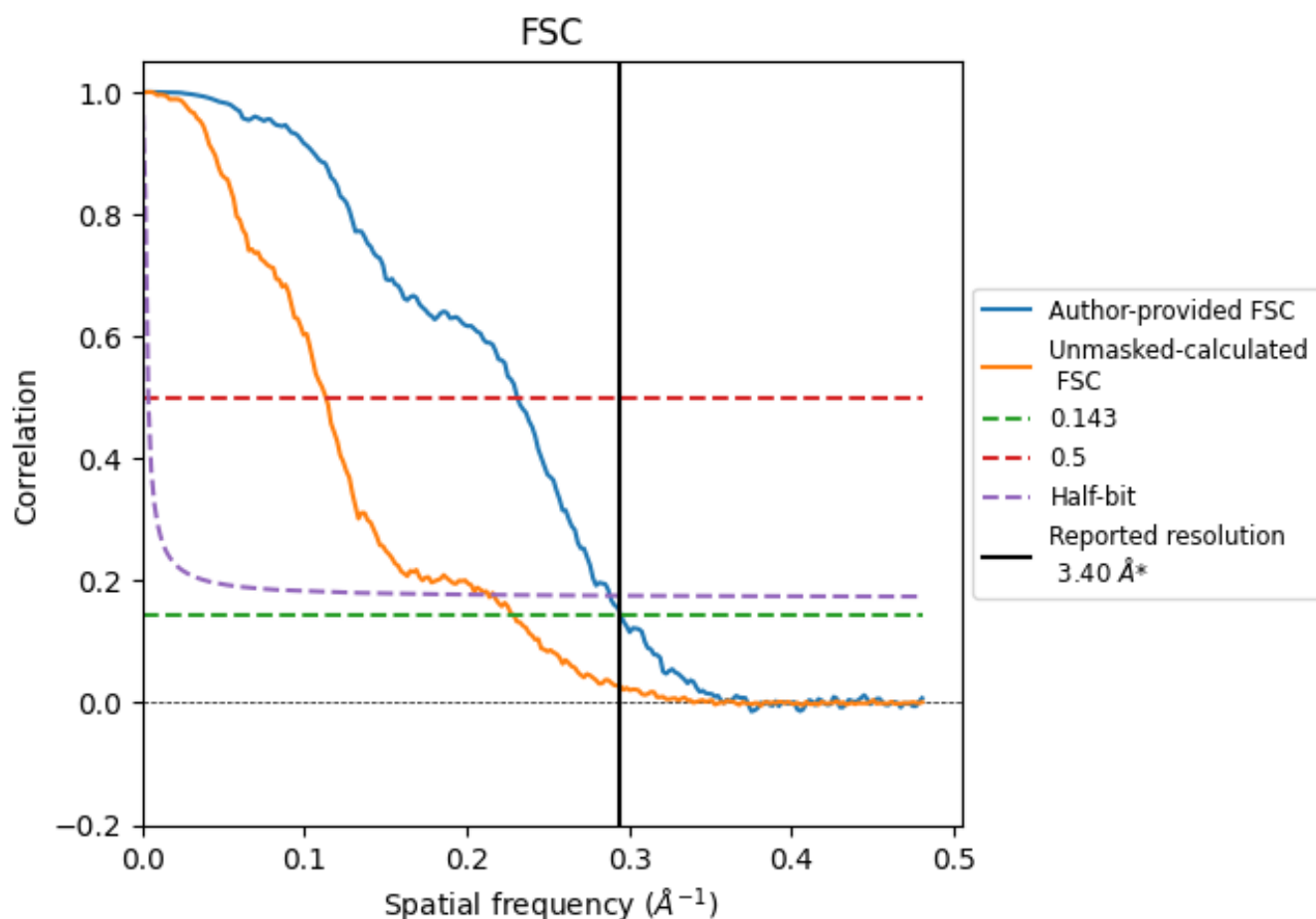


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

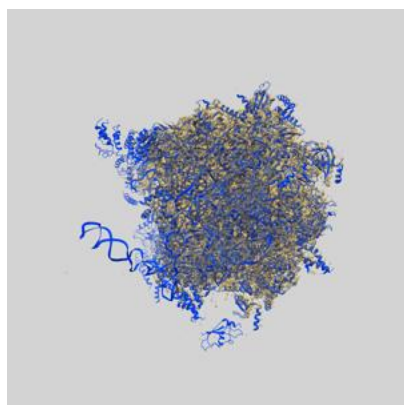
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	4.32	3.47
Unmasked-calculated*	4.36	8.83	4.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.36 differs from the reported value 3.4 by more than 10 %

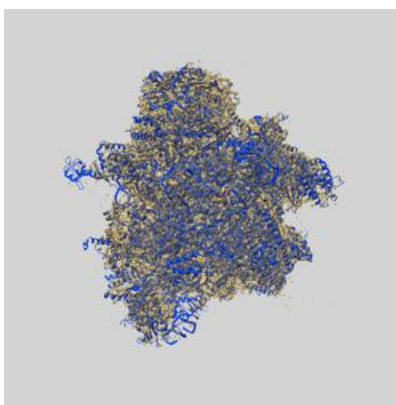
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13329 and PDB model 7PD3. Per-residue inclusion information can be found in section 3 on page 17.

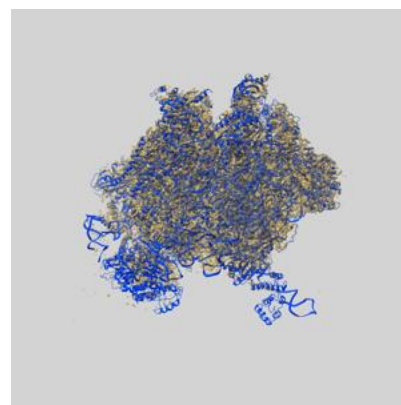
9.1 Map-model overlay [i](#)



X



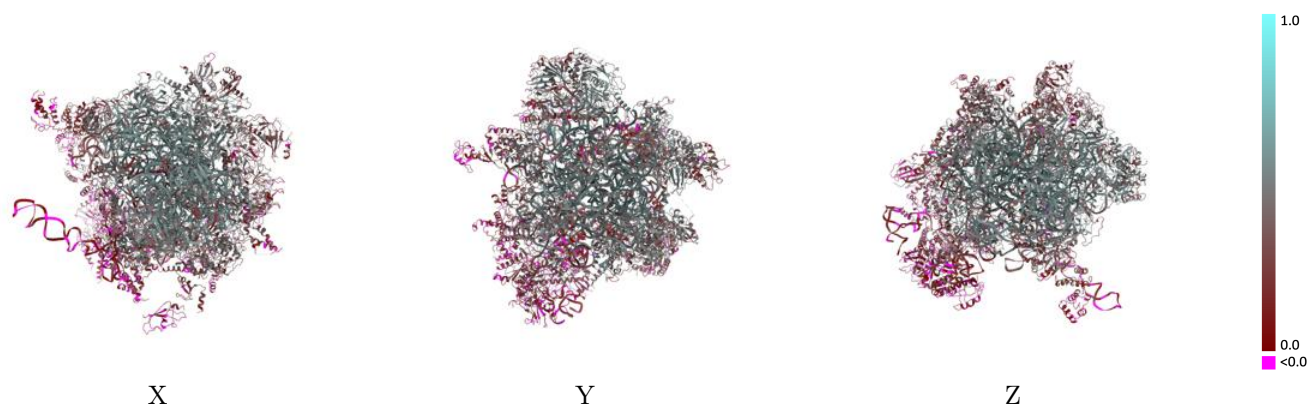
Y



Z

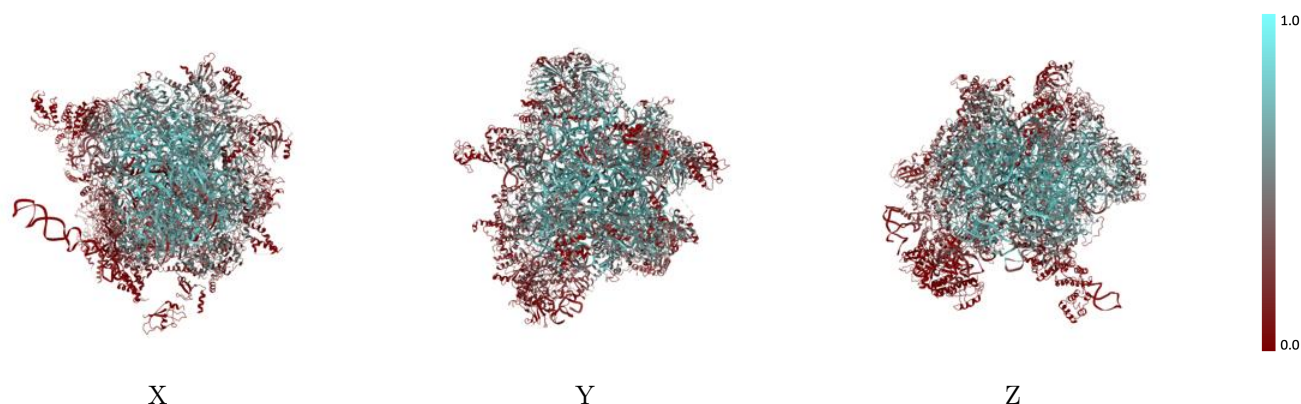
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



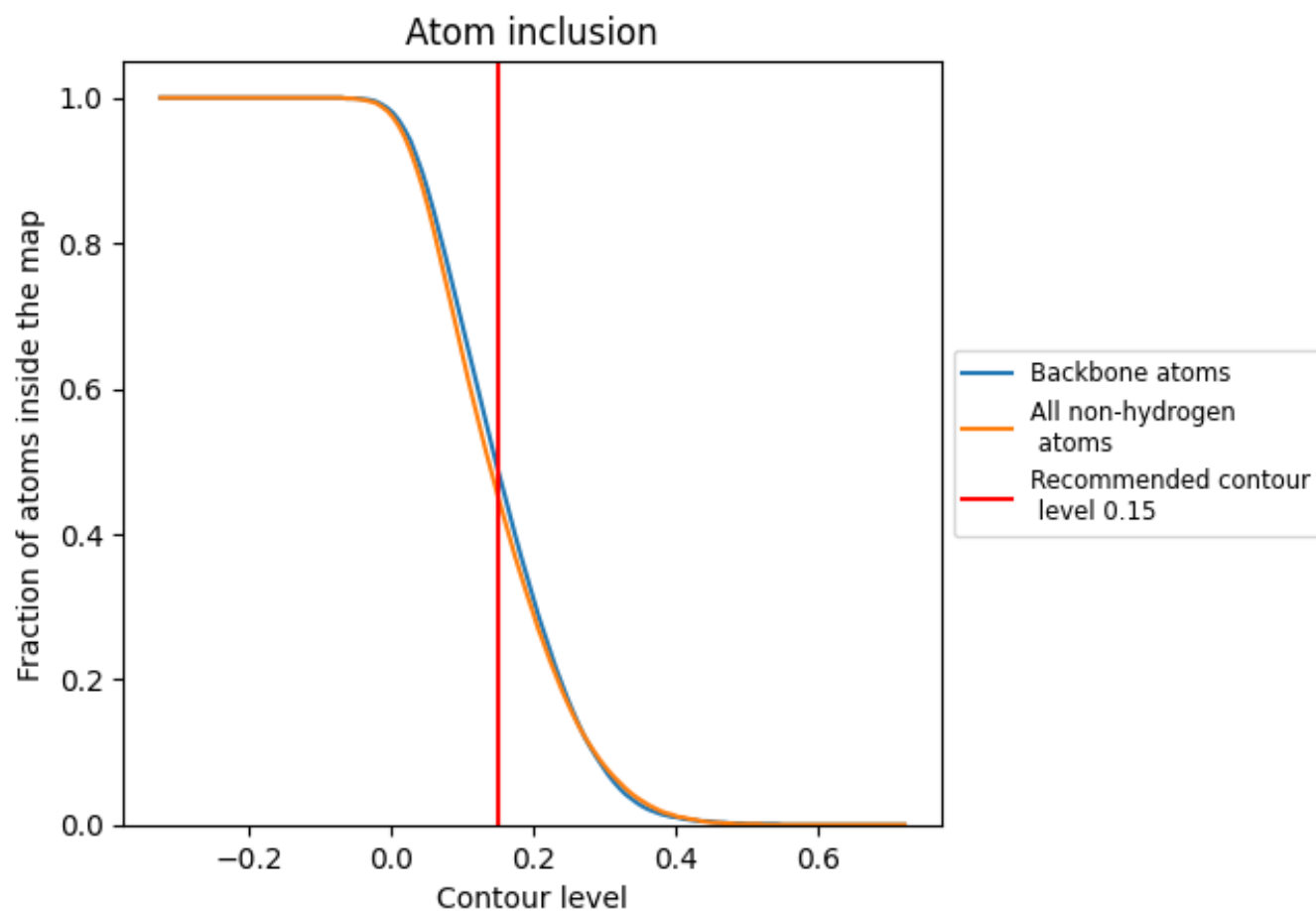
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4530	 0.3940
0	 0.4700	 0.4540
1	 0.4090	 0.3450
2	 0.7920	 0.5740
3	 0.6970	 0.5170
4	 0.6630	 0.5020
5	 0.4340	 0.4320
6	 0.1970	 0.2300
7	 0.2710	 0.3720
8	 0.0150	 0.1150
9	 0.3970	 0.4020
A	 0.6810	 0.4870
B	 0.0850	 0.0760
C	 0.0000	 0.0800
D	 0.5610	 0.4640
E	 0.5880	 0.5090
F	 0.4920	 0.3980
G	 0.1230	 0.2610
H	 0.2780	 0.3450
J	 0.0230	 0.1270
K	 0.6210	 0.4960
L	 0.5140	 0.4630
M	 0.4450	 0.3600
N	 0.4210	 0.4090
O	 0.6060	 0.5050
P	 0.2560	 0.2330
Q	 0.4930	 0.4680
R	 0.6070	 0.4720
S	 0.5160	 0.4470
T	 0.6200	 0.4990
U	 0.4750	 0.4460
V	 0.2210	 0.3090
W	 0.5490	 0.4580
X	 0.4000	 0.3780
Y	 0.5200	 0.4550



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Chain	Atom inclusion	Q-score
Z	 0.5010	 0.4380
a	 0.4990	 0.4620
b	 0.4940	 0.4110
c	 0.3350	 0.3890
d	 0.1740	 0.2970
e	 0.0040	 0.0830
f	 0.1060	 0.1740
g	 0.3540	 0.3140
h	 0.1340	 0.2180
i	 0.6530	 0.4910
j	 0.3900	 0.3370
k	 0.1140	 0.2240
l	 0.1990	 0.2890
m	 0.0000	 0.0580
o	 0.4740	 0.4140
p	 0.1250	 0.1890
q	 0.1320	 0.1760
r	 0.5410	 0.4520
s	 0.5100	 0.4700
t	 0.0000	 0.2160
u	 0.1440	 0.3250
v	 0.0330	 0.2480
w	 0.0000	 0.1020
x	 0.2020	 0.2730
y	 0.2960	 0.3400
z	 0.2960	 0.3550