



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 10:30 AM UTC

PDB ID : 8PK0 / pdb_00008pk0
EMDB ID : EMD-17719
Title : human mitoribosomal large subunit assembly intermediate 1 with GTPBP10-GTPBP7
Authors : Kummer, E.; Nguyen, T.G.; Ritter, C.
Deposited on : 2023-06-23
Resolution : 3.03 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

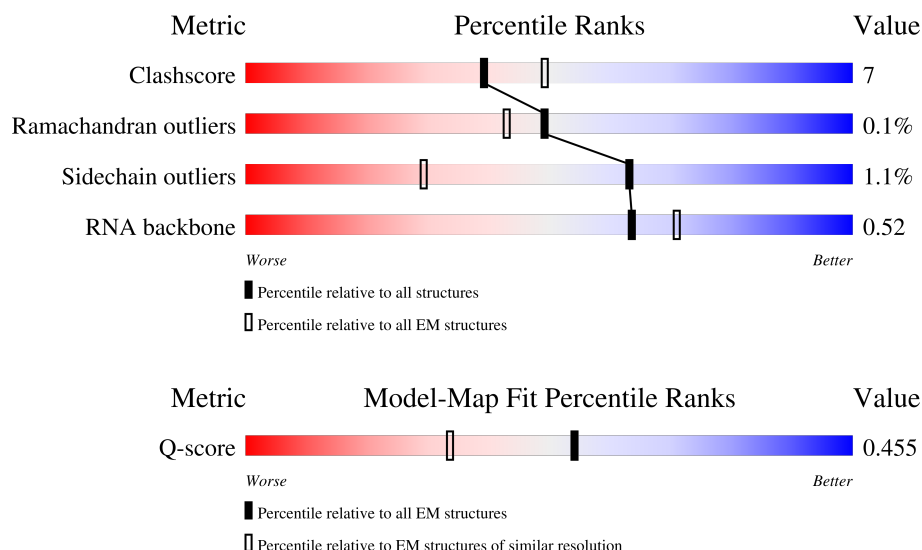
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.03 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	13929 (2.53 - 3.53)

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	T	206	
3	u	234	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	1	65	
5	U	153	
6	v	70	
7	2	92	
8	V	216	
9	w	156	
10	3	188	
11	W	148	
12	x	384	
13	5	423	
14	X	256	
15	y	381	
16	6	380	
17	Y	250	
18	z	334	
19	7	338	
20	Z	161	
21	8	206	
22	a	142	
23	9	137	
24	b	215	
25	A	1589	
26	c	332	
27	B	72	
28	d	306	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	D	305	
30	e	279	
31	E	348	
32	f	212	
33	F	311	
34	g	166	
35	H	267	
36	h	158	
37	I	261	
38	i	128	
39	J	192	
40	j	123	
41	K	178	
42	k	112	
43	L	145	
44	l	138	
45	M	296	
46	m	128	
47	N	251	
48	o	102	
49	O	175	
50	p	206	
51	P	180	
52	q	222	
53	Q	292	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	r	196	19% 65% 17% • 17%
55	R	149	79% 15% • 6%
56	s	439	73% 15% 12%
57	S	205	69% 10% 21%
58	t	387	40% 73% 11% 16%

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 108702 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	110	Total	C	N	O	S	0	0
			898	554	176	162	6		

- Molecule 2 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 3 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	u	126	Total	C	N	O	S	0	0
			1044	671	172	191	10		

- Molecule 4 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	55	Total	C	N	O	S	0	0
			455	290	87	76	2		

- Molecule 5 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 6 is a protein called MIEF1 upstream open reading frame protein.

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

- Molecule 7 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2	46	Total	C	N	O	S	0	0
			377	233	83	60	1		

- Molecule 8 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 9 is a protein called Acyl carrier protein, mitochondrial.

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

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

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

- Molecule 11 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 12 is a protein called 5-methylcytosine rRNA methyltransferase NSUN4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	x	338	Total	C	N	O	S	0	0
			2676	1703	467	489	17		

- Molecule 13 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	5	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 14 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 15 is a protein called Transcription termination factor 4, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 17 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 18 is a protein called Mitochondrial ribosome-associated GTPase 1.

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

- Molecule 19 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	7	294	Total	C	N	O	S	0	0
			2390	1529	405	438	18		

- Molecule 20 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	8	102	Total	C	N	O	S	0	0
			860	543	152	163	2		

- Molecule 22 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 24 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	150	Total	C	N	O	S	0	0
			1189	739	230	217	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	2	ACE	-	acetylation	UNP Q8N983

- Molecule 25 is a RNA chain called 16S rRNA + pre-H68-71 segment.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	1423	Total	C	N	O	P	0	0
			30199	13555	5442	9779	1423		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2737	A	G	conflict	GB 1858624182
A	3138	U	-	insertion	GB 1858624182

- Molecule 26 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 27 is a RNA chain called CP tRNA-Val.

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

- Molecule 28 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	255	Total	C	N	O	S	0	0
			2088	1335	360	379	14		

- Molecule 29 is a protein called 39S ribosomal protein L2, mitochondrial.

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

- Molecule 30 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 31 is a protein called 39S ribosomal protein L3, mitochondrial.

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

- Molecule 32 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 33 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	I	158	Total	C	N	O	S	0	0
			871	533	169	166	3		

- Molecule 38 is a protein called 39S ribosomal protein L51, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	J	162	Total	C	N	O	S	0	0
			798	474	162	162			

- Molecule 40 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	90	Total	C	N	O	S	0	0
			722	449	140	131	2		

- Molecule 41 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	k	101	Total	C	N	O	0	0
			502	299	101	102		

- Molecule 43 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	l	72	Total	C	N	O	0	0
			353	209	72	72		

- Molecule 45 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 46 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 47 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	N	144	Total	C	N	O	S	0	0
			799	485	157	156	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	80	Total	C	N	O	S	0	0
			677	426	134	114	3		

- Molecule 49 is a protein called 39S ribosomal protein L17, mitochondrial.

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

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

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

- Molecule 51 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 52 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

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

- Molecule 53 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 54 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	r	162	Total	C	N	O	S	0	0
			1251	791	243	209	8		

- Molecule 55 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 56 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 57 is a protein called 39S ribosomal protein L21, mitochondrial.

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

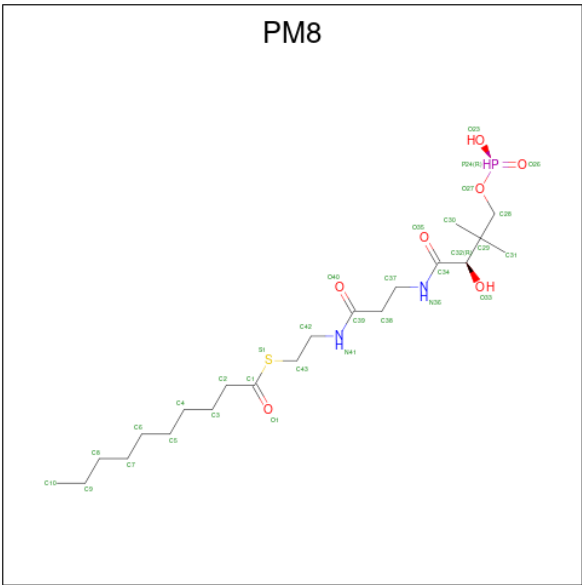
- Molecule 58 is a protein called GTP-binding protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	t	325	Total	C	N	O	S	0	0
			1958	1202	380	372	4		

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

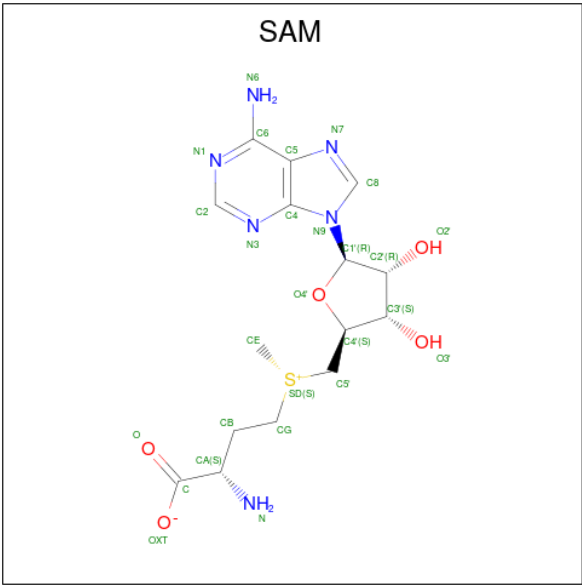
Mol	Chain	Residues	Atoms		AltConf
59	0	1	Total	Zn	0
			1	1	

- Molecule 60 is S-(2-{[N-(2-HYDROXY-4-{[HYDROXY(OXIDO)PHOSPHINO]OXY}-3,3-DIMETHYLBUTANOYL)-BETA-ALANYL]AMINO}ETHYL) DECANETHIOATE (CCD ID: PM8) (formula: C₂₁H₄₁N₂O₇PS).



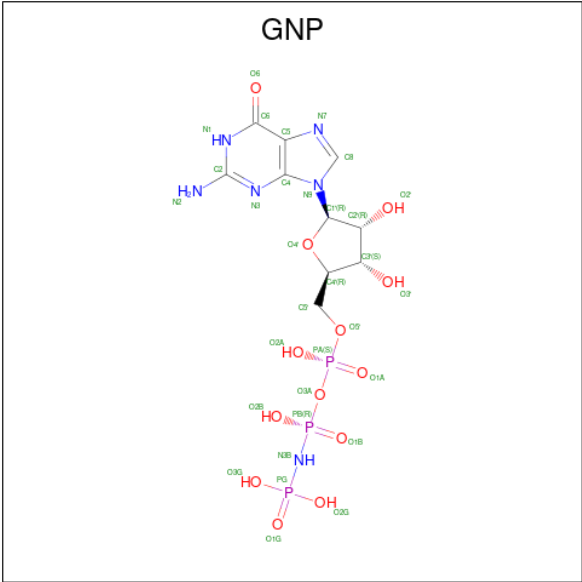
Mol	Chain	Residues	Atoms					AltConf	
60	w	1	Total	C	N	O	P	S	0
			32	21	2	7	1	1	

- Molecule 61 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



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

- Molecule 62 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
62	z	1	Total	C	N	O	P	0
			32	10	6	13	3	
62	t	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 63 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
63	z	1	Total	Mg	0
			1	1	
63	A	92	Total	Mg	0
			92	92	
63	E	1	Total	Mg	0
			1	1	
63	g	1	Total	Mg	0
			1	1	
63	t	1	Total	Mg	0
			1	1	

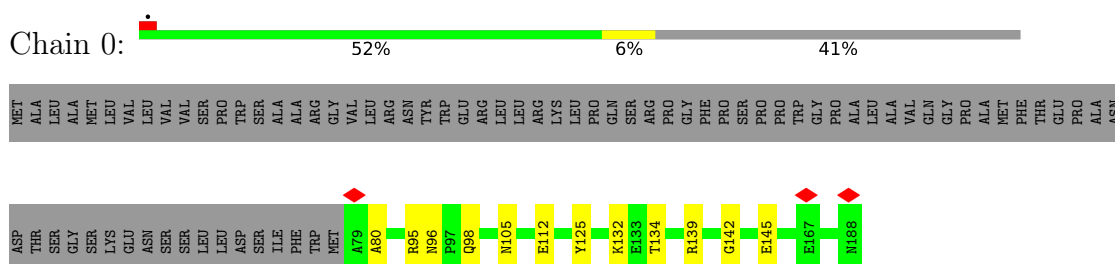
- Molecule 64 is POTASSIUM ION (CCD ID: K) (formula: K).

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

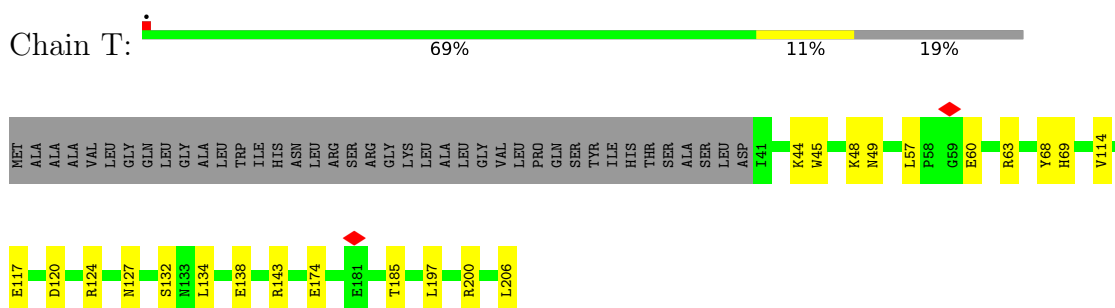
3 Residue-property plots

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

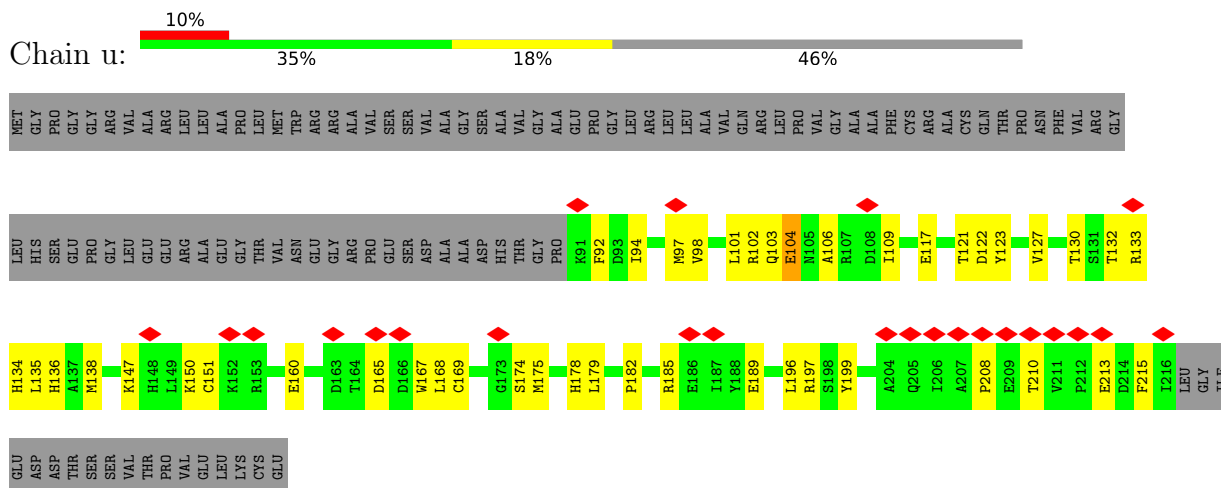
- Molecule 1: 39S ribosomal protein L32, mitochondrial

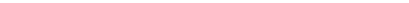


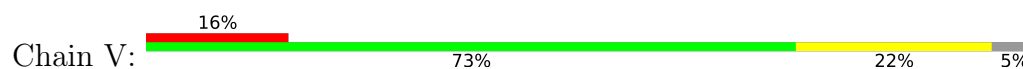
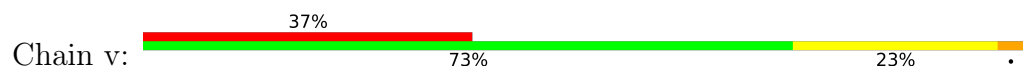
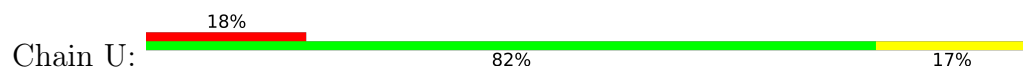
- Molecule 2: 39S ribosomal protein L22, mitochondrial

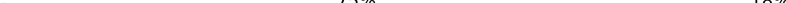


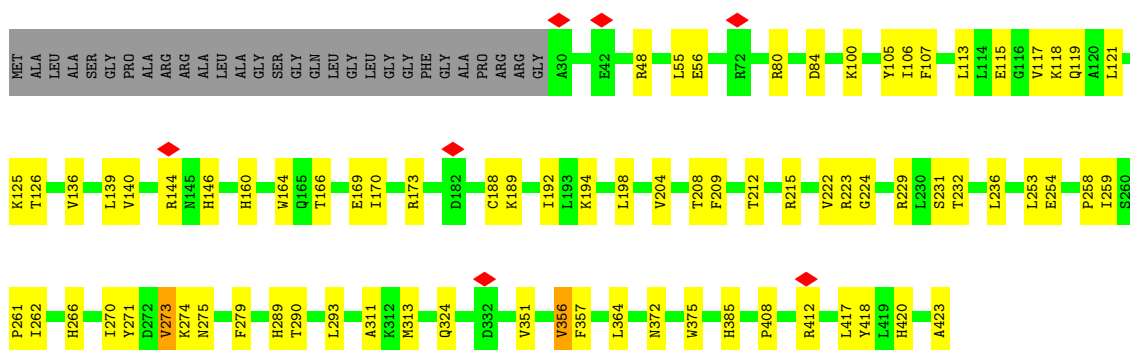
- Molecule 3: Mitochondrial assembly of ribosomal large subunit protein 1

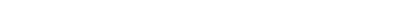


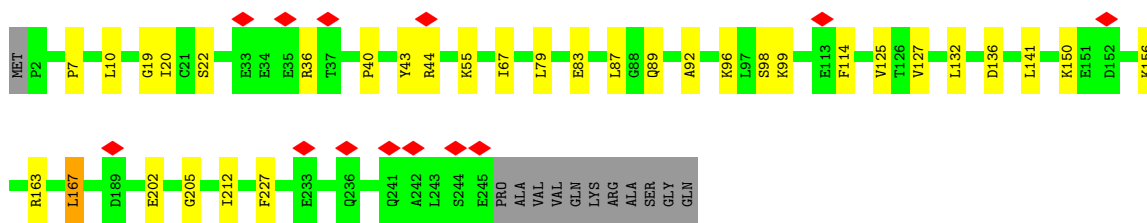
- Chain 1: 

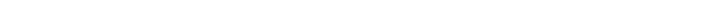


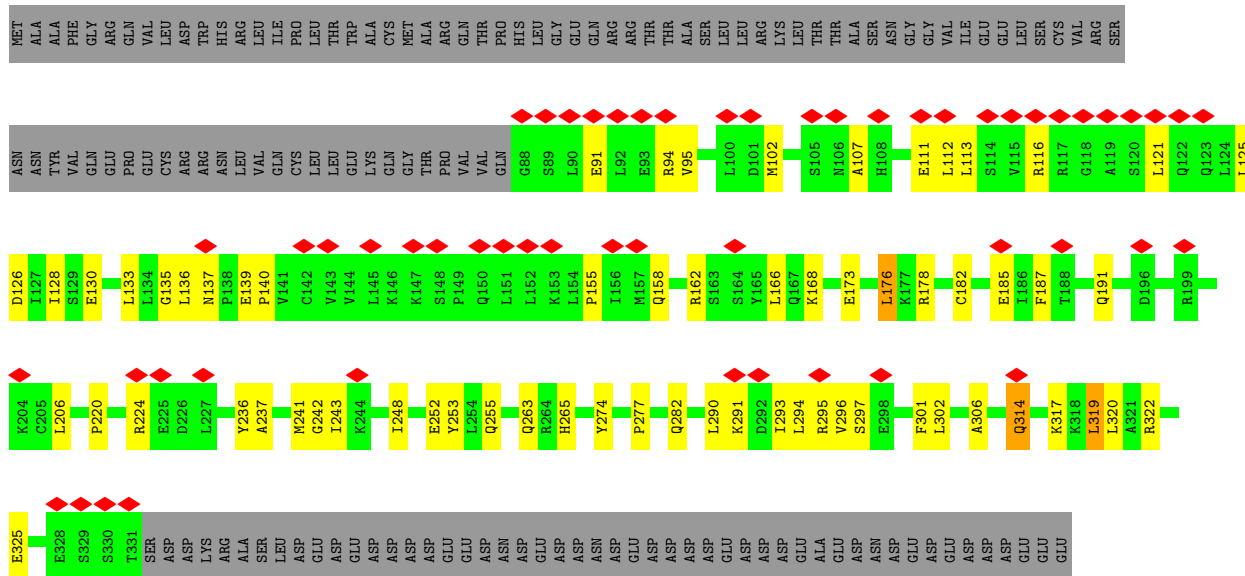
- Chain 5:  75% 18% 7%

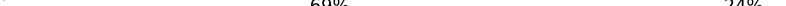


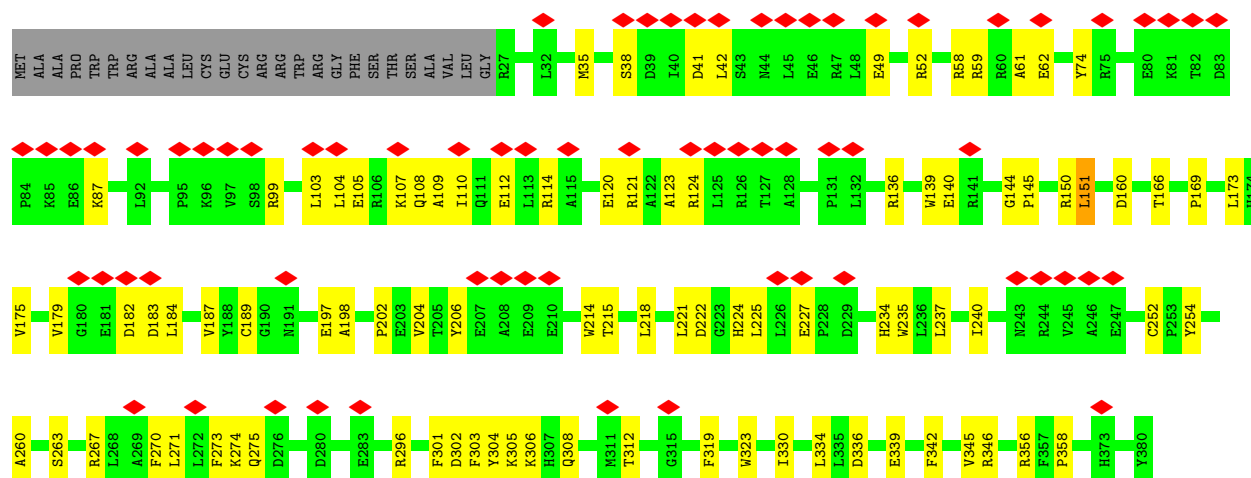
- Chain X: 



- Chain y: 

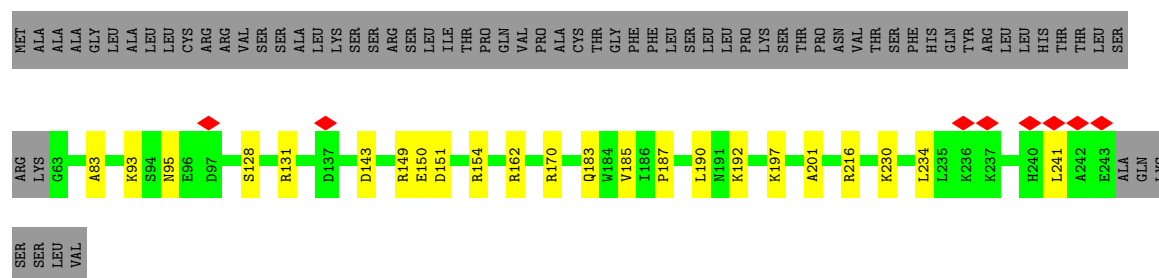


- Chain 6: 



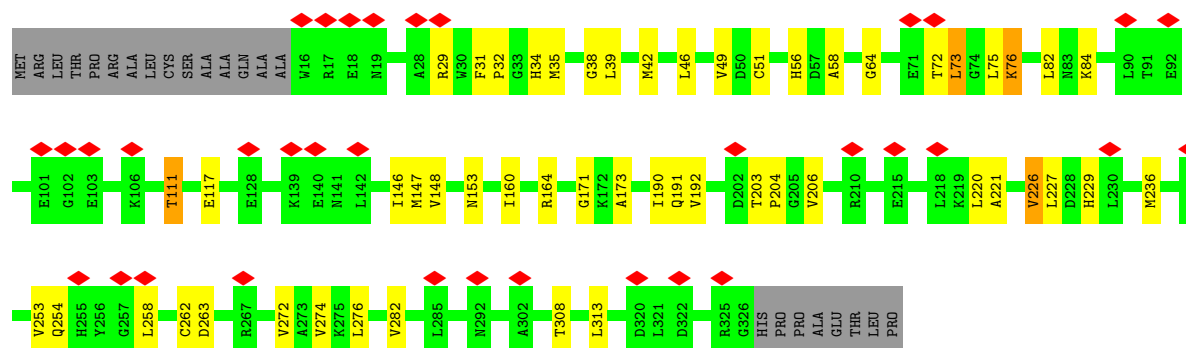
- Molecule 17: 39S ribosomal protein L47, mitochondrial

Chain Y: 63% 9% 28%



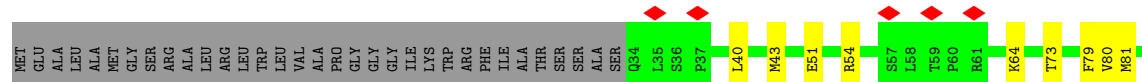
- Molecule 18: Mitochondrial ribosome-associated GTPase 1

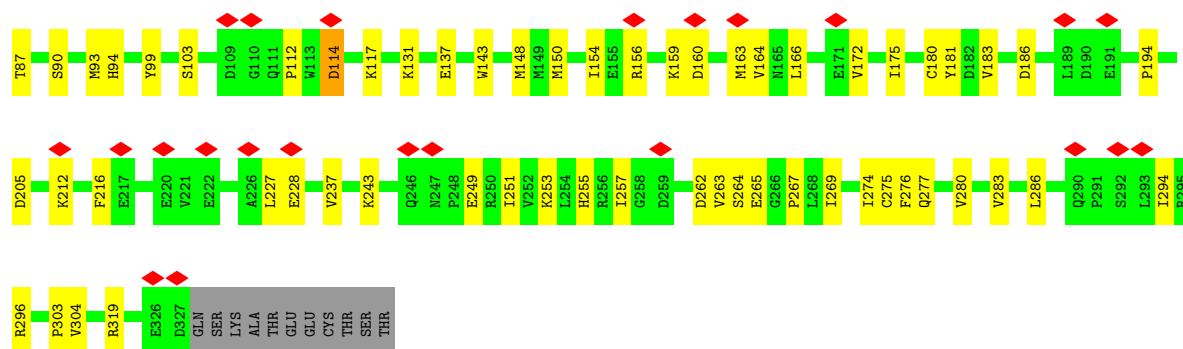
Chain z: 10% 77% 15% 7%



- Molecule 19: 39S ribosomal protein L39, mitochondrial

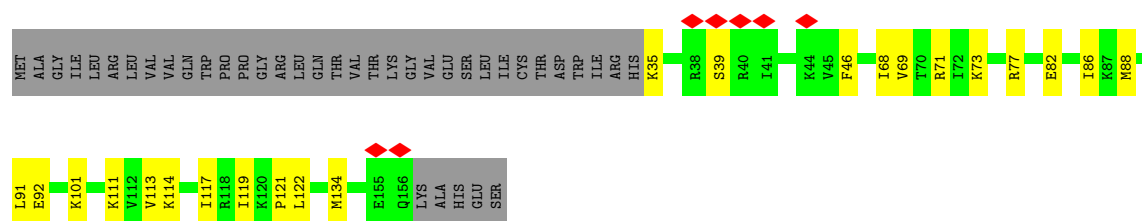
Chain 7: 8% 67% 20% 13%





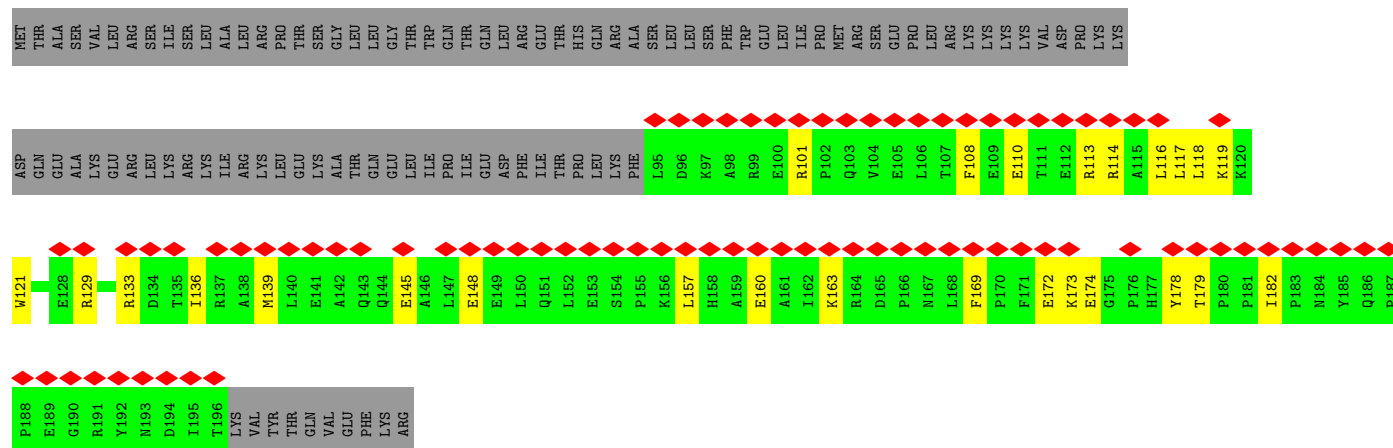
- Molecule 20: 39S ribosomal protein L30, mitochondrial

Chain Z:



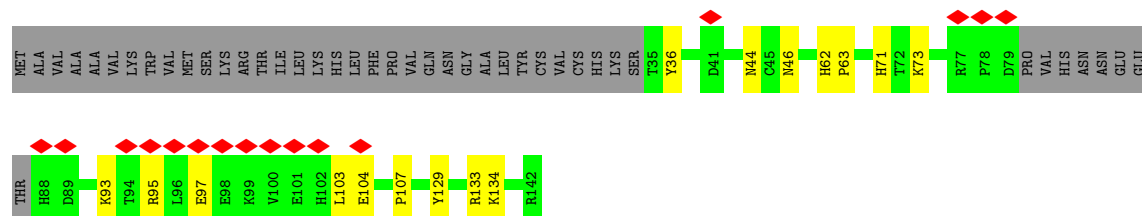
- Molecule 21: 39S ribosomal protein L40, mitochondrial

Chain 8:

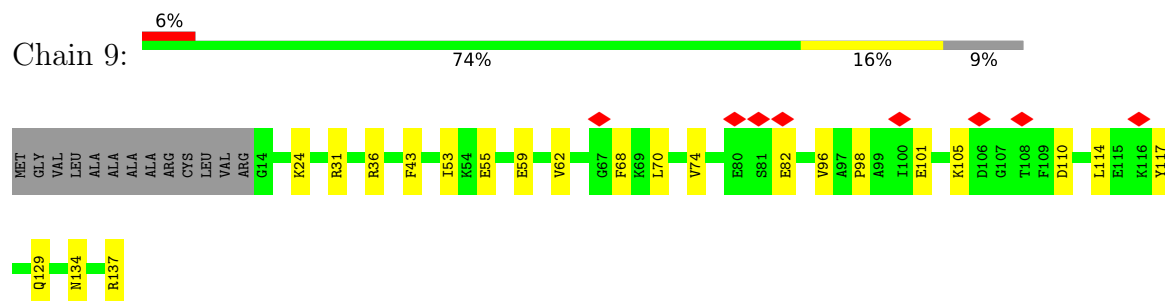


- Molecule 22: 39S ribosomal protein L42, mitochondrial

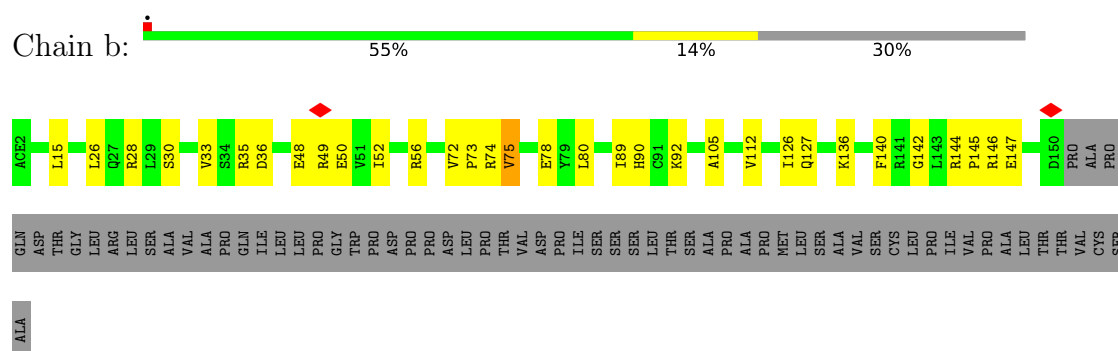
Chain a:



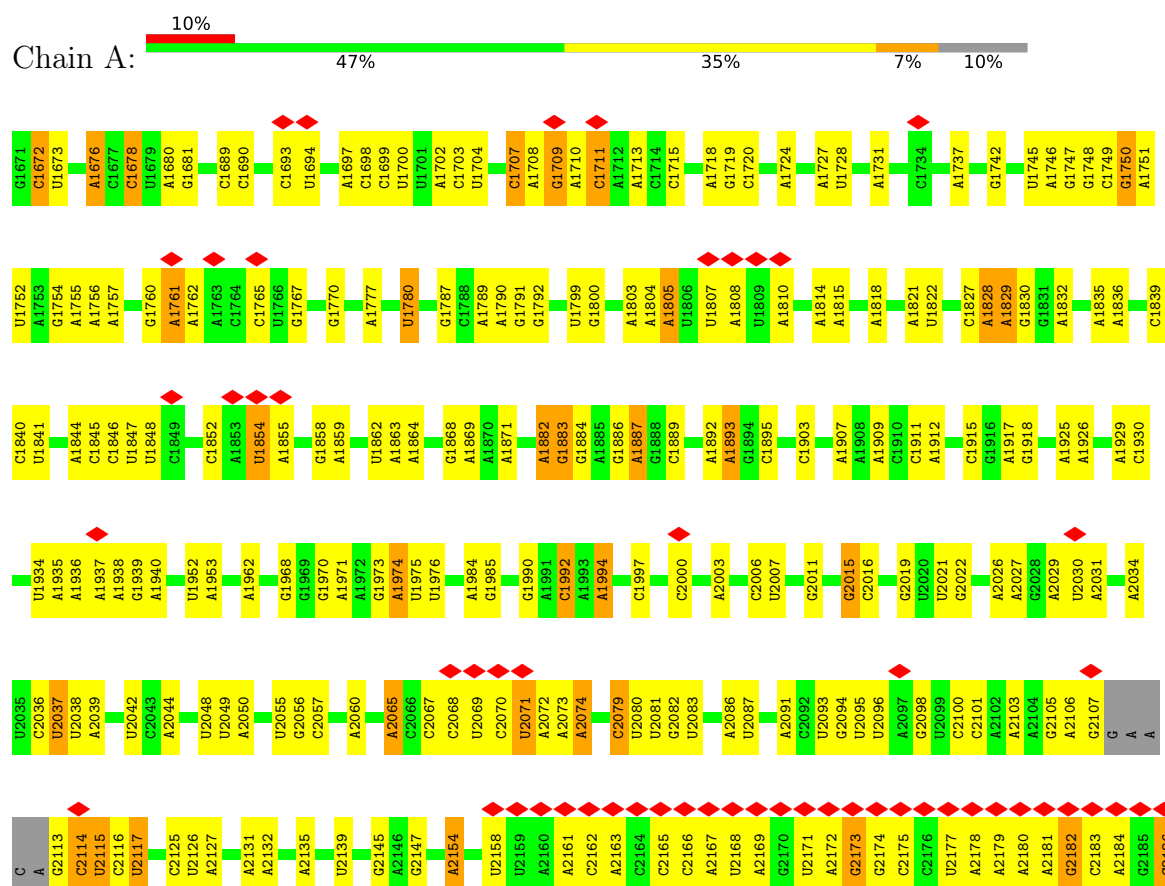
- Molecule 23: 39S ribosomal protein L41, mitochondrial

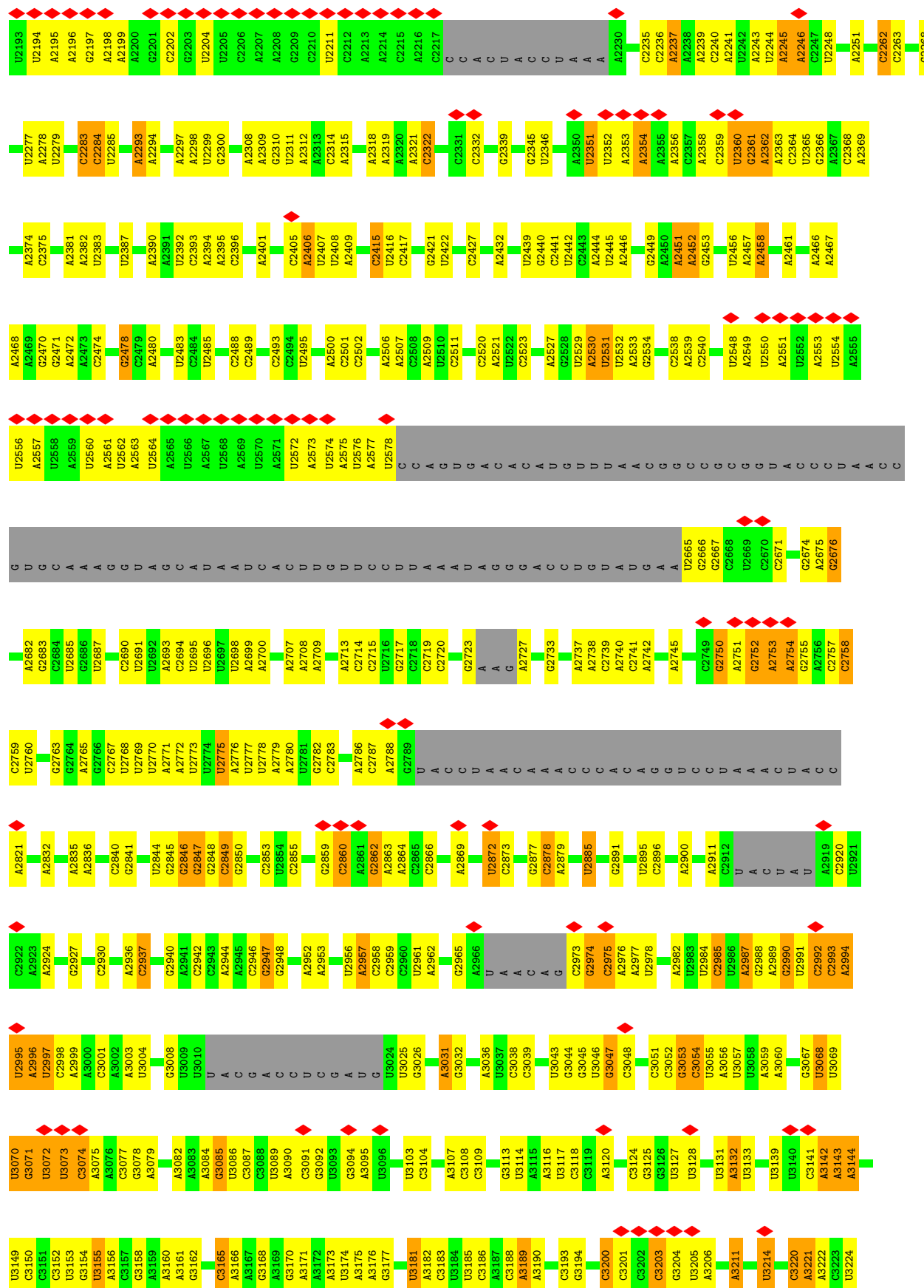


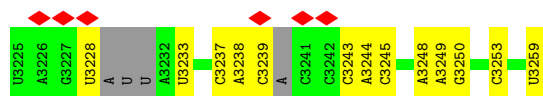
- Molecule 24: Large ribosomal subunit protein mL43



- Molecule 25: 16S rRNA + pre-H68-71 segment

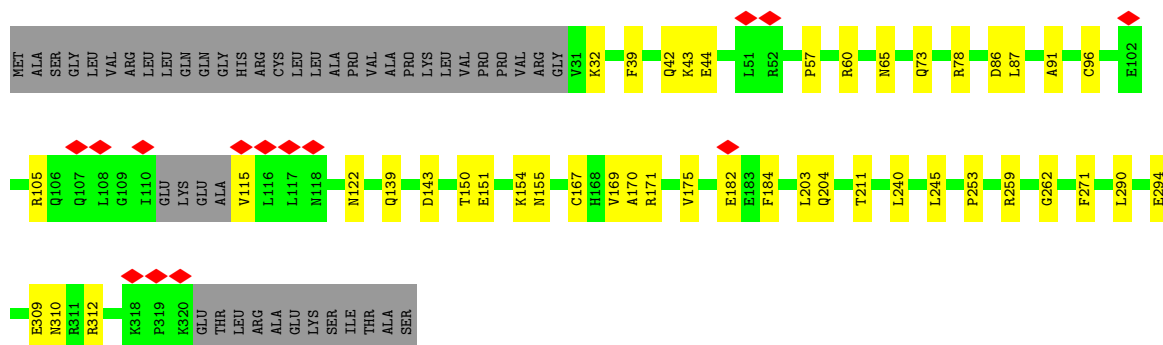






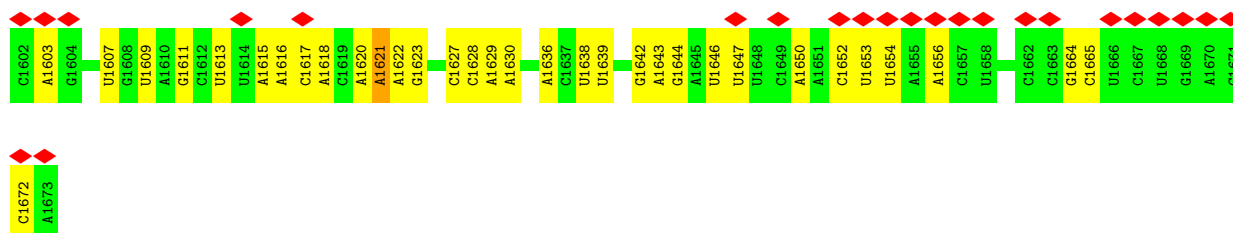
- Molecule 26: 39S ribosomal protein L44, mitochondrial

Chain c: 73% 13% 14%



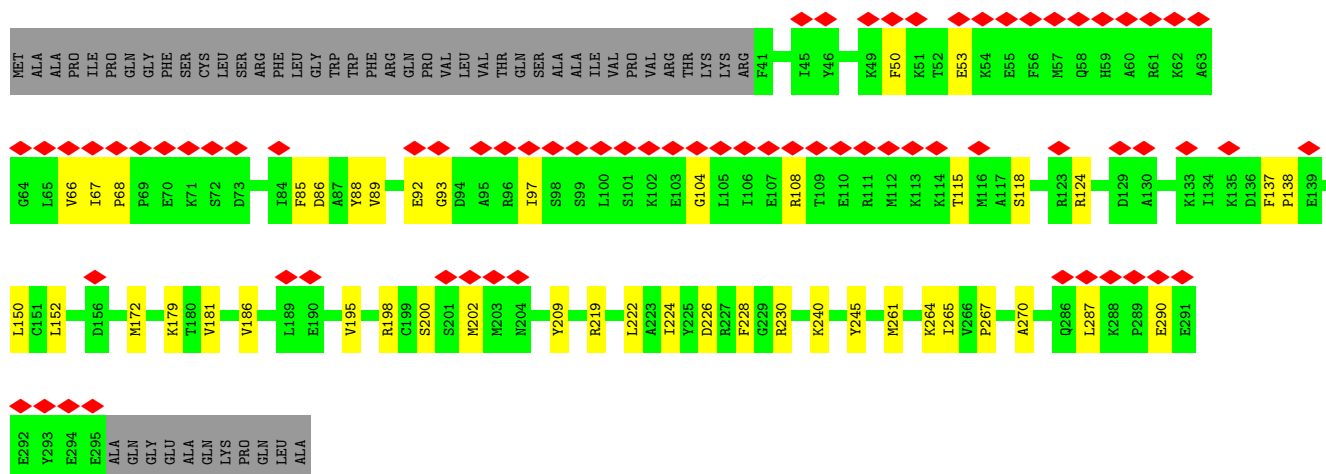
- Molecule 27: CP tRNA-Val

Chain B: 33% 54% 44%



- Molecule 28: 39S ribosomal protein L45, mitochondrial

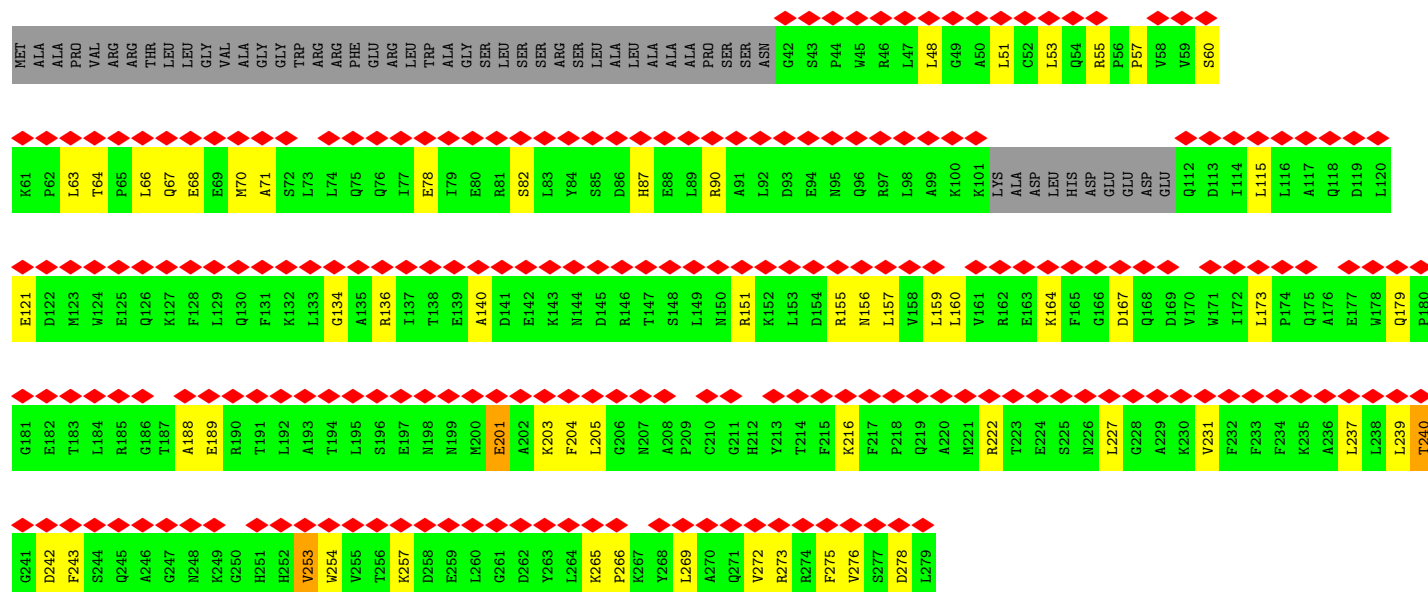
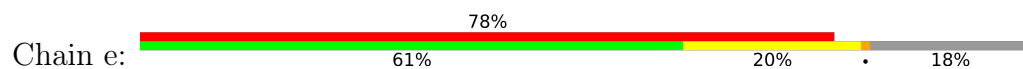
Chain d: 24% 69% 15% 17%



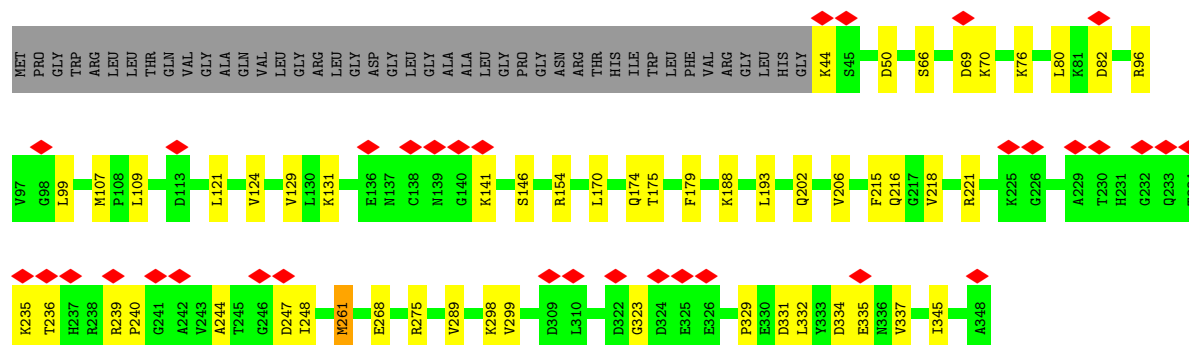
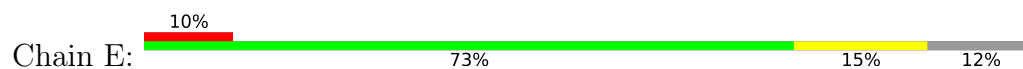
- Molecule 29: 39S ribosomal protein L2, mitochondrial



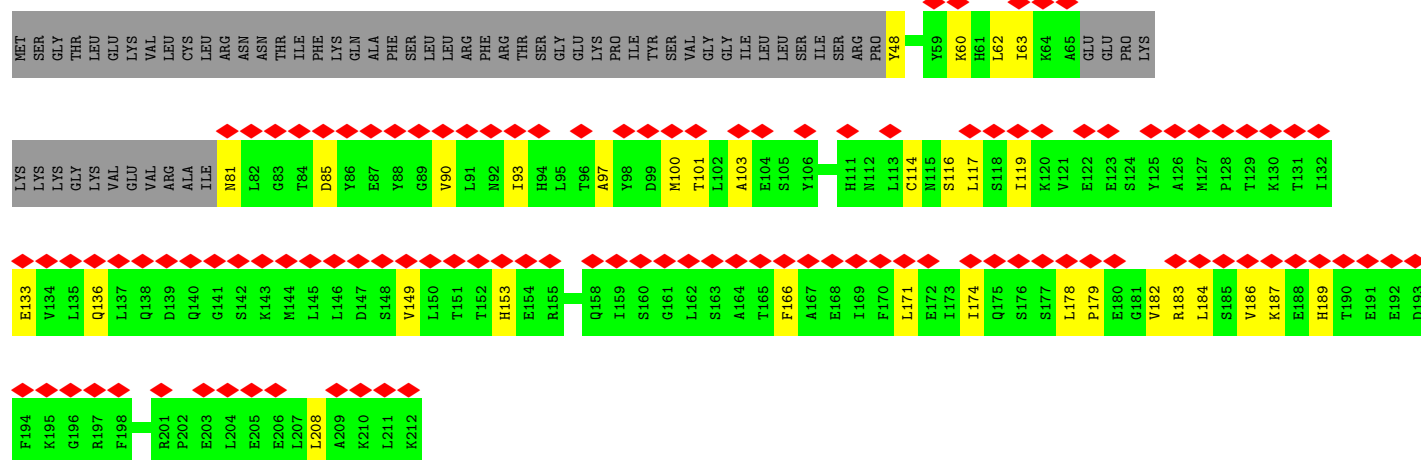
- Molecule 30: 39S ribosomal protein L46, mitochondrial



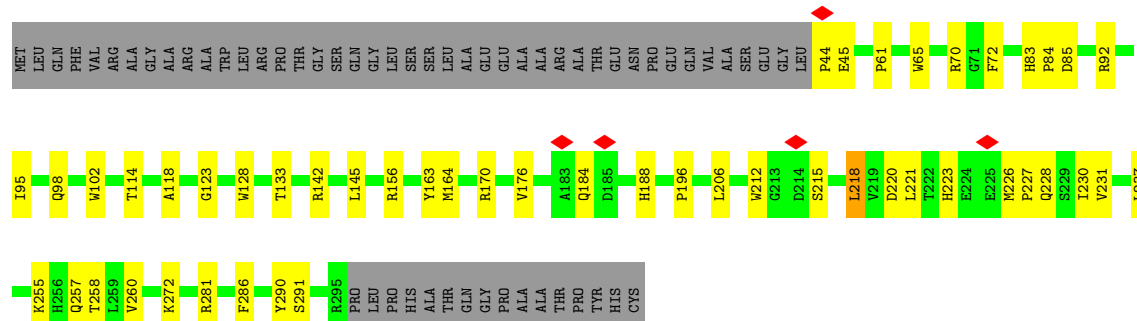
- Molecule 31: 39S ribosomal protein L3, mitochondrial



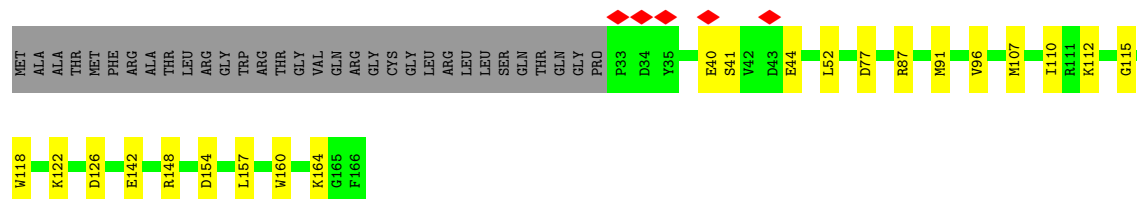
- Molecule 32: 39S ribosomal protein L48, mitochondrial



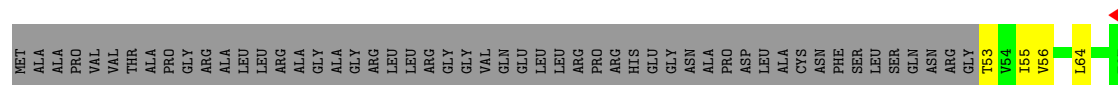
• Molecule 33: 39S ribosomal protein L4, mitochondrial



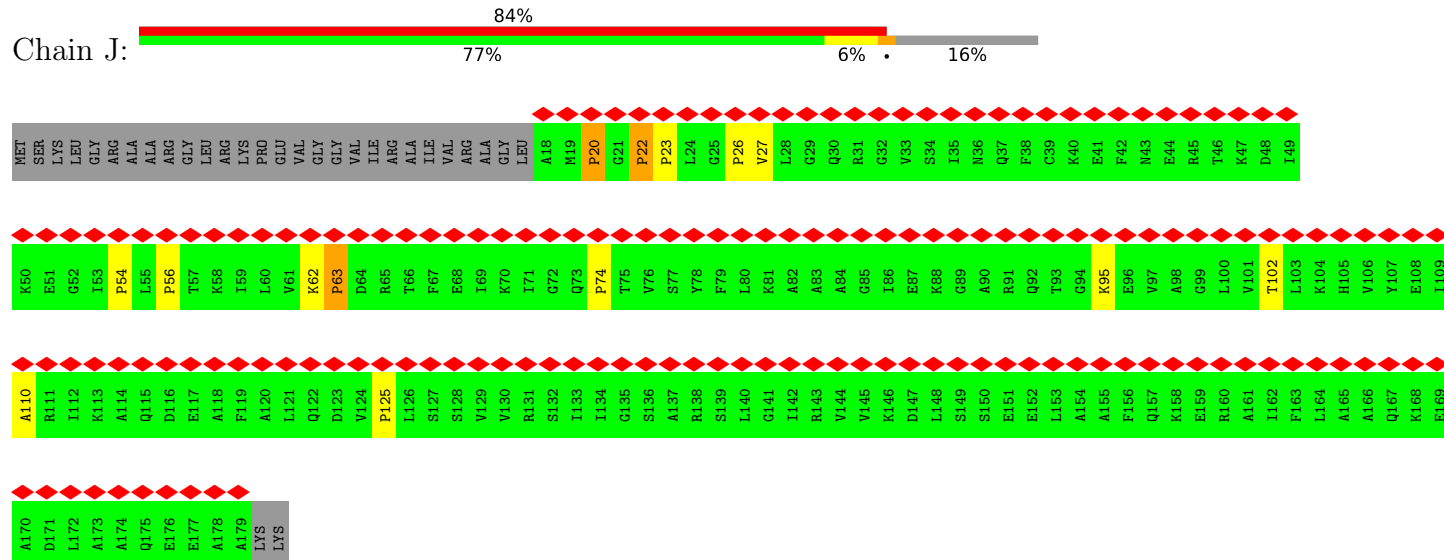
• Molecule 34: 39S ribosomal protein L49, mitochondrial



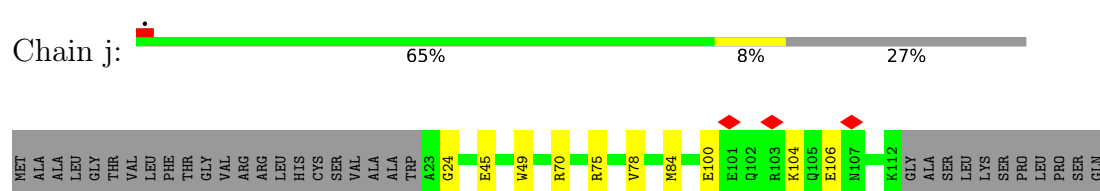
• Molecule 35: 39S ribosomal protein L9, mitochondrial



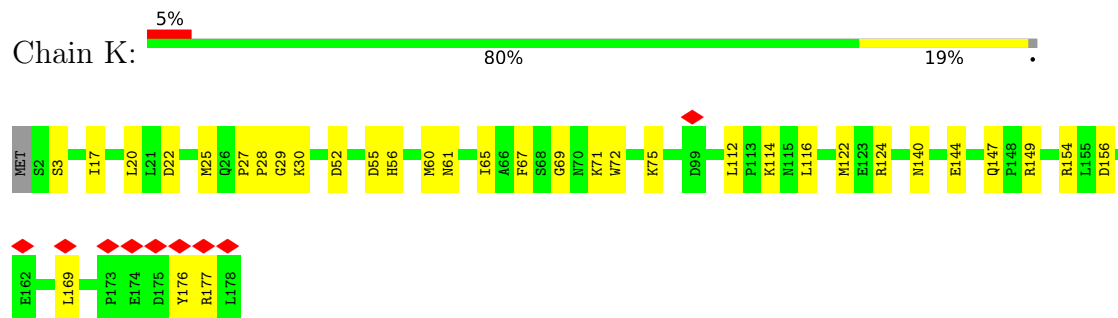
- Molecule 39: 39S ribosomal protein L11, mitochondrial



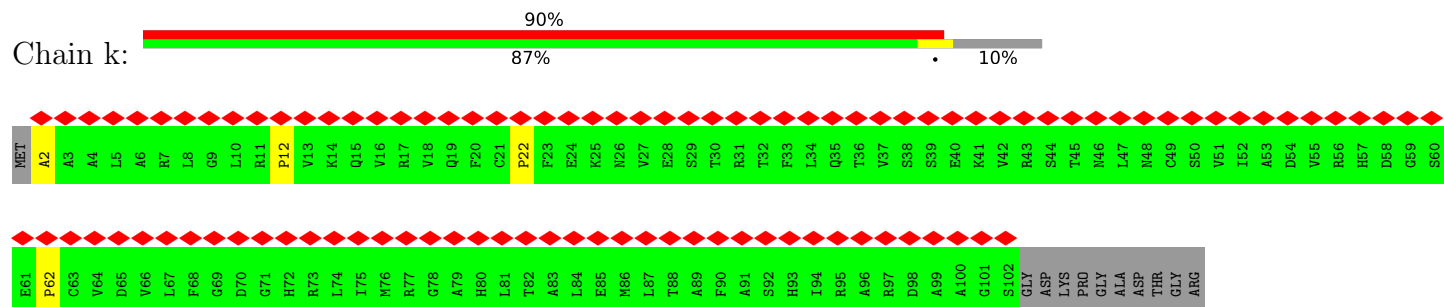
- Molecule 40: 39S ribosomal protein L52, mitochondrial



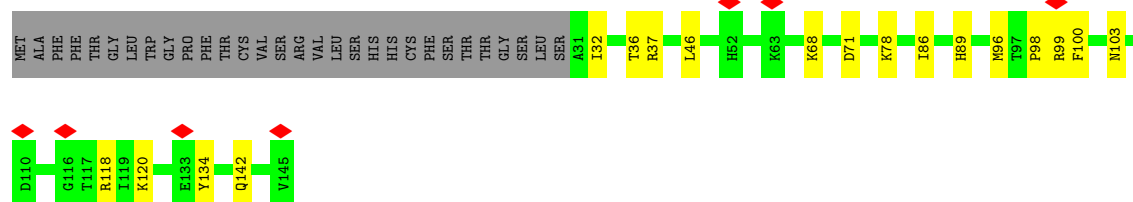
- Molecule 41: 39S ribosomal protein L13, mitochondrial



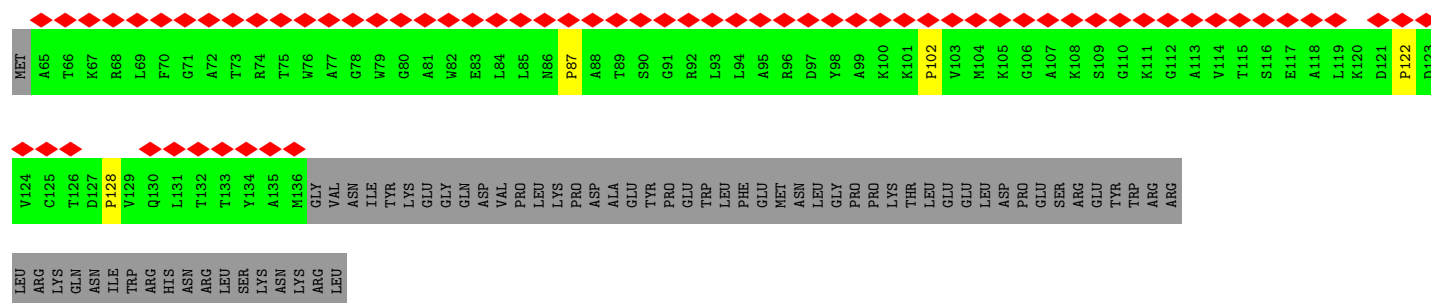
- Molecule 42: 39S ribosomal protein L53, mitochondrial



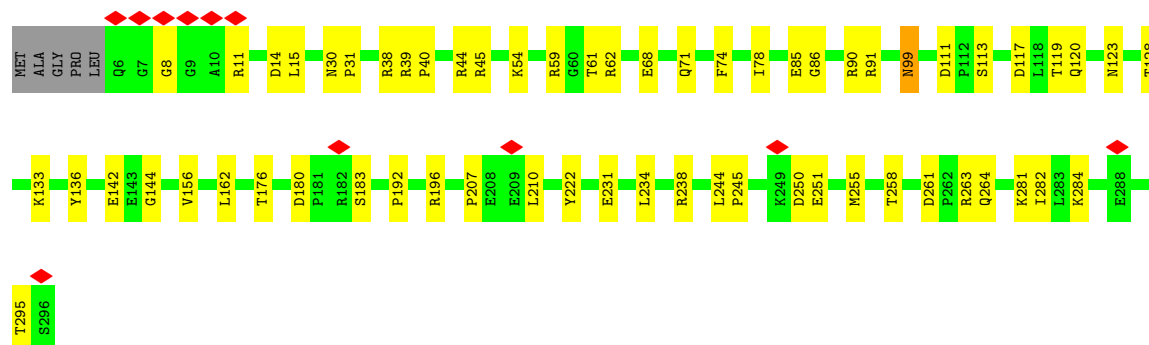
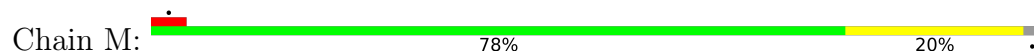
- Molecule 43: 39S ribosomal protein L14, mitochondrial



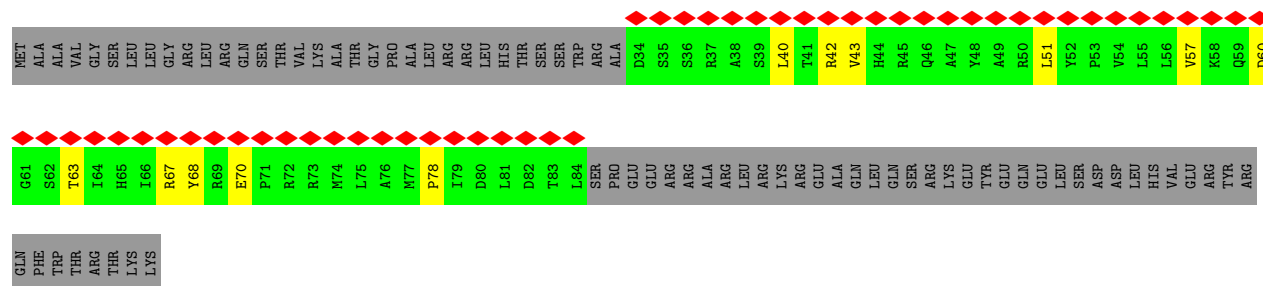
- Molecule 44: 39S ribosomal protein L54, mitochondrial



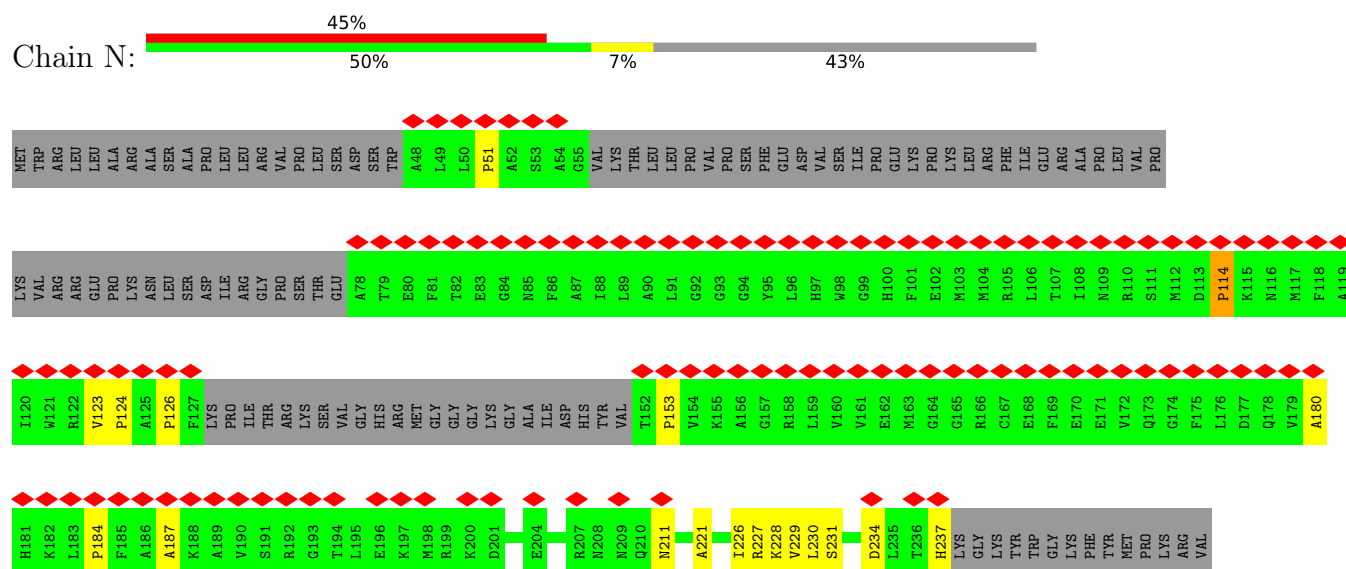
- Molecule 45: 39S ribosomal protein L15, mitochondrial



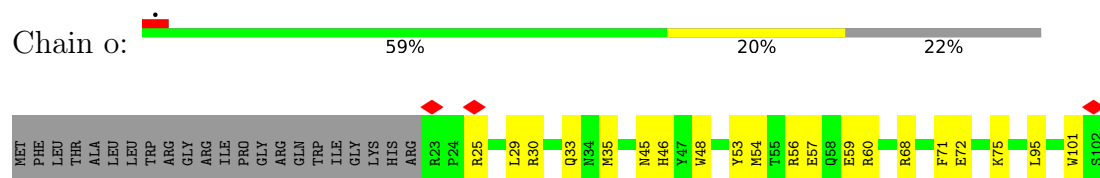
- Molecule 46: 39S ribosomal protein L55, mitochondrial



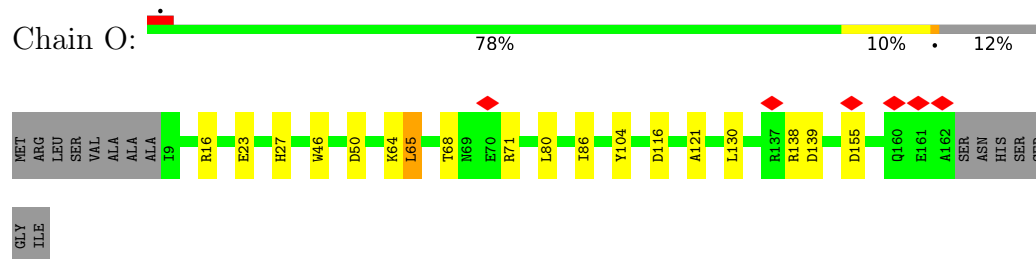
- Molecule 47: 39S ribosomal protein L16, mitochondrial



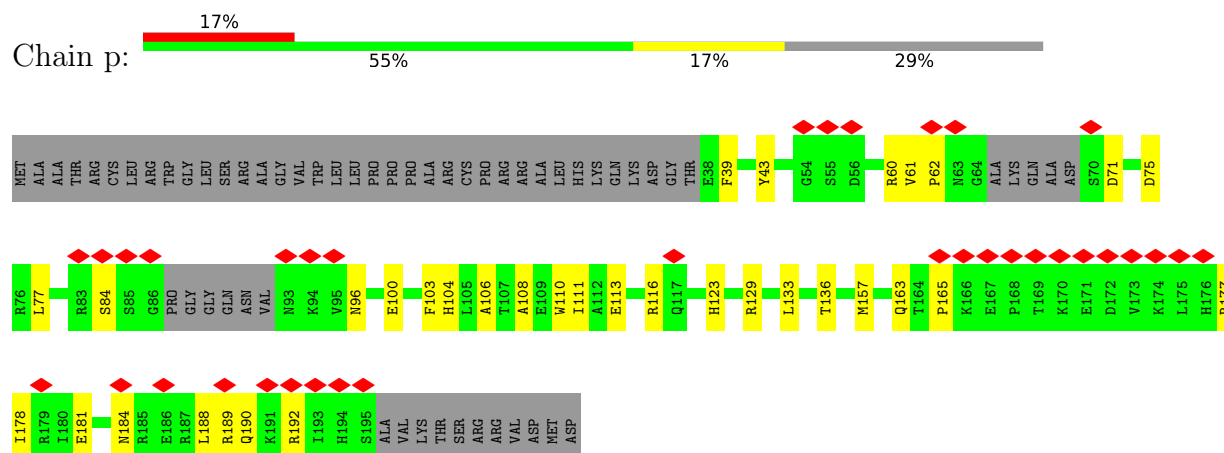
- Molecule 48: Ribosomal protein 63, mitochondrial

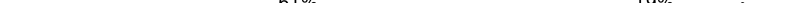


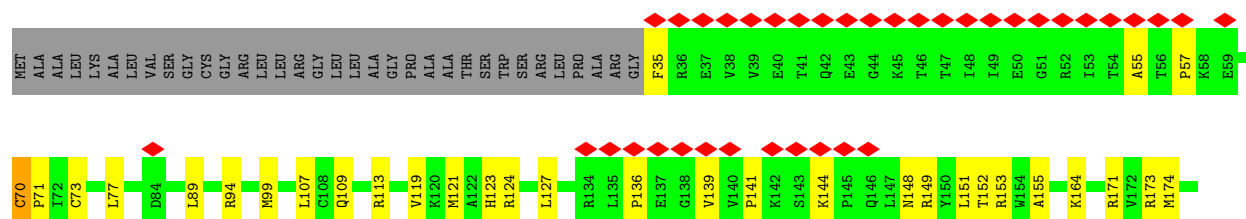
- Molecule 49: 39S ribosomal protein L17, mitochondrial

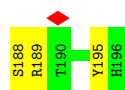


- Molecule 50: Peptidyl-tRNA hydrolase ICT1, mitochondrial

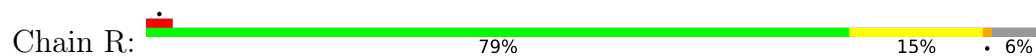


- Chain P: 

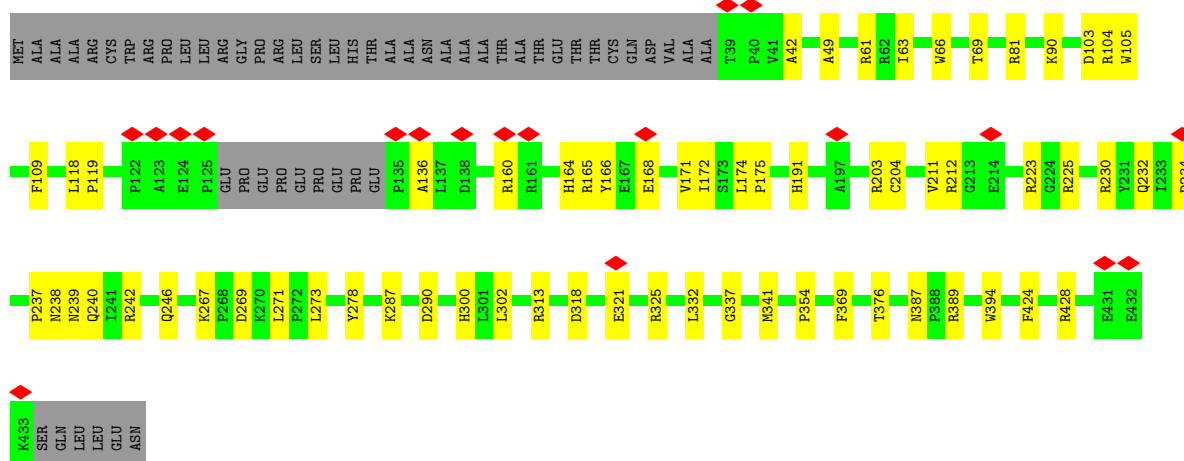




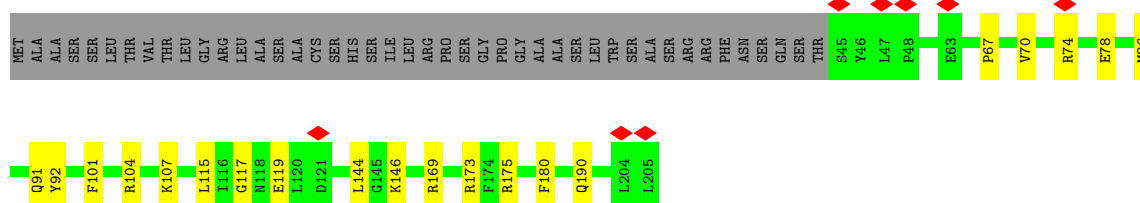
- Molecule 55: 39S ribosomal protein L20, mitochondrial



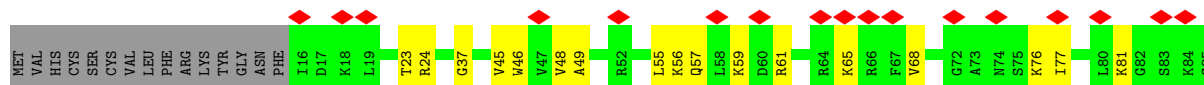
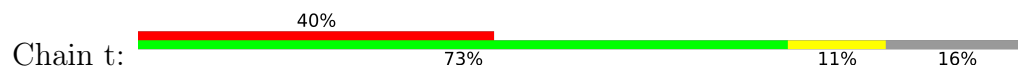
- Molecule 56: 39S ribosomal protein S30, mitochondrial

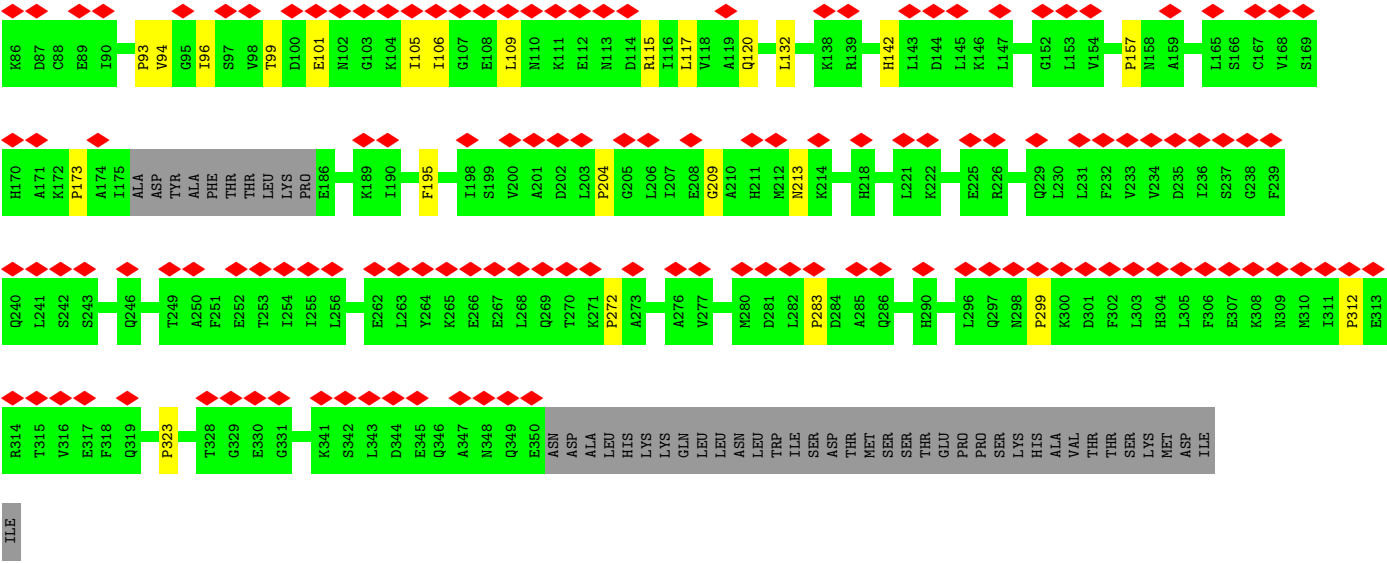


- Molecule 57: 39S ribosomal protein L21, mitochondrial



- Molecule 58: GTP-binding protein 10





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31656	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	4.028	Depositor
Minimum map value	-2.106	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.160	Depositor
Recommended contour level	0.747	Depositor
Map size (Å)	518.4, 518.4, 518.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.11	0/913	0.22	0/1224
2	T	0.11	0/1403	0.24	0/1886
3	u	0.12	0/1069	0.30	0/1447
4	1	0.10	0/460	0.23	0/610
5	U	0.11	0/1274	0.24	0/1723
6	v	0.14	0/597	0.34	0/796
7	2	0.11	0/383	0.22	0/507
8	V	0.09	0/1721	0.22	0/2333
9	w	0.12	0/647	0.37	0/871
10	3	0.11	0/853	0.23	0/1136
11	W	0.11	0/857	0.22	0/1155
12	x	0.11	0/2737	0.26	0/3714
13	5	0.11	0/3305	0.25	0/4502
14	X	0.10	0/2099	0.22	0/2837
15	y	0.11	0/2011	0.25	0/2702
16	6	0.10	0/3043	0.26	0/4140
17	Y	0.11	0/1593	0.21	0/2136
18	z	0.11	0/2484	0.26	0/3349
19	7	0.10	0/2447	0.23	0/3310
20	Z	0.10	0/1021	0.24	0/1378
21	8	0.10	0/880	0.31	0/1188
22	a	0.11	0/866	0.25	0/1174
23	9	0.11	0/1025	0.24	0/1379
24	b	0.14	0/1211	0.26	0/1639
25	A	0.12	0/33779	0.25	0/52552
26	c	0.10	0/2347	0.23	0/3171
27	B	0.08	0/1700	0.17	0/2641
28	d	0.09	0/2145	0.23	0/2903
29	D	0.11	0/1910	0.25	0/2569
30	e	0.08	0/1885	0.25	0/2542
31	E	0.10	0/2475	0.24	0/3355
32	f	0.09	0/1216	0.24	0/1638

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	F	0.12	0/2090	0.27	0/2842
34	g	0.11	0/1151	0.25	0/1569
35	H	0.10	0/816	0.23	0/1097
36	h	0.09	0/918	0.21	0/1249
37	I	0.22	0/880	0.75	9/1220 (0.7%)
38	i	0.12	0/850	0.23	0/1135
39	J	0.26	0/797	0.90	11/1107 (1.0%)
40	j	0.10	0/737	0.19	0/992
41	K	0.11	0/1490	0.24	0/2021
42	k	0.25	0/493	0.70	3/685 (0.4%)
43	L	0.11	0/905	0.26	0/1218
44	l	0.22	0/352	0.77	4/487 (0.8%)
45	M	0.11	0/2381	0.24	0/3212
46	m	0.07	0/426	0.19	0/575
47	N	0.22	0/803	0.75	6/1105 (0.5%)
48	o	0.11	0/694	0.24	0/931
49	O	0.11	0/1283	0.24	0/1727
50	p	0.09	0/1223	0.22	0/1641
51	P	0.10	0/1199	0.24	0/1623
52	q	0.10	0/1208	0.21	0/1633
53	Q	0.10	0/1884	0.22	0/2535
54	r	0.13	0/1289	0.31	1/1752 (0.1%)
55	R	0.12	0/1175	0.23	0/1572
56	s	0.12	0/3239	0.25	0/4400
57	S	0.12	0/1320	0.27	0/1789
58	t	0.19	0/1971	0.56	8/2684 (0.3%)
All	All	0.12	0/113930	0.28	42/161308 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
21	8	0	1

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	t	173	PRO	N-CA-CB	10.84	110.49	103.23
42	k	62	PRO	N-CA-CB	10.45	110.23	103.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	J	63	PRO	N-CA-CB	9.72	113.45	103.25
58	t	157	PRO	N-CA-CB	8.61	110.97	103.31
47	N	153	PRO	N-CA-CB	8.50	110.41	103.36
39	J	22	PRO	N-CA-CB	8.32	111.15	103.08
42	k	12	PRO	N-CA-CB	8.24	110.20	101.88
37	I	69	PRO	N-CA-CB	7.97	110.40	103.31
37	I	127	PRO	N-CA-CB	7.90	110.34	103.31
47	N	126	PRO	N-CA-CB	7.89	110.66	103.33
58	t	272	PRO	N-CA-CB	7.76	110.22	103.31
47	N	51	PRO	N-CA-CB	7.73	110.52	103.33
47	N	124	PRO	N-CA-CB	7.60	110.77	102.72
39	J	26	PRO	N-CA-CB	7.58	110.09	103.27
47	N	114	PRO	N-CA-CB	7.57	111.20	103.25
54	r	57	PRO	N-CA-CB	7.57	110.37	103.33
39	J	20	PRO	N-CA-CB	7.50	111.13	103.25
39	J	23	PRO	N-CA-CB	7.42	111.04	103.25
37	I	175	PRO	N-CA-CB	7.38	110.71	102.67
44	l	87	PRO	N-CA-CB	7.38	110.99	103.25
37	I	71	PRO	N-CA-CB	7.29	110.15	103.08
58	t	323	PRO	N-CA-CB	7.08	110.68	103.25
37	I	172	PRO	N-CA-CB	7.04	110.27	103.51
37	I	159	PRO	N-CA-CB	6.94	110.54	103.25
44	l	102	PRO	N-CA-CB	6.89	110.49	103.25
58	t	312	PRO	N-CA-CB	6.89	110.61	103.38
39	J	125	PRO	N-CA-CB	6.87	109.87	103.41
37	I	72	PRO	N-CA-CB	6.83	110.42	103.25
47	N	184	PRO	N-CA-CB	6.79	109.98	103.19
58	t	204	PRO	N-CA-CB	6.74	110.85	103.23
58	t	299	PRO	N-CA-CB	6.64	110.23	103.25
37	I	145	PRO	N-CA-CB	6.61	110.09	103.48
39	J	62	LYS	CA-C-N	6.56	128.04	119.84
39	J	62	LYS	C-N-CA	6.56	128.04	119.84
39	J	74	PRO	N-CA-CB	6.54	110.02	103.48
39	J	56	PRO	N-CA-CB	6.48	110.06	103.25
42	k	22	PRO	N-CA-CB	6.42	110.32	103.52
39	J	54	PRO	N-CA-CB	6.21	110.16	103.33
44	l	128	PRO	N-CA-CB	6.17	110.12	103.33
37	I	133	PRO	N-CA-CB	6.17	110.12	103.33
44	l	122	PRO	N-CA-CB	6.11	110.05	103.33
58	t	283	PRO	N-CA-CB	6.05	109.99	103.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	8	169	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	898	0	916	14	0
2	T	1369	0	1410	16	0
3	u	1044	0	1035	31	0
4	1	455	0	498	10	0
5	U	1251	0	1232	23	0
6	v	588	0	604	12	0
7	2	377	0	406	2	0
8	V	1676	0	1687	29	0
9	w	638	0	636	15	0
10	3	832	0	883	9	0
11	W	835	0	858	10	0
12	x	2676	0	2652	58	0
13	5	3210	0	3206	49	0
14	X	2044	0	2060	28	0
15	y	1980	0	2066	51	0
16	6	2948	0	2841	70	0
17	Y	1556	0	1597	22	0
18	z	2443	0	2545	40	0
19	7	2390	0	2397	46	0
20	Z	996	0	1044	18	0
21	8	860	0	852	26	0
22	a	840	0	810	14	0
23	9	997	0	987	20	0
24	b	1189	0	1188	24	0
25	A	30199	0	15338	427	0
26	c	2299	0	2320	30	0
27	B	1522	0	776	21	0
28	d	2088	0	2079	32	0
29	D	1872	0	1932	39	0
30	e	1848	0	1849	40	0
31	E	2406	0	2415	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	f	1196	0	1212	27	0
33	F	2031	0	2065	31	0
34	g	1113	0	1097	17	0
35	H	802	0	846	22	0
36	h	895	0	881	10	0
37	I	871	0	506	5	0
38	i	828	0	857	12	0
39	J	798	0	389	2	0
40	j	722	0	722	7	0
41	K	1455	0	1452	28	0
42	k	502	0	244	0	0
43	L	890	0	941	14	0
44	l	353	0	179	0	0
45	M	2327	0	2395	43	0
46	m	419	0	435	8	0
47	N	799	0	503	9	0
48	o	677	0	676	18	0
49	O	1259	0	1294	14	0
50	p	1205	0	1223	25	0
51	P	1173	0	1165	25	0
52	q	1177	0	1154	14	0
53	Q	1843	0	1878	27	0
54	r	1251	0	1204	28	0
55	R	1154	0	1214	18	0
56	s	3155	0	3139	44	0
57	S	1293	0	1365	15	0
58	t	1958	0	1486	24	0
59	0	1	0	0	0	0
60	w	32	0	39	2	0
61	x	27	0	22	4	0
62	t	32	0	13	0	0
62	z	32	0	13	2	0
63	A	92	0	0	0	0
63	E	1	0	0	0	0
63	g	1	0	0	0	0
63	t	1	0	0	0	0
63	z	1	0	0	0	0
64	A	10	0	0	0	0
All	All	108702	0	91728	1425	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 7.

All (1425) 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)
25:A:2354:A:N6	25:A:2361:G:H1	1.42	1.18
27:B:1607:U:H3	27:B:1664:G:H1	1.05	1.02
25:A:2351:U:H3	25:A:2362:A:H62	1.11	0.91
25:A:2351:U:H3	25:A:2362:A:N6	1.75	0.85
13:5:126:THR:HG22	13:5:372:ASN:HB2	1.62	0.80
16:6:104:LEU:HD23	16:6:107:LYS:HZ3	1.48	0.79
54:r:70:CYS:N	54:r:73:CYS:SG	2.56	0.78
25:A:1777:A:N6	25:A:1780:U:OP2	2.17	0.77
30:e:51:LEU:HD12	30:e:188:ALA:HB1	1.65	0.77
29:D:296:VAL:HG23	29:D:297:LYS:HG2	1.67	0.77
25:A:2846:G:H2'	25:A:2847:G:C8	2.20	0.75
15:y:248:ILE:HG13	15:y:253:TYR:HB3	1.68	0.75
6:v:17:LEU:HG	9:w:120:MET:HE3	1.69	0.74
45:M:44:ARG:HG3	45:M:45:ARG:HG3	1.70	0.74
25:A:2248:U:OP1	55:R:99:ARG:NH2	2.20	0.74
16:6:160:ASP:OD2	16:6:267:ARG:NH2	2.20	0.73
12:x:153:MET:HB2	12:x:220:TYR:HE1	1.54	0.73
25:A:1737:A:H4'	38:i:97:MET:HE2	1.70	0.73
12:x:103:ILE:HA	12:x:106:TRP:HD1	1.53	0.73
3:u:92:PHE:H	3:u:150:LYS:HE3	1.54	0.72
13:5:106:ILE:HD13	13:5:223:ARG:HH12	1.55	0.72
6:v:9:VAL:HG22	6:v:55:LEU:HD21	1.72	0.72
12:x:42:ARG:HH12	29:D:299:PRO:HD2	1.55	0.72
33:F:188:HIS:HB2	33:F:260:VAL:HG12	1.72	0.72
24:b:126:ILE:O	26:c:310:ASN:ND2	2.24	0.71
9:w:138:LEU:HD11	9:w:144:ILE:HG12	1.72	0.70
9:w:100:VAL:HB	9:w:142:GLN:HB2	1.73	0.70
6:v:45:LEU:HD11	6:v:51:ARG:HB3	1.72	0.70
21:8:114:ARG:HE	21:8:117:LEU:HD21	1.54	0.70
15:y:297:SER:HB3	25:A:2562:U:H4'	1.73	0.70
3:u:150:LYS:NZ	3:u:151:CYS:SG	2.65	0.70
25:A:2976:A:H2'	25:A:2977:A:C8	2.27	0.70
37:I:47:LEU:HD22	47:N:226:ILE:HG12	1.72	0.70
20:Z:77:ARG:O	47:N:228:LYS:NZ	2.24	0.70
24:b:49:ARG:HG3	24:b:50:GLU:HG3	1.74	0.70
25:A:2975:C:H2'	25:A:2976:A:H8	1.58	0.69
34:g:41:SER:OG	45:M:284:LYS:NZ	2.25	0.69
3:u:135:LEU:HG	3:u:179:LEU:HB3	1.74	0.69
8:V:145:ARG:HG3	8:V:154:ILE:HG13	1.73	0.69
25:A:2240:C:H5'	41:K:29:GLY:HA3	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:259:ARG:HB2	26:c:271:PHE:HB2	1.73	0.69
33:F:128:TRP:HB2	33:F:133:THR:HG21	1.74	0.69
56:s:49:ALA:O	56:s:61:ARG:NH1	2.26	0.69
30:e:257:LYS:HD3	30:e:278:ASP:HB2	1.75	0.69
45:M:119:THR:O	45:M:123:ASN:ND2	2.25	0.69
30:e:48:LEU:HB2	30:e:231:VAL:HG12	1.75	0.68
12:x:45:LEU:HD21	12:x:64:ARG:HH21	1.56	0.68
19:7:148:MET:HE2	19:7:262:ASP:HB3	1.74	0.68
25:A:1710:A:H5''	25:A:1711:C:H5'	1.74	0.68
14:X:7:PRO:HD2	14:X:10:LEU:HD12	1.75	0.68
25:A:2576:U:H2'	25:A:2577:A:C8	2.28	0.68
8:V:93:THR:HG22	8:V:112:GLU:HG3	1.76	0.68
25:A:2177:U:O2'	25:A:2180:A:N7	2.24	0.68
53:Q:120:THR:HB	53:Q:173:GLU:HG3	1.76	0.68
16:6:49:GLU:HG3	16:6:52:ARG:HH22	1.59	0.68
35:H:53:THR:N	35:H:86:THR:HG1	1.91	0.68
1:0:96:ASN:OD1	25:A:2739:C:O2'	2.11	0.67
16:6:136:ARG:NH1	16:6:140:GLU:OE2	2.27	0.67
8:V:131:THR:HG21	8:V:152:ARG:HH22	1.57	0.67
18:z:164:ARG:NH1	18:z:171:GLY:O	2.27	0.67
30:e:273:ARG:HA	30:e:276:VAL:HG12	1.76	0.67
13:5:115:GLU:HB2	13:5:119:GLN:HB2	1.77	0.66
19:7:148:MET:HE1	19:7:255:HIS:HB2	1.77	0.66
25:A:2154:A:H5'	48:o:30:ARG:HH21	1.59	0.66
25:A:2975:C:H2'	25:A:2976:A:C8	2.31	0.66
4:1:20:MET:HE1	4:1:41:LEU:HB2	1.78	0.66
25:A:1761:A:OP1	25:A:1887:A:N6	2.29	0.66
1:0:125:TYR:OH	28:d:287:LEU:O	2.14	0.65
8:V:105:ARG:NH1	8:V:106:GLY:O	2.30	0.65
14:X:99:LYS:NZ	25:A:2773:U:O2	2.29	0.65
34:g:87:ARG:HG3	34:g:112:LYS:HE2	1.79	0.65
53:Q:121:THR:HG22	53:Q:171:VAL:HA	1.79	0.65
25:A:2055:U:H2'	25:A:2056:G:H8	1.62	0.65
41:K:27:PRO:HG2	41:K:30:LYS:HB2	1.78	0.65
24:b:28:ARG:NH1	24:b:78:GLU:OE1	2.30	0.64
25:A:2416:U:OP2	56:s:165:ARG:NH2	2.30	0.64
56:s:267:LYS:NZ	56:s:269:ASP:OD2	2.29	0.64
25:A:2016:C:OP2	45:M:59:ARG:NH1	2.31	0.64
25:A:2674:G:O2'	25:A:2676:G:OP2	2.16	0.64
46:m:57:VAL:HG22	46:m:63:THR:HG22	1.78	0.64
25:A:2771:A:N3	25:A:2952:A:O2'	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:5:118:LYS:HD3	13:5:254:GLU:HG3	1.80	0.64
50:p:177:ARG:NH1	51:P:60:SER:OG	2.31	0.64
25:A:2976:A:H2'	25:A:2977:A:H8	1.62	0.64
12:x:70:GLU:O	12:x:371:ASN:ND2	2.31	0.64
18:z:51:CYS:HB3	18:z:146:ILE:HG13	1.80	0.64
11:W:48:GLY:HA3	25:A:2866:C:H5''	1.80	0.63
18:z:49:VAL:HG21	18:z:147:MET:HE3	1.79	0.63
25:A:2081:U:H2'	25:A:2082:G:C8	2.34	0.63
25:A:2754:A:H2'	25:A:2755:G:H8	1.64	0.63
29:D:113:ARG:O	29:D:147:ARG:NH2	2.30	0.63
31:E:69:ASP:OD1	31:E:154:ARG:NH1	2.31	0.63
25:A:1787:G:N2	25:A:1790:A:OP2	2.25	0.63
3:u:197:ARG:NH2	43:L:142:GLN:O	2.31	0.63
45:M:238:ARG:NH2	50:p:71:ASP:OD1	2.32	0.63
56:s:376:THR:HB	56:s:389:ARG:HG3	1.81	0.63
12:x:187:LYS:NZ	61:x:401:SAM:O	2.28	0.63
19:7:276:PHE:HB2	19:7:304:VAL:HG22	1.80	0.63
25:A:3214:U:H3	41:K:177:ARG:HB3	1.63	0.63
2:T:63:ARG:NH1	28:d:228:PHE:O	2.32	0.63
29:D:281:TRP:O	29:D:285:LYS:HB2	1.97	0.63
10:3:108:LYS:NZ	25:A:1745:U:O4	2.31	0.63
25:A:1974:A:H5'	29:D:261:GLY:HA2	1.81	0.63
40:j:24:GLY:HA3	55:R:91:VAL:HG11	1.80	0.63
2:T:143:ARG:O	25:A:1672:C:O2'	2.14	0.62
29:D:126:VAL:HA	29:D:142:VAL:HG12	1.80	0.62
16:6:58:ARG:HH12	51:P:73:PRO:HD3	1.64	0.62
12:x:139:ILE:O	15:y:322:ARG:NH2	2.32	0.62
30:e:90:ARG:NH2	30:e:115:LEU:O	2.32	0.62
16:6:336:ASP:OD1	50:p:129:ARG:NH2	2.30	0.62
53:Q:127:SER:OG	53:Q:129:LYS:NZ	2.33	0.62
24:b:72:VAL:HG13	24:b:90:HIS:HB2	1.80	0.62
15:y:162:ARG:NH1	15:y:191:GLN:OE1	2.32	0.62
56:s:191:HIS:O	56:s:428:ARG:NH2	2.32	0.62
55:R:85:ALA:O	55:R:89:ASN:ND2	2.33	0.62
16:6:346:ARG:NH2	51:P:178:ILE:O	2.33	0.62
3:u:196:LEU:HB3	3:u:199:TYR:HB2	1.81	0.62
32:f:97:ALA:HB3	32:f:103:ALA:HB2	1.82	0.62
17:Y:216:ARG:NH1	25:A:1690:C:O2	2.32	0.61
30:e:55:ARG:HD3	30:e:157:LEU:HD12	1.82	0.61
1:0:145:GLU:OE2	25:A:2321:A:N6	2.33	0.61
25:A:3155:U:H2'	25:A:3156:A:C8	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2576:U:H2'	25:A:2577:A:H8	1.65	0.61
56:s:211:VAL:HG22	56:s:230:ARG:HG2	1.83	0.61
12:x:274:LYS:HD2	12:x:277:ARG:HH12	1.66	0.61
21:8:133:ARG:HH22	32:f:116:SER:HB3	1.64	0.61
50:p:133:LEU:HD21	50:p:157:MET:HE1	1.81	0.61
15:y:91:GLU:HG2	15:y:94:ARG:HH22	1.65	0.61
23:9:129:GLN:OE1	23:9:134:ASN:ND2	2.30	0.61
43:L:100:PHE:HB3	53:Q:158:GLN:HE22	1.64	0.61
3:u:133:ARG:HH11	58:t:195:PHE:HB3	1.66	0.61
8:V:64:ILE:HD11	8:V:88:VAL:HG21	1.83	0.61
12:x:209:ARG:HG2	12:x:212:ARG:HH21	1.64	0.61
19:7:143:TRP:HE1	19:7:172:VAL:HG13	1.66	0.61
25:A:3113:G:N2	25:A:3116:A:OP2	2.26	0.61
43:L:96:MET:HE3	53:Q:168:ASN:HD22	1.64	0.61
43:L:99:ARG:NH2	53:Q:161:GLU:OE1	2.34	0.61
25:A:2860:C:N4	25:A:2869:A:OP2	2.34	0.61
31:E:206:VAL:HG12	31:E:299:VAL:HG22	1.83	0.61
27:B:1621:A:OP1	51:P:113:LYS:NZ	2.32	0.61
25:A:2358:A:H2'	25:A:2361:G:H2'	1.83	0.61
31:E:82:ASP:O	31:E:188:LYS:NZ	2.33	0.61
19:7:79:PHE:HB3	19:7:81:MET:HE2	1.84	0.60
19:7:159:LYS:HD3	22:a:93:LYS:HG2	1.82	0.60
16:6:175:VAL:HG11	16:6:270:PHE:HE2	1.66	0.60
16:6:237:LEU:HB3	16:6:240:ILE:HD11	1.82	0.60
25:A:3155:U:H2'	25:A:3156:A:H8	1.66	0.60
25:A:2351:U:O4	25:A:2362:A:N7	2.34	0.60
5:U:18:ARG:NH1	23:9:59:GLU:OE1	2.35	0.60
25:A:2279:U:OP2	38:i:46:ARG:NH1	2.33	0.60
1:0:105:ASN:ND2	31:E:44:LYS:O	2.34	0.60
25:A:2237:A:OP1	54:r:171:ARG:NH2	2.35	0.60
25:A:2453:G:O2'	49:O:116:ASP:OD2	2.17	0.60
8:V:181:ASP:O	17:Y:93:LYS:NZ	2.34	0.60
25:A:1990:G:OP1	29:D:269:ARG:NH2	2.33	0.60
34:g:115:GLY:HA2	45:M:8:GLY:H	1.66	0.60
50:p:108:ALA:O	50:p:116:ARG:NH1	2.34	0.60
18:z:282:VAL:HG12	25:A:2682:A:H4'	1.82	0.60
25:A:1962:A:OP2	25:A:2501:C:N4	2.35	0.60
19:7:73:THR:OG1	19:7:99:TYR:OH	2.20	0.60
25:A:2069:U:H1'	25:A:2071:U:H1'	1.84	0.60
50:p:163:GLN:HG3	50:p:165:PRO:HD3	1.84	0.60
16:6:123:ALA:HA	51:P:123:VAL:HG21	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:p:184:ASN:ND2	51:P:142:ASN:OD1	2.35	0.59
16:6:252:CYS:SG	16:6:296:ARG:NH1	2.74	0.59
25:A:2562:U:H2'	25:A:2563:A:C8	2.37	0.59
19:7:243:LYS:NZ	19:7:265:GLU:OE1	2.35	0.59
26:c:105:ARG:NH2	26:c:115:VAL:O	2.34	0.59
12:x:271:ASN:O	12:x:277:ARG:NH1	2.35	0.59
25:A:2236:C:OP1	54:r:164:LYS:NZ	2.34	0.59
21:8:129:ARG:HG2	27:B:1627:C:H5''	1.85	0.59
20:Z:71:ARG:NH2	20:Z:92:GLU:O	2.35	0.59
25:A:2961:U:H2'	25:A:2962:A:H8	1.68	0.59
28:d:267:PRO:HG2	28:d:270:ALA:HB2	1.85	0.59
13:5:274:LYS:NZ	13:5:275:ASN:O	2.35	0.59
25:A:1886:G:N7	33:F:170:ARG:NH2	2.50	0.59
25:A:3158:G:N2	25:A:3161:A:OP2	2.36	0.59
5:U:79:ARG:NH1	25:A:2366:G:OP1	2.30	0.59
13:5:229:ARG:NH1	13:5:231:SER:OG	2.36	0.59
25:A:2771:A:H2'	25:A:2772:A:C8	2.38	0.59
33:F:215:SER:N	33:F:257:GLN:OE1	2.34	0.59
19:7:175:ILE:O	19:7:319:ARG:NH2	2.36	0.59
26:c:262:GLY:HA2	41:K:140:ASN:HB2	1.85	0.59
30:e:151:ARG:NH2	30:e:254:TRP:O	2.35	0.59
31:E:221:ARG:HA	31:E:261:MET:HE2	1.84	0.59
46:m:51:LEU:HB3	46:m:67:ARG:HB3	1.84	0.59
18:z:35:MET:HB2	18:z:206:VAL:HG22	1.85	0.58
25:A:2360:U:H3'	25:A:2361:G:H4'	1.84	0.58
12:x:153:MET:HB2	12:x:220:TYR:CE1	2.36	0.58
25:A:3107:A:N1	25:A:3124:C:N4	2.51	0.58
27:B:1672:C:O2'	30:e:216:LYS:O	2.20	0.58
16:6:221:LEU:HB2	16:6:267:ARG:HG3	1.85	0.58
18:z:64:GLY:HA3	18:z:220:LEU:HD21	1.85	0.58
21:8:110:GLU:OE2	21:8:114:ARG:NH1	2.35	0.58
5:U:150:TRP:O	28:d:264:LYS:NZ	2.28	0.58
25:A:2065:A:OP1	32:f:48:TYR:N	2.35	0.58
21:8:178:TYR:O	30:e:136:ARG:NH1	2.36	0.58
25:A:2067:C:H4'	32:f:60:LYS:HD3	1.85	0.58
37:I:52:GLU:O	47:N:211:ASN:ND2	2.36	0.58
48:o:29:LEU:O	48:o:33:GLN:HG2	2.04	0.58
20:Z:77:ARG:NH1	25:A:2139:U:O4	2.37	0.58
12:x:67:LEU:HD23	12:x:262:ARG:HH21	1.69	0.58
17:Y:162:ARG:HH22	25:A:1693:C:H42	1.50	0.58
34:g:110:ILE:HD11	34:g:157:LEU:HD13	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:Q:182:ARG:HG3	53:Q:187:LEU:HD11	1.85	0.58
18:z:29:ARG:NH2	25:A:3077:C:O3'	2.37	0.58
19:7:205:ASP:OD2	22:a:95:ARG:NH2	2.36	0.58
25:A:1822:U:O2	25:A:2738:A:O2'	2.22	0.58
55:R:90:LEU:HD12	55:R:95:VAL:HB	1.86	0.58
58:t:99:THR:HG22	58:t:105:ILE:HA	1.85	0.58
20:Z:71:ARG:NH1	20:Z:73:LYS:O	2.36	0.57
25:A:1814:A:N3	25:A:1862:U:O2'	2.37	0.57
58:t:117:LEU:HD21	58:t:120:GLN:HG2	1.85	0.57
14:X:136:ASP:OD2	35:H:120:ARG:NH2	2.36	0.57
19:7:286:LEU:HB2	19:7:294:ILE:HB	1.86	0.57
25:A:2387:U:O2'	25:A:2406:A:N7	2.37	0.57
25:A:3044:G:H1	25:A:3055:U:H3	1.52	0.57
16:6:150:ARG:NH1	51:P:104:SER:OG	2.34	0.57
22:a:73:LYS:NZ	24:b:142:GLY:O	2.37	0.57
41:K:169:LEU:HD21	54:r:77:LEU:HD12	1.87	0.57
16:6:99:ARG:NH2	27:B:1621:A:O5'	2.37	0.57
56:s:63:ILE:HA	56:s:66:TRP:CD1	2.38	0.57
41:K:25:MET:O	41:K:149:ARG:NH1	2.37	0.57
20:Z:82:GLU:HG3	20:Z:113:VAL:HG12	1.85	0.57
22:a:97:GLU:N	22:a:97:GLU:OE1	2.38	0.57
15:y:112:LEU:HD21	15:y:128:ILE:HD11	1.87	0.57
25:A:2283:C:H4'	25:A:2284:C:H5''	1.86	0.57
25:A:2754:A:H2'	25:A:2755:G:C8	2.40	0.57
1:0:98:GLN:OE1	25:A:2740:A:O2'	2.22	0.57
24:b:74:ARG:NH1	25:A:2284:C:OP2	2.35	0.57
25:A:3183:C:OP1	53:Q:141:SER:OG	2.21	0.57
15:y:237:ALA:HB1	15:y:243:ILE:HD11	1.86	0.57
25:A:2961:U:H2'	25:A:2962:A:C8	2.40	0.57
50:p:111:ILE:HB	50:p:116:ARG:HD3	1.86	0.57
25:A:2550:U:H2'	25:A:2551:A:H8	1.70	0.56
52:q:37:PRO:HG2	52:q:68:SER:HA	1.86	0.56
16:6:198:ALA:O	16:6:254:TYR:OH	2.22	0.56
16:6:206:TYR:HH	16:6:214:TRP:CD1	2.22	0.56
52:q:102:SER:OG	52:q:106:LYS:NZ	2.38	0.56
2:T:127:ASN:O	28:d:230:ARG:NH2	2.39	0.56
13:5:140:VAL:O	13:5:146:HIS:NE2	2.28	0.56
21:8:173:LYS:NZ	21:8:174:GLU:O	2.38	0.56
28:d:181:VAL:HG22	28:d:224:ILE:HG12	1.85	0.56
53:Q:155:ILE:HG22	53:Q:156:GLU:HG2	1.87	0.56
13:5:289:HIS:ND1	13:5:290:THR:OG1	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2294:A:OP2	45:M:39:ARG:NH2	2.38	0.56
25:A:2339:G:H21	25:A:2427:C:H5'	1.70	0.56
25:A:2351:U:N3	25:A:2362:A:N6	2.42	0.56
25:A:3114:U:OP1	29:D:297:LYS:NZ	2.34	0.56
35:H:117:SER:O	35:H:121:ASN:ND2	2.36	0.56
53:Q:205:LYS:HD3	53:Q:206:PRO:HD2	1.86	0.56
54:r:149:ARG:HD3	54:r:152:THR:HG21	1.87	0.56
2:T:69:HIS:NE2	2:T:117:GLU:OE2	2.35	0.56
19:7:114:ASP:HB2	19:7:117:LYS:HB2	1.87	0.56
25:A:1698:C:O2'	25:A:1702:A:N3	2.37	0.56
26:c:245:LEU:HD12	26:c:253:PRO:HD3	1.87	0.56
53:Q:148:THR:HG22	53:Q:165:GLU:HG2	1.88	0.56
18:z:42:MET:HE1	18:z:203:THR:HB	1.88	0.56
25:A:1747:G:N2	25:A:1750:G:O2'	2.38	0.56
25:A:2039:A:N6	25:A:2760:U:O2	2.38	0.56
25:A:1800:G:N1	25:A:1803:A:OP2	2.37	0.56
26:c:139:GLN:NE2	26:c:143:ASP:OD2	2.39	0.56
28:d:50:PHE:HA	28:d:53:GLU:HG3	1.86	0.56
51:P:102:VAL:HG12	51:P:103:VAL:HG13	1.88	0.56
19:7:269:ILE:HD12	19:7:274:ILE:HB	1.87	0.56
25:A:1882:A:N6	25:A:1893:A:O4'	2.39	0.56
25:A:3142:A:H2'	25:A:3143:A:H5''	1.88	0.56
13:5:100:LYS:NZ	13:5:271:TYR:O	2.36	0.56
14:X:87:LEU:O	35:H:78:ARG:NH1	2.39	0.56
25:A:2468:A:H61	25:A:2690:C:H42	1.52	0.56
26:c:44:GLU:HG3	55:R:19:PHE:HE1	1.71	0.56
50:p:60:ARG:HH12	50:p:62:PRO:HA	1.71	0.56
5:U:21:ARG:HH12	17:Y:143:ASP:HA	1.71	0.56
27:B:1630:A:OP1	46:m:42:ARG:NH2	2.32	0.56
56:s:242:ARG:NH1	56:s:290:ASP:OD2	2.37	0.56
2:T:57:LEU:N	2:T:60:GLU:OE2	2.38	0.55
13:5:166:THR:O	56:s:287:LYS:NZ	2.32	0.55
60:w:200:PM8:O40	60:w:200:PM8:N36	2.39	0.55
22:a:134:LYS:NZ	25:A:1835:A:O2'	2.38	0.55
5:U:7:TYR:O	17:Y:183:GLN:NE2	2.40	0.55
25:A:2835:A:H2'	25:A:2836:A:H8	1.70	0.55
30:e:201:GLU:OE2	30:e:240:THR:OG1	2.24	0.55
1:0:139:ARG:NH1	25:A:2322:C:OP1	2.40	0.55
19:7:112:PRO:HB2	19:7:267:PRO:HG2	1.87	0.55
25:A:2086:A:H2'	25:A:2087:U:C6	2.42	0.55
41:K:20:LEU:HD11	41:K:60:MET:HE3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:K:22:ASP:HB3	41:K:147:GLN:HE21	1.72	0.55
33:F:70:ARG:HA	33:F:196:PRO:HD3	1.89	0.55
49:O:16:ARG:NH2	49:O:50:ASP:OD2	2.40	0.55
24:b:48:GLU:OE2	48:o:101:TRP:NE1	2.38	0.55
25:A:2262:C:OP2	57:S:173:ARG:NH1	2.40	0.55
25:A:2699:A:H2'	25:A:2700:A:C8	2.41	0.55
18:z:171:GLY:HA2	25:A:2667:G:H5''	1.89	0.55
25:A:2782:G:H2'	25:A:2783:C:C6	2.42	0.55
25:A:2998:C:H2'	25:A:2999:A:O4'	2.07	0.55
40:j:49:TRP:HB3	57:S:101:PHE:HE2	1.71	0.55
56:s:271:LEU:HD23	56:s:273:LEU:HD13	1.88	0.55
3:u:182:PRO:HA	3:u:185:ARG:HD3	1.88	0.55
5:U:143:ARG:HG2	19:7:80:VAL:HG21	1.88	0.55
37:I:47:LEU:O	37:I:51:THR:HG22	2.06	0.55
25:A:1697:A:N3	25:A:1703:C:O2'	2.40	0.55
25:A:1884:G:N3	25:A:1895:C:O2'	2.40	0.55
25:A:2346:U:OP1	56:s:223:ARG:NH2	2.39	0.55
32:f:81:ASN:HD22	32:f:90:VAL:HG23	1.72	0.55
35:H:134:PRO:HA	35:H:137:LYS:HG2	1.89	0.55
5:U:23:ASN:HB3	23:9:137:ARG:NH1	2.21	0.55
18:z:42:MET:HB2	18:z:73:LEU:HD11	1.88	0.55
25:A:2354:A:N1	25:A:2361:G:N2	2.43	0.55
25:A:3250:G:O2'	25:A:3253:C:N4	2.37	0.55
27:B:1628:C:H2'	27:B:1629:A:H8	1.72	0.55
32:f:101:THR:HG21	46:m:43:VAL:HG22	1.88	0.55
16:6:114:ARG:NH2	27:B:1643:A:OP1	2.40	0.54
16:6:224:HIS:CE1	16:6:227:GLU:H	2.25	0.54
24:b:136:LYS:O	26:c:259:ARG:NH2	2.35	0.54
25:A:1737:A:N6	25:A:1760:G:H1'	2.22	0.54
52:q:146:ALA:O	52:q:150:LYS:HG2	2.07	0.54
5:U:146:GLY:O	28:d:179:LYS:NZ	2.40	0.54
6:v:23:LEU:HG	6:v:70:ILE:HA	1.89	0.54
9:w:100:VAL:HA	9:w:141:PRO:HG2	1.89	0.54
9:w:103:HIS:ND1	9:w:106:LYS:HG2	2.23	0.54
12:x:72:LYS:H	12:x:371:ASN:HB3	1.70	0.54
19:7:150:MET:HE2	19:7:280:VAL:HG12	1.89	0.54
20:Z:88:MET:HE3	25:A:2082:G:H21	1.72	0.54
25:A:2187:C:H2'	25:A:2188:A:C8	2.42	0.54
25:A:2987:A:N6	25:A:2999:A:O2'	2.39	0.54
26:c:42:GLN:NE2	38:i:36:LEU:O	2.40	0.54
27:B:1643:A:H62	51:P:120:ARG:HH12	1.54	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:E:275:ARG:NH1	31:E:331:ASP:OD2	2.40	0.54
3:u:189:GLU:O	43:L:118:ARG:NH2	2.39	0.54
3:u:208:PRO:HA	43:L:120:LYS:HE3	1.89	0.54
35:H:99:THR:HA	35:H:108:ARG:HG3	1.89	0.54
3:u:147:LYS:NZ	25:A:3154:G:OP2	2.39	0.54
12:x:81:ALA:HA	12:x:150:LEU:HD22	1.88	0.54
34:g:41:SER:OG	34:g:44:GLU:OE2	2.19	0.54
6:v:18:ARG:HH22	9:w:120:MET:HG3	1.72	0.54
24:b:145:PRO:HB3	41:K:144:GLU:HB2	1.88	0.54
25:A:2115:U:O2'	25:A:2869:A:N6	2.33	0.54
25:A:2853:C:O2'	25:A:2946:C:OP2	2.26	0.54
28:d:86:ASP:HB3	28:d:198:ARG:HD2	1.90	0.54
31:E:99:LEU:HD13	31:E:124:VAL:HG21	1.89	0.54
50:p:77:LEU:HD13	50:p:103:PHE:HB3	1.88	0.54
21:8:163:LYS:NZ	32:f:85:ASP:OD1	2.31	0.54
37:I:45:GLN:NE2	48:o:25:ARG:O	2.37	0.54
45:M:180:ASP:OD1	45:M:183:SER:OG	2.19	0.54
58:t:57:GLN:O	58:t:61:ARG:HG2	2.07	0.54
8:V:23:MET:HE2	8:V:114:PRO:HG3	1.89	0.54
9:w:103:HIS:CE1	9:w:105:MET:HB2	2.43	0.54
12:x:79:ASN:N	12:x:193:GLN:OE1	2.39	0.54
25:A:2365:U:H2'	25:A:2366:G:H8	1.71	0.54
25:A:3043:U:H2'	25:A:3044:G:H8	1.73	0.54
14:X:114:PHE:HE2	14:X:127:VAL:HG11	1.73	0.54
17:Y:83:ALA:N	23:9:74:VAL:O	2.37	0.54
41:K:28:PRO:HG3	41:K:65:ILE:HD12	1.89	0.54
51:P:55:ASN:OD1	51:P:56:LEU:N	2.39	0.54
53:Q:233:TRP:HB3	53:Q:240:ILE:HD12	1.89	0.54
11:W:148:LEU:OXT	16:6:339:GLU:N	2.40	0.54
16:6:225:LEU:HB3	51:P:44:VAL:HG13	1.89	0.54
45:M:244:LEU:HD12	45:M:245:PRO:HD2	1.90	0.54
6:v:63:ASN:O	6:v:68:ARG:NH2	2.41	0.54
25:A:1789:A:N3	25:A:1915:C:O2'	2.40	0.54
25:A:1936:A:H1'	25:A:1938:A:C6	2.43	0.54
25:A:2467:A:O2'	25:A:3185:U:H4'	2.08	0.54
45:M:255:MET:O	45:M:258:THR:OG1	2.27	0.54
8:V:48:PRO:HD3	17:Y:234:LEU:HD21	1.89	0.53
18:z:164:ARG:HG2	18:z:192:VAL:HA	1.90	0.53
4:1:19:ARG:NH1	25:A:2937:C:N3	2.55	0.53
12:x:181:CYS:HB3	61:x:401:SAM:H5'2	1.89	0.53
19:7:180:CYS:SG	19:7:296:ARG:NH1	2.81	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1676:A:H4'	38:i:35:ARG:HA	1.90	0.53
14:X:55:LYS:NZ	25:A:1746:A:OP1	2.33	0.53
19:7:275:CYS:HA	19:7:303:PRO:HA	1.89	0.53
25:A:1862:U:H2'	25:A:1863:A:H8	1.73	0.53
28:d:152:LEU:HD21	28:d:172:MET:HE2	1.91	0.53
34:g:44:GLU:HG2	45:M:282:ILE:HD12	1.90	0.53
35:H:138:LYS:O	35:H:141:GLU:HG2	2.08	0.53
49:O:68:THR:HA	56:s:42:ALA:HB2	1.89	0.53
24:b:48:GLU:OE2	36:h:139:LYS:NZ	2.39	0.53
25:A:1992:C:C4	29:D:274:ARG:HB2	2.43	0.53
25:A:2855:C:O2'	25:A:2924:A:O2'	2.22	0.53
31:E:216:GLN:HG3	31:E:261:MET:HE3	1.90	0.53
32:f:179:PRO:HD2	32:f:182:VAL:HG21	1.90	0.53
8:V:144:VAL:HG21	8:V:153:ILE:HD12	1.91	0.53
9:w:93:ILE:HB	9:w:108:LEU:HD23	1.90	0.53
9:w:116:VAL:HG12	9:w:120:MET:HE1	1.89	0.53
14:X:227:PHE:HE1	23:9:96:VAL:HG21	1.73	0.53
16:6:218:LEU:HG	16:6:234:HIS:HB2	1.91	0.53
16:6:323:TRP:NE1	16:6:339:GLU:OE2	2.41	0.53
27:B:1622:A:H2'	27:B:1623:G:C8	2.43	0.53
28:d:88:TYR:HB2	28:d:198:ARG:HH22	1.73	0.53
8:V:52:GLU:O	8:V:143:ARG:NH2	2.41	0.53
10:3:188:VAL:O	16:6:356:ARG:NH2	2.38	0.53
16:6:215:THR:HG1	16:6:275:GLN:HE21	1.54	0.53
33:F:114:THR:O	33:F:156:ARG:NH1	2.41	0.53
16:6:109:ALA:O	16:6:112:GLU:HG2	2.09	0.53
25:A:3222:A:H4'	54:r:123:HIS:HB3	1.90	0.53
14:X:96:LYS:O	25:A:1728:U:O2'	2.21	0.53
19:7:64:LYS:HD2	19:7:80:VAL:HG12	1.91	0.53
25:A:1883:G:H5'	34:g:91:MET:HG3	1.91	0.53
25:A:1917:A:N1	25:A:1997:C:H1'	2.23	0.53
25:A:2456:U:OP1	49:O:16:ARG:NH1	2.41	0.53
25:A:2985:C:H41	25:A:3001:C:N4	2.07	0.53
6:v:12:LEU:HD11	6:v:59:LEU:HD22	1.91	0.53
12:x:296:LEU:HD23	12:x:305:VAL:HG21	1.91	0.53
16:6:222:ASP:OD2	16:6:267:ARG:NH1	2.42	0.53
25:A:1749:C:OP2	25:A:2930:C:O2'	2.27	0.53
25:A:2994:A:H5''	25:A:2995:U:OP1	2.09	0.53
34:g:118:TRP:NE1	34:g:142:GLU:OE2	2.37	0.53
45:M:156:VAL:O	45:M:176:THR:HA	2.09	0.53
45:M:234:LEU:HD21	50:p:61:VAL:HG13	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:u:117:GLU:N	3:u:117:GLU:OE1	2.41	0.52
12:x:178:LEU:HB2	12:x:249:TYR:CD2	2.44	0.52
25:A:2533:A:H2'	25:A:2534:G:H8	1.74	0.52
25:A:2771:A:H2'	25:A:2772:A:H8	1.73	0.52
25:A:1678:C:OP1	38:i:35:ARG:NH2	2.42	0.52
32:f:97:ALA:HB2	32:f:182:VAL:HG12	1.89	0.52
8:V:64:ILE:HA	8:V:120:VAL:HG12	1.92	0.52
15:y:166:LEU:HD13	15:y:176:LEU:HD21	1.92	0.52
15:y:290:LEU:HA	15:y:293:ILE:HG22	1.91	0.52
18:z:111:THR:OG1	18:z:117:GLU:O	2.22	0.52
25:A:2786:A:OP2	35:H:91:LYS:NZ	2.41	0.52
25:A:3174:U:H2'	25:A:3175:A:H8	1.74	0.52
12:x:141:ARG:HH22	15:y:322:ARG:HD3	1.74	0.52
15:y:236:TYR:OH	15:y:265:HIS:ND1	2.26	0.52
19:7:114:ASP:OD1	19:7:114:ASP:N	2.42	0.52
35:H:140:PHE:O	35:H:143:GLU:HG3	2.09	0.52
23:9:114:LEU:HD23	23:9:117:TYR:HD2	1.75	0.52
35:H:104:ASN:OD1	35:H:105:VAL:N	2.43	0.52
13:5:208:THR:OG1	56:s:160:ARG:NH1	2.38	0.52
47:N:231:SER:HB3	47:N:234:ASP:HB2	1.92	0.52
51:P:158:MET:O	51:P:162:GLN:HG2	2.10	0.52
3:u:101:LEU:HA	3:u:104:GLU:HB2	1.91	0.52
47:N:221:ALA:HB1	48:o:46:HIS:HE1	1.75	0.52
51:P:107:THR:HA	51:P:112:ILE:HD11	1.92	0.52
2:T:143:ARG:NH1	25:A:1673:U:O2'	2.43	0.52
45:M:261:ASP:HB3	45:M:264:GLN:HB2	1.91	0.52
12:x:83:TRP:HE1	52:q:153:ARG:HG3	1.74	0.52
25:A:2733:G:H5'	41:K:114:LYS:HE2	1.92	0.52
32:f:136:GLN:HG2	46:m:78:PRO:HG3	1.92	0.52
35:H:53:THR:N	35:H:86:THR:OG1	2.43	0.52
16:6:87:LYS:HD3	16:6:166:THR:HG21	1.92	0.52
25:A:3074:C:O2'	25:A:3075:A:H5''	2.10	0.52
26:c:151:GLU:O	26:c:155:ASN:ND2	2.37	0.52
30:e:53:LEU:HD23	30:e:159:LEU:HD22	1.92	0.52
3:u:132:THR:O	3:u:136:HIS:ND1	2.34	0.51
4:1:63:ARG:NH1	25:A:2940:G:OP1	2.34	0.51
13:5:56:GLU:OE1	13:5:56:GLU:N	2.39	0.51
29:D:289:LEU:HB3	29:D:291:PRO:HD2	1.91	0.51
49:O:80:LEU:HD12	49:O:86:ILE:HG12	1.92	0.51
56:s:63:ILE:HA	56:s:66:TRP:HD1	1.76	0.51
14:X:92:ALA:O	14:X:98:SER:OG	2.27	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:y:314:GLN:HG3	15:y:317:LYS:HZ1	1.73	0.51
19:7:249:GLU:HB3	19:7:251:ILE:HG12	1.92	0.51
25:A:2056:G:H2'	25:A:2057:C:H6	1.74	0.51
25:A:3108:C:H2'	25:A:3109:C:C6	2.45	0.51
26:c:91:ALA:O	26:c:122:ASN:ND2	2.34	0.51
31:E:50:ASP:O	49:O:138:ARG:NH2	2.44	0.51
15:y:242:GLY:HA3	15:y:277:PRO:HG2	1.92	0.51
25:A:1719:G:H2'	25:A:1720:C:H6	1.75	0.51
50:p:100:GLU:HB3	50:p:136:THR:HG22	1.93	0.51
53:Q:123:ASP:HB3	53:Q:126:ALA:HB3	1.91	0.51
12:x:178:LEU:HD22	12:x:249:TYR:HD2	1.76	0.51
19:7:81:MET:HE1	19:7:94:HIS:CD2	2.45	0.51
25:A:1868:G:H2'	45:M:40:PRO:HG3	1.92	0.51
41:K:154:ARG:HG2	54:r:127:LEU:HA	1.91	0.51
55:R:148:TYR:OH	57:S:146:LYS:O	2.26	0.51
3:u:123:TYR:HB2	3:u:175:MET:HG3	1.92	0.51
25:A:2186:C:O2'	25:A:2187:C:OP1	2.27	0.51
25:A:2245:A:H4'	25:A:2246:A:OP1	2.11	0.51
25:A:2682:A:H2'	25:A:2683:G:C8	2.45	0.51
56:s:164:HIS:O	56:s:168:GLU:HG2	2.10	0.51
11:W:65:ASN:OD1	25:A:2891:G:O2'	2.20	0.51
15:y:139:GLU:HG3	15:y:140:PRO:HD3	1.93	0.51
15:y:293:ILE:HG23	15:y:294:LEU:HG	1.92	0.51
21:8:157:LEU:HA	21:8:160:GLU:HG2	1.93	0.51
25:A:1911:C:H2'	25:A:1912:A:H8	1.75	0.51
25:A:2472:A:O2'	25:A:2478:G:N7	2.32	0.51
18:z:46:LEU:O	18:z:76:LYS:NZ	2.42	0.51
25:A:2458:A:O2'	31:E:215:PHE:O	2.28	0.51
27:B:1622:A:H2'	27:B:1623:G:H8	1.74	0.51
45:M:14:ASP:OD1	45:M:15:LEU:N	2.44	0.51
16:6:260:ALA:O	16:6:263:SER:OG	2.28	0.51
25:A:2015:G:N2	25:A:2038:U:OP1	2.44	0.51
31:E:244:ALA:HB1	31:E:248:ILE:HD11	1.93	0.51
53:Q:278:ILE:O	53:Q:282:ILE:HG12	2.10	0.51
30:e:78:GLU:O	30:e:82:SER:OG	2.17	0.51
33:F:220:ASP:OD1	33:F:221:LEU:N	2.44	0.51
33:F:231:VAL:HG23	52:q:26:ARG:HD2	1.91	0.51
33:F:237:LEU:O	52:q:25:TYR:N	2.44	0.51
12:x:76:LEU:HD21	12:x:193:GLN:HG3	1.92	0.51
13:5:173:ARG:NH2	25:A:2395:A:OP1	2.44	0.51
14:X:36:ARG:H	14:X:36:ARG:HD3	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2985:C:H41	25:A:3001:C:H42	1.59	0.51
26:c:309:GLU:N	26:c:309:GLU:OE1	2.42	0.51
33:F:223:HIS:HA	33:F:226:MET:HE3	1.92	0.51
13:5:204:VAL:HG11	13:5:279:PHE:HZ	1.76	0.50
21:8:121:TRP:CE2	30:e:70:MET:HG2	2.46	0.50
25:A:2177:U:N3	25:A:2180:A:OP2	2.40	0.50
25:A:2768:U:OP1	29:D:278:LYS:NZ	2.44	0.50
25:A:2988:G:H2'	25:A:2989:A:C8	2.45	0.50
36:h:82:LEU:HD23	36:h:89:ILE:HD11	1.93	0.50
41:K:72:TRP:NE1	54:r:148:ASN:O	2.40	0.50
50:p:84:SER:OG	50:p:96:ASN:O	2.28	0.50
8:V:102:MET:SD	8:V:102:MET:N	2.83	0.50
25:A:1863:A:H2'	25:A:1864:A:C8	2.46	0.50
25:A:3085:G:H2'	25:A:3086:U:C6	2.46	0.50
25:A:3177:G:N2	31:E:268:GLU:OE2	2.33	0.50
25:A:3203:C:O2'	25:A:3204:G:N2	2.44	0.50
25:A:3205:U:H2'	25:A:3206:A:H8	1.76	0.50
16:6:215:THR:OG1	16:6:275:GLN:NE2	2.34	0.50
16:6:302:ASP:OD1	16:6:306:LYS:NZ	2.42	0.50
17:Y:197:LYS:NZ	25:A:1699:C:OP2	2.34	0.50
53:Q:152:ARG:NH1	53:Q:161:GLU:OE2	2.43	0.50
55:R:95:VAL:HG12	55:R:97:LEU:HG	1.93	0.50
24:b:127:GLN:OE1	55:R:111:LYS:HB2	2.11	0.50
25:A:3071:G:H4'	25:A:3072:U:OP1	2.11	0.50
31:E:66:SER:OG	31:E:70:LYS:NZ	2.45	0.50
56:s:246:GLN:NE2	56:s:354:PRO:O	2.44	0.50
8:V:80:ILE:HD12	8:V:85:TRP:HE3	1.76	0.50
11:W:103:VAL:HG11	16:6:61:ALA:HB1	1.94	0.50
15:y:155:PRO:HB2	15:y:158:GLN:HG2	1.92	0.50
16:6:175:VAL:HG22	16:6:204:VAL:HG22	1.92	0.50
25:A:2127:A:H4'	25:A:2251:A:C5	2.45	0.50
12:x:297:LEU:HD21	12:x:332:TYR:HD2	1.77	0.50
14:X:20:ILE:HG23	14:X:212:ILE:HD12	1.92	0.50
15:y:302:LEU:HA	15:y:306:ALA:HB3	1.93	0.50
25:A:1761:A:H1'	25:A:1762:A:C8	2.47	0.50
25:A:2310:G:N2	25:A:2707:A:OP2	2.38	0.50
50:p:178:ILE:O	50:p:181:GLU:HG2	2.11	0.50
58:t:48:VAL:HG22	58:t:115:ARG:HG2	1.92	0.50
3:u:167:TRP:HD1	3:u:168:LEU:H	1.60	0.50
5:U:114:LYS:O	5:U:117:SER:OG	2.25	0.50
15:y:95:VAL:HG11	15:y:121:LEU:HG	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:z:72:THR:HG22	18:z:73:LEU:HD13	1.94	0.50
19:7:194:PRO:HG2	19:7:283:VAL:HG21	1.94	0.50
20:Z:35:LYS:N	25:A:2103:A:HO2'	2.10	0.50
24:b:89:ILE:HA	24:b:92:LYS:HD2	1.94	0.50
25:A:1911:C:H2'	25:A:1912:A:C8	2.47	0.50
25:A:2100:C:H1'	25:A:2135:A:C8	2.47	0.50
38:i:69:HIS:HB3	38:i:72:GLU:HG3	1.93	0.50
2:T:44:LYS:O	2:T:48:LYS:HG3	2.12	0.50
25:A:2115:U:H2'	25:A:2116:C:C6	2.47	0.50
25:A:2752:G:N2	25:A:2753:A:O4'	2.45	0.50
29:D:109:PHE:HB3	29:D:204:ALA:HB3	1.94	0.50
3:u:104:GLU:HG3	3:u:138:MET:HG2	1.93	0.50
10:3:163:THR:HG23	10:3:165:PHE:H	1.77	0.50
13:5:126:THR:HG21	13:5:357:PHE:CE1	2.47	0.50
14:X:156:LYS:NZ	14:X:205:GLY:O	2.45	0.50
16:6:150:ARG:HD2	51:P:101:VAL:HG13	1.92	0.50
16:6:304:TYR:O	16:6:308:GLN:HB3	2.12	0.50
9:w:103:HIS:CE1	9:w:105:MET:HE2	2.47	0.49
12:x:252:VAL:HG13	12:x:305:VAL:HG13	1.93	0.49
23:9:24:LYS:NZ	25:A:2422:U:OP2	2.45	0.49
25:A:2042:U:OP1	45:M:62:ARG:NH2	2.43	0.49
25:A:2240:C:O3'	41:K:30:LYS:NZ	2.45	0.49
25:A:2472:A:N3	25:A:2474:C:N4	2.60	0.49
25:A:2548:U:H2'	25:A:2549:A:H8	1.77	0.49
25:A:2778:U:H2'	25:A:2779:A:H8	1.77	0.49
45:M:111:ASP:OD2	45:M:113:SER:OG	2.25	0.49
56:s:232:GLN:NE2	56:s:234:ASP:OD1	2.45	0.49
4:1:16:ILE:HG23	4:1:36:ARG:HG2	1.93	0.49
6:v:48:ALA:HA	6:v:51:ARG:HG2	1.93	0.49
25:A:3222:A:HO2'	54:r:123:HIS:HD1	1.58	0.49
27:B:1664:G:H2'	27:B:1665:C:H6	1.77	0.49
31:E:221:ARG:HG3	31:E:261:MET:HG3	1.94	0.49
13:5:113:LEU:HD12	13:5:311:ALA:HB1	1.94	0.49
25:A:2392:U:H2'	25:A:2394:A:H62	1.77	0.49
25:A:3039:C:O2'	25:A:3082:A:N3	2.41	0.49
33:F:72:PHE:HA	33:F:206:LEU:HD13	1.94	0.49
34:g:77:ASP:OD1	34:g:77:ASP:N	2.45	0.49
53:Q:221:LYS:NZ	53:Q:241:LYS:O	2.37	0.49
12:x:247:ASP:HA	12:x:300:LYS:HA	1.94	0.49
21:8:145:GLU:O	21:8:148:GLU:HG2	2.12	0.49
25:A:1756:A:H2'	25:A:1757:A:H8	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:3182:A:N1	25:A:3194:G:O2'	2.40	0.49
52:q:112:GLN:OE1	52:q:115:ARG:NH2	2.46	0.49
1:0:142:GLY:HA2	1:0:145:GLU:HG2	1.94	0.49
16:6:302:ASP:HA	16:6:305:LYS:HB3	1.94	0.49
25:A:2244:U:O3'	54:r:189:ARG:NH1	2.45	0.49
41:K:69:GLY:HA2	54:r:152:THR:HA	1.95	0.49
8:V:60:ASP:OD2	8:V:145:ARG:NH2	2.45	0.49
11:W:120:LEU:HD23	32:f:63:ILE:HD11	1.95	0.49
12:x:79:ASN:OD1	12:x:130:ARG:NH1	2.45	0.49
13:5:106:ILE:HD13	13:5:223:ARG:NH1	2.23	0.49
13:5:125:LYS:HA	13:5:253:LEU:HD11	1.94	0.49
15:y:206:LEU:HD13	29:D:284:ARG:HA	1.95	0.49
19:7:166:LEU:HD23	19:7:183:VAL:HG13	1.95	0.49
34:g:96:VAL:HG22	34:g:110:ILE:HG12	1.93	0.49
12:x:67:LEU:HB3	12:x:265:LEU:HD12	1.95	0.49
24:b:80:LEU:HD11	26:c:78:ARG:HD3	1.95	0.49
25:A:2993:C:OP1	25:A:2995:U:O2'	2.24	0.49
48:o:68:ARG:O	48:o:72:GLU:HG2	2.12	0.49
7:2:85:LYS:NZ	25:A:1792:G:OP2	2.45	0.49
15:y:133:LEU:HG	29:D:225:ILE:HD11	1.94	0.49
25:A:2318:A:H2'	25:A:2319:A:C8	2.48	0.49
25:A:2562:U:H2'	25:A:2563:A:H8	1.76	0.49
18:z:272:VAL:O	18:z:276:LEU:HG	2.13	0.49
25:A:2532:U:H2'	25:A:2533:A:H8	1.77	0.49
25:A:3181:U:C2	25:A:3182:A:C8	3.01	0.49
12:x:182:ALA:HB1	12:x:188:THR:HG21	1.94	0.49
15:y:168:LYS:HG2	29:D:232:ARG:NH2	2.28	0.49
19:7:87:THR:O	19:7:90:SER:OG	2.21	0.49
24:b:127:GLN:NE2	55:R:109:GLU:OE2	2.46	0.49
25:A:2723:G:N1	25:A:2727:A:OP2	2.41	0.49
14:X:44:ARG:HD3	35:H:55:ILE:HD13	1.95	0.48
16:6:218:LEU:HD13	16:6:270:PHE:CE1	2.47	0.48
20:Z:86:ILE:HG23	20:Z:91:LEU:HB2	1.95	0.48
25:A:1737:A:H61	25:A:1760:G:H1'	1.76	0.48
25:A:2957:A:O2'	25:A:3118:C:OP1	2.20	0.48
28:d:186:VAL:HG23	28:d:219:ARG:HB3	1.93	0.48
56:s:337:GLY:O	56:s:341:MET:HG2	2.13	0.48
9:w:117:GLU:HA	9:w:120:MET:HE2	1.95	0.48
12:x:38:PHE:HB3	12:x:43:LEU:HD21	1.94	0.48
12:x:267:GLU:HG2	12:x:269:GLU:H	1.78	0.48
25:A:2992:C:O2	25:A:2992:C:H2'	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:3244:A:H2'	25:A:3245:C:H6	1.78	0.48
32:f:187:LYS:HE2	32:f:189:HIS:NE2	2.28	0.48
33:F:61:PRO:HA	33:F:84:PRO:HD3	1.96	0.48
45:M:263:ARG:HH21	50:p:43:TYR:HE2	1.60	0.48
11:W:102:GLU:OE2	16:6:74:TYR:N	2.46	0.48
15:y:168:LYS:HG2	29:D:232:ARG:HH22	1.78	0.48
21:8:110:GLU:O	21:8:114:ARG:HG2	2.14	0.48
25:A:2044:A:H61	25:A:2096:U:H3	1.59	0.48
31:E:329:PRO:HD2	31:E:332:LEU:HD21	1.95	0.48
43:L:98:PRO:HA	53:Q:162:ILE:HG12	1.96	0.48
12:x:345:ARG:HG3	12:x:354:PHE:CG	2.49	0.48
13:5:105:TYR:CZ	13:5:262:ILE:HD12	2.49	0.48
13:5:139:LEU:HD13	13:5:423:ALA:HB3	1.94	0.48
14:X:40:PRO:HB3	14:X:43:TYR:CZ	2.49	0.48
25:A:2990:G:H21	25:A:2996:A:H62	1.62	0.48
30:e:87:HIS:NE2	30:e:121:GLU:OE2	2.45	0.48
33:F:291:SER:OG	34:g:52:LEU:O	2.31	0.48
57:S:119:GLU:OE1	57:S:119:GLU:N	2.34	0.48
14:X:167:LEU:HD21	14:X:202:GLU:HA	1.95	0.48
25:A:1858:G:H2'	25:A:1859:A:C8	2.48	0.48
25:A:2145:G:N3	57:S:104:ARG:NH2	2.61	0.48
25:A:2548:U:H2'	25:A:2549:A:C8	2.49	0.48
25:A:3200:C:H2'	25:A:3201:C:O2	2.13	0.48
45:M:180:ASP:OD1	45:M:180:ASP:N	2.46	0.48
25:A:1829:A:H2'	25:A:1830:G:H8	1.79	0.48
25:A:1863:A:H2'	25:A:1864:A:H8	1.77	0.48
25:A:1907:A:N3	25:A:2961:U:O2'	2.43	0.48
25:A:3149:U:H2'	25:A:3150:C:H6	1.79	0.48
29:D:115:GLU:HB2	29:D:118:LYS:HG2	1.96	0.48
30:e:64:THR:HB	30:e:67:GLN:HG3	1.96	0.48
30:e:66:LEU:O	30:e:70:MET:HG3	2.14	0.48
30:e:242:ASP:OD1	30:e:243:PHE:N	2.47	0.48
45:M:38:ARG:HH21	45:M:45:ARG:NH2	2.12	0.48
53:Q:120:THR:HG22	53:Q:172:GLN:HB2	1.96	0.48
9:w:91:ASP:OD1	9:w:91:ASP:N	2.39	0.48
12:x:312:LEU:HD23	12:x:363:LEU:HD21	1.95	0.48
17:Y:185:VAL:HG21	25:A:1707:C:C4	2.48	0.48
18:z:38:GLY:O	18:z:42:MET:HG2	2.14	0.48
25:A:2574:U:H2'	25:A:2575:A:H8	1.78	0.48
25:A:2835:A:H2'	25:A:2836:A:C8	2.49	0.48
32:f:133:GLU:HG3	32:f:149:VAL:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:F:102:TRP:NE1	33:F:163:TYR:O	2.46	0.48
33:F:281:ARG:HH22	45:M:128:THR:HG1	1.57	0.48
45:M:99:ASN:N	45:M:99:ASN:OD1	2.46	0.48
58:t:49:ALA:HB2	58:t:109:LEU:HD23	1.95	0.48
10:3:152:LYS:NZ	25:A:2091:A:OP2	2.38	0.48
16:6:121:ARG:HD2	21:8:108:PHE:CZ	2.49	0.48
25:A:1862:U:H2'	25:A:1863:A:C8	2.49	0.48
30:e:71:ALA:HB2	46:m:40:LEU:HD22	1.96	0.48
3:u:106:ALA:HB3	3:u:109:ILE:HD11	1.96	0.48
8:V:69:ASP:OD1	8:V:69:ASP:N	2.46	0.48
8:V:84:ASN:HB3	8:V:117:HIS:HD2	1.78	0.48
15:y:322:ARG:O	15:y:325:GLU:HG3	2.14	0.48
18:z:84:LYS:HG2	62:z:401:GNP:C5	2.43	0.48
20:Z:134:MET:HE1	40:j:78:VAL:HG21	1.95	0.48
23:9:68:PHE:CE2	23:9:70:LEU:HB2	2.48	0.48
29:D:128:GLN:HE22	29:D:130:ARG:HB3	1.79	0.48
4:1:44:LEU:HG	4:1:53:ARG:HD2	1.96	0.48
8:V:48:PRO:HD2	17:Y:241:LEU:HD11	1.96	0.48
25:A:2739:C:H2'	25:A:2740:A:H8	1.79	0.48
25:A:3244:A:H2'	25:A:3245:C:C6	2.48	0.48
56:s:66:TRP:O	56:s:69:THR:OG1	2.26	0.48
56:s:90:LYS:HD2	56:s:232:GLN:HB2	1.96	0.48
56:s:203:ARG:HA	56:s:237:PRO:O	2.14	0.48
58:t:99:THR:HA	58:t:106:ILE:H	1.78	0.48
58:t:209:GLY:O	58:t:213:ASN:N	2.25	0.48
15:y:136:LEU:HD21	15:y:176:LEU:HB3	1.96	0.47
24:b:35:ARG:HG2	48:o:101:TRP:HB2	1.96	0.47
25:A:2778:U:H2'	25:A:2779:A:C8	2.49	0.47
29:D:211:GLY:H	29:D:247:VAL:HB	1.79	0.47
56:s:376:THR:OG1	56:s:387:ASN:ND2	2.46	0.47
15:y:185:GLU:OE1	15:y:224:ARG:NH2	2.46	0.47
18:z:75:LEU:HD21	58:t:37:GLY:HA2	1.95	0.47
25:A:2277:U:H2'	25:A:2278:A:H8	1.79	0.47
26:c:60:ARG:NH2	26:c:65:ASN:O	2.46	0.47
27:B:1609:U:O2	27:B:1616:A:N6	2.47	0.47
28:d:137:PHE:N	28:d:138:PRO:HD2	2.29	0.47
1:0:142:GLY:HA3	25:A:2321:A:N7	2.29	0.47
16:6:121:ARG:HD2	21:8:108:PHE:HZ	1.80	0.47
17:Y:143:ASP:OD2	23:9:137:ARG:NH2	2.43	0.47
19:7:262:ASP:OD1	19:7:263:VAL:N	2.48	0.47
28:d:115:THR:HG22	28:d:118:SER:H	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:265:LYS:HG2	30:e:266:PRO:HD2	1.95	0.47
3:u:127:VAL:HB	3:u:179:LEU:HD13	1.95	0.47
12:x:204:ASP:O	12:x:235:SER:HA	2.15	0.47
13:5:80:ARG:NH2	25:A:1707:C:O2	2.48	0.47
25:A:2003:A:OP2	25:A:2765:A:O2'	2.27	0.47
41:K:22:ASP:OD1	41:K:61:ASN:ND2	2.44	0.47
47:N:227:ARG:HA	47:N:230:LEU:HB2	1.95	0.47
55:R:72:ILE:HD11	55:R:102:LEU:C	2.40	0.47
1:0:132:LYS:HZ2	28:d:290:GLU:HB2	1.80	0.47
2:T:49:ASN:ND2	2:T:68:TYR:O	2.31	0.47
2:T:69:HIS:HD2	2:T:114:VAL:HG13	1.79	0.47
5:U:153:LEU:HD11	28:d:240:LYS:HB2	1.96	0.47
14:X:67:ILE:HD13	35:H:56:VAL:HG23	1.97	0.47
25:A:2777:U:H2'	25:A:2778:U:C6	2.50	0.47
25:A:3055:U:H2'	25:A:3056:A:H8	1.78	0.47
28:d:124:ARG:NH2	28:d:202:MET:SD	2.82	0.47
54:r:109:GLN:O	54:r:113:ARG:HG2	2.15	0.47
3:u:169:CYS:HG	3:u:178:HIS:CE1	2.31	0.47
21:8:116:LEU:HA	21:8:119:LYS:HG2	1.96	0.47
25:A:1994:A:H61	25:A:2767:C:H4'	1.78	0.47
25:A:2015:G:H22	25:A:2037:U:H5''	1.80	0.47
25:A:2113:G:N2	25:A:2973:C:O5'	2.47	0.47
25:A:2240:C:OP2	41:K:71:LYS:NZ	2.39	0.47
25:A:2408:U:H2'	25:A:2409:A:H8	1.78	0.47
25:A:2550:U:H2'	25:A:2551:A:C8	2.48	0.47
25:A:2973:C:O2'	25:A:2974:G:OP2	2.27	0.47
25:A:3095:A:H2'	25:A:3132:A:N6	2.29	0.47
36:h:95:ARG:O	36:h:99:ASN:ND2	2.30	0.47
48:o:71:PHE:CE2	48:o:75:LYS:HD2	2.49	0.47
5:U:66:ALA:HB2	5:U:100:ALA:HA	1.96	0.47
8:V:73:GLN:HE22	8:V:128:ARG:HB3	1.78	0.47
11:W:74:ARG:HE	25:A:2065:A:H5'	1.79	0.47
15:y:95:VAL:HG21	15:y:121:LEU:HD11	1.97	0.47
15:y:139:GLU:CG	15:y:140:PRO:HD3	2.45	0.47
17:Y:230:LYS:HE2	25:A:1680:A:OP1	2.13	0.47
25:A:2243:A:H5''	54:r:188:SER:HB3	1.97	0.47
25:A:2483:U:O2	25:A:2683:G:N2	2.48	0.47
25:A:3175:A:H2'	25:A:3176:A:H8	1.78	0.47
25:A:3205:U:H2'	25:A:3206:A:C8	2.49	0.47
26:c:39:PHE:O	26:c:43:LYS:HG2	2.15	0.47
27:B:1638:U:H2'	27:B:1639:U:H6	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:109:PHE:HE1	29:D:152:ILE:HD11	1.79	0.47
33:F:102:TRP:HE1	33:F:164:MET:HA	1.80	0.47
34:g:122:LYS:NZ	34:g:126:ASP:OD2	2.47	0.47
36:h:116:ARG:O	36:h:120:MET:HG2	2.15	0.47
53:Q:182:ARG:HD2	53:Q:218:ASN:HB3	1.97	0.47
57:S:115:LEU:HD11	57:S:190:GLN:HB3	1.96	0.47
58:t:56:LYS:HE3	58:t:56:LYS:HB3	1.71	0.47
3:u:133:ARG:NH2	25:A:3161:A:OP1	2.48	0.47
9:w:124:ASP:OD1	9:w:125:GLU:N	2.48	0.47
13:5:136:VAL:HG22	13:5:420:HIS:CD2	2.50	0.47
19:7:286:LEU:HD21	19:7:296:ARG:HE	1.80	0.47
24:b:73:PRO:HB2	24:b:89:ILE:HG13	1.96	0.47
25:A:2093:U:H4'	38:i:126:LYS:HE2	1.95	0.47
31:E:235:LYS:O	31:E:239:ARG:NH1	2.31	0.47
34:g:154:ASP:OD1	34:g:154:ASP:N	2.41	0.47
8:V:54:TRP:NE1	8:V:56:LEU:O	2.46	0.47
13:5:144:ARG:O	13:5:194:LYS:NZ	2.41	0.47
25:A:1742:G:O2'	25:A:1754:G:O6	2.31	0.47
25:A:2166:C:H2'	25:A:2167:A:C8	2.50	0.47
52:q:137:GLN:N	52:q:140:ARG:HH21	2.13	0.47
3:u:121:THR:OG1	3:u:174:SER:O	2.33	0.47
19:7:131:LYS:NZ	49:O:139:ASP:OD2	2.46	0.47
19:7:156:ARG:O	22:a:93:LYS:NZ	2.43	0.47
25:A:1839:C:H2'	25:A:1840:C:C6	2.50	0.47
25:A:2072:A:H2'	25:A:2073:A:C8	2.50	0.47
25:A:2787:C:H2'	25:A:2788:A:C8	2.50	0.47
25:A:2992:C:H5''	25:A:2993:C:C5	2.50	0.47
28:d:92:GLU:OE1	28:d:92:GLU:N	2.42	0.47
29:D:215:VAL:HG13	29:D:227:GLN:HB3	1.96	0.47
12:x:315:LEU:HD13	12:x:319:TYR:CD2	2.50	0.46
16:6:41:ASP:OD1	16:6:42:LEU:N	2.48	0.46
26:c:312:ARG:NH2	57:S:92:TYR:O	2.48	0.46
27:B:1628:C:H2'	27:B:1629:A:C8	2.49	0.46
34:g:160:TRP:CE2	34:g:164:LYS:HD2	2.50	0.46
8:V:65:LEU:HD11	8:V:121:LYS:HB2	1.97	0.46
13:5:136:VAL:HG11	13:5:417:LEU:HD23	1.97	0.46
14:X:227:PHE:CZ	23:9:96:VAL:HG11	2.51	0.46
22:a:46:ASN:O	22:a:63:PRO:HD2	2.16	0.46
24:b:52:ILE:HG22	24:b:56:ARG:HE	1.80	0.46
25:A:2529:U:H2'	29:D:208:ARG:HB2	1.96	0.46
25:A:2788:A:H2	25:A:2821:A:H5'	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:60:SER:O	30:e:136:ARG:NH2	2.48	0.46
2:T:132:SER:OG	19:7:93:MET:O	2.30	0.46
11:W:143:LYS:HE2	16:6:345:VAL:HB	1.97	0.46
12:x:77:VAL:HB	12:x:130:ARG:HB2	1.97	0.46
25:A:2553:A:H2'	25:A:2554:U:C6	2.50	0.46
33:F:218:LEU:HA	33:F:260:VAL:HG23	1.96	0.46
20:Z:101:LYS:HG2	40:j:84:MET:HE2	1.95	0.46
38:i:83:TRP:HZ3	38:i:90:ARG:HG2	1.80	0.46
39:J:95:LYS:CB	39:J:110:ALA:HB1	2.45	0.46
54:r:121:MET:HE3	54:r:151:LEU:HA	1.97	0.46
18:z:148:VAL:O	18:z:203:THR:OG1	2.27	0.46
25:A:1884:G:H1'	25:A:1895:C:H1'	1.98	0.46
25:A:1952:U:H2'	25:A:1953:A:C8	2.51	0.46
25:A:3175:A:H2'	25:A:3176:A:C8	2.51	0.46
45:M:85:GLU:N	45:M:85:GLU:OE1	2.48	0.46
56:s:237:PRO:HB3	56:s:300:HIS:CE1	2.51	0.46
3:u:130:THR:HG22	3:u:134:HIS:ND1	2.30	0.46
16:6:42:LEU:HD11	32:f:62:LEU:HA	1.97	0.46
16:6:187:VAL:HG13	16:6:319:PHE:HB3	1.98	0.46
25:A:2034:A:H4'	25:A:2947:G:N7	2.30	0.46
25:A:2956:U:O2'	25:A:2958:C:OP1	2.30	0.46
32:f:114:CYS:SG	32:f:119:ILE:HB	2.55	0.46
34:g:40:GLU:HG3	45:M:281:LYS:HE3	1.96	0.46
35:H:138:LYS:O	35:H:142:GLU:HG2	2.15	0.46
2:T:134:LEU:HD23	2:T:174:GLU:HA	1.97	0.46
8:V:49:ILE:HD11	8:V:117:HIS:CE1	2.51	0.46
16:6:35:MET:HB3	16:6:38:SER:HB3	1.97	0.46
18:z:308:THR:HG23	18:z:313:LEU:HD12	1.97	0.46
19:7:216:PHE:CG	19:7:257:ILE:HD11	2.51	0.46
23:9:101:GLU:O	23:9:105:LYS:HG2	2.15	0.46
25:A:2449:G:OP2	56:s:225:ARG:NH2	2.42	0.46
29:D:115:GLU:H	29:D:118:LYS:HE2	1.80	0.46
31:E:131:LYS:H	31:E:146:SER:HG	1.64	0.46
48:o:56:ARG:HA	48:o:59:GLU:HG2	1.96	0.46
1:0:134:THR:HG23	49:O:130:LEU:HD22	1.97	0.46
10:3:94:LEU:N	25:A:1752:U:OP1	2.48	0.46
12:x:259:THR:HG22	12:x:272:ILE:HG21	1.97	0.46
13:5:55:LEU:HD21	14:X:163:ARG:HH21	1.81	0.46
20:Z:68:ILE:HD11	20:Z:122:LEU:HD13	1.98	0.46
25:A:1975:U:H2'	25:A:1976:U:C6	2.50	0.46
25:A:2757:C:H2'	25:A:2758:C:H6	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:L:46:LEU:HD12	43:L:78:LYS:HD2	1.98	0.46
52:q:40:PRO:HG2	52:q:51:GLN:HB3	1.98	0.46
17:Y:192:LYS:HD3	25:A:1709:G:H4'	1.98	0.46
21:8:101:ARG:NE	30:e:82:SER:O	2.43	0.46
25:A:2308:A:OP2	25:A:2309:A:O2'	2.28	0.46
25:A:2415:C:H41	56:s:166:TYR:HE2	1.63	0.46
28:d:85:PHE:CZ	28:d:200:SER:HB3	2.51	0.46
56:s:171:VAL:HG13	56:s:172:ILE:HG13	1.97	0.46
2:T:197:LEU:O	2:T:200:ARG:HG2	2.16	0.46
3:u:132:THR:HG21	3:u:165:ASP:HB2	1.98	0.46
12:x:150:LEU:HD23	52:q:150:LYS:HE2	1.98	0.46
16:6:120:GLU:OE2	21:8:119:LYS:NZ	2.31	0.46
25:A:2529:U:OP2	29:D:208:ARG:NE	2.48	0.46
25:A:2699:A:H2'	25:A:2700:A:H8	1.80	0.46
25:A:2788:A:C2	25:A:2821:A:H5'	2.51	0.46
26:c:86:ASP:OD1	26:c:87:LEU:N	2.49	0.46
27:B:1638:U:H2'	27:B:1639:U:C6	2.51	0.46
43:L:68:LYS:N	43:L:71:ASP:OD2	2.41	0.46
55:R:18:TYR:O	55:R:22:GLN:HG2	2.16	0.46
25:A:2750:G:H2'	25:A:2750:G:N3	2.30	0.45
25:A:3222:A:O2'	54:r:123:HIS:ND1	2.47	0.45
36:h:148:LEU:HD22	36:h:152:LEU:HD23	1.97	0.45
56:s:105:TRP:CG	56:s:271:LEU:HD13	2.51	0.45
57:S:70:VAL:HG12	57:S:74:ARG:HH12	1.81	0.45
12:x:71:GLN:HB3	12:x:262:ARG:NH1	2.31	0.45
12:x:345:ARG:O	12:x:349:MET:HG2	2.16	0.45
15:y:182:CYS:HB2	15:y:220:PRO:HG2	1.97	0.45
25:A:2182:G:H1'	25:A:2199:A:H2'	1.98	0.45
32:f:171:LEU:HD12	32:f:174:ILE:HD11	1.97	0.45
58:t:59:LYS:HD2	58:t:65:LYS:HE2	1.98	0.45
11:W:102:GLU:HB2	11:W:130:PHE:CD1	2.51	0.45
13:5:232:THR:HG22	13:5:289:HIS:HB2	1.98	0.45
14:X:19:GLY:O	14:X:22:SER:OG	2.33	0.45
25:A:1803:A:H4'	25:A:1804:A:H3'	1.98	0.45
25:A:2173:G:H2'	25:A:2174:G:C8	2.51	0.45
30:e:63:LEU:HG	30:e:67:GLN:HB2	1.98	0.45
43:L:32:ILE:HD11	43:L:103:ASN:HB3	1.99	0.45
51:P:164:ALA:O	51:P:167:GLU:HG2	2.17	0.45
8:V:159:PHE:CD1	8:V:160:PRO:HD2	2.51	0.45
12:x:244:LEU:HD11	32:f:208:LEU:HG	1.99	0.45
12:x:363:LEU:HG	12:x:376:TYR:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:83:GLU:OE2	35:H:53:THR:OG1	2.30	0.45
19:7:276:PHE:CD2	19:7:277:GLN:HG3	2.51	0.45
20:Z:121:PRO:HG3	48:o:48:TRP:CH2	2.51	0.45
25:A:1829:A:H2'	25:A:1830:G:C8	2.52	0.45
25:A:2847:G:H2'	25:A:2848:G:H8	1.80	0.45
29:D:115:GLU:HG3	29:D:118:LYS:HE2	1.99	0.45
29:D:155:GLU:HA	29:D:248:SER:HA	1.99	0.45
31:E:96:ARG:HH21	31:E:202:GLN:HE22	1.64	0.45
31:E:218:VAL:HG11	31:E:240:PRO:HB3	1.98	0.45
53:Q:290:LYS:HE3	53:Q:291:ARG:HH22	1.80	0.45
57:S:86:MET:HG3	57:S:91:GLN:HB2	1.97	0.45
5:U:131:GLU:O	5:U:135:GLN:HG2	2.17	0.45
22:a:103:LEU:HG	22:a:107:PRO:HB2	1.99	0.45
25:A:2572:U:H2'	25:A:2573:A:H8	1.81	0.45
25:A:2693:A:OP1	25:A:3190:A:O2'	2.30	0.45
58:t:23:THR:HB	58:t:45:VAL:HG11	1.98	0.45
12:x:82:ALA:HA	52:q:153:ARG:HH21	1.81	0.45
17:Y:150:GLU:OE1	17:Y:154:ARG:NH1	2.49	0.45
25:A:2556:U:H2'	25:A:2557:A:H8	1.81	0.45
25:A:2770:U:O4	29:D:297:LYS:NZ	2.46	0.45
29:D:176:ALA:HB1	29:D:244:VAL:HG11	1.98	0.45
30:e:140:ALA:HB1	30:e:151:ARG:HB2	1.98	0.45
45:M:207:PRO:HD2	45:M:210:LEU:HD12	1.97	0.45
3:u:160:GLU:OE2	43:L:134:TYR:N	2.50	0.45
5:U:150:TRP:HZ2	28:d:261:MET:HE2	1.82	0.45
12:x:69:SER:HB3	15:y:319:LEU:HD22	1.99	0.45
12:x:86:VAL:HG11	12:x:154:GLU:HB3	1.98	0.45
17:Y:162:ARG:NH2	25:A:1693:C:H42	2.14	0.45
18:z:46:LEU:HD11	18:z:73:LEU:HA	1.97	0.45
18:z:58:ALA:HA	18:z:82:LEU:HD12	1.98	0.45
19:7:160:ASP:OD1	19:7:160:ASP:N	2.49	0.45
24:b:30:SER:O	24:b:75:VAL:HA	2.17	0.45
25:A:2451:A:N7	25:A:2452:A:N6	2.65	0.45
30:e:203:LYS:HB3	30:e:237:LEU:HB2	1.98	0.45
17:Y:128:SER:HB2	17:Y:131:ARG:NE	2.32	0.45
20:Z:117:ILE:O	48:o:45:ASN:ND2	2.50	0.45
25:A:1814:A:C4	25:A:1815:A:C8	3.05	0.45
25:A:1939:G:O2'	25:A:1973:G:H4'	2.16	0.45
25:A:2531:U:O2'	29:D:210:ALA:O	2.32	0.45
47:N:234:ASP:HA	47:N:237:HIS:HB3	1.99	0.45
51:P:136:CYS:HB3	51:P:141:ILE:HG13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:15:LEU:HD11	26:c:169:VAL:HA	1.99	0.45
25:A:1711:C:H2'	25:A:1711:C:O2	2.17	0.45
25:A:2173:G:H2'	25:A:2174:G:H8	1.82	0.45
25:A:2992:C:H3'	25:A:2993:C:C6	2.51	0.45
25:A:3026:G:OP1	25:A:3073:U:O2'	2.34	0.45
35:H:56:VAL:HB	35:H:80:TYR:HB3	1.98	0.45
49:O:46:TRP:CD1	49:O:121:ALA:HB2	2.52	0.45
58:t:93:PRO:HG2	58:t:96:ILE:HD11	1.98	0.45
1:0:96:ASN:ND2	1:0:98:GLN:H	2.14	0.45
8:V:147:SER:OG	8:V:152:ARG:NH1	2.50	0.45
10:3:138:PRO:HG2	25:A:2885:U:H4'	1.98	0.45
15:y:113:LEU:HG	15:y:116:ARG:HH12	1.82	0.45
18:z:39:LEU:HA	18:z:42:MET:HG2	1.99	0.45
18:z:221:ALA:HA	18:z:226:VAL:HG22	1.99	0.45
25:A:1755:A:O2'	35:H:64:LEU:O	2.29	0.45
25:A:2314:C:H2'	25:A:2315:A:C8	2.52	0.45
25:A:2708:A:H2'	25:A:2709:A:C8	2.53	0.45
25:A:2847:G:H2'	25:A:2848:G:C8	2.52	0.45
30:e:55:ARG:CG	30:e:157:LEU:HB2	2.47	0.45
54:r:124:ARG:NH1	54:r:153:ARG:O	2.50	0.45
56:s:238:ASN:O	56:s:239:ASN:ND2	2.49	0.45
16:6:182:ASP:O	50:p:192:ARG:HG3	2.17	0.44
24:b:144:ARG:HB2	24:b:147:GLU:HG2	1.98	0.44
25:A:2135:A:N3	25:A:2135:A:H2'	2.32	0.44
25:A:2779:A:H2'	25:A:2780:A:C8	2.52	0.44
26:c:203:LEU:HA	26:c:211:THR:OG1	2.17	0.44
33:F:228:GLN:HA	33:F:231:VAL:HG12	2.00	0.44
3:u:147:LYS:NZ	25:A:3152:C:OP2	2.33	0.44
18:z:84:LYS:HG2	62:z:401:GNP:N7	2.32	0.44
25:A:2877:G:H5''	25:A:2878:C:H5''	1.99	0.44
27:B:1613:U:O2'	27:B:1615:A:OP1	2.26	0.44
48:o:57:GLU:CD	48:o:57:GLU:H	2.26	0.44
2:T:206:LEU:HD11	57:S:107:LYS:HD2	2.00	0.44
25:A:2284:C:H5'	26:c:39:PHE:CE2	2.52	0.44
25:A:3224:U:OP2	54:r:144:LYS:NZ	2.48	0.44
29:D:210:ALA:HB1	29:D:249:ASN:HB2	2.00	0.44
31:E:109:LEU:HD21	31:E:337:VAL:HG22	1.99	0.44
49:O:65:LEU:HD21	49:O:71:ARG:HH21	1.82	0.44
21:8:136:ILE:HA	21:8:139:MET:HE3	1.98	0.44
25:A:2074:A:N6	32:f:48:TYR:OH	2.44	0.44
25:A:2488:C:H2'	25:A:2489:C:H6	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2713:A:OP1	55:R:34:ARG:NH2	2.50	0.44
26:c:170:ALA:HB1	26:c:175:VAL:HB	1.99	0.44
5:U:48:MET:HE2	5:U:53:LEU:HA	1.98	0.44
5:U:151:PHE:HB3	28:d:222:LEU:HD21	1.99	0.44
13:5:258:PRO:HG2	13:5:259:ILE:HD12	2.00	0.44
16:6:145:PRO:HA	16:6:169:PRO:HG2	1.99	0.44
25:A:1737:A:O2'	38:i:93:ARG:NH2	2.51	0.44
25:A:2416:U:OP1	56:s:313:ARG:NH1	2.50	0.44
25:A:2533:A:H2'	25:A:2534:G:C8	2.51	0.44
25:A:2665:U:H2'	25:A:2666:G:C8	2.52	0.44
25:A:2848:G:C2'	25:A:2849:C:H5'	2.47	0.44
28:d:104:GLY:O	28:d:108:ARG:HG2	2.18	0.44
28:d:226:ASP:OD1	28:d:230:ARG:N	2.50	0.44
30:e:57:PRO:HG3	30:e:155:ARG:C	2.42	0.44
45:M:91:ARG:HG2	45:M:136:TYR:CD1	2.52	0.44
52:q:117:ARG:O	52:q:121:ILE:HG12	2.17	0.44
53:Q:100:LEU:HD21	53:Q:286:ILE:HG12	1.99	0.44
55:R:72:ILE:HD13	55:R:72:ILE:HA	1.85	0.44
56:s:174:LEU:HB3	56:s:175:PRO:HD3	2.00	0.44
4:1:39:GLU:H	4:1:39:GLU:CD	2.26	0.44
5:U:81:ASP:HB3	5:U:87:ILE:HD11	1.99	0.44
13:5:126:THR:HG21	13:5:357:PHE:HE1	1.81	0.44
16:6:173:LEU:HD21	16:6:175:VAL:HG23	1.99	0.44
21:8:172:GLU:OE1	21:8:172:GLU:N	2.51	0.44
25:A:2927:G:C6	25:A:2946:C:H1'	2.53	0.44
36:h:143:LEU:O	36:h:146:SER:OG	2.34	0.44
51:P:88:HIS:O	51:P:119:THR:OG1	2.32	0.44
15:y:158:GLN:O	15:y:162:ARG:HG3	2.18	0.44
18:z:29:ARG:NH2	25:A:3077:C:O2'	2.51	0.44
25:A:2195:A:H2'	25:A:2196:A:C2	2.53	0.44
25:A:2777:U:H2'	25:A:2778:U:H6	1.83	0.44
25:A:3124:C:H2'	25:A:3125:G:C8	2.53	0.44
30:e:156:ASN:OD1	30:e:157:LEU:N	2.51	0.44
45:M:192:PRO:O	45:M:196:ARG:HG3	2.18	0.44
4:1:20:MET:HB3	4:1:56:PHE:HB3	2.00	0.44
15:y:293:ILE:HG13	15:y:301:PHE:HE1	1.83	0.44
16:6:136:ARG:HE	51:P:138:GLU:CD	2.26	0.44
16:6:139:TRP:CE2	16:6:144:GLY:HA2	2.53	0.44
24:b:26:LEU:HD22	24:b:105:ALA:HA	2.00	0.44
40:j:100:GLU:O	40:j:104:LYS:HG2	2.18	0.44
45:M:99:ASN:OD1	45:M:144:GLY:HA3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:r:35:PHE:N	54:r:55:ALA:O	2.51	0.44
5:U:130:LEU:HD12	28:d:66:VAL:HG13	2.00	0.44
7:2:60:ARG:NH1	7:2:92:HIS:O	2.51	0.44
12:x:258:CYS:HA	12:x:284:LEU:HD21	2.00	0.44
14:X:79:LEU:HB2	14:X:127:VAL:HG12	2.00	0.44
16:6:179:VAL:O	16:6:183:ASP:HB2	2.18	0.44
25:A:2236:C:N4	25:A:2719:C:O2	2.51	0.44
25:A:2468:A:H61	25:A:2690:C:N4	2.15	0.44
26:c:290:LEU:O	26:c:294:GLU:HG2	2.18	0.44
31:E:129:VAL:HG23	31:E:193:LEU:HD11	1.99	0.44
56:s:119:PRO:HG3	56:s:394:TRP:CD2	2.52	0.44
4:1:16:ILE:HG22	4:1:64:SER:HA	2.00	0.43
8:V:133:ILE:HA	8:V:147:SER:HA	2.00	0.43
9:w:148:ILE:HG22	9:w:152:LYS:HE2	2.00	0.43
15:y:237:ALA:HB2	15:y:253:TYR:CE2	2.53	0.43
17:Y:95:ASN:OD1	17:Y:149:ARG:NH1	2.45	0.43
21:8:172:GLU:HG3	32:f:183:ARG:HH22	1.82	0.43
22:a:71:HIS:CD2	24:b:140:PHE:HA	2.53	0.43
25:A:2293:A:C6	45:M:39:ARG:HD2	2.53	0.43
25:A:2442:U:OP1	56:s:81:ARG:NH2	2.45	0.43
25:A:2751:A:H8	25:A:2751:A:P	2.41	0.43
25:A:3233:U:OP1	31:E:141:LYS:HD2	2.18	0.43
28:d:245:TYR:HB2	28:d:265:ILE:HB	1.99	0.43
30:e:189:GLU:HG2	30:e:204:PHE:HE2	1.83	0.43
32:f:93:ILE:HG12	32:f:186:VAL:HG13	2.00	0.43
33:F:272:LYS:NZ	38:i:65:ASN:OD1	2.34	0.43
3:u:167:TRP:HD1	3:u:168:LEU:N	2.15	0.43
5:U:11:ARG:HH22	13:5:84:ASP:CG	2.25	0.43
15:y:241:MET:O	15:y:274:TYR:OH	2.33	0.43
18:z:42:MET:HE1	18:z:204:PRO:HD2	2.01	0.43
19:7:154:ILE:HG22	19:7:164:VAL:HG11	2.00	0.43
21:8:117:LEU:HD12	21:8:118:LEU:N	2.33	0.43
25:A:2995:U:O2'	25:A:2996:A:O5'	2.35	0.43
26:c:73:GLN:HE21	26:c:73:GLN:HB3	1.70	0.43
28:d:93:GLY:O	28:d:97:ILE:HG13	2.18	0.43
45:M:86:GLY:O	45:M:90:ARG:HG3	2.18	0.43
51:P:77:PHE:CE1	51:P:80:ARG:HB2	2.54	0.43
53:Q:95:GLU:OE2	53:Q:144:GLY:HA3	2.18	0.43
56:s:109:PHE:O	56:s:212:ARG:HD3	2.17	0.43
56:s:321:GLU:O	56:s:325:ARG:HG2	2.18	0.43
58:t:101:GLU:CD	58:t:142:HIS:HE2	2.25	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:6:301:PHE:C	16:6:303:PHE:H	2.26	0.43
23:9:82:GLU:CD	23:9:82:GLU:H	2.27	0.43
25:A:2779:A:H2'	25:A:2780:A:H8	1.83	0.43
25:A:3078:G:H2'	25:A:3079:A:C8	2.53	0.43
25:A:3089:U:O3'	31:E:247:ASP:HB2	2.17	0.43
26:c:57:PRO:HB2	26:c:184:PHE:HE2	1.83	0.43
26:c:309:GLU:OE1	41:K:3:SER:HA	2.19	0.43
31:E:107:MET:HE3	31:E:121:LEU:HD11	2.00	0.43
38:i:98:VAL:O	38:i:102:MET:HG3	2.19	0.43
50:p:188:LEU:HD21	51:P:137:LEU:HB3	2.00	0.43
56:s:90:LYS:NZ	56:s:278:TYR:O	2.44	0.43
2:T:200:ARG:NH1	41:K:52:ASP:O	2.47	0.43
12:x:224:GLU:HG2	12:x:225:ILE:HD12	2.00	0.43
12:x:296:LEU:HD13	12:x:328:LEU:HD11	2.00	0.43
16:6:103:LEU:HG	16:6:107:LYS:NZ	2.33	0.43
25:A:2538:C:H2'	25:A:2539:A:O4'	2.18	0.43
25:A:2878:C:H2'	25:A:2879:A:O4'	2.19	0.43
25:A:3031:A:H2'	25:A:3032:G:C8	2.54	0.43
25:A:3173:A:H2'	25:A:3174:U:C6	2.54	0.43
28:d:67:ILE:HG22	28:d:68:PRO:O	2.18	0.43
31:E:334:ASP:HB3	31:E:337:VAL:HG23	2.00	0.43
41:K:176:TYR:OH	54:r:94:ARG:NH2	2.52	0.43
5:U:150:TRP:CZ2	28:d:264:LYS:HE2	2.54	0.43
6:v:23:LEU:HB3	6:v:28:ARG:HH12	1.84	0.43
17:Y:128:SER:HB2	17:Y:131:ARG:HE	1.83	0.43
18:z:29:ARG:HH22	25:A:3078:G:H5'	1.83	0.43
18:z:262:CYS:SG	18:z:263:ASP:N	2.91	0.43
25:A:2080:U:O2'	48:o:60:ARG:HA	2.18	0.43
25:A:2759:C:H2'	25:A:2760:U:H6	1.83	0.43
33:F:212:TRP:O	33:F:258:THR:OG1	2.37	0.43
11:W:66:ILE:HD12	11:W:88:CYS:SG	2.58	0.43
13:5:169:GLU:HG3	13:5:170:ILE:HG13	2.00	0.43
13:5:215:ARG:NH1	13:5:364:LEU:O	2.51	0.43
15:y:178:ARG:HD3	25:A:2578:U:H4'	2.00	0.43
16:6:175:VAL:HG11	16:6:270:PHE:CE2	2.51	0.43
25:A:1889:C:OP1	45:M:133:LYS:HE2	2.19	0.43
25:A:2364:C:C2	25:A:2365:U:C5	3.07	0.43
25:A:2775:U:O2'	25:A:2777:U:O4	2.30	0.43
25:A:3074:C:O2'	25:A:3075:A:H8	2.01	0.43
29:D:196:VAL:HG22	29:D:206:TYR:HB2	2.01	0.43
31:E:80:LEU:HD12	31:E:323:GLY:HA3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:3:140:ARG:HA	10:3:143:ARG:HE	1.82	0.43
12:x:49:ASP:OD1	12:x:60:TRP:NE1	2.47	0.43
12:x:139:ILE:HG13	15:y:322:ARG:CZ	2.48	0.43
15:y:102:MET:HE2	29:D:220:VAL:HG13	2.00	0.43
15:y:126:ASP:O	15:y:130:GLU:HG2	2.19	0.43
16:6:105:GLU:O	16:6:108:GLN:HG2	2.19	0.43
25:A:1852:C:O2'	25:A:1854:U:OP2	2.36	0.43
25:A:2416:U:N3	56:s:166:TYR:HB3	2.33	0.43
27:B:1627:C:C2	27:B:1642:G:N2	2.87	0.43
31:E:334:ASP:OD1	31:E:335:GLU:N	2.49	0.43
33:F:44:PRO:HB2	33:F:45:GLU:H	1.64	0.43
46:m:68:TYR:HD2	46:m:70:GLU:H	1.67	0.43
57:S:117:GLY:HA2	57:S:190:GLN:HG2	2.00	0.43
4:1:47:ASP:HB3	4:1:50:VAL:HG22	2.01	0.43
16:6:52:ARG:HD3	27:B:1636:A:H4'	2.00	0.43
16:6:184:LEU:N	50:p:190:GLN:O	2.35	0.43
19:7:137:GLU:H	19:7:137:GLU:CD	2.26	0.43
25:A:1934:U:H2'	25:A:1935:A:O4'	2.19	0.43
45:M:8:GLY:HA2	45:M:11:ARG:HG2	2.00	0.43
45:M:295:THR:HG22	50:p:39:PHE:HE1	1.84	0.43
51:P:40:GLU:OE1	51:P:40:GLU:N	2.43	0.43
3:u:94:ILE:HA	3:u:97:MET:HE2	2.01	0.43
18:z:173:ALA:HB1	18:z:190:ILE:HD13	2.01	0.43
19:7:163:MET:H	19:7:186:ASP:HB2	1.84	0.43
25:A:2019:G:N7	45:M:54:LYS:NZ	2.67	0.43
25:A:2070:C:H3'	25:A:2862:G:N2	2.34	0.43
30:e:164:LYS:HE3	30:e:167:ASP:HA	2.01	0.43
30:e:201:GLU:HG3	30:e:239:LEU:HB2	2.01	0.43
30:e:253:VAL:C	30:e:254:TRP:HD1	2.26	0.43
36:h:87:GLN:HB3	36:h:124:ARG:HB2	2.01	0.43
41:K:17:ILE:O	41:K:55:ASP:HB3	2.19	0.43
53:Q:153:ASN:OD1	53:Q:154:VAL:N	2.47	0.43
55:R:81:LEU:HD12	55:R:117:ALA:HB1	2.00	0.43
1:0:80:ALA:H	25:A:2750:G:H21	1.67	0.43
12:x:183:ALA:O	61:x:401:SAM:HB1	2.18	0.43
61:x:401:SAM:H8	61:x:401:SAM:H2'	1.79	0.43
13:5:223:ARG:NH1	25:A:2409:A:H5''	2.34	0.43
14:X:36:ARG:NH2	14:X:150:LYS:HG2	2.34	0.43
25:A:1939:G:C8	29:D:259:LYS:HD2	2.54	0.43
25:A:2757:C:H2'	25:A:2758:C:C6	2.54	0.43
25:A:3055:U:H2'	25:A:3056:A:C8	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:111:ARG:NH2	29:D:165:ASN:OD1	2.39	0.43
32:f:93:ILE:HG12	32:f:186:VAL:HG22	2.01	0.43
51:P:136:CYS:SG	51:P:144:MET:HE1	2.59	0.43
58:t:24:ARG:HH21	58:t:68:VAL:HG11	1.84	0.43
1:0:112:GLU:OE1	1:0:112:GLU:N	2.51	0.42
14:X:125:VAL:HG23	14:X:127:VAL:HG13	2.01	0.42
18:z:56:HIS:O	18:z:82:LEU:HA	2.19	0.42
25:A:3068:U:H2'	25:A:3069:U:C6	2.53	0.42
25:A:3221:A:H4'	54:r:124:ARG:HH21	1.84	0.42
26:c:150:THR:O	26:c:154:LYS:HG2	2.18	0.42
31:E:76:LYS:HG3	31:E:170:LEU:HD21	2.00	0.42
41:K:75:LYS:HB2	54:r:174:MET:HE1	2.00	0.42
54:r:89:LEU:HD12	54:r:119:VAL:HG23	2.00	0.42
14:X:132:LEU:HD22	35:H:120:ARG:HD3	2.02	0.42
15:y:162:ARG:NE	15:y:187:PHE:HA	2.34	0.42
16:6:59:ARG:O	16:6:62:GLU:HG3	2.19	0.42
16:6:342:PHE:CE1	51:P:48:PHE:HB2	2.54	0.42
25:A:1829:A:H5''	55:R:31:PHE:CE1	2.54	0.42
25:A:2026:A:H2'	25:A:2027:A:C8	2.54	0.42
25:A:2279:U:OP1	33:F:255:LYS:NZ	2.42	0.42
25:A:2530:A:H4'	25:A:2531:U:O5'	2.19	0.42
25:A:2532:U:H2'	25:A:2533:A:C8	2.53	0.42
25:A:3070:U:H3'	25:A:3071:G:C8	2.54	0.42
25:A:3174:U:H2'	25:A:3175:A:C8	2.54	0.42
27:B:1664:G:H2'	27:B:1665:C:C6	2.54	0.42
33:F:65:TRP:CD1	36:h:117:LEU:HD11	2.54	0.42
5:U:37:GLU:OE1	5:U:37:GLU:N	2.45	0.42
10:3:154:GLN:O	10:3:158:LEU:HG	2.18	0.42
13:5:209:PHE:CZ	13:5:224:GLY:HA3	2.54	0.42
15:y:252:GLU:O	15:y:255:GLN:HG2	2.19	0.42
20:Z:39:SER:HA	47:N:227:ARG:HH22	1.84	0.42
23:9:110:ASP:OD1	23:9:110:ASP:N	2.50	0.42
25:A:1828:A:H4'	25:A:1829:A:C8	2.54	0.42
25:A:2530:A:H5''	29:D:212:THR:HG21	2.00	0.42
28:d:85:PHE:HZ	28:d:209:TYR:HB2	1.84	0.42
3:u:215:PHE:HZ	18:z:274:VAL:HG22	1.85	0.42
12:x:171:LEU:HD13	12:x:251:ARG:HG3	1.99	0.42
14:X:227:PHE:HZ	23:9:96:VAL:HG11	1.84	0.42
15:y:139:GLU:CD	15:y:140:PRO:HD3	2.44	0.42
16:6:121:ARG:HA	16:6:124:ARG:HG2	2.00	0.42
16:6:274:LYS:HE3	16:6:274:LYS:HB3	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1760:G:OP2	52:q:55:ARG:NH2	2.52	0.42
25:A:3165:C:H5'	25:A:3166:A:OP2	2.19	0.42
50:p:113:GLU:HA	50:p:116:ARG:HE	1.84	0.42
6:v:6:ARG:HH12	6:v:9:VAL:HG11	1.85	0.42
13:5:119:GLN:NE2	13:5:261:PRO:O	2.39	0.42
15:y:314:GLN:HG3	15:y:317:LYS:NZ	2.33	0.42
17:Y:151:ASP:OD1	17:Y:154:ARG:NH2	2.38	0.42
19:7:51:GLU:OE2	19:7:54:ARG:NH2	2.45	0.42
20:Z:69:VAL:HG12	20:Z:119:ILE:HG12	2.01	0.42
25:A:2049:U:H2'	25:A:2050:A:C8	2.55	0.42
25:A:3211:A:O2'	54:r:99:MET:O	2.37	0.42
25:A:3220:C:HO2'	54:r:155:ALA:H	1.57	0.42
32:f:178:LEU:HD13	32:f:184:LEU:HD23	2.02	0.42
34:g:107:MET:SD	34:g:148:ARG:HD3	2.60	0.42
36:h:74:VAL:HA	36:h:77:VAL:HG22	2.00	0.42
37:I:46:LYS:HB3	48:o:35:MET:SD	2.59	0.42
5:U:153:LEU:HD23	28:d:222:LEU:HB2	2.00	0.42
12:x:187:LYS:HD3	12:x:253:LEU:HD21	2.02	0.42
13:5:48:ARG:NH1	14:X:125:VAL:HG12	2.34	0.42
17:Y:170:ARG:HH21	17:Y:201:ALA:HB3	1.84	0.42
20:Z:134:MET:HE3	40:j:75:ARG:HH11	1.84	0.42
22:a:62:HIS:O	22:a:62:HIS:ND1	2.47	0.42
25:A:1718:A:H2'	25:A:1719:G:O4'	2.19	0.42
25:A:1756:A:H2'	25:A:1757:A:C8	2.55	0.42
25:A:1800:G:H1'	25:A:1805:A:H61	1.84	0.42
25:A:1845:C:H2'	25:A:1846:C:H6	1.85	0.42
25:A:3045:G:H2'	25:A:3046:U:O4'	2.19	0.42
25:A:3047:G:C6	25:A:3053:G:C6	3.08	0.42
25:A:3170:G:H2'	25:A:3171:A:C8	2.54	0.42
25:A:3189:A:H2'	25:A:3190:A:C8	2.54	0.42
26:c:96:CYS:HB2	26:c:182:GLU:HG2	2.01	0.42
28:d:88:TYR:CZ	28:d:195:VAL:HG11	2.54	0.42
33:F:92:ARG:HB2	33:F:176:VAL:HG21	2.01	0.42
56:s:136:ALA:O	56:s:191:HIS:NE2	2.42	0.42
56:s:302:LEU:HD13	56:s:302:LEU:HA	1.94	0.42
58:t:46:TRP:HE3	58:t:115:ARG:HB3	1.84	0.42
2:T:45:TRP:HB2	25:A:1672:C:OP1	2.19	0.42
6:v:6:ARG:NH1	60:w:200:PM8:H372	2.34	0.42
6:v:14:ARG:O	6:v:18:ARG:HG2	2.19	0.42
16:6:151:LEU:HD22	16:6:189:CYS:SG	2.59	0.42
19:7:40:LEU:O	19:7:43:MET:HG3	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:129:TYR:CZ	22:a:133:ARG:HD2	2.55	0.42
23:9:31:ARG:HD2	25:A:2421:G:H4'	2.01	0.42
24:b:146:ARG:NH2	41:K:22:ASP:OD2	2.52	0.42
25:A:1925:A:H2'	25:A:1926:A:C8	2.55	0.42
25:A:2006:C:H2'	25:A:2007:U:C6	2.55	0.42
25:A:2782:G:H2'	25:A:2783:C:H6	1.83	0.42
25:A:3054:C:H1'	58:t:61:ARG:NH1	2.35	0.42
29:D:125:LYS:HE2	29:D:160:GLY:HA2	2.01	0.42
31:E:345:ILE:HG12	53:Q:169:PRO:HB2	2.01	0.42
48:o:53:TYR:HD2	48:o:54:MET:HG3	1.84	0.42
50:p:123:HIS:CG	50:p:157:MET:HE3	2.55	0.42
56:s:332:LEU:HD13	56:s:332:LEU:HA	1.91	0.42
8:V:116:LEU:H	8:V:119:GLN:HB2	1.84	0.42
8:V:197:GLU:CD	17:Y:95:ASN:HD22	2.28	0.42
22:a:104:GLU:HB2	22:a:107:PRO:HD2	2.02	0.42
25:A:2351:U:C2	25:A:2362:A:N6	2.88	0.42
25:A:2382:A:H2'	25:A:2383:U:C6	2.55	0.42
25:A:2461:A:C2	25:A:2698:U:H1'	2.55	0.42
25:A:2665:U:H2'	25:A:2666:G:H8	1.85	0.42
25:A:3070:U:H3'	25:A:3071:G:H8	1.84	0.42
26:c:167:CYS:HB3	26:c:171:ARG:NH1	2.35	0.42
31:E:179:PHE:CE2	31:E:298:LYS:HE3	2.54	0.42
36:h:77:VAL:HG23	36:h:78:PHE:CD1	2.54	0.42
52:q:61:PHE:HB2	52:q:70:VAL:HB	2.00	0.42
15:y:137:ASN:C	15:y:140:PRO:HD2	2.45	0.42
25:A:2070:C:H3'	25:A:2862:G:H22	1.83	0.42
25:A:2466:A:OP1	53:Q:235:ARG:NH1	2.49	0.42
25:A:3046:U:H2'	25:A:3047:G:C8	2.55	0.42
41:K:154:ARG:NH1	41:K:156:ASP:OD1	2.53	0.42
45:M:68:GLU:OE1	45:M:71:GLN:NE2	2.53	0.42
12:x:221:VAL:HB	12:x:226:ARG:HD3	2.02	0.42
12:x:304:HIS:CE1	12:x:381:ARG:HE	2.38	0.42
13:5:356:VAL:HG13	13:5:375:TRP:HB2	2.01	0.42
15:y:263:GLN:HA	15:y:320:LEU:HD23	2.01	0.42
16:6:197:GLU:OE2	50:p:189:ARG:NH2	2.53	0.42
18:z:227:LEU:HD23	18:z:229:HIS:NE2	2.34	0.42
22:a:36:TYR:HB3	57:S:67:PRO:HG3	2.02	0.42
25:A:1840:C:H2'	25:A:1841:U:C6	2.55	0.42
25:A:2056:G:H2'	25:A:2057:C:C6	2.54	0.42
25:A:2100:C:H2'	25:A:2101:C:C6	2.54	0.42
56:s:103:ASP:OD1	56:s:104:ARG:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:u:121:THR:OG1	3:u:122:ASP:N	2.53	0.41
13:5:293:LEU:HD12	13:5:313:MET:HG2	2.02	0.41
19:7:166:LEU:HD22	19:7:181:TYR:HE2	1.85	0.41
21:8:113:ARG:NH2	21:8:114:ARG:HH22	2.18	0.41
25:A:2094:G:H2'	25:A:2095:U:C6	2.55	0.41
25:A:2988:G:H2'	25:A:2989:A:H8	1.85	0.41
25:A:3053:G:H21	58:t:61:ARG:NH2	2.18	0.41
47:N:180:ALA:HB1	47:N:187:ALA:C	2.45	0.41
3:u:98:VAL:O	3:u:102:ARG:HG2	2.21	0.41
12:x:260:THR:HG22	12:x:310:CYS:HB3	2.02	0.41
16:6:218:LEU:HB3	16:6:235:TRP:HB3	2.01	0.41
16:6:271:LEU:HB3	16:6:273:PHE:CE1	2.55	0.41
23:9:36:ARG:HA	23:9:36:ARG:HD2	1.80	0.41
23:9:98:PRO:O	23:9:101:GLU:HG3	2.20	0.41
25:A:2182:G:N3	25:A:2199:A:O2'	2.35	0.41
25:A:3070:U:H2'	25:A:3071:G:O4'	2.21	0.41
43:L:86:ILE:HD11	43:L:89:HIS:HB3	2.02	0.41
45:M:117:ASP:OD1	45:M:120:GLN:HG2	2.20	0.41
45:M:142:GLU:HG3	45:M:162:LEU:HD23	2.01	0.41
54:r:71:PRO:HD2	54:r:107:LEU:HD23	2.02	0.41
57:S:175:ARG:HB2	57:S:180:PHE:HB3	2.01	0.41
3:u:106:ALA:HB1	3:u:127:VAL:HG13	2.03	0.41
12:x:251:ARG:HD3	12:x:304:HIS:HB2	2.02	0.41
15:y:291:LYS:HA	15:y:295:ARG:HG3	2.02	0.41
16:6:215:THR:HG1	16:6:275:GLN:NE2	2.16	0.41
18:z:32:PRO:HD2	18:z:35:MET:HE3	2.03	0.41
26:c:290:LEU:HD12	26:c:290:LEU:H	1.85	0.41
54:r:173:ARG:HB3	54:r:195:TYR:HB3	2.02	0.41
2:T:120:ASP:OD1	2:T:124:ARG:NH2	2.53	0.41
8:V:98:ILE:HD12	8:V:98:ILE:HA	1.92	0.41
8:V:210:TYR:HD2	23:9:134:ASN:HD22	1.67	0.41
13:5:266:HIS:HD1	25:A:2408:U:HO2'	1.63	0.41
15:y:95:VAL:HG12	15:y:125:LEU:HD22	2.02	0.41
16:6:330:ILE:HG12	16:6:334:LEU:HD12	2.01	0.41
25:A:1968:G:N3	25:A:2675:A:H2	2.19	0.41
25:A:1970:G:H2'	25:A:1971:A:O4'	2.20	0.41
25:A:2048:U:H2'	25:A:2049:U:C6	2.55	0.41
32:f:100:MET:HB2	32:f:153:HIS:CD2	2.55	0.41
35:H:134:PRO:O	35:H:138:LYS:HD3	2.21	0.41
40:j:45:GLU:OE2	40:j:70:ARG:NH2	2.44	0.41
50:p:75:ASP:OD1	50:p:75:ASP:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:Q:77:SER:HB3	53:Q:80:PHE:HD1	1.85	0.41
13:5:117:VAL:O	13:5:121:LEU:HG	2.21	0.41
15:y:162:ARG:HG2	15:y:191:GLN:OE1	2.20	0.41
18:z:82:LEU:HA	18:z:82:LEU:HD13	1.93	0.41
25:A:2849:C:H2'	25:A:2850:G:O4'	2.21	0.41
25:A:3053:G:H21	58:t:61:ARG:HH22	1.69	0.41
28:d:226:ASP:OD2	28:d:230:ARG:NE	2.46	0.41
29:D:132:ASP:HB3	29:D:135:ARG:HG2	2.02	0.41
30:e:203:LYS:HB2	30:e:239:LEU:HD11	2.02	0.41
31:E:206:VAL:HG21	31:E:289:VAL:HG12	2.02	0.41
35:H:145:LEU:O	35:H:148:GLN:HG3	2.19	0.41
49:O:64:LYS:HZ2	49:O:104:TYR:HH	1.59	0.41
55:R:57:ARG:HE	57:S:169:ARG:NH1	2.18	0.41
14:X:89:GLN:HB2	35:H:79:VAL:HG22	2.01	0.41
16:6:107:LYS:HA	16:6:110:ILE:HG12	2.03	0.41
22:a:44:ASN:HB3	55:R:114:LYS:HD2	2.03	0.41
25:A:1929:A:H2'	25:A:1930:C:C6	2.56	0.41
25:A:1952:U:H2'	25:A:1953:A:H8	1.85	0.41
25:A:3043:U:H2'	25:A:3044:G:C8	2.53	0.41
25:A:3224:U:OP1	54:r:141:PRO:HB3	2.21	0.41
33:F:95:ILE:HD13	33:F:98:GLN:NE2	2.35	0.41
12:x:341:LEU:HD11	12:x:379:LYS:HB3	2.02	0.41
20:Z:114:LYS:HD2	48:o:46:HIS:CD2	2.55	0.41
25:A:2354:A:N6	25:A:2361:G:N1	2.25	0.41
25:A:2365:U:H2'	25:A:2366:G:C8	2.52	0.41
25:A:2859:G:H3'	25:A:2860:C:H5'	2.02	0.41
31:E:174:GLN:HG2	31:E:175:THR:HG23	2.03	0.41
41:K:56:HIS:CE1	41:K:124:ARG:HG2	2.55	0.41
45:M:74:PHE:O	45:M:78:ILE:HG12	2.20	0.41
56:s:318:ASP:OD1	56:s:318:ASP:N	2.54	0.41
58:t:101:GLU:HA	58:t:142:HIS:NE2	2.36	0.41
58:t:101:GLU:OE1	58:t:142:HIS:NE2	2.48	0.41
5:U:74:HIS:HB2	23:9:24:LYS:HE3	2.02	0.41
10:3:149:PHE:HB2	16:6:358:PRO:O	2.21	0.41
15:y:107:ALA:O	15:y:111:GLU:HG2	2.21	0.41
20:Z:46:PHE:CE2	20:Z:111:LYS:HE3	2.56	0.41
25:A:2268:G:N7	45:M:44:ARG:NH2	2.55	0.41
25:A:2560:U:H2'	25:A:2561:A:H8	1.86	0.41
25:A:2768:U:H2'	25:A:2769:U:C6	2.55	0.41
32:f:93:ILE:HG23	32:f:186:VAL:HG22	2.03	0.41
33:F:286:PHE:HA	33:F:290:TYR:HE2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:O:23:GLU:OE2	49:O:27:HIS:NE2	2.53	0.41
4:1:40:LYS:HE2	4:1:40:LYS:HB3	1.90	0.41
5:U:137:ARG:HE	5:U:137:ARG:HB3	1.73	0.41
8:V:168:GLU:OE1	8:V:169:THR:OG1	2.36	0.41
13:5:107:PHE:HB3	13:5:222:VAL:HG22	2.02	0.41
13:5:188:CYS:HB3	13:5:418:TYR:CD2	2.56	0.41
13:5:236:LEU:HD21	13:5:289:HIS:CD2	2.56	0.41
13:5:356:VAL:CG1	13:5:375:TRP:HB2	2.50	0.41
13:5:408:PRO:HG2	13:5:412:ARG:HH12	1.86	0.41
19:7:99:TYR:O	19:7:103:SER:HB2	2.20	0.41
21:8:117:LEU:HD13	21:8:121:TRP:CZ2	2.54	0.41
24:b:35:ARG:HD2	24:b:36:ASP:OD1	2.21	0.41
25:A:1799:U:H2'	25:A:1800:G:O4'	2.21	0.41
25:A:2049:U:H2'	25:A:2050:A:H8	1.86	0.41
25:A:2354:A:H61	25:A:2361:G:H1	0.61	0.41
25:A:2997:U:H2'	25:A:2998:C:C6	2.56	0.41
25:A:3160:A:H2'	25:A:3161:A:O4'	2.21	0.41
30:e:222:ARG:HG3	30:e:227:LEU:HD12	2.03	0.41
30:e:272:VAL:HA	30:e:275:PHE:CZ	2.56	0.41
32:f:117:LEU:HD13	32:f:166:PHE:CZ	2.56	0.41
41:K:67:PHE:HB3	41:K:71:LYS:HB2	2.03	0.41
58:t:45:VAL:O	58:t:117:LEU:HD12	2.21	0.41
14:X:114:PHE:HB3	14:X:141:LEU:HD22	2.03	0.41
15:y:135:GLY:O	15:y:173:GLU:HG2	2.21	0.41
19:7:81:MET:HE1	19:7:94:HIS:HD2	1.86	0.41
25:A:3143:A:H3'	25:A:3144:A:H5''	2.03	0.41
25:A:3221:A:H2'	25:A:3222:A:C8	2.56	0.41
29:D:182:HIS:HB2	29:D:187:LEU:HD21	2.03	0.41
32:f:178:LEU:HD22	32:f:184:LEU:HD23	2.02	0.41
49:O:116:ASP:N	49:O:116:ASP:OD1	2.53	0.41
51:P:118:SER:HB3	51:P:121:ASN:ND2	2.36	0.41
58:t:76:LYS:HG3	58:t:77:ILE:H	1.86	0.41
16:6:175:VAL:HG13	16:6:202:PRO:HB2	2.03	0.40
19:7:319:ARG:NH1	49:O:155:ASP:OD2	2.54	0.40
21:8:182:ILE:N	46:m:60:ASP:O	2.53	0.40
25:A:1847:U:H2'	25:A:1848:U:C6	2.56	0.40
25:A:2235:C:H2'	25:A:2236:C:O4'	2.21	0.40
25:A:2439:U:H2'	25:A:2440:G:H8	1.86	0.40
25:A:2456:U:H2'	25:A:2457:A:O4'	2.21	0.40
25:A:2719:C:H2'	25:A:2720:C:C6	2.56	0.40
30:e:55:ARG:HG3	30:e:157:LEU:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:205:LEU:HD22	32:f:171:LEU:HD23	2.02	0.40
50:p:104:HIS:HE1	50:p:106:ALA:HB3	1.85	0.40
50:p:110:TRP:H	50:p:110:TRP:CD1	2.38	0.40
55:R:71:ARG:HD3	55:R:107:ILE:HD11	2.02	0.40
56:s:204:CYS:SG	56:s:240:GLN:NE2	2.94	0.40
58:t:76:LYS:HZ2	58:t:77:ILE:HG22	1.86	0.40
1:0:95:ARG:NH2	25:A:1818:A:OP1	2.52	0.40
19:7:212:LYS:HA	19:7:212:LYS:HD3	1.88	0.40
19:7:243:LYS:HD3	19:7:243:LYS:HA	1.82	0.40
25:A:2011:G:C8	33:F:118:ALA:HB2	2.55	0.40
25:A:2113:G:H4'	25:A:2114:C:O5'	2.21	0.40
25:A:2694:C:H2'	25:A:2695:U:H6	1.86	0.40
25:A:3085:G:H2'	25:A:3086:U:H6	1.87	0.40
34:g:160:TRP:O	34:g:164:LYS:HG3	2.21	0.40
35:H:112:VAL:HG12	35:H:114:VAL:HG13	2.03	0.40
12:x:72:LYS:HD2	12:x:372:PHE:CZ	2.55	0.40
13:5:385:HIS:HB2	25:A:2395:A:H1'	2.03	0.40
15:y:282:GLN:NE2	18:z:191:GLN:OE1	2.39	0.40
18:z:32:PRO:HG2	18:z:34:HIS:CD2	2.56	0.40
21:8:129:ARG:HA	21:8:129:ARG:HD2	1.95	0.40
25:A:2311:U:H2'	25:A:2312:A:H8	1.87	0.40
25:A:2470:G:H4'	43:L:36:THR:HG23	2.04	0.40
25:A:2471:G:P	43:L:37:ARG:HH21	2.44	0.40
25:A:2563:A:H2'	25:A:2564:U:C6	2.56	0.40
25:A:3068:U:H2'	25:A:3069:U:H6	1.87	0.40
31:E:99:LEU:HD21	31:E:193:LEU:HB3	2.03	0.40
33:F:123:GLY:HA3	33:F:142:ARG:HG2	2.02	0.40
41:K:122:MET:HE2	41:K:122:MET:HA	2.04	0.40
45:M:30:ASN:OD1	45:M:31:PRO:HD2	2.21	0.40
45:M:231:GLU:OE1	45:M:231:GLU:N	2.51	0.40
48:o:95:LEU:HD13	48:o:95:LEU:HA	1.96	0.40
51:P:89:HIS:CE1	51:P:108:ARG:HG3	2.57	0.40
56:s:118:LEU:HD13	56:s:118:LEU:HA	1.95	0.40
13:5:212:THR:HG21	13:5:273:VAL:HG23	2.03	0.40
15:y:135:GLY:HA2	29:D:218:ARG:NH1	2.37	0.40
18:z:31:PHE:HA	18:z:35:MET:SD	2.61	0.40
18:z:160:ILE:O	18:z:164:ARG:HG3	2.21	0.40
19:7:227:LEU:HD22	19:7:237:VAL:HG13	2.03	0.40
19:7:253:LYS:NZ	19:7:264:SER:O	2.54	0.40
23:9:43:PHE:HE1	23:9:53:ILE:HD11	1.86	0.40
25:A:2079:C:H41	48:o:56:ARG:HH21	1.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2116:C:H2'	25:A:2117:U:C6	2.56	0.40
25:A:2178:A:H3'	25:A:2179:A:H8	1.86	0.40
25:A:2298:A:N6	33:F:145:LEU:HD22	2.36	0.40
25:A:2368:C:C2	25:A:2369:A:C8	3.09	0.40
25:A:2495:U:O4	25:A:2509:A:H2	2.05	0.40
25:A:2695:U:H2'	25:A:2696:U:C6	2.56	0.40
25:A:3025:U:O2'	25:A:3072:U:O2	2.31	0.40
25:A:3056:A:H2'	25:A:3057:U:H6	1.86	0.40
30:e:160:LEU:HD23	30:e:173:LEU:HD23	2.02	0.40
30:e:269:LEU:O	30:e:273:ARG:HG2	2.21	0.40
33:F:83:HIS:CE1	33:F:85:ASP:HB2	2.56	0.40
45:M:250:ASP:OD1	45:M:251:GLU:N	2.55	0.40
54:r:136:PRO:HG2	54:r:139:VAL:HG21	2.04	0.40
56:s:369:PHE:HB3	56:s:424:PHE:CE2	2.57	0.40
9:w:93:ILE:HG22	9:w:110:LEU:HD21	2.03	0.40
13:5:160:HIS:HA	13:5:164:TRP:HB2	2.02	0.40
13:5:189:LYS:O	13:5:192:ILE:HG13	2.21	0.40
13:5:192:ILE:HG12	13:5:198:LEU:HB2	2.04	0.40
17:Y:187:PRO:HD2	17:Y:190:LEU:HD12	2.04	0.40
18:z:76:LYS:HE2	18:z:76:LYS:HB2	1.96	0.40
21:8:121:TRP:CZ2	30:e:70:MET:HA	2.56	0.40
21:8:179:THR:HB	30:e:134:GLY:HA3	2.03	0.40
25:A:2100:C:H2'	25:A:2101:C:H6	1.85	0.40
25:A:2175:C:O4'	39:J:102:THR:HA	2.22	0.40
25:A:2741:C:O2	25:A:2742:A:C8	2.75	0.40
25:A:2872:U:H2'	25:A:2873:C:C6	2.56	0.40
26:c:32:LYS:NZ	38:i:33:GLY:O	2.54	0.40
27:B:1618:A:O2'	27:B:1620:A:N7	2.48	0.40
33:F:227:PRO:O	33:F:230:ILE:HG22	2.22	0.40
41:K:112:LEU:HD23	41:K:112:LEU:HA	1.94	0.40
53:Q:103:ARG:NH2	53:Q:167:TYR:OH	2.54	0.40
57:S:74:ARG:O	57:S:78:GLU:HG2	2.21	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	108/188 (57%)	108 (100%)	0	0	100	100
2	T	164/206 (80%)	162 (99%)	2 (1%)	0	100	100
3	u	124/234 (53%)	117 (94%)	7 (6%)	0	100	100
4	1	53/65 (82%)	53 (100%)	0	0	100	100
5	U	150/153 (98%)	148 (99%)	2 (1%)	0	100	100
6	v	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
7	2	44/92 (48%)	44 (100%)	0	0	100	100
8	V	203/216 (94%)	201 (99%)	2 (1%)	0	100	100
9	w	77/156 (49%)	70 (91%)	7 (9%)	0	100	100
10	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
11	W	104/148 (70%)	102 (98%)	2 (2%)	0	100	100
12	x	334/384 (87%)	324 (97%)	10 (3%)	0	100	100
13	5	392/423 (93%)	385 (98%)	7 (2%)	0	100	100
14	X	242/256 (94%)	239 (99%)	3 (1%)	0	100	100
15	y	242/381 (64%)	238 (98%)	4 (2%)	0	100	100
16	6	352/380 (93%)	340 (97%)	12 (3%)	0	100	100
17	Y	179/250 (72%)	178 (99%)	1 (1%)	0	100	100
18	z	309/334 (92%)	302 (98%)	7 (2%)	0	100	100
19	7	292/338 (86%)	281 (96%)	11 (4%)	0	100	100
20	Z	120/161 (74%)	118 (98%)	2 (2%)	0	100	100
21	8	100/206 (48%)	98 (98%)	2 (2%)	0	100	100
22	a	96/142 (68%)	95 (99%)	1 (1%)	0	100	100
23	9	122/137 (89%)	118 (97%)	4 (3%)	0	100	100
24	b	148/215 (69%)	143 (97%)	5 (3%)	0	100	100
26	c	282/332 (85%)	276 (98%)	6 (2%)	0	100	100
28	d	253/306 (83%)	251 (99%)	2 (1%)	0	100	100
29	D	238/305 (78%)	227 (95%)	11 (5%)	0	100	100
30	e	224/279 (80%)	221 (99%)	3 (1%)	0	100	100
31	E	303/348 (87%)	296 (98%)	7 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	f	146/212 (69%)	142 (97%)	4 (3%)	0	100	100
33	F	250/311 (80%)	248 (99%)	2 (1%)	0	100	100
34	g	132/166 (80%)	129 (98%)	3 (2%)	0	100	100
35	H	95/267 (36%)	95 (100%)	0	0	100	100
36	h	108/158 (68%)	104 (96%)	4 (4%)	0	100	100
37	I	156/261 (60%)	153 (98%)	3 (2%)	0	100	100
38	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
39	J	160/192 (83%)	149 (93%)	7 (4%)	4 (2%)	4	20
40	j	88/123 (72%)	87 (99%)	1 (1%)	0	100	100
41	K	175/178 (98%)	171 (98%)	4 (2%)	0	100	100
42	k	99/112 (88%)	97 (98%)	2 (2%)	0	100	100
43	L	113/145 (78%)	110 (97%)	3 (3%)	0	100	100
44	l	70/138 (51%)	67 (96%)	3 (4%)	0	100	100
45	M	289/296 (98%)	288 (100%)	1 (0%)	0	100	100
46	m	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
47	N	138/251 (55%)	132 (96%)	4 (3%)	2 (1%)	9	33
48	o	78/102 (76%)	78 (100%)	0	0	100	100
49	O	152/175 (87%)	148 (97%)	4 (3%)	0	100	100
50	p	141/206 (68%)	136 (96%)	5 (4%)	0	100	100
51	P	142/180 (79%)	141 (99%)	1 (1%)	0	100	100
52	q	139/222 (63%)	139 (100%)	0	0	100	100
53	Q	219/292 (75%)	217 (99%)	2 (1%)	0	100	100
54	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
55	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
56	s	382/439 (87%)	374 (98%)	8 (2%)	0	100	100
57	S	159/205 (78%)	158 (99%)	1 (1%)	0	100	100
58	t	321/387 (83%)	307 (96%)	14 (4%)	0	100	100
All	All	9609/12512 (77%)	9399 (98%)	204 (2%)	6 (0%)	49	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	J	22	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	J	63	PRO
47	N	114	PRO
39	J	20	PRO
39	J	27	VAL
47	N	123	VAL

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	99/164 (60%)	99 (100%)	0	100	100
2	T	146/176 (83%)	144 (99%)	2 (1%)	59	78
3	u	118/200 (59%)	114 (97%)	4 (3%)	32	63
4	1	52/60 (87%)	52 (100%)	0	100	100
5	U	134/135 (99%)	134 (100%)	0	100	100
6	v	59/60 (98%)	55 (93%)	4 (7%)	14	42
7	2	40/72 (56%)	40 (100%)	0	100	100
8	V	183/191 (96%)	178 (97%)	5 (3%)	39	68
9	w	73/136 (54%)	72 (99%)	1 (1%)	59	78
10	3	88/166 (53%)	87 (99%)	1 (1%)	65	80
11	W	86/119 (72%)	86 (100%)	0	100	100
12	x	293/328 (89%)	287 (98%)	6 (2%)	48	73
13	5	353/368 (96%)	348 (99%)	5 (1%)	59	78
14	X	220/229 (96%)	219 (100%)	1 (0%)	81	86
15	y	226/350 (65%)	222 (98%)	4 (2%)	51	74
16	6	313/332 (94%)	311 (99%)	2 (1%)	78	85
17	Y	163/223 (73%)	163 (100%)	0	100	100
18	z	270/287 (94%)	261 (97%)	9 (3%)	33	64
19	7	270/303 (89%)	268 (99%)	2 (1%)	76	84
20	Z	113/147 (77%)	113 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	8	93/190 (49%)	93 (100%)	0	100	100
22	a	96/133 (72%)	96 (100%)	0	100	100
23	9	104/112 (93%)	102 (98%)	2 (2%)	50	73
24	b	131/185 (71%)	128 (98%)	3 (2%)	44	70
26	c	251/288 (87%)	249 (99%)	2 (1%)	73	83
28	d	233/274 (85%)	231 (99%)	2 (1%)	70	82
29	D	194/245 (79%)	194 (100%)	0	100	100
30	e	198/236 (84%)	193 (98%)	5 (2%)	42	69
31	E	260/290 (90%)	258 (99%)	2 (1%)	73	83
32	f	133/188 (71%)	133 (100%)	0	100	100
33	F	219/262 (84%)	217 (99%)	2 (1%)	70	82
34	g	124/148 (84%)	124 (100%)	0	100	100
35	H	88/228 (39%)	88 (100%)	0	100	100
36	h	104/148 (70%)	104 (100%)	0	100	100
37	I	27/232 (12%)	27 (100%)	0	100	100
38	i	86/110 (78%)	85 (99%)	1 (1%)	63	79
40	j	72/97 (74%)	71 (99%)	1 (1%)	59	78
41	K	154/155 (99%)	153 (99%)	1 (1%)	78	85
43	L	98/124 (79%)	98 (100%)	0	100	100
45	M	246/249 (99%)	243 (99%)	3 (1%)	63	79
46	m	46/113 (41%)	46 (100%)	0	100	100
47	N	25/211 (12%)	24 (96%)	1 (4%)	28	59
48	o	69/87 (79%)	69 (100%)	0	100	100
49	O	134/150 (89%)	133 (99%)	1 (1%)	76	84
50	p	135/181 (75%)	135 (100%)	0	100	100
51	P	126/155 (81%)	125 (99%)	1 (1%)	73	83
52	q	119/178 (67%)	118 (99%)	1 (1%)	73	83
53	Q	203/256 (79%)	201 (99%)	2 (1%)	68	81
54	r	126/169 (75%)	125 (99%)	1 (1%)	73	83
55	R	118/126 (94%)	117 (99%)	1 (1%)	73	83
56	s	340/381 (89%)	340 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	S	146/180 (81%)	145 (99%)	1 (1%)	76	84
58	t	106/331 (32%)	102 (96%)	4 (4%)	29	60
All	All	7903/10458 (76%)	7820 (99%)	83 (1%)	63	80

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	T	138	GLU
2	T	185	THR
3	u	103	GLN
3	u	104	GLU
3	u	210	THR
3	u	213	GLU
6	v	10	LEU
6	v	23	LEU
6	v	59	LEU
6	v	69	ILE
8	V	29	VAL
8	V	44	VAL
8	V	76	VAL
8	V	86	VAL
8	V	152	ARG
9	w	112	SER
10	3	173	VAL
12	x	55	GLN
12	x	139	ILE
12	x	180	LEU
12	x	233	VAL
12	x	320	VAL
12	x	360	VAL
13	5	270	ILE
13	5	273	VAL
13	5	324	GLN
13	5	351	VAL
13	5	356	VAL
14	X	167	LEU
15	y	176	LEU
15	y	296	VAL
15	y	314	GLN
15	y	319	LEU
16	6	151	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	6	312	THR
18	z	73	LEU
18	z	76	LYS
18	z	111	THR
18	z	153	ASN
18	z	226	VAL
18	z	236	MET
18	z	253	VAL
18	z	254	GLN
18	z	258	LEU
19	7	114	ASP
19	7	228	GLU
23	9	55	GLU
23	9	62	VAL
24	b	33	VAL
24	b	75	VAL
24	b	112	VAL
26	c	204	GLN
26	c	240	LEU
28	d	89	VAL
28	d	150	LEU
30	e	68	GLU
30	e	179	GLN
30	e	201	GLU
30	e	240	THR
30	e	253	VAL
31	E	236	THR
31	E	261	MET
33	F	184	GLN
33	F	218	LEU
38	i	43	VAL
40	j	106	GLU
41	K	116	LEU
45	M	61	THR
45	M	99	ASN
45	M	222	TYR
47	N	229	VAL
49	O	65	LEU
51	P	101	VAL
52	q	84	GLU
53	Q	246	ASP
53	Q	275	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	r	70	CYS
55	R	90	LEU
57	S	144	LEU
58	t	55	LEU
58	t	81	LYS
58	t	94	VAL
58	t	132	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	118	GLN
2	T	56	GLN
5	U	27	GLN
5	U	55	ASN
5	U	77	ASN
5	U	84	ASN
8	V	73	GLN
8	V	82	GLN
8	V	117	HIS
11	W	62	HIS
12	x	218	HIS
12	x	314	HIS
12	x	371	ASN
13	5	160	HIS
13	5	384	GLN
14	X	4	HIS
14	X	76	GLN
15	y	284	GLN
15	y	287	ASN
16	6	69	HIS
17	Y	117	GLN
17	Y	179	HIS
18	z	43	GLN
18	z	153	ASN
18	z	290	ASN
18	z	307	GLN
23	9	123	GLN
24	b	25	GLN
24	b	123	ASN
24	b	135	ASN
26	c	204	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	d	119	GLN
28	d	157	HIS
29	D	195	ASN
29	D	235	GLN
29	D	271	ASN
32	f	112	ASN
33	F	223	HIS
34	g	93	ASN
38	i	59	ASN
38	i	111	ASN
38	i	120	HIS
38	i	124	HIS
40	j	105	GLN
41	K	9	GLN
43	L	104	ASN
43	L	113	ASN
45	M	53	HIS
45	M	130	GLN
47	N	210	GLN
48	o	58	GLN
49	O	141	HIS
49	O	150	GLN
50	p	96	ASN
50	p	184	ASN
50	p	194	HIS
51	P	142	ASN
53	Q	209	GLN
54	r	131	HIS
55	R	89	ASN
56	s	238	ASN
56	s	239	ASN
56	s	240	GLN
56	s	298	GLN
56	s	386	ASN
56	s	387	ASN
58	t	51	ASN
58	t	57	GLN
58	t	197	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	A	1409/1589 (88%)	295 (20%)	11 (0%)
27	B	71/72 (98%)	12 (16%)	0
All	All	1480/1661 (89%)	307 (20%)	11 (0%)

All (307) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
25	A	1672	C
25	A	1676	A
25	A	1678	C
25	A	1681	G
25	A	1689	C
25	A	1694	U
25	A	1700	U
25	A	1704	U
25	A	1707	C
25	A	1708	A
25	A	1709	G
25	A	1711	C
25	A	1713	A
25	A	1715	C
25	A	1724	A
25	A	1727	A
25	A	1731	A
25	A	1748	G
25	A	1750	G
25	A	1751	A
25	A	1761	A
25	A	1765	C
25	A	1767	G
25	A	1770	G
25	A	1780	U
25	A	1791	G
25	A	1805	A
25	A	1807	U
25	A	1808	A
25	A	1810	A
25	A	1821	A
25	A	1827	C
25	A	1828	A
25	A	1829	A
25	A	1832	A
25	A	1836	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	1844	A
25	A	1854	U
25	A	1855	A
25	A	1869	A
25	A	1871	A
25	A	1882	A
25	A	1883	G
25	A	1887	A
25	A	1892	A
25	A	1893	A
25	A	1903	C
25	A	1909	A
25	A	1918	G
25	A	1937	A
25	A	1940	A
25	A	1974	A
25	A	1984	A
25	A	1985	G
25	A	1992	C
25	A	1994	A
25	A	2000	C
25	A	2015	G
25	A	2021	U
25	A	2022	G
25	A	2029	A
25	A	2030	U
25	A	2031	A
25	A	2036	C
25	A	2037	U
25	A	2060	A
25	A	2065	A
25	A	2068	C
25	A	2071	U
25	A	2074	A
25	A	2079	C
25	A	2083	U
25	A	2098	G
25	A	2105	G
25	A	2106	A
25	A	2107	G
25	A	2114	C
25	A	2115	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	2117	U
25	A	2125	C
25	A	2126	U
25	A	2131	A
25	A	2132	A
25	A	2147	G
25	A	2154	A
25	A	2158	U
25	A	2161	A
25	A	2162	C
25	A	2163	A
25	A	2165	C
25	A	2168	U
25	A	2169	A
25	A	2171	U
25	A	2172	A
25	A	2173	G
25	A	2181	A
25	A	2182	G
25	A	2183	C
25	A	2184	A
25	A	2187	C
25	A	2194	U
25	A	2197	G
25	A	2198	A
25	A	2202	C
25	A	2204	U
25	A	2211	U
25	A	2237	A
25	A	2239	A
25	A	2241	A
25	A	2245	A
25	A	2246	A
25	A	2262	C
25	A	2263	C
25	A	2283	C
25	A	2284	C
25	A	2285	U
25	A	2293	A
25	A	2297	A
25	A	2299	U
25	A	2300	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	2322	C
25	A	2332	C
25	A	2345	G
25	A	2351	U
25	A	2352	U
25	A	2353	A
25	A	2354	A
25	A	2356	A
25	A	2359	C
25	A	2360	U
25	A	2361	G
25	A	2362	A
25	A	2363	A
25	A	2374	A
25	A	2375	C
25	A	2381	A
25	A	2390	A
25	A	2393	C
25	A	2396	C
25	A	2401	A
25	A	2405	C
25	A	2406	A
25	A	2407	U
25	A	2415	C
25	A	2417	C
25	A	2432	A
25	A	2441	C
25	A	2444	A
25	A	2445	U
25	A	2446	A
25	A	2451	A
25	A	2452	A
25	A	2458	A
25	A	2478	G
25	A	2480	A
25	A	2485	U
25	A	2493	C
25	A	2500	A
25	A	2502	C
25	A	2506	A
25	A	2507	A
25	A	2511	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	2520	C
25	A	2521	A
25	A	2523	C
25	A	2527	A
25	A	2531	U
25	A	2540	C
25	A	2671	C
25	A	2676	G
25	A	2685	U
25	A	2687	U
25	A	2691	U
25	A	2714	C
25	A	2715	C
25	A	2717	G
25	A	2737	A
25	A	2745	A
25	A	2750	G
25	A	2752	G
25	A	2753	A
25	A	2754	A
25	A	2758	C
25	A	2763	G
25	A	2775	U
25	A	2776	A
25	A	2832	A
25	A	2840	C
25	A	2841	G
25	A	2844	U
25	A	2845	G
25	A	2846	G
25	A	2847	G
25	A	2849	C
25	A	2860	C
25	A	2862	G
25	A	2863	A
25	A	2864	A
25	A	2872	U
25	A	2878	C
25	A	2885	U
25	A	2895	U
25	A	2896	C
25	A	2900	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	2911	A
25	A	2920	C
25	A	2937	C
25	A	2942	C
25	A	2944	A
25	A	2947	G
25	A	2948	G
25	A	2953	A
25	A	2957	A
25	A	2959	C
25	A	2965	G
25	A	2974	G
25	A	2975	C
25	A	2978	U
25	A	2982	A
25	A	2984	U
25	A	2985	C
25	A	2987	A
25	A	2990	G
25	A	2991	U
25	A	2992	C
25	A	2993	C
25	A	2994	A
25	A	2995	U
25	A	2996	A
25	A	2997	U
25	A	3003	A
25	A	3004	U
25	A	3008	G
25	A	3031	A
25	A	3036	A
25	A	3038	C
25	A	3047	G
25	A	3048	C
25	A	3051	C
25	A	3052	C
25	A	3053	G
25	A	3054	C
25	A	3059	A
25	A	3060	A
25	A	3067	G
25	A	3068	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	3070	U
25	A	3072	U
25	A	3073	U
25	A	3074	C
25	A	3084	A
25	A	3085	G
25	A	3087	C
25	A	3090	A
25	A	3091	C
25	A	3092	G
25	A	3094	G
25	A	3103	U
25	A	3104	C
25	A	3117	U
25	A	3120	A
25	A	3127	U
25	A	3128	U
25	A	3131	U
25	A	3132	A
25	A	3133	U
25	A	3139	U
25	A	3141	C
25	A	3142	A
25	A	3143	A
25	A	3144	A
25	A	3153	U
25	A	3155	U
25	A	3162	G
25	A	3165	C
25	A	3168	G
25	A	3181	U
25	A	3186	C
25	A	3188	C
25	A	3189	A
25	A	3193	C
25	A	3200	C
25	A	3203	C
25	A	3211	A
25	A	3214	U
25	A	3220	C
25	A	3221	A
25	A	3228	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	A	3237	C
25	A	3238	A
25	A	3239	C
25	A	3243	C
25	A	3248	A
25	A	3249	A
25	A	3259	U
27	B	1603	A
27	B	1611	G
27	B	1617	C
27	B	1621	A
27	B	1644	G
27	B	1646	U
27	B	1647	U
27	B	1650	A
27	B	1652	C
27	B	1653	U
27	B	1654	U
27	B	1656	A

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	2030	U
25	A	2182	G
25	A	2186	C
25	A	2245	A
25	A	2530	A
25	A	2846	G
25	A	2936	A
25	A	2994	A
25	A	2995	U
25	A	3071	G
25	A	3073	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
5	AYA	U	2	5	6,7,8	1.33	1 (16%)	6,8,10	1.01	1 (16%)
42	AYA	k	2	42	6,7,8	1.24	1 (16%)	6,8,10	1.09	1 (16%)
41	SAC	K	2	41	7,8,9	1.02	0	7,9,11	0.97	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
5	AYA	U	2	5	-	2/5/6/8	-
42	AYA	k	2	42	-	0/5/6/8	-
41	SAC	K	2	41	-	3/7/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	2	AYA	CA-N	-2.60	1.43	1.46
42	k	2	AYA	CA-N	-2.19	1.44	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	k	2	AYA	CB-CA-N	2.48	112.48	109.68
5	U	2	AYA	CB-CA-N	2.33	112.31	109.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	U	2	AYA	O-C-CA-CB
41	K	2	SAC	O-C-CA-CB
41	K	2	SAC	N-CA-CB-OG
41	K	2	SAC	C-CA-CB-OG
5	U	2	AYA	C-CA-N-CT

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 111 ligands modelled in this entry, 107 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PM8	w	200	9	26,31,31	1.81	6 (23%)	30,38,38	1.83	9 (30%)
62	GNP	z	401	63	34,34,34	1.27	5 (14%)	47,54,54	0.65	0
61	SAM	x	401	-	27,29,29	1.10	4 (14%)	34,42,42	2.00	9 (26%)
62	GNP	t	1000	63	34,34,34	1.32	5 (14%)	47,54,54	0.62	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
60	PM8	w	200	9	-	17/36/38/38	-
62	GNP	z	401	63	-	6/18/38/38	0/3/3/3
61	SAM	x	401	-	-	8/17/33/33	0/3/3/3
62	GNP	t	1000	63	-	3/18/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	w	200	PM8	C34-N36	5.66	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	w	200	PM8	C39-N41	5.01	1.45	1.33
62	t	1000	GNP	PB-O3A	4.61	1.64	1.59
62	z	401	GNP	PB-O3A	4.32	1.64	1.59
62	t	1000	GNP	PB-O1B	3.29	1.51	1.46
62	z	401	GNP	PB-O1B	3.10	1.50	1.46
62	t	1000	GNP	PG-N3B	2.97	1.71	1.63
62	z	401	GNP	PG-N3B	2.87	1.70	1.63
62	t	1000	GNP	PG-O1G	2.79	1.50	1.46
62	z	401	GNP	PG-O1G	2.72	1.50	1.46
61	x	401	SAM	C2-N3	2.60	1.38	1.33
61	x	401	SAM	C2-N1	2.52	1.38	1.33
60	w	200	PM8	O35-C34	-2.50	1.18	1.23
60	w	200	PM8	C1-S1	2.36	1.81	1.76
62	t	1000	GNP	PB-O2B	-2.27	1.50	1.56
61	x	401	SAM	OXT-C	-2.23	1.23	1.30
62	z	401	GNP	PB-O2B	-2.21	1.50	1.56
60	w	200	PM8	O40-C39	-2.13	1.19	1.23
60	w	200	PM8	C2-C1	2.09	1.53	1.50
61	x	401	SAM	C8-N7	2.01	1.35	1.31

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	w	200	PM8	C2-C1-S1	5.66	120.14	113.40
61	x	401	SAM	N3-C2-N1	-5.46	120.31	128.58
61	x	401	SAM	C5-C4-N3	-4.61	120.37	126.72
61	x	401	SAM	N9-C8-N7	-3.75	108.62	113.94
61	x	401	SAM	C2-N3-C4	3.41	120.16	111.83
60	w	200	PM8	O1-C1-C2	-3.39	120.07	123.98
61	x	401	SAM	C5-N7-C8	3.35	108.72	103.45
60	w	200	PM8	C37-C38-C39	3.16	117.66	112.39
61	x	401	SAM	N3-C4-N9	3.13	132.48	127.17
60	w	200	PM8	C32-C34-N36	3.08	122.32	116.48
61	x	401	SAM	OXT-C-O	-2.76	117.81	124.08
60	w	200	PM8	O40-C39-N41	-2.39	118.34	123.03
61	x	401	SAM	C4-C5-N7	-2.29	107.96	110.58
61	x	401	SAM	C3'-C2'-C1'	2.29	105.79	101.46
60	w	200	PM8	O1-C1-S1	-2.27	119.79	122.68
60	w	200	PM8	C43-S1-C1	2.26	108.53	101.84
60	w	200	PM8	C38-C39-N41	2.18	120.32	116.34
60	w	200	PM8	C37-N36-C34	-2.04	118.89	122.55

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	w	200	PM8	O27-C28-C29-C30
60	w	200	PM8	O27-C28-C29-C31
60	w	200	PM8	O27-C28-C29-C32
60	w	200	PM8	C32-C34-N36-C37
60	w	200	PM8	N36-C37-C38-C39
60	w	200	PM8	N41-C42-C43-S1
60	w	200	PM8	C1-C2-C3-C4
61	x	401	SAM	N-CA-CB-CG
61	x	401	SAM	C-CA-CB-CG
61	x	401	SAM	CB-CG-SD-CE
61	x	401	SAM	CB-CG-SD-C5'
61	x	401	SAM	C4'-C5'-SD-CE
62	z	401	GNP	PG-N3B-PB-O1B
62	z	401	GNP	PG-N3B-PB-O3A
62	z	401	GNP	PA-O3A-PB-O2B
62	t	1000	GNP	PG-N3B-PB-O1B
60	w	200	PM8	C38-C39-N41-C42
60	w	200	PM8	O35-C34-N36-C37
60	w	200	PM8	O40-C39-N41-C42
62	z	401	GNP	O4'-C4'-C5'-O5'
62	z	401	GNP	C3'-C4'-C5'-O5'
61	x	401	SAM	C2'-C1'-N9-C8
60	w	200	PM8	C3-C4-C5-C6
60	w	200	PM8	O1-C1-S1-C43
60	w	200	PM8	C2-C1-S1-C43
60	w	200	PM8	C5-C6-C7-C8
60	w	200	PM8	O33-C32-C34-O35
60	w	200	PM8	C6-C7-C8-C9
61	x	401	SAM	C2'-C1'-N9-C4
61	x	401	SAM	O4'-C1'-N9-C8
62	t	1000	GNP	O4'-C4'-C5'-O5'
62	z	401	GNP	PA-O3A-PB-O1B
60	w	200	PM8	O33-C32-C34-N36
62	t	1000	GNP	PB-O3A-PA-O1A

There are no ring outliers.

3 monomers are involved in 8 short contacts:

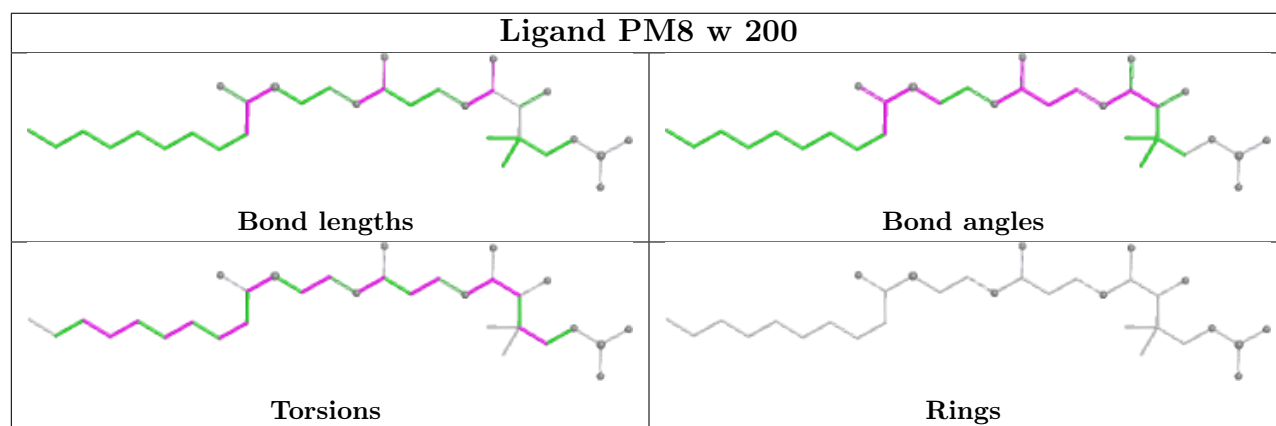
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	w	200	PM8	2	0

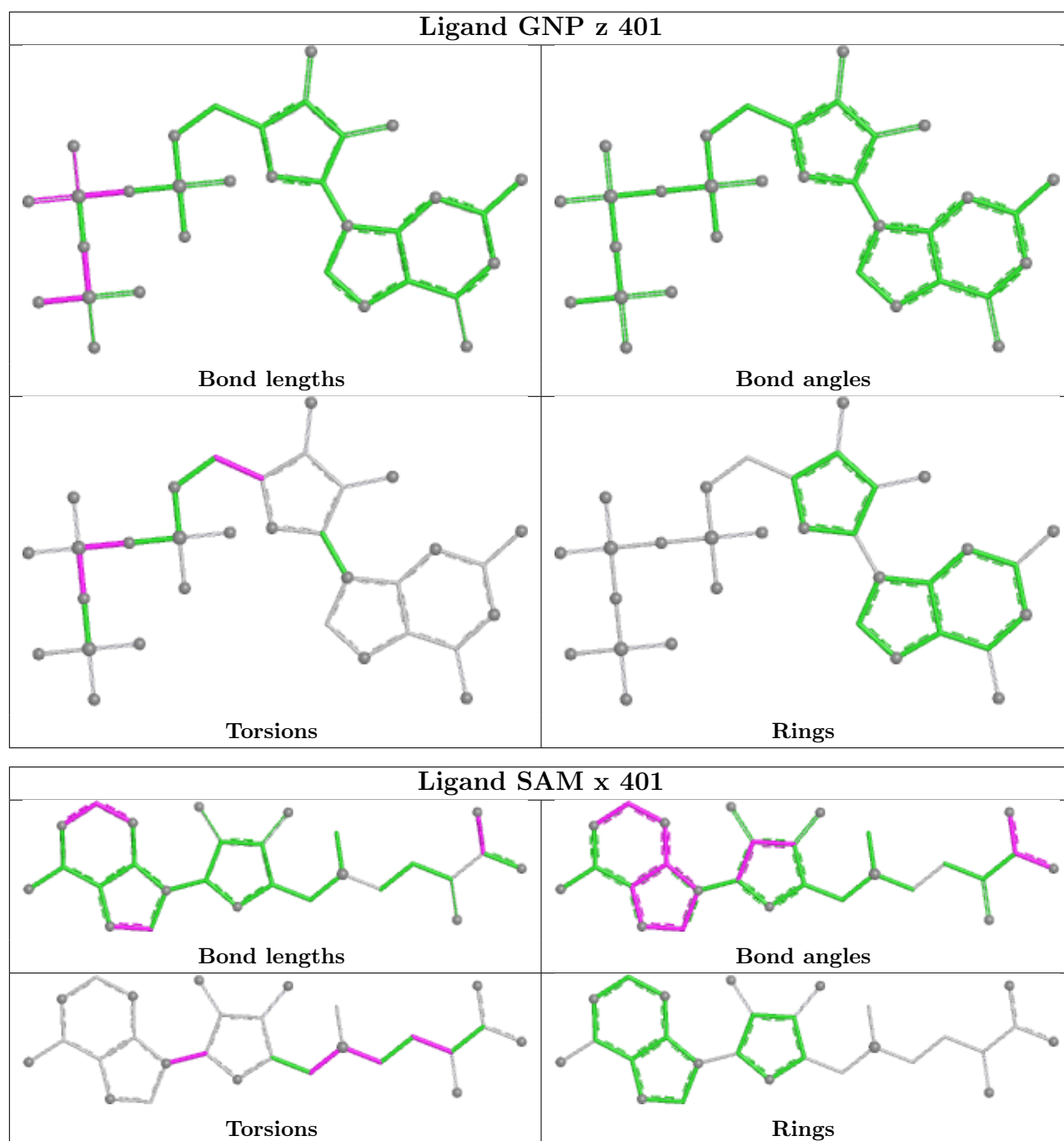
Continued on next page...

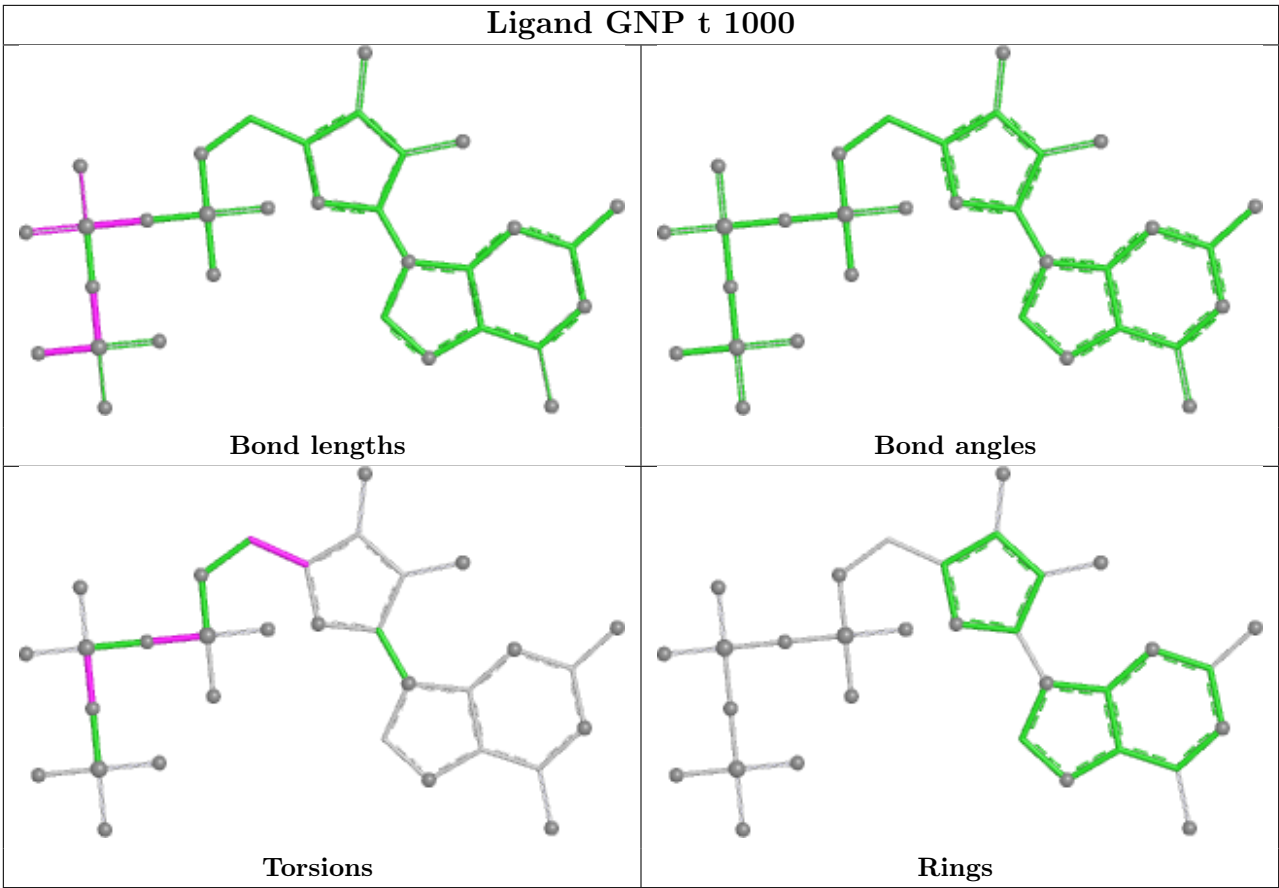
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	z	401	GNP	2	0
61	x	401	SAM	4	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2554:U	O3'	2555:A	P	17.72
1	A	2570:U	O3'	2571:A	P	17.44
1	A	2547:C	O3'	2548:U	P	12.62

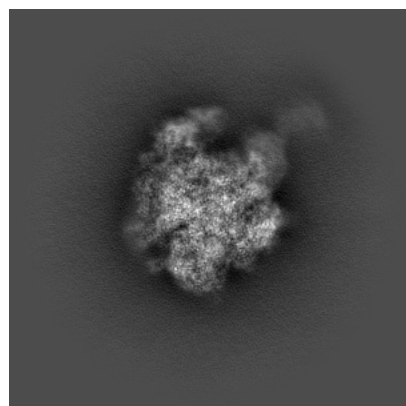
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17719. These allow visual inspection of the internal detail of the map and identification of artifacts.

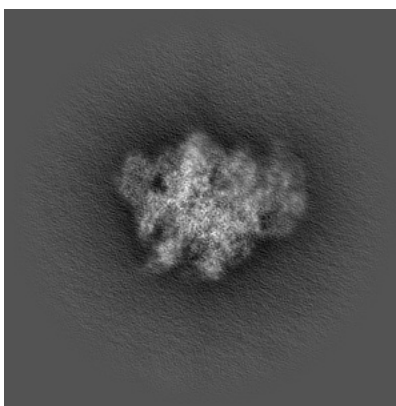
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

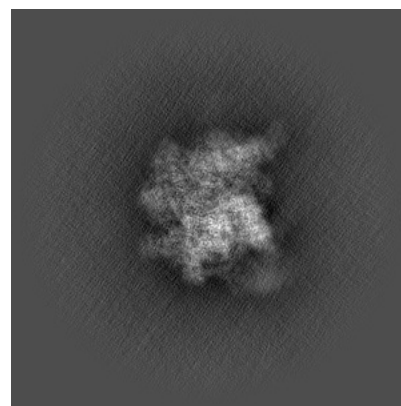
6.1.1 Primary map



X

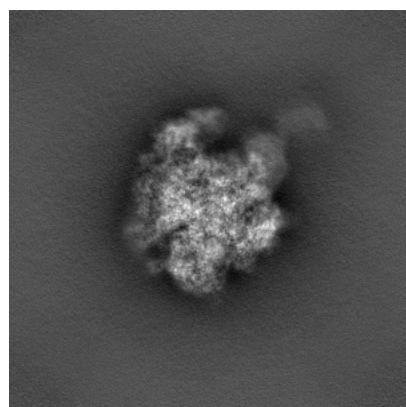


Y

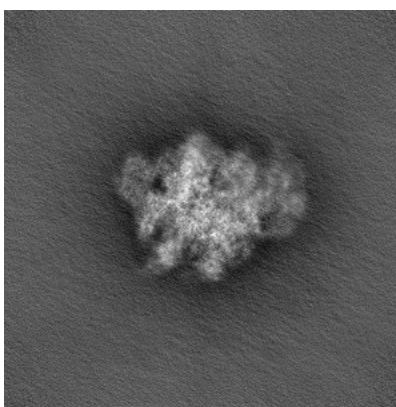


Z

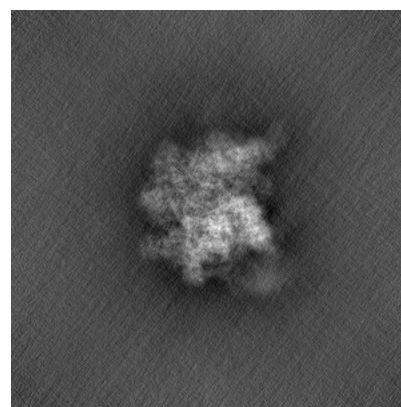
6.1.2 Raw map



X



Y

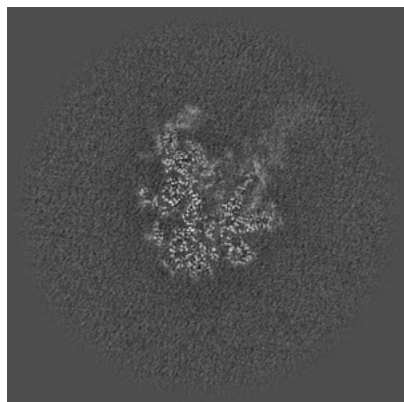


Z

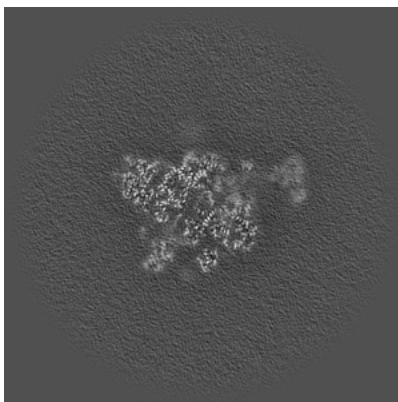
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

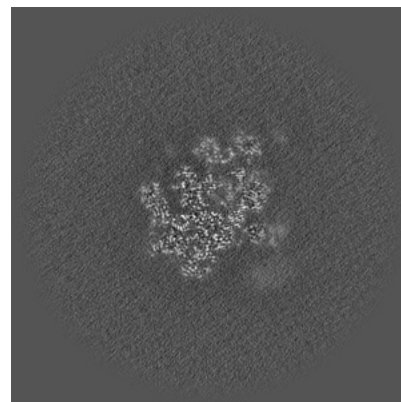
6.2.1 Primary map



X Index: 240

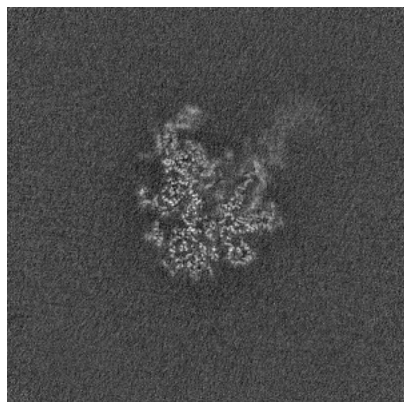


Y Index: 240

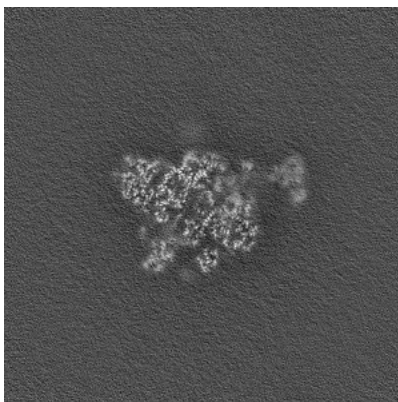


Z Index: 240

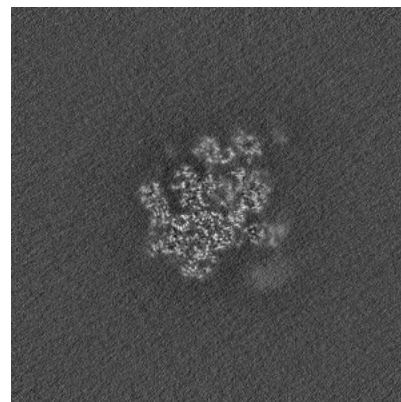
6.2.2 Raw map



X Index: 240



Y Index: 240

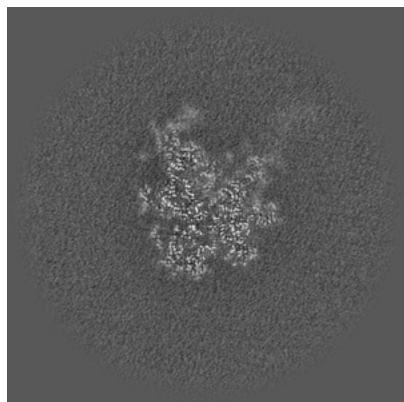


Z Index: 240

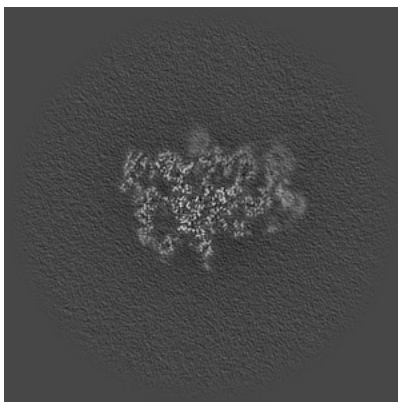
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

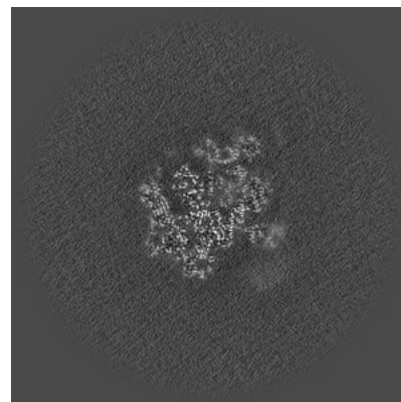
6.3.1 Primary map



X Index: 237

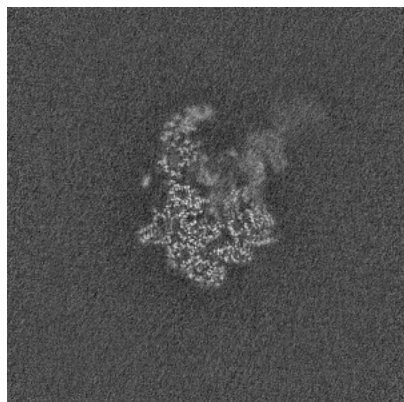


Y Index: 217

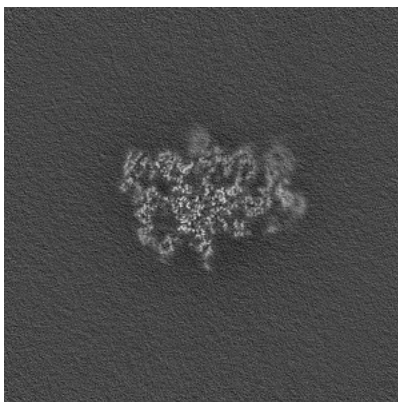


Z Index: 242

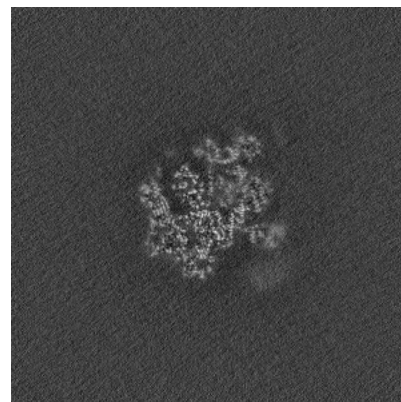
6.3.2 Raw map



X Index: 250



Y Index: 217

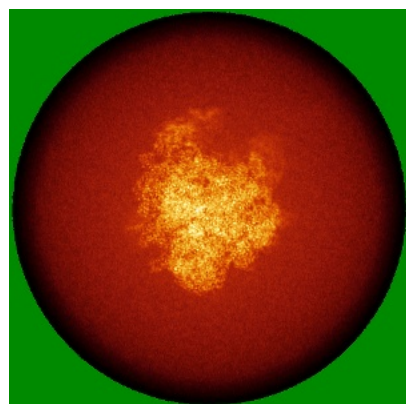


Z Index: 242

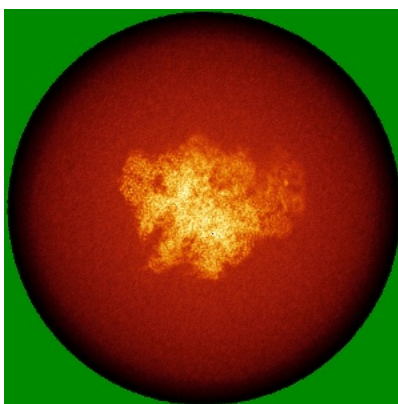
The images above show the largest variance slices of the map in three orthogonal directions.

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

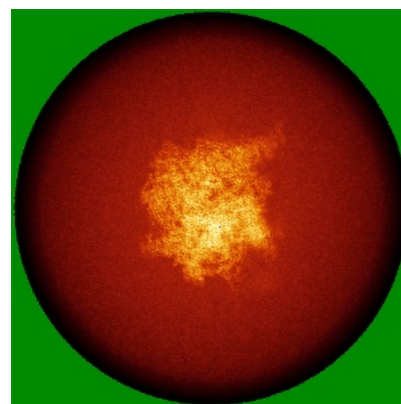
6.4.1 Primary map



X

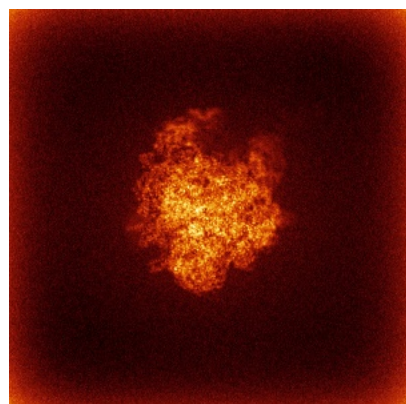


Y

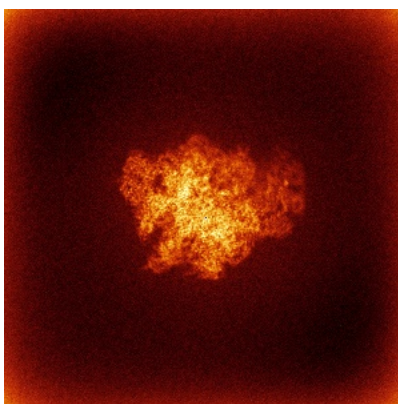


Z

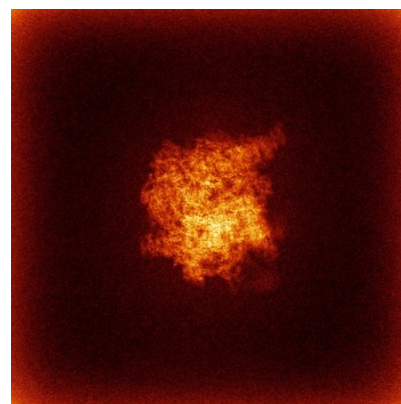
6.4.2 Raw map



X



Y

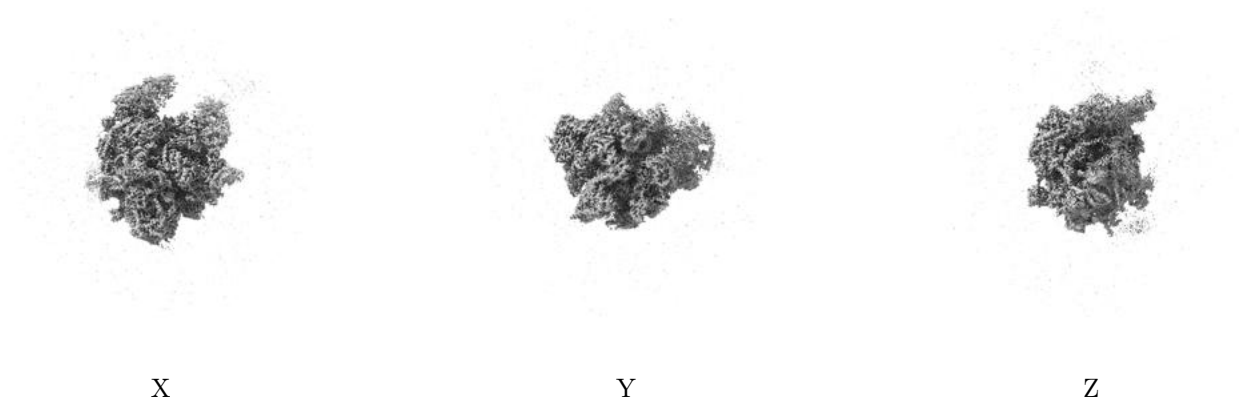


Z

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

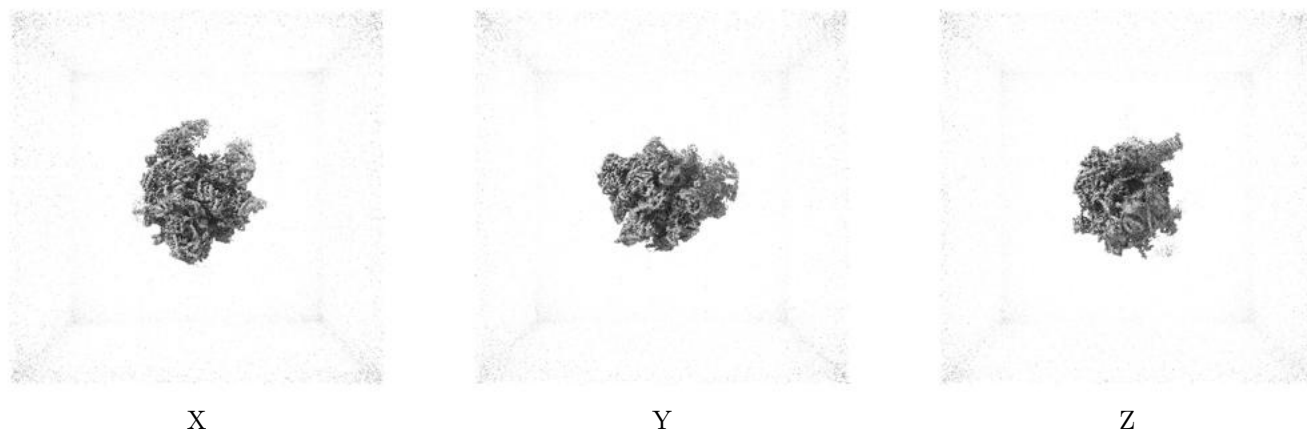
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.747. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

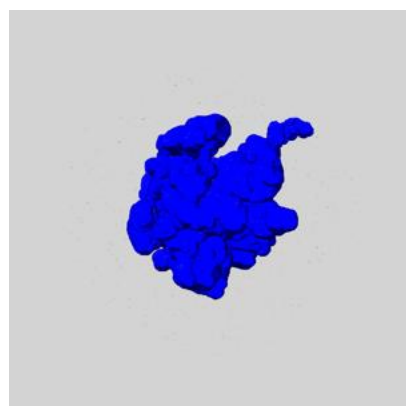
6.6 Mask visualisation [i](#)

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

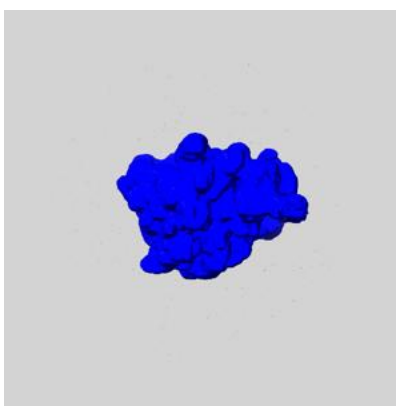
A mask typically either:

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

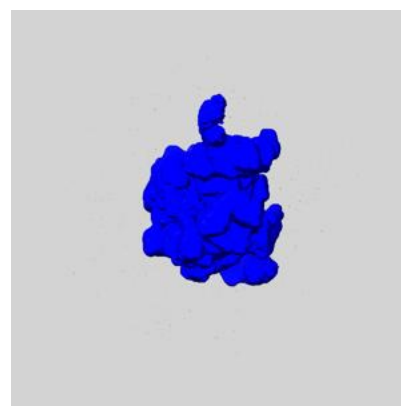
6.6.1 emd_17719_msk_1.map [i](#)



X



Y

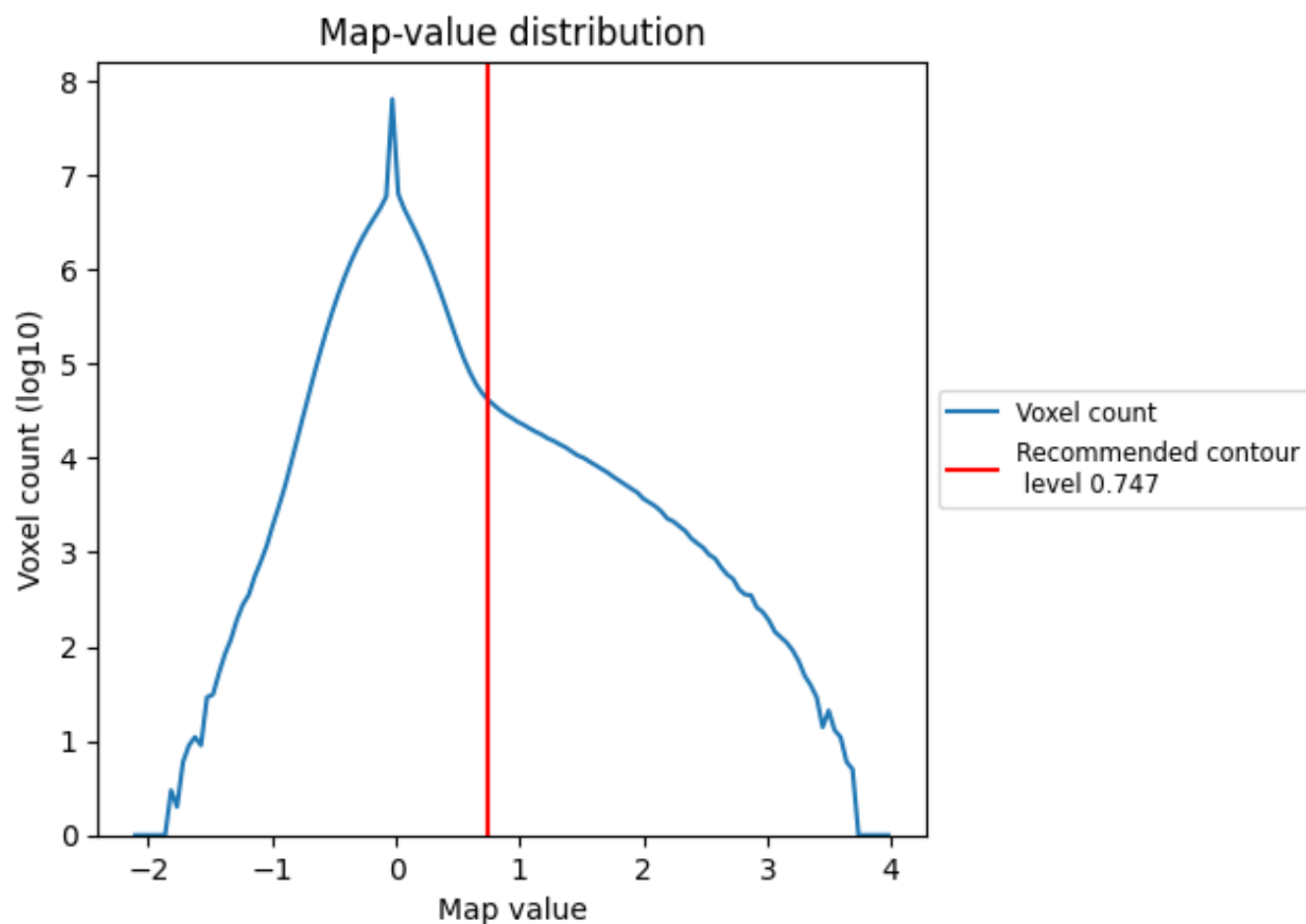


Z

7 Map analysis [i](#)

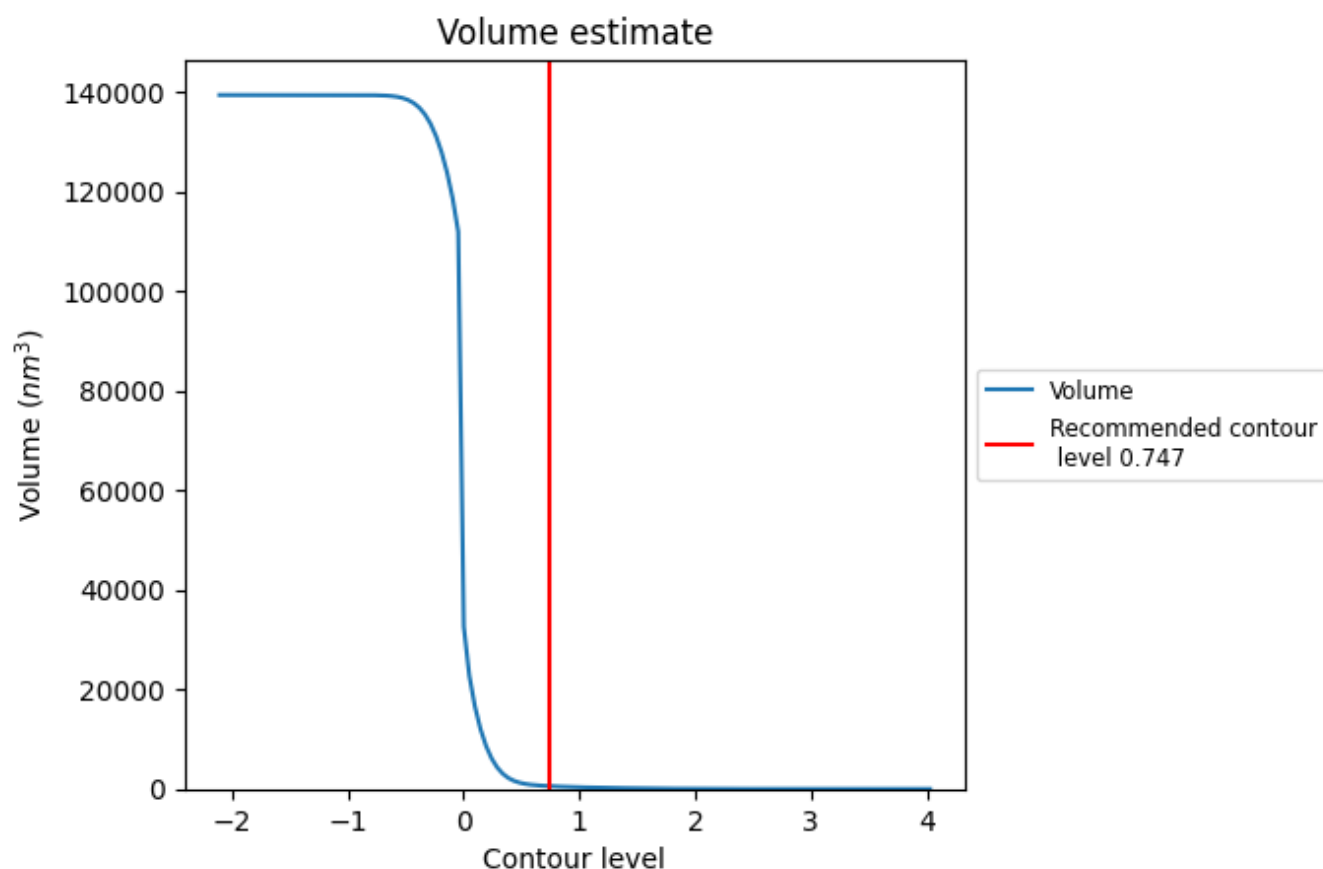
This section contains the results of statistical analysis of the map.

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.

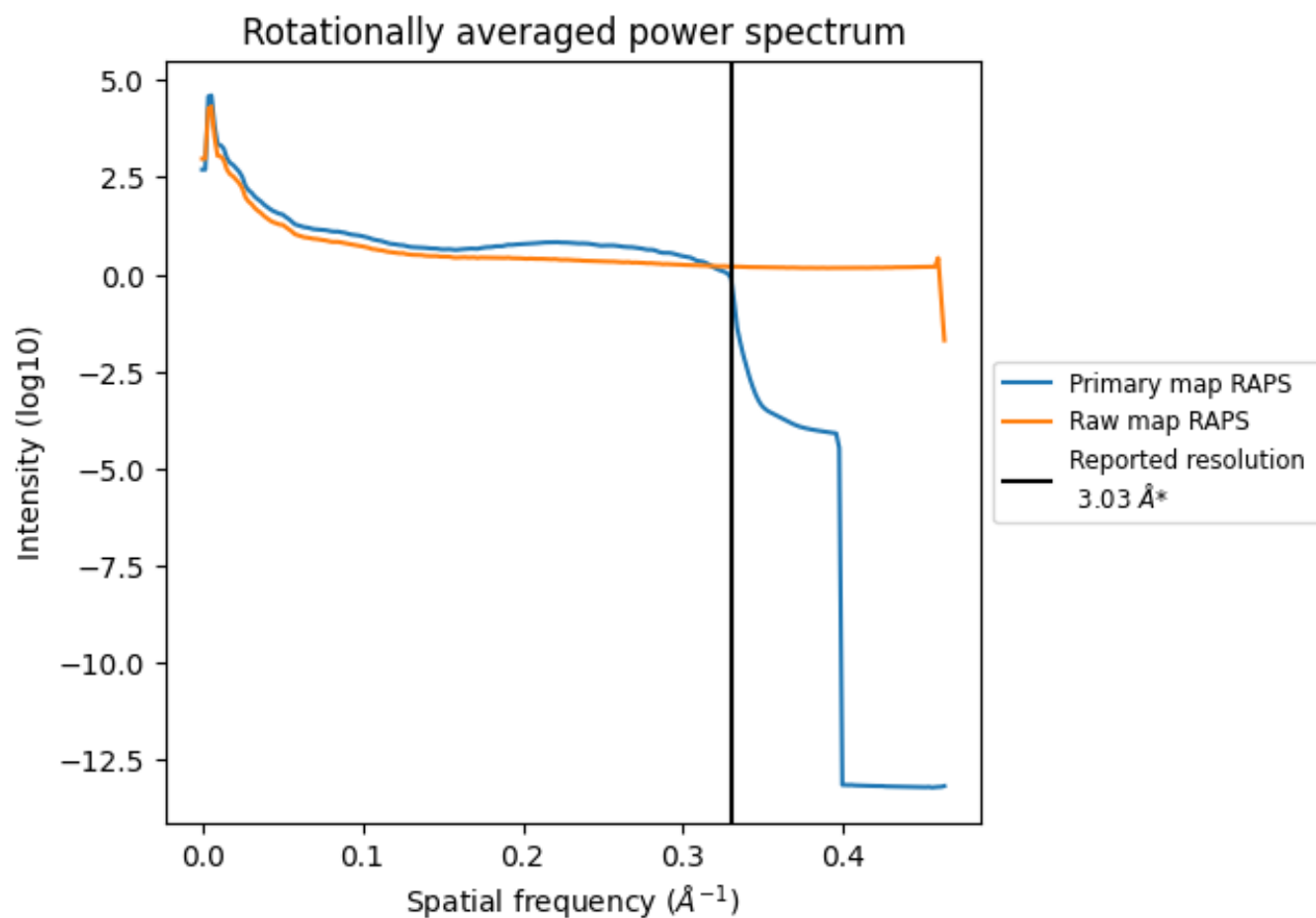
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 564 nm³; this corresponds to an approximate mass of 510 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 ⓘ

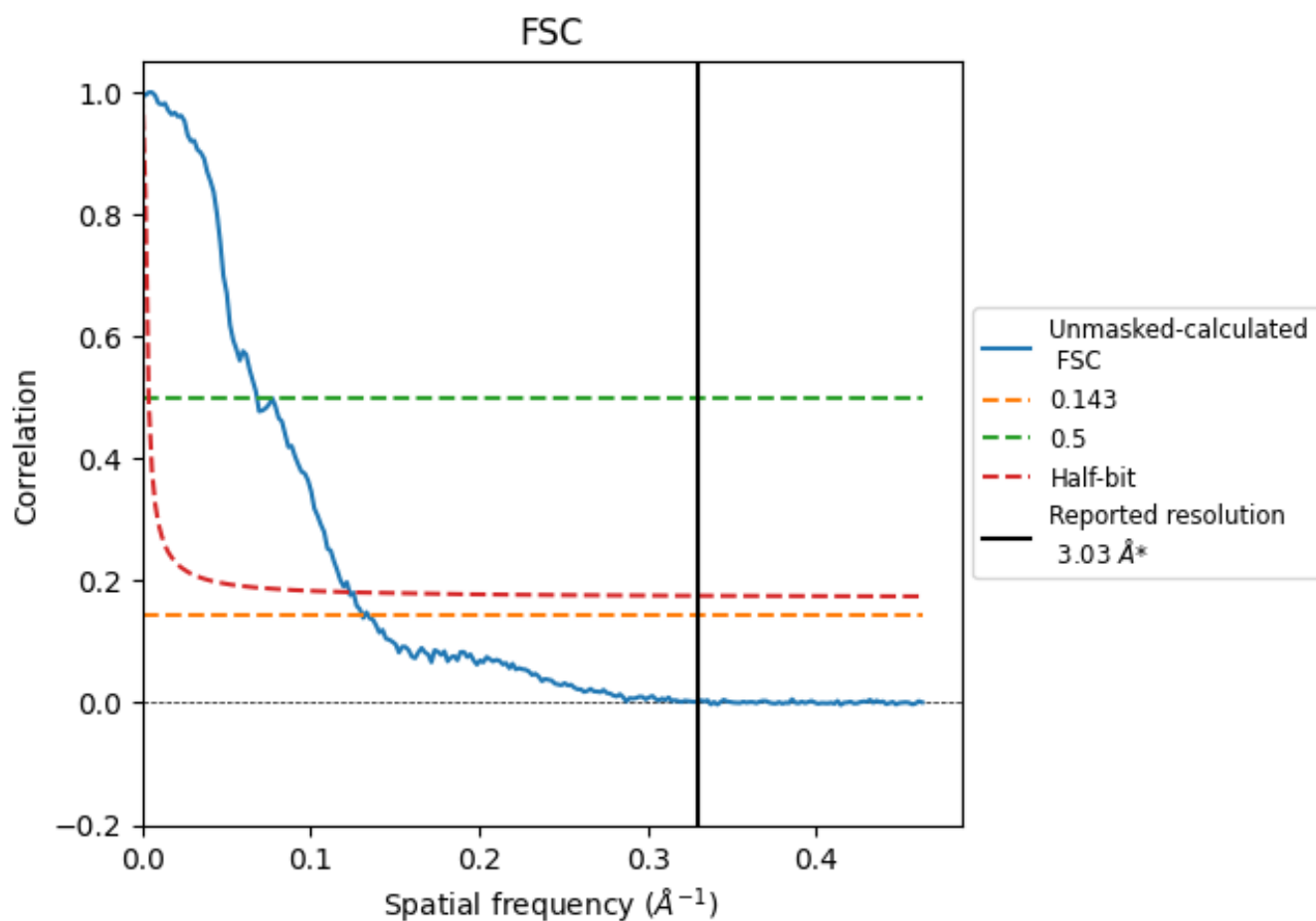


*Reported resolution corresponds to spatial frequency of 0.330 Å⁻¹

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 0.330 Å⁻¹

8.2 Resolution estimates [i](#)

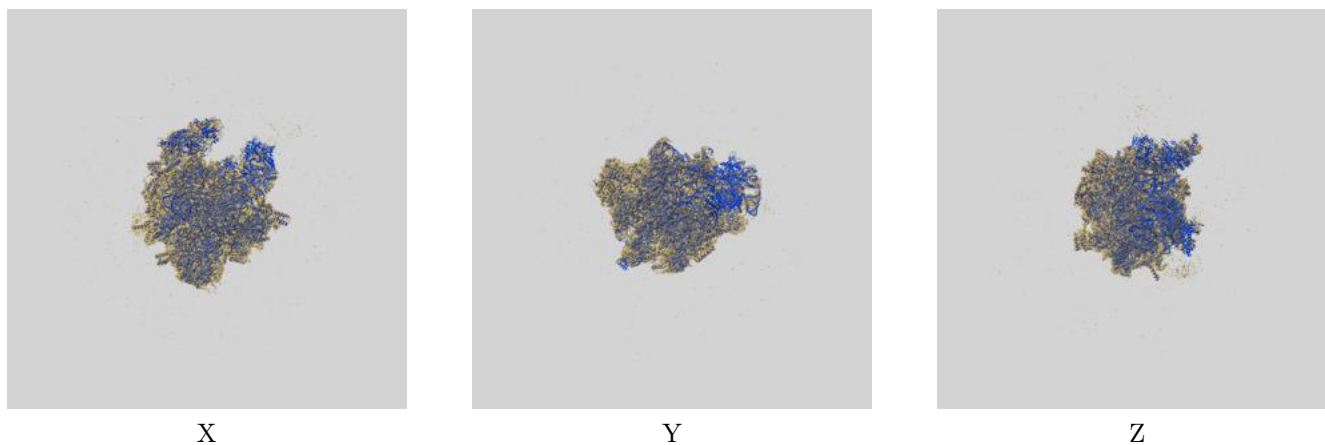
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.66	14.68	8.13

*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 7.66 differs from the reported value 3.03 by more than 10 %

9 Map-model fit [i](#)

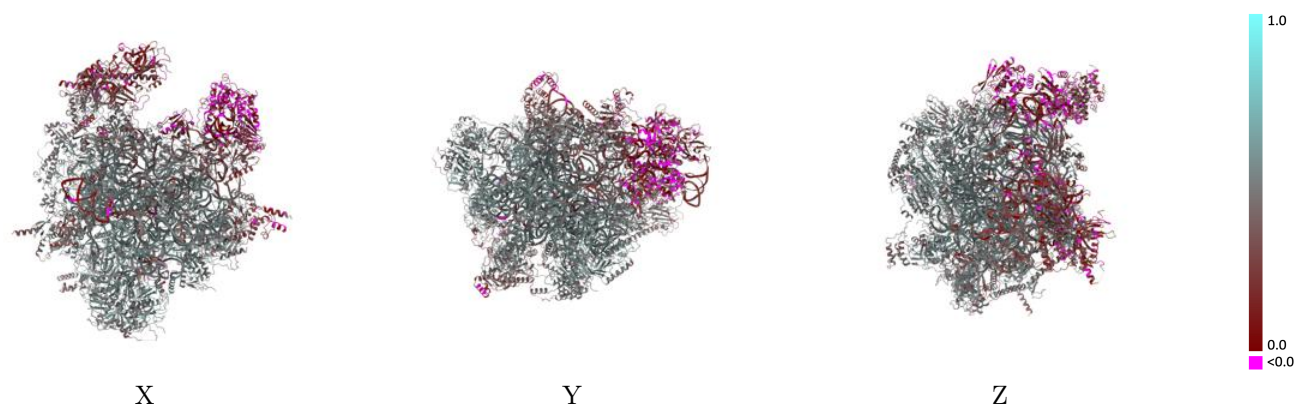
This section contains information regarding the fit between EMDB map EMD-17719 and PDB model 8PK0. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



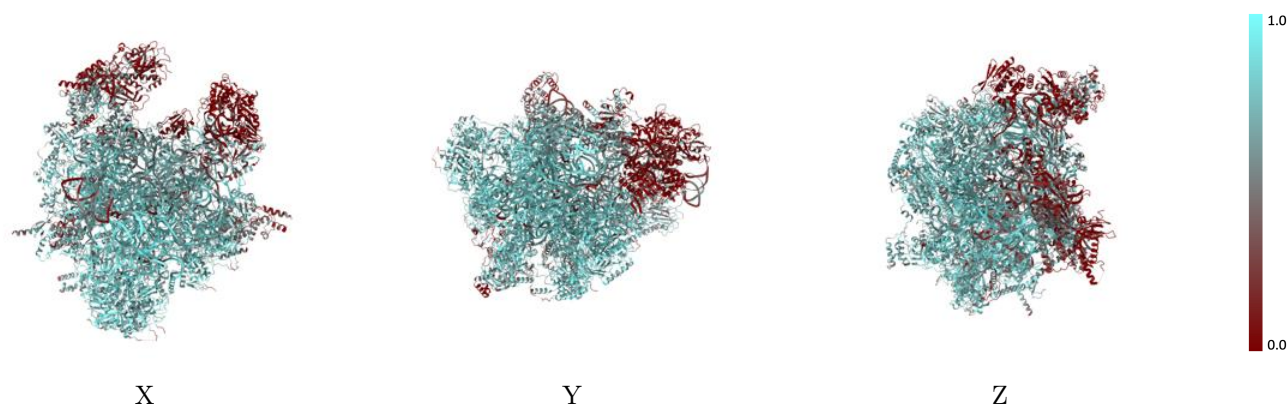
The images above show the 3D surface view of the map at the recommended contour level 0.747 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



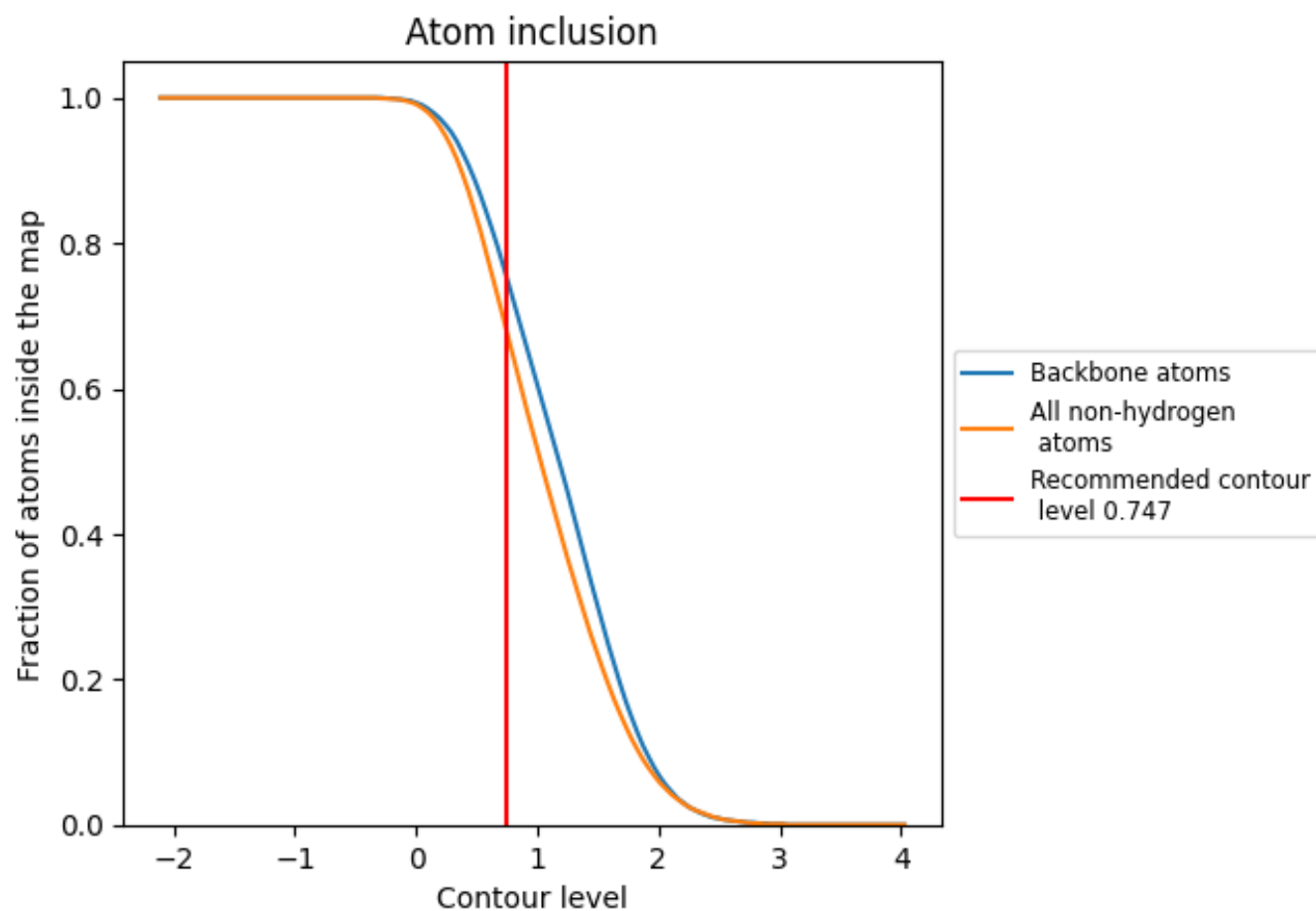
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.747).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 68% 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 (0.747) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6800	 0.4550
0	 0.7520	 0.5190
1	 0.6810	 0.4910
2	 0.8310	 0.5780
3	 0.8300	 0.5760
5	 0.7690	 0.5100
6	 0.6210	 0.4180
7	 0.6830	 0.4410
8	 0.2150	 0.2230
9	 0.7520	 0.4980
A	 0.7870	 0.4750
B	 0.5510	 0.2720
D	 0.7420	 0.5150
E	 0.7180	 0.5090
F	 0.8000	 0.5360
H	 0.6490	 0.4750
I	 0.1430	 0.1430
J	 0.0260	 0.0530
K	 0.7580	 0.5220
L	 0.6800	 0.5140
M	 0.7890	 0.5310
N	 0.2550	 0.2650
O	 0.7900	 0.5300
P	 0.6860	 0.4740
Q	 0.7310	 0.4990
R	 0.7900	 0.5420
S	 0.7460	 0.5270
T	 0.7920	 0.5460
U	 0.7050	 0.4860
V	 0.6440	 0.4490
W	 0.7180	 0.5200
X	 0.7470	 0.5140
Y	 0.7580	 0.5170
Z	 0.7330	 0.5180
a	 0.6920	 0.4900



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.8000	 0.5300
c	 0.7260	 0.4860
d	 0.5370	 0.3870
e	 0.1180	 0.1790
f	 0.2380	 0.2840
g	 0.7950	 0.5290
h	 0.6800	 0.4390
i	 0.8130	 0.5580
j	 0.7450	 0.4930
k	 0.0380	 0.1050
l	 0.0960	 0.1110
m	 0.0750	 0.1910
o	 0.7440	 0.5120
p	 0.5680	 0.4360
q	 0.6560	 0.4470
r	 0.6340	 0.4350
s	 0.7750	 0.5270
t	 0.4460	 0.3430
u	 0.5710	 0.4150
v	 0.4910	 0.3380
w	 0.2540	 0.2030
x	 0.5790	 0.4350
y	 0.5700	 0.4320
z	 0.6520	 0.4700