



## Full wwPDB EM Validation Report ⓘ

Oct 12, 2021 – 10:08 am BST

PDB ID : 7OI6  
EMDB ID : EMD-12919  
Title : Cryo-EM structure of late human 39S mitoribosome assembly intermediates, state 1  
Authors : Cheng, J.; Berninghausen, O.; Beckmann, R.  
Deposited on : 2021-05-11  
Resolution : 5.70 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](mailto: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.

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

EMDB validation analysis : 0.0.0.dev97  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

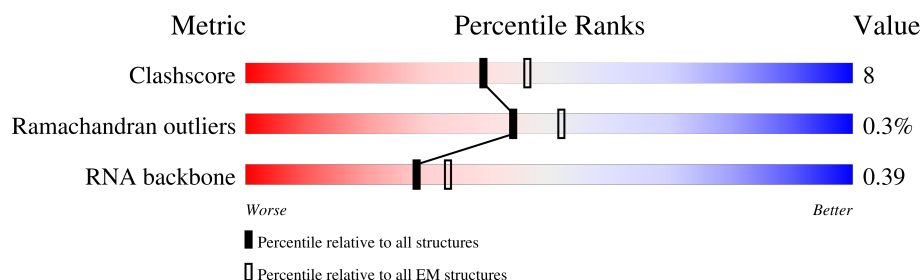
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.70 Å.

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




























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
RNA backbone	4643	859

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  $\geq 3$ , 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	D	305	<div> <div>8%</div> <div>62%</div> <div>10%</div> <div>28%</div> </div>
2	E	348	<div> <div>73%</div> <div>9%</div> <div>18%</div> </div>
3	F	311	<div> <div>75%</div> <div>5%</div> <div>20%</div> </div>
4	H	267	<div> <div>33%</div> <div>64%</div> </div>
5	K	178	<div> <div>93%</div> <div>6%</div> </div>
6	L	145	<div> <div>72%</div> <div>7%</div> <div>21%</div> </div>
7	M	296	<div> <div>82%</div> <div>13%</div> </div>
8	N	251	<div> <div>9%</div> <div>75%</div> <div>7%</div> <div>18%</div> </div>





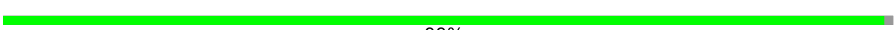





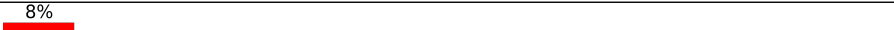

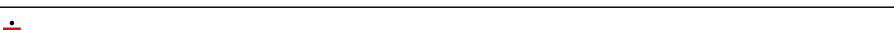






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Mol	Chain	Length	Quality of chain
9	O	175	
10	Q	292	
11	R	149	
12	S	205	
13	T	206	
14	U	153	
15	V	216	
16	X	256	
17	Y	250	
18	Z	161	
19	0	188	
20	2	92	
21	5	423	
22	7	338	
23	9	137	
24	a	142	
25	b	215	
26	c	332	
27	d	306	
28	g	166	
29	h	158	
30	i	128	
31	j	123	
32	o	102	
33	p	206	

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Mol	Chain	Length	Quality of chain
34	q	222	
35	r	196	
36	s	439	
37	u	234	
38	v	70	
39	w	156	
40	A	1559	
41	x	540	
42	y	387	
43	1	420	
43	z	420	
44	B	69	
45	P	180	
46	W	148	
47	6	380	
48	I	261	
49	J	192	
50	k	112	
51	l	138	

## 2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 69386 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 L2, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	D	220	Total	C	N	O	0	0
			1076	636	220	220		

- Molecule 2 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	285	Total	C	N	O	0	0
			1399	829	285	285		

- Molecule 3 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	250	Total	C	N	O	0	0
			1233	733	250	250		

- Molecule 4 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	95	Total	C	N	O	0	0
			469	279	95	95		

- Molecule 5 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	177	Total	C	N	O	0	0
			876	522	177	177		

- Molecule 6 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	115	Total	C	N	O	0	0
			565	335	115	115		

- Molecule 7 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	257	Total	C	N	O	0	0
			1266	752	257	257		

- Molecule 8 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	N	205	Total	C	N	O	0	0
			1006	596	205	205		

- Molecule 9 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	O	152	Total	C	N	O	0	0
			749	445	152	152		

- Molecule 10 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	Q	217	Total	C	N	O	0	0
			1075	641	217	217		

- Molecule 11 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	R	140	Total	C	N	O	0	0
			693	413	140	140		

- Molecule 12 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	S	156	Total	C	N	O	0	0
			772	460	156	156		

- Molecule 13 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	T	159	Total	C	N	O	0	0
			788	470	159	159		

- Molecule 14 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	U	139	Total	C	N	O	0	0
			686	408	139	139		

- Molecule 15 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	V	192	Total	C	N	O	0	0
			946	562	192	192		

- Molecule 16 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	X	243	Total	C	N	O	0	0
			1202	716	243	243		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Y	176	Total	C	N	O	0	0
			874	522	176	176		

- Molecule 18 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Z	120	Total	C	N	O	0	0
			595	355	120	120		

- Molecule 19 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	0	108	Total	C	N	O	0	0
			534	318	108	108		

- Molecule 20 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	2	43	Total	C	N	O	0	0
			211	125	43	43		

- Molecule 21 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	5	387	Total	C	N	O	0	0
			1916	1142	387	387		

- Molecule 22 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	7	287	Total	C	N	O	0	0
			1426	852	287	287		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
23	9	117	Total	C	N	O	0	0
			575	341	117	117		

- Molecule 24 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	a	82	Total	C	N	O	0	0
			407	243	82	82		

- Molecule 25 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	b	148	Total	C	N	O	0	0
			730	434	148	148		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
26	c	275	Total	C	N	O	0	0
			1360	810	275	275		

- Molecule 27 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	d	211	Total	C	N	O	0	0
			1048	626	211	211		

- Molecule 28 is a protein called 39S ribosomal protein L49, mitochondrial.



Mol	Chain	Residues	Atoms				AltConf	Trace
28	g	129	Total	C	N	O	0	0
			638	380	129	129		

- Molecule 29 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	h	100	Total	C	N	O	0	0
			499	299	100	100		

- Molecule 30 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	i	97	Total	C	N	O	0	0
			476	282	97	97		

- Molecule 31 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	j	85	Total	C	N	O	0	0
			417	247	85	85		

- Molecule 32 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	o	79	Total	C	N	O	0	0
			394	236	79	79		

- Molecule 33 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	p	107	Total	C	N	O	0	0
			533	319	107	107		

- Molecule 34 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	q	99	Total	C	N	O	0	0
			490	292	99	99		

- Molecule 35 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	r	146	Total	C	N	O	0	0
			721	429	146	146		

- Molecule 36 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	s	370	Total	C	N	O	0	0
			1838	1098	370	370		

- Molecule 37 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	u	111	Total	C	N	O	0	0
			552	330	111	111		

- Molecule 38 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	v	69	Total	C	N	O	0	0
			341	203	69	69		

- Molecule 39 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	w	79	Total	C	N	O	0	0
			392	234	79	79		

- Molecule 40 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A	1208	Total	C	N	O	P	0	0
			25636	11507	4620	8301	1208		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1437	U	UNK	conflict	GB 1025814679

- Molecule 41 is a protein called Probable ATP-dependent RNA helicase DDX28.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	x	374	Total	C	N	O	0	0
			1843	1095	374	374		

- Molecule 42 is a protein called GTP-binding protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	y	331	Total	C	N	O	0	0
			1621	959	331	331		

- Molecule 43 is a protein called rRNA methyltransferase 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	z	253	Total	C	N	O	0	0
			1242	736	253	253		
43	1	257	Total	C	N	O	0	0
			1262	748	257	257		

- Molecule 44 is a RNA chain called mitochondrial Val tRNA.

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

- Molecule 45 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	P	133	Total	C	N	O	0	0
			659	393	133	133		

- Molecule 46 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	W	98	Total	C	N	O	0	0
			481	285	98	98		

- Molecule 47 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	6	325	Total	C	N	O	0	0
			1611	961	325	325		

- Molecule 48 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	I	158	Total	C	N	O	0	0
			785	469	158	158		

- Molecule 49 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	J	140	Total	C	N	O	0	0
			686	406	140	140		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	k	84	Total	C	N	O	0	0
			416	248	84	84		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
51	l	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

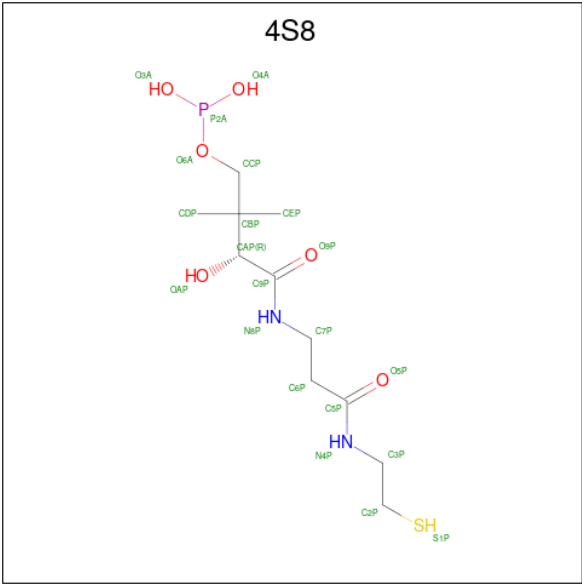
Mol	Chain	Residues	Atoms		AltConf
52	F	1	Total	Mg	0
			1	1	
52	g	1	Total	Mg	0
			1	1	
52	A	44	Total	Mg	0
			44	44	
52	x	1	Total	Mg	0
			1	1	
52	W	1	Total	Mg	0
			1	1	

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	0	1	Total	Zn	0
			1	1	

- Molecule 54 is N 3 -{(2R)-4-[(dihydroxyphosphanyl)oxy]-2-hydroxy-3,3-dimethylbutanoyl}-

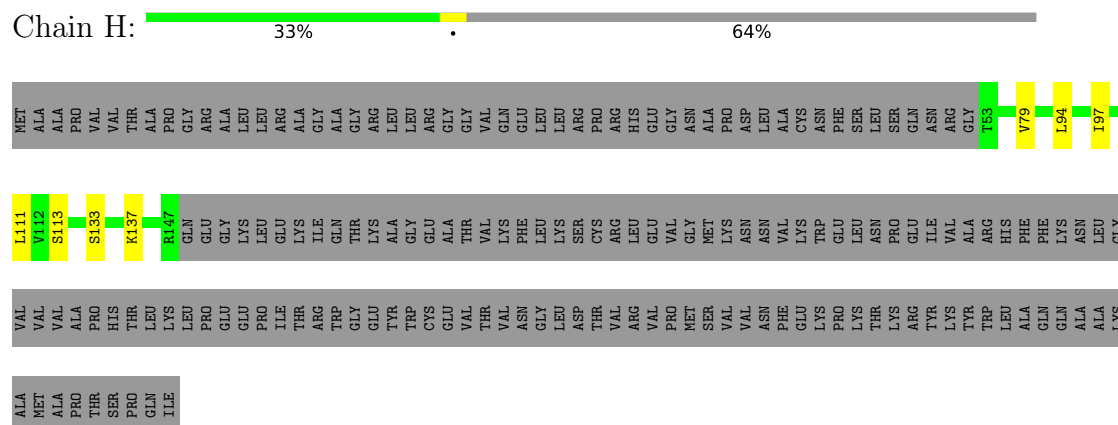
N-(2-sulfanylethyl)-beta-alaninamide (three-letter code: 4S8) (formula: C<sub>11</sub>H<sub>23</sub>N<sub>2</sub>O<sub>6</sub>PS).



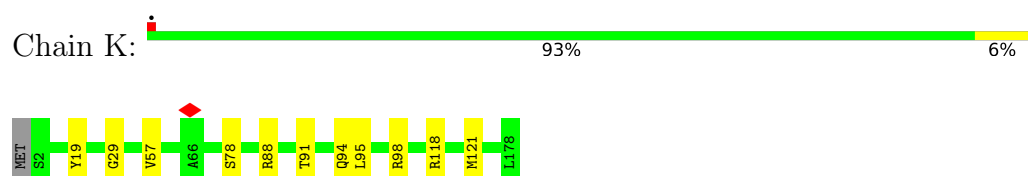
Mol	Chain	Residues	Atoms						AltConf
54	v	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	



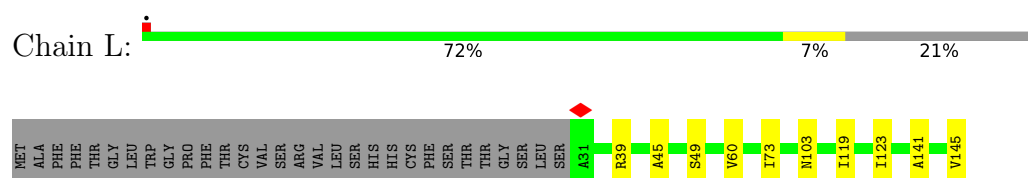
- Molecule 4: 39S ribosomal protein L9, mitochondrial



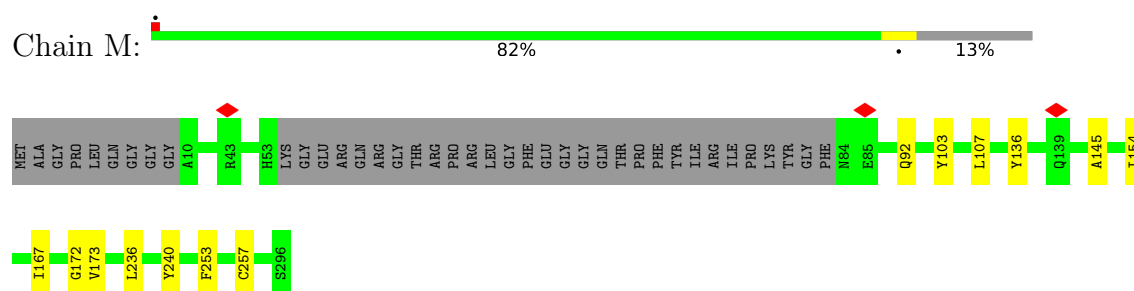
- Molecule 5: 39S ribosomal protein L13, mitochondrial



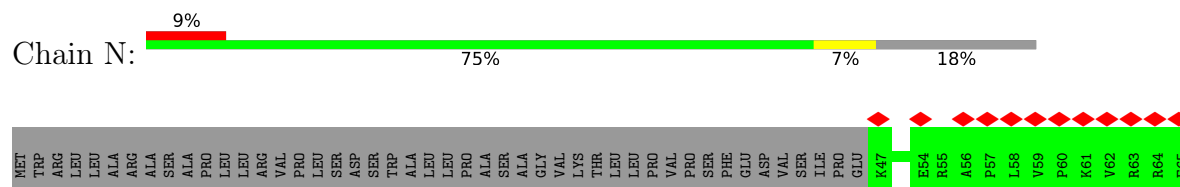
- Molecule 6: 39S ribosomal protein L14, mitochondrial

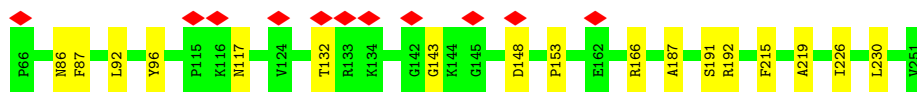


- Molecule 7: 39S ribosomal protein L15, mitochondrial



- Molecule 8: 39S ribosomal protein L16, mitochondrial





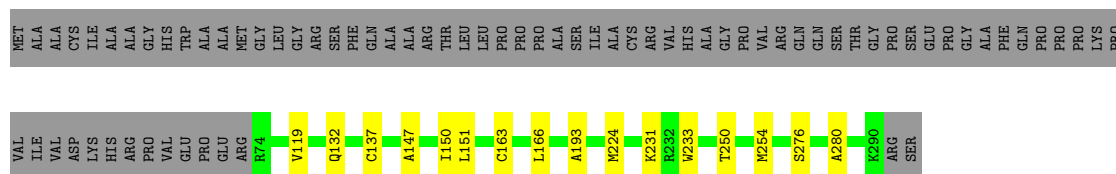
- Molecule 9: 39S ribosomal protein L17, mitochondrial

Chain O: 84% 13%



- Molecule 10: 39S ribosomal protein L19, mitochondrial

Chain Q: 69% 5% 26%



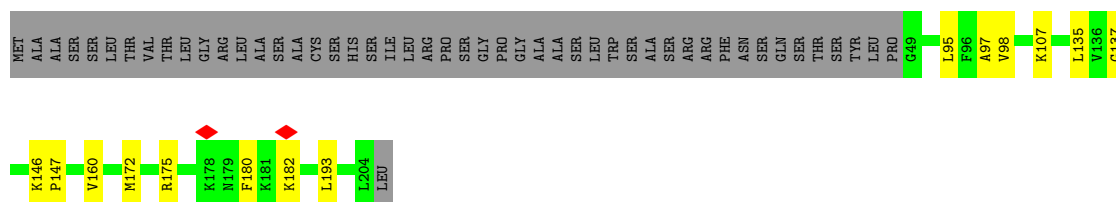
- Molecule 11: 39S ribosomal protein L20, mitochondrial

Chain R: 91% 6%



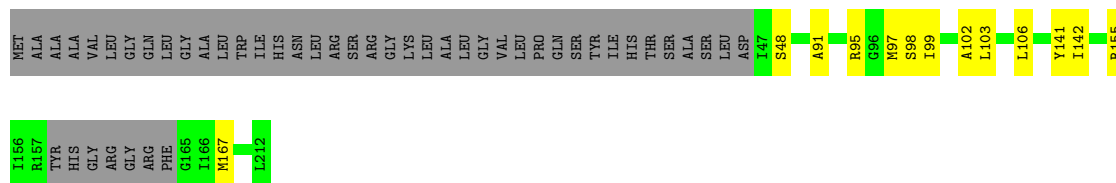
- Molecule 12: 39S ribosomal protein L21, mitochondrial

Chain S: 69% 7% 24%




- Molecule 13: 39S ribosomal protein L22, mitochondrial

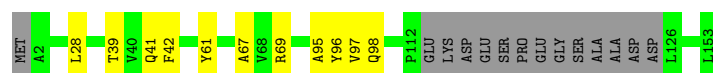
Chain T: 71% 6% 23%




- Molecule 14: 39S ribosomal protein L23, mitochondrial



Chain U:  84% 7% 9%



- Molecule 15: 39S ribosomal protein L24, mitochondrial

Chain V:  84% 5% 11%



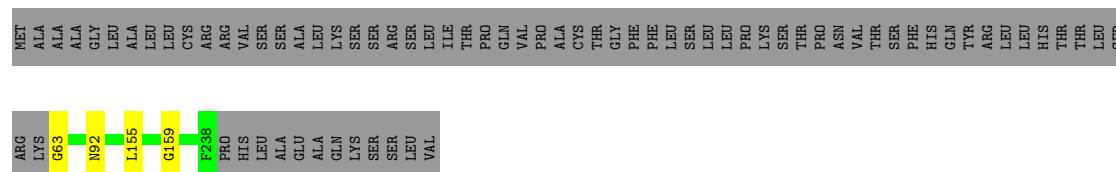
- Molecule 16: 39S ribosomal protein L28, mitochondrial

Chain X:  90% 5% 5%



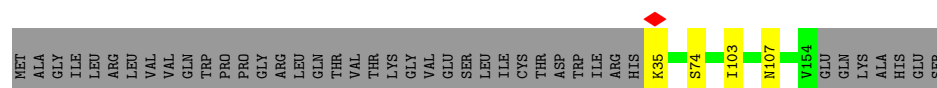
- Molecule 17: 39S ribosomal protein L47, mitochondrial

Chain Y:  69% 30% 1%



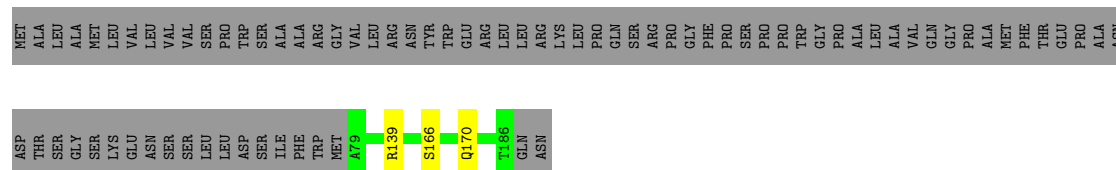
- Molecule 18: 39S ribosomal protein L30, mitochondrial

Chain Z:  72% 25% 3%



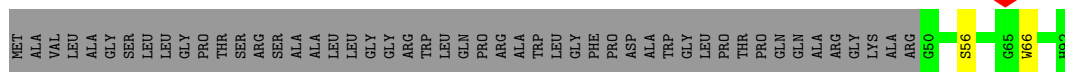
- Molecule 19: 39S ribosomal protein L32, mitochondrial

Chain 0:  56% 43% 1%



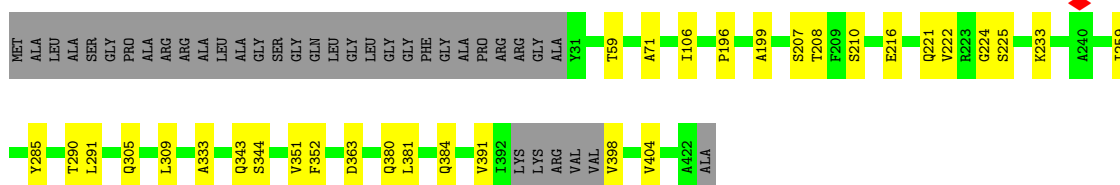
- Molecule 20: 39S ribosomal protein L34, mitochondrial

Chain 2:  45% 53% 2%



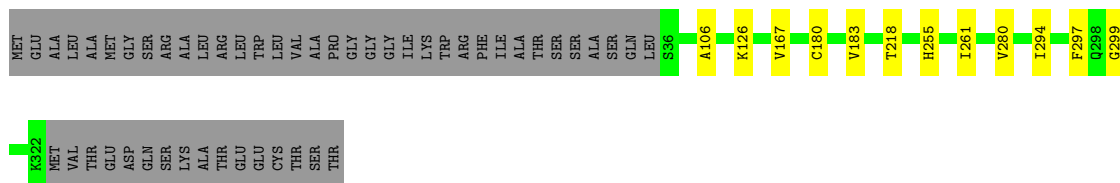
- Molecule 21: 39S ribosomal protein L37, mitochondrial

Chain 5: 84% 8% 9%



- Molecule 22: 39S ribosomal protein L39, mitochondrial

Chain 7: 81% 15%



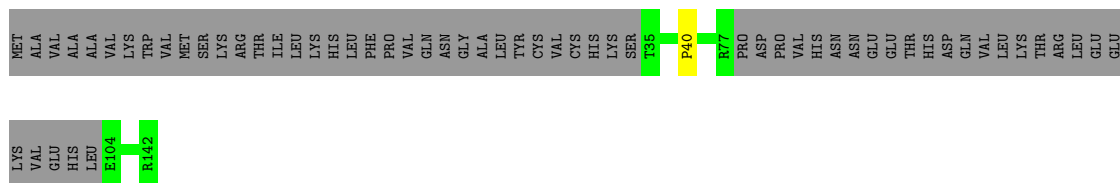
- Molecule 23: 39S ribosomal protein L41, mitochondrial

Chain 9: 82% 15%



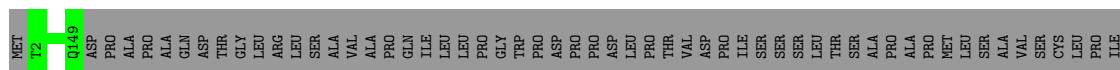
- Molecule 24: 39S ribosomal protein L42, mitochondrial

Chain a: 57% 42%




- Molecule 25: 39S ribosomal protein L43, mitochondrial

Chain b: 69% 31%



VAL  
PRO  
ALA  
SER  
GLY  
LEU  
THR  
THR  
VAL  
VAL  
CYS  
SER  
ALA

- Molecule 26: 39S ribosomal protein L44, mitochondrial

Chain c:  83% 17%

MET  
ALA  
SER  
GLY  
LEU  
VAL  
VAL  
ARG  
LEU  
LEU  
GLN  
GLN  
HIS  
ARG  
CYS  
LEU  
LEU  
ALA  
PRO  
VAL  
ALA  
LYS  
PRO  
LEU  
VAL  
VAL  
PRO  
VAL  
VAL  
GLY  
V31  
Q107  
LEU  
GLY  
ILE  
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LYS  
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LEU  
ASN  
L119  
Y316  
SER  
LYS  
PRO  
LYS  
GLU  
THR  
LEU  
ARG  
ALA  
GLU  
LYS  
SER  
ILE

THR  
ALA  
SER


- Molecule 27: 39S ribosomal protein L45, mitochondrial

Chain d:  69% 31%

MET  
ALA  
ALA  
PRO  
ILE  
ILE  
SER  
GLN  
GLY  
PHE  
SER  
CYS  
GLY  
LEU  
SER  
ARG  
PHE  
GLY  
THR  
PHE  
PHE  
GLN  
PRO  
VAL  
VAL  
THR  
GLN  
SER  
SER  
SER  
ALA  
ILE  
VAL  
VAL  
PRO  
VAL  
N207  
L252  
THR  
LYS  
ASN  
P255  
E294  
GLU  
ALA  
GLN  
TYR  
GLN  
PRO  
LYS  
LYS  
F50  
H59  
AGO  
R61  
K62  
L65  
P91  
GLU

GLY  
ASP  
ALA  
THR  
MET  
SER  
SER  
LEU  
SER  
LYS  
GLY  
GLY  
LEU  
ILE  
GLU  
THR  
GLU  
MET  
LYS  
LYS  
THR  
MET  
VAL  
A117  
C199  
SER  
SER  
MET  
MET  
ASN  
GLN  
N207  
L252  
THR  
LYS  
ASN  
P255  
E294  
GLU  
ALA  
GLN  
TYR  
GLN  
PRO  
LYS  
LYS  
PRO  
GLN  
LEU  
ALA

- Molecule 28: 39S ribosomal protein L49, mitochondrial

Chain g:  78% 22%

MET  
ALA  
ALA  
THR  
MET  
PHE  
ARG  
ALA  
THR  
LEU  
ARG  
GLY  
THR  
ARG  
THR  
VAL  
GLN  
ARG  
GLY  
CYS  
GLY  
LEU  
ARG  
LEU  
LEU  
SER  
GLN  
THR  
GLN  
GLY  
PRO  
PRO  
ASP  
TYR  
PRO  
ARG  
F38  
F166

- Molecule 29: 39S ribosomal protein L50, mitochondrial

Chain h:  63% 37%

MET  
ALA  
ALA  
ARG  
SER  
VAL  
SER  
GLY  
ILE  
THR  
THR  
ARG  
VAL  
PHE  
MET  
TRP  
TRP  
VAL  
PRO  
SER  
GLY  
THR  
CYS  
PRO  
ARG  
GLY  
PHE  
TRP  
SER  
PHE  
ARG  
LYS  
GLU  
LYS  
GLY  
PRO  
VAL  
VAL  
VAL  
THR  
GLY  
GLY  
LYS  
PRO  
PRO  
PRO  
ILE  
LEU  
VAL  
CYS  
PRO  
PRO  
LEU  
R56  
F78  
GLY  
SER

SER  
L62  
Y158

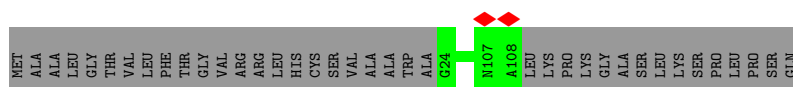
- Molecule 30: 39S ribosomal protein L51, mitochondrial

Chain i:  76% 24%


MET  
ALA  
GLY  
ASN  
LEU  
LEU  
SER  
GLY  
ALA  
GLY  
ARG  
ARG  
LEU  
TRP  
ASP  
VAL  
PRO  
LEU  
ALA  
CYS  
ARG  
SER  
PHE  
SER  
LEU  
GLY  
VAL  
PRO  
ARG  
LEU  
I32  
O61  
G125  
R128

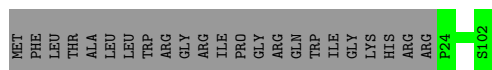
- Molecule 31: 39S ribosomal protein L52, mitochondrial

Chain j:  69% 31%



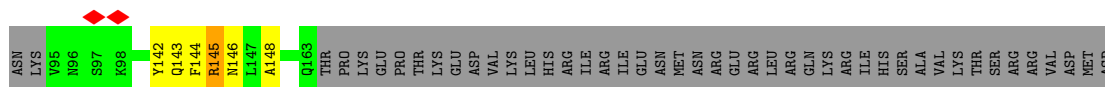
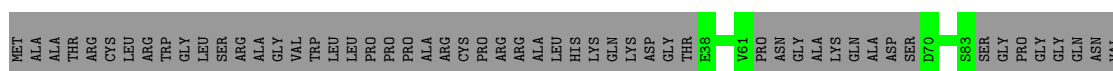
- Molecule 32: Ribosomal protein 63, mitochondrial

Chain o:  77% 23%



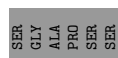
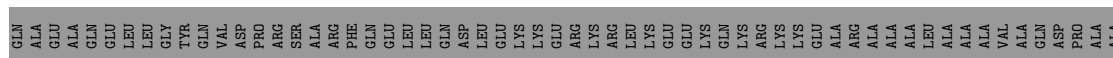
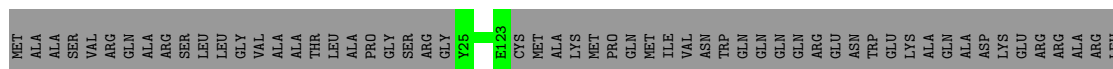
- Molecule 33: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:  49% 48%



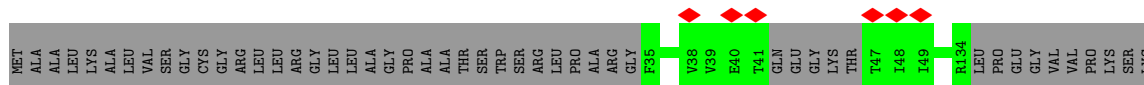
- Molecule 34: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:  45% 55%




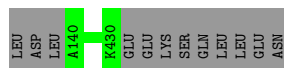
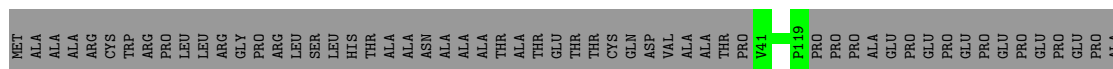
- Molecule 35: 39S ribosomal protein S18a, mitochondrial

Chain r:  74% 26%



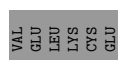
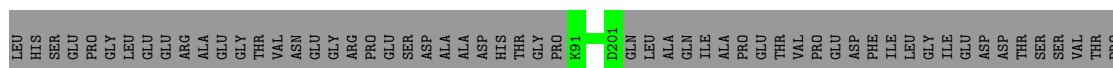
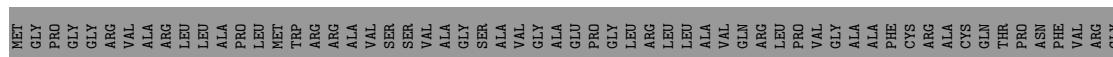
- Molecule 36: 39S ribosomal protein S30, mitochondrial

Chain s:  84% 16%



- Molecule 37: Mitochondrial assembly of ribosomal large subunit protein 1

Chain u: 47% 53%



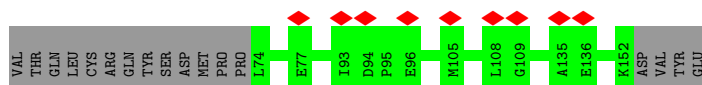
- Molecule 38: MIEF1 upstream open reading frame protein

Chain v: 99% .



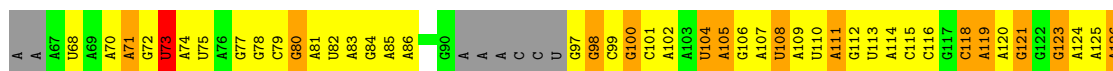
- Molecule 39: Acyl carrier protein, mitochondrial

Chain w: 6% 51% 49%

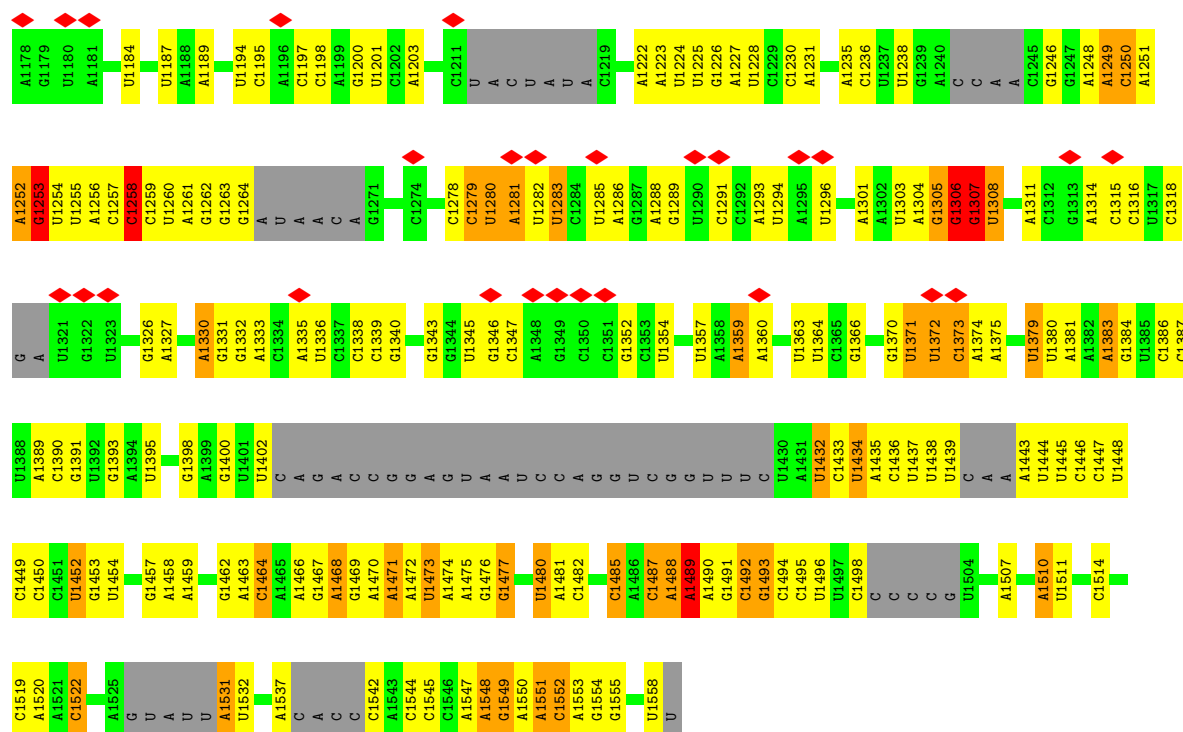


- Molecule 40: 16S rRNA

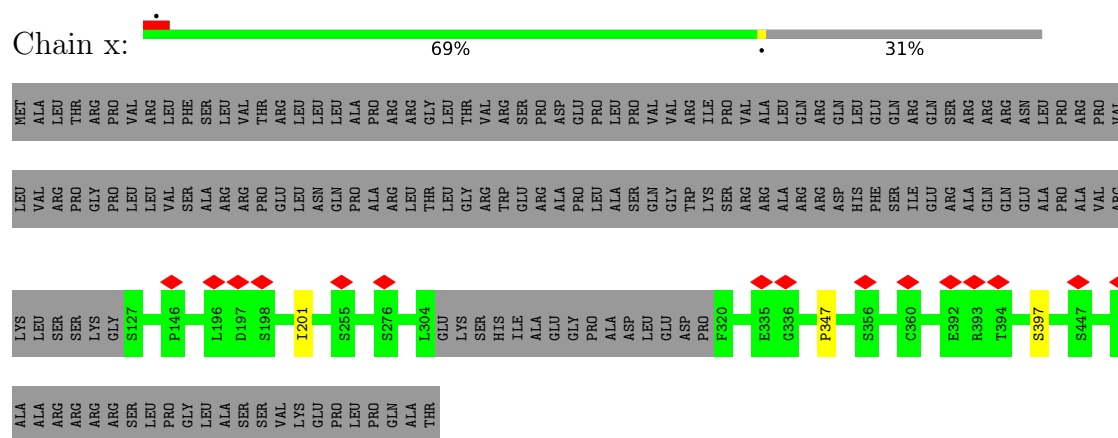
Chain A: 26% 37% 13% 23%



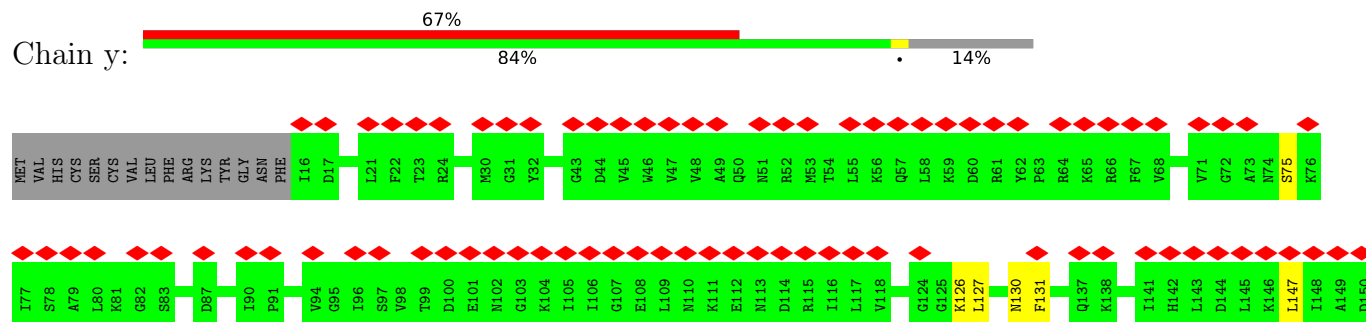


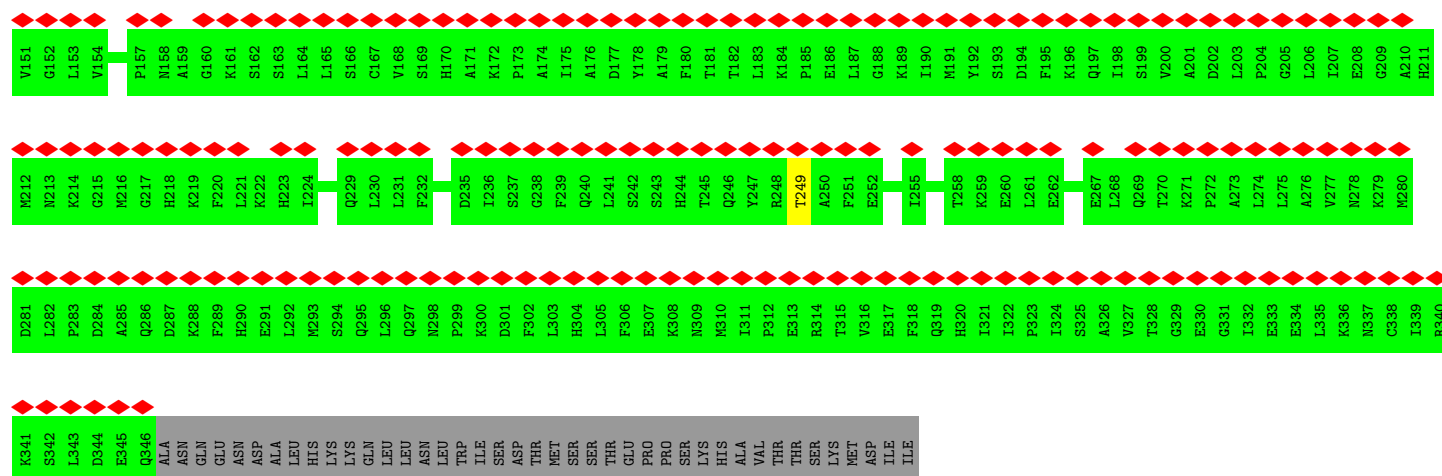


- Molecule 41: Probable ATP-dependent RNA helicase DDX28

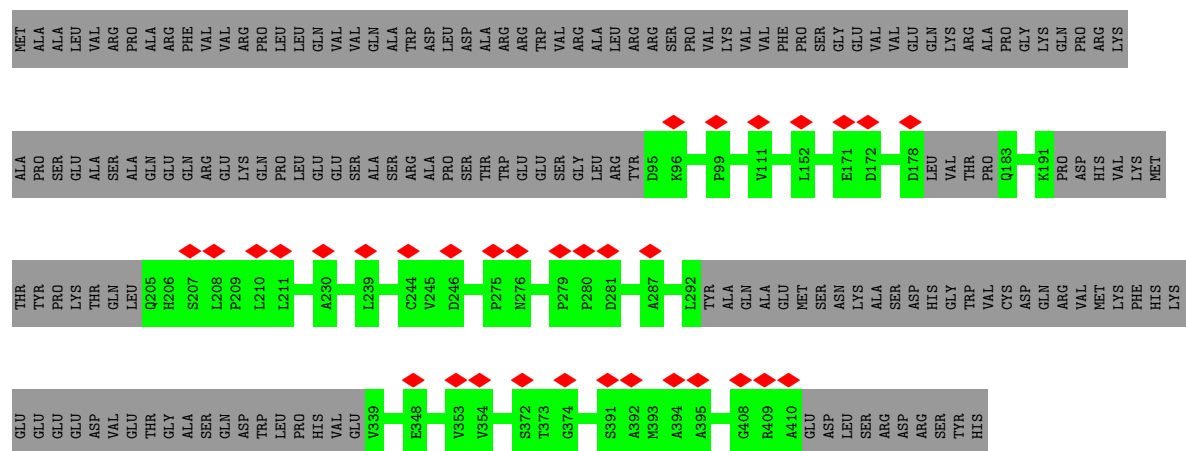


- Molecule 42: GTP-binding protein 10

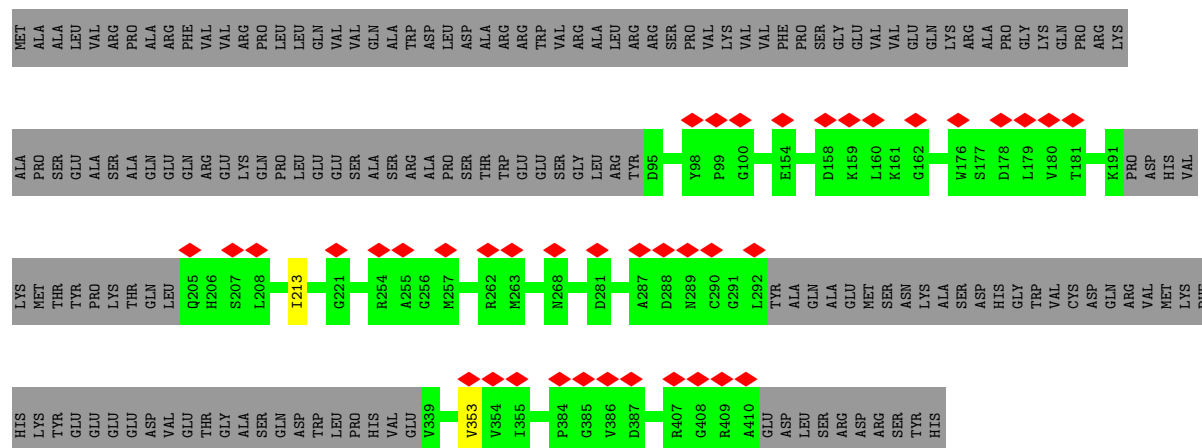




• Molecule 43: rRNA methyltransferase 3, mitochondrial

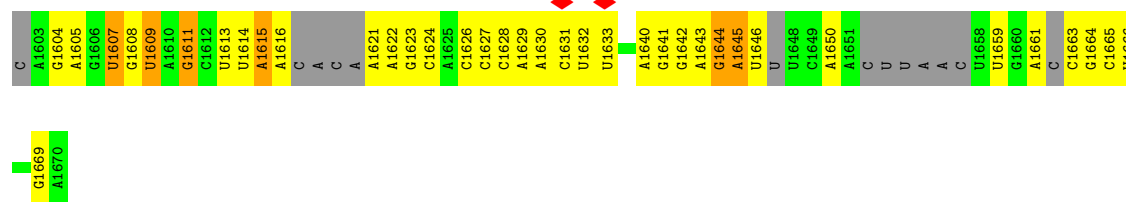


• Molecule 43: rRNA methyltransferase 3, mitochondrial

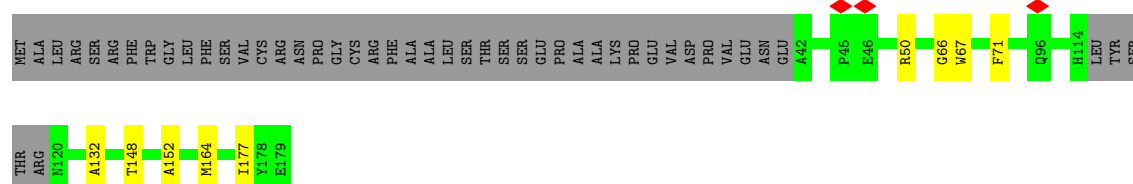


• Molecule 44: mitochondrial Val tRNA

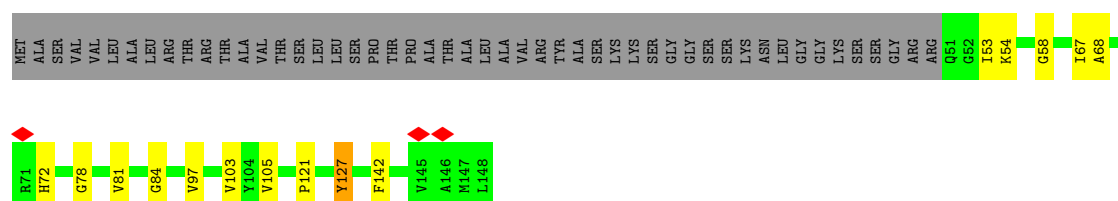




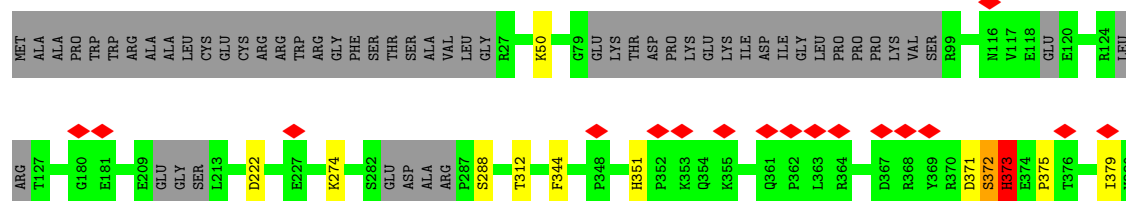
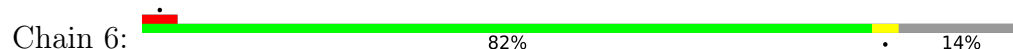
- Molecule 45: 39S ribosomal protein L18, mitochondrial



- Molecule 46: 39S ribosomal protein L27, mitochondrial

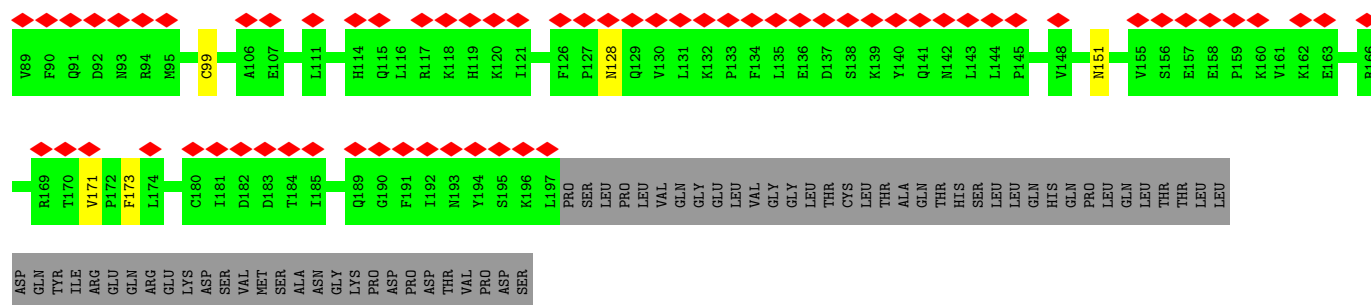


- Molecule 47: 39S ribosomal protein L38, mitochondrial

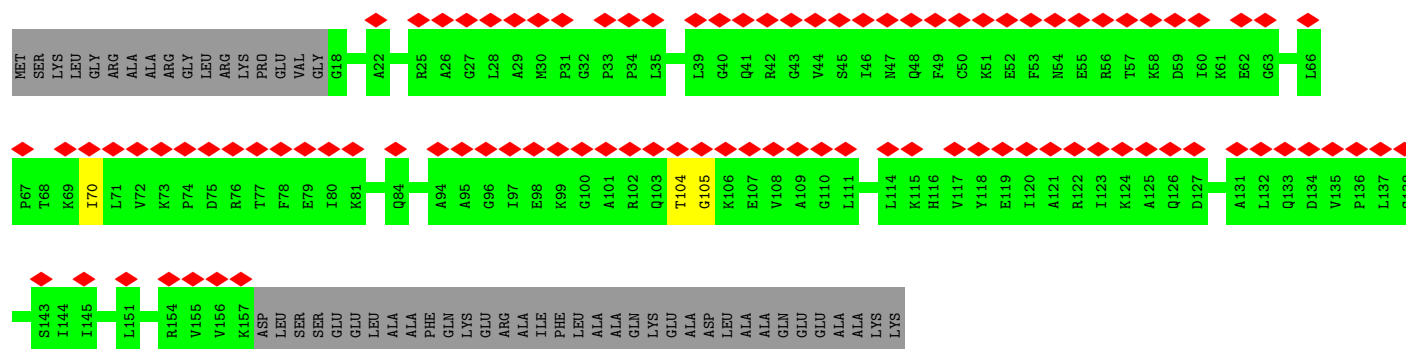


- Molecule 48: 39S ribosomal protein L10, mitochondrial

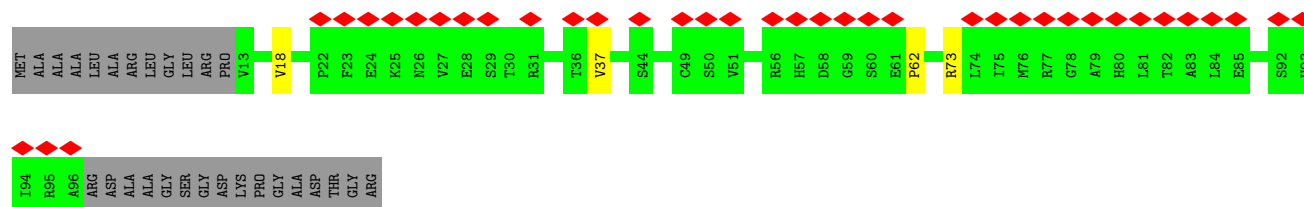




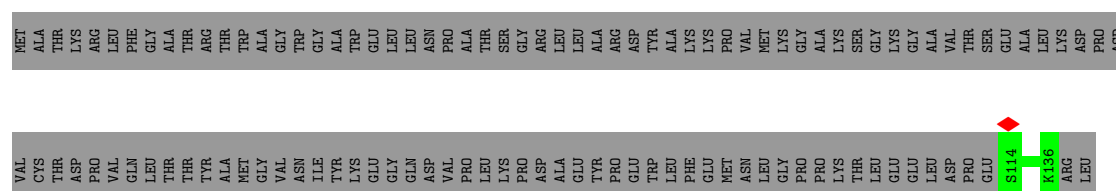
- Molecule 49: 39S ribosomal protein L11, mitochondrial



- Molecule 50: 39S ribosomal protein L53, mitochondrial



- Molecule 51: 39S ribosomal protein L54, mitochondrial



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18134	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.478	Depositor
Minimum map value	-0.383	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.084, 1.084, 1.084	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 4S8

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	D	0.26	0/1074	0.47	0/1486
2	E	0.31	0/1397	0.49	0/1937
3	F	0.33	0/1232	0.50	0/1713
4	H	0.26	0/468	0.46	0/650
5	K	0.34	0/875	0.50	0/1218
6	L	0.27	0/564	0.48	0/782
7	M	0.31	0/1264	0.48	0/1755
8	N	0.26	0/1005	0.45	0/1394
9	O	0.29	0/748	0.45	0/1039
10	Q	0.28	0/1074	0.45	0/1496
11	R	0.34	0/692	0.49	0/963
12	S	0.32	0/771	0.53	0/1073
13	T	0.33	0/786	0.51	0/1093
14	U	0.32	0/684	0.49	0/949
15	V	0.29	0/944	0.47	0/1310
16	X	0.28	0/1201	0.42	0/1672
17	Y	0.31	0/873	0.41	0/1217
18	Z	0.32	0/594	0.49	0/827
19	0	0.32	0/533	0.46	0/741
20	2	0.35	0/210	0.50	0/290
21	5	0.27	0/1914	0.46	0/2665
22	7	0.28	0/1425	0.45	0/1988
23	9	0.30	0/573	0.49	0/793
24	a	0.33	0/405	0.55	0/562
25	b	0.38	0/729	0.52	0/1013
26	c	0.30	0/1358	0.43	0/1889
27	d	0.27	0/1044	0.48	0/1451
28	g	0.33	0/637	0.48	0/886
29	h	0.27	0/497	0.41	0/692
30	i	0.34	0/475	0.52	0/658
31	j	0.30	0/416	0.41	0/576
32	o	0.28	0/393	0.40	0/548

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	p	0.97	4/530 (0.8%)	1.02	7/736 (1.0%)
34	q	0.30	0/489	0.39	0/680
35	r	0.29	0/718	0.45	0/995
36	s	0.29	0/1836	0.46	0/2560
37	u	0.26	0/551	0.42	0/768
38	v	0.23	0/340	0.36	0/472
39	w	0.22	0/391	0.43	0/544
40	A	0.76	11/28659 (0.0%)	1.29	306/44547 (0.7%)
41	x	0.26	0/1841	0.43	0/2558
42	y	0.30	0/1620	0.51	0/2246
43	l	0.25	0/1259	0.42	0/1744
43	z	0.25	0/1238	0.43	0/1713
44	B	0.32	0/1328	1.08	5/2056 (0.2%)
45	P	0.25	0/657	0.45	0/913
46	W	0.25	0/480	0.45	0/665
47	6	0.34	1/1605 (0.1%)	0.66	7/2229 (0.3%)
48	I	0.25	0/783	0.41	0/1090
49	J	0.25	0/685	0.41	0/949
50	k	0.23	0/415	0.44	0/577
51	l	0.21	0/114	0.26	0/158
All	All	0.54	16/72394 (0.0%)	0.92	325/105526 (0.3%)

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
3	F	0	1
24	a	0	1
33	p	0	2
42	y	0	3
47	6	0	3
All	All	0	10

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	A	1281	A	N9-C4	11.65	1.44	1.37
33	p	145	ARG	C-N	11.26	1.59	1.34
40	A	1281	A	N7-C5	-10.98	1.32	1.39
33	p	146	ASN	N-CA	10.48	1.67	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	A	1306	G	P-O5'	7.89	1.67	1.59
40	A	148	A	N9-C4	-7.02	1.33	1.37
40	A	1281	A	C8-N7	-6.27	1.27	1.31
40	A	239	A	C6-N1	-6.07	1.31	1.35
40	A	158	A	N9-C4	-6.03	1.34	1.37
47	6	373	HIS	CA-C	5.81	1.68	1.52
33	p	146	ASN	CA-C	5.80	1.68	1.52
40	A	193	A	N9-C4	-5.72	1.34	1.37
40	A	1306	G	C5'-C4'	5.37	1.57	1.51
40	A	340	U	N3-C4	-5.36	1.33	1.38
33	p	145	ARG	N-CA	5.04	1.56	1.46
40	A	476	A	N9-C4	-5.02	1.34	1.37

All (325) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	A	340	U	C5-C4-O4	20.32	138.09	125.90
40	A	340	U	N3-C4-O4	-18.56	106.41	119.40
40	A	1281	A	C4-C5-C6	16.63	125.32	117.00
40	A	1281	A	N3-C4-N9	13.60	138.28	127.40
40	A	1305	G	O4'-C1'-N9	13.39	118.92	108.20
40	A	1281	A	N3-C4-C5	-13.19	117.57	126.80
40	A	1281	A	C6-C5-N7	-13.00	123.20	132.30
33	p	145	ARG	C-N-CA	11.19	149.67	121.70
40	A	1305	G	N1-C6-O6	-11.03	113.28	119.90
40	A	1281	A	C4-N9-C1'	10.73	145.62	126.30
40	A	239	A	N1-C6-N6	-10.37	112.38	118.60
40	A	1305	G	N9-C4-C5	10.07	109.43	105.40
40	A	1281	A	C8-N9-C4	-9.90	101.84	105.80
40	A	1253	G	C5-C6-O6	9.70	134.42	128.60
40	A	1139	C	C2-N3-C4	-9.69	115.05	119.90
40	A	1315	C	N1-C2-O2	9.62	124.67	118.90
40	A	1279	C	C6-N1-C2	-9.56	116.48	120.30
47	6	373	HIS	N-CA-CB	-9.55	93.41	110.60
40	A	1542	C	C2-N1-C1'	9.21	128.93	118.80
40	A	108	U	C2-N1-C1'	9.15	128.68	117.70
40	A	582	C	N1-C2-O2	9.13	124.38	118.90
40	A	1305	G	C4-C5-N7	-8.98	107.21	110.80
40	A	1303	U	C2-N3-C4	-8.82	121.71	127.00
40	A	1253	G	N1-C6-O6	-8.80	114.62	119.90
40	A	709	C	C6-N1-C2	-8.80	116.78	120.30
40	A	1139	C	N3-C4-C5	8.71	125.39	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	A	1258	C	N1-C2-O2	8.69	124.11	118.90
40	A	108	U	N3-C2-O2	-8.66	116.14	122.20
47	6	373	HIS	N-CA-C	8.64	134.32	111.00
40	A	118	C	N1-C2-O2	8.60	124.06	118.90
40	A	15	C	N1-C2-O2	8.54	124.02	118.90
40	A	1258	C	C2-N1-C1'	8.52	128.18	118.80
40	A	1279	C	N3-C2-O2	-8.47	115.97	121.90
40	A	23	C	C2-N1-C1'	8.44	128.08	118.80
40	A	1281	A	C8-N9-C1'	-8.43	112.53	127.70
40	A	641	U	C2-N1-C1'	8.43	127.81	117.70
40	A	582	C	C2-N1-C1'	8.38	128.02	118.80
40	A	523	U	C5-C4-O4	8.37	130.92	125.90
40	A	1305	G	C8-N9-C1'	8.33	137.83	127.00
40	A	1228	U	C2-N1-C1'	8.32	127.68	117.70
40	A	1305	G	C5-C6-O6	8.24	133.54	128.60
40	A	1305	G	C6-C5-N7	8.24	135.34	130.40
47	6	373	HIS	C-N-CA	8.08	141.89	121.70
40	A	23	C	N1-C2-O2	8.06	123.74	118.90
40	A	1073	U	C2-N1-C1'	8.05	127.36	117.70
40	A	1281	A	C6-N1-C2	-7.94	113.83	118.60
40	A	423	U	N3-C2-O2	-7.90	116.67	122.20
40	A	709	C	N3-C2-O2	-7.77	116.46	121.90
40	A	195	C	N1-C2-O2	7.75	123.55	118.90
40	A	149	U	O4'-C1'-N1	7.72	114.38	108.20
40	A	1432	U	C2-N1-C1'	7.71	126.96	117.70
40	A	1017	C	C2-N1-C1'	7.68	127.25	118.80
40	A	1138	U	N1-C2-O2	7.64	128.15	122.80
40	A	15	C	N3-C2-O2	-7.63	116.56	121.90
47	6	372	SER	C-N-CA	7.62	140.76	121.70
40	A	161	G	N9-C4-C5	-7.60	102.36	105.40
40	A	55	C	N1-C2-O2	7.59	123.45	118.90
40	A	997	U	N3-C2-O2	-7.57	116.90	122.20
40	A	1522	C	N1-C2-O2	7.47	123.38	118.90
40	A	188	G	C4-N9-C1'	7.47	136.21	126.50
40	A	170	C	C2-N1-C1'	7.46	127.01	118.80
40	A	118	C	N3-C2-O2	-7.44	116.69	121.90
40	A	1487	C	C2-N1-C1'	7.43	126.97	118.80
40	A	12	C	C6-N1-C2	-7.42	117.33	120.30
40	A	423	U	N1-C2-O2	7.42	127.99	122.80
44	B	1627	C	N3-C2-O2	-7.41	116.71	121.90
40	A	195	C	N3-C2-O2	-7.37	116.74	121.90
40	A	50	C	N1-C2-O2	7.35	123.31	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	A	24	U	N1-C2-O2	7.31	127.92	122.80
40	A	709	C	N1-C2-O2	7.28	123.27	118.90
40	A	523	U	N3-C4-O4	-7.28	114.31	119.40
40	A	641	U	N1-C2-O2	7.26	127.88	122.80
40	A	169	C	N3-C2-O2	-7.26	116.82	121.90
40	A	108	U	N1-C2-O2	7.25	127.87	122.80
40	A	373	C	C2-N1-C1'	7.24	126.77	118.80
40	A	466	C	N1-C2-O2	7.22	123.23	118.90
40	A	1307	G	O5'-P-OP1	-7.19	99.23	105.70
40	A	582	C	C6-N1-C1'	-7.17	112.19	120.80
40	A	355	C	N1-C2-O2	7.17	123.20	118.90
40	A	108	U	C6-N1-C2	-7.12	116.73	121.00
40	A	423	U	C2-N1-C1'	7.10	126.22	117.70
40	A	188	G	N3-C4-C5	-7.09	125.06	128.60
40	A	1305	G	C4-N9-C1'	-7.06	117.32	126.50
40	A	377	U	C2-N1-C1'	7.05	126.16	117.70
33	p	145	ARG	CA-C-O	-7.04	105.31	120.10
40	A	659	C	C2-N1-C1'	7.03	126.54	118.80
40	A	986	U	N3-C2-O2	-7.03	117.28	122.20
40	A	800	G	N1-C6-O6	-7.03	115.68	119.90
40	A	1306	G	O5'-P-OP1	7.03	119.13	110.70
40	A	1278	C	N1-C2-O2	7.01	123.11	118.90
40	A	1258	C	N3-C2-O2	-7.00	117.00	121.90
40	A	425	U	C5-C6-N1	6.99	126.19	122.70
40	A	377	U	N3-C2-O2	-6.97	117.32	122.20
40	A	1315	C	N3-C2-O2	-6.96	117.03	121.90
40	A	592	C	C6-N1-C2	-6.93	117.53	120.30
40	A	1487	C	N1-C2-O2	6.93	123.06	118.90
40	A	239	A	C5-C6-N6	6.93	129.24	123.70
40	A	1542	C	N1-C2-O2	6.90	123.04	118.90
47	6	373	HIS	CA-C-N	6.89	132.37	117.20
40	A	143	C	C2-N1-C1'	6.86	126.35	118.80
40	A	601	C	N3-C2-O2	-6.85	117.11	121.90
40	A	188	G	N3-C4-N9	6.84	130.10	126.00
40	A	787	A	P-O3'-C3'	6.82	127.88	119.70
40	A	24	U	N3-C2-O2	-6.81	117.44	122.20
40	A	1306	G	O5'-C5'-C4'	6.81	124.64	111.70
40	A	1306	G	C5'-C4'-C3'	6.80	126.88	116.00
40	A	12	C	C2-N1-C1'	6.80	126.28	118.80
40	A	169	C	N1-C2-O2	6.80	122.98	118.90
40	A	705	C	N1-C2-O2	6.78	122.97	118.90
40	A	1315	C	C2-N1-C1'	6.75	126.23	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	A	161	G	C6-C5-N7	-6.75	126.35	130.40
40	A	377	U	N1-C2-O2	6.72	127.51	122.80
40	A	1434	U	N3-C2-O2	-6.71	117.50	122.20
40	A	23	C	N3-C2-O2	-6.67	117.23	121.90
40	A	1281	A	N7-C8-N9	6.65	117.12	113.80
40	A	1487	C	C6-N1-C1'	-6.65	112.83	120.80
40	A	588	A	N1-C2-N3	6.63	132.62	129.30
40	A	709	C	C2-N1-C1'	6.63	126.10	118.80
40	A	1138	U	N3-C2-O2	-6.63	117.56	122.20
40	A	55	C	N3-C2-O2	-6.62	117.26	121.90
40	A	1531	A	P-O3'-C3'	6.60	127.62	119.70
40	A	641	U	N3-C2-O2	-6.60	117.58	122.20
40	A	161	G	C4-C5-N7	6.59	113.44	110.80
40	A	1542	C	C5-C6-N1	6.58	124.29	121.00
40	A	1138	U	C2-N1-C1'	6.55	125.56	117.70
40	A	1164	C	N1-C2-O2	6.55	122.83	118.90
47	6	373	HIS	O-C-N	-6.53	112.25	122.70
40	A	143	C	N1-C2-O2	6.53	122.82	118.90
40	A	239	A	C8-N9-C1'	-6.53	115.94	127.70
40	A	50	C	C2-N1-C1'	6.52	125.97	118.80
40	A	239	A	C4-N9-C1'	6.51	138.03	126.30
40	A	1542	C	C6-N1-C2	-6.51	117.69	120.30
40	A	1305	G	P-O3'-C3'	6.51	127.51	119.70
40	A	1522	C	N3-C2-O2	-6.50	117.35	121.90
40	A	12	C	N3-C2-O2	-6.48	117.36	121.90
40	A	447	U	N1-C2-O2	6.47	127.33	122.80
40	A	188	G	C8-N9-C1'	-6.45	118.61	127.00
40	A	50	C	N3-C2-O2	-6.42	117.40	121.90
40	A	360	U	P-O3'-C3'	6.42	127.40	119.70
40	A	422	C	C6-N1-C2	-6.42	117.73	120.30
40	A	610	C	N3-C2-O2	-6.42	117.41	121.90
40	A	726	C	N1-C2-O2	6.39	122.73	118.90
40	A	1306	G	C6-C5-N7	-6.39	126.56	130.40
40	A	422	C	N1-C2-O2	6.39	122.73	118.90
40	A	28	C	C6-N1-C2	-6.38	117.75	120.30
40	A	355	C	C2-N1-C1'	6.36	125.80	118.80
40	A	1011	G	C4-C5-N7	6.35	113.34	110.80
40	A	1373	C	N1-C2-O2	6.34	122.70	118.90
44	B	1624	C	N1-C2-O2	6.33	122.70	118.90
40	A	1011	G	N9-C4-C5	-6.32	102.87	105.40
40	A	1432	U	C5-C6-N1	6.32	125.86	122.70
40	A	192	U	N3-C2-O2	-6.29	117.80	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	A	577	C	N1-C2-O2	6.29	122.67	118.90
40	A	396	C	N1-C2-O2	6.29	122.67	118.90
40	A	1017	C	N1-C2-O2	6.28	122.67	118.90
40	A	670	C	N1-C2-O2	6.27	122.66	118.90
40	A	239	A	N9-C4-C5	-6.26	103.30	105.80
40	A	1283	U	C2-N1-C1'	6.24	125.18	117.70
40	A	459	G	N1-C6-O6	-6.22	116.17	119.90
33	p	146	ASN	O-C-N	-6.21	112.77	122.70
40	A	1542	C	C6-N1-C1'	-6.20	113.36	120.80
40	A	121	G	C6-C5-N7	-6.20	126.68	130.40
40	A	169	C	C2-N1-C1'	6.19	125.61	118.80
40	A	355	C	N3-C2-O2	-6.19	117.57	121.90
40	A	12	C	N1-C2-O2	6.19	122.61	118.90
40	A	1258	C	C6-N1-C1'	-6.18	113.39	120.80
40	A	641	U	C6-N1-C1'	-6.17	112.56	121.20
40	A	161	G	C8-N9-C1'	-6.16	119.00	127.00
40	A	396	C	N3-C2-O2	-6.14	117.60	121.90
40	A	1464	C	N1-C2-O2	6.13	122.58	118.90
40	A	705	C	C2-N1-C1'	6.12	125.54	118.80
40	A	1544	C	N1-C2-O2	6.12	122.57	118.90
40	A	582	C	N3-C2-O2	-6.06	117.66	121.90
40	A	44	C	N1-C2-O2	6.05	122.53	118.90
40	A	153	A	C8-N9-C4	-6.05	103.38	105.80
40	A	1032	G	N3-C4-N9	6.02	129.61	126.00
40	A	176	C	C2-N3-C4	-6.00	116.90	119.90
40	A	330	C	N1-C2-O2	5.99	122.50	118.90
40	A	1228	U	N1-C2-O2	5.98	126.99	122.80
40	A	24	U	C2-N1-C1'	5.98	124.87	117.70
33	p	146	ASN	N-CA-C	5.97	127.11	111.00
40	A	153	A	P-O3'-C3'	5.97	126.86	119.70
40	A	670	C	N3-C2-O2	-5.95	117.73	121.90
40	A	153	A	N7-C8-N9	5.94	116.77	113.80
33	p	144	PHE	C-N-CA	5.94	136.54	121.70
40	A	675	G	N3-C4-N9	5.93	129.56	126.00
40	A	1022	G	N3-C2-N2	-5.91	115.76	119.90
40	A	1038	C	C6-N1-C2	-5.91	117.94	120.30
40	A	447	U	N3-C2-O2	-5.90	118.07	122.20
40	A	23	C	C6-N1-C2	-5.90	117.94	120.30
33	p	143	GLN	C-N-CA	5.90	136.45	121.70
40	A	195	C	C2-N1-C1'	5.89	125.28	118.80
40	A	1432	U	C6-N1-C2	-5.89	117.46	121.00
44	B	1626	C	N1-C2-O2	5.89	122.43	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	A	50	C	C6-N1-C2	-5.88	117.95	120.30
40	A	1552	C	N3-C2-O2	-5.86	117.80	121.90
40	A	997	U	N1-C2-O2	5.86	126.90	122.80
40	A	422	C	N3-C2-O2	-5.86	117.80	121.90
40	A	1017	C	C6-N1-C1'	-5.86	113.77	120.80
40	A	577	C	N3-C2-O2	-5.84	117.81	121.90
40	A	108	U	C5-C6-N1	5.84	125.62	122.70
40	A	1011	G	C8-N9-C1'	-5.82	119.43	127.00
40	A	466	C	N3-C2-O2	-5.81	117.83	121.90
40	A	1228	U	C6-N1-C1'	-5.81	113.07	121.20
40	A	1473	U	N3-C2-O2	-5.78	118.15	122.20
40	A	143	C	N3-C2-O2	-5.76	117.87	121.90
40	A	1291	C	N1-C2-O2	5.74	122.34	118.90
40	A	1032	G	C8-N9-C1'	-5.73	119.55	127.00
33	p	145	ARG	CA-C-N	5.73	129.80	117.20
40	A	1123	C	N1-C2-O2	5.69	122.32	118.90
40	A	628	A	C4-N9-C1'	5.69	136.54	126.30
40	A	23	C	C6-N1-C1'	-5.69	113.98	120.80
40	A	987	C	N1-C2-O2	5.68	122.31	118.90
40	A	379	U	C2-N1-C1'	5.66	124.49	117.70
40	A	73	U	N1-C2-O2	5.65	126.75	122.80
40	A	153	A	C4-N9-C1'	5.64	136.46	126.30
40	A	373	C	N1-C2-O2	5.64	122.28	118.90
40	A	1522	C	C2-N1-C1'	5.64	125.00	118.80
44	B	1627	C	C6-N1-C2	-5.61	118.06	120.30
40	A	1339	C	C2-N1-C1'	5.61	124.97	118.80
40	A	210	C	C2-N1-C1'	5.61	124.97	118.80
40	A	592	C	C5-C6-N1	5.60	123.80	121.00
44	B	1624	C	N3-C2-O2	-5.57	118.00	121.90
40	A	1009	U	N3-C2-O2	-5.57	118.30	122.20
40	A	1073	U	C6-N1-C1'	-5.56	113.42	121.20
40	A	610	C	N1-C2-O2	5.56	122.23	118.90
40	A	19	C	N1-C2-O2	5.55	122.23	118.90
40	A	170	C	N1-C2-O2	5.54	122.22	118.90
40	A	1464	C	C2-N1-C1'	5.54	124.89	118.80
40	A	524	U	N1-C2-O2	5.53	126.67	122.80
40	A	1073	U	N1-C2-O2	5.52	126.67	122.80
40	A	1473	U	C2-N1-C1'	5.52	124.33	117.70
40	A	73	U	C2-N1-C1'	5.52	124.32	117.70
40	A	447	U	C2-N1-C1'	5.52	124.32	117.70
40	A	1434	U	N1-C2-O2	5.51	126.66	122.80
40	A	1531	A	O4'-C1'-N9	5.50	112.60	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	A	1029	C	C2-N1-C1'	5.48	124.83	118.80
40	A	1315	C	C5-C6-N1	5.48	123.74	121.00
40	A	466	C	C2-N1-C1'	5.44	124.78	118.80
40	A	1011	G	C6-C5-N7	-5.43	127.14	130.40
40	A	19	C	C2-N1-C1'	5.43	124.78	118.80
40	A	248	G	N3-C4-C5	-5.43	125.88	128.60
40	A	1373	C	N3-C2-O2	-5.43	118.10	121.90
40	A	986	U	N1-C2-O2	5.42	126.60	122.80
40	A	675	G	N9-C4-C5	-5.42	103.23	105.40
40	A	118	C	C2-N1-C1'	5.41	124.75	118.80
40	A	1464	C	C6-N1-C2	-5.40	118.14	120.30
40	A	248	G	N3-C4-N9	5.40	129.24	126.00
40	A	170	C	C5-C6-N1	5.38	123.69	121.00
40	A	1011	G	N3-C4-N9	5.38	129.23	126.00
40	A	1004	U	C2-N1-C1'	5.37	124.15	117.70
40	A	609	U	N3-C2-O2	-5.36	118.45	122.20
40	A	44	C	N3-C2-O2	-5.35	118.16	121.90
40	A	210	C	N1-C2-O2	5.34	122.11	118.90
40	A	330	C	C2-N1-C1'	5.34	124.68	118.80
40	A	1032	G	C4-N9-C1'	5.34	133.45	126.50
40	A	1027	G	C8-N9-C1'	-5.34	120.06	127.00
40	A	98	G	N3-C4-N9	5.33	129.20	126.00
40	A	601	C	N1-C2-O2	5.32	122.09	118.90
40	A	1306	G	OP1-P-OP2	-5.32	111.63	119.60
40	A	1489	A	P-O3'-C3'	5.31	126.07	119.70
40	A	1303	U	N3-C4-C5	5.30	117.78	114.60
40	A	628	A	C8-N9-C1'	-5.30	118.17	127.70
40	A	980	C	N1-C2-O2	5.30	122.08	118.90
40	A	239	A	N3-C4-N9	5.29	131.63	127.40
40	A	456	U	N1-C2-O2	5.28	126.49	122.80
40	A	373	C	C5-C6-N1	5.27	123.64	121.00
40	A	573	A	P-O3'-C3'	5.27	126.03	119.70
40	A	659	C	C6-N1-C1'	-5.27	114.48	120.80
40	A	587	C	C2-N1-C1'	5.26	124.59	118.80
40	A	1552	C	N1-C2-O2	5.26	122.06	118.90
40	A	1048	C	C6-N1-C2	-5.25	118.20	120.30
40	A	55	C	C6-N1-C2	-5.25	118.20	120.30
40	A	1238	U	N1-C2-O2	5.25	126.47	122.80
40	A	726	C	N3-C2-O2	-5.24	118.23	121.90
40	A	1228	U	N3-C2-O2	-5.23	118.54	122.20
40	A	216	G	N1-C6-O6	5.23	123.04	119.90
40	A	170	C	C6-N1-C1'	-5.23	114.53	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	A	1164	C	C2-N1-C1'	5.23	124.55	118.80
40	A	747	C	C2-N1-C1'	5.22	124.54	118.80
40	A	1281	A	C2-N3-C4	5.20	113.20	110.60
40	A	1487	C	O4'-C1'-N1	5.20	112.36	108.20
40	A	396	C	C2-N1-C1'	5.20	124.52	118.80
40	A	1011	G	C4-N9-C1'	5.19	133.25	126.50
40	A	1464	C	N3-C2-O2	-5.19	118.27	121.90
40	A	171	U	N3-C4-O4	5.19	123.03	119.40
40	A	73	U	N3-C2-O2	-5.18	118.58	122.20
47	6	371	ASP	C-N-CA	5.18	134.64	121.70
40	A	349	G	N3-C4-N9	5.17	129.10	126.00
40	A	1164	C	N3-C2-O2	-5.17	118.28	121.90
40	A	1432	U	N3-C2-O2	-5.17	118.58	122.20
40	A	1452	U	C2-N1-C1'	5.17	123.90	117.70
40	A	785	U	N3-C2-O2	-5.16	118.58	122.20
40	A	566	C	P-O3'-C3'	5.16	125.89	119.70
40	A	1279	C	N3-C4-C5	-5.16	119.84	121.90
40	A	640	G	C4-C5-N7	5.14	112.86	110.80
40	A	1306	G	N3-C4-N9	5.14	129.08	126.00
40	A	1434	U	C2-N1-C1'	5.14	123.87	117.70
40	A	687	C	C6-N1-C2	-5.13	118.25	120.30
40	A	726	C	C2-N1-C1'	5.13	124.45	118.80
40	A	670	C	C2-N1-C1'	5.13	124.44	118.80
40	A	8	C	O4'-C1'-N1	-5.11	104.11	108.20
40	A	753	C	C2-N1-C1'	5.11	124.42	118.80
40	A	43	A	P-O3'-C3'	5.11	125.83	119.70
40	A	771	C	C6-N1-C2	-5.10	118.26	120.30
40	A	376	C	N3-C2-O2	-5.10	118.33	121.90
40	A	588	A	C2-N3-C4	-5.09	108.06	110.60
40	A	349	G	N3-C4-C5	-5.09	126.06	128.60
40	A	783	G	C5-C6-N1	5.09	114.04	111.50
40	A	188	G	C6-C5-N7	-5.08	127.35	130.40
40	A	171	U	C2-N1-C1'	5.08	123.80	117.70
40	A	104	U	O4'-C1'-N1	-5.08	104.14	108.20
40	A	1073	U	C5-C6-N1	5.07	125.24	122.70
40	A	170	C	C6-N1-C2	-5.07	118.27	120.30
40	A	98	G	C6-C5-N7	-5.06	127.36	130.40
40	A	705	C	C6-N1-C1'	-5.05	114.74	120.80
40	A	1006	A	C6-N1-C2	-5.05	115.57	118.60
40	A	410	U	N1-C2-O2	5.04	126.33	122.80
40	A	422	C	C2-N1-C1'	5.04	124.34	118.80
40	A	1542	C	O4'-C1'-N1	5.04	112.23	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	A	56	C	N1-C2-O2	5.03	121.92	118.90
40	A	373	C	C6-N1-C2	-5.02	118.29	120.30
40	A	1305	G	N3-C4-N9	-5.02	122.99	126.00
40	A	705	C	N3-C2-O2	-5.01	118.39	121.90
40	A	575	A	C8-N9-C4	-5.00	103.80	105.80

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	6	372	SER	Peptide
47	6	373	HIS	Peptide,Mainchain
3	F	151	VAL	Peptide
24	a	40	PRO	Peptide
33	p	145	ARG	Peptide
33	p	148	ALA	Peptide
42	y	127	LEU	Peptide
42	y	130	ASN	Peptide
42	y	131	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	D	1076	0	502	19	0
2	E	1399	0	611	19	0
3	F	1233	0	543	8	0
4	H	469	0	199	4	0
5	K	876	0	386	6	0
6	L	565	0	252	5	0
7	M	1266	0	559	7	0
8	N	1006	0	456	10	0
9	O	749	0	329	3	0
10	Q	1075	0	453	8	0
11	R	693	0	328	2	0
12	S	772	0	330	7	0
13	T	788	0	344	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	U	686	0	292	6	0
15	V	946	0	398	6	0
16	X	1202	0	513	8	0
17	Y	874	0	383	3	0
18	Z	595	0	245	3	0
19	0	534	0	228	2	0
20	2	211	0	90	2	0
21	5	1916	0	819	16	0
22	7	1426	0	610	7	0
23	9	575	0	257	3	0
24	a	407	0	158	0	0
25	b	730	0	320	0	0
26	c	1360	0	604	0	0
27	d	1048	0	442	0	0
28	g	638	0	257	0	0
29	h	499	0	204	0	0
30	i	476	0	203	0	0
31	j	417	0	198	0	0
32	o	394	0	185	0	0
33	p	533	0	234	0	0
34	q	490	0	219	0	0
35	r	721	0	294	0	0
36	s	1838	0	825	0	0
37	u	552	0	229	0	0
38	v	341	0	158	0	0
39	w	392	0	166	0	0
40	A	25636	0	13040	386	0
41	x	1843	0	825	0	0
42	y	1621	0	735	0	0
43	1	1262	0	579	1	0
43	z	1242	0	571	0	0
44	B	1191	0	607	19	0
45	P	659	0	300	6	0
46	W	481	0	221	10	0
47	6	1611	0	701	5	0
48	I	785	0	332	3	0
49	J	686	0	323	2	0
50	k	416	0	187	0	0
51	l	115	0	45	0	0
52	A	44	0	0	0	0
52	F	1	0	0	0	0
52	W	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	g	1	0	0	0	0
52	x	1	0	0	0	0
53	0	1	0	0	0	0
54	v	21	0	0	0	0
All	All	69386	0	32289	566	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 8.

All (566) 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)
40:A:1446:C:N4	40:A:1470:A:H61	1.50	1.08
40:A:1446:C:H42	40:A:1470:A:N6	1.51	1.07
2:E:106:MET:HA	2:E:119:VAL:O	1.57	1.04
40:A:238:A:H62	40:A:342:A:N6	1.55	1.04
40:A:130:G:N2	40:A:135:A:H62	1.55	1.02
40:A:1454:U:N3	40:A:1463:A:C8	2.26	1.02
40:A:662:C:C2	40:A:774:A:N6	2.26	1.02
40:A:51:C:N4	40:A:60:U:H3	1.57	1.01
40:A:662:C:N4	40:A:772:U:H3	1.58	1.01
40:A:238:A:N6	40:A:342:A:H61	1.63	0.96
22:7:106:ALA:HA	22:7:126:LYS:O	1.64	0.95
40:A:1343:G:H1	40:A:1354:U:H3	1.07	0.94
40:A:1065:G:H1	40:A:1254:U:H3	1.02	0.94
40:A:130:G:H21	40:A:135:A:N6	1.67	0.91
40:A:238:A:H62	40:A:342:A:H61	0.93	0.91
40:A:114:A:H62	40:A:123:G:N2	1.70	0.90
40:A:114:A:H62	40:A:123:G:H21	0.89	0.89
40:A:482:A:H62	40:A:579:G:N2	1.71	0.87
40:A:130:G:H21	40:A:135:A:H62	0.88	0.86
40:A:114:A:N6	40:A:123:G:H21	1.72	0.85
44:B:1607:U:H3	44:B:1664:G:H1	1.22	0.85
1:D:129:VAL:HA	1:D:139:ILE:O	1.78	0.84
12:S:95:LEU:HA	12:S:137:GLY:O	1.78	0.83
40:A:482:A:N6	40:A:579:G:H21	1.78	0.82
16:X:85:TRP:HA	16:X:105:TRP:O	1.80	0.81
2:E:215:PHE:HA	2:E:259:GLY:O	1.80	0.81
40:A:662:C:H42	40:A:772:U:H3	0.84	0.81
40:A:802:A:H62	40:A:984:U:H3	1.27	0.79
2:E:106:MET:CA	2:E:119:VAL:O	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A:662:C:N4	40:A:772:U:N3	2.25	0.78
40:A:482:A:N6	40:A:579:G:N2	2.32	0.78
40:A:74:A:N6	40:A:84:G:H21	1.81	0.77
40:A:1371:U:H4'	40:A:1372:U:OP1	1.84	0.77
40:A:991:U:H2'	40:A:992:A:H8	1.51	0.74
22:7:183:VAL:O	22:7:294:ILE:HA	1.86	0.74
12:S:172:MET:HA	12:S:182:LYS:O	1.87	0.74
44:B:1622:A:N6	44:B:1645:A:C2	2.56	0.74
40:A:74:A:N6	40:A:84:G:N2	2.36	0.73
40:A:51:C:N4	40:A:60:U:N3	2.26	0.73
40:A:74:A:H62	40:A:84:G:N2	1.85	0.73
40:A:988:U:H3'	40:A:989:C:H2'	1.69	0.72
8:N:92:LEU:H	8:N:187:ALA:HA	1.55	0.71
40:A:237:A:C8	40:A:343:U:N3	2.59	0.71
40:A:51:C:H42	40:A:60:U:H3	1.09	0.71
40:A:1454:U:C2	40:A:1463:A:N7	2.59	0.71
40:A:438:G:H21	40:A:442:A:H62	1.37	0.70
40:A:1139:C:N3	40:A:1254:U:O4	2.25	0.70
5:K:19:TYR:O	5:K:57:VAL:HA	1.90	0.70
40:A:1457:G:H2'	40:A:1458:A:H2'	1.73	0.69
21:5:207:SER:O	21:5:225:SER:HA	1.93	0.68
40:A:1363:U:H5''	40:A:1364:U:H5'	1.76	0.68
40:A:111:A:H62	40:A:125:A:H62	1.42	0.67
40:A:738:U:H2'	40:A:739:A:H8	1.57	0.67
40:A:73:U:H3	40:A:85:A:H62	1.41	0.67
40:A:1336:U:O2	40:A:1338:C:N4	2.28	0.67
40:A:1446:C:N3	40:A:1470:A:N1	2.42	0.67
40:A:385:U:H2'	40:A:386:G:H8	1.60	0.67
44:B:1622:A:N6	44:B:1645:A:H2	1.92	0.66
21:5:196:PRO:O	21:5:199:ALA:HB3	1.95	0.66
40:A:153:A:H8	40:A:1036:A:HO2'	1.44	0.66
40:A:1480:U:H2'	40:A:1481:A:H8	1.59	0.66
44:B:1628:C:H42	44:B:1640:A:H61	1.43	0.66
1:D:129:VAL:CA	1:D:139:ILE:O	2.44	0.66
40:A:1454:U:O2	40:A:1463:A:N7	2.28	0.66
21:5:106:ILE:HA	21:5:221:GLN:O	1.96	0.65
40:A:113:U:H2'	40:A:114:A:H8	1.61	0.65
16:X:116:SER:O	16:X:120:ASP:N	2.30	0.65
40:A:480:U:H2'	40:A:481:A:H8	1.61	0.65
9:O:9:ILE:N	40:A:788:A:OP1	2.29	0.65
23:9:40:GLY:O	40:A:35:A:N6	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A:1203:A:H5''	46:W:84:GLY:HA3	1.78	0.64
40:A:647:G:H2'	40:A:648:A:H8	1.63	0.64
40:A:519:C:H5'	40:A:520:C:H5'	1.78	0.64
40:A:159:A:H2'	40:A:160:G:H8	1.62	0.63
40:A:1379:U:O2	40:A:1383:A:N7	2.32	0.63
21:5:290:THR:HA	21:5:343:GLN:O	1.98	0.63
40:A:798:A:H61	40:A:989:C:N4	1.96	0.63
40:A:1446:C:H42	40:A:1470:A:H61	0.73	0.63
40:A:523:U:C4	40:A:526:A:N1	2.66	0.62
40:A:662:C:N4	40:A:772:U:C4	2.66	0.62
40:A:70:A:H3'	40:A:71:A:H2'	1.82	0.62
40:A:482:A:N6	40:A:579:G:C2	2.67	0.62
40:A:850:C:O2	40:A:858:G:N2	2.30	0.62
14:U:69:ARG:O	14:U:95:ALA:HA	1.99	0.62
21:5:210:SER:HA	21:5:222:VAL:O	2.00	0.62
40:A:632:U:H2'	40:A:633:A:H8	1.65	0.62
40:A:1549:G:N2	40:A:1551:A:OP1	2.33	0.61
40:A:802:A:N6	40:A:984:U:H3	1.97	0.61
13:T:98:SER:HA	13:T:141:TYR:HA	1.83	0.61
40:A:1433:C:H2'	40:A:1434:U:H6	1.65	0.61
40:A:388:C:N3	40:A:411:U:O4	2.34	0.61
5:K:91:THR:O	5:K:95:LEU:N	2.34	0.60
40:A:497:A:N6	40:A:542:C:OP2	2.34	0.60
40:A:1139:C:C4	40:A:1254:U:O4	2.54	0.60
44:B:1616:A:N6	44:B:1646:U:C2	2.69	0.60
40:A:241:C:H2'	40:A:242:A:H8	1.67	0.60
40:A:769:U:H2'	40:A:770:G:H8	1.66	0.60
40:A:571:A:N6	40:A:572:U:O4	2.34	0.60
40:A:1398:G:N2	40:A:1398:G:OP2	2.32	0.60
21:5:391:VAL:O	21:5:398:VAL:N	2.35	0.60
40:A:256:A:H2	40:A:308:A:H61	1.49	0.60
2:E:103:LYS:HA	2:E:122:LEU:HA	1.84	0.60
40:A:118:C:HI'	40:A:248:G:N1	2.17	0.60
40:A:1160:A:N6	40:A:1167:A:OP2	2.35	0.59
40:A:391:C:N4	40:A:408:C:O2'	2.35	0.59
40:A:73:U:O4	40:A:85:A:N7	2.36	0.59
40:A:478:A:H2'	40:A:479:G:H8	1.68	0.59
40:A:1257:C:H2'	40:A:1258:C:H4'	1.85	0.59
40:A:523:U:O4	40:A:526:A:C6	2.55	0.58
10:Q:193:ALA:HA	10:Q:224:MET:HA	1.85	0.58
14:U:39:THR:HA	14:U:98:GLN:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ILE:HA	1:D:186:ALA:HB2	1.84	0.58
40:A:180:U:O2'	40:A:464:A:N1	2.37	0.58
40:A:130:G:C2	40:A:135:A:N6	2.72	0.58
40:A:603:A:N1	40:A:623:A:O2'	2.36	0.57
40:A:225:C:H2'	40:A:226:U:H6	1.70	0.57
40:A:53:A:N6	40:A:57:A:OP2	2.37	0.57
11:R:98:ASN:O	11:R:102:LEU:N	2.32	0.57
40:A:632:U:H2'	40:A:633:A:C8	2.40	0.57
2:E:110:TRP:HA	2:E:116:LYS:HA	1.86	0.57
10:Q:250:THR:O	10:Q:254:MET:N	2.36	0.57
13:T:99:ILE:O	13:T:103:LEU:CB	2.53	0.57
40:A:1359:A:H4'	40:A:1360:A:H5'	1.87	0.57
40:A:163:C:N4	40:A:166:A:OP1	2.38	0.56
40:A:802:A:N7	40:A:984:U:O4	2.38	0.56
2:E:134:SER:O	2:E:138:CYS:N	2.37	0.56
40:A:152:U:O2	40:A:1037:A:O2'	2.21	0.56
40:A:160:G:H2'	40:A:161:G:C8	2.39	0.56
40:A:105:A:H2'	40:A:106:G:C8	2.41	0.56
40:A:796:A:O2'	40:A:1485:C:OP2	2.23	0.56
44:B:1611:G:O6	44:B:1644:G:N2	2.22	0.56
40:A:160:G:H2'	40:A:161:G:H8	1.70	0.56
9:O:21:GLY:O	9:O:25:ARG:N	2.37	0.56
5:K:118:ARG:O	5:K:121:MET:N	2.40	0.55
40:A:517:C:O2'	49:J:104:THR:O	2.25	0.55
7:M:92:GLN:O	7:M:136:TYR:N	2.31	0.55
18:Z:35:LYS:N	40:A:433:A:HO2'	2.03	0.55
40:A:747:C:H4'	40:A:748:A:H5'	1.87	0.55
21:5:305:GLN:O	21:5:309:LEU:N	2.35	0.55
40:A:158:A:N6	40:A:1013:C:O2'	2.39	0.55
8:N:132:THR:HA	8:N:148:ASP:H	1.71	0.55
40:A:567:A:H2'	40:A:568:A:C8	2.42	0.55
2:E:203:TYR:HA	2:E:272:LYS:HA	1.88	0.55
40:A:526:A:O2'	40:A:543:A:N1	2.38	0.55
40:A:415:A:H2'	40:A:416:A:H8	1.71	0.55
40:A:1043:C:H2'	40:A:1044:A:C4	2.42	0.55
40:A:1454:U:N3	40:A:1463:A:H8	2.00	0.55
40:A:583:U:H2'	40:A:584:C:H6	1.72	0.55
40:A:343:U:N3	40:A:344:A:N7	2.55	0.55
40:A:1040:C:H2'	40:A:1041:A:H8	1.72	0.55
7:M:253:PHE:O	7:M:257:CYS:N	2.40	0.54
14:U:61:TYR:O	17:Y:63:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A:1345:U:OP2	40:A:1347:C:N4	2.41	0.54
40:A:7:C:N3	40:A:128:A:O2'	2.34	0.54
46:W:53:ILE:HA	46:W:68:ALA:HA	1.90	0.54
40:A:774:A:H1'	40:A:775:U:C2	2.42	0.54
22:7:280:VAL:HA	22:7:299:GLY:HA3	1.89	0.54
40:A:583:U:H2'	40:A:584:C:C6	2.43	0.54
40:A:101:C:C4	40:A:102:A:N6	2.75	0.54
40:A:459:G:H2'	40:A:460:A:H8	1.72	0.54
16:X:207:THR:O	16:X:211:ALA:N	2.38	0.54
40:A:130:G:N2	40:A:135:A:N6	2.36	0.54
44:B:1642:G:H2'	44:B:1643:A:H8	1.72	0.54
40:A:998:A:H2'	40:A:999:A:H8	1.72	0.53
40:A:159:A:H2'	40:A:160:G:C8	2.42	0.53
40:A:237:A:N7	40:A:343:U:C2	2.76	0.53
40:A:1139:C:N3	40:A:1254:U:C4	2.77	0.53
3:F:67:GLU:O	3:F:191:ASP:N	2.40	0.53
13:T:48:SER:N	40:A:3:U:OP2	2.41	0.53
40:A:193:A:H2'	40:A:194:A:H8	1.73	0.53
40:A:1338:C:O2'	40:A:1381:A:N3	2.36	0.53
3:F:218:LEU:O	3:F:242:LEU:HA	2.09	0.53
21:5:208:THR:HA	21:5:224:GLY:O	2.08	0.53
40:A:1326:G:H2'	40:A:1327:A:H8	1.73	0.53
44:B:1642:G:H2'	44:B:1643:A:C8	2.44	0.53
40:A:5:A:H3'	40:A:6:A:H8	1.73	0.53
40:A:597:U:H2'	40:A:598:G:H8	1.72	0.53
40:A:113:U:H2'	40:A:114:A:C8	2.43	0.53
8:N:215:PHE:O	8:N:219:ALA:CB	2.57	0.53
40:A:241:C:H2'	40:A:242:A:C8	2.44	0.53
44:B:1609:U:O2	44:B:1616:A:N6	2.41	0.53
40:A:985:G:N2	40:A:989:C:O2	2.42	0.53
1:D:235:GLN:O	1:D:295:TYR:N	2.42	0.53
40:A:105:A:H2'	40:A:106:G:H8	1.73	0.53
40:A:390:A:N6	40:A:408:C:O2'	2.42	0.52
2:E:128:HIS:HA	2:E:192:PRO:HA	1.92	0.52
40:A:1155:G:H1'	40:A:1223:A:H1'	1.91	0.52
2:E:251:VAL:O	40:A:1435:A:O2'	2.27	0.52
44:B:1663:C:N4	44:B:1664:G:O6	2.42	0.52
40:A:97:G:H2'	40:A:98:G:C8	2.44	0.52
40:A:336:C:H2'	40:A:337:U:C6	2.44	0.52
22:7:167:VAL:H	22:7:183:VAL:HA	1.75	0.52
40:A:101:C:N4	40:A:102:A:N6	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A:1059:U:H2'	40:A:1060:A:C8	2.45	0.52
40:A:79:C:H4'	40:A:80:G:H8	1.74	0.52
40:A:698:C:H2'	40:A:699:A:H8	1.75	0.52
40:A:1074:U:O2	40:A:1075:A:N6	2.37	0.52
46:W:121:PRO:HA	47:6:50:LYS:HA	1.91	0.52
40:A:615:U:H2'	40:A:616:A:H8	1.75	0.51
40:A:459:G:H2'	40:A:460:A:C8	2.46	0.51
2:E:106:MET:CB	2:E:119:VAL:O	2.58	0.51
16:X:10:LEU:O	16:X:14:LEU:N	2.40	0.51
40:A:345:G:N2	40:A:370:G:N3	2.58	0.51
14:U:28:LEU:HA	14:U:42:PHE:HA	1.91	0.51
40:A:647:G:H2'	40:A:648:A:C8	2.43	0.51
40:A:1260:U:H2'	40:A:1261:A:H8	1.75	0.51
40:A:309:U:H2'	40:A:310:A:H8	1.75	0.51
40:A:311:G:H2'	40:A:312:G:H8	1.75	0.51
40:A:841:C:H3'	40:A:842:A:H8	1.76	0.51
8:N:226:ILE:O	8:N:230:LEU:N	2.44	0.51
45:P:132:ALA:HB2	45:P:164:MET:HA	1.93	0.51
7:M:236:LEU:O	7:M:240:TYR:N	2.40	0.51
11:R:82:LYS:O	11:R:85:ALA:N	2.43	0.51
18:Z:103:ILE:O	18:Z:107:ASN:N	2.40	0.51
40:A:751:G:H2'	40:A:752:U:O4'	2.11	0.51
40:A:1380:U:N3	40:A:1383:A:OP2	2.40	0.51
9:O:110:ILE:H	9:O:121:ALA:HA	1.76	0.51
14:U:41:GLN:HA	14:U:96:TYR:HA	1.92	0.51
40:A:607:U:H2'	40:A:608:A:H8	1.76	0.51
40:A:801:G:N2	40:A:985:G:OP2	2.44	0.51
45:P:148:THR:O	45:P:152:ALA:N	2.41	0.50
40:A:618:A:H2'	40:A:619:G:H8	1.77	0.50
40:A:1488:A:H2'	40:A:1489:A:C8	2.46	0.50
40:A:1491:G:N3	40:A:1492:C:O2'	2.43	0.50
12:S:160:VAL:HA	12:S:193:LEU:HA	1.94	0.50
20:2:56:SER:HA	40:A:669:G:H5''	1.92	0.50
12:S:98:VAL:HA	12:S:107:LYS:HA	1.93	0.50
40:A:615:U:H2'	40:A:616:A:C8	2.47	0.50
8:N:96:TYR:HA	8:N:153:PRO:HA	1.94	0.50
40:A:12:C:H1'	40:A:106:G:N2	2.27	0.50
19:O:139:ARG:HA	40:A:651:A:C8	2.47	0.50
40:A:101:C:H2'	40:A:102:A:C8	2.47	0.50
40:A:227:A:H2'	40:A:228:A:H8	1.76	0.50
6:L:123:ILE:O	6:L:145:VAL:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:119:VAL:O	10:Q:132:GLN:HA	2.12	0.49
13:T:102:ALA:O	13:T:106:LEU:CB	2.61	0.49
44:B:1607:U:O2	44:B:1664:G:N2	2.36	0.49
1:D:126:VAL:HA	1:D:142:VAL:HA	1.95	0.49
40:A:220:C:H2'	40:A:221:A:H8	1.76	0.49
40:A:1176:G:H21	40:A:1225:U:H3	1.60	0.49
8:N:86:ASN:O	8:N:192:ARG:N	2.45	0.49
40:A:169:C:H2'	40:A:170:C:C6	2.48	0.49
10:Q:147:ALA:O	10:Q:166:LEU:N	2.43	0.49
40:A:501:U:C2	40:A:503:G:H4'	2.48	0.49
3:F:262:THR:O	3:F:266:VAL:N	2.44	0.49
40:A:53:A:H5''	40:A:54:A:H4'	1.95	0.49
40:A:618:A:H2'	40:A:619:G:C8	2.47	0.49
44:B:1622:A:H2'	44:B:1623:G:C8	2.48	0.49
40:A:430:C:H2'	40:A:431:C:C6	2.47	0.49
40:A:1481:A:N1	40:A:1493:G:O2'	2.36	0.49
40:A:12:C:H1'	40:A:106:G:H21	1.78	0.49
40:A:193:A:H2'	40:A:194:A:C8	2.48	0.49
40:A:991:U:H2'	40:A:992:A:C8	2.40	0.49
40:A:1371:U:O2'	40:A:1372:U:O5'	2.27	0.49
40:A:424:G:H2'	40:A:425:U:C5	2.48	0.49
40:A:1029:C:H2'	40:A:1030:G:H8	1.78	0.49
2:E:158:ALA:O	2:E:162:LEU:N	2.42	0.48
40:A:309:U:H2'	40:A:310:A:C8	2.48	0.48
40:A:70:A:OP2	40:A:71:A:O2'	2.28	0.48
40:A:1330:A:H2'	40:A:1331:G:C8	2.48	0.48
40:A:1364:U:OP2	40:A:1383:A:O2'	2.31	0.48
46:W:58:GLY:N	46:W:97:VAL:O	2.44	0.48
15:V:186:THR:N	17:Y:92:ASN:O	2.45	0.48
46:W:103:VAL:HA	46:W:127:TYR:HA	1.94	0.48
46:W:142:PHE:HA	47:6:344:PHE:H	1.78	0.48
40:A:374:A:H2'	40:A:375:A:C8	2.48	0.48
40:A:402:A:H2'	40:A:403:A:C8	2.49	0.48
40:A:85:A:H2'	40:A:86:A:C8	2.49	0.48
40:A:348:G:H2'	40:A:349:G:H8	1.79	0.48
19:O:166:SER:O	19:O:170:GLN:N	2.47	0.48
21:5:351:VAL:HA	21:5:381:LEU:HA	1.95	0.48
40:A:249:C:H42	40:A:327:C:H4'	1.79	0.48
40:A:381:A:H2'	40:A:382:A:H8	1.79	0.48
40:A:450:G:H2'	40:A:451:G:C8	2.48	0.48
40:A:605:U:H2'	40:A:606:C:H6	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A:1279:C:H2'	40:A:1280:U:C4	2.48	0.48
3:F:84:PRO:HA	3:F:88:ALA:HB3	1.95	0.48
40:A:478:A:H2'	40:A:479:G:C8	2.49	0.48
40:A:637:U:H2'	40:A:638:A:C8	2.49	0.48
40:A:1488:A:H2'	40:A:1489:A:H8	1.79	0.48
40:A:792:A:H2'	40:A:793:A:H8	1.79	0.47
45:P:71:PHE:N	46:W:105:VAL:O	2.45	0.47
40:A:337:U:H2'	40:A:338:G:C8	2.49	0.47
40:A:371:U:H2'	40:A:372:U:H6	1.78	0.47
40:A:656:C:H2'	40:A:657:U:H6	1.79	0.47
7:M:154:ILE:N	7:M:173:VAL:O	2.47	0.47
40:A:514:A:H2'	40:A:515:G:H8	1.79	0.47
40:A:626:U:H2'	40:A:627:A:C5	2.49	0.47
40:A:1332:G:H2'	40:A:1333:A:C8	2.50	0.47
7:M:167:ILE:O	7:M:172:GLY:N	2.46	0.47
40:A:101:C:N3	40:A:102:A:C6	2.82	0.47
1:D:129:VAL:CB	1:D:139:ILE:O	2.63	0.47
15:V:135:TRP:HA	15:V:145:ARG:HA	1.96	0.47
40:A:377:U:H3'	40:A:378:U:H6	1.79	0.47
10:Q:276:SER:O	10:Q:280:ALA:N	2.46	0.47
18:Z:74:SER:N	40:A:469:U:OP2	2.47	0.47
40:A:208:U:O4	40:A:227:A:N6	2.48	0.47
40:A:783:G:O6	40:A:1002:A:N6	2.48	0.47
40:A:1029:C:H2'	40:A:1030:G:C8	2.49	0.47
40:A:1288:A:H3'	40:A:1289:G:H8	1.79	0.47
44:B:1665:C:H2'	44:B:1666:U:C6	2.49	0.47
8:N:87:PHE:HA	8:N:191:SER:HA	1.97	0.47
16:X:149:PRO:O	16:X:153:LEU:N	2.48	0.47
22:7:180:CYS:HA	22:7:297:PHE:O	2.14	0.47
40:A:998:A:H2'	40:A:999:A:C8	2.49	0.47
40:A:1139:C:N3	40:A:1253:G:C6	2.83	0.47
40:A:1343:G:N2	40:A:1354:U:O2	2.33	0.47
45:P:67:TRP:N	46:W:78:GLY:O	2.47	0.47
3:F:63:GLN:HA	3:F:81:ASP:HA	1.97	0.47
40:A:547:C:OP1	48:I:128:ASN:N	2.47	0.47
40:A:769:U:H2'	40:A:770:G:C8	2.46	0.47
40:A:1019:C:H2'	40:A:1020:G:C8	2.50	0.47
7:M:103:TYR:O	7:M:107:LEU:N	2.34	0.47
16:X:86:ILE:O	16:X:104:VAL:HA	2.15	0.47
21:5:333:ALA:HB1	21:5:363:ASP:HA	1.97	0.47
1:D:145:GLY:H	21:5:259:ILE:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:P:50:ARG:H	47:6:222:ASP:HA	1.80	0.47
2:E:212:GLY:N	40:A:1548:A:OP1	2.47	0.46
5:K:29:GLY:HA3	40:A:569:A:O3'	2.15	0.46
40:A:332:G:C2	40:A:1257:C:N3	2.83	0.46
40:A:993:C:H2'	40:A:994:U:C6	2.50	0.46
40:A:1036:A:O2'	40:A:1037:A:H5'	2.14	0.46
40:A:1139:C:N3	40:A:1254:U:C5	2.83	0.46
13:T:97:MET:O	13:T:142:ILE:N	2.38	0.46
15:V:76:VAL:HA	15:V:87:VAL:O	2.14	0.46
21:5:384:GLN:N	21:5:404:VAL:O	2.46	0.46
40:A:240:C:H2'	40:A:241:C:C6	2.50	0.46
40:A:786:U:H2'	40:A:787:A:H8	1.80	0.46
21:5:352:PHE:O	21:5:380:GLN:N	2.45	0.46
40:A:1450:C:H42	40:A:1466:A:H61	1.64	0.46
13:T:91:ALA:O	13:T:95:ARG:N	2.48	0.46
40:A:220:C:H2'	40:A:221:A:C8	2.51	0.46
40:A:224:G:H2'	40:A:225:C:C6	2.50	0.46
40:A:1306:G:O2'	40:A:1307:G:H5'	2.15	0.46
40:A:1371:U:H6	40:A:1371:U:H5'	1.80	0.46
15:V:76:VAL:HA	15:V:88:VAL:HA	1.97	0.46
40:A:467:C:H2'	40:A:468:U:H6	1.81	0.46
40:A:1078:A:H2'	40:A:1079:A:H8	1.81	0.46
40:A:1332:G:H2'	40:A:1333:A:H8	1.81	0.46
40:A:339:G:C8	40:A:340:U:H2'	2.50	0.46
40:A:510:A:O2'	40:A:536:C:O3'	2.33	0.46
48:I:99:CYS:O	48:I:151:ASN:HA	2.16	0.46
40:A:1065:G:N2	40:A:1254:U:O2	2.31	0.46
21:5:59:THR:HA	21:5:71:ALA:HB3	1.97	0.46
40:A:11:G:N1	40:A:102:A:C2	2.84	0.46
40:A:432:A:N6	40:A:450:G:O6	2.49	0.46
40:A:213:G:H2'	40:A:214:G:H8	1.80	0.46
40:A:332:G:C6	40:A:1257:C:C2	3.03	0.46
40:A:586:U:H2'	40:A:587:C:C6	2.51	0.46
40:A:1259:C:H2'	40:A:1260:U:C6	2.51	0.46
1:D:193:ILE:N	1:D:214:GLY:O	2.44	0.46
6:L:60:VAL:HA	6:L:73:ILE:HA	1.98	0.46
13:T:155:ARG:O	13:T:167:MET:CB	2.64	0.45
40:A:348:G:H2'	40:A:349:G:C8	2.51	0.45
2:E:274:TRP:N	2:E:284:TYR:O	2.42	0.45
40:A:125:A:H2'	40:A:126:A:C4	2.51	0.45
40:A:495:C:H1'	40:A:546:A:H61	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:B:1616:A:C6	44:B:1646:U:N3	2.84	0.45
40:A:227:A:H2'	40:A:228:A:C8	2.50	0.45
40:A:450:G:H2'	40:A:451:G:H8	1.81	0.45
40:A:644:C:H2'	40:A:645:A:C8	2.52	0.45
1:D:196:VAL:N	1:D:206:TYR:O	2.46	0.45
40:A:97:G:H2'	40:A:98:G:H8	1.80	0.45
40:A:521:A:N6	40:A:527:G:OP2	2.38	0.45
40:A:1078:A:H2'	40:A:1079:A:C8	2.51	0.45
40:A:100:G:H2'	40:A:101:C:H6	1.81	0.45
40:A:1379:U:C2	40:A:1383:A:N7	2.85	0.45
40:A:566:C:O2'	40:A:567:A:O5'	2.31	0.45
40:A:631:U:H2'	40:A:632:U:C6	2.52	0.45
40:A:748:A:H2'	40:A:749:C:C6	2.52	0.45
40:A:1138:U:H1'	40:A:1251:A:H2'	1.99	0.45
40:A:1470:A:H2'	40:A:1471:A:C8	2.51	0.45
12:S:146:LYS:HA	12:S:147:PRO:HA	1.78	0.45
40:A:205:C:H2'	40:A:206:U:C6	2.52	0.45
40:A:594:A:H2'	40:A:595:A:C8	2.52	0.45
40:A:696:G:H2'	40:A:697:A:C8	2.52	0.45
40:A:699:A:H2'	40:A:700:A:H8	1.82	0.45
40:A:786:U:H2'	40:A:787:A:C8	2.51	0.45
40:A:1454:U:OP2	40:A:1462:G:N1	2.49	0.45
40:A:164:U:H2'	40:A:165:A:C8	2.52	0.45
40:A:225:C:H2'	40:A:226:U:C6	2.51	0.45
45:P:66:GLY:HA3	46:W:81:VAL:H	1.81	0.45
1:D:230:SER:N	40:A:849:G:O6	2.50	0.45
40:A:82:U:H2'	40:A:83:A:C8	2.52	0.45
40:A:242:A:H2'	40:A:243:G:H8	1.82	0.45
40:A:429:U:H2'	40:A:430:C:C6	2.51	0.45
12:S:175:ARG:O	12:S:180:PHE:CB	2.65	0.45
40:A:21:C:H2'	40:A:22:A:N3	2.32	0.45
40:A:415:A:H2'	40:A:416:A:C8	2.51	0.45
40:A:999:A:H2'	40:A:1000:C:C6	2.53	0.45
40:A:313:U:O2	40:A:318:G:O2'	2.35	0.44
40:A:1026:A:N7	40:A:1029:C:N4	2.65	0.44
1:D:196:VAL:O	1:D:206:TYR:N	2.50	0.44
40:A:457:A:H2'	40:A:458:G:H8	1.82	0.44
40:A:616:A:H2'	40:A:617:U:C6	2.52	0.44
40:A:1475:A:H2'	40:A:1476:G:C8	2.52	0.44
2:E:216:GLN:O	2:E:258:PRO:HA	2.16	0.44
40:A:1454:U:C4	40:A:1463:A:C8	3.03	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A:1481:A:H61	40:A:1493:G:H1'	1.82	0.44
47:6:274:LYS:N	47:6:312:THR:O	2.47	0.44
2:E:158:ALA:HB3	2:E:161:ILE:H	1.83	0.44
3:F:206:LEU:O	3:F:210:ARG:N	2.49	0.44
40:A:648:A:H2'	40:A:649:A:C8	2.52	0.44
40:A:850:C:C2	40:A:858:G:N2	2.78	0.44
1:D:181:ALA:HA	1:D:243:THR:HA	2.00	0.44
40:A:11:G:C2	40:A:102:A:C2	3.05	0.44
40:A:51:C:N4	40:A:60:U:C4	2.84	0.44
40:A:696:G:H2'	40:A:697:A:H8	1.83	0.44
40:A:258:A:H2'	40:A:259:A:C8	2.53	0.44
40:A:430:C:H2'	40:A:431:C:H6	1.83	0.44
8:N:117:ASN:O	8:N:166:ARG:N	2.51	0.44
22:7:255:HIS:O	22:7:261:ILE:HA	2.17	0.44
40:A:161:G:N1	40:A:162:A:N3	2.65	0.44
40:A:993:C:H2'	40:A:994:U:H6	1.82	0.44
8:N:215:PHE:O	8:N:219:ALA:HB3	2.18	0.44
20:2:66:TRP:H	40:A:32:A:P	2.41	0.44
40:A:1139:C:N4	40:A:1253:G:O6	2.50	0.44
40:A:1389:A:OP1	40:A:1391:G:O2'	2.24	0.44
40:A:1554:G:H2'	40:A:1555:G:H8	1.83	0.44
4:H:79:VAL:HA	16:X:89:GLN:H	1.83	0.44
40:A:460:A:H2'	40:A:463:A:H61	1.82	0.44
40:A:1446:C:H2'	40:A:1447:C:C6	2.52	0.44
2:E:208:ALA:O	2:E:265:TYR:HA	2.18	0.43
6:L:119:ILE:H	6:L:141:ALA:HA	1.83	0.43
40:A:238:A:N6	40:A:342:A:N6	2.37	0.43
40:A:672:U:N3	40:A:701:U:O4	2.51	0.43
40:A:1040:C:H2'	40:A:1041:A:C8	2.51	0.43
40:A:1197:C:H2'	40:A:1198:C:O4'	2.18	0.43
22:7:218:THR:HA	22:7:255:HIS:HA	1.99	0.43
23:9:29:SER:O	23:9:32:GLY:N	2.50	0.43
40:A:1447:C:H2'	40:A:1448:U:C6	2.53	0.43
2:E:99:LEU:CB	2:E:299:VAL:O	2.66	0.43
4:H:94:LEU:O	4:H:113:SER:HA	2.18	0.43
15:V:93:THR:HA	15:V:112:GLU:HA	2.00	0.43
16:X:116:SER:O	16:X:120:ASP:CA	2.67	0.43
40:A:424:G:H2'	40:A:425:U:C6	2.53	0.43
6:L:39:ARG:N	6:L:103:ASN:O	2.50	0.43
4:H:133:SER:O	4:H:137:LYS:N	2.49	0.43
17:Y:155:LEU:HA	17:Y:159:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A:71:A:H4'	40:A:72:G:H4'	2.00	0.43
40:A:224:G:H2'	40:A:225:C:H6	1.84	0.43
40:A:699:A:H2'	40:A:700:A:C8	2.53	0.43
40:A:792:A:H2'	40:A:793:A:C8	2.53	0.43
40:A:994:U:H2'	40:A:995:U:C6	2.53	0.43
3:F:222:THR:O	3:F:226:MET:N	2.52	0.43
40:A:213:G:H2'	40:A:214:G:C8	2.53	0.43
40:A:228:A:H2'	40:A:229:G:C8	2.53	0.43
40:A:242:A:H2'	40:A:243:G:C8	2.54	0.43
40:A:785:U:H2'	40:A:786:U:H6	1.83	0.43
4:H:97:ILE:HA	4:H:111:LEU:HA	2.00	0.43
5:K:94:GLN:O	5:K:98:ARG:CB	2.66	0.43
40:A:512:G:H1'	40:A:529:A:H2'	2.01	0.43
40:A:862:U:H2'	40:A:863:A:H8	1.82	0.43
48:I:171:VAL:O	48:I:173:PHE:N	2.51	0.43
40:A:605:U:H2'	40:A:606:C:C6	2.54	0.43
1:D:83:GLY:HA2	1:D:97:GLY:HA3	2.01	0.43
10:Q:137:CYS:HA	10:Q:151:LEU:HA	2.00	0.43
40:A:1081:G:H2'	40:A:1082:C:C6	2.54	0.43
40:A:47:U:H2'	40:A:48:A:C8	2.54	0.43
40:A:413:U:H2'	40:A:414:A:C8	2.54	0.43
49:J:104:THR:HA	49:J:105:GLY:HA2	1.58	0.43
1:D:190:GLY:N	1:D:216:LEU:O	2.49	0.42
40:A:43:A:H2'	40:A:44:C:C2	2.54	0.42
40:A:741:U:H2'	40:A:742:A:H8	1.84	0.42
40:A:1493:G:H2'	40:A:1494:C:H6	1.84	0.42
40:A:1080:U:H3'	40:A:1081:G:H8	1.84	0.42
40:A:1474:A:H2'	40:A:1475:A:C8	2.54	0.42
40:A:467:C:H2'	40:A:468:U:C6	2.54	0.42
1:D:155:GLU:N	1:D:246:ARG:O	2.53	0.42
40:A:115:C:H2'	40:A:116:C:C6	2.55	0.42
40:A:1076:U:H2'	40:A:1077:U:C6	2.54	0.42
40:A:1476:G:H2'	40:A:1477:G:O4'	2.19	0.42
5:K:78:SER:HA	5:K:88:ARG:O	2.19	0.42
40:A:381:A:H2'	40:A:382:A:C8	2.54	0.42
40:A:431:C:N3	40:A:451:G:N1	2.68	0.42
40:A:847:U:H2'	40:A:848:A:C8	2.55	0.42
40:A:1307:G:H4'	40:A:1308:U:H5''	2.01	0.42
43:1:213:ILE:N	43:1:353:VAL:O	2.43	0.42
1:D:192:LEU:O	1:D:245:GLY:N	2.44	0.42
8:N:143:GLY:HA2	40:A:437:G:H4'	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A:610:C:H42	40:A:615:U:H3	1.65	0.42
40:A:616:A:H2'	40:A:617:U:H6	1.83	0.42
40:A:768:A:H2'	40:A:769:U:C6	2.54	0.42
15:V:198:VAL:O	15:V:202:MET:N	2.42	0.42
40:A:170:C:H2'	40:A:171:U:C6	2.54	0.42
40:A:258:A:H2'	40:A:259:A:H8	1.84	0.42
40:A:326:C:H2'	40:A:327:C:C6	2.54	0.42
40:A:1260:U:H2'	40:A:1261:A:C8	2.53	0.42
44:B:1609:U:O2'	44:B:1645:A:N3	2.43	0.42
6:L:45:ALA:O	6:L:49:SER:N	2.52	0.42
40:A:259:A:H2'	40:A:260:C:C6	2.55	0.42
40:A:1125:U:H2'	40:A:1126:G:H8	1.85	0.42
40:A:1289:G:N2	40:A:1296:U:O4	2.52	0.42
44:B:1661:A:H2'	44:B:1663:C:C6	2.55	0.42
46:W:54:LYS:N	46:W:67:ILE:O	2.53	0.42
40:A:337:U:H2'	40:A:338:G:H8	1.84	0.42
40:A:521:A:N6	40:A:528:A:OP2	2.53	0.42
40:A:523:U:O4	40:A:526:A:N1	2.51	0.42
40:A:1436:C:H2'	40:A:1437:U:C6	2.55	0.42
40:A:1467:G:H2'	40:A:1468:A:C8	2.55	0.42
40:A:1386:C:H2'	40:A:1387:C:C6	2.54	0.42
40:A:1448:U:H2'	40:A:1449:C:C6	2.55	0.42
2:E:151:THR:HA	2:E:173:LYS:HA	2.02	0.41
40:A:252:C:H2'	40:A:253:C:H6	1.85	0.41
40:A:1252:A:H2'	40:A:1253:G:H8	1.84	0.41
40:A:29:C:H5''	40:A:30:U:H5	1.85	0.41
40:A:533:G:H21	40:A:538:A:H62	1.67	0.41
40:A:748:A:H2'	40:A:749:C:H6	1.85	0.41
40:A:1454:U:C4	40:A:1463:A:H8	2.38	0.41
1:D:85:ARG:HA	1:D:91:ILE:HA	2.01	0.41
23:9:93:SER:O	23:9:97:ALA:HB2	2.20	0.41
40:A:119:A:H2'	40:A:120:A:C8	2.55	0.41
40:A:1374:A:H2'	40:A:1375:A:H8	1.85	0.41
40:A:201:A:N6	40:A:230:A:H2'	2.35	0.41
40:A:402:A:H2'	40:A:403:A:H8	1.86	0.41
40:A:530:A:H2'	40:A:531:G:C8	2.55	0.41
1:D:121:PRO:HA	1:D:165:ASN:O	2.20	0.41
10:Q:231:LYS:O	10:Q:233:TRP:N	2.52	0.41
40:A:317:G:H2'	40:A:318:G:C8	2.55	0.41
12:S:97:ALA:HA	12:S:135:LEU:O	2.20	0.41
40:A:212:A:H4'	40:A:213:G:H5'	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A:620:A:H2'	40:A:621:A:C8	2.56	0.41
40:A:1140:G:H2'	40:A:1141:G:C8	2.56	0.41
44:B:1664:G:H2'	44:B:1665:C:C6	2.56	0.41
3:F:144:PRO:HA	3:F:150:GLY:H	1.86	0.41
40:A:656:C:H2'	40:A:657:U:C6	2.56	0.41
40:A:1495:C:H2'	40:A:1496:U:C6	2.56	0.41
40:A:411:U:H2'	40:A:412:G:C8	2.56	0.41
40:A:862:U:H2'	40:A:863:A:C8	2.55	0.41
40:A:1020:G:N1	40:A:1030:G:C6	2.89	0.41
40:A:1070:A:H2'	40:A:1071:A:C8	2.56	0.41
40:A:1083:A:H3'	40:A:1084:A:H8	1.86	0.41
40:A:1249:A:O2'	40:A:1250:C:O4'	2.38	0.41
40:A:1254:U:H2'	40:A:1255:U:C6	2.55	0.41
44:B:1615:A:N1	44:B:1621:A:O2'	2.37	0.41
2:E:146:SER:HA	2:E:178:ILE:HA	2.03	0.41
40:A:1:G:O2'	40:A:2:C:O4'	2.38	0.41
40:A:154:U:O2'	40:A:155:A:O5'	2.37	0.41
40:A:425:U:H2'	40:A:426:U:C6	2.56	0.41
40:A:570:C:O2'	40:A:572:U:OP2	2.38	0.41
40:A:586:U:H2'	40:A:587:C:H6	1.86	0.41
40:A:990:U:H2'	40:A:991:U:C6	2.56	0.41
40:A:1006:A:H2'	40:A:1007:A:C8	2.56	0.41
40:A:1494:C:H2'	40:A:1495:C:H6	1.85	0.41
44:B:1604:G:H2'	44:B:1605:A:C8	2.56	0.41
21:5:233:LYS:HA	21:5:285:TYR:HA	2.02	0.41
40:A:366:C:H4'	40:A:367:U:C5	2.56	0.41
40:A:741:U:H2'	40:A:742:A:C8	2.56	0.41
40:A:1076:U:H2'	40:A:1077:U:H6	1.86	0.41
40:A:1263:G:H2'	40:A:1264:G:C8	2.56	0.41
40:A:1493:G:H2'	40:A:1494:C:C6	2.56	0.41
40:A:1510:A:H2'	40:A:1511:U:O4'	2.21	0.41
40:A:1340:G:H1	40:A:1357:U:H3	1.70	0.40
40:A:83:A:H2'	40:A:84:G:C8	2.57	0.40
40:A:332:G:H1'	40:A:333:A:C5	2.56	0.40
40:A:345:G:H21	40:A:370:G:H1'	1.86	0.40
40:A:421:A:H2'	40:A:422:C:C6	2.56	0.40
10:Q:150:ILE:HA	10:Q:163:CYS:HA	2.03	0.40
21:5:291:LEU:O	21:5:344:SER:HA	2.22	0.40
40:A:662:C:N3	40:A:774:A:C6	2.89	0.40
1:D:183:PRO:HA	1:D:241:VAL:HA	2.03	0.40
40:A:729:A:H2'	40:A:730:C:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A:1446:C:H2'	40:A:1447:C:H6	1.85	0.40
7:M:145:ALA:HA	47:6:379:ILE:HA	2.01	0.40
14:U:67:ALA:O	14:U:97:VAL:HA	2.21	0.40
40:A:1445:U:H2'	40:A:1446:C:C6	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	216/305 (71%)	204 (94%)	12 (6%)	0	100	100
2	E	281/348 (81%)	249 (89%)	32 (11%)	0	100	100
3	F	248/311 (80%)	221 (89%)	27 (11%)	0	100	100
4	H	93/267 (35%)	84 (90%)	9 (10%)	0	100	100
5	K	175/178 (98%)	154 (88%)	21 (12%)	0	100	100
6	L	113/145 (78%)	107 (95%)	6 (5%)	0	100	100
7	M	253/296 (86%)	226 (89%)	27 (11%)	0	100	100
8	N	203/251 (81%)	195 (96%)	8 (4%)	0	100	100
9	O	150/175 (86%)	138 (92%)	12 (8%)	0	100	100
10	Q	215/292 (74%)	196 (91%)	19 (9%)	0	100	100
11	R	138/149 (93%)	126 (91%)	12 (9%)	0	100	100
12	S	154/205 (75%)	141 (92%)	13 (8%)	0	100	100
13	T	155/206 (75%)	143 (92%)	12 (8%)	0	100	100
14	U	135/153 (88%)	123 (91%)	12 (9%)	0	100	100
15	V	188/216 (87%)	176 (94%)	12 (6%)	0	100	100
16	X	241/256 (94%)	227 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	174/250 (70%)	161 (92%)	13 (8%)	0	100	100
18	Z	118/161 (73%)	107 (91%)	11 (9%)	0	100	100
19	0	106/188 (56%)	100 (94%)	6 (6%)	0	100	100
20	2	41/92 (45%)	36 (88%)	5 (12%)	0	100	100
21	5	383/423 (90%)	361 (94%)	21 (6%)	1 (0%)	41	76
22	7	285/338 (84%)	252 (88%)	33 (12%)	0	100	100
23	9	113/137 (82%)	99 (88%)	14 (12%)	0	100	100
24	a	78/142 (55%)	67 (86%)	11 (14%)	0	100	100
25	b	146/215 (68%)	127 (87%)	19 (13%)	0	100	100
26	c	271/332 (82%)	256 (94%)	15 (6%)	0	100	100
27	d	203/306 (66%)	189 (93%)	14 (7%)	0	100	100
28	g	127/166 (76%)	120 (94%)	7 (6%)	0	100	100
29	h	96/158 (61%)	92 (96%)	4 (4%)	0	100	100
30	i	95/128 (74%)	83 (87%)	12 (13%)	0	100	100
31	j	83/123 (68%)	78 (94%)	5 (6%)	0	100	100
32	o	77/102 (76%)	71 (92%)	6 (8%)	0	100	100
33	p	101/206 (49%)	93 (92%)	7 (7%)	1 (1%)	15	54
34	q	97/222 (44%)	93 (96%)	4 (4%)	0	100	100
35	r	140/196 (71%)	129 (92%)	11 (8%)	0	100	100
36	s	366/439 (83%)	341 (93%)	25 (7%)	0	100	100
37	u	109/234 (47%)	100 (92%)	9 (8%)	0	100	100
38	v	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
39	w	77/156 (49%)	73 (95%)	4 (5%)	0	100	100
41	x	370/540 (68%)	351 (95%)	16 (4%)	3 (1%)	19	60
42	y	329/387 (85%)	276 (84%)	49 (15%)	4 (1%)	13	49
43	1	251/420 (60%)	239 (95%)	12 (5%)	0	100	100
43	z	245/420 (58%)	233 (95%)	12 (5%)	0	100	100
45	P	129/180 (72%)	124 (96%)	4 (3%)	1 (1%)	19	60
46	W	96/148 (65%)	92 (96%)	2 (2%)	2 (2%)	7	36
47	6	313/380 (82%)	286 (91%)	23 (7%)	4 (1%)	12	48
48	I	154/261 (59%)	145 (94%)	8 (5%)	1 (1%)	25	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	J	138/192 (72%)	129 (94%)	8 (6%)	1 (1%)	22	62
50	k	82/112 (73%)	73 (89%)	5 (6%)	4 (5%)	2	20
51	l	21/138 (15%)	21 (100%)	0	0	100	100
All	All	8439/11715 (72%)	7771 (92%)	646 (8%)	22 (0%)	44	76

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
41	x	201	ILE
41	x	347	PRO
42	y	75	SER
47	6	373	HIS
50	k	62	PRO
33	p	142	TYR
42	y	126	LYS
46	W	72	HIS
21	5	216	GLU
42	y	147	LEU
42	y	249	THR
46	W	127	TYR
49	J	70	ILE
50	k	73	ARG
41	x	397	SER
45	P	177	ILE
47	6	351	HIS
47	6	375	PRO
48	I	61	HIS
50	k	37	VAL
50	k	18	VAL
47	6	288	SER

### 5.3.2 Protein sidechains ⓘ

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

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
40	A	1183/1559 (75%)	457 (38%)	20 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	B	51/69 (73%)	18 (35%)	1 (1%)
All	All	1234/1628 (75%)	475 (38%)	21 (1%)

All (475) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
40	A	2	C
40	A	5	A
40	A	6	A
40	A	8	C
40	A	9	U
40	A	10	A
40	A	11	G
40	A	12	C
40	A	14	C
40	A	15	C
40	A	19	C
40	A	22	A
40	A	23	C
40	A	24	U
40	A	29	C
40	A	30	U
40	A	31	U
40	A	32	A
40	A	34	U
40	A	36	C
40	A	37	C
40	A	38	A
40	A	43	A
40	A	44	C
40	A	45	C
40	A	46	U
40	A	47	U
40	A	49	G
40	A	50	C
40	A	52	A
40	A	54	A
40	A	55	C
40	A	57	A
40	A	59	U
40	A	61	A
40	A	68	U

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Mol	Chain	Res	Type
40	A	71	A
40	A	73	U
40	A	75	U
40	A	77	G
40	A	78	G
40	A	80	G
40	A	81	A
40	A	99	C
40	A	100	G
40	A	104	U
40	A	105	A
40	A	107	A
40	A	108	U
40	A	109	A
40	A	110	U
40	A	111	A
40	A	112	G
40	A	119	A
40	A	121	G
40	A	123	G
40	A	124	A
40	A	126	A
40	A	133	A
40	A	134	A
40	A	136	U
40	A	142	C
40	A	143	C
40	A	144	A
40	A	149	U
40	A	150	A
40	A	151	A
40	A	152	U
40	A	153	A
40	A	154	U
40	A	155	A
40	A	156	G
40	A	157	C
40	A	158	A
40	A	162	A
40	A	163	C
40	A	167	C
40	A	169	C

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Mol	Chain	Res	Type
40	A	170	C
40	A	173	U
40	A	174	A
40	A	175	C
40	A	177	U
40	A	178	U
40	A	179	C
40	A	180	U
40	A	187	U
40	A	192	U
40	A	195	C
40	A	197	A
40	A	198	G
40	A	199	A
40	A	200	A
40	A	201	A
40	A	202	U
40	A	204	A
40	A	205	C
40	A	208	U
40	A	210	C
40	A	212	A
40	A	213	G
40	A	216	G
40	A	217	A
40	A	218	G
40	A	222	A
40	A	223	A
40	A	231	C
40	A	232	C
40	A	233	C
40	A	237	A
40	A	239	A
40	A	244	A
40	A	247	A
40	A	248	G
40	A	303	G
40	A	305	U
40	A	315	G
40	A	316	A
40	A	317	G
40	A	322	C

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Mol	Chain	Res	Type
40	A	324	A
40	A	325	A
40	A	328	U
40	A	329	A
40	A	330	C
40	A	332	G
40	A	333	A
40	A	340	U
40	A	341	G
40	A	343	U
40	A	345	G
40	A	346	C
40	A	351	U
40	A	352	G
40	A	358	G
40	A	360	U
40	A	361	A
40	A	366	C
40	A	367	U
40	A	369	A
40	A	374	A
40	A	377	U
40	A	378	U
40	A	379	U
40	A	383	U
40	A	385	U
40	A	386	G
40	A	389	C
40	A	390	A
40	A	391	C
40	A	395	A
40	A	404	A
40	A	409	C
40	A	413	U
40	A	414	A
40	A	415	A
40	A	416	A
40	A	417	U
40	A	418	U
40	A	420	A
40	A	422	C
40	A	423	U

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Mol	Chain	Res	Type
40	A	427	A
40	A	432	A
40	A	439	A
40	A	441	C
40	A	443	G
40	A	444	C
40	A	446	C
40	A	447	U
40	A	454	A
40	A	455	C
40	A	456	U
40	A	460	A
40	A	461	A
40	A	464	A
40	A	465	A
40	A	471	U
40	A	472	A
40	A	473	G
40	A	477	G
40	A	481	A
40	A	483	A
40	A	484	A
40	A	485	A
40	A	487	U
40	A	489	U
40	A	490	A
40	A	495	C
40	A	496	C
40	A	499	A
40	A	500	G
40	A	501	U
40	A	502	A
40	A	503	G
40	A	504	G
40	A	510	A
40	A	511	A
40	A	512	G
40	A	513	C
40	A	514	A
40	A	516	C
40	A	517	C
40	A	522	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
40	A	523	U
40	A	524	U
40	A	525	A
40	A	527	G
40	A	528	A
40	A	530	A
40	A	531	G
40	A	532	C
40	A	534	U
40	A	540	C
40	A	541	U
40	A	546	A
40	A	564	C
40	A	565	C
40	A	566	C
40	A	567	A
40	A	571	A
40	A	572	U
40	A	573	A
40	A	574	U
40	A	575	A
40	A	577	C
40	A	580	A
40	A	582	C
40	A	583	U
40	A	587	C
40	A	589	C
40	A	591	C
40	A	592	C
40	A	593	C
40	A	594	A
40	A	599	G
40	A	602	C
40	A	604	A
40	A	609	U
40	A	610	C
40	A	613	C
40	A	614	C
40	A	615	U
40	A	620	A
40	A	622	G
40	A	624	A

*Continued on next page...*

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Mol	Chain	Res	Type
40	A	626	U
40	A	627	A
40	A	628	A
40	A	629	U
40	A	630	G
40	A	631	U
40	A	639	A
40	A	640	G
40	A	641	U
40	A	642	A
40	A	645	A
40	A	646	U
40	A	647	G
40	A	652	C
40	A	653	A
40	A	654	U
40	A	662	C
40	A	675	G
40	A	679	G
40	A	680	A
40	A	702	U
40	A	703	A
40	A	704	A
40	A	705	C
40	A	709	C
40	A	711	A
40	A	717	U
40	A	718	A
40	A	720	A
40	A	723	C
40	A	724	A
40	A	727	C
40	A	731	A
40	A	734	U
40	A	736	A
40	A	737	U
40	A	744	C
40	A	745	C
40	A	746	U
40	A	748	A
40	A	752	U
40	A	753	C

*Continued on next page...*

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Mol	Chain	Res	Type
40	A	756	C
40	A	757	C
40	A	758	C
40	A	759	A
40	A	761	C
40	A	765	G
40	A	771	C
40	A	773	C
40	A	774	A
40	A	776	A
40	A	782	A
40	A	788	A
40	A	798	A
40	A	838	C
40	A	841	C
40	A	842	A
40	A	850	C
40	A	851	A
40	A	853	C
40	A	854	A
40	A	856	C
40	A	857	A
40	A	985	G
40	A	986	U
40	A	990	U
40	A	997	U
40	A	1004	U
40	A	1011	G
40	A	1013	C
40	A	1014	C
40	A	1015	U
40	A	1016	G
40	A	1027	G
40	A	1035	U
40	A	1036	A
40	A	1037	A
40	A	1038	C
40	A	1039	A
40	A	1040	C
40	A	1044	A
40	A	1046	G
40	A	1048	C

*Continued on next page...*



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Mol	Chain	Res	Type
40	A	1049	G
40	A	1055	A
40	A	1061	U
40	A	1069	U
40	A	1070	A
40	A	1071	A
40	A	1073	U
40	A	1075	A
40	A	1078	A
40	A	1080	U
40	A	1081	G
40	A	1083	A
40	A	1084	A
40	A	1085	A
40	A	1129	U
40	A	1131	A
40	A	1134	A
40	A	1138	U
40	A	1140	G
40	A	1155	G
40	A	1161	G
40	A	1162	A
40	A	1163	A
40	A	1167	A
40	A	1168	A
40	A	1169	C
40	A	1174	G
40	A	1177	C
40	A	1184	U
40	A	1187	U
40	A	1189	A
40	A	1194	U
40	A	1195	C
40	A	1200	G
40	A	1201	U
40	A	1222	A
40	A	1224	U
40	A	1226	G
40	A	1227	A
40	A	1230	C
40	A	1231	A
40	A	1236	C

*Continued on next page...*

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Mol	Chain	Res	Type
40	A	1246	G
40	A	1248	A
40	A	1249	A
40	A	1250	C
40	A	1252	A
40	A	1253	G
40	A	1256	A
40	A	1258	C
40	A	1262	G
40	A	1280	U
40	A	1281	A
40	A	1282	U
40	A	1283	U
40	A	1285	U
40	A	1286	A
40	A	1293	A
40	A	1294	U
40	A	1301	A
40	A	1304	A
40	A	1305	G
40	A	1306	G
40	A	1307	G
40	A	1308	U
40	A	1311	A
40	A	1314	A
40	A	1316	C
40	A	1318	C
40	A	1330	A
40	A	1335	A
40	A	1346	G
40	A	1352	G
40	A	1359	A
40	A	1366	G
40	A	1370	G
40	A	1371	U
40	A	1372	U
40	A	1373	C
40	A	1379	U
40	A	1383	A
40	A	1384	G
40	A	1390	C
40	A	1393	G

*Continued on next page...*

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Mol	Chain	Res	Type
40	A	1395	U
40	A	1400	G
40	A	1402	U
40	A	1432	U
40	A	1438	U
40	A	1439	U
40	A	1444	U
40	A	1452	U
40	A	1453	G
40	A	1459	A
40	A	1464	C
40	A	1468	A
40	A	1469	G
40	A	1471	A
40	A	1472	A
40	A	1473	U
40	A	1477	G
40	A	1480	U
40	A	1482	C
40	A	1485	C
40	A	1487	C
40	A	1488	A
40	A	1490	A
40	A	1492	C
40	A	1493	G
40	A	1498	C
40	A	1507	A
40	A	1510	A
40	A	1514	C
40	A	1519	C
40	A	1520	A
40	A	1522	C
40	A	1532	U
40	A	1537	A
40	A	1545	C
40	A	1547	A
40	A	1548	A
40	A	1549	G
40	A	1550	A
40	A	1551	A
40	A	1552	C
40	A	1553	A

*Continued on next page...*

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Mol	Chain	Res	Type
40	A	1558	U
44	B	1607	U
44	B	1608	G
44	B	1609	U
44	B	1611	G
44	B	1613	U
44	B	1614	U
44	B	1615	A
44	B	1629	A
44	B	1630	A
44	B	1631	C
44	B	1632	U
44	B	1633	U
44	B	1641	G
44	B	1644	G
44	B	1645	A
44	B	1650	A
44	B	1659	U
44	B	1669	G

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
40	A	43	A
40	A	135	A
40	A	149	U
40	A	153	A
40	A	173	U
40	A	360	U
40	A	495	C
40	A	516	C
40	A	566	C
40	A	573	A
40	A	628	A
40	A	641	U
40	A	787	A
40	A	837	A
40	A	1235	A
40	A	1249	A
40	A	1371	U
40	A	1443	A
40	A	1489	A

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Mol	Chain	Res	Type
40	A	1531	A
44	B	1607	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 49 are monoatomic - leaving 1 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	$\# Z  > 2$
54	4S8	v	101	-	14,20,20	2.25	4 (28%)	18,26,26	1.14	1 (5%)

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
54	4S8	v	101	-	-	5/24/26/26	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	v	101	4S8	C9P-N8P	5.40	1.45	1.33
54	v	101	4S8	C5P-N4P	5.35	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	v	101	4S8	O5P-C5P	-2.19	1.18	1.23
54	v	101	4S8	O9P-C9P	-2.14	1.19	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	v	101	4S8	C6P-C7P-N8P	-2.93	105.98	111.90

There are no chirality outliers.

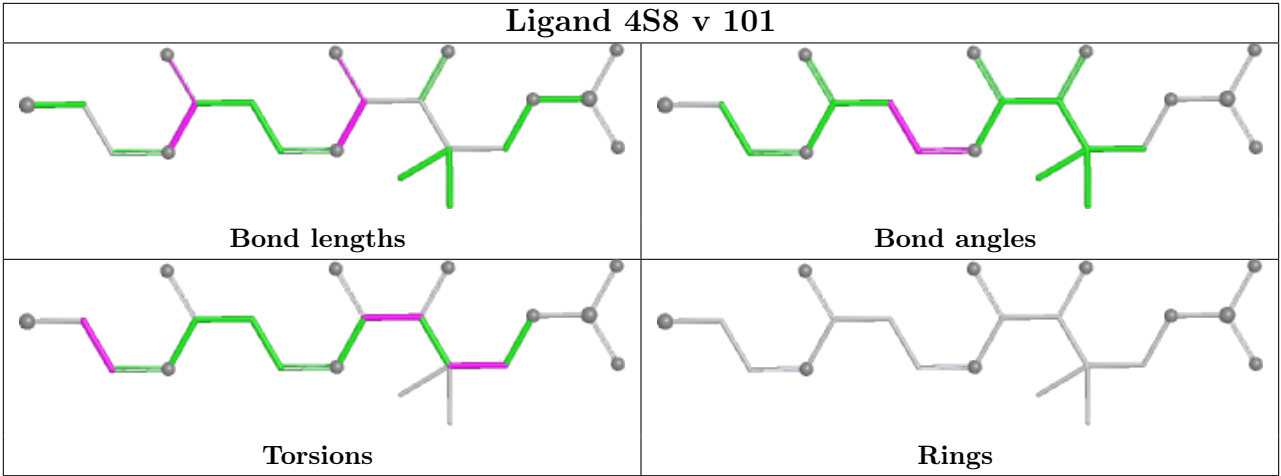
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	v	101	4S8	N8P-C9P-CAP-OAP
54	v	101	4S8	O9P-C9P-CAP-OAP
54	v	101	4S8	O9P-C9P-CAP-CBP
54	v	101	4S8	S1P-C2P-C3P-N4P
54	v	101	4S8	CDP-CBP-CCP-O6A

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
40	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1182:C	O3'	1183:A	P	11.06

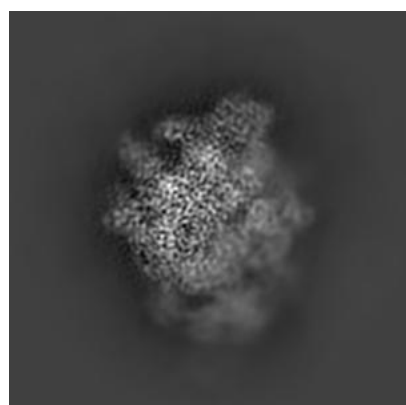
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12919. These allow visual inspection of the internal detail of the map and identification of artifacts.

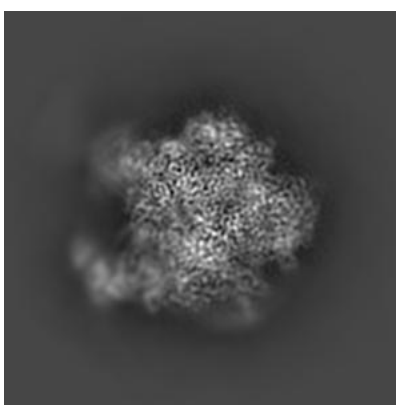
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

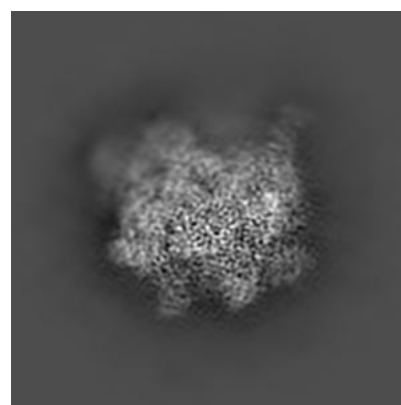
#### 6.1.1 Primary map



X



Y

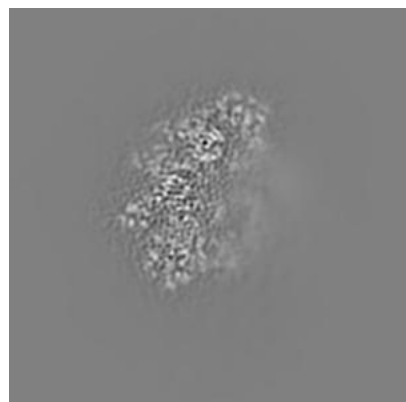


Z

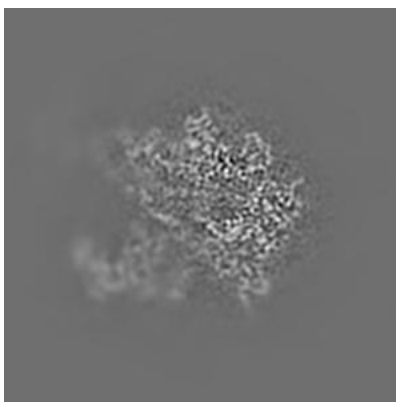
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

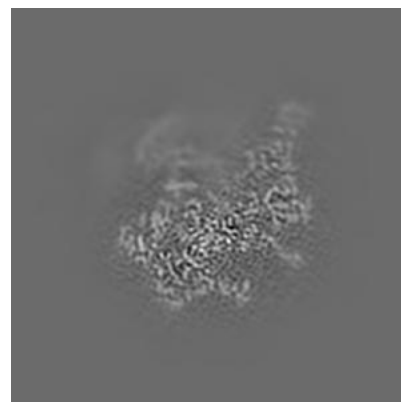
#### 6.2.1 Primary map



X Index: 180



Y Index: 180



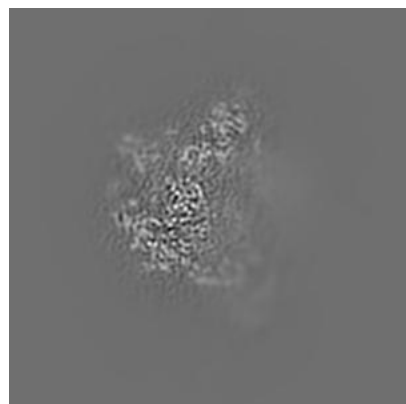
Z Index: 180



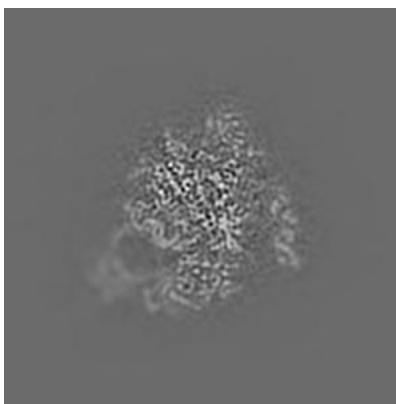
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

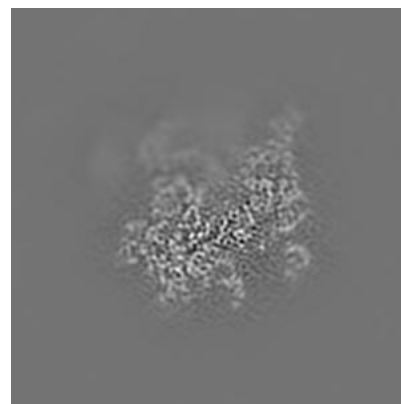
### 6.3.1 Primary map



X Index: 196



Y Index: 145

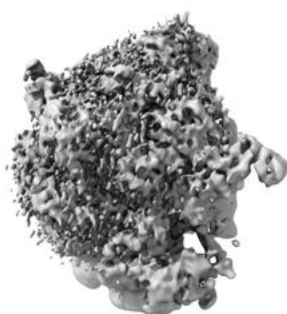


Z Index: 186

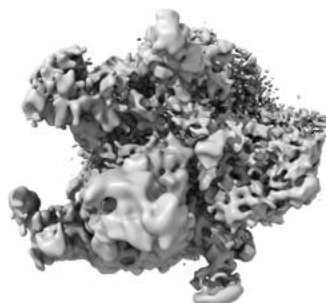
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

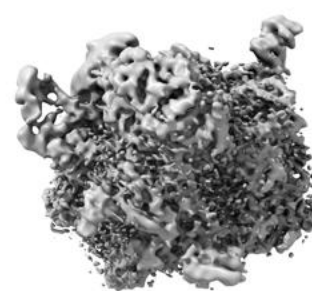
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

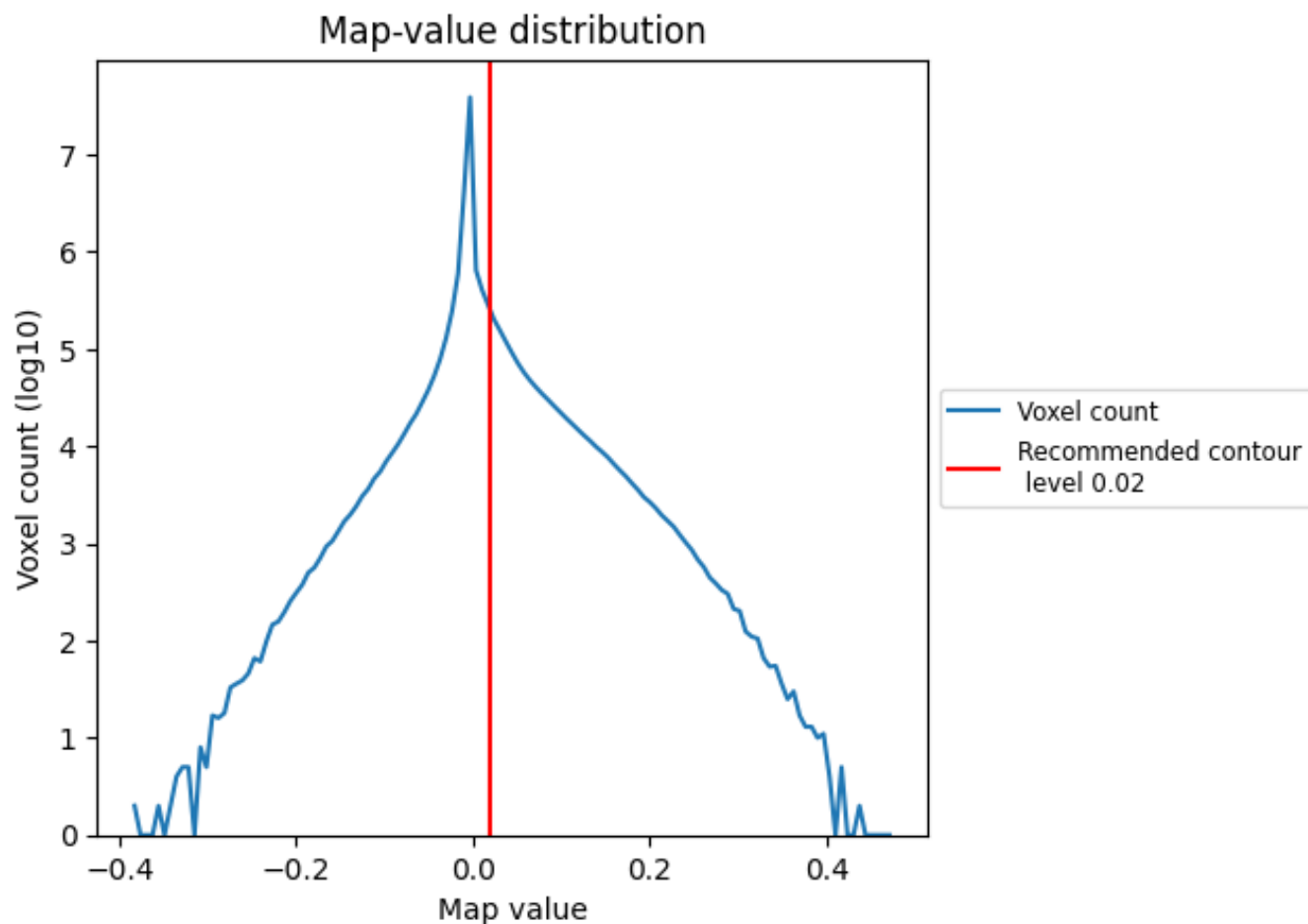
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

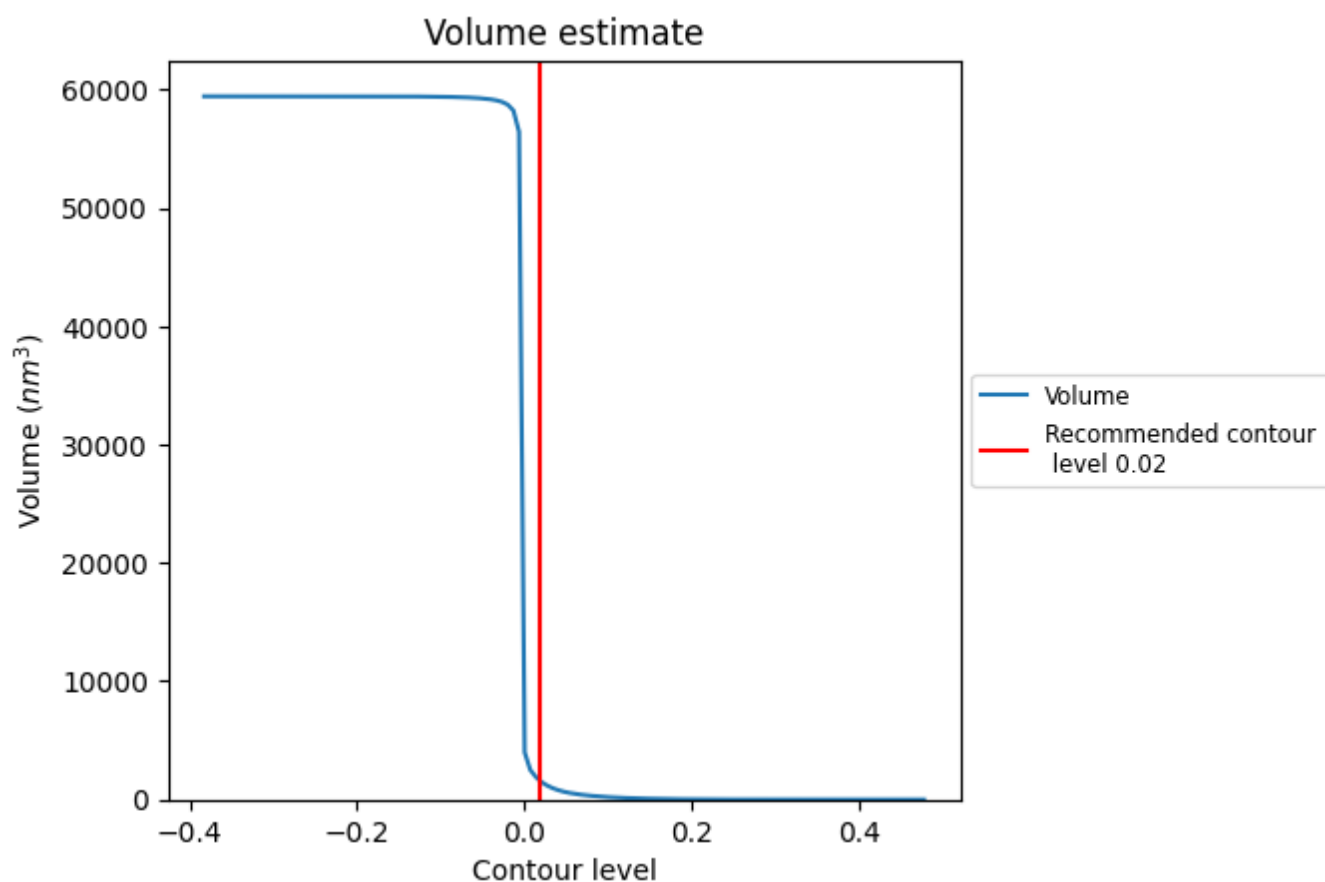
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

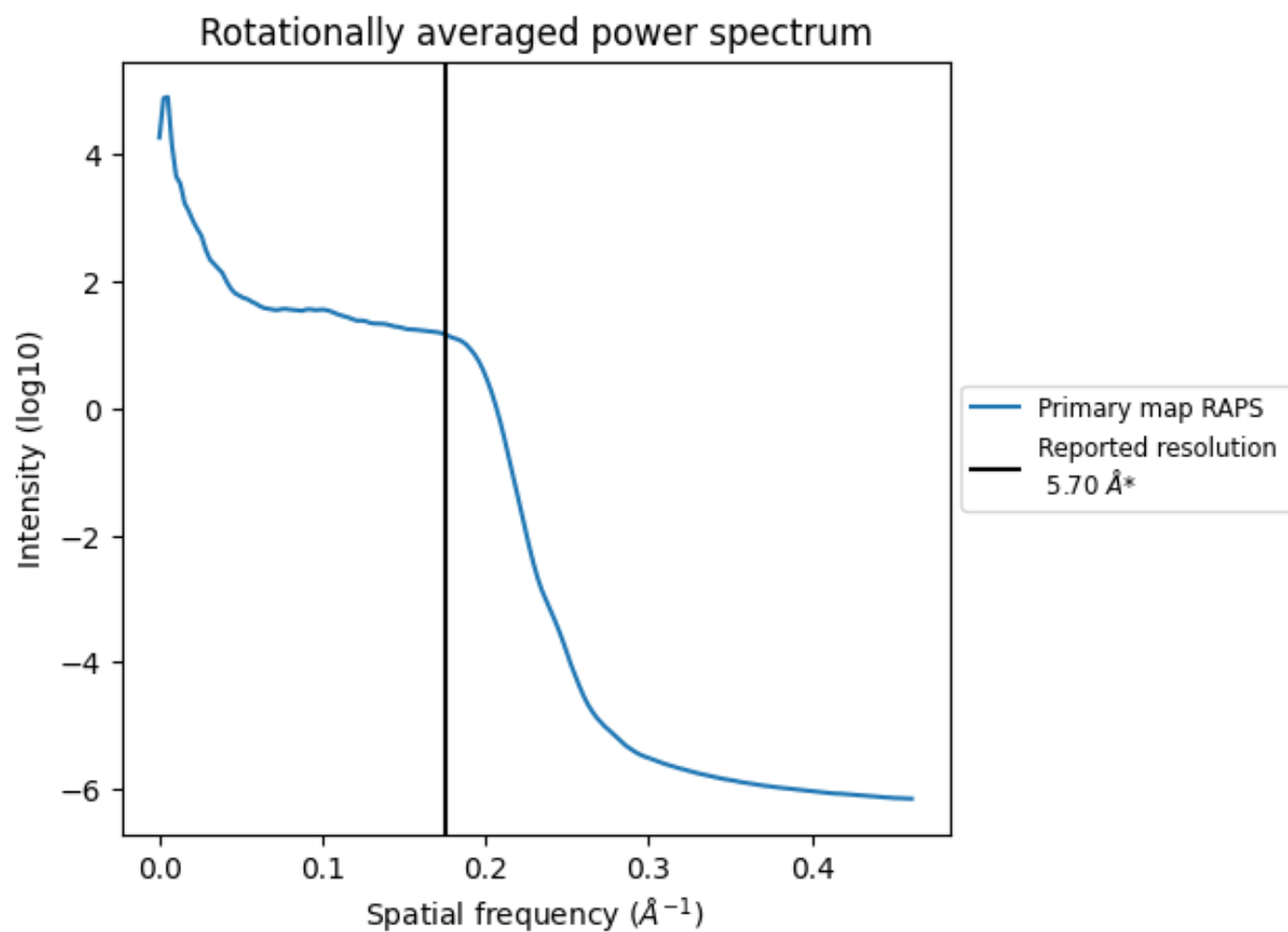
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1540  $\text{nm}^3$ ; this corresponds to an approximate mass of 1391 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 ⓘ

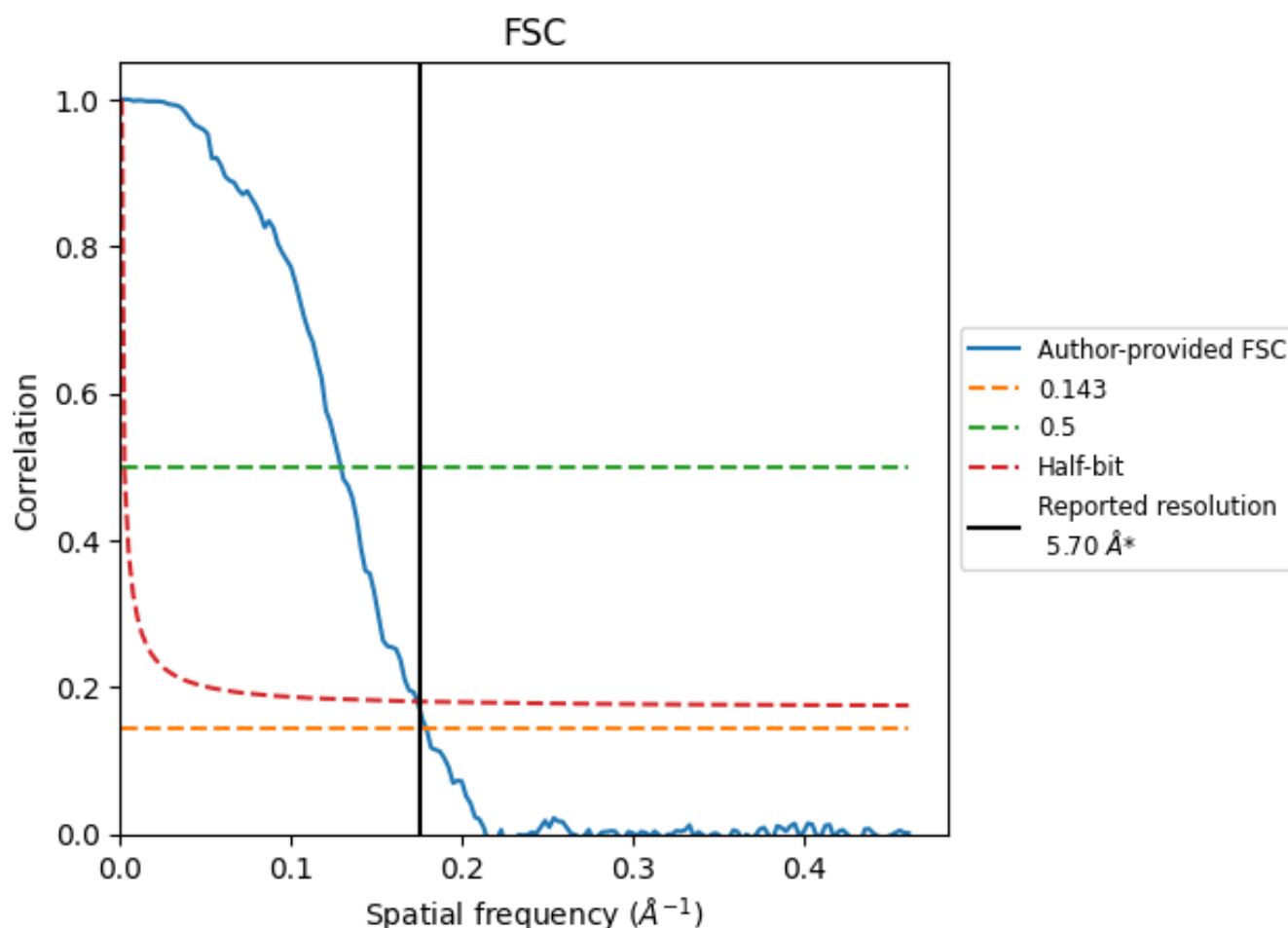


\*Reported resolution corresponds to spatial frequency of 0.175 Å<sup>-1</sup>

## 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 0.175 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

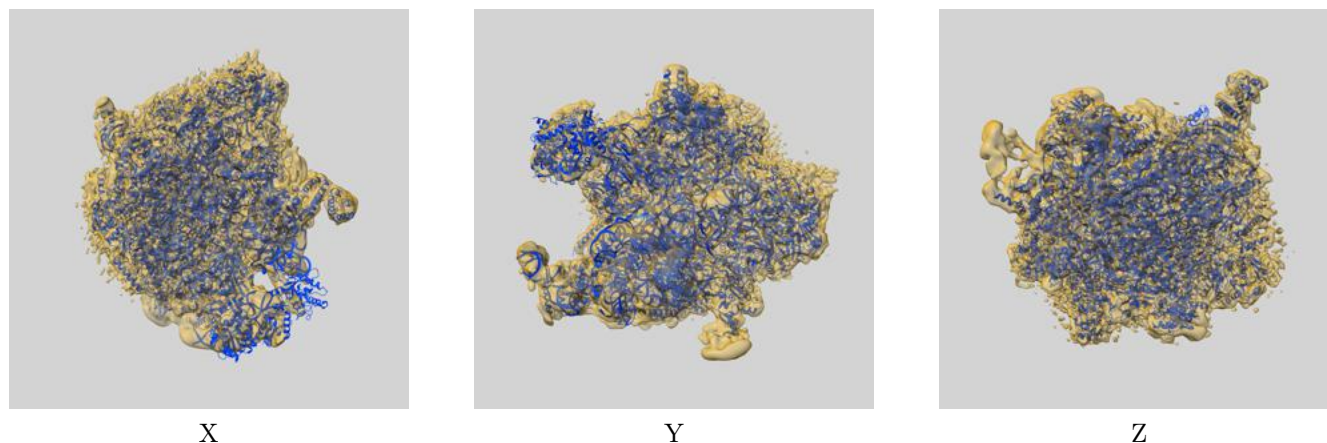
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.70	-	-
Author-provided FSC curve	5.58	7.75	5.75
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12919 and PDB model 7OI6. Per-residue inclusion information can be found in section 3 on page 14.

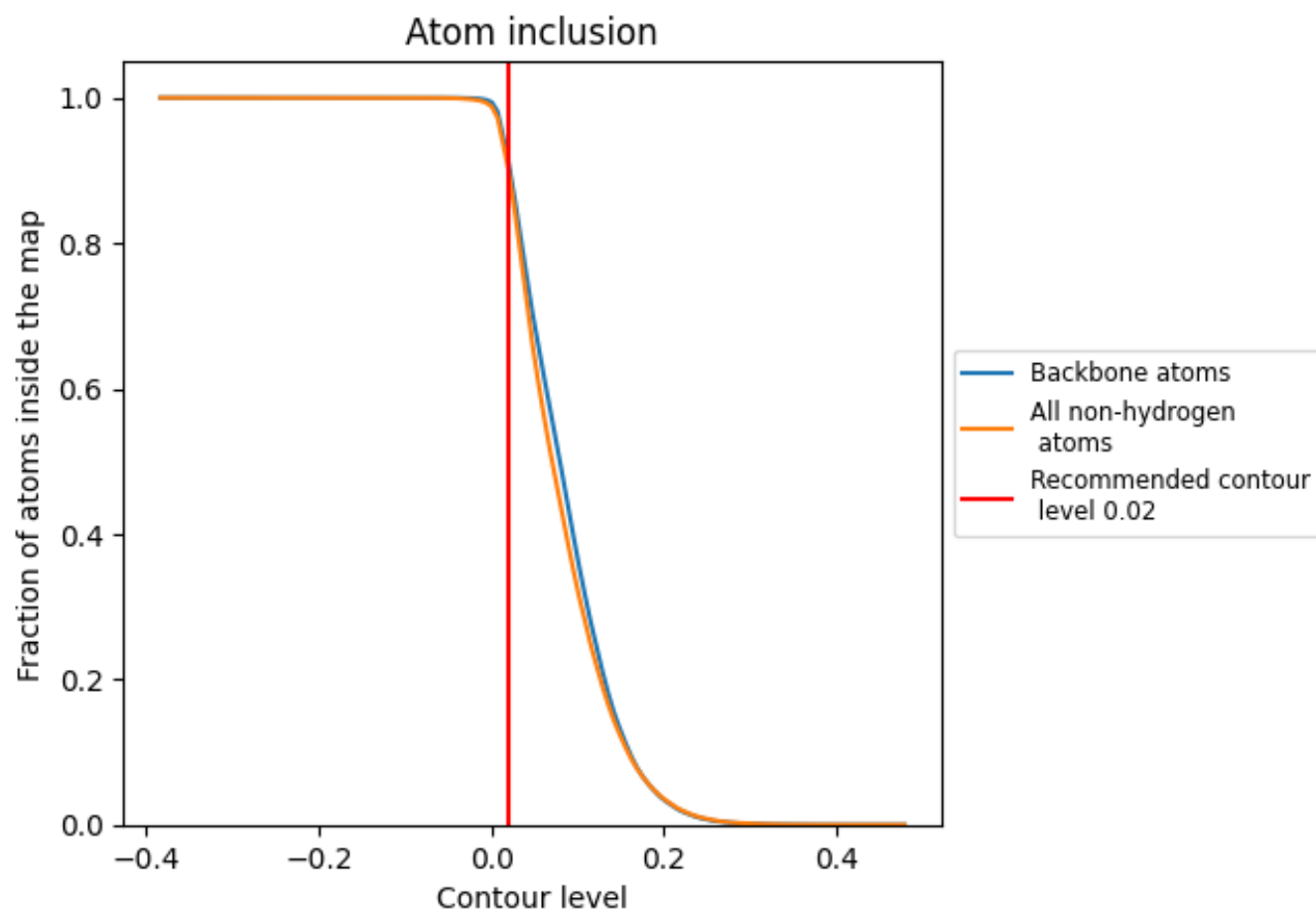
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.02 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 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.