



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:45 PM UTC

PDB ID : 7OF4 / pdb_00007of4
EMDB ID : EMD-12869
Title : Structure of mature human mitochondrial ribosome large subunit in complex with GTPBP6 (PTC conformation 1).
Authors : Hillen, H.S.; Lavdovskaia, E.; Nadler, F.; Hanitsch, E.; Linden, A.; Bohnsack, K.E.; Urlaub, H.; Richter-Dennerlein, R.
Deposited on : 2021-05-04
Resolution : 2.70 Å (reported)
Based on initial model : 5OOL

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:

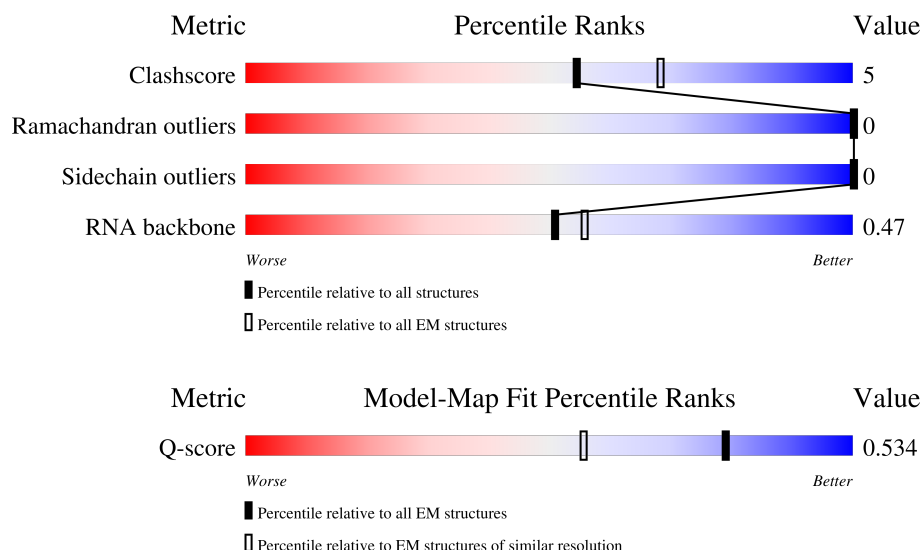
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.70 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	10327 (2.20 - 3.20)

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	
2	1	65	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	2	92	
4	3	188	
5	4	103	
6	5	423	
7	6	380	
8	7	338	
9	8	206	
10	9	137	
11	A	1559	
12	B	69	
13	C	516	
14	D	305	
15	E	348	
16	F	311	
17	H	267	
18	I	261	
19	J	192	
20	K	178	
21	L	145	
22	M	296	
23	N	251	
24	O	175	
25	P	180	
26	Q	292	
27	R	149	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	S	205	
29	T	206	
30	U	153	
31	V	216	
32	W	148	
33	X	256	
34	Y	250	
35	Z	161	
36	a	142	
37	b	215	
38	c	332	
39	d	306	
40	e	279	
41	f	212	
42	g	166	
43	h	158	
44	i	128	
45	j	123	
46	k	112	
47	l	138	
48	m	128	
49	o	102	
50	p	206	
51	q	222	
52	r	196	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	s	439	 73% 12% 16%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 100322 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
			2723	1743	488	484	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	77	Total	C	N	O	S	0	0
			651	413	113	123	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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1463	Total	C	N	O	P	0	0
			31075	13943	5609	10060	1463		

- Molecule 12 is a RNA chain called mitochondrial tRNA^{Val}.

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

- Molecule 13 is a protein called Putative GTP-binding protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	422	Total	C	N	O	S	0	0
			3313	2097	607	596	13		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	305	Total	C	N	O	S	0	0
			2405	1545	418	431	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 L9, mitochondrial.

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

- Molecule 18 is a protein called 39S ribosomal protein L10, mitochondrial.

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

- Molecule 19 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 25 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 26 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 28 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 29 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 30 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 31 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	191	Total	C	N	O	S	0	0
			1568	999	280	281	8		

- Molecule 32 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 33 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L44, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	d	208	Total	C	N	O	S	0	0
			1731	1121	295	306	9		

- Molecule 40 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	e	197	Total	C	N	O	S	0	0
			1599	1027	277	290	5		

- Molecule 41 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	f	105	Total	C	N	O	S	0	0
			834	535	136	160	3		

- Molecule 42 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	105	Total	C	N	O	S	0	0
			862	548	151	160	3		

- Molecule 44 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 45 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	j	84	Total	C	N	O	S	0	0
			679	420	132	125	2		

- Molecule 46 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 47 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 48 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 49 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	o	94	Total	C	N	O	S	0	0
			797	501	165	128	3		

- Molecule 50 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 51 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	q	120	Total	C	N	O	S	0	0
			1011	633	194	179	5		

- Molecule 52 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	r	157	Total	C	N	O	S	0	0
			1287	817	247	215	8		

- Molecule 53 is a protein called 39S ribosomal protein S30, mitochondrial.

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

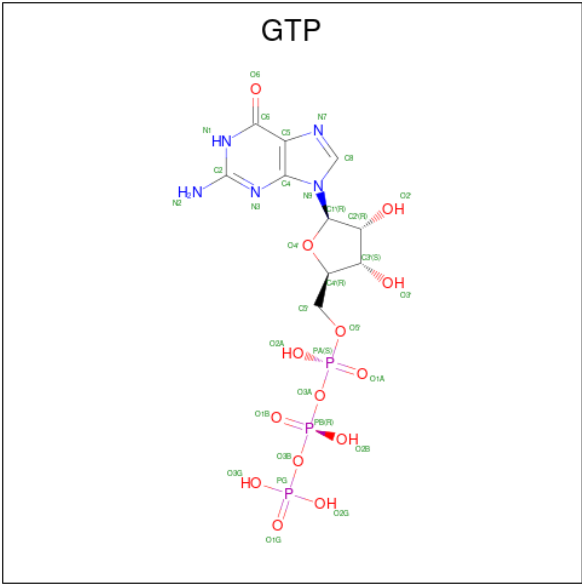
- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

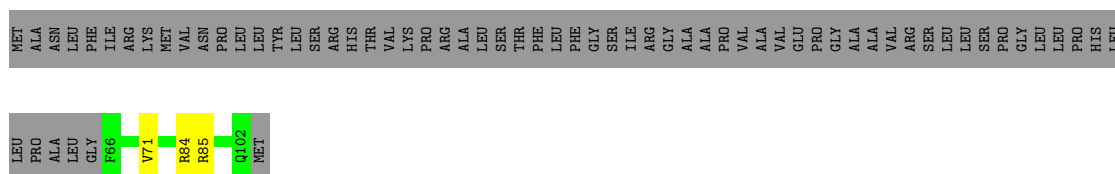
Mol	Chain	Residues	Atoms		AltConf
54	0	1	Total	Zn	0
			1	1	
54	4	1	Total	Zn	0
			1	1	
54	r	1	Total	Zn	0
			1	1	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

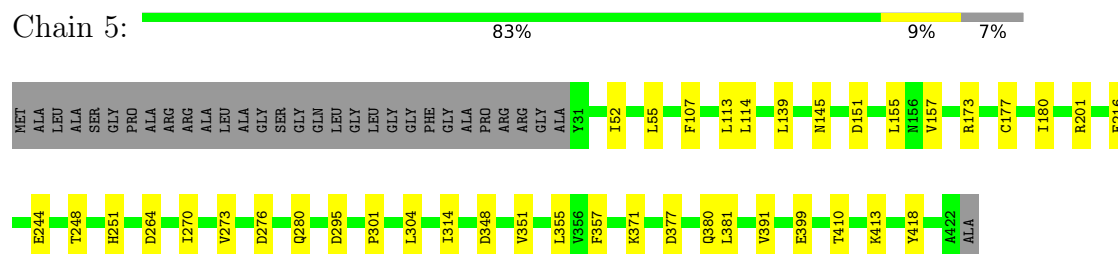
Mol	Chain	Residues	Atoms		AltConf
55	A	86	Total	Mg	0
			86	86	
55	C	1	Total	Mg	0
			1	1	
55	E	1	Total	Mg	0
			1	1	
55	g	1	Total	Mg	0
			1	1	

- Molecule 56 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

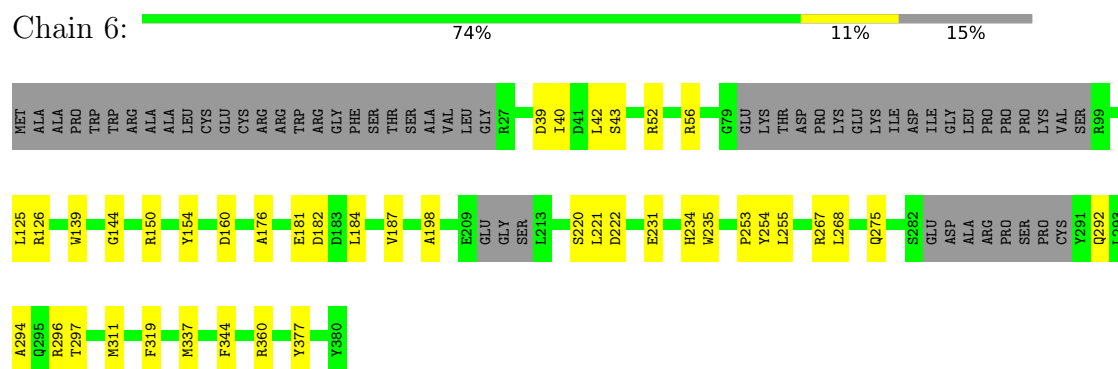




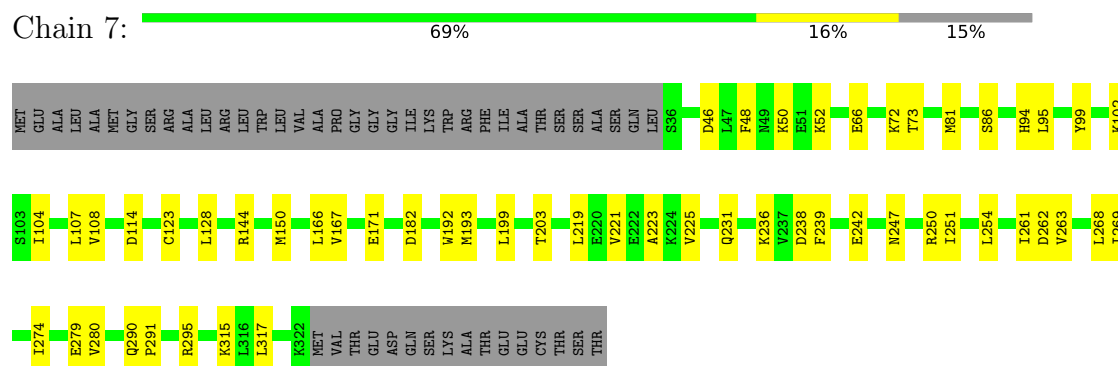
- Molecule 6: 39S ribosomal protein L37, mitochondrial



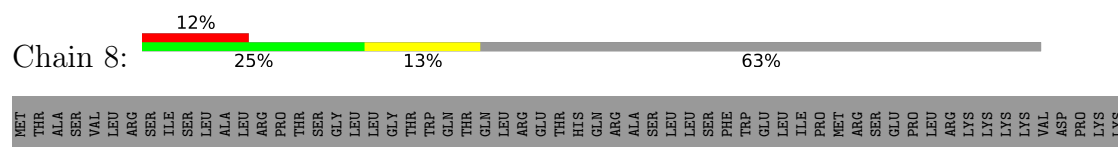
- Molecule 7: 39S ribosomal protein L38, mitochondrial

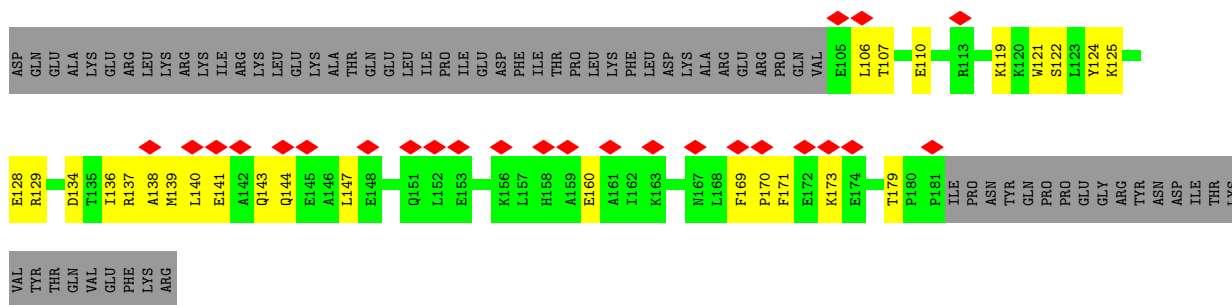


- Molecule 8: 39S ribosomal protein L39, mitochondrial

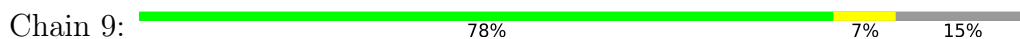


- Molecule 9: 39S ribosomal protein L40, mitochondrial

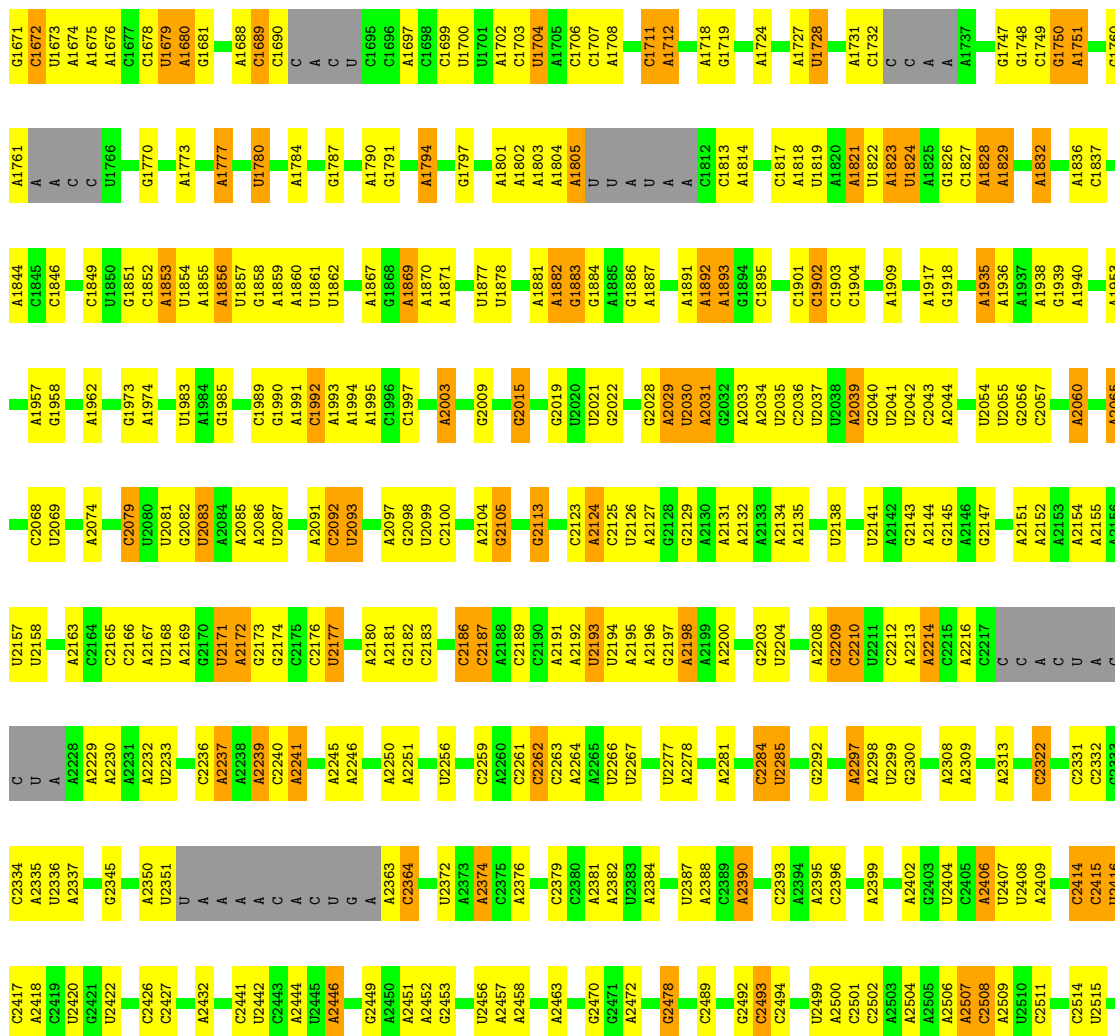


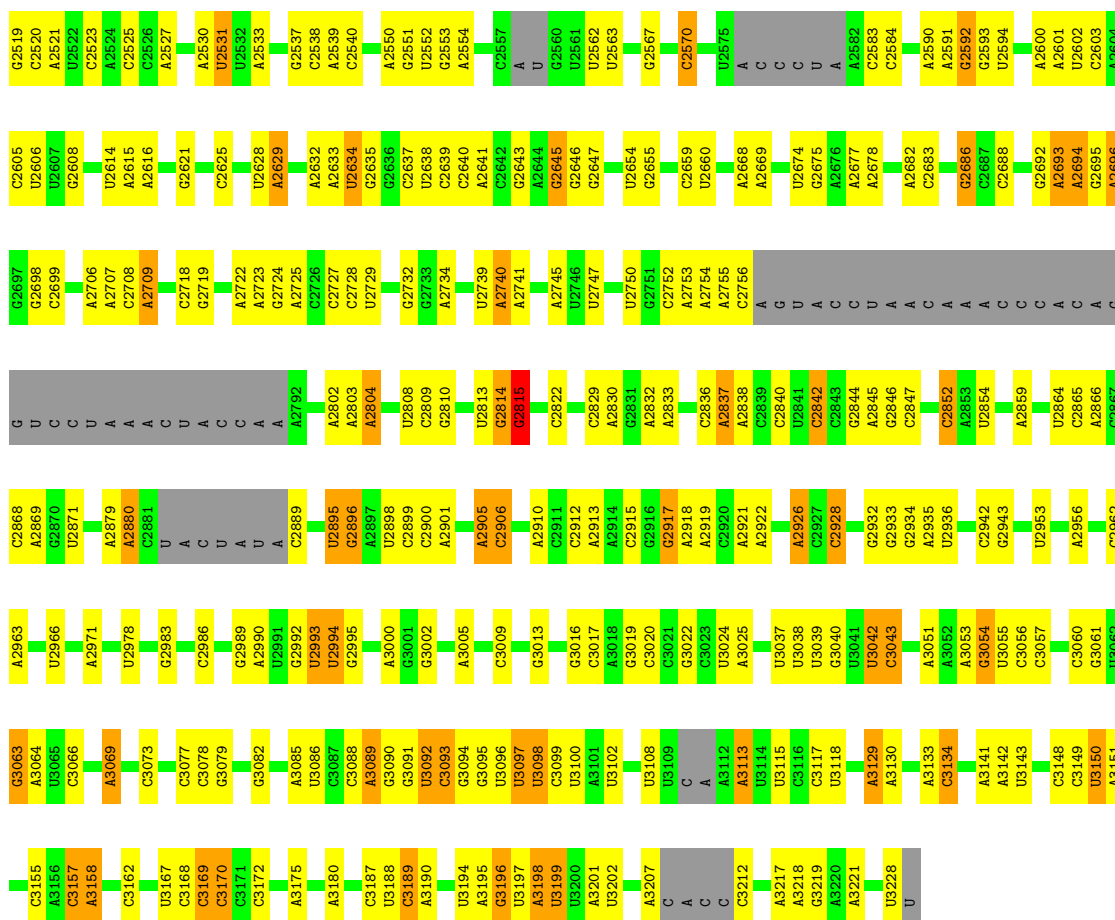


- Molecule 10: 39S ribosomal protein L41, mitochondrial



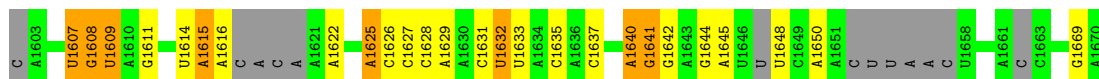
- Molecule 11: 16S ribosomal RNA





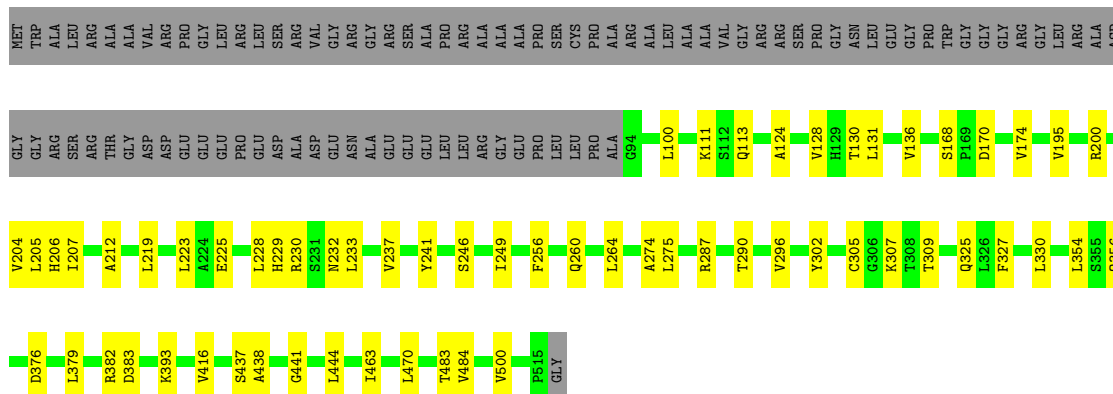
• Molecule 12: mitochondrial tRNA^{Val}

Chain B: 43% 26% 12% 19%



• Molecule 13: Putative GTP-binding protein 6

Chain C: 70% 12% 18%

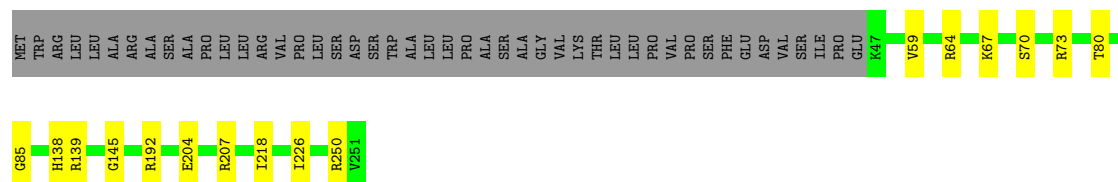


- Chain M:  88% 9%

S296

- Molecule 23: 39S ribosomal protein L16, mitochondrial

Chain N:  75% 6% 18%



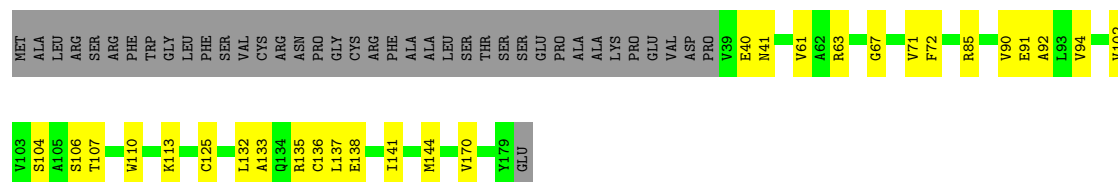
- Molecule 24: 39S ribosomal protein L17, mitochondrial

Chain O:  78% 9% 13%



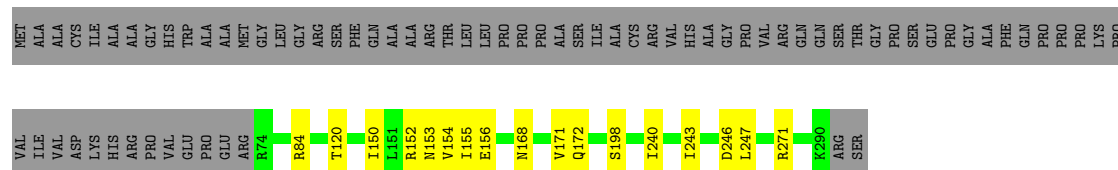
- Molecule 25: 39S ribosomal protein L18, mitochondrial

Chain P:  63% 16% 22%



- Molecule 26: 39S ribosomal protein L19, mitochondrial

Chain Q:  68% 6% 26%



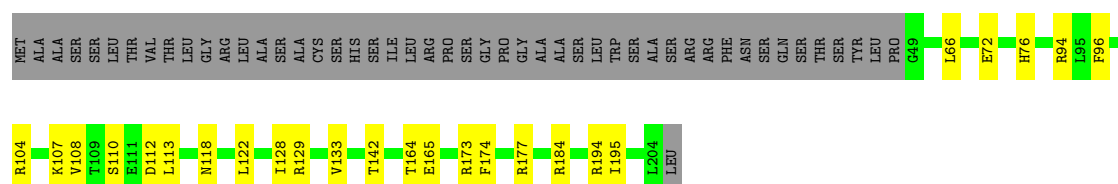
- Molecule 27: 39S ribosomal protein L20, mitochondrial

Chain R:  88% 6% 6%



- Molecule 28: 39S ribosomal protein L21, mitochondrial

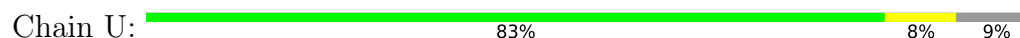
Chain S:  64% 12% 24%



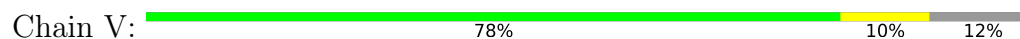
- Molecule 29: 39S ribosomal protein L22, mitochondrial



- Molecule 30: 39S ribosomal protein L23, mitochondrial



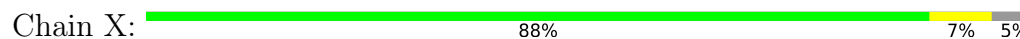
- Molecule 31: 39S ribosomal protein L24, mitochondrial



- Molecule 32: 39S ribosomal protein L27, mitochondrial

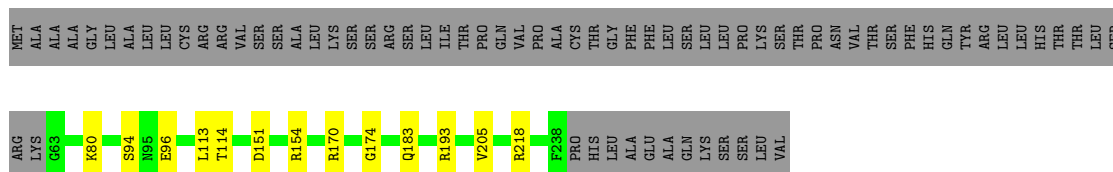


- Molecule 33: 39S ribosomal protein L28, mitochondrial



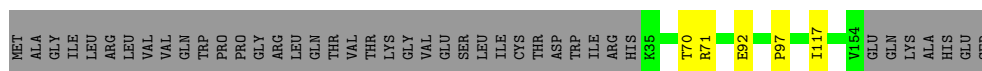
- Molecule 34: 39S ribosomal protein L47, mitochondrial

Chain Y:  65% 5% 30%



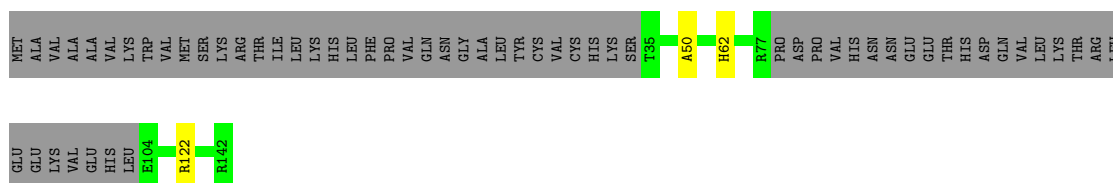
- Molecule 35: 39S ribosomal protein L30, mitochondrial

Chain Z:  71% 25%



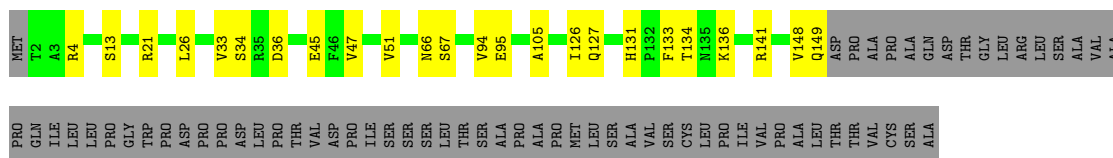
- Molecule 36: 39S ribosomal protein L42, mitochondrial

Chain a:  56% 42%



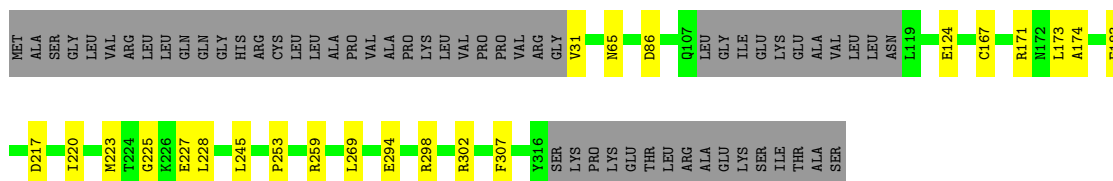
- Molecule 37: 39S ribosomal protein L43, mitochondrial

Chain b:  58% 11% 31%



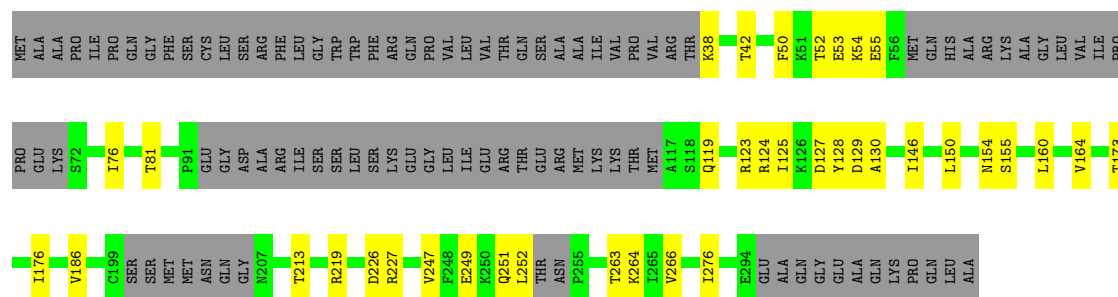
- Molecule 38: 39S ribosomal protein L44, mitochondrial

Chain c:  76% 7% 17%

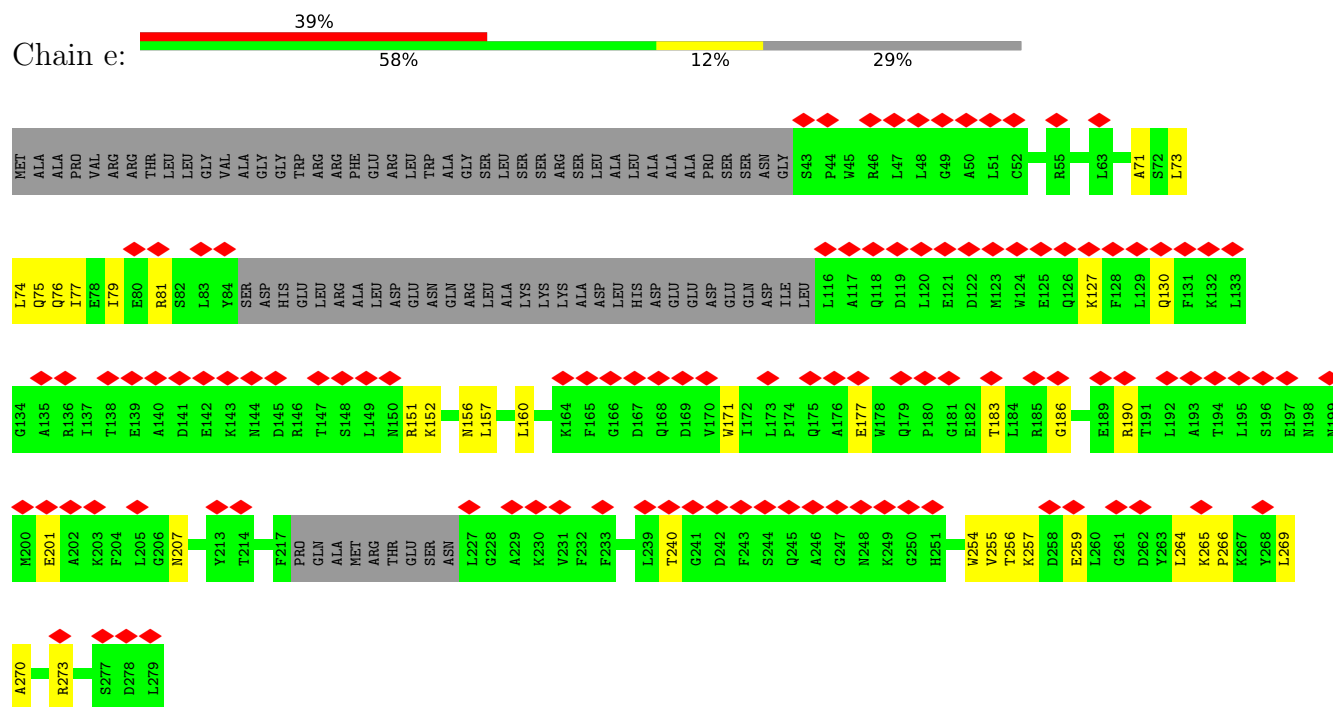


- Molecule 39: 39S ribosomal protein L45, mitochondrial

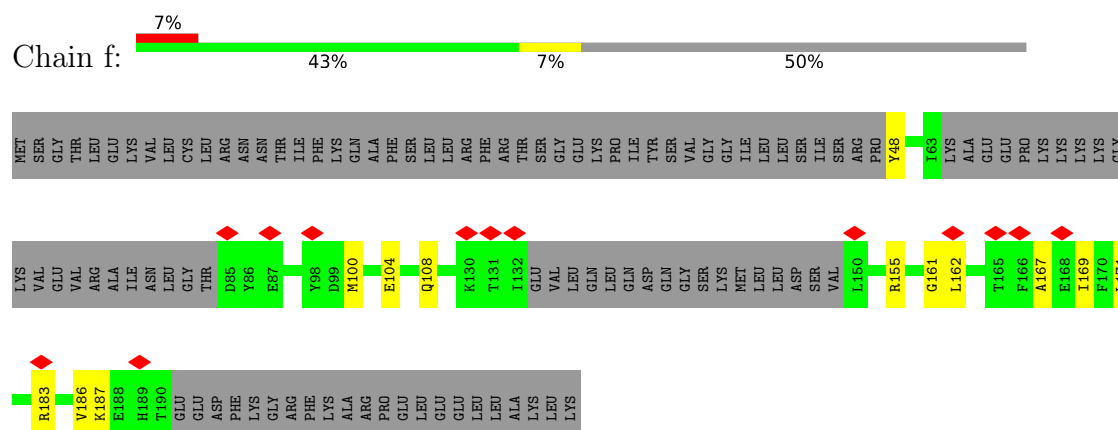
Chain d:  56% 12% 32%



• Molecule 40: 39S ribosomal protein L46, mitochondrial

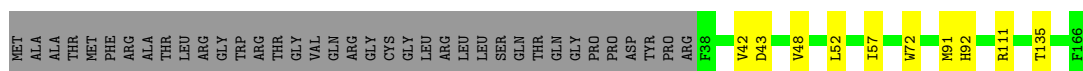


• Molecule 41: 39S ribosomal protein L48, mitochondrial

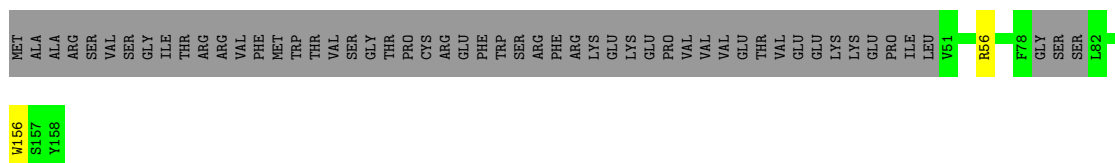


• Molecule 42: 39S ribosomal protein L49, mitochondrial

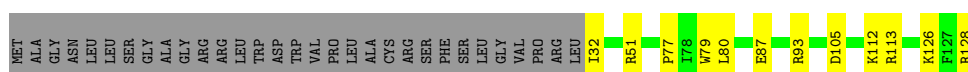




- Molecule 43: 39S ribosomal protein L50, mitochondrial



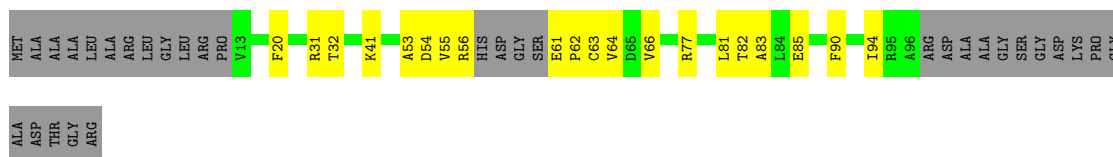
- Molecule 44: 39S ribosomal protein L51, mitochondrial



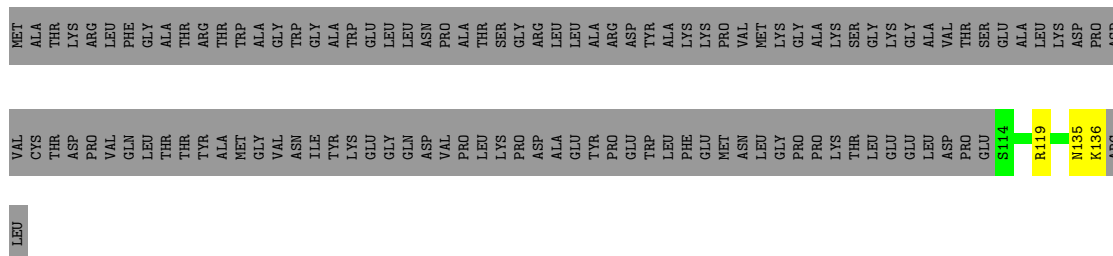
- Molecule 45: 39S ribosomal protein L52, mitochondrial



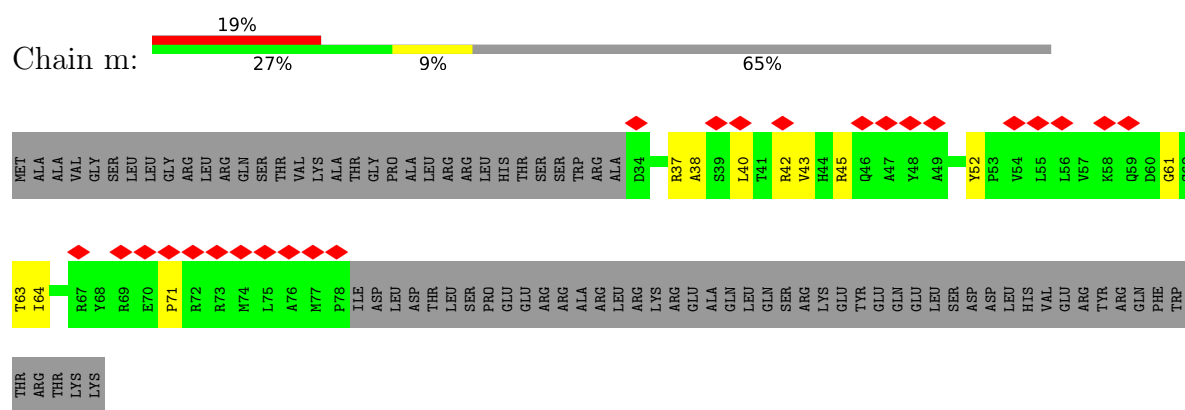
- Molecule 46: 39S ribosomal protein L53, mitochondrial



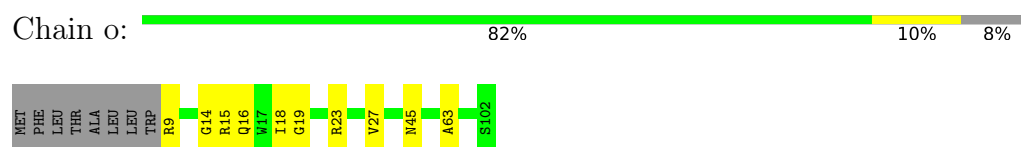
- Molecule 47: 39S ribosomal protein L54, mitochondrial



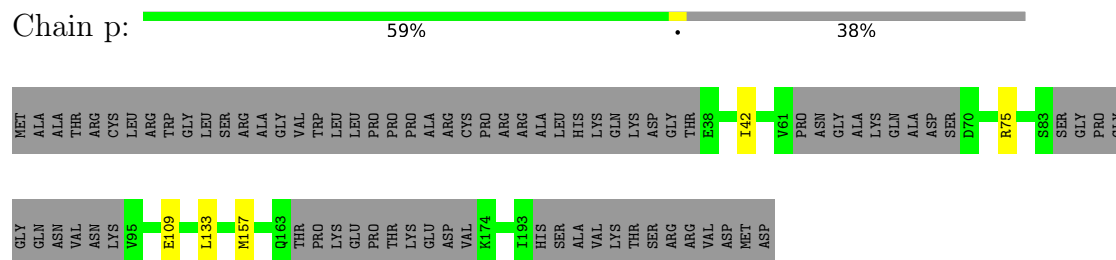
- Molecule 48: 39S ribosomal protein L55, mitochondrial



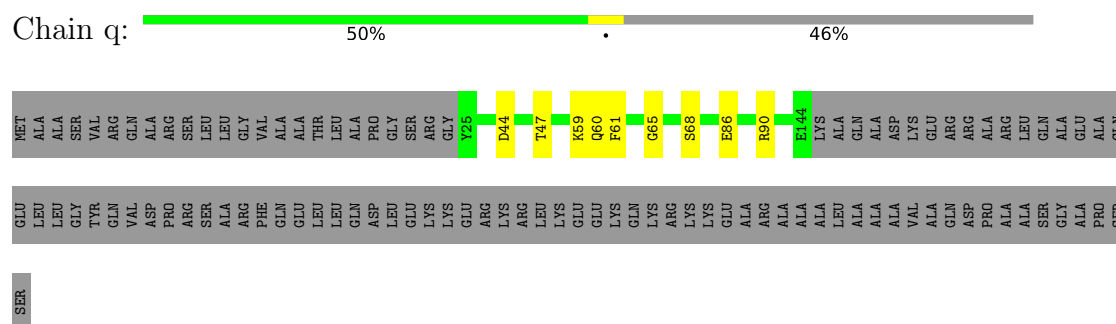
- Molecule 49: Ribosomal protein 63, mitochondrial



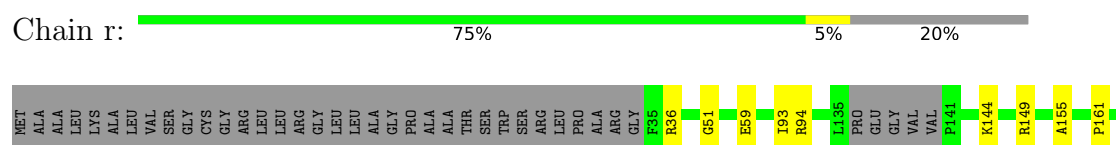
- Molecule 50: Peptidyl-tRNA hydrolase ICT1, mitochondrial



- Molecule 51: Growth arrest and DNA damage-inducible proteins-interacting protein 1

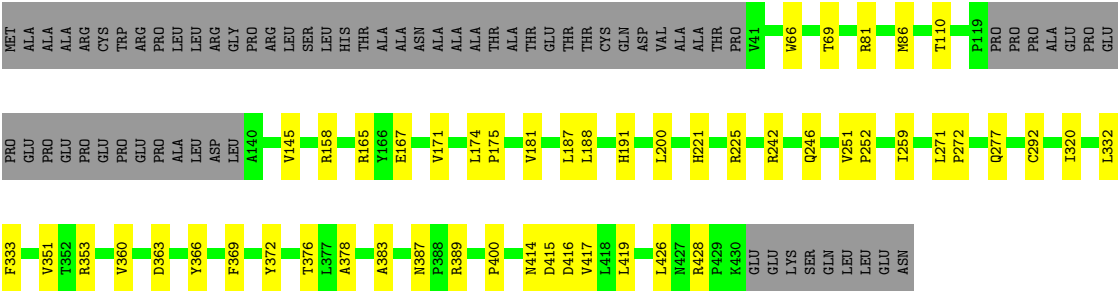


- Molecule 52: 39S ribosomal protein S18a, mitochondrial





- Molecule 53: 39S ribosomal protein S30, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137890	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 ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	367.49997, 367.49997, 367.49997	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, MG, ZN, GTP, 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	0.18	0/895	0.31	0/1201
2	1	0.16	0/438	0.25	0/583
3	2	0.22	0/373	0.27	0/496
4	3	0.21	0/852	0.24	0/1136
5	4	0.20	0/341	0.27	0/451
6	5	0.18	0/3294	0.28	0/4488
7	6	0.15	0/2809	0.28	0/3818
8	7	0.16	0/2391	0.28	0/3234
9	8	0.11	0/665	0.28	0/894
10	9	0.17	0/972	0.23	0/1306
11	A	0.24	0/34684	0.29	0/53971
12	B	0.11	0/1328	0.21	0/2056
13	C	0.14	0/3375	0.27	0/4571
14	D	0.19	0/1879	0.27	0/2527
15	E	0.20	0/2474	0.30	0/3355
16	F	0.20	0/2071	0.30	0/2817
17	H	0.15	0/798	0.27	0/1073
18	I	0.15	0/1308	0.32	0/1761
19	J	0.11	0/1077	0.28	0/1452
20	K	0.20	0/1495	0.26	0/2029
21	L	0.18	0/904	0.26	0/1218
22	M	0.20	0/2359	0.27	0/3185
23	N	0.19	0/1697	0.29	0/2281
24	O	0.19	0/1269	0.29	0/1708
25	P	0.17	0/1173	0.25	0/1588
26	Q	0.18	0/1846	0.26	0/2487
27	R	0.21	0/1174	0.26	0/1572
28	S	0.21	0/1276	0.31	0/1729
29	T	0.20	0/1402	0.26	0/1886
30	U	0.18	0/1183	0.25	0/1600
31	V	0.14	0/1609	0.24	0/2179
32	W	0.21	0/881	0.23	0/1188

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	X	0.17	0/2090	0.23	0/2825
34	Y	0.19	0/1552	0.22	0/2079
35	Z	0.19	0/1003	0.29	0/1354
36	a	0.18	0/709	0.25	0/963
37	b	0.19	0/1202	0.28	0/1626
38	c	0.18	0/2264	0.25	0/3059
39	d	0.14	0/1781	0.27	0/2410
40	e	0.09	0/1633	0.26	0/2204
41	f	0.12	0/850	0.28	0/1150
42	g	0.19	0/1102	0.28	0/1503
43	h	0.14	0/884	0.25	0/1203
44	i	0.21	0/849	0.25	0/1135
45	j	0.17	0/693	0.27	0/933
46	k	0.11	0/635	0.25	0/855
47	l	0.10	0/226	0.20	0/299
48	m	0.09	0/379	0.28	0/510
49	o	0.19	0/818	0.30	0/1097
50	p	0.14	0/1071	0.22	0/1433
51	q	0.15	0/1042	0.23	0/1413
52	r	0.17	0/1325	0.26	0/1793
53	s	0.20	0/3114	0.27	0/4225
All	All	0.20	0/105514	0.28	0/149909

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	880	0	902	12	0
2	1	433	0	475	8	0
3	2	367	0	393	3	0
4	3	831	0	883	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	4	333	0	352	5	0
6	5	3199	0	3196	27	0
7	6	2723	0	2615	31	0
8	7	2334	0	2343	36	0
9	8	651	0	649	23	0
10	9	947	0	949	9	0
11	A	31075	0	15786	340	0
12	B	1191	0	607	17	0
13	C	3313	0	3415	43	0
14	D	1842	0	1896	22	0
15	E	2405	0	2415	19	0
16	F	2013	0	2044	25	0
17	H	784	0	832	6	0
18	I	1283	0	1369	33	0
19	J	1061	0	1141	28	0
20	K	1451	0	1448	15	0
21	L	889	0	941	14	0
22	M	2305	0	2378	21	0
23	N	1654	0	1681	12	0
24	O	1245	0	1283	12	0
25	P	1148	0	1148	20	0
26	Q	1805	0	1841	13	0
27	R	1153	0	1214	12	0
28	S	1251	0	1322	26	0
29	T	1368	0	1410	19	0
30	U	1154	0	1154	11	0
31	V	1568	0	1576	20	0
32	W	859	0	888	6	0
33	X	2035	0	2054	13	0
34	Y	1517	0	1561	10	0
35	Z	978	0	1030	3	0
36	a	686	0	658	3	0
37	b	1178	0	1180	20	0
38	c	2217	0	2220	19	0
39	d	1731	0	1716	27	0
40	e	1599	0	1604	24	0
41	f	834	0	828	14	0
42	g	1067	0	1056	7	0
43	h	862	0	845	3	0
44	i	827	0	857	10	0
45	j	679	0	668	3	0
46	k	627	0	636	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	l	221	0	227	2	0
48	m	372	0	387	9	0
49	o	797	0	804	9	0
50	p	1058	0	1083	4	0
51	q	1011	0	982	6	0
52	r	1287	0	1314	9	0
53	s	3036	0	3022	35	0
54	0	1	0	0	0	0
54	4	1	0	0	0	0
54	r	1	0	0	0	0
55	A	86	0	0	0	0
55	C	1	0	0	0	0
55	E	1	0	0	0	0
55	g	1	0	0	0	0
56	A	64	0	24	0	0
56	C	32	0	12	2	0
All	All	100322	0	85314	928	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 (928) 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)
11:A:2643:G:O2'	11:A:2645:G:OP2	1.84	0.95
8:7:247:ASN:ND2	8:7:251:ILE:O	2.00	0.94
11:A:1777:A:N6	11:A:1780:U:OP2	2.03	0.91
11:A:3198:A:O2'	11:A:3199:U:OP2	1.89	0.88
30:U:11:ARG:NH1	31:V:212:LYS:O	2.07	0.88
22:M:62:ARG:O	44:i:128:ARG:NH1	2.07	0.87
7:6:160:ASP:OD2	7:6:267:ARG:NH2	2.08	0.87
14:D:138:ASP:OD1	14:D:248:SER:OG	1.94	0.85
41:f:100:MET:SD	41:f:155:ARG:NH2	2.49	0.85
10:9:28:ARG:NH1	11:A:2376:A:O2'	2.10	0.84
14:D:194:ASN:OD1	14:D:243:THR:OG1	1.94	0.83
15:E:63:GLN:NE2	15:E:67:ASP:OD2	2.11	0.83
20:K:3:SER:O	38:c:302:ARG:NH1	2.11	0.83
11:A:2284:C:O2'	11:A:2285:U:OP2	1.95	0.83
18:I:128:ASN:OD1	18:I:151:ASN:ND2	2.12	0.83
37:b:136:LYS:O	38:c:259:ARG:NH2	2.12	0.82
11:A:2993:U:O2'	11:A:2994:U:O5'	1.97	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1823:A:O2'	11:A:1824:U:OP2	1.96	0.81
31:V:126:MET:SD	31:V:152:ARG:NH1	2.53	0.81
11:A:1837:C:OP1	37:b:4:ARG:NH2	2.15	0.80
11:A:2192:A:O2'	19:J:134:ASP:OD2	1.99	0.80
11:A:2191:A:OP1	19:J:142:ARG:NH2	2.15	0.79
15:E:69:ASP:OD1	15:E:154:ARG:NH1	2.15	0.79
11:A:1822:U:O2	11:A:2707:A:O2'	2.01	0.78
12:B:1607:U:O2'	12:B:1608:G:OP1	2.01	0.77
25:P:85:ARG:NH1	25:P:125:CYS:SG	2.58	0.77
11:A:1881:A:OP2	42:g:111:ARG:NH2	2.16	0.76
11:A:2562:U:O2'	14:D:284:ARG:O	2.01	0.76
18:I:101:ASN:O	18:I:109:LYS:NZ	2.19	0.76
11:A:2537:G:O2'	11:A:2634:U:OP2	2.03	0.76
11:A:3157:C:O2'	26:Q:84:ARG:O	2.03	0.75
11:A:2926:A:N6	13:C:246:SER:O	2.20	0.75
13:C:233:LEU:O	13:C:237:VAL:HG22	1.86	0.75
18:I:51:THR:OG1	23:N:250:ARG:NH2	2.19	0.75
21:L:41:VAL:HG11	21:L:121:THR:OG1	1.86	0.75
11:A:1711:C:O2'	11:A:1712:A:OP2	2.03	0.74
29:T:55:ASN:ND2	29:T:74:TYR:O	2.20	0.74
38:c:294:GLU:OE2	38:c:298:ARG:NE	2.19	0.74
11:A:2458:A:O2'	15:E:215:PHE:O	2.03	0.74
16:F:175:LYS:O	16:F:179:THR:HG23	1.88	0.73
41:f:104:GLU:OE2	41:f:108:GLN:NE2	2.22	0.73
53:s:246:GLN:OE1	53:s:353:ARG:NH1	2.22	0.73
16:F:126:LYS:NZ	16:F:130:GLN:OE1	2.15	0.73
38:c:167:CYS:SG	38:c:171:ARG:NH1	2.61	0.73
11:A:2515:U:O2'	14:D:282:ALA:O	2.07	0.73
28:S:112:ASP:OD1	28:S:113:LEU:N	2.22	0.72
21:L:101:ASP:OD2	26:Q:152:ARG:NH2	2.22	0.72
16:F:49:ARG:NH1	16:F:81:ASP:O	2.23	0.71
11:A:1867:A:N1	11:A:2019:G:O2'	2.22	0.71
18:I:128:ASN:ND2	18:I:149:GLY:O	2.22	0.71
5:4:85:ARG:N	11:A:3189:C:OP1	2.24	0.71
38:c:183:GLU:OE1	38:c:183:GLU:N	2.24	0.71
45:j:63:GLN:OE1	45:j:66:ARG:NH1	2.24	0.71
40:e:81:ARG:NH1	48:m:45:ARG:O	2.24	0.71
15:E:111:THR:OG1	15:E:113:ASP:OD1	2.09	0.71
40:e:177:GLU:O	40:e:190:ARG:NH2	2.23	0.71
40:e:75:GLN:O	40:e:79:ILE:HD12	1.91	0.70
11:A:2187:C:O2'	19:J:103:GLN:O	2.07	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2259:C:O2'	11:A:2261:C:OP2	2.02	0.70
26:Q:155:ILE:HG22	26:Q:156:GLU:OE1	1.91	0.70
39:d:129:ASP:OD1	39:d:130:ALA:N	2.24	0.70
11:A:1794:A:OP1	16:F:142:ARG:NH2	2.25	0.69
11:A:2169:A:OP1	19:J:69:LYS:NZ	2.25	0.69
9:8:179:THR:OG1	48:m:61:GLY:O	2.10	0.69
11:A:1747:G:OP2	11:A:1749:C:N4	2.26	0.69
6:5:270:ILE:O	11:A:2409:A:O2'	2.11	0.69
23:N:85:GLY:O	23:N:192:ARG:NH1	2.26	0.69
8:7:144:ARG:NE	8:7:171:GLU:OE2	2.26	0.68
19:J:23:ILE:HD11	19:J:86:THR:HG22	1.73	0.68
11:A:2694:A:O2'	11:A:2942:C:O2'	2.10	0.68
15:E:133:THR:OG1	15:E:144:THR:OG1	2.11	0.68
18:I:148:VAL:O	46:k:31:ARG:NH1	2.25	0.68
22:M:264:GLN:NE2	22:M:267:PHE:O	2.26	0.68
13:C:223:LEU:HD22	13:C:275:LEU:HD22	1.75	0.68
16:F:184:GLN:NE2	22:M:20:PRO:O	2.27	0.68
11:A:2191:A:N6	11:A:2198:A:OP2	2.27	0.67
50:p:133:LEU:HD21	50:p:157:MET:HE1	1.75	0.67
6:5:114:LEU:N	6:5:264:ASP:OD2	2.27	0.67
27:R:112:THR:OG1	37:b:127:GLN:NE2	2.28	0.67
29:T:202:GLN:OE1	36:a:122:ARG:NH2	2.28	0.67
11:A:2602:U:O4'	11:A:3078:C:O2'	2.10	0.67
11:A:3158:A:O2'	24:O:11:HIS:O	2.09	0.67
28:S:94:ARG:NH2	28:S:110:SER:O	2.27	0.67
9:8:129:ARG:NH1	12:B:1627:C:O4'	2.28	0.67
11:A:3020:C:OP1	11:A:3133:A:O2'	2.13	0.66
11:A:2895:U:O2'	11:A:2896:G:O5'	2.13	0.66
33:X:81:GLY:N	33:X:131:THR:OG1	2.29	0.66
11:A:2933:G:N2	11:A:2936:U:O2	2.25	0.66
8:7:231:GLN:N	8:7:231:GLN:OE1	2.29	0.66
6:5:295:ASP:OD2	6:5:304:LEU:N	2.29	0.65
38:c:227:GLU:OE2	38:c:302:ARG:NE	2.26	0.65
33:X:35:GLU:N	33:X:35:GLU:OE1	2.30	0.65
29:T:155:ARG:NH2	39:d:55:GLU:OE1	2.30	0.65
33:X:61:ARG:NH2	33:X:63:GLU:OE2	2.30	0.65
11:A:2195:A:OP1	47:l:119:ARG:NH2	2.30	0.65
26:Q:152:ARG:NH1	26:Q:198:SER:OG	2.30	0.65
7:6:176:ALA:HB3	7:6:184:LEU:HD12	1.79	0.64
11:A:2145:G:N3	28:S:104:ARG:NH2	2.45	0.64
11:A:2472:A:O2'	11:A:2478:G:N7	2.21	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2696:A:O2'	11:A:2698:G:OP2	2.15	0.64
18:I:82:LEU:HD11	18:I:130:VAL:HG21	1.80	0.64
11:A:1953:A:O2'	11:A:2463:A:OP1	2.15	0.64
6:5:276:ASP:OD1	53:s:158:ARG:NH1	2.31	0.64
11:A:2191:A:O2'	19:J:143:SER:OG	2.12	0.64
15:E:325:GLU:OE1	15:E:325:GLU:N	2.30	0.64
4:3:169:ARG:NH2	11:A:1892:A:N7	2.45	0.64
11:A:1679:U:O2'	11:A:1680:A:OP2	2.14	0.64
11:A:1749:C:OP2	11:A:2899:C:O2'	2.15	0.64
11:A:1860:A:O2'	11:A:2682:A:OP1	2.15	0.64
11:A:1750:G:O2'	11:A:1751:A:OP2	2.14	0.63
14:D:113:ARG:O	14:D:147:ARG:NH2	2.31	0.63
34:Y:94:SER:OG	34:Y:96:GLU:OE1	2.16	0.63
11:A:1853:A:OP2	28:S:177:ARG:NH2	2.30	0.63
25:P:94:VAL:HG21	25:P:136:CYS:SG	2.39	0.63
20:K:110:GLY:O	20:K:114:LYS:NZ	2.24	0.63
40:e:151:ARG:NH1	40:e:254:TRP:O	2.31	0.63
18:I:101:ASN:OD1	18:I:174:LEU:HD21	1.99	0.63
11:A:2507:A:O2'	11:A:2508:C:OP1	2.14	0.63
8:7:193:MET:SD	8:7:295:ARG:NH2	2.72	0.62
11:A:2040:G:O2'	22:M:56:GLU:OE1	2.17	0.62
11:A:2191:A:HO2'	19:J:143:SER:HG	1.47	0.62
31:V:171:ILE:O	34:Y:80:LYS:NZ	2.32	0.62
11:A:2932:G:OP1	16:F:137:ARG:NH1	2.31	0.62
6:5:377:ASP:OD1	6:5:380:GLN:NE2	2.33	0.62
11:A:2822:C:O2'	11:A:2915:C:OP2	2.17	0.62
18:I:181:ILE:O	18:I:184:THR:OG1	2.18	0.62
8:7:114:ASP:OD1	8:7:268:LEU:N	2.33	0.62
11:A:2029:A:O2'	11:A:2030:U:OP2	2.15	0.62
53:s:191:HIS:O	53:s:428:ARG:NH2	2.31	0.62
19:J:127:ASP:O	19:J:133:GLN:NE2	2.32	0.62
48:m:37:ARG:NH1	48:m:38:ALA:HB3	2.15	0.62
11:A:1672:C:O2'	29:T:149:ARG:O	2.16	0.62
11:A:3017:C:O2'	11:A:3019:G:OP2	2.15	0.62
13:C:327:PHE:CZ	13:C:354:LEU:HD23	2.35	0.61
11:A:1962:A:OP2	11:A:2501:C:N4	2.34	0.61
11:A:2256:U:O2'	28:S:118:ASN:ND2	2.33	0.61
16:F:94:ASP:OD1	16:F:95:ILE:N	2.33	0.61
24:O:64:LYS:NZ	24:O:100:GLN:O	2.32	0.61
40:e:201:GLU:OE1	40:e:240:THR:OG1	2.17	0.61
8:7:315:LYS:NZ	15:E:68:GLU:OE1	2.29	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:C:437:SER:O	13:C:441:GLY:N	2.33	0.61
11:A:2104:A:OP1	23:N:73:ARG:NH1	2.31	0.61
14:D:132:ASP:OD2	14:D:135:ARG:NH1	2.33	0.61
11:A:2065:A:OP1	41:f:48:TYR:N	2.34	0.60
29:T:156:ILE:HB	39:d:52:THR:HG21	1.84	0.60
10:9:71:LYS:H	31:V:177:THR:HG22	1.66	0.60
11:A:2740:A:N3	11:A:2921:A:O2'	2.30	0.60
35:Z:71:ARG:NH2	35:Z:92:GLU:O	2.34	0.60
6:5:201:ARG:NH1	6:5:418:TYR:O	2.34	0.60
11:A:1884:G:N3	11:A:1895:C:O2'	2.35	0.60
16:F:91:PRO:HB3	22:M:16:LEU:HD11	1.84	0.60
7:6:176:ALA:CB	7:6:184:LEU:HD12	2.32	0.60
8:7:203:THR:HG22	8:7:280:VAL:H	1.67	0.60
29:T:94:ILE:HD11	29:T:174:TYR:OH	2.03	0.59
13:C:200:ARG:NH1	13:C:356:GLN:O	2.35	0.59
11:A:2363:A:O2'	11:A:2364:C:OP2	2.20	0.59
28:S:142:THR:HG23	36:a:62:HIS:NE2	2.18	0.59
21:L:84:ALA:HB1	21:L:105:VAL:HG22	1.84	0.59
35:Z:117:ILE:O	49:o:45:ASN:ND2	2.34	0.59
11:A:2472:A:OP1	21:L:56:ARG:NH2	2.36	0.58
13:C:249:ILE:O	13:C:249:ILE:HG22	2.01	0.58
40:e:270:ALA:O	40:e:273:ARG:NH1	2.35	0.58
23:N:59:VAL:O	23:N:59:VAL:HG13	2.03	0.58
8:7:199:LEU:O	8:7:203:THR:HG23	2.04	0.58
11:A:2727:C:O2'	11:A:2815:OMG:N2	2.36	0.58
11:A:2567:G:OP1	14:D:277:ARG:NH2	2.37	0.58
40:e:74:LEU:HD13	48:m:42:ARG:HD3	1.85	0.58
9:8:121:TRP:HZ3	12:B:1628:C:HO2'	1.50	0.58
9:8:160:GLU:OE1	40:e:207:ASN:ND2	2.36	0.58
11:A:2277:U:O2	16:F:104:LYS:NZ	2.37	0.58
15:E:121:LEU:HD22	15:E:284:TYR:CE1	2.39	0.58
46:k:77:ARG:O	46:k:81:LEU:HD13	2.04	0.58
1:0:96:ASN:ND2	11:A:2709:A:O4'	2.37	0.57
11:A:1787:G:N2	11:A:1790:A:OP2	2.31	0.57
12:B:1607:U:HO2'	12:B:1608:G:P	2.24	0.57
23:N:204:GLU:OE1	23:N:207:ARG:NH1	2.35	0.57
37:b:21:ARG:NE	38:c:217:ASP:OD2	2.37	0.57
42:g:72:TRP:NE1	42:g:92:HIS:O	2.34	0.57
18:I:188:ARG:NE	46:k:55:VAL:HG13	2.19	0.57
4:3:153:THR:HG21	11:A:2044:A:OP1	2.04	0.57
11:A:2692:G:N1	11:A:2696:A:OP2	2.26	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S:164:THR:HG22	28:S:165:GLU:N	2.19	0.57
50:p:75:ARG:NH1	50:p:109:GLU:OE1	2.36	0.57
1:0:139:ARG:NH2	11:A:2322:C:OP1	2.35	0.57
29:T:133:ASN:ND2	39:d:226:ASP:OD2	2.37	0.57
11:A:1760:G:OP2	51:q:59:LYS:NZ	2.30	0.57
11:A:3194:U:OP2	52:r:144:LYS:NZ	2.38	0.57
32:W:67:ILE:HG21	32:W:131:VAL:HG11	1.87	0.57
8:7:81:MET:HE1	8:7:94:HIS:HD2	1.70	0.57
7:6:220:SER:HA	7:6:268:LEU:HD23	1.85	0.56
15:E:203:TYR:CD1	15:E:307:TYR:CE1	2.93	0.56
11:A:1877:U:O3'	22:M:30:ASN:ND2	2.38	0.56
11:A:2499:U:OP2	11:A:2504:A:N6	2.24	0.56
7:6:268:LEU:HD12	7:6:319:PHE:CZ	2.40	0.56
11:A:2029:A:HO2'	11:A:2030:U:P	2.27	0.56
13:C:230:ARG:HA	13:C:233:LEU:HD23	1.87	0.56
13:C:260:GLN:O	13:C:264:LEU:HD23	2.05	0.56
11:A:1731:A:OP1	17:H:74:HIS:NE2	2.38	0.56
11:A:1832:A:N6	11:A:1837:C:OP2	2.38	0.56
6:5:216:GLU:N	6:5:216:GLU:OE1	2.39	0.56
11:A:1697:A:N3	11:A:1703:C:O2'	2.38	0.56
18:I:113:ARG:NH1	18:I:123:MET:O	2.38	0.56
53:s:415:ASP:O	53:s:419:LEU:HD23	2.06	0.56
20:K:73:GLU:OE2	52:r:149:ARG:NH2	2.37	0.56
33:X:116:SER:O	33:X:120:ASP:N	2.38	0.56
11:A:2105:G:OP1	23:N:70:SER:OG	2.24	0.56
11:A:2442:U:O2'	53:s:86:MET:SD	2.63	0.56
11:A:2638:U:O4	11:A:2639:C:N4	2.39	0.56
11:A:2966:U:OP1	11:A:3024:U:O2'	2.17	0.56
26:Q:84:ARG:NH2	26:Q:271:ARG:O	2.38	0.56
13:C:205:LEU:HD13	13:C:228:LEU:HD22	1.87	0.55
1:0:85:ARG:NH2	11:A:2308:A:OP1	2.38	0.55
1:0:112:GLU:OE1	8:7:72:LYS:NZ	2.37	0.55
11:A:1678:C:O2'	11:A:1679:U:OP2	2.17	0.55
11:A:1773:A:OP2	38:c:31:VAL:N	2.39	0.55
48:m:40:LEU:HD23	48:m:40:LEU:H	1.71	0.55
53:s:360:VAL:HG12	53:s:369:PHE:CD2	2.42	0.55
11:A:2086:A:H2'	11:A:2087:U:C6	2.42	0.55
11:A:2525:C:O2'	11:A:2533:A:O2'	2.24	0.55
19:J:138:SER:HA	19:J:141:VAL:HG12	1.89	0.55
13:C:233:LEU:HD11	13:C:264:LEU:HD21	1.89	0.55
11:A:1856:A:OP2	11:A:2986:C:O2'	2.25	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:d:50:PHE:HA	39:d:53:GLU:HG3	1.89	0.55
13:C:205:LEU:HD11	13:C:225:GLU:HA	1.88	0.55
22:M:54:LYS:N	22:M:58:GLN:OE1	2.35	0.55
24:O:38:ARG:NH2	24:O:82:GLU:OE1	2.39	0.55
13:C:136:VAL:HG23	13:C:136:VAL:O	2.06	0.55
11:A:1702:A:HO2'	11:A:1704:U:H5	1.55	0.55
18:I:132:LYS:NZ	18:I:147:PHE:O	2.27	0.55
37:b:66:ASN:ND2	38:c:65:ASN:OD1	2.39	0.55
39:d:42:THR:O	39:d:42:THR:HG23	2.07	0.54
11:A:2171:U:O2'	11:A:2172:A:OP2	2.23	0.54
37:b:33:VAL:HG12	37:b:34:SER:H	1.72	0.54
11:A:2131:A:OP1	49:o:23:ARG:NH1	2.39	0.54
7:6:235:TRP:HB3	7:6:254:TYR:HA	1.90	0.54
28:S:108:VAL:HG13	28:S:195:ILE:HG13	1.88	0.54
11:A:2387:U:O2'	11:A:2406:A:N7	2.41	0.54
31:V:138:THR:OG1	31:V:141:GLY:O	2.22	0.54
46:k:81:LEU:HD11	52:r:51:GLY:N	2.23	0.54
15:E:96:ARG:NH1	15:E:315:PRO:O	2.38	0.53
7:6:181:GLU:N	7:6:181:GLU:OE1	2.41	0.53
11:A:1671:G:O2'	11:A:1672:C:O5'	2.25	0.53
11:A:2132:A:N6	49:o:16:GLN:OE1	2.41	0.53
22:M:111:ASP:O	22:M:116:ILE:HD11	2.08	0.53
11:A:2523:C:O2	11:A:2523:C:H2'	2.08	0.53
44:i:80:LEU:HD12	44:i:80:LEU:O	2.09	0.53
34:Y:151:ASP:OD1	34:Y:154:ARG:NH2	2.39	0.53
9:8:125:LYS:NZ	12:B:1628:C:O4'	2.40	0.53
11:A:1849:C:O2'	11:A:1851:G:N7	2.33	0.53
24:O:33:LEU:HD21	24:O:59:LEU:CD1	2.39	0.53
31:V:122:LEU:HD12	31:V:133:ILE:HG13	1.89	0.53
8:7:95:LEU:O	29:T:137:ARG:NH2	2.41	0.53
11:A:1728:U:O2'	33:X:96:LYS:O	2.10	0.53
12:B:1632:U:N3	12:B:1635:C:OP2	2.41	0.53
18:I:164:MET:O	18:I:168:LEU:HD23	2.08	0.53
47:l:135:ASN:OD1	47:l:136:LYS:N	2.42	0.53
10:9:71:LYS:N	31:V:177:THR:HG22	2.24	0.53
11:A:3113:A:OP1	11:A:3167:U:O2'	2.27	0.53
11:A:2489:C:O2'	11:A:2621:G:OP1	2.27	0.53
14:D:124:GLU:HB3	14:D:142:VAL:HG22	1.90	0.53
53:s:400:PRO:O	53:s:414:ASN:ND2	2.41	0.53
11:A:2236:C:OP1	49:o:9:ARG:NH2	2.43	0.52
11:A:2402:A:OP2	14:D:131:TYR:OH	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2829:C:OP2	11:A:2830:A:O2'	2.14	0.52
17:H:107:VAL:HG13	17:H:108:ARG:H	1.73	0.52
27:R:122:ARG:NH1	28:S:66:LEU:HD22	2.25	0.52
11:A:1751:A:OP1	22:M:75:TYR:OH	2.22	0.52
11:A:2449:G:OP2	53:s:225:ARG:NH2	2.40	0.52
11:A:3092:U:HO2'	11:A:3093:C:P	2.31	0.52
53:s:378:ALA:HB1	53:s:383:ALA:HB1	1.91	0.52
10:9:73:TYR:O	31:V:177:THR:HG23	2.09	0.52
17:H:138:LYS:O	17:H:142:GLU:OE1	2.28	0.52
38:c:228:LEU:HB2	38:c:307:PHE:CD2	2.45	0.52
14:D:193:ILE:HD11	14:D:226:ILE:HD12	1.90	0.52
19:J:103:GLN:O	19:J:104:THR:OG1	2.23	0.52
11:A:2240:C:OP2	20:K:71:LYS:NZ	2.43	0.52
40:e:81:ARG:NH2	48:m:43:VAL:O	2.38	0.52
52:r:93:ILE:HG22	52:r:94:ARG:O	2.09	0.52
25:P:94:VAL:HG22	25:P:144:MET:SD	2.50	0.52
7:6:292:GLN:NE2	25:P:40:GLU:OE2	2.42	0.52
9:8:129:ARG:NE	12:B:1626:C:O2'	2.43	0.52
11:A:2458:A:OP2	24:O:9:ILE:N	2.43	0.52
46:k:82:THR:HG23	46:k:85:GLU:H	1.74	0.52
11:A:2003:A:OP2	11:A:2734:A:O2'	2.26	0.52
11:A:2442:U:OP1	53:s:81:ARG:NH2	2.36	0.52
14:D:117:THR:HG22	14:D:117:THR:O	2.10	0.52
10:9:103:ASP:OD2	10:9:116:LYS:NZ	2.43	0.52
37:b:33:VAL:HG12	37:b:34:SER:N	2.25	0.52
13:C:100:LEU:HD11	13:C:124:ALA:HB3	1.92	0.51
28:S:164:THR:HG22	28:S:165:GLU:H	1.74	0.51
11:A:2414:C:OP1	11:A:2415:C:N4	2.43	0.51
40:e:156:ASN:C	40:e:157:LEU:HD12	2.36	0.51
11:A:2144:A:OP1	27:R:57:ARG:NH1	2.39	0.51
11:A:3009:C:O2'	11:A:3115:U:OP1	2.25	0.51
16:F:211:ARG:NH1	43:h:56:ARG:O	2.44	0.51
25:P:144:MET:HE2	25:P:170:VAL:HG11	1.91	0.51
11:A:1784:A:O2'	30:U:84:ASN:ND2	2.43	0.51
11:A:2374:A:N6	53:s:272:PRO:O	2.41	0.51
24:O:38:ARG:NE	24:O:82:GLU:OE1	2.43	0.51
25:P:91:GLU:OE1	25:P:106:SER:HB3	2.11	0.51
46:k:66:VAL:HG11	46:k:90:PHE:HE1	1.75	0.51
7:6:39:ASP:OD1	7:6:40:ILE:N	2.43	0.51
8:7:223:ALA:N	8:7:250:ARG:O	2.42	0.51
20:K:171:THR:HG22	52:r:59:GLU:H	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:90:VAL:H	25:P:107:THR:HG22	1.76	0.51
26:Q:246:ASP:OD1	26:Q:247:LEU:N	2.42	0.51
11:A:2694:A:N3	11:A:2942:C:O2'	2.43	0.51
13:C:219:LEU:HD21	13:C:274:ALA:HB1	1.92	0.51
6:5:280:GLN:OE1	53:s:158:ARG:NE	2.44	0.51
11:A:2905:A:O2'	11:A:2906:C:P	2.69	0.51
14:D:232:ARG:HE	14:D:290:PRO:HB2	1.75	0.51
53:s:416:ASP:OD1	53:s:417:VAL:N	2.43	0.51
1:0:163:GLU:OE2	1:0:181:ARG:NE	2.37	0.50
8:7:150:MET:HE2	8:7:280:VAL:HG13	1.93	0.50
11:A:1805:A:OP2	31:V:94:HIS:NE2	2.34	0.50
11:A:2261:C:O2'	28:S:184:ARG:NH1	2.43	0.50
46:k:20:PHE:O	46:k:55:VAL:HG23	2.11	0.50
11:A:2186:C:O2'	11:A:2187:C:P	2.69	0.50
23:N:138:HIS:ND1	23:N:139:ARG:O	2.44	0.50
53:s:351:VAL:O	53:s:389:ARG:NH1	2.42	0.50
6:5:381:LEU:HD23	6:5:381:LEU:H	1.76	0.50
11:A:1852:C:H2'	11:A:1852:C:O2	2.11	0.50
15:E:307:TYR:HD1	15:E:310:LEU:HD12	1.75	0.50
39:d:213:THR:HG22	39:d:247:VAL:HG22	1.93	0.50
11:A:2030:U:H2'	11:A:2030:U:O2	2.10	0.50
11:A:3189:C:O2'	52:r:155:ALA:N	2.39	0.50
1:0:113:CYS:O	8:7:73:THR:OG1	2.27	0.50
18:I:119:HIS:NE2	18:I:158:GLU:O	2.43	0.50
19:J:32:GLY:O	19:J:36:GLY:N	2.44	0.50
19:J:84:GLN:N	19:J:127:ASP:OD2	2.34	0.50
4:3:148:VAL:HG13	7:6:360:ARG:HA	1.94	0.50
18:I:101:ASN:N	18:I:152:MET:HE2	2.27	0.50
18:I:139:LYS:HD2	18:I:139:LYS:O	2.12	0.50
51:q:44:ASP:O	51:q:47:THR:HG22	2.12	0.50
28:S:96:PHE:HB3	37:b:126:ILE:HD13	1.94	0.50
42:g:48:VAL:O	42:g:52:LEU:HD23	2.12	0.50
6:5:273:VAL:O	6:5:273:VAL:HG13	2.11	0.50
9:8:136:ILE:HD13	41:f:169:ILE:HD11	1.93	0.49
12:B:1607:U:O2'	12:B:1608:G:P	2.68	0.49
12:B:1628:C:N4	12:B:1640:A:N1	2.59	0.49
18:I:125:VAL:HG22	18:I:152:MET:HG3	1.94	0.49
26:Q:240:ILE:HG21	26:Q:243:ILE:HD12	1.93	0.49
7:6:139:TRP:O	7:6:144:GLY:N	2.41	0.49
11:A:1882:A:N1	11:A:1891:A:O2'	2.44	0.49
17:H:107:VAL:HG13	17:H:108:ARG:N	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:I:188:ARG:NH2	46:k:55:VAL:HG22	2.27	0.49
27:R:112:THR:HG23	28:S:142:THR:HG21	1.93	0.49
11:A:1823:A:O2'	11:A:1824:U:P	2.70	0.49
31:V:133:ILE:HD12	31:V:154:ILE:HD12	1.93	0.49
6:5:177:CYS:O	6:5:180:ILE:HG22	2.12	0.49
9:8:136:ILE:O	9:8:140:LEU:HD23	2.12	0.49
37:b:47:VAL:O	37:b:51:VAL:HG12	2.13	0.49
13:C:174:VAL:HG13	13:C:195:VAL:HG21	1.95	0.49
39:d:266:VAL:HG13	39:d:266:VAL:O	2.13	0.49
40:e:264:LEU:HD23	40:e:269:LEU:HB3	1.94	0.49
37:b:67:SER:HB3	43:h:156:TRP:CD1	2.47	0.49
13:C:484:VAL:HG12	13:C:500:VAL:HG12	1.95	0.49
40:e:152:LYS:HB2	40:e:157:LEU:HD11	1.95	0.49
39:d:160:LEU:O	39:d:164:VAL:HG22	2.13	0.49
11:A:1814:A:C8	44:i:32:ILE:HG21	2.48	0.49
6:5:251:HIS:O	6:5:371:LYS:NZ	2.36	0.48
11:A:1882:A:N6	11:A:1893:A:O4'	2.46	0.48
11:A:2615:A:C6	21:L:58:ILE:HG23	2.48	0.48
41:f:161:GLY:C	41:f:162:LEU:HD22	2.37	0.48
6:5:107:PHE:CE1	6:5:113:LEU:HD11	2.48	0.48
7:6:182:ASP:OD1	7:6:182:ASP:N	2.47	0.48
8:7:192:TRP:O	8:7:295:ARG:NH2	2.46	0.48
2:1:53:ARG:NH2	11:A:2879:A:O2'	2.38	0.48
8:7:279:GLU:HG2	8:7:317:LEU:HD22	1.95	0.48
25:P:63:ARG:NH2	32:W:137:LYS:O	2.37	0.48
28:S:76:HIS:CD2	36:a:50:ALA:HA	2.47	0.48
40:e:74:LEU:HD12	40:e:75:GLN:N	2.29	0.48
11:A:3150:U:C2	11:A:3151:A:C8	3.00	0.48
15:E:206:VAL:HG11	15:E:289:VAL:HG11	1.94	0.48
31:V:47:GLU:OE2	31:V:117:HIS:NE2	2.45	0.48
7:6:294:ALA:O	7:6:297:THR:HG22	2.14	0.48
11:A:2123:C:C3'	11:A:2124:A:H5''	2.44	0.48
11:A:2754:A:OP1	17:H:91:LYS:NZ	2.46	0.48
19:J:23:ILE:HG23	19:J:23:ILE:O	2.13	0.48
7:6:187:VAL:HG12	7:6:187:VAL:O	2.14	0.48
11:A:2209:G:C2'	11:A:2210:C:OP1	2.61	0.48
11:A:2693:A:H1'	11:A:2694:A:OP2	2.14	0.48
30:U:22:THR:HG22	30:U:24:PHE:H	1.79	0.48
33:X:16:LEU:HD21	33:X:208:LEU:HD11	1.95	0.48
44:i:79:TRP:O	44:i:93:ARG:NE	2.42	0.48
1:0:167:GLU:OE1	1:0:167:GLU:N	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:262:ASP:OD1	8:7:263:VAL:N	2.46	0.48
11:A:1706:C:OP1	34:Y:193:ARG:NH1	2.43	0.48
11:A:1859:A:OP1	11:A:2299:U:O2'	2.26	0.48
11:A:2895:U:O2'	11:A:2896:G:P	2.71	0.48
11:A:3088:C:H3'	11:A:3089:A:H5''	1.94	0.48
11:A:3092:U:O2'	11:A:3093:C:P	2.71	0.48
34:Y:218:ARG:NH2	44:i:105:ASP:OD1	2.47	0.48
1:0:91:ARG:NE	11:A:1818:A:OP2	2.44	0.48
13:C:382:ARG:HH12	13:C:393:LYS:HB2	1.79	0.48
30:U:9:LEU:N	34:Y:183:GLN:OE1	2.47	0.48
33:X:53:ASN:ND2	33:X:56:ASN:OD1	2.41	0.48
11:A:2081:U:OP1	49:o:63:ALA:N	2.42	0.47
11:A:2506:A:H1'	11:A:2601:A:N6	2.29	0.47
29:T:52:GLU:OE1	29:T:52:GLU:N	2.45	0.47
6:5:139:LEU:O	6:5:145:ASN:ND2	2.45	0.47
11:A:1849:C:OP2	22:M:53:HIS:NE2	2.47	0.47
13:C:483:THR:HG23	13:C:483:THR:O	2.14	0.47
9:8:140:LEU:O	9:8:144:GLN:OE1	2.31	0.47
11:A:2898:U:H2'	11:A:2899:C:O4'	2.14	0.47
17:H:110:ASP:OD1	17:H:110:ASP:N	2.47	0.47
19:J:26:ALA:HB1	19:J:57:THR:HG23	1.95	0.47
6:5:377:ASP:OD2	6:5:413:LYS:NZ	2.46	0.47
11:A:1869:A:N6	11:A:1904:C:OP1	2.47	0.47
11:A:3092:U:O2'	11:A:3093:C:OP1	2.23	0.47
13:C:307:LYS:N	56:C:601:GTP:O1B	2.37	0.47
20:K:15:ALA:CB	38:c:269:LEU:HD22	2.44	0.47
21:L:32:ILE:HG23	21:L:36:THR:OG1	2.15	0.47
2:1:62:ILE:HD12	2:1:62:ILE:H	1.80	0.47
10:9:24:LYS:NZ	11:A:2422:U:OP2	2.46	0.47
11:A:1688:A:H2'	11:A:1689:C:H4'	1.97	0.47
11:A:2138:U:O2'	11:A:2151:A:N3	2.43	0.47
11:A:2203:G:O2'	11:A:2208:A:N6	2.42	0.47
25:P:92:ALA:HB1	25:P:132:LEU:HD22	1.96	0.47
38:c:124:GLU:OE1	38:c:124:GLU:N	2.41	0.47
39:d:127:ASP:OD1	39:d:128:TYR:N	2.47	0.47
2:1:34:ARG:NH1	2:1:38:ARG:O	2.48	0.47
3:2:82:ARG:HD3	11:A:1791:G:OP2	2.15	0.47
8:7:52:LYS:HG3	8:7:219:LEU:HD11	1.97	0.47
11:A:2166:C:OP2	46:k:41:LYS:NZ	2.44	0.47
11:A:3195:A:OP2	11:A:3196:G:O2'	2.26	0.47
13:C:463:ILE:HG23	13:C:463:ILE:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:I:96:ILE:HG22	18:I:180:CYS:O	2.15	0.47
53:s:242:ARG:NH1	53:s:292:CYS:O	2.46	0.47
11:A:2198:A:N1	19:J:150:SER:OG	2.37	0.47
11:A:2278:A:OP1	44:i:51:ARG:NE	2.41	0.47
16:F:102:TRP:O	16:F:106:PHE:HD1	1.98	0.47
16:F:277:ASP:O	16:F:278:SER:OG	2.13	0.47
23:N:64:ARG:NH1	23:N:145:GLY:O	2.48	0.47
23:N:218:ILE:HG22	23:N:226:ILE:CD1	2.45	0.47
11:A:2079:C:O4'	11:A:2079:C:O2	2.33	0.47
11:A:2135:A:N3	11:A:2135:A:H2'	2.29	0.47
21:L:38:VAL:CG1	21:L:75:LEU:HD11	2.45	0.47
31:V:103:ASP:OD1	31:V:104:TYR:N	2.44	0.47
39:d:127:ASP:OD1	39:d:127:ASP:C	2.57	0.47
53:s:110:THR:HG22	53:s:110:THR:O	2.15	0.47
53:s:251:VAL:HG22	53:s:252:PRO:HD2	1.97	0.47
1:O:108:ASP:OD1	1:O:109:VAL:N	2.44	0.47
5:4:84:ARG:NE	11:A:3188:U:OP2	2.44	0.47
7:6:52:ARG:HB3	12:B:1637:C:H5'	1.97	0.47
7:6:56:ARG:NH1	12:B:1625:A:OP1	2.42	0.47
11:A:2055:U:H2'	11:A:2056:G:H8	1.79	0.47
11:A:2388:A:N3	14:D:128:GLN:NE2	2.62	0.47
53:s:174:LEU:HB3	53:s:175:PRO:HD3	1.97	0.47
13:C:470:LEU:HD23	19:J:40:GLY:HA3	1.96	0.46
39:d:263:THR:HG22	39:d:264:LYS:N	2.31	0.46
11:A:1861:U:H2'	11:A:1862:U:C6	2.51	0.46
11:A:2334:C:OP1	53:s:221:HIS:NE2	2.48	0.46
13:C:383:ASP:N	13:C:383:ASP:OD1	2.46	0.46
7:6:377:TYR:CD1	22:M:141:VAL:HG11	2.50	0.46
11:A:3169:C:H2'	11:A:3170:C:O2	2.16	0.46
14:D:139:ILE:HD12	14:D:150:TRP:CE3	2.50	0.46
31:V:139:GLU:OE1	31:V:139:GLU:N	2.41	0.46
6:5:151:ASP:O	6:5:155:LEU:HD23	2.15	0.46
11:A:2802:A:H2'	11:A:2803:A:O4'	2.15	0.46
11:A:3082:G:N2	11:A:3085:A:OP2	2.38	0.46
12:B:1609:U:O2	12:B:1616:A:N6	2.49	0.46
15:E:316:PHE:HB3	15:E:317:PRO:HD3	1.97	0.46
20:K:175:ASP:OD1	52:r:36:ARG:NH1	2.39	0.46
21:L:96:MET:HE1	26:Q:171:VAL:CG1	2.46	0.46
28:S:108:VAL:CG1	28:S:195:ILE:HG21	2.44	0.46
28:S:133:VAL:O	28:S:133:VAL:HG13	2.16	0.46
29:T:97:MET:HE1	29:T:105:GLN:HG3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:d:125:ILE:HG22	39:d:129:ASP:OD2	2.15	0.46
11:A:2028:G:N1	11:A:2264:A:OP2	2.31	0.46
16:F:92:ARG:HE	16:F:95:ILE:CD1	2.29	0.46
7:6:275:GLN:CD	7:6:311:MET:HE1	2.41	0.46
11:A:2267:U:OP1	44:i:126:LYS:NZ	2.49	0.46
11:A:2531:U:O4	14:D:246:ARG:NH2	2.48	0.46
11:A:2677:A:H2'	11:A:2678:A:C8	2.50	0.46
13:C:205:LEU:HD21	13:C:225:GLU:HG2	1.98	0.46
16:F:220:ASP:O	16:F:245:ALA:N	2.48	0.46
27:R:141:ILE:H	27:R:141:ILE:HD12	1.80	0.46
7:6:42:LEU:HD23	7:6:43:SER:N	2.30	0.46
13:C:287:ARG:O	13:C:290:THR:OG1	2.28	0.46
26:Q:168:ASN:O	26:Q:171:VAL:HG22	2.16	0.46
18:I:171:VAL:HG23	18:I:171:VAL:O	2.15	0.46
53:s:363:ASP:OD1	53:s:366:TYR:N	2.44	0.46
11:A:2124:A:H5'	11:A:2125:C:H5''	1.98	0.46
15:E:204:VAL:HG21	15:E:299:VAL:CG1	2.46	0.46
19:J:57:THR:O	19:J:60:ILE:O	2.34	0.46
38:c:307:PHE:CD2	38:c:307:PHE:O	2.69	0.46
39:d:81:THR:HG22	39:d:249:GLU:OE2	2.15	0.46
23:N:80:THR:O	23:N:80:THR:HG22	2.17	0.45
11:A:2039:A:N6	11:A:2729:U:O2	2.49	0.45
11:A:2754:A:N3	33:X:108:GLN:NE2	2.61	0.45
19:J:39:LEU:HB3	19:J:44:VAL:HG21	1.98	0.45
20:K:7:ALA:HB3	20:K:8:PRO:HD3	1.98	0.45
25:P:110:TRP:HA	25:P:113:LYS:HG2	1.98	0.45
39:d:173:THR:HA	39:d:176:ILE:HG22	1.97	0.45
51:q:61:PHE:O	51:q:65:GLY:N	2.46	0.45
7:6:154:TYR:CD2	25:P:102:VAL:HG13	2.51	0.45
11:A:1747:G:N2	11:A:1750:G:O2'	2.50	0.45
11:A:2186:C:O2'	11:A:2187:C:O5'	2.32	0.45
40:e:73:LEU:O	40:e:76:GLN:HG3	2.17	0.45
41:f:169:ILE:HD12	41:f:172:GLU:OE2	2.16	0.45
10:9:75:SER:OG	31:V:177:THR:O	2.21	0.45
11:A:1828:A:H4'	11:A:1829:A:C8	2.52	0.45
11:A:2494:C:O2	11:A:2494:C:H2'	2.16	0.45
11:A:3092:U:H2'	11:A:3093:C:C6	2.52	0.45
11:A:3092:U:H2'	11:A:3093:C:H6	1.81	0.45
13:C:212:ALA:HA	13:C:330:LEU:HD23	1.98	0.45
21:L:32:ILE:HD11	21:L:89:HIS:HB3	1.98	0.45
40:e:74:LEU:HA	40:e:77:ILE:HG12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:i:87:GLU:OE2	44:i:113:ARG:NE	2.47	0.45
7:6:234:HIS:ND1	7:6:255:LEU:O	2.35	0.45
11:A:2889:C:OP2	32:W:85:LYS:NZ	2.45	0.45
8:7:254:LEU:HD11	8:7:261:ILE:HG22	1.99	0.45
35:Z:70:THR:HG22	35:Z:97:PRO:HA	1.99	0.45
4:3:148:VAL:HG12	4:3:149:PHE:O	2.16	0.45
6:5:391:VAL:HG22	6:5:399:GLU:HB2	1.98	0.45
28:S:107:LYS:HE3	29:T:212:LEU:HD22	1.98	0.45
51:q:47:THR:HG23	51:q:47:THR:O	2.17	0.45
8:7:48:PHE:CE1	8:7:219:LEU:HD12	2.52	0.45
9:8:140:LEU:HD21	41:f:169:ILE:HG12	1.99	0.45
11:A:1990:G:OP1	14:D:269:ARG:NH1	2.49	0.45
11:A:2416:U:O2	11:A:2416:U:C2'	2.64	0.45
11:A:2993:U:H4'	11:A:2994:U:OP1	2.16	0.45
20:K:90:VAL:HG22	20:K:94:GLN:HB2	1.99	0.45
38:c:86:ASP:OD1	38:c:86:ASP:N	2.50	0.45
53:s:259:ILE:HD12	53:s:259:ILE:H	1.81	0.45
11:A:1939:G:O2'	11:A:1973:G:H4'	2.17	0.45
11:A:2134:A:N6	11:A:2135:A:H62	2.14	0.45
11:A:2457:A:O2'	24:O:17:ARG:NH1	2.41	0.45
11:A:2605:C:OP2	11:A:2606:U:O2'	2.23	0.45
13:C:441:GLY:HA2	13:C:444:LEU:HD23	1.99	0.45
27:R:64:MET:HE1	29:T:210:HIS:CG	2.52	0.45
37:b:26:LEU:HD22	37:b:105:ALA:HA	1.99	0.45
45:j:96:GLN:O	45:j:97:LYS:C	2.59	0.45
53:s:271:LEU:O	53:s:272:PRO:C	2.60	0.45
7:6:344:PHE:CE2	25:P:61:VAL:HG11	2.52	0.45
8:7:81:MET:HB3	8:7:86:SER:OG	2.17	0.45
11:A:2554:A:O2'	14:D:285:LYS:NZ	2.50	0.45
11:A:2615:A:C5	21:L:58:ILE:HD12	2.52	0.45
11:A:2740:A:H2'	11:A:2741:A:C8	2.52	0.45
11:A:3064:A:O4'	11:A:3099:C:N4	2.50	0.45
28:S:122:LEU:HD22	28:S:128:ILE:HD11	1.98	0.45
41:f:186:VAL:HG12	41:f:186:VAL:O	2.17	0.45
8:7:107:LEU:HG	8:7:128:LEU:HD11	1.98	0.44
11:A:1750:G:O2'	11:A:1751:A:P	2.75	0.44
11:A:2134:A:H62	11:A:2135:A:H62	1.65	0.44
19:J:20:ILE:HB	19:J:70:ILE:HG23	1.98	0.44
23:N:67:LYS:O	23:N:67:LYS:HG3	2.17	0.44
26:Q:153:ASN:OD1	26:Q:154:VAL:N	2.51	0.44
32:W:61:VAL:HG21	32:W:97:VAL:CG2	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:s:167:GLU:O	53:s:171:VAL:HG22	2.17	0.44
53:s:376:THR:HG23	53:s:387:ASN:HD21	1.83	0.44
5:4:71:VAL:O	5:4:71:VAL:HG13	2.17	0.44
16:F:89:THR:H	16:F:179:THR:HG21	1.82	0.44
25:P:102:VAL:HG11	25:P:141:ILE:HD11	1.99	0.44
30:U:28:LEU:O	34:Y:114:THR:HG23	2.17	0.44
40:e:256:THR:OG1	40:e:257:LYS:N	2.50	0.44
53:s:145:VAL:HG21	53:s:187:LEU:HD11	1.98	0.44
4:3:113:ARG:NH2	11:A:2898:U:O2'	2.45	0.44
8:7:167:VAL:HG12	8:7:182:ASP:O	2.18	0.44
8:7:238:ASP:O	8:7:242:GLU:HG2	2.17	0.44
8:7:238:ASP:OD1	8:7:239:PHE:N	2.50	0.44
11:A:2538:C:H2'	11:A:2539:A:O4'	2.17	0.44
11:A:2646:G:H4'	11:A:3093:C:H4'	1.99	0.44
11:A:2905:A:O2'	11:A:2906:C:O5'	2.28	0.44
14:D:157:MET:HE2	14:D:163:ILE:HD11	1.97	0.44
25:P:94:VAL:HG13	25:P:144:MET:SD	2.57	0.44
53:s:181:VAL:HG11	53:s:200:LEU:HD11	1.99	0.44
1:0:96:ASN:OD1	1:0:97:PRO:HD2	2.17	0.44
11:A:1823:A:C2'	11:A:1824:U:OP2	2.65	0.44
11:A:2470:G:H4'	21:L:36:THR:HG22	1.98	0.44
11:A:2727:C:H2'	11:A:2728:C:C6	2.53	0.44
13:C:204:VAL:HA	13:C:207:ILE:HG12	1.99	0.44
19:J:135:VAL:N	19:J:136:PRO:HD2	2.33	0.44
37:b:131:HIS:O	37:b:134:THR:OG1	2.29	0.44
5:4:71:VAL:HG12	11:A:2953:U:H5''	1.99	0.44
6:5:348:ASP:OD1	6:5:351:VAL:N	2.41	0.44
11:A:2041:U:H2'	11:A:2042:U:C6	2.53	0.44
11:A:2129:G:O4'	11:A:2152:A:H2	2.00	0.44
11:A:2134:A:OP1	49:o:15:ARG:NH2	2.51	0.44
11:A:2232:A:O2'	11:A:3002:G:N3	2.48	0.44
11:A:2262:C:OP1	28:S:173:ARG:NH1	2.50	0.44
33:X:124:THR:HG23	33:X:124:THR:O	2.18	0.44
41:f:167:ALA:O	41:f:171:LEU:HD23	2.18	0.44
9:8:107:THR:O	9:8:110:GLU:HG3	2.17	0.44
11:A:1671:G:O2'	11:A:1672:C:P	2.75	0.44
11:A:2167:A:N6	11:A:2212:C:OP2	2.44	0.44
13:C:256:PHE:O	13:C:260:GLN:HG2	2.18	0.44
46:k:54:ASP:OD2	46:k:56:ARG:NH1	2.44	0.44
9:8:169:PHE:HB2	9:8:170:PRO:HD3	1.99	0.44
11:A:2379:C:O2	11:A:2379:C:O4'	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2728:C:H4'	11:A:2815:OMG:HM22	1.99	0.44
11:A:3054:G:H2'	11:A:3055:U:C6	2.52	0.44
18:I:89:VAL:CG1	18:I:155:VAL:HG11	2.47	0.44
8:7:102:LYS:O	8:7:104:ILE:HD12	2.17	0.44
11:A:1857:U:H2'	11:A:1858:G:C8	2.52	0.44
11:A:2696:A:HO2'	11:A:2698:G:P	2.41	0.44
21:L:33:GLN:H	21:L:36:THR:HG21	1.83	0.44
11:A:1851:G:H2'	11:A:2693:A:N7	2.33	0.44
11:A:1962:A:N7	11:A:2501:C:C2	2.86	0.44
16:F:292:ASP:OD1	16:F:292:ASP:N	2.49	0.44
11:A:2674:U:H2'	11:A:2675:G:O4'	2.17	0.43
11:A:2868:C:H2'	11:A:2869:A:O4'	2.18	0.43
18:I:132:LYS:HB2	18:I:133:PRO:HD3	1.99	0.43
29:T:174:TYR:CE2	29:T:176:VAL:HG13	2.53	0.43
46:k:66:VAL:HG11	46:k:90:PHE:CE1	2.53	0.43
53:s:188:LEU:HD12	53:s:426:LEU:HD21	2.00	0.43
11:A:1917:A:N1	11:A:1997:C:H1'	2.33	0.43
11:A:2151:A:H2'	11:A:2152:A:C8	2.52	0.43
11:A:2629:A:N3	11:A:3079:G:O2'	2.37	0.43
11:A:2803:A:H2'	11:A:2804:A:O4'	2.18	0.43
13:C:131:LEU:HA	13:C:207:ILE:HG22	2.01	0.43
18:I:168:LEU:HD11	18:I:174:LEU:HD23	1.98	0.43
11:A:2492:G:N2	11:A:2494:C:H5''	2.33	0.43
11:A:2514:C:H2'	11:A:2515:U:H6	1.83	0.43
11:A:2550:A:C6	11:A:2590:A:C6	3.06	0.43
13:C:111:LYS:O	13:C:113:GLN:NE2	2.51	0.43
13:C:438:ALA:HB3	56:C:601:GTP:N2	2.32	0.43
29:T:55:ASN:O	39:d:227:ARG:NE	2.51	0.43
29:T:157:ARG:HB2	29:T:167:MET:HG3	2.00	0.43
6:5:355:LEU:HD21	6:5:357:PHE:HB2	2.00	0.43
10:9:41:ILE:HG23	10:9:57:VAL:HG22	2.00	0.43
11:A:1917:A:C8	11:A:1983:U:C4	3.06	0.43
11:A:3219:G:O2'	11:A:3221:A:OP2	2.29	0.43
13:C:168:SER:OG	13:C:170:ASP:OD1	2.33	0.43
16:F:177:ALA:O	16:F:181:LYS:HG2	2.19	0.43
20:K:154:ARG:NH2	20:K:157:GLU:OE2	2.51	0.43
4:3:127:ALA:HA	22:M:79:PRO:HD3	2.01	0.43
4:3:169:ARG:NH2	4:3:182:ASP:OD2	2.51	0.43
6:5:301:PRO:HD3	11:A:2390:A:H4'	2.00	0.43
11:A:2416:U:H2'	53:s:165:ARG:NH2	2.34	0.43
11:A:2838:A:C6	11:A:2840:C:C5	3.07	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:F:62:VAL:HG13	16:F:82:LEU:HB2	2.00	0.43
26:Q:171:VAL:O	26:Q:171:VAL:HG23	2.18	0.43
30:U:42:PHE:HB3	30:U:44:ILE:HD11	2.00	0.43
39:d:76:ILE:HD12	39:d:76:ILE:H	1.83	0.43
4:3:116:ARG:NH1	4:3:159:ASP:OD1	2.52	0.43
7:6:187:VAL:HG13	7:6:319:PHE:HB3	2.00	0.43
8:7:108:VAL:HG13	8:7:123:CYS:SG	2.58	0.43
11:A:2015:G:O4'	22:M:56:GLU:HG3	2.19	0.43
11:A:2060:A:C8	11:A:2079:C:C4	3.07	0.43
11:A:2842:C:OP1	23:N:64:ARG:NE	2.43	0.43
11:A:2978:U:O2'	11:A:3057:C:OP1	2.29	0.43
20:K:6:ARG:NH2	38:c:225:GLY:O	2.52	0.43
20:K:91:THR:HG22	52:r:161:PRO:HB3	2.00	0.43
31:V:141:GLY:O	31:V:142:GLU:C	2.61	0.43
46:k:61:GLU:N	46:k:62:PRO:HD2	2.33	0.43
7:6:125:LEU:C	7:6:126:ARG:HG2	2.43	0.43
11:A:2845:A:O2'	11:A:2846:G:H5'	2.19	0.43
11:A:3201:A:H2'	11:A:3202:U:O4'	2.19	0.43
19:J:60:ILE:HG23	19:J:61:LYS:O	2.19	0.43
26:Q:120:THR:O	26:Q:172:GLN:N	2.51	0.43
30:U:80:ARG:NH1	30:U:84:ASN:O	2.52	0.43
2:1:19:ARG:HB2	2:1:62:ILE:HD11	2.01	0.43
7:6:253:PRO:O	7:6:296:ARG:NH2	2.52	0.43
11:A:1718:A:H2'	11:A:1719:G:O4'	2.19	0.43
11:A:1883:G:H5'	42:g:91:MET:HG3	2.01	0.43
11:A:2213:A:H2'	11:A:2214:A:H5'	1.99	0.43
11:A:2836:C:H5'	11:A:2837:A:OP1	2.19	0.43
11:A:3198:A:HO2'	11:A:3199:U:P	2.27	0.43
16:F:87:PHE:HA	16:F:179:THR:HG22	2.01	0.43
22:M:110:VAL:HG13	22:M:116:ILE:HD12	2.01	0.43
39:d:119:GLN:OE1	39:d:123:ARG:NE	2.52	0.43
8:7:66:GLU:OE2	30:U:143:ARG:NH2	2.52	0.43
18:I:151:ASN:OD1	18:I:151:ASN:N	2.52	0.43
37:b:45:GLU:HB2	37:b:94:VAL:HG22	2.01	0.43
1:0:85:ARG:HE	11:A:2308:A:H5''	1.84	0.43
6:5:113:LEU:HD12	6:5:113:LEU:H	1.84	0.43
7:6:221:LEU:HA	7:6:231:GLU:OE1	2.19	0.43
11:A:2113:G:H22	11:A:2693:A:P	2.42	0.43
11:A:3198:A:C2'	11:A:3199:U:OP2	2.66	0.43
12:B:1628:C:H2'	12:B:1629:A:H8	1.84	0.43
16:F:193:LEU:HD22	16:F:218:LEU:HD23	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:b:95:GLU:OE1	37:b:95:GLU:N	2.49	0.43
11:A:2614:U:O2'	11:A:2616:A:N7	2.48	0.42
11:A:3013:G:O6	11:A:3025:A:C6	2.72	0.42
38:c:220:ILE:O	38:c:223:MET:HG2	2.19	0.42
39:d:263:THR:HG22	39:d:264:LYS:H	1.84	0.42
41:f:161:GLY:O	41:f:162:LEU:HD22	2.19	0.42
50:p:42:ILE:H	50:p:42:ILE:HD12	1.84	0.42
2:1:45:HIS:ND1	11:A:2852:C:O2'	2.35	0.42
11:A:1679:U:O2'	11:A:1680:A:P	2.77	0.42
11:A:1935:A:H2'	11:A:1936:A:O4'	2.19	0.42
11:A:1991:A:H5''	11:A:1992:C:OP1	2.19	0.42
11:A:2334:C:O2	53:s:277:GLN:NE2	2.47	0.42
11:A:2813:U:H3'	11:A:2814:G:C5'	2.49	0.42
11:A:2814:G:O2'	11:A:2983:G:OP1	2.32	0.42
11:A:3212:C:O2	11:A:3212:C:O4'	2.36	0.42
13:C:219:LEU:HD21	13:C:274:ALA:CB	2.49	0.42
16:F:191:ASP:OD1	16:F:192:SER:N	2.50	0.42
39:d:124:ARG:O	39:d:127:ASP:OD1	2.37	0.42
11:A:2387:U:H3'	14:D:75:THR:HG22	2.02	0.42
11:A:2928:C:OP1	39:d:38:LYS:N	2.52	0.42
14:D:247:VAL:HG12	14:D:248:SER:N	2.35	0.42
31:V:204:ILE:HD12	31:V:204:ILE:H	1.84	0.42
39:d:50:PHE:O	39:d:54:LYS:HG3	2.20	0.42
40:e:160:LEU:HD21	40:e:264:LEU:HD11	2.01	0.42
48:m:43:VAL:HG12	48:m:45:ARG:H	1.84	0.42
4:3:138:PRO:HG2	11:A:2854:U:H4'	2.02	0.42
6:5:173:ARG:NH2	11:A:2395:A:OP1	2.40	0.42
8:7:46:ASP:O	8:7:50:LYS:HG2	2.20	0.42
11:A:1871:A:N7	11:A:1902:C:N4	2.66	0.42
11:A:2446:A:N6	53:s:66:TRP:NE1	2.67	0.42
11:A:3089:A:O4'	13:C:241:TYR:OH	2.33	0.42
13:C:130:THR:HG23	13:C:325:GLN:HB3	2.01	0.42
15:E:204:VAL:HG21	15:E:299:VAL:HG12	2.02	0.42
18:I:188:ARG:CZ	46:k:55:VAL:HG22	2.49	0.42
19:J:60:ILE:HG13	19:J:61:LYS:H	1.84	0.42
37:b:141:ARG:NH1	37:b:149:GLN:O	2.48	0.42
39:d:154:ASN:O	39:d:155:SER:OG	2.29	0.42
5:4:84:ARG:C	5:4:85:ARG:HG2	2.43	0.42
8:7:290:GLN:CG	8:7:291:PRO:HD3	2.50	0.42
11:A:1826:G:N2	11:A:2686:G:N7	2.67	0.42
11:A:2728:C:H2'	11:A:2729:U:H6	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:3150:U:C5	15:E:118:VAL:HG11	2.55	0.42
39:d:276:ILE:HD12	39:d:276:ILE:H	1.83	0.42
7:6:126:ARG:NH2	12:B:1641:G:OP1	2.52	0.42
9:8:119:LYS:NZ	12:B:1642:G:O2'	2.49	0.42
11:A:2099:U:H2'	11:A:2100:C:C6	2.55	0.42
11:A:2236:C:N4	11:A:2688:C:O2	2.53	0.42
11:A:2241:A:OP2	20:K:68:SER:OG	2.25	0.42
11:A:2994:U:H5	11:A:3069:A:N1	2.17	0.42
11:A:3091:G:C2'	11:A:3092:U:H5'	2.50	0.42
19:J:134:ASP:OD2	19:J:139:SER:OG	2.36	0.42
25:P:67:GLY:HA3	32:W:78:GLY:O	2.19	0.42
8:7:269:ILE:HD12	8:7:274:ILE:HB	2.02	0.42
11:A:2091:A:H2'	11:A:2092:C:O4'	2.19	0.42
11:A:2127:A:H4'	11:A:2251:A:C5	2.55	0.42
11:A:2209:G:H2'	11:A:2210:C:OP1	2.20	0.42
11:A:2281:A:H5''	37:b:36:ASP:HB3	2.02	0.42
11:A:2752:C:C2	11:A:2753:A:C8	3.08	0.42
11:A:3078:C:N4	11:A:3079:G:O6	2.53	0.42
13:C:131:LEU:HD11	13:C:206:HIS:ND1	2.35	0.42
11:A:2029:A:O2'	11:A:2124:A:N6	2.53	0.42
11:A:2453:G:O2'	24:O:116:ASP:OD2	2.32	0.42
11:A:3097:U:C4'	11:A:3098:U:OP2	2.67	0.42
13:C:309:THR:HG22	13:C:438:ALA:HB1	2.02	0.42
19:J:23:ILE:HD11	19:J:86:THR:CG2	2.44	0.42
20:K:143:GLU:OE1	37:b:136:LYS:NZ	2.45	0.42
22:M:255:MET:O	22:M:258:THR:OG1	2.37	0.42
39:d:251:GLN:OE1	39:d:252:LEU:N	2.53	0.42
8:7:73:THR:HG23	8:7:99:TYR:OH	2.20	0.42
9:8:106:LEU:HB3	9:8:110:GLU:OE2	2.20	0.42
11:A:2570:C:C5	11:A:2592:G:H2'	2.55	0.42
13:C:302:TYR:HB3	13:C:305:CYS:SG	2.59	0.42
16:F:75:GLU:OE1	43:h:56:ARG:NH1	2.53	0.42
33:X:80:TRP:CD1	33:X:80:TRP:N	2.88	0.42
40:e:160:LEU:HG	40:e:171:TRP:CD1	2.55	0.42
49:o:18:ILE:HG13	49:o:19:GLY:N	2.34	0.42
7:6:150:ARG:NH2	25:P:104:SER:OG	2.42	0.42
11:A:2854:U:C2	11:A:2889:C:C5	3.08	0.42
11:A:3134:C:O2	11:A:3134:C:O4'	2.38	0.42
14:D:189:VAL:HG13	14:D:217:LEU:O	2.20	0.42
22:M:229:PHE:N	22:M:230:PRO:HD2	2.35	0.42
24:O:30:ARG:HD2	24:O:78:PHE:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:k:63:CYS:SG	46:k:64:VAL:N	2.93	0.42
9:8:129:ARG:HD3	12:B:1627:C:H5'	2.02	0.41
11:A:1957:A:OP2	29:T:163:ARG:NH2	2.53	0.41
11:A:2056:G:H2'	11:A:2057:C:H6	1.85	0.41
11:A:2298:A:N6	16:F:145:LEU:HD22	2.35	0.41
11:A:2745:A:O2'	33:X:102:LYS:O	2.27	0.41
11:A:3063:G:O2'	11:A:3066:C:OP2	2.27	0.41
18:I:79:ILE:O	18:I:83:ARG:HG3	2.19	0.41
28:S:108:VAL:CG1	28:S:195:ILE:HG13	2.49	0.41
53:s:110:THR:HG23	53:s:333:PHE:CD1	2.54	0.41
3:2:78:VAL:HG22	3:2:81:ARG:NH2	2.35	0.41
9:8:139:MET:SD	41:f:169:ILE:HD13	2.60	0.41
11:A:2009:G:OP1	44:i:112:LYS:HD3	2.20	0.41
11:A:2239:A:O3'	20:K:29:GLY:HA3	2.19	0.41
11:A:2284:C:C2'	11:A:2285:U:OP2	2.68	0.41
11:A:2493:C:O2	11:A:2493:C:O4'	2.37	0.41
11:A:3228:U:OP1	15:E:153:SER:OG	2.36	0.41
18:I:86:ILE:HD11	18:I:126:PHE:CD2	2.55	0.41
25:P:71:VAL:HG12	25:P:72:PHE:N	2.35	0.41
29:T:87:MET:HE3	29:T:117:ILE:CG1	2.50	0.41
42:g:135:THR:O	42:g:135:THR:HG23	2.20	0.41
48:m:52:TYR:CG	48:m:71:PRO:HG3	2.54	0.41
9:8:124:TYR:OH	9:8:128:GLU:OE2	2.29	0.41
11:A:1852:C:O2	11:A:1852:C:C2'	2.68	0.41
11:A:2043:C:C2	11:A:2044:A:C8	3.08	0.41
11:A:2507:A:HO2'	11:A:2508:C:P	2.38	0.41
11:A:2899:C:H2'	11:A:2900:C:O4'	2.20	0.41
18:I:86:ILE:HG21	18:I:134:PHE:CD2	2.55	0.41
18:I:128:ASN:O	18:I:132:LYS:HG2	2.21	0.41
28:S:194:ARG:NH2	37:b:13:SER:OG	2.53	0.41
37:b:148:VAL:HG23	37:b:149:GLN:N	2.35	0.41
39:d:146:ILE:O	39:d:150:LEU:HD23	2.20	0.41
42:g:57:ILE:HD13	42:g:91:MET:HE2	2.02	0.41
46:k:90:PHE:CZ	46:k:94:ILE:HD11	2.55	0.41
51:q:60:GLN:O	51:q:68:SER:OG	2.38	0.41
53:s:332:LEU:HD13	53:s:372:TYR:HB2	2.02	0.41
11:A:2030:U:C4'	11:A:2031:A:OP2	2.69	0.41
11:A:2093:U:O2	11:A:2266:U:O2'	2.38	0.41
11:A:2157:U:OP1	52:r:182:ARG:NH1	2.52	0.41
11:A:2236:C:O2'	11:A:2237:A:O5'	2.35	0.41
11:A:3117:C:H2'	11:A:3118:U:H6	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:I:181:ILE:O	18:I:182:ASP:OD1	2.38	0.41
37:b:133:PHE:CE2	38:c:269:LEU:HD23	2.56	0.41
39:d:186:VAL:HG12	39:d:219:ARG:O	2.20	0.41
46:k:32:THR:OG1	46:k:83:ALA:HB2	2.20	0.41
9:8:122:SER:HA	9:8:125:LYS:HE3	2.02	0.41
9:8:138:ALA:O	9:8:141:GLU:HG3	2.20	0.41
11:A:2698:G:OP1	11:A:2699:C:N4	2.46	0.41
13:C:379:LEU:HD11	13:C:416:VAL:HG13	2.01	0.41
19:J:40:GLY:HA2	19:J:44:VAL:HG22	2.03	0.41
45:j:96:GLN:O	45:j:100:GLU:OE1	2.38	0.41
2:1:53:ARG:NH2	11:A:2880:A:O5'	2.49	0.41
4:3:111:ILE:O	22:M:84:ASN:ND2	2.51	0.41
11:A:1989:C:O2	11:A:1995:A:N1	2.54	0.41
11:A:2172:A:C5	19:J:23:ILE:HG22	2.56	0.41
11:A:2552:U:C2	11:A:2553:G:C8	3.08	0.41
11:A:3042:U:H5'	11:A:3043:C:OP2	2.21	0.41
28:S:128:ILE:HG22	28:S:129:ARG:N	2.36	0.41
30:U:27:GLN:HG2	34:Y:113:LEU:HB3	2.03	0.41
30:U:130:LEU:HD23	31:V:107:THR:HG21	2.03	0.41
31:V:126:MET:SD	31:V:127:ASP:N	2.94	0.41
34:Y:205:VAL:O	34:Y:205:VAL:HG12	2.21	0.41
2:1:41:LEU:HG	2:1:43:LEU:CD2	2.50	0.41
6:5:244:GLU:O	6:5:248:THR:HG23	2.21	0.41
6:5:380:GLN:HB3	6:5:410:THR:HG22	2.01	0.41
7:6:337:MET:HE2	25:P:41:ASN:HB3	2.02	0.41
9:8:173:LYS:H	41:f:183:ARG:HH22	1.68	0.41
11:A:2363:A:HO2'	11:A:2364:C:P	2.43	0.41
11:A:2507:A:O2'	11:A:2508:C:P	2.79	0.41
11:A:2808:U:H2'	11:A:2809:C:O4'	2.21	0.41
15:E:196:ALA:HB3	15:E:319:TYR:CD2	2.56	0.41
27:R:141:ILE:HD13	28:S:72:GLU:OE1	2.20	0.41
40:e:183:THR:HG23	40:e:186:GLY:H	1.86	0.41
53:s:110:THR:HG23	53:s:333:PHE:CG	2.56	0.41
6:5:52:ILE:HG21	6:5:55:LEU:CD2	2.51	0.41
11:A:3129:A:H2'	11:A:3130:A:O4'	2.21	0.41
13:C:229:HIS:O	13:C:232:ASN:N	2.52	0.41
13:C:296:VAL:HG13	13:C:376:ASP:H	1.86	0.41
16:F:218:LEU:N	16:F:218:LEU:HD12	2.35	0.41
18:I:121:ILE:HD11	18:I:154:LEU:O	2.21	0.41
22:M:296:SER:HA	50:p:42:ILE:HD13	2.03	0.41
38:c:173:LEU:O	38:c:174:ALA:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:171:PHE:O	41:f:187:LYS:NZ	2.54	0.41
11:A:1689:C:O2	11:A:1689:C:O4'	2.39	0.41
11:A:1803:A:H4'	11:A:1804:A:H3'	2.03	0.41
11:A:1846:C:H5'	11:A:2297:A:N6	2.35	0.41
11:A:2034:A:H2'	11:A:2035:U:O4'	2.20	0.41
11:A:2082:G:H2'	11:A:2083:U:O4'	2.21	0.41
11:A:2171:U:OP1	19:J:87:VAL:HG12	2.20	0.41
11:A:2284:C:HO2'	11:A:2285:U:P	2.32	0.41
11:A:2292:G:C8	27:R:11:ARG:HB2	2.56	0.41
11:A:2456:U:O2'	11:A:2457:A:H5'	2.21	0.41
11:A:2508:C:H2'	11:A:2509:A:O4'	2.21	0.41
11:A:2668:A:H2'	11:A:2669:A:C8	2.56	0.41
11:A:2896:G:N2	11:A:2917:G:O4'	2.54	0.41
11:A:2943:G:H5''	49:o:14:GLY:N	2.36	0.41
11:A:3148:C:O2'	11:A:3149:C:H5'	2.21	0.41
12:B:1615:A:C6	12:B:1622:A:C5	3.09	0.41
19:J:25:ARG:HA	19:J:65:PRO:HA	2.01	0.41
21:L:47:GLY:HA2	21:L:77:ILE:HD11	2.03	0.41
22:M:119:THR:OG1	22:M:187:VAL:HG22	2.21	0.41
25:P:133:ALA:O	25:P:137:LEU:HD13	2.21	0.41
27:R:51:VAL:HG21	28:S:174:PHE:HB3	2.03	0.41
27:R:122:ARG:NH2	28:S:72:GLU:OE2	2.53	0.41
29:T:190:LYS:NZ	29:T:198:GLU:OE1	2.51	0.41
31:V:55:TYR:O	31:V:122:LEU:HD11	2.20	0.41
34:Y:170:ARG:NH1	34:Y:174:GLY:O	2.54	0.41
41:f:167:ALA:O	41:f:171:LEU:CD2	2.69	0.41
53:s:320:ILE:H	53:s:320:ILE:HD12	1.85	0.41
8:7:166:LEU:O	8:7:236:LYS:NZ	2.52	0.41
11:A:2336:U:C2	11:A:2337:A:C8	3.08	0.41
11:A:2550:A:C6	11:A:2551:G:N7	2.89	0.41
11:A:3170:C:O2	11:A:3170:C:O4'	2.36	0.41
18:I:96:ILE:HG13	18:I:155:VAL:HG12	2.03	0.41
25:P:135:ARG:HA	25:P:138:GLU:HG2	2.03	0.41
27:R:43:VAL:HG13	27:R:44:ARG:N	2.36	0.41
30:U:42:PHE:CB	30:U:44:ILE:HD11	2.51	0.41
31:V:151:GLY:O	31:V:152:ARG:HB2	2.20	0.41
44:i:77:PRO:HD2	44:i:80:LEU:HD11	2.03	0.41
1:0:134:THR:HG23	24:O:130:LEU:HD22	2.04	0.40
6:5:157:VAL:HG12	6:5:180:ILE:HD12	2.03	0.40
6:5:314:ILE:HG12	6:5:355:LEU:HD11	2.03	0.40
8:7:221:VAL:HG12	8:7:225:VAL:HB	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:2081:U:H2'	11:A:2082:G:C8	2.56	0.40
11:A:2519:G:N7	14:D:230:SER:OG	2.49	0.40
11:A:2655:G:N2	11:A:2659:C:O2'	2.54	0.40
18:I:173:PHE:HA	46:k:53:ALA:HB3	2.03	0.40
40:e:265:LYS:N	40:e:266:PRO:HD2	2.36	0.40
53:s:66:TRP:O	53:s:69:THR:OG1	2.32	0.40
3:2:62:ASN:O	3:2:68:ARG:HD2	2.21	0.40
7:6:222:ASP:OD1	7:6:222:ASP:N	2.53	0.40
9:8:134:ASP:OD1	9:8:137:ARG:NH2	2.43	0.40
11:A:1821:A:H2'	11:A:1822:U:O4'	2.22	0.40
11:A:2591:A:H2'	11:A:2592:G:O4'	2.21	0.40
11:A:3142:A:H2'	11:A:3143:U:C6	2.57	0.40
15:E:230:THR:O	15:E:231:HIS:HB2	2.21	0.40
18:I:130:VAL:O	18:I:130:VAL:HG22	2.21	0.40
24:O:99:ASP:OD1	24:O:100:GLN:N	2.54	0.40
27:R:64:MET:HE1	29:T:210:HIS:ND1	2.36	0.40
32:W:70:GLN:OE1	32:W:74:ARG:N	2.52	0.40
40:e:71:ALA:O	40:e:74:LEU:HG	2.20	0.40
40:e:255:VAL:HG22	40:e:259:GLU:HB2	2.02	0.40
4:3:127:ALA:N	11:A:2869:A:OP1	2.49	0.40
7:6:198:ALA:O	7:6:254:TYR:OH	2.32	0.40
11:A:3094:G:H2'	11:A:3095:G:O4'	2.21	0.40
33:X:80:TRP:O	33:X:82:GLY:N	2.52	0.40
33:X:176:LEU:HD23	33:X:176:LEU:C	2.47	0.40
38:c:245:LEU:HD12	38:c:253:PRO:HD3	2.02	0.40
48:m:63:THR:O	48:m:64:ILE:HD13	2.21	0.40
11:A:2143:G:OP1	28:S:173:ARG:NH2	2.54	0.40
11:A:2176:C:H2'	11:A:2177:U:C1'	2.52	0.40
11:A:3175:A:OP2	11:A:3187:C:N4	2.45	0.40
13:C:128:VAL:HG21	13:C:136:VAL:HG13	2.03	0.40
16:F:87:PHE:C	16:F:179:THR:HG22	2.46	0.40
22:M:211:VAL:N	22:M:212:PRO:HD2	2.36	0.40
22:M:233:ARG:HB3	22:M:244:LEU:HD11	2.04	0.40
26:Q:150:ILE:O	26:Q:150:ILE:HG23	2.19	0.40
40:e:71:ALA:HA	40:e:74:LEU:HG	2.04	0.40
40:e:127:LYS:O	40:e:130:GLN:HG3	2.21	0.40
49:o:27:VAL:O	49:o:27:VAL:HG23	2.20	0.40
2:1:47:ASP:O	2:1:51:LYS:N	2.55	0.40
8:7:52:LYS:CG	8:7:219:LEU:HD11	2.51	0.40
8:7:81:MET:HE1	8:7:94:HIS:CD2	2.53	0.40
9:8:143:GLN:O	9:8:147:LEU:HD23	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:9:31:ARG:O	11:A:2420:U:O2'	2.35	0.40
11:A:2033:A:H1'	11:A:2866:A:N7	2.36	0.40
11:A:2192:A:H2'	11:A:2193:U:O4'	2.21	0.40
11:A:2550:A:C2	11:A:2551:G:C8	3.09	0.40
11:A:2928:C:OP2	11:A:3073:C:O2'	2.31	0.40
21:L:123:ILE:CG2	21:L:127:LEU:HD12	2.50	0.40
24:O:110:ILE:HG23	24:O:111:PRO:HD2	2.02	0.40
42:g:42:VAL:HG22	42:g:43:ASP:H	1.85	0.40
51:q:86:GLU:OE1	51:q:90:ARG:NH2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	106/188 (56%)	106 (100%)	0	0	100	100
2	1	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
3	2	43/92 (47%)	42 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	89 (96%)	4 (4%)	0	100	100
5	4	35/103 (34%)	34 (97%)	1 (3%)	0	100	100
6	5	390/423 (92%)	380 (97%)	10 (3%)	0	100	100
7	6	316/380 (83%)	304 (96%)	12 (4%)	0	100	100
8	7	285/338 (84%)	268 (94%)	17 (6%)	0	100	100
9	8	75/206 (36%)	71 (95%)	4 (5%)	0	100	100
10	9	113/137 (82%)	113 (100%)	0	0	100	100
13	C	420/516 (81%)	405 (96%)	15 (4%)	0	100	100
14	D	234/305 (77%)	227 (97%)	7 (3%)	0	100	100
15	E	303/348 (87%)	290 (96%)	13 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	F	248/311 (80%)	241 (97%)	7 (3%)	0	100	100
17	H	93/267 (35%)	90 (97%)	3 (3%)	0	100	100
18	I	154/261 (59%)	141 (92%)	13 (8%)	0	100	100
19	J	138/192 (72%)	123 (89%)	15 (11%)	0	100	100
20	K	175/178 (98%)	170 (97%)	5 (3%)	0	100	100
21	L	113/145 (78%)	109 (96%)	4 (4%)	0	100	100
22	M	285/296 (96%)	279 (98%)	6 (2%)	0	100	100
23	N	203/251 (81%)	200 (98%)	3 (2%)	0	100	100
24	O	150/175 (86%)	149 (99%)	1 (1%)	0	100	100
25	P	139/180 (77%)	135 (97%)	4 (3%)	0	100	100
26	Q	215/292 (74%)	209 (97%)	6 (3%)	0	100	100
27	R	138/149 (93%)	135 (98%)	3 (2%)	0	100	100
28	S	154/205 (75%)	148 (96%)	6 (4%)	0	100	100
29	T	164/206 (80%)	160 (98%)	4 (2%)	0	100	100
30	U	135/153 (88%)	132 (98%)	3 (2%)	0	100	100
31	V	187/216 (87%)	180 (96%)	7 (4%)	0	100	100
32	W	107/148 (72%)	106 (99%)	1 (1%)	0	100	100
33	X	241/256 (94%)	238 (99%)	3 (1%)	0	100	100
34	Y	174/250 (70%)	171 (98%)	3 (2%)	0	100	100
35	Z	118/161 (73%)	116 (98%)	2 (2%)	0	100	100
36	a	78/142 (55%)	77 (99%)	1 (1%)	0	100	100
37	b	146/215 (68%)	143 (98%)	3 (2%)	0	100	100
38	c	271/332 (82%)	267 (98%)	4 (2%)	0	100	100
39	d	198/306 (65%)	190 (96%)	8 (4%)	0	100	100
40	e	191/279 (68%)	179 (94%)	12 (6%)	0	100	100
41	f	99/212 (47%)	89 (90%)	10 (10%)	0	100	100
42	g	127/166 (76%)	124 (98%)	3 (2%)	0	100	100
43	h	101/158 (64%)	96 (95%)	5 (5%)	0	100	100
44	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
45	j	82/123 (67%)	80 (98%)	2 (2%)	0	100	100
46	k	76/112 (68%)	75 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	l	21/138 (15%)	21 (100%)	0	0	100	100
48	m	43/128 (34%)	36 (84%)	7 (16%)	0	100	100
49	o	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
50	p	119/206 (58%)	116 (98%)	3 (2%)	0	100	100
51	q	118/222 (53%)	117 (99%)	1 (1%)	0	100	100
52	r	153/196 (78%)	149 (97%)	4 (3%)	0	100	100
53	s	366/439 (83%)	359 (98%)	7 (2%)	0	100	100
All	All	8170/11185 (73%)	7911 (97%)	259 (3%)	0	100	100

There are no Ramachandran outliers to report.

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
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	286/332 (86%)	286 (100%)	0	100	100
8	7	263/303 (87%)	263 (100%)	0	100	100
9	8	70/190 (37%)	70 (100%)	0	100	100
10	9	99/112 (88%)	99 (100%)	0	100	100
13	C	360/424 (85%)	360 (100%)	0	100	100
14	D	190/245 (78%)	190 (100%)	0	100	100
15	E	260/290 (90%)	260 (100%)	0	100	100
16	F	217/262 (83%)	217 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	H	86/228 (38%)	86 (100%)	0	100	100
18	I	145/232 (62%)	145 (100%)	0	100	100
19	J	113/150 (75%)	113 (100%)	0	100	100
20	K	155/156 (99%)	155 (100%)	0	100	100
21	L	98/124 (79%)	98 (100%)	0	100	100
22	M	245/249 (98%)	245 (100%)	0	100	100
23	N	172/211 (82%)	172 (100%)	0	100	100
24	O	133/150 (89%)	133 (100%)	0	100	100
25	P	123/155 (79%)	123 (100%)	0	100	100
26	Q	199/256 (78%)	199 (100%)	0	100	100
27	R	118/126 (94%)	118 (100%)	0	100	100
28	S	141/180 (78%)	141 (100%)	0	100	100
29	T	146/176 (83%)	146 (100%)	0	100	100
30	U	124/135 (92%)	124 (100%)	0	100	100
31	V	171/191 (90%)	171 (100%)	0	100	100
32	W	89/119 (75%)	89 (100%)	0	100	100
33	X	219/229 (96%)	219 (100%)	0	100	100
34	Y	159/223 (71%)	159 (100%)	0	100	100
35	Z	111/147 (76%)	111 (100%)	0	100	100
36	a	78/133 (59%)	78 (100%)	0	100	100
37	b	130/186 (70%)	130 (100%)	0	100	100
38	c	241/288 (84%)	241 (100%)	0	100	100
39	d	193/274 (70%)	193 (100%)	0	100	100
40	e	171/236 (72%)	171 (100%)	0	100	100
41	f	93/188 (50%)	93 (100%)	0	100	100
42	g	119/148 (80%)	119 (100%)	0	100	100
43	h	100/148 (68%)	100 (100%)	0	100	100
44	i	86/110 (78%)	86 (100%)	0	100	100
45	j	68/97 (70%)	68 (100%)	0	100	100
46	k	71/90 (79%)	71 (100%)	0	100	100
47	l	23/116 (20%)	23 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	m	40/113 (35%)	40 (100%)	0	100	100
49	o	80/87 (92%)	80 (100%)	0	100	100
50	p	117/181 (65%)	117 (100%)	0	100	100
51	q	104/178 (58%)	104 (100%)	0	100	100
52	r	143/169 (85%)	143 (100%)	0	100	100
53	s	326/381 (86%)	326 (100%)	0	100	100
All	All	7337/9637 (76%)	7337 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
6	5	94	HIS
8	7	305	HIS
13	C	96	GLN
13	C	239	HIS
13	C	335	HIS
13	C	356	GLN
15	E	88	HIS
15	E	227	GLN
15	E	294	ASN
16	F	228	GLN
21	L	33	GLN
21	L	89	HIS
22	M	219	ASN
26	Q	139	GLN
27	R	149	HIS
28	S	118	ASN
29	T	151	GLN
30	U	103	GLN
33	X	27	HIS
33	X	76	GLN
33	X	93	ASN
33	X	240	GLN
34	Y	147	GLN
37	b	16	HIS
37	b	102	GLN
37	b	135	ASN
38	c	69	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	c	123	GLN
38	c	155	ASN
38	c	222	GLN
39	d	47	GLN
40	e	75	GLN
40	e	251	HIS
42	g	155	GLN
44	i	120	HIS
50	p	152	GLN
50	p	184	ASN
51	q	60	GLN
51	q	139	GLN
53	s	107	GLN
53	s	281	HIS
53	s	387	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1450/1559 (93%)	328 (22%)	17 (1%)
12	B	52/69 (75%)	17 (32%)	1 (1%)
All	All	1502/1628 (92%)	345 (22%)	18 (1%)

All (345) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1672	C
11	A	1673	U
11	A	1674	A
11	A	1675	A
11	A	1676	A
11	A	1679	U
11	A	1680	A
11	A	1681	G
11	A	1689	C
11	A	1690	C
11	A	1699	C
11	A	1700	U
11	A	1704	U
11	A	1707	C
11	A	1708	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	1711	C
11	A	1712	A
11	A	1724	A
11	A	1727	A
11	A	1728	U
11	A	1732	C
11	A	1748	G
11	A	1750	G
11	A	1751	A
11	A	1761	A
11	A	1770	G
11	A	1777	A
11	A	1780	U
11	A	1794	A
11	A	1797	G
11	A	1801	A
11	A	1802	A
11	A	1805	A
11	A	1813	C
11	A	1817	C
11	A	1819	U
11	A	1821	A
11	A	1823	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	1844	A
11	A	1853	A
11	A	1854	U
11	A	1855	A
11	A	1856	A
11	A	1869	A
11	A	1870	A
11	A	1878	U
11	A	1882	A
11	A	1883	G
11	A	1886	G
11	A	1887	A
11	A	1892	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	1893	A
11	A	1901	C
11	A	1902	C
11	A	1903	C
11	A	1909	A
11	A	1918	G
11	A	1935	A
11	A	1938	A
11	A	1940	A
11	A	1958	G
11	A	1974	A
11	A	1985	G
11	A	1992	C
11	A	1993	A
11	A	1994	A
11	A	2003	A
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	2036	C
11	A	2037	U
11	A	2039	A
11	A	2054	U
11	A	2060	A
11	A	2065	A
11	A	2068	C
11	A	2069	U
11	A	2074	A
11	A	2079	C
11	A	2083	U
11	A	2085	A
11	A	2092	C
11	A	2093	U
11	A	2097	A
11	A	2098	G
11	A	2105	G
11	A	2113	G
11	A	2124	A
11	A	2126	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2141	U
11	A	2147	G
11	A	2154	A
11	A	2155	A
11	A	2158	U
11	A	2163	A
11	A	2165	C
11	A	2168	U
11	A	2171	U
11	A	2172	A
11	A	2173	G
11	A	2174	G
11	A	2177	U
11	A	2180	A
11	A	2181	A
11	A	2182	G
11	A	2183	C
11	A	2187	C
11	A	2189	C
11	A	2193	U
11	A	2194	U
11	A	2196	A
11	A	2197	G
11	A	2198	A
11	A	2200	A
11	A	2204	U
11	A	2210	C
11	A	2214	A
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	2245	A
11	A	2246	A
11	A	2250	A
11	A	2262	C
11	A	2263	C
11	A	2284	C
11	A	2285	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2297	A
11	A	2300	G
11	A	2309	A
11	A	2313	A
11	A	2322	C
11	A	2331	C
11	A	2332	C
11	A	2335	A
11	A	2345	G
11	A	2350	A
11	A	2351	U
11	A	2364	C
11	A	2372	U
11	A	2374	A
11	A	2381	A
11	A	2382	A
11	A	2384	A
11	A	2390	A
11	A	2393	C
11	A	2396	C
11	A	2399	A
11	A	2404	U
11	A	2406	A
11	A	2407	U
11	A	2408	U
11	A	2414	C
11	A	2415	C
11	A	2416	U
11	A	2417	C
11	A	2418	A
11	A	2426	C
11	A	2427	C
11	A	2432	A
11	A	2441	C
11	A	2444	A
11	A	2446	A
11	A	2451	A
11	A	2452	A
11	A	2478	G
11	A	2493	C
11	A	2500	A
11	A	2502	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2507	A
11	A	2508	C
11	A	2511	C
11	A	2520	C
11	A	2521	A
11	A	2527	A
11	A	2531	U
11	A	2540	C
11	A	2563	U
11	A	2570	C
11	A	2583	C
11	A	2584	C
11	A	2592	G
11	A	2593	G
11	A	2594	U
11	A	2600	A
11	A	2603	C
11	A	2608	G
11	A	2625	C
11	A	2628	U
11	A	2629	A
11	A	2632	A
11	A	2633	A
11	A	2634	U
11	A	2635	G
11	A	2637	C
11	A	2640	C
11	A	2641	A
11	A	2645	G
11	A	2647	G
11	A	2654	U
11	A	2660	U
11	A	2683	C
11	A	2686	G
11	A	2693	A
11	A	2694	A
11	A	2695	G
11	A	2696	A
11	A	2706	A
11	A	2708	C
11	A	2709	A
11	A	2718	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2719	G
11	A	2722	A
11	A	2723	A
11	A	2724	G
11	A	2725	A
11	A	2732	G
11	A	2739	U
11	A	2740	A
11	A	2747	U
11	A	2750	U
11	A	2755	A
11	A	2756	C
11	A	2804	A
11	A	2810	G
11	A	2814	G
11	A	2815	OMG
11	A	2832	A
11	A	2833	A
11	A	2837	A
11	A	2842	C
11	A	2844	G
11	A	2847	C
11	A	2852	C
11	A	2859	A
11	A	2864	U
11	A	2865	C
11	A	2871	U
11	A	2880	A
11	A	2895	U
11	A	2896	G
11	A	2901	A
11	A	2906	C
11	A	2910	A
11	A	2912	C
11	A	2913	A
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	2934	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2935	A
11	A	2956	A
11	A	2962	C
11	A	2963	A
11	A	2971	A
11	A	2989	G
11	A	2990	A
11	A	2992	G
11	A	2994	U
11	A	2995	G
11	A	3000	A
11	A	3005	A
11	A	3016	G
11	A	3022	G
11	A	3037	U
11	A	3038	U
11	A	3042	U
11	A	3043	C
11	A	3051	A
11	A	3053	A
11	A	3054	G
11	A	3056	C
11	A	3060	C
11	A	3061	G
11	A	3063	G
11	A	3069	A
11	A	3077	C
11	A	3086	U
11	A	3089	A
11	A	3090	G
11	A	3092	U
11	A	3093	C
11	A	3096	U
11	A	3097	U
11	A	3098	U
11	A	3100	U
11	A	3102	U
11	A	3108	U
11	A	3113	A
11	A	3129	A
11	A	3134	C
11	A	3141	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	3150	U
11	A	3155	C
11	A	3157	C
11	A	3158	A
11	A	3162	C
11	A	3168	C
11	A	3169	C
11	A	3170	C
11	A	3172	C
11	A	3180	A
11	A	3189	C
11	A	3190	A
11	A	3196	G
11	A	3197	U
11	A	3198	A
11	A	3199	U
11	A	3207	A
11	A	3217	A
11	A	3218	A
12	B	1607	U
12	B	1608	G
12	B	1609	U
12	B	1611	G
12	B	1614	U
12	B	1615	A
12	B	1625	A
12	B	1631	C
12	B	1632	U
12	B	1633	U
12	B	1640	A
12	B	1641	G
12	B	1644	G
12	B	1645	A
12	B	1648	U
12	B	1650	A
12	B	1669	G

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	1823	A
11	A	2030	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2186	C
11	A	2209	G
11	A	2245	A
11	A	2284	C
11	A	2507	A
11	A	2530	A
11	A	2693	A
11	A	2694	A
11	A	2814	G
11	A	2895	U
11	A	2905	A
11	A	2993	U
11	A	3092	U
11	A	3097	U
11	A	3198	A
12	B	1607	U

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

3 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	3040	11	23,26,27	1.27	4 (17%)	32,38,41	1.86	6 (18%)
11	OMG	A	2815	11	23,26,27	1.20	3 (13%)	32,38,41	2.01	6 (18%)
11	OMU	A	3039	11	19,22,23	1.30	3 (15%)	25,31,34	2.04	7 (28%)

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	3040	11	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OMG	A	2815	11	-	5/9/27/28	0/3/3/3
11	OMU	A	3039	11	-	0/9/27/28	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	3039	OMU	C4-N3	-3.01	1.33	1.38
11	A	2815	OMG	C5-C4	2.93	1.46	1.38
11	A	3040	OMG	C5-C4	2.76	1.46	1.38
11	A	2815	OMG	C6-N1	-2.63	1.33	1.38
11	A	3039	OMU	C2-N3	-2.54	1.33	1.38
11	A	3040	OMG	C5-N7	-2.51	1.34	1.39
11	A	3040	OMG	C4-N9	-2.48	1.31	1.38
11	A	3040	OMG	C6-N1	-2.45	1.34	1.38
11	A	3039	OMU	C5-C4	-2.32	1.38	1.43
11	A	2815	OMG	C5-N7	-2.26	1.34	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	2815	OMG	C5-C4-N3	-6.29	118.38	128.39
11	A	2815	OMG	C2-N3-C4	5.08	121.05	112.30
11	A	3040	OMG	C5-C4-N3	-4.90	120.59	128.39
11	A	2815	OMG	N9-C4-N3	4.63	135.21	125.95
11	A	3040	OMG	C2-N3-C4	4.57	120.18	112.30
11	A	3039	OMU	C4-N3-C2	-4.53	120.99	126.61
11	A	3039	OMU	N3-C2-N1	4.17	120.33	114.89
11	A	3039	OMU	C5-C4-N3	4.12	120.57	114.80
11	A	3040	OMG	N9-C4-N3	4.06	134.08	125.95
11	A	3039	OMU	C2'-C1'-N1	-3.49	107.62	114.24
11	A	3039	OMU	O4-C4-C5	-3.16	119.70	125.16
11	A	2815	OMG	C6-C5-N7	3.15	136.03	130.29
11	A	3040	OMG	C6-C5-N7	3.07	135.87	130.29
11	A	3040	OMG	C2'-C1'-N9	-2.92	108.70	114.24
11	A	2815	OMG	C4-C5-N7	-2.55	106.63	110.67
11	A	3039	OMU	O4'-C1'-N1	2.50	114.02	108.36
11	A	3040	OMG	O6-C6-C5	-2.47	120.01	126.53
11	A	2815	OMG	O6-C6-C5	-2.18	120.78	126.53
11	A	3039	OMU	C6-N1-C2	-2.02	118.53	121.00

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2815	OMG	O4'-C4'-C5'-O5'
11	A	2815	OMG	C3'-C2'-O2'-CM2
11	A	2815	OMG	C4'-C5'-O5'-P
11	A	2815	OMG	C1'-C2'-O2'-CM2
11	A	2815	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	2815	OMG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 95 ligands modelled in this entry, 92 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	GTP	C	601	55	33,34,34	0.56	0	50,54,54	0.60	0
56	GTP	A	3388	-	33,34,34	0.58	0	50,54,54	0.58	0
56	GTP	A	3387	-	33,34,34	0.58	0	50,54,54	0.58	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
56	GTP	C	601	55	-	3/22/38/38	0/3/3/3
56	GTP	A	3388	-	-	0/22/38/38	0/3/3/3
56	GTP	A	3387	-	-	0/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

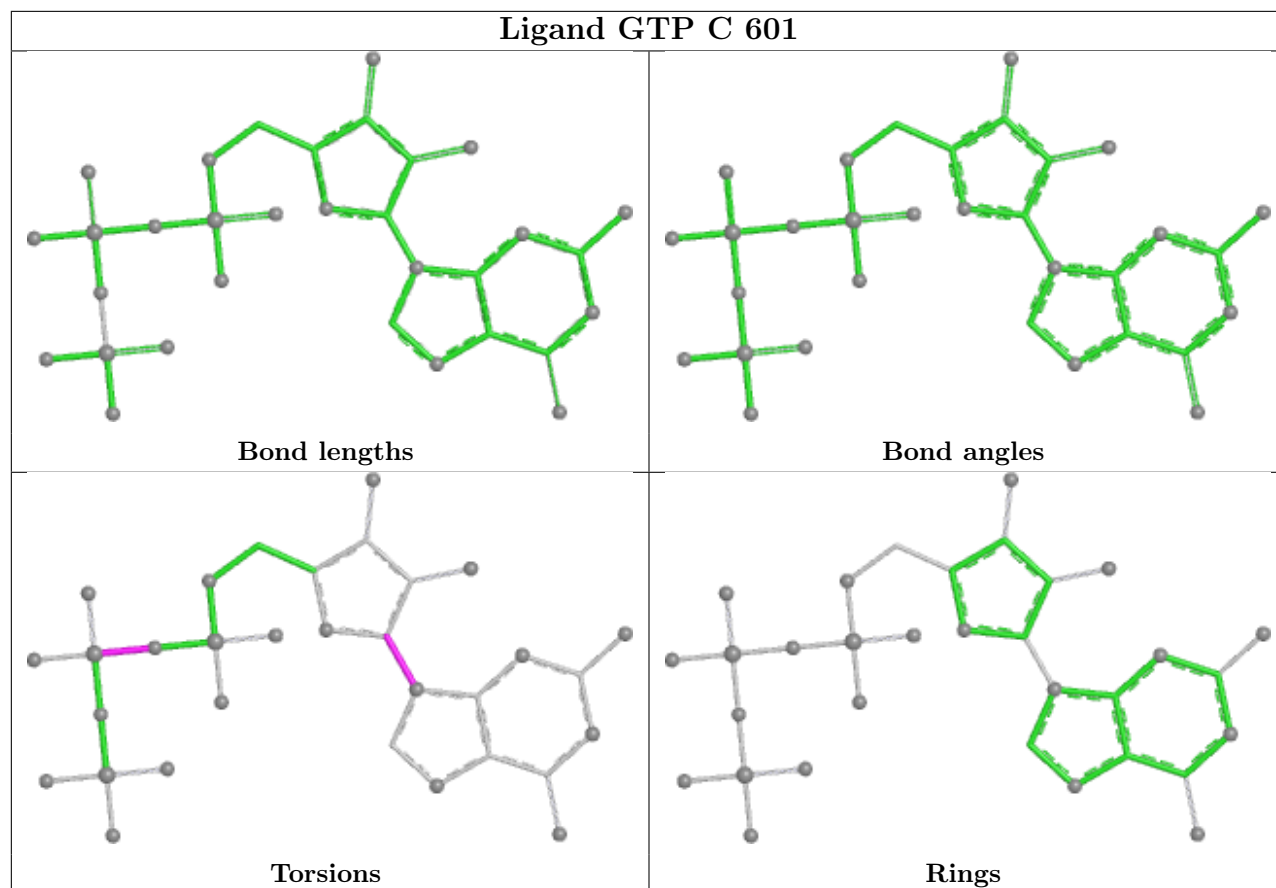
Mol	Chain	Res	Type	Atoms
56	C	601	GTP	O4'-C1'-N9-C4
56	C	601	GTP	O4'-C1'-N9-C8
56	C	601	GTP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	C	601	GTP	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

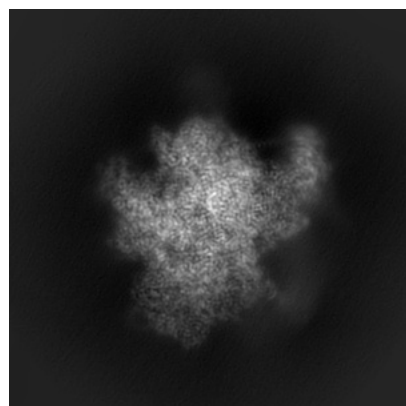
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12869. These allow visual inspection of the internal detail of the map and identification of artifacts.

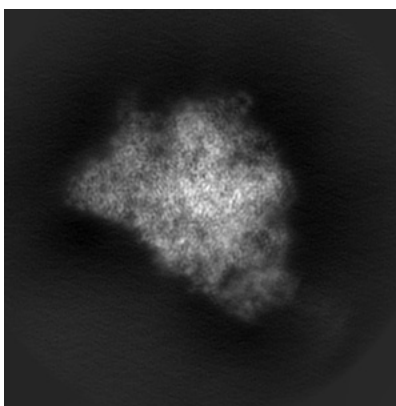
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

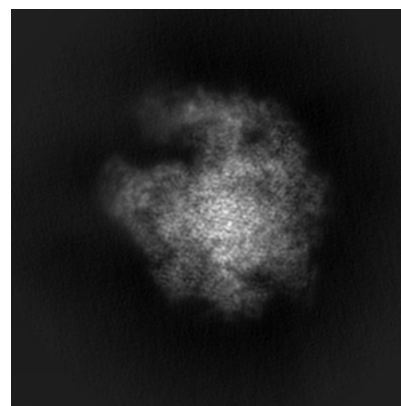
6.1.1 Primary map



X

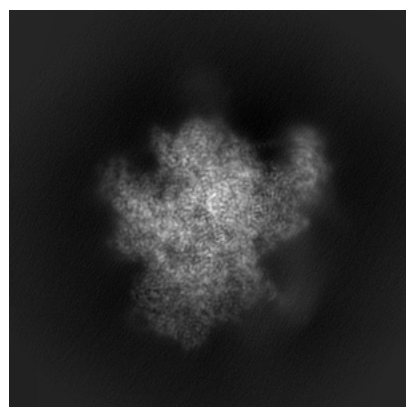


Y

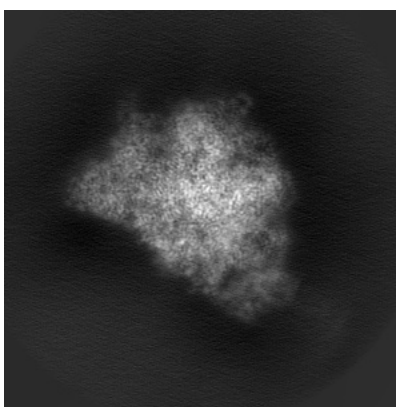


Z

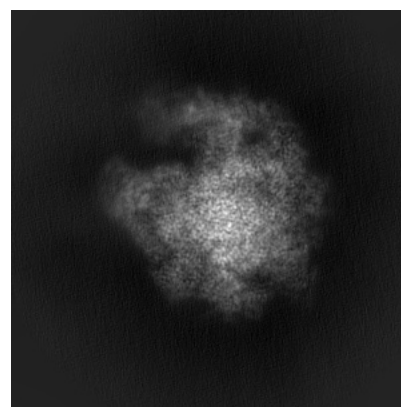
6.1.2 Raw map



X



Y

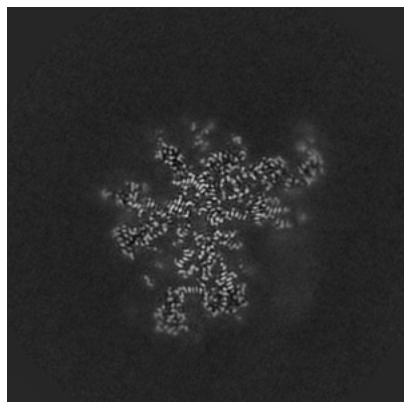


Z

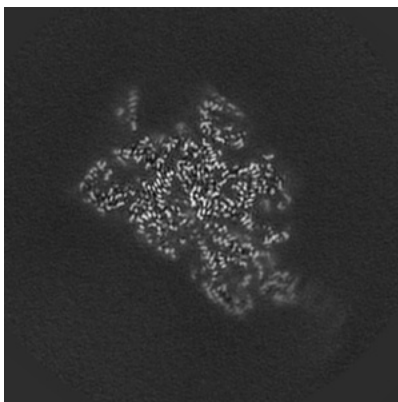
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

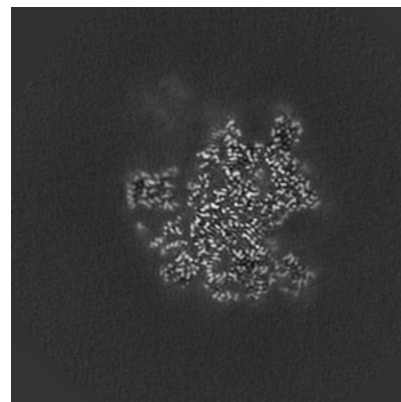
6.2.1 Primary map



X Index: 175

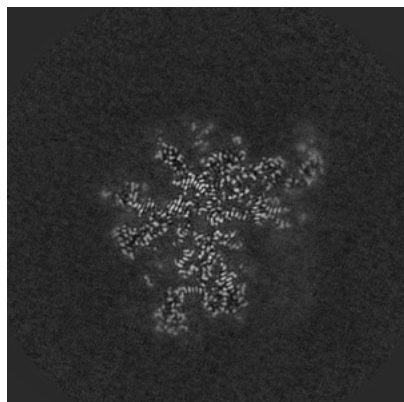


Y Index: 175

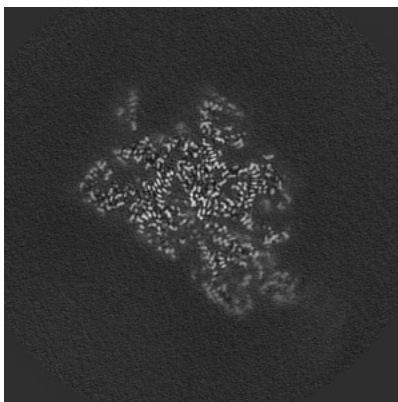


Z Index: 175

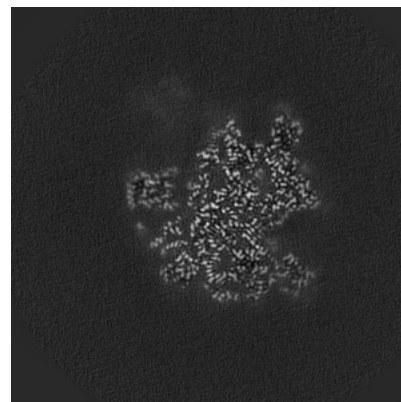
6.2.2 Raw map



X Index: 175



Y Index: 175

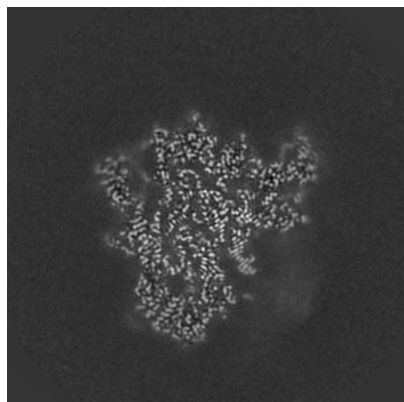


Z Index: 175

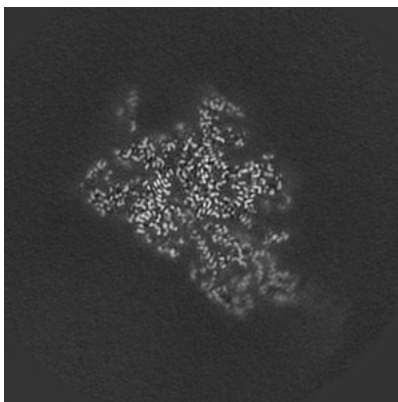
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

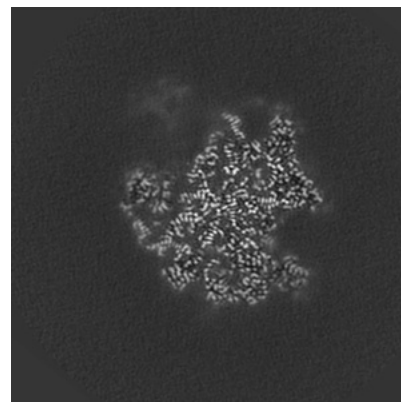
6.3.1 Primary map



X Index: 187

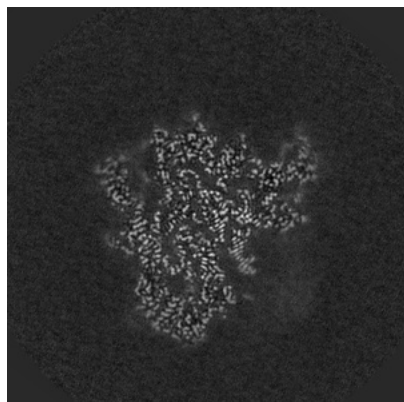


Y Index: 176

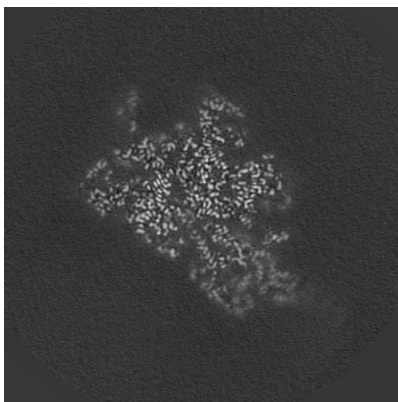


Z Index: 179

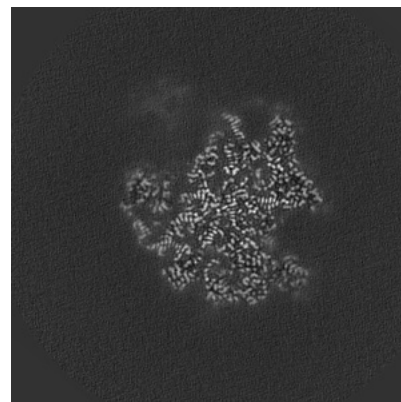
6.3.2 Raw map



X Index: 187



Y Index: 176

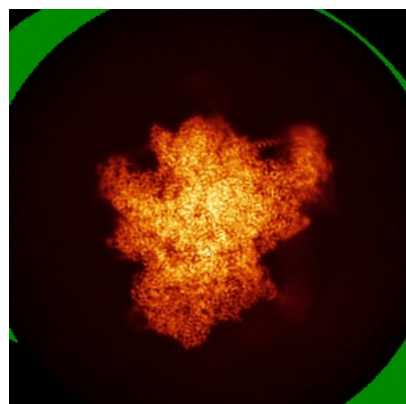


Z Index: 179

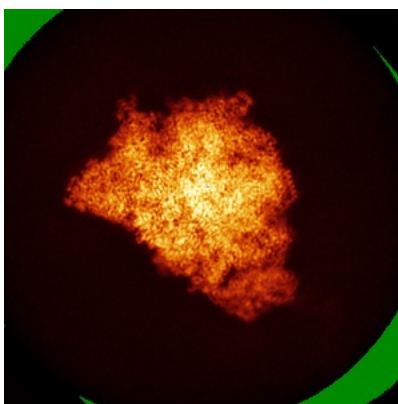
The images above show the largest variance slices of the map in three orthogonal directions.

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

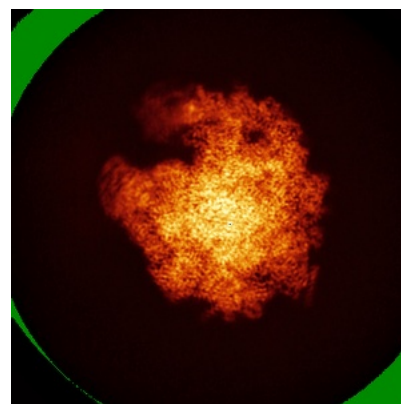
6.4.1 Primary map



X

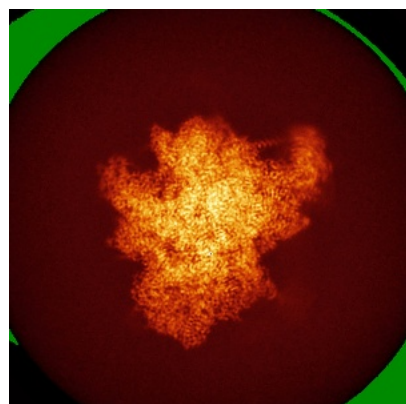


Y

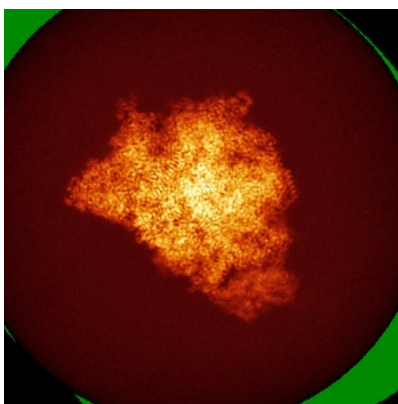


Z

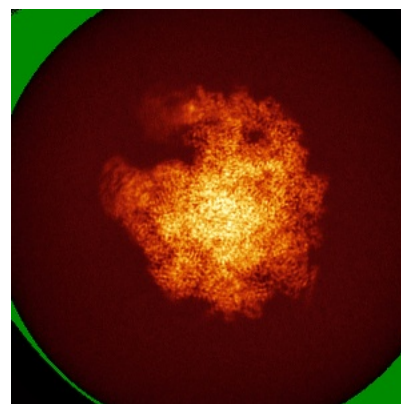
6.4.2 Raw map



X



Y



Z

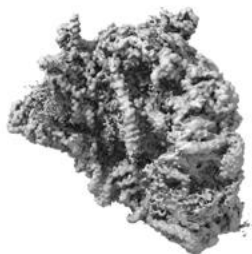
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

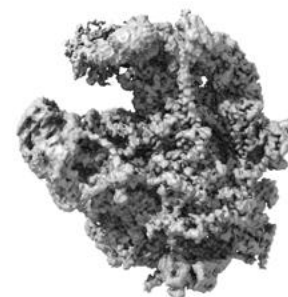
6.5.1 Primary map



X



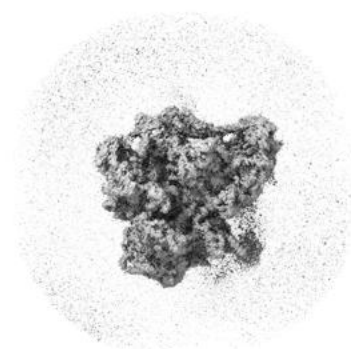
Y



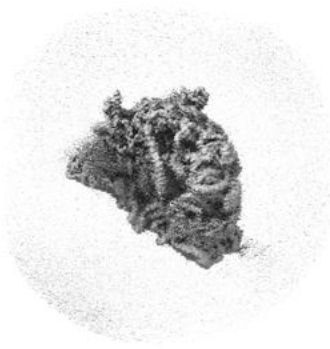
Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

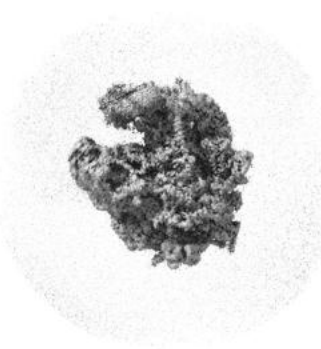
6.5.2 Raw map



X



Y



Z

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

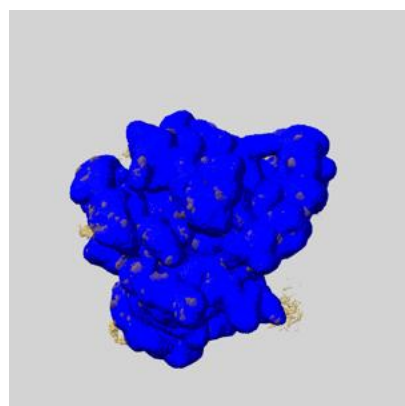
6.6 Mask visualisation [i](#)

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

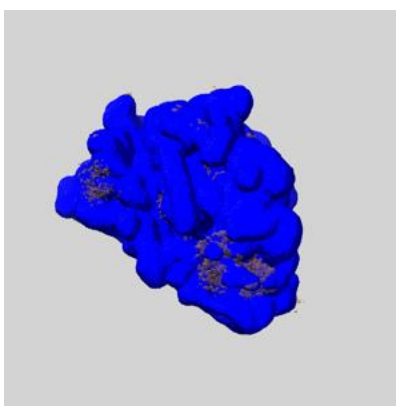
A mask typically either:

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

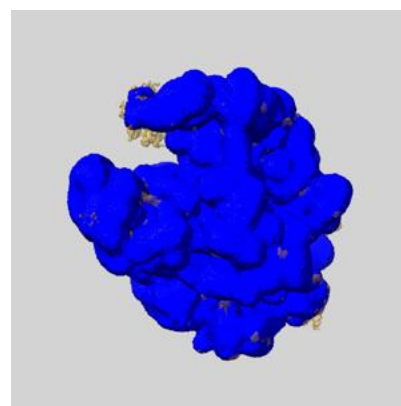
6.6.1 emd_12869_msk_1.map [i](#)



X



Y

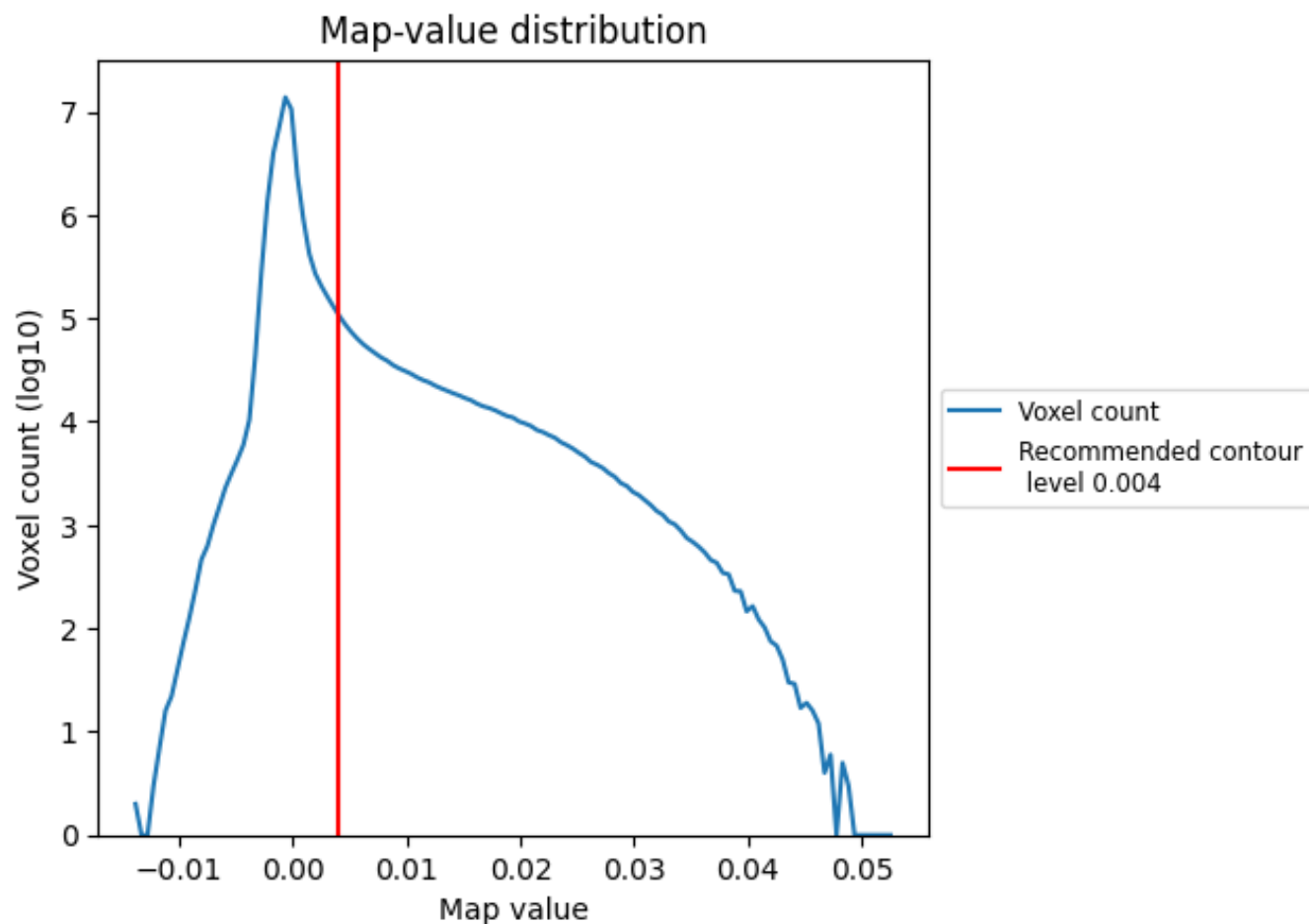


Z

7 Map analysis [i](#)

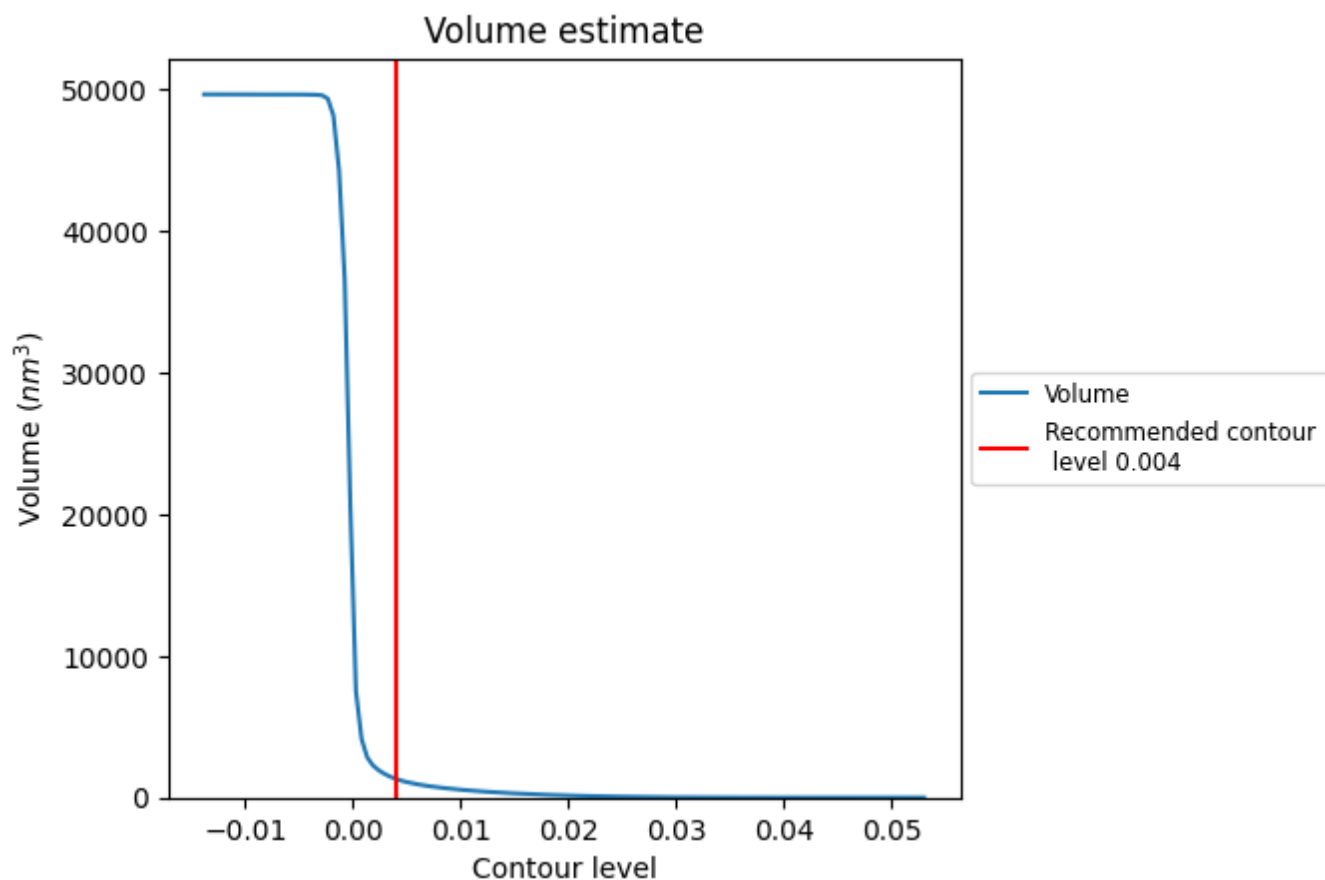
This section contains the results of statistical analysis of the map.

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.

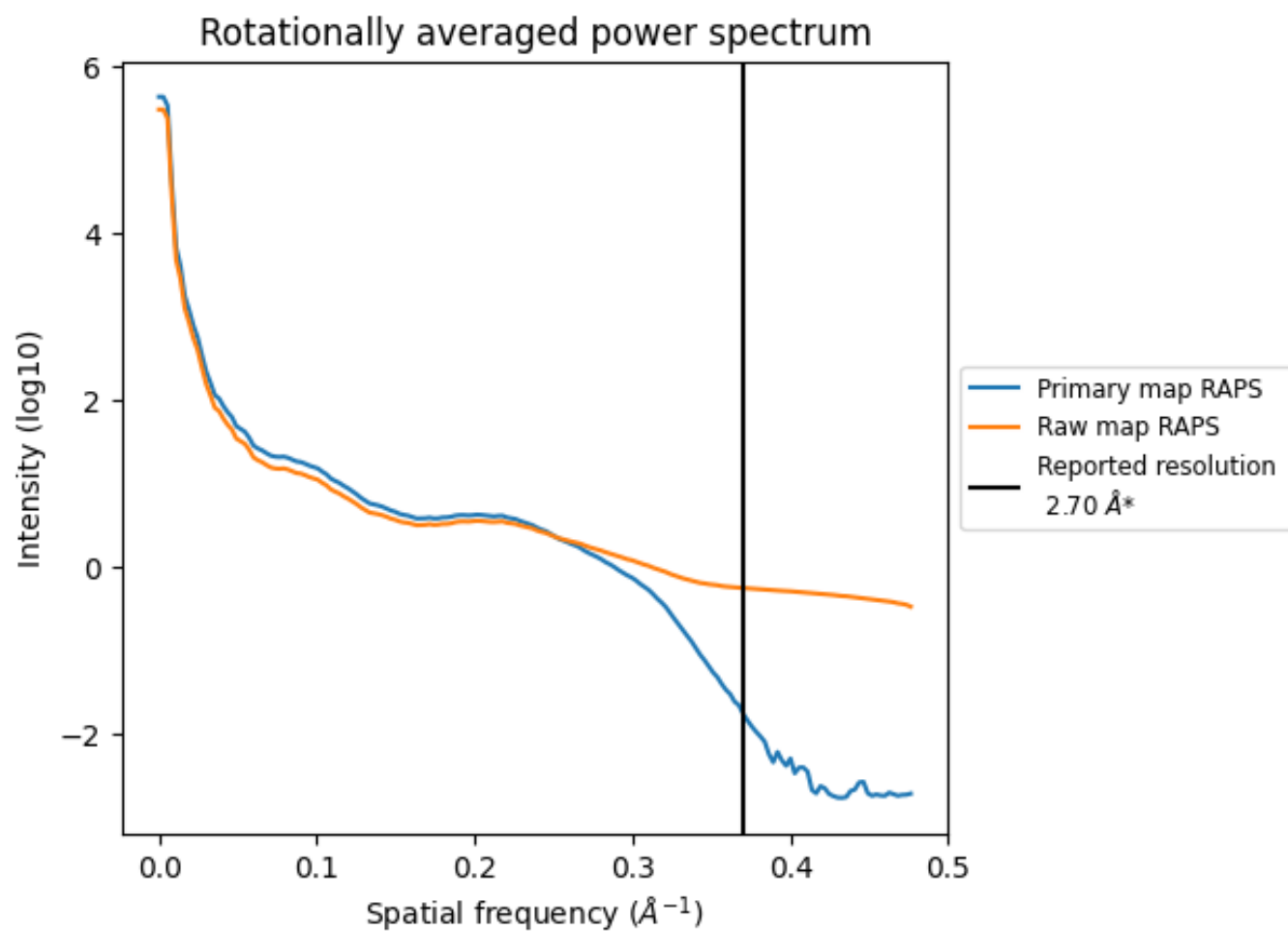
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1320 nm^3 ; this corresponds to an approximate mass of 1193 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 ⓘ

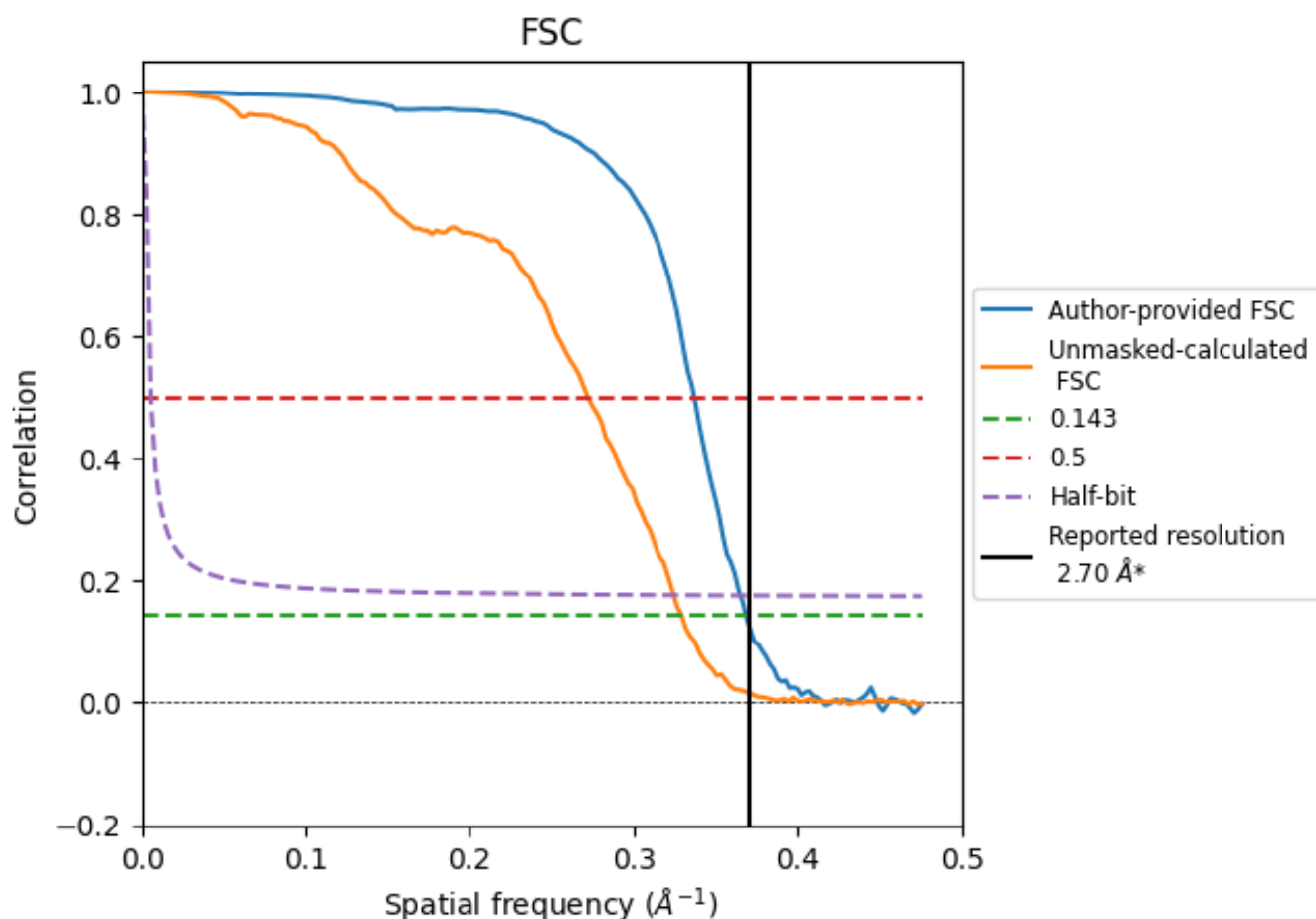


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 $0.370 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

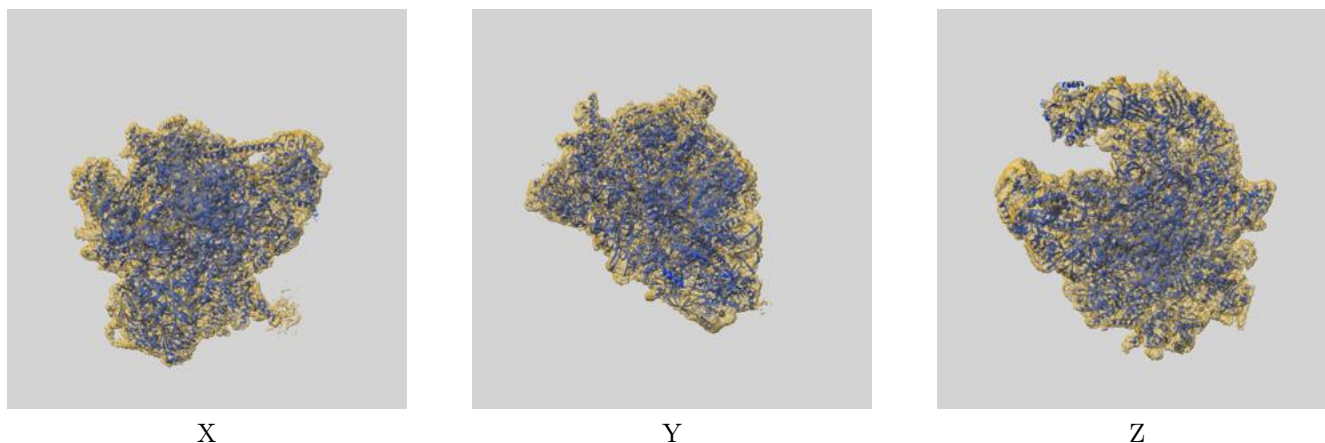
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	2.97	2.74
Unmasked-calculated*	3.04	3.68	3.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.04 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

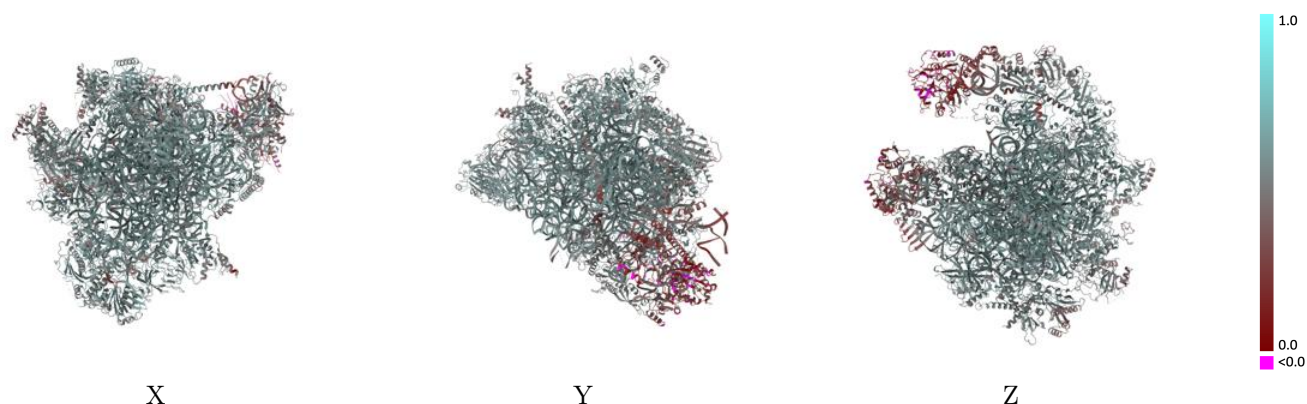
This section contains information regarding the fit between EMDB map EMD-12869 and PDB model 7OF4. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



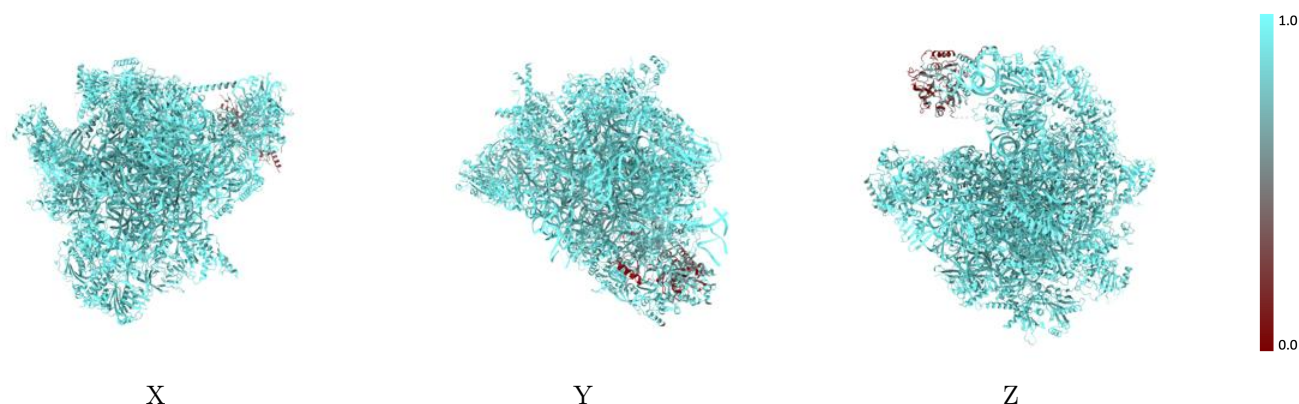
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



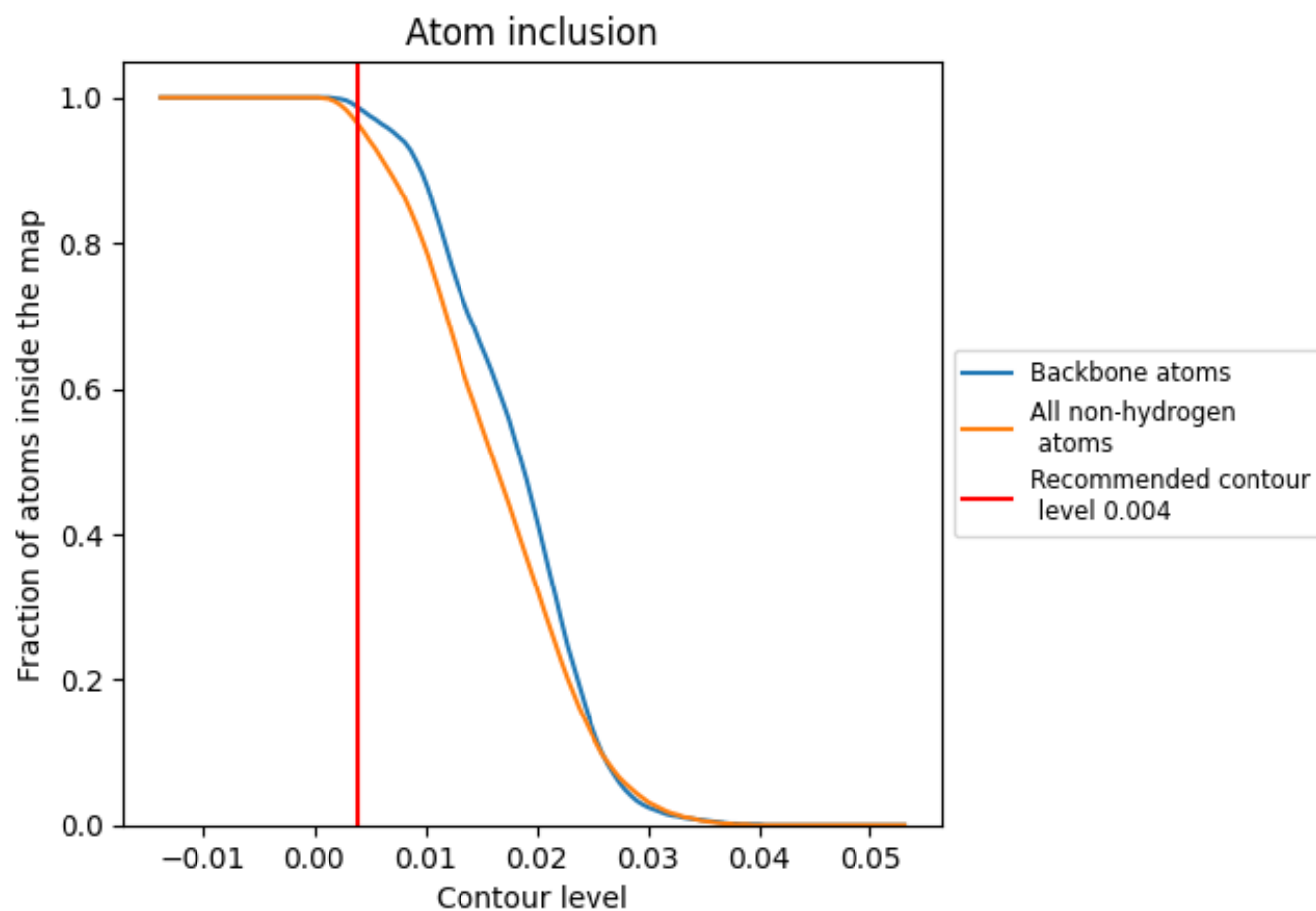
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).

9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9630	 0.5340
0	 0.9730	 0.5530
1	 0.9710	 0.5390
2	 1.0000	 0.6020
3	 0.9910	 0.6010
4	 0.9810	 0.5850
5	 0.9730	 0.5450
6	 0.9670	 0.4900
7	 0.9540	 0.4970
8	 0.5740	 0.2220
9	 0.9740	 0.5470
A	 1.0000	 0.5710
B	 0.9890	 0.3580
C	 0.9470	 0.4840
D	 0.9800	 0.5720
E	 0.9780	 0.5640
F	 0.9880	 0.5780
H	 0.9350	 0.5100
I	 0.9190	 0.3560
J	 0.8810	 0.3040
K	 0.9870	 0.5760
L	 0.9840	 0.5690
M	 0.9810	 0.5720
N	 0.9720	 0.5660
O	 0.9890	 0.5680
P	 0.9780	 0.5240
Q	 0.9740	 0.5510
R	 0.9780	 0.5750
S	 0.9780	 0.5680
T	 0.9800	 0.5820
U	 0.9700	 0.5550
V	 0.9550	 0.5100
W	 0.9910	 0.5880
X	 0.9680	 0.5460
Y	 0.9760	 0.5640



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Z	 0.9750	 0.5800
a	 0.9770	 0.5660
b	 0.9800	 0.5790
c	 0.9710	 0.5360
d	 0.9540	 0.5010
e	 0.3740	 0.1520
f	 0.7030	 0.3190
g	 0.9850	 0.5630
h	 0.9630	 0.5070
i	 0.9890	 0.5920
j	 0.9530	 0.5350
k	 0.9450	 0.3660
l	 0.9850	 0.4110
m	 0.4390	 0.1930
o	 0.9800	 0.5800
p	 0.9610	 0.4980
q	 0.9590	 0.4850
r	 0.9830	 0.5480
s	 0.9800	 0.5600