



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 11:18 PM UTC

PDB ID : 6I9R / pdb_00006i9r
EMDB ID : EMD-4434
Title : Large subunit of the human mitochondrial ribosome in complex with Virginiamycin M and Quinupristin
Authors : Modelska, A.; Aibara, S.; Amunts, A.
Deposited on : 2018-11-25
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

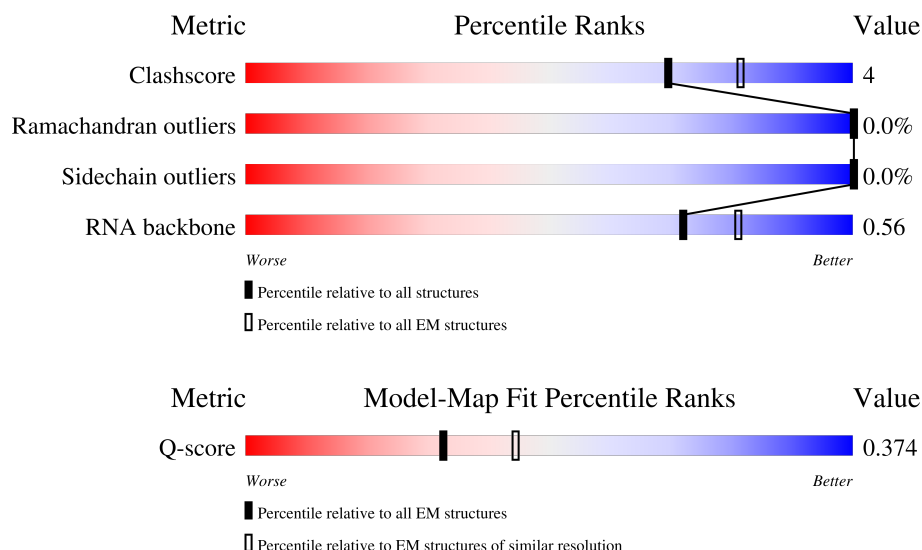
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



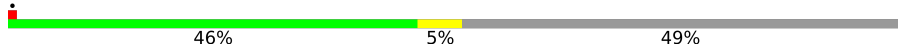
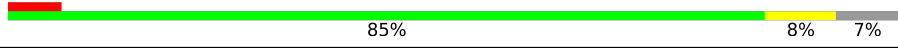
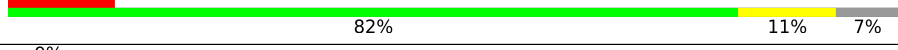
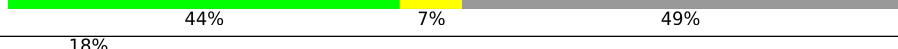
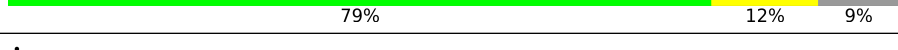
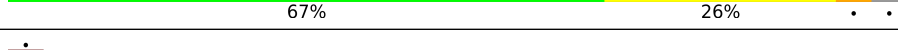
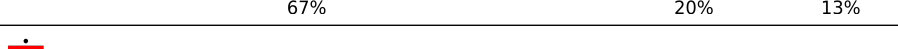
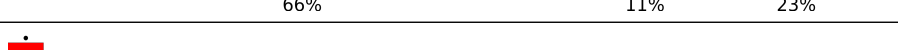
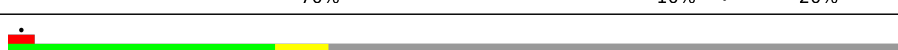
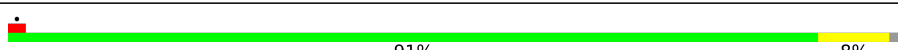
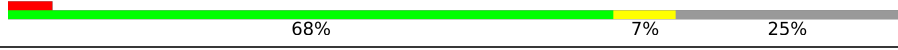
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

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

Mol	Chain	Length	Quality of chain
1	0	188	
2	1	65	
3	2	92	

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Mol	Chain	Length	Quality of chain
4	3	188	
5	4	103	
6	5	423	
7	6	380	
8	7	338	
9	8	206	
10	9	137	
11	A	1558	
12	B	69	
13	D	305	
14	E	348	
15	F	311	
16	H	267	
17	I	261	
18	J	192	
19	K	178	
20	L	145	
21	M	296	
22	N	251	
23	O	175	
24	P	179	
25	Q	292	
26	R	149	
27	S	205	
28	T	212	

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Mol	Chain	Length	Quality of chain
29	U	153	
30	V	216	
31	W	148	
32	X	256	
33	Y	250	
34	Z	161	
35	a	142	
36	b	215	
37	c	332	
38	d	306	
39	e	279	
40	f	212	
41	g	166	
42	h	158	
43	i	128	
44	j	123	
45	k	112	
46	l	138	
47	m	128	
48	o	102	
49	p	206	
50	q	222	
51	r	196	
52	s	439	
53	C	8	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 100274 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	53	Total	C	N	O	S	0	0
			439	281	84	72	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			376	233	83	59	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			341	217	72	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	393	Total	C	N	O	S	0	0
			3204	2070	559	564	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	354	Total	C	N	O	S	0	0
			2947	1881	525	532	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	291	Total	C	N	O	S	0	0
			2365	1514	401	432	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	105	Total	C	N	O	S	0	0
			886	568	152	164	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	124	Total	C	N	O	S	0	0
			996	644	170	180	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1502	Total	C	N	O	P	0	0
			31898	14316	5763	10317	1502		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4118	A	U	conflict	GB 1765886256
A	4119	C	G	conflict	GB 1765886256

- Molecule 12 is a RNA chain called tRNA Val.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	60	Total	C	N	O	P	0	0
			1275	572	230	413	60		

- Molecule 13 is a protein called 39S ribosomal protein L2, mitochondrial.

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

- Molecule 14 is a protein called 39S ribosomal protein L3, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L9, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	167	Total	C	N	O	S	0	0
			1350	869	245	226	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	170	Total	C	N	O	S	0	0
			1294	826	230	236	2		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	221	Total	C	N	O	S	0	0
			1778	1138	325	305	10		

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

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

- Molecule 24 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	143	Total	C	N	O	S	0	0
			1164	729	223	207	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	219	Total	C	N	O	S	0	0
			1822	1168	322	323	9		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	160	Total	C	N	O	S	0	0
			1284	829	226	225	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	141	Total	C	N	O	S	0	0
			1171	743	222	203	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	202	Total	C	N	O	S	0	0
			1652	1053	294	297	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	111	Total	C	N	O	S	0	0
			871	558	164	146	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X	243	Total	C	N	O	S	0	0
			2027	1310	350	362	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	148	ALA	THR	conflict	UNP Q13084
X	149	SER	PRO	conflict	UNP Q13084
X	150	GLY	LYS	conflict	UNP Q13084

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	178	Total	C	N	O	S	0	0
			1534	981	295	254	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	83	Total	C	N	O	S	0	0
			693	440	124	124	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	214	Total	C	N	O	S	0	0
			1736	1113	303	307	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	62	PHE	GLU	conflict	UNP Q9BRJ2
d	63	ALA	PHE	conflict	UNP Q9BRJ2

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	125	Total	C	N	O	S	0	0
			999	640	159	196	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	131	Total	C	N	O	S	0	0
			1085	701	190	192	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	109	Total	C	N	O	S	0	0
			886	562	155	166	3		

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

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

- Molecule 44 is a protein called cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	86	Total	C	N	O	S	0	0
			689	426	134	127	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	95	Total	C	N	O	S	0	0
			732	456	139	132	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	l	80	Total	C	N	O	S	0	0
			675	428	118	126	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	60	Total	C	N	O	S	0	0
			499	309	103	85	2		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	130	Total	C	N	O	S	0	0
			1092	680	213	194	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	153	Total	C	N	O	S	0	0
			1256	797	241	210	8		

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

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

- Molecule 53 is a protein called Quinupristin.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	C	8	Total	C	N	O	S	0	0
			73	53	9	10	1		

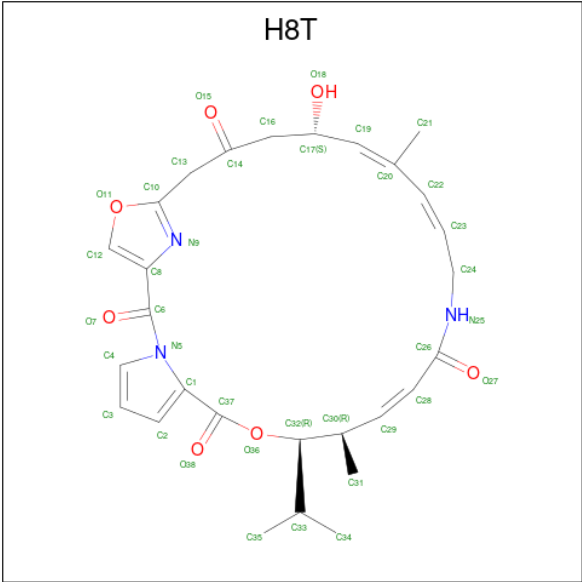
- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

Mol	Chain	Residues	Atoms		AltConf
55	9	1	Total	Mg	0
			1	1	
55	A	128	Total	Mg	0
			128	128	
55	D	1	Total	Mg	0
			1	1	
55	L	1	Total	Mg	0
			1	1	
55	M	1	Total	Mg	0
			1	1	
55	g	1	Total	Mg	0
			1	1	
55	o	1	Total	Mg	0
			1	1	

- Molecule 56 is Virginiamycin M (CCD ID: H8T) (formula: C₂₈H₃₃N₃O₇).



Mol	Chain	Residues	Atoms				AltConf
56	A	1	Total	C	N	O	0
			38	28	3	7	

- Molecule 5: 39S ribosomal protein L36, mitochondrial

Chain 4: 

MET ALA ASN LEU PHE ARG LYS MET VAL ASN PRO LEU LEU TYR SER ARG HIS THR VAL LYS PRO ARG ALA LEU SER THR PHE LEU PHE GLY SER ILE ARG GLY ALA PRO VAL VAL VAL PRO GLY ALA VAL ARG SER LEU SER PRO GLY LEU LEU HIS LEU

LEU PRO ALA LEU LEU GLY F66 R84 M103

- Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5: 

MET ALA LEU ALA SER GLY PRO ALA ARG ARG ALA LEU LEU GLY SER GLY GLN LEU LEU GLY LEU LEU GLY PHE LEU ARG ALA PRO ARG ARG GLY A30 D47 Y50 E51 G54 L55 E56 R72 R80 G81 Y82 D101 C104 Y105 G131 E134 L137 V140 D141 D142

P143 R144 N145 H146 N149 P408 E152 L155 D182 K194 R201 I202 E243 E244 I245 E246 A247 T248 K249 Y257 H266 G282 Y285 R300 R303 E337 Q343 T347 V351 D365 C366 N367 E368 D377 S378 D379 Q380 L381 Q384 K393

K394 R395 V396 K407 P408 E409 L417 Y418 A422 ALA

- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6: 

MET ALA ALA PRO TRP ARG ALA ALA LEU CYS GLU CYS ARG ARG TRP ARG GLY TRP ARG GLY GLY PHE SER THR SER ALA VAL LEU GLY R27 R28 T29 D39 I40 R47 E62 D63 E64 H69 E80 R81 T82 D83 P84 R85 E86 D89 R96 R114 A115 E119 E120 R121 A122

A123 R124 L125 R126 T127 D133 D160 T166 F167 A176 Y177 A178 V179 G180 E181 D182 D183 L184 E197 A198 Y206 E207 A208 E209 E210 V214 L226 D229 A230 E231 N239 G242 N243 R244 V245 A246 E247 C252 P253 Y254 I265 R266 R267 F270 L271 L272

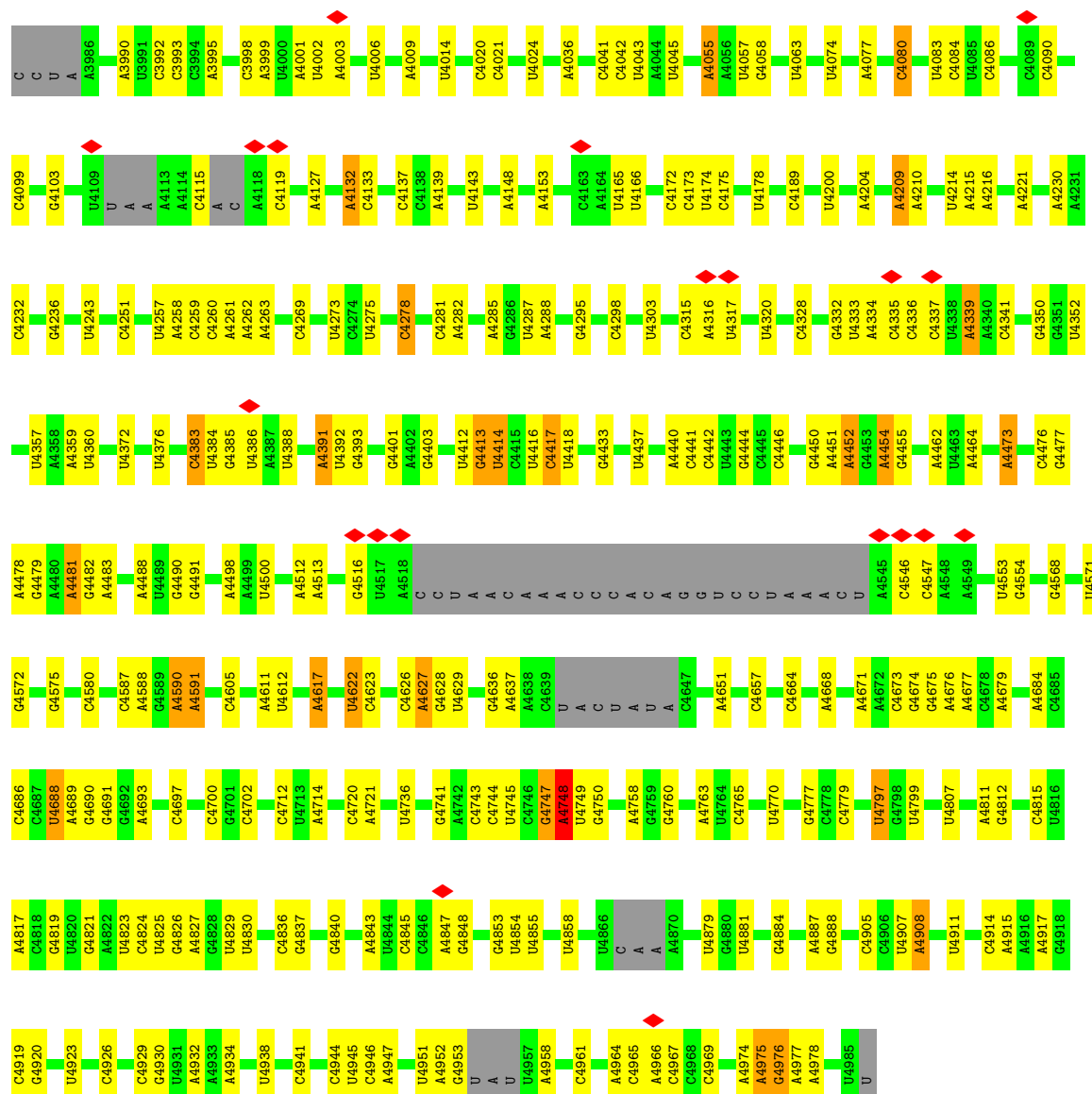
F273 R274 Q275 E276 S282 D283 D284 A285 R286 C290 R299 D302 K306 R307 Q308 M311 S317 D325 E339 R360 R364 D367 R368 Y369 R370 H373 E374 Y380

- Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7: 

MET GLU ALA LEU LEU MET GLY SER ARG ARG ALA LEU ARG LEU TRP VAL ALA PRO PRO GLY GLY ILE LYS TRP ARG PHE ILE ALA THR SER SER ALA SER GLN LEU S36 E51 L58 T59 P60 T62 T63 E63 E66 V67 R68 V78 N82 S86 Y99 S103

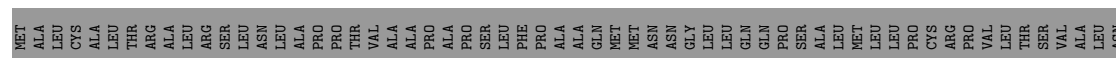
D114 G133 R144 E155 R156 N165 E171 D182 S187 R188 E191 K204 E220 E241 A244 S245 Q246 N247 R250 I251 I257 Q258 D259 F260 I261 D262 V263 I269 I274 S281 A282 L286 T289 Q290 P291 G299 R309 D314

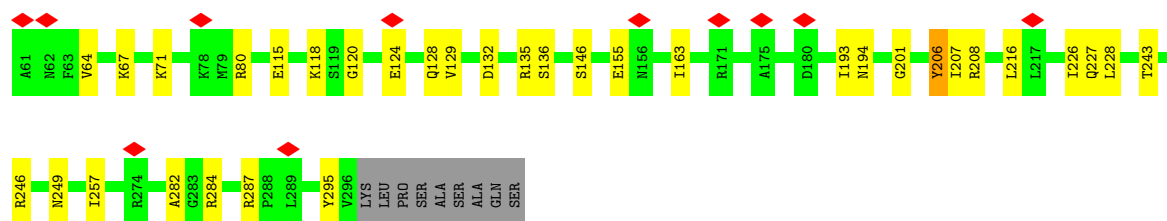


• Molecule 12: tRNA Val



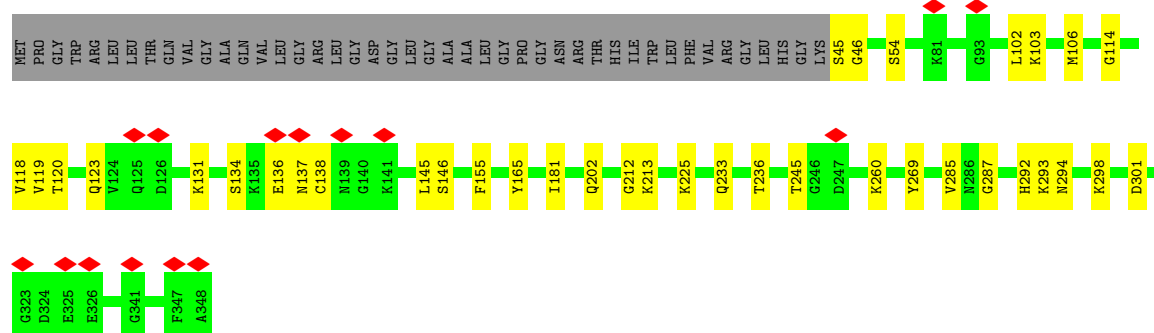
• Molecule 13: 39S ribosomal protein L2, mitochondrial





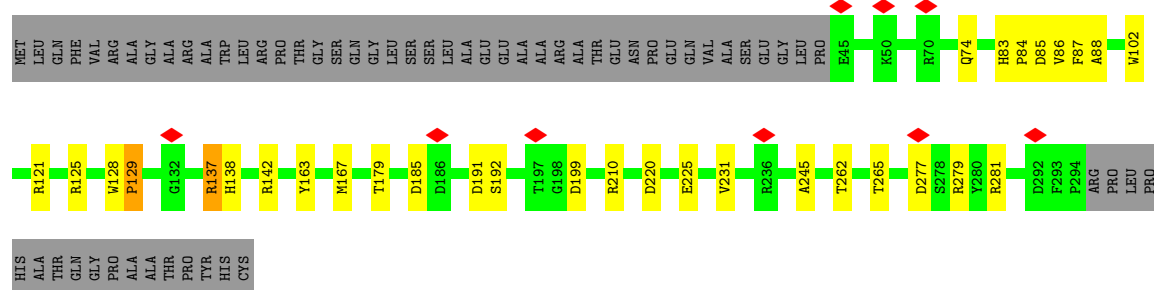
- Molecule 14: 39S ribosomal protein L3, mitochondrial

Chain E: 77% 11% 13%



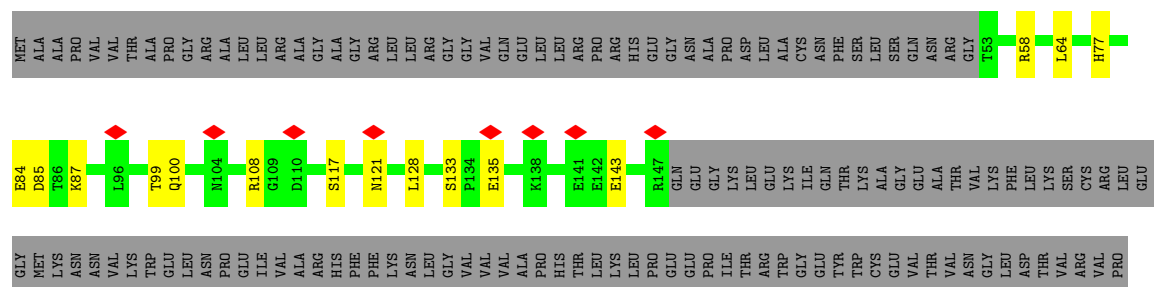
- Molecule 15: 39S ribosomal protein L4, mitochondrial

Chain F: 70% 10% 20%



- Molecule 16: 39S ribosomal protein L9, mitochondrial

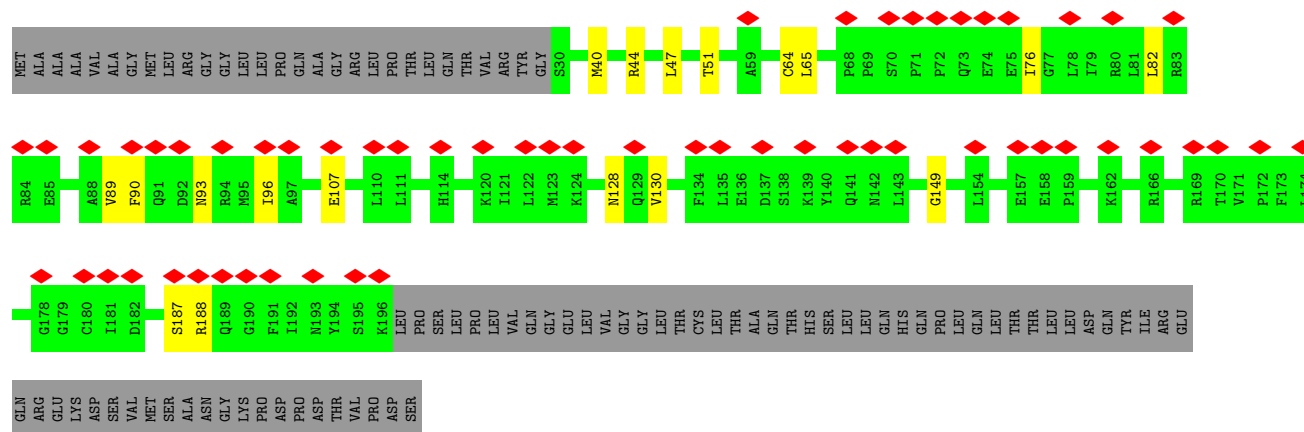
Chain H: 30% 6% 64%



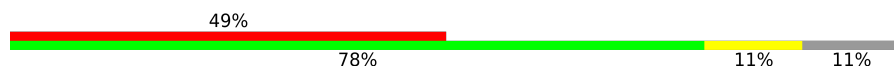
MET SER VAL VAL PHE GLY LYS PRO LYS THR LYS ARG TYR LYS THR TRP ALA GLN ALA ALA LYS MET ALA ALA PRO THR SER PRO GLN ILE

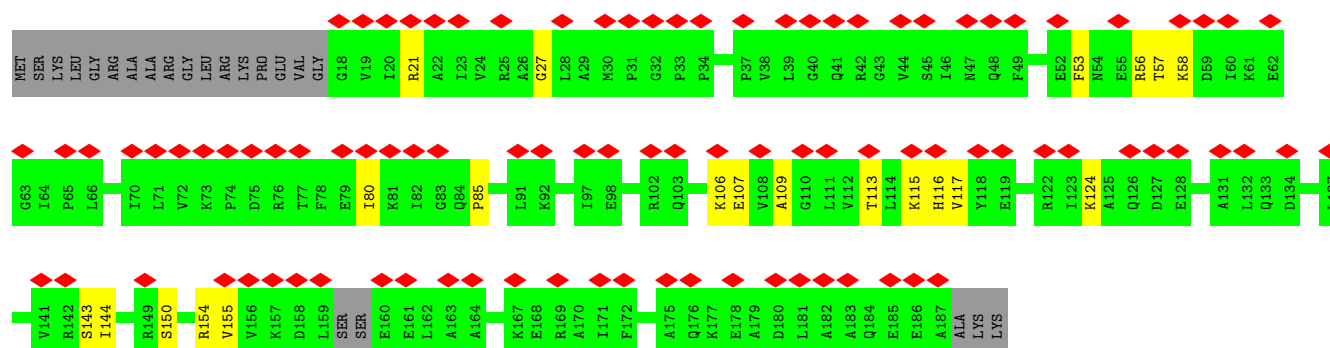
- Molecule 17: 39S ribosomal protein L10, mitochondrial

Chain I: 

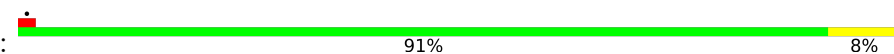


- Molecule 18: 39S ribosomal protein L11, mitochondrial

Chain J: 



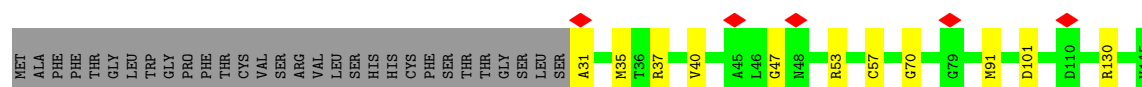
- Molecule 19: 39S ribosomal protein L13, mitochondrial

Chain K: 



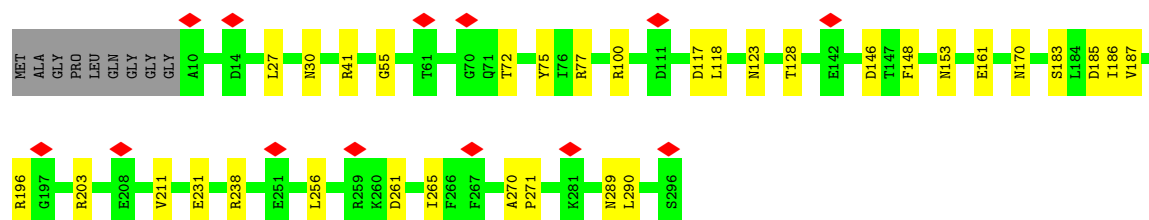
- Molecule 20: 39S ribosomal protein L14, mitochondrial

Chain L: 



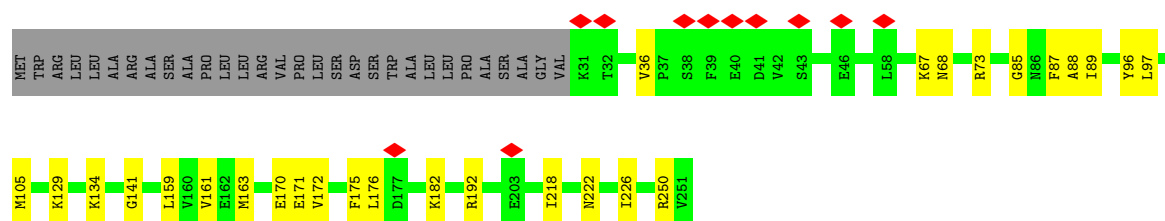
- Molecule 21: 39S ribosomal protein L15, mitochondrial

Chain M:  86% 11%



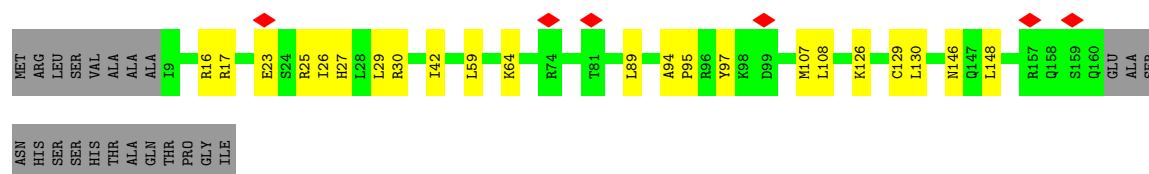
- Molecule 22: 39S ribosomal protein L16, mitochondrial

Chain N:  77% 11% 12%



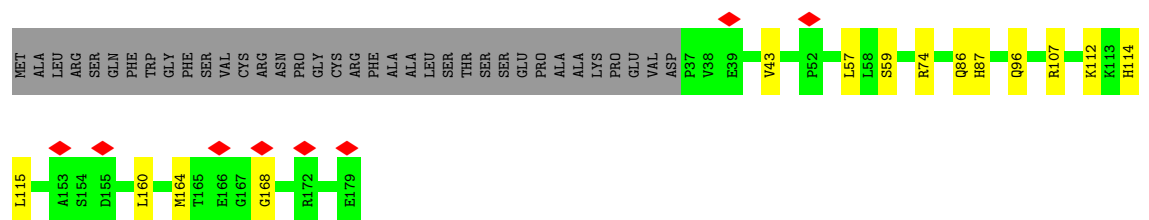
- Molecule 23: 39S ribosomal protein L17, mitochondrial

Chain O:  74% 13% 13%



- Molecule 24: Mitochondrial ribosomal protein L18, isoform CRA_b

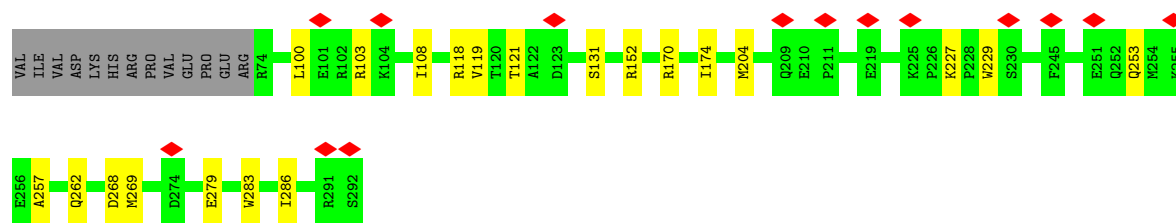
Chain P:  72% 8% 20%



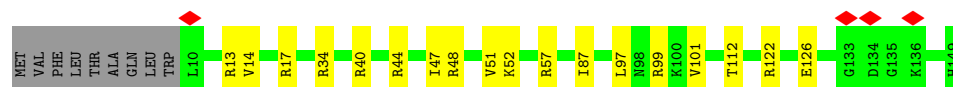
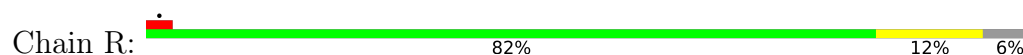
- Molecule 25: 39S ribosomal protein L19, mitochondrial

Chain Q:  5% 68% 7% 25%

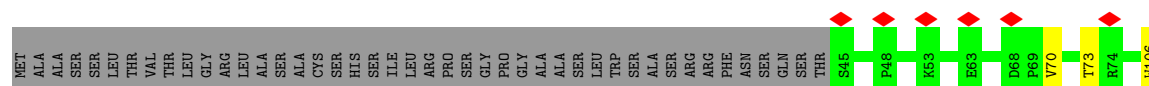




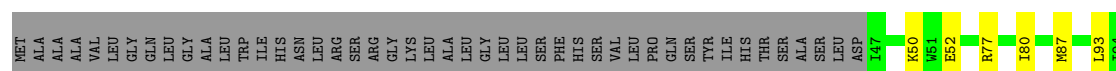
- Molecule 26: 39S ribosomal protein L20, mitochondrial



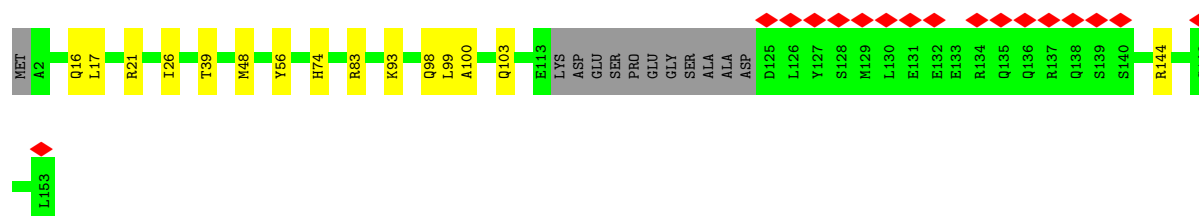
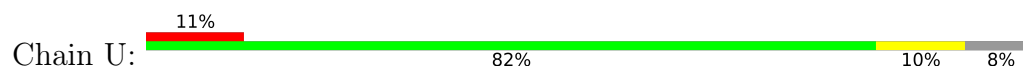
- Molecule 27: 39S ribosomal protein L21, mitochondrial



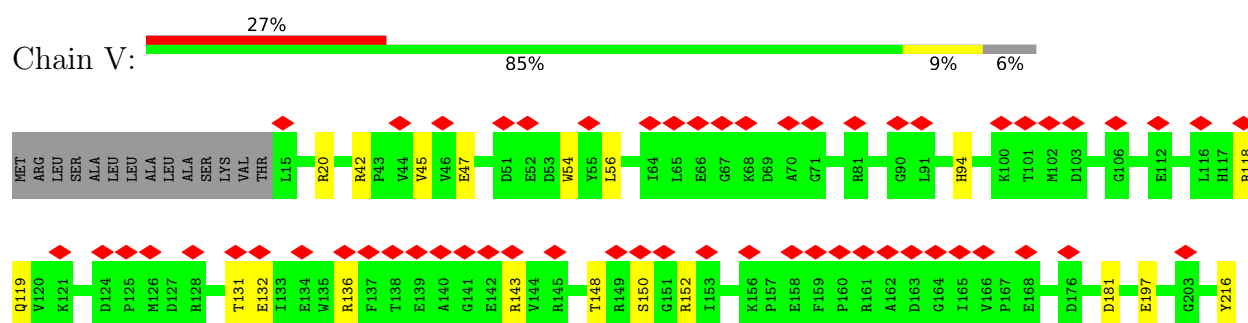
- Molecule 28: 39S ribosomal protein L22, mitochondrial



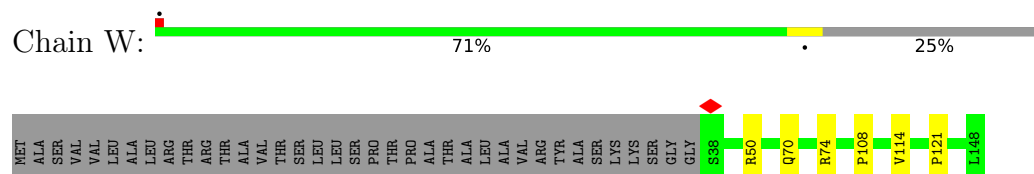
- Molecule 29: 39S ribosomal protein L23, mitochondrial



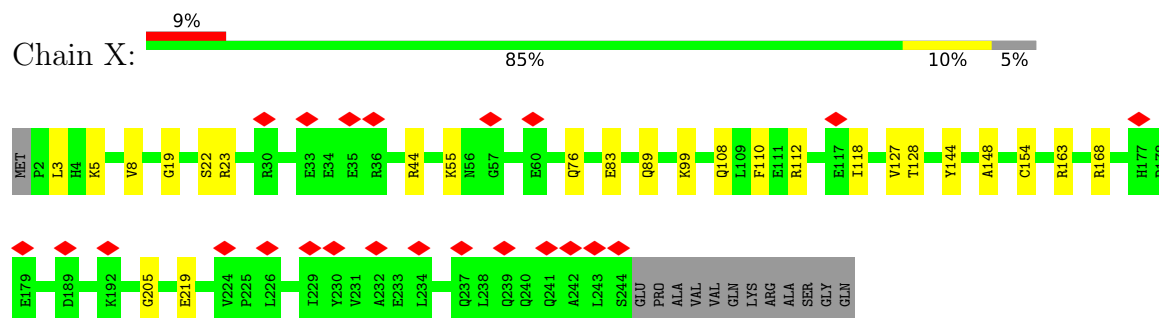
- Molecule 30: 39S ribosomal protein L24, mitochondrial



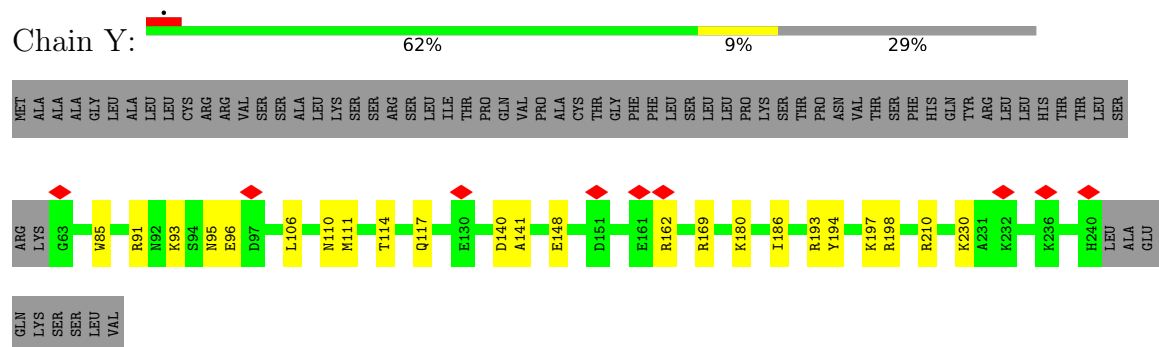
- Molecule 31: 39S ribosomal protein L27, mitochondrial



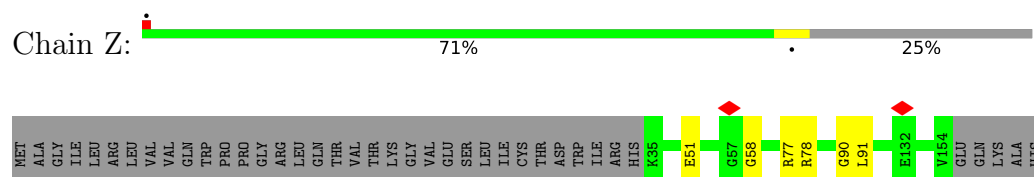
- Molecule 32: 39S ribosomal protein L28, mitochondrial



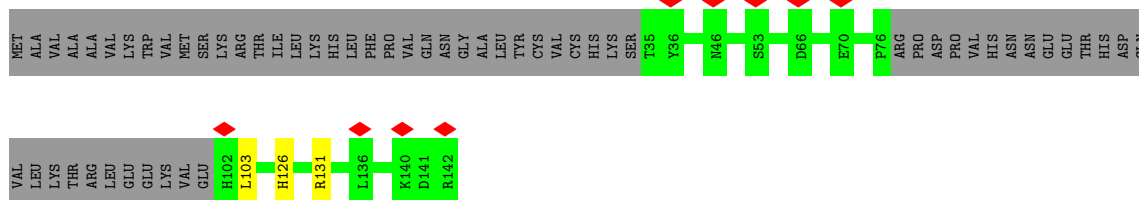
- Molecule 33: 39S ribosomal protein L47, mitochondrial



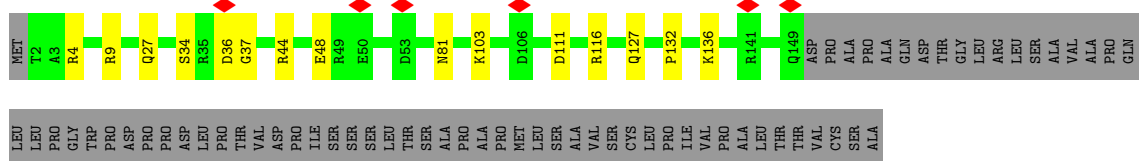
- Molecule 34: 39S ribosomal protein L30, mitochondrial



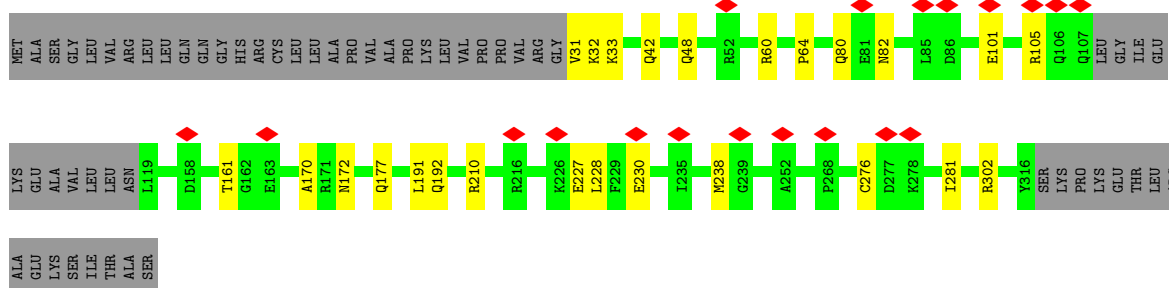
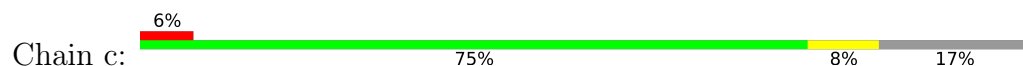
- Molecule 35: 39S ribosomal protein L42, mitochondrial



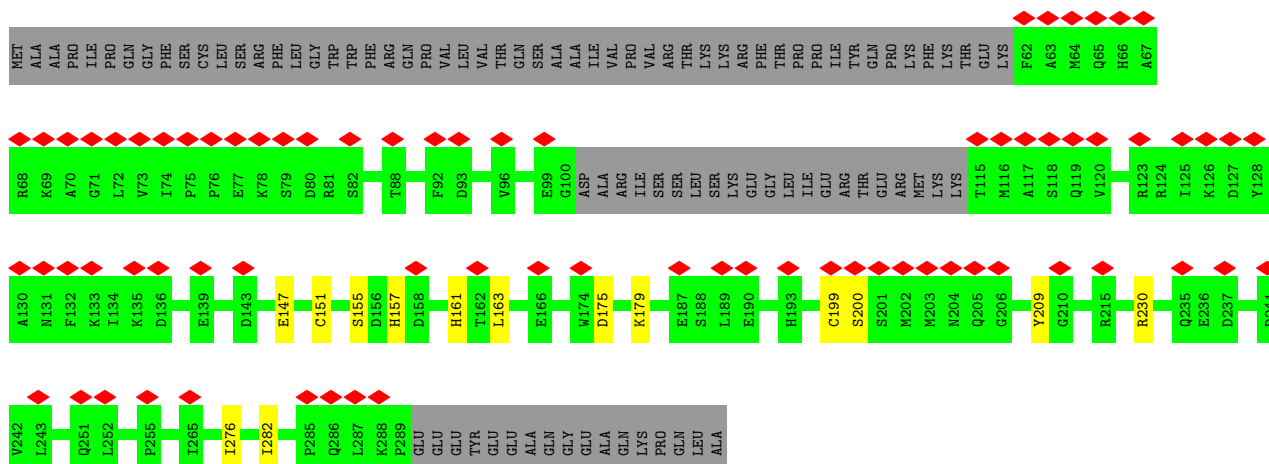
- Molecule 36: 39S ribosomal protein L43, mitochondrial



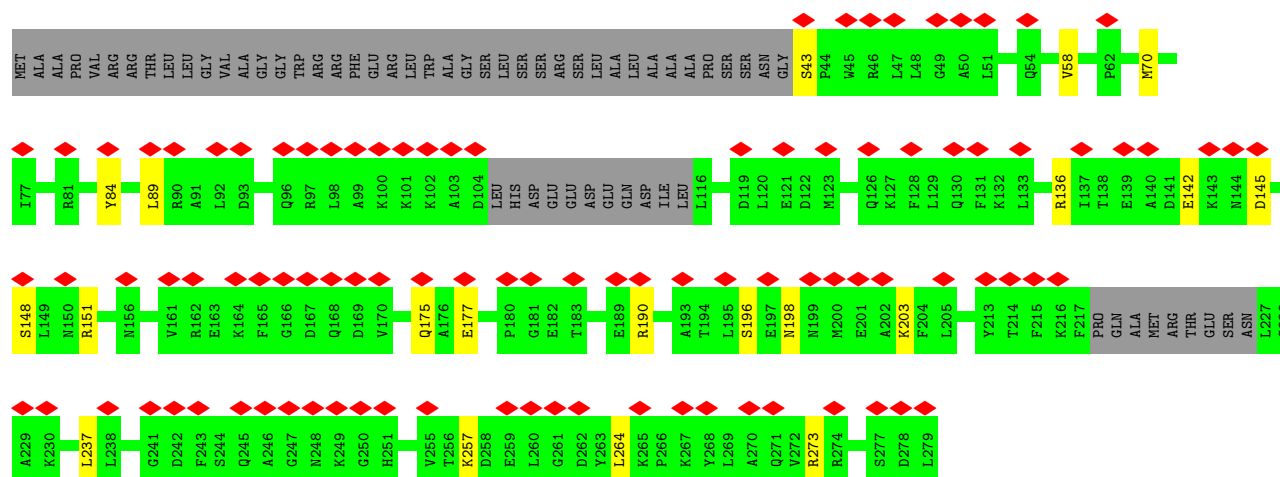
- Molecule 37: 39S ribosomal protein L44, mitochondrial



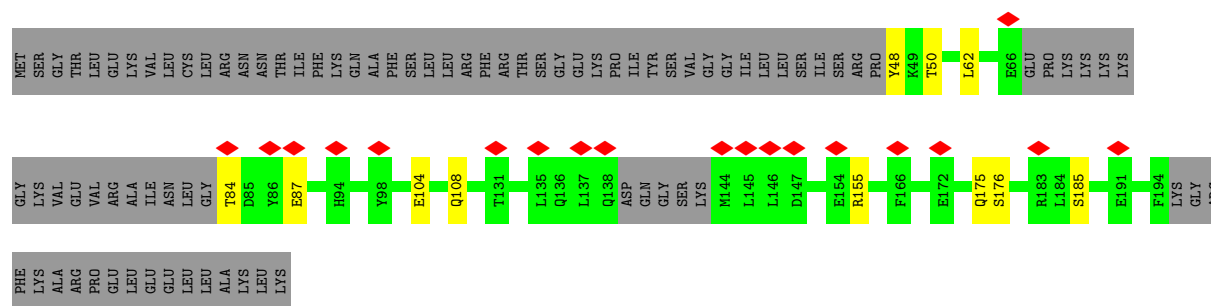
- Molecule 38: 39S ribosomal protein L45, mitochondrial



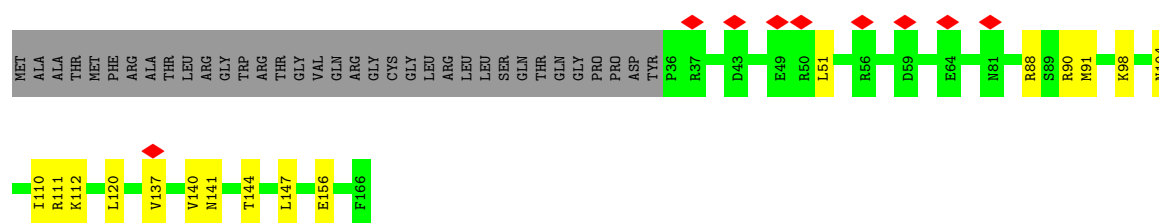
Chain e: 35% 71% 7% 22%



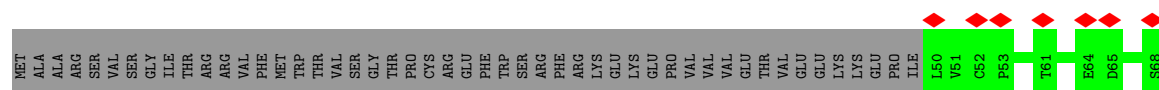
Chain f:

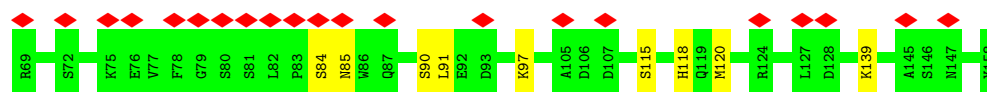


Chain g:

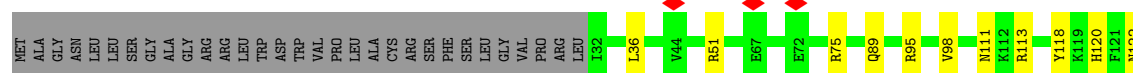


Chain h:





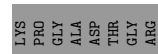
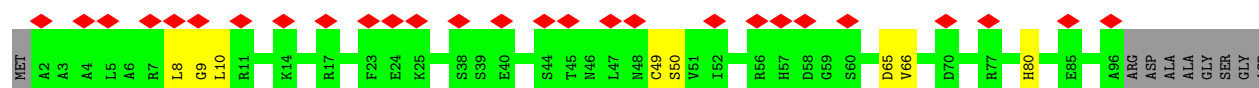
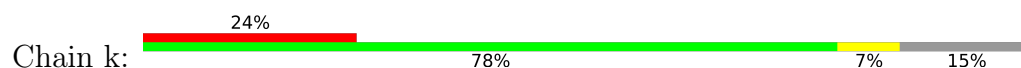
- Molecule 43: 39S ribosomal protein L51, mitochondrial



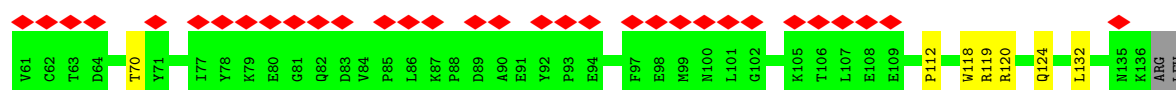
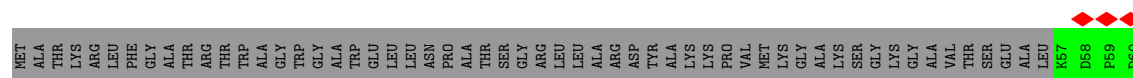
- Molecule 44: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA



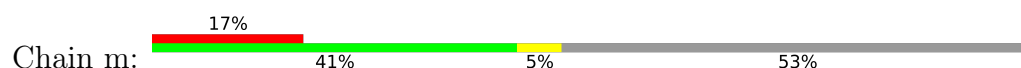
- Molecule 45: 39S ribosomal protein L53, mitochondrial

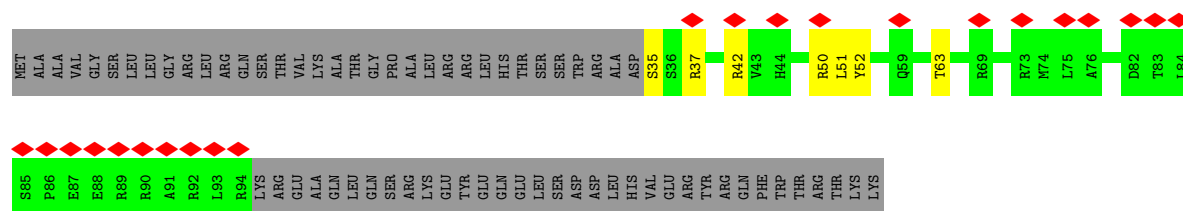


- Molecule 46: 39S ribosomal protein L54, mitochondrial

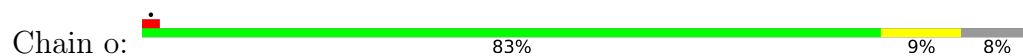


- Molecule 47: 39S ribosomal protein L55, mitochondrial

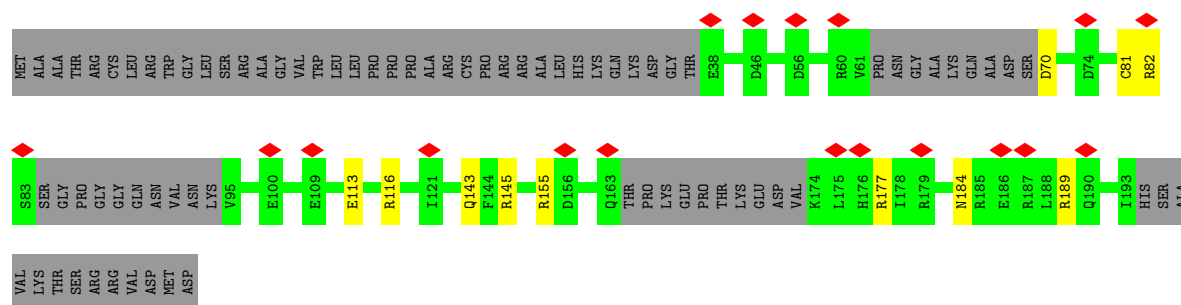




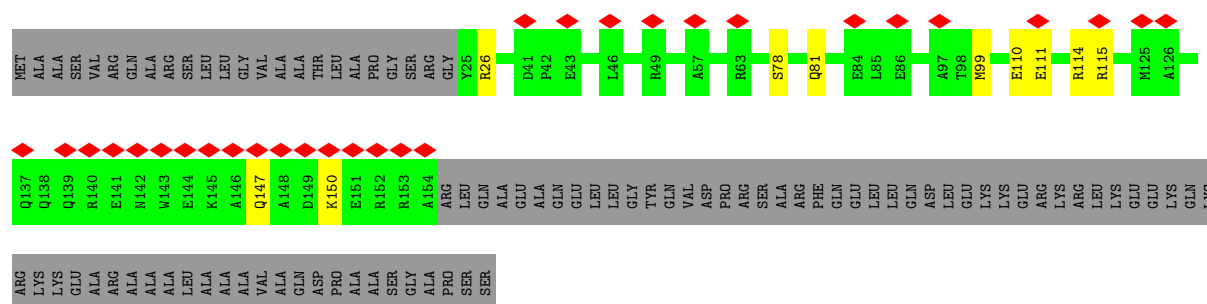
- Molecule 48: Ribosomal protein 63, mitochondrial



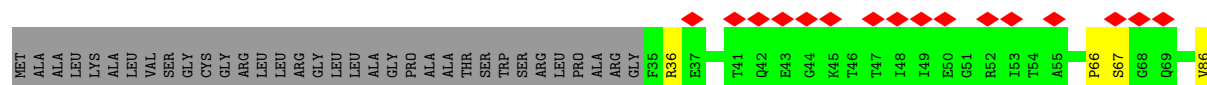
- Molecule 49: Peptidyl-tRNA hydrolase ICT1, mitochondrial

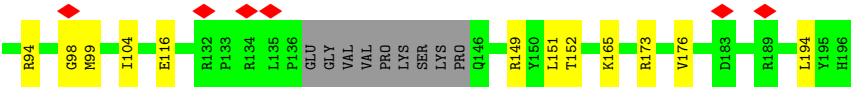


- Molecule 50: Growth arrest and DNA damage-inducible proteins-interacting protein 1

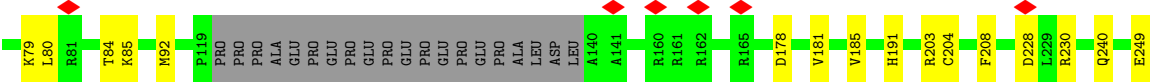
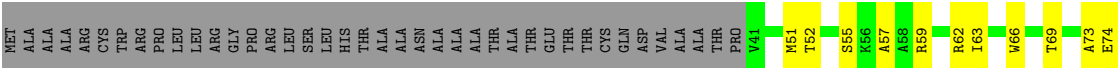


- Molecule 51: 39S ribosomal protein S18a, mitochondrial

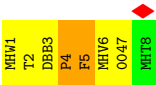
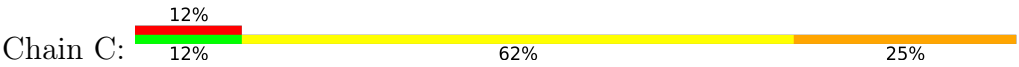




• Molecule 52: 39S ribosomal protein S30, mitochondrial



• Molecule 53: Quinupristin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.166	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	525.0, 525.0, 525.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 5MC, MHU, 2MU, MHT, 004, 2MA, ZN, MHW, MHV, H8T, MG, DBB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.17	0/895	0.34	0/1201
2	1	0.16	0/444	0.39	0/591
3	2	0.21	0/382	0.40	0/507
4	3	0.15	0/852	0.37	0/1136
5	4	0.17	0/348	0.36	0/458
6	5	0.16	0/3296	0.35	0/4486
7	6	0.18	0/3039	0.41	0/4131
8	7	0.17	0/2419	0.38	0/3267
9	8	0.18	0/909	0.38	0/1228
10	9	0.16	0/1024	0.36	0/1379
11	A	0.11	4/35588 (0.0%)	0.21	2/55382 (0.0%)
12	B	0.07	0/1422	0.18	0/2202
13	D	0.18	0/1879	0.40	0/2527
14	E	0.15	0/2464	0.34	0/3341
15	F	0.54	2/2071 (0.1%)	0.73	7/2817 (0.2%)
16	H	0.17	0/798	0.37	0/1073
17	I	0.18	0/1380	0.40	0/1864
18	J	0.18	0/1312	0.36	0/1768
19	K	0.18	0/1495	0.36	0/2029
20	L	0.16	0/904	0.37	0/1218
21	M	0.20	0/2359	0.42	0/3185
22	N	0.17	0/1825	0.37	0/2458
23	O	0.17	0/1269	0.39	0/1708
24	P	0.17	0/1189	0.41	0/1608
25	Q	0.18	0/1863	0.37	0/2509
26	R	0.16	0/1174	0.36	0/1572
27	S	0.19	0/1311	0.40	0/1778
28	T	0.17	0/1402	0.38	0/1886
29	U	0.18	0/1200	0.40	0/1623
30	V	0.20	0/1696	0.43	0/2299
31	W	0.16	0/893	0.36	0/1204
32	X	0.17	0/2081	0.37	0/2812

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Y	0.16	0/1571	0.35	0/2106
34	Z	0.17	0/1003	0.36	0/1354
35	a	0.15	0/717	0.39	0/975
36	b	0.17	0/1202	0.38	0/1626
37	c	0.16	0/2264	0.33	0/3059
38	d	0.17	0/1783	0.34	0/2415
39	e	0.19	0/1797	0.35	0/2422
40	f	0.13	0/1016	0.28	0/1374
41	g	0.18	0/1121	0.40	0/1528
42	h	0.17	0/908	0.38	0/1235
43	i	0.17	0/849	0.39	0/1135
44	j	0.13	0/703	0.39	0/947
45	k	0.18	0/743	0.36	0/1003
46	l	0.16	0/694	0.37	0/942
47	m	0.20	0/507	0.39	0/682
48	o	0.18	0/818	0.41	0/1097
49	p	0.17	0/1071	0.31	0/1433
50	q	0.18	0/1123	0.36	0/1519
51	r	0.17	0/1291	0.37	0/1746
52	s	0.16	0/3114	0.37	0/4225
53	C	0.59	0/13	1.38	0/15
All	All	0.17	6/105491 (0.0%)	0.33	9/150085 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	D	0	1
15	F	0	1
53	C	2	3
All	All	2	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	129	PRO	N-CA	19.12	1.70	1.47
15	F	128	TRP	C-N	9.93	1.47	1.33
11	A	4688	U	O3'-P	7.08	1.71	1.61
11	A	4745	U	O3'-P	6.39	1.70	1.61
11	A	3773	G	O3'-P	5.54	1.69	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	4478	A	O3'-P	5.17	1.69	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	128	TRP	CA-C-N	17.14	137.44	119.78
15	F	128	TRP	C-N-CA	17.14	137.44	119.78
15	F	129	PRO	CA-N-CD	-10.41	97.43	112.00
11	A	4745	U	P-O3'-C3'	6.63	130.15	120.20
11	A	4055	A	P-O3'-C3'	6.16	129.44	120.20
15	F	128	TRP	O-C-N	-5.82	117.99	121.71
15	F	138	HIS	CA-C-N	5.53	127.25	120.22
15	F	138	HIS	C-N-CA	5.53	127.25	120.22
15	F	129	PRO	N-CA-CB	5.47	108.11	103.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	C	2	THR	CB
53	C	4	PRO	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
53	C	3	DBB	Peptide
53	C	4	PRO	Peptide
53	C	5	MHU	Peptide
13	D	206	TYR	Peptide
15	F	137	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	880	0	904	8	0
2	1	439	0	480	2	0
3	2	376	0	406	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3	831	0	883	7	0
5	4	341	0	361	1	0
6	5	3204	0	3198	19	0
7	6	2947	0	2838	30	0
8	7	2365	0	2371	12	0
9	8	886	0	889	14	0
10	9	996	0	987	13	0
11	A	31898	0	16211	235	0
12	B	1275	0	651	5	0
13	D	1842	0	1896	22	0
14	E	2396	0	2401	27	0
15	F	2013	0	2044	21	0
16	H	784	0	832	10	0
17	I	1350	0	1429	12	0
18	J	1294	0	1366	13	0
19	K	1451	0	1448	14	0
20	L	889	0	941	7	0
21	M	2305	0	2378	25	0
22	N	1778	0	1808	21	0
23	O	1245	0	1283	14	0
24	P	1164	0	1161	11	0
25	Q	1822	0	1859	12	0
26	R	1153	0	1214	16	0
27	S	1284	0	1354	15	0
28	T	1368	0	1410	16	0
29	U	1171	0	1164	12	0
30	V	1652	0	1657	12	0
31	W	871	0	898	5	0
32	X	2027	0	2040	17	0
33	Y	1534	0	1575	19	0
34	Z	978	0	1030	5	0
35	a	693	0	663	2	0
36	b	1178	0	1180	12	0
37	c	2217	0	2220	18	0
38	d	1736	0	1727	9	0
39	e	1762	0	1767	14	0
40	f	999	0	995	12	0
41	g	1085	0	1077	15	0
42	h	886	0	869	6	0
43	i	827	0	857	14	0
44	j	689	0	678	7	0
45	k	732	0	745	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	l	675	0	658	8	0
47	m	499	0	523	6	0
48	o	797	0	804	9	0
49	p	1058	0	1083	9	0
50	q	1092	0	1067	6	0
51	r	1256	0	1275	12	0
52	s	3036	0	3022	24	0
53	C	73	0	65	0	0
54	0	1	0	0	0	0
54	4	1	0	0	0	0
54	I	1	0	0	0	0
55	9	1	0	0	0	0
55	A	128	0	0	0	0
55	D	1	0	0	0	0
55	L	1	0	0	0	0
55	M	1	0	0	0	0
55	g	1	0	0	0	0
55	o	1	0	0	0	0
56	A	38	0	0	1	0
All	All	100274	0	84642	642	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 4.

All (642) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:4797:2MU:C4	11:A:4797:2MU:C5	1.81	1.57
11:A:3663:C:C2	11:A:3776:G:N2	1.80	1.46
15:F:129:PRO:N	15:F:129:PRO:CA	1.70	1.36
11:A:4488:A:C2	11:A:4689:A:C2	2.28	1.22
11:A:3663:C:O2	11:A:3776:G:N2	1.75	1.18
11:A:4748:2MA:O2'	56:A:5129:H8T:O18	1.75	1.03
11:A:4437:U:H5''	11:A:4479:G:OP1	1.65	0.96
11:A:3615:U:O2'	11:A:4747:G:C6	2.28	0.86
11:A:3663:C:C2	11:A:3776:G:C2	2.65	0.84
38:d:199:CYS:HG	38:d:200:SER:N	1.81	0.79
1:0:139:ARG:NH2	11:A:4080:C:OP1	2.18	0.77
11:A:3663:C:N3	11:A:3776:G:C2	2.54	0.76
11:A:4006:U:OP1	26:R:99:ARG:NH2	2.19	0.76
27:S:138:ALA:O	36:b:127:GLN:NE2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:3904:A:N6	36:b:116:ARG:O	2.21	0.73
11:A:4488:A:C6	11:A:4689:A:N1	2.56	0.73
4:3:102:GLY:O	43:i:89:GLN:NE2	2.22	0.73
11:A:3639:A:OP2	41:g:111:ARG:NH2	2.21	0.73
11:A:3949:A:N6	11:A:3956:A:OP2	2.21	0.73
11:A:4257:U:OP2	11:A:4262:A:N6	2.20	0.73
11:A:3438:A:OP1	33:Y:230:LYS:NZ	2.21	0.72
11:A:4488:A:N1	11:A:4689:A:C2	2.57	0.72
11:A:3711:A:O2'	11:A:4221:A:OP1	2.07	0.72
4:3:104:ARG:NH1	4:3:160:LYS:O	2.22	0.72
11:A:4821:G:O2'	11:A:4824:C:OP2	2.07	0.72
36:b:9:ARG:NH1	36:b:111:ASP:O	2.22	0.72
11:A:3930:A:OP2	18:J:21:ARG:NH1	2.23	0.71
39:e:177:GLU:O	39:e:190:ARG:NH2	2.23	0.71
11:A:3535:A:N6	11:A:3538:U:OP2	2.22	0.71
20:L:31:ALA:N	20:L:91:MET:SD	2.63	0.71
11:A:3454:C:OP2	33:Y:180:LYS:NZ	2.23	0.71
11:A:3769:G:O6	43:i:113:ARG:NH1	2.23	0.71
1:0:95:ARG:NH1	11:A:3579:A:OP2	2.24	0.71
11:A:3507:C:OP2	11:A:4657:C:O2'	2.08	0.70
3:2:82:ARG:NH2	11:A:3549:G:OP2	2.24	0.70
11:A:3772:A:H2'	11:A:3774:C:N3	2.06	0.70
52:s:51:MET:O	52:s:62:ARG:NH2	2.25	0.70
14:E:114:GLY:O	25:Q:170:ARG:NH1	2.24	0.70
15:F:167:MET:SD	15:F:279:ARG:NH1	2.65	0.70
9:8:132:GLU:OE2	47:m:37:ARG:NH2	2.25	0.70
11:A:3519:A:O2'	11:A:3520:A:O5'	2.08	0.70
7:6:368:ARG:NH2	11:A:4617:A:OP2	2.25	0.70
11:A:4063:U:OP1	28:T:149:ARG:NH1	2.25	0.70
11:A:4488:A:C2	11:A:4689:A:N3	2.60	0.70
29:U:16:GLN:NE2	29:U:17:LEU:O	2.25	0.70
36:b:44:ARG:NH2	48:o:99:LYS:O	2.25	0.69
4:3:113:ARG:NH1	21:M:75:TYR:O	2.24	0.69
11:A:4840:G:N2	11:A:4843:A:OP2	2.25	0.69
11:A:4488:A:N1	11:A:4689:A:N1	2.41	0.69
37:c:161:THR:O	37:c:192:GLN:NE2	2.25	0.69
11:A:3495:A:N6	11:A:3518:G:O2'	2.26	0.69
11:A:4275:U:OP1	13:D:287:ARG:NH2	2.26	0.69
11:A:4580:C:O2'	11:A:4673:C:OP2	2.11	0.69
28:T:133:ASN:O	38:d:230:ARG:NH2	2.26	0.69
37:c:80:GLN:O	37:c:210:ARG:NH2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:27:ARG:N	11:A:3831:A:OP2	2.26	0.69
11:A:4826:G:N2	11:A:4826:G:OP2	2.25	0.69
27:S:132:LYS:NZ	44:j:48:ASP:OD1	2.26	0.69
4:3:179:LYS:NZ	7:6:373:HIS:O	2.25	0.69
11:A:4278:C:OP2	13:D:295:TYR:OH	2.09	0.68
24:P:168:GLY:O	49:p:184:ASN:ND2	2.26	0.68
11:A:3457:C:OP1	33:Y:197:LYS:NZ	2.27	0.68
13:D:128:GLN:NE2	13:D:129:VAL:O	2.27	0.68
7:6:308:GLN:NE2	7:6:311:MET:SD	2.67	0.68
11:A:3925:A:N6	11:A:3970:C:OP2	2.26	0.68
11:A:4488:A:N3	11:A:4689:A:C2	2.60	0.68
35:a:126:HIS:O	35:a:131:ARG:NH2	2.27	0.68
7:6:160:ASP:OD2	7:6:267:ARG:NH1	2.27	0.68
11:A:4295:G:O2'	11:A:4392:U:OP2	2.12	0.68
36:b:132:PRO:O	36:b:136:LYS:NZ	2.26	0.68
11:A:4174:U:OP1	52:s:313:ARG:NH1	2.27	0.68
20:L:70:GLY:O	20:L:130:ARG:NH1	2.27	0.67
17:I:40:MET:SD	17:I:44:ARG:NH1	2.67	0.67
18:J:154:ARG:NH1	18:J:155:VAL:O	2.28	0.67
11:A:3447:C:OP2	32:X:5:LYS:NZ	2.27	0.67
11:A:3531:A:OP2	37:c:31:VAL:N	2.27	0.67
36:b:37:GLY:O	48:o:100:LYS:NZ	2.27	0.67
6:5:30:ALA:N	13:D:201:GLY:O	2.27	0.67
9:8:164:ARG:NH1	40:f:87:GLU:O	2.27	0.67
6:5:245:ILE:O	6:5:248:THR:OG1	2.12	0.67
11:A:3869:C:HO2'	11:A:4702:C:HO2'	1.42	0.67
9:8:93:LYS:O	39:e:84:TYR:OH	2.13	0.67
13:D:227:GLN:NE2	13:D:228:LEU:O	2.28	0.67
4:3:124:ARG:NH2	11:A:4626:C:OP1	2.28	0.66
13:D:132:ASP:OD2	13:D:135:ARG:NH1	2.28	0.66
11:A:3713:G:O2'	11:A:3716:G:O2'	2.12	0.66
11:A:3474:U:O2	32:X:89:GLN:NE2	2.28	0.66
11:A:4712:C:O2	22:N:182:LYS:NZ	2.28	0.66
8:7:247:ASN:ND2	8:7:251:ILE:O	2.28	0.66
18:J:85:PRO:O	18:J:124:LYS:NZ	2.29	0.66
11:A:4622:U:O5'	31:W:50:ARG:NH1	2.29	0.66
11:A:4977:A:OP1	14:E:260:LYS:NZ	2.28	0.66
11:A:4451:A:OP1	48:o:15:ARG:NH2	2.29	0.66
11:A:4975:A:OP2	14:E:212:GLY:N	2.29	0.65
14:E:102:LEU:N	14:E:123:GLN:O	2.29	0.65
40:f:176:SER:O	47:m:35:SER:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:4572:G:O2'	11:A:4741:G:OP1	2.10	0.65
30:V:150:SER:OG	30:V:152:ARG:NH1	2.29	0.65
7:6:367:ASP:OD1	7:6:370:ARG:NH1	2.30	0.65
11:A:4437:U:C5'	11:A:4479:G:OP1	2.42	0.65
11:A:4917:A:OP1	14:E:213:LYS:NZ	2.30	0.65
13:D:136:SER:O	13:D:249:ASN:ND2	2.30	0.65
11:A:3513:A:O2'	16:H:64:LEU:O	2.10	0.65
3:2:57:ASN:ND2	10:9:25:ARG:O	2.30	0.65
52:s:419:LEU:O	52:s:423:HIS:ND1	2.30	0.65
16:H:99:THR:OG1	16:H:100:GLN:OE1	2.14	0.65
10:9:22:THR:OG1	10:9:36:ARG:NH1	2.31	0.64
11:A:4817:A:OP1	11:A:4819:G:O2'	2.14	0.64
52:s:204:CYS:SG	52:s:240:GLN:NE2	2.69	0.64
11:A:3431:U:O2'	28:T:149:ARG:NH2	2.29	0.64
18:J:56:ARG:NH1	18:J:80:ILE:O	2.31	0.64
34:Z:58:GLY:O	48:o:47:TYR:OH	2.15	0.64
9:8:179:THR:OG1	47:m:63:THR:OG1	2.11	0.64
11:A:3615:U:O2'	11:A:4747:G:C5	2.49	0.64
29:U:48:MET:O	29:U:93:LYS:NZ	2.28	0.64
52:s:358:GLN:NE2	52:s:424:PHE:O	2.31	0.64
10:9:31:ARG:O	11:A:4178:U:O2'	2.11	0.64
11:A:4143:U:OP1	13:D:71:LYS:NZ	2.30	0.64
7:6:198:ALA:O	7:6:254:TYR:OH	2.15	0.64
11:A:3623:C:OP1	26:R:13:ARG:NE	2.30	0.64
16:H:133:SER:OG	16:H:135:GLU:OE1	2.16	0.64
13:D:115:GLU:OE2	13:D:146:SER:OG	2.12	0.63
7:6:252:CYS:SG	7:6:286:ARG:NH2	2.71	0.63
32:X:118:ILE:O	32:X:168:ARG:NH1	2.31	0.63
49:p:113:GLU:OE1	49:p:116:ARG:NH2	2.31	0.63
39:e:257:LYS:NZ	39:e:273:ARG:O	2.28	0.63
5:4:84:ARG:NE	11:A:4945:U:OP2	2.31	0.63
23:O:97:TYR:OH	23:O:126:LYS:O	2.15	0.63
29:U:39:THR:OG1	29:U:98:GLN:OE1	2.11	0.63
11:A:3832:A:N6	40:f:48:TYR:OH	2.31	0.63
11:A:3962:U:O2'	11:A:3965:A:N7	2.29	0.63
13:D:155:GLU:OE2	13:D:246:ARG:NH1	2.32	0.63
7:6:27:ARG:N	11:A:4590:A:N1	2.46	0.63
11:A:3897:U:O4	34:Z:77:ARG:NH1	2.31	0.63
52:s:228:ASP:O	52:s:230:ARG:NH1	2.32	0.63
29:U:56:TYR:OH	33:Y:106:LEU:HD21	1.99	0.62
37:c:42:GLN:NE2	43:i:36:LEU:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:F:220:ASP:O	15:F:245:ALA:N	2.31	0.62
14:E:145:LEU:HD13	14:E:181:ILE:HG21	1.81	0.62
11:A:4571:U:N3	11:A:4575:G:OP2	2.33	0.62
39:e:196:SER:OG	39:e:198:ASN:OD1	2.07	0.62
11:A:3452:U:O4'	33:Y:162:ARG:NH2	2.32	0.62
6:5:381:LEU:O	6:5:407:LYS:NZ	2.31	0.62
9:8:134:ASP:OD1	9:8:137:ARG:NH1	2.33	0.61
11:A:3622:A:O3'	26:R:13:ARG:NH1	2.33	0.61
11:A:3635:U:O3'	21:M:30:ASN:ND2	2.33	0.61
11:A:3518:G:OP1	21:M:196:ARG:NE	2.33	0.61
24:P:114:HIS:O	24:P:115:LEU:N	2.34	0.61
43:i:95:ARG:NH1	43:i:111:ASN:OD1	2.34	0.61
9:8:121:TRP:CD2	39:e:70:MET:HE1	2.35	0.61
21:M:72:THR:OG1	21:M:77:ARG:NH2	2.34	0.61
28:T:77:ARG:NH2	28:T:119:GLU:OE1	2.34	0.61
9:8:178:TYR:O	39:e:136:ARG:NE	2.34	0.61
11:A:3613:A:N6	11:A:4455:G:OP1	2.34	0.61
11:A:3912:A:N7	48:o:30:ARG:NH2	2.48	0.61
11:A:4282:A:OP1	13:D:67:LYS:NZ	2.33	0.61
19:K:10:GLN:NE2	28:T:206:ARG:O	2.34	0.60
15:F:121:ARG:O	15:F:142:ARG:NE	2.34	0.60
25:Q:103:ARG:CZ	25:Q:108:ILE:HD11	2.31	0.60
39:e:145:ASP:O	39:e:148:SER:OG	2.12	0.60
3:2:49:ARG:NH2	11:A:4258:A:N1	2.49	0.60
11:A:3660:C:O2	43:i:126:LYS:N	2.34	0.60
11:A:3505:G:OP2	11:A:3507:C:N4	2.34	0.60
11:A:4961:C:OP1	14:E:298:LYS:NZ	2.33	0.60
7:6:114:ARG:NH1	12:B:1643:A:OP1	2.35	0.60
30:V:181:ASP:O	33:Y:93:LYS:NZ	2.35	0.60
4:3:169:ARG:NH2	11:A:3650:A:OP1	2.34	0.59
11:A:3614:A:OP2	11:A:4744:C:O2'	2.10	0.59
11:A:3663:C:N3	11:A:3776:G:N1	2.50	0.59
11:A:4691:G:O5'	11:A:4691:G:H8	1.85	0.59
11:A:3896:U:O2'	11:A:3909:A:N3	2.32	0.59
11:A:3523:C:O3'	43:i:75:ARG:NH1	2.35	0.59
11:A:3558:G:N1	11:A:3561:A:OP2	2.35	0.59
11:A:3545:G:N2	11:A:3548:A:OP2	2.33	0.59
11:A:3615:U:O2'	11:A:4747:G:O6	2.20	0.59
27:S:166:SER:OG	27:S:188:THR:N	2.36	0.59
1:0:133:GLU:OE1	1:0:179:ARG:NH2	2.36	0.59
11:A:3869:C:O2'	11:A:4702:C:O2'	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:F:74:GLN:O	15:F:210:ARG:NH2	2.36	0.59
7:6:360:ARG:NH2	11:A:4627:A:N7	2.51	0.58
11:A:3909:A:O3'	48:o:38:ARG:NH1	2.36	0.58
11:A:4462:A:OP2	19:K:109:TYR:OH	2.15	0.58
11:A:4401:G:O2'	11:A:4403:G:OP2	2.18	0.58
14:E:45:SER:OG	14:E:46:GLY:N	2.36	0.58
1:0:163:GLU:OE1	1:0:181:ARG:NH2	2.36	0.58
24:P:74:ARG:O	24:P:96:GLN:NE2	2.36	0.58
52:s:73:ALA:O	52:s:79:LYS:NZ	2.31	0.58
26:R:14:VAL:O	37:c:32:LYS:NZ	2.32	0.58
11:A:3611:A:H61	11:A:4450:G:H21	1.52	0.58
11:A:4823:U:HO2'	14:E:236:THR:HG1	1.50	0.58
18:J:27:GLY:O	18:J:58:LYS:NZ	2.37	0.58
44:j:30:GLN:OE1	44:j:31:GLN:NE2	2.37	0.58
11:A:3529:C:OP1	37:c:33:LYS:NZ	2.37	0.57
41:g:110:ILE:HD13	41:g:147:LEU:HD12	1.85	0.57
11:A:3833:U:O2'	11:A:4591:A:N7	2.28	0.57
11:A:4553:U:O2	16:H:87:LYS:NZ	2.37	0.57
11:A:4320:U:O2'	13:D:284:ARG:O	2.11	0.57
11:A:3862:A:OP1	22:N:73:ARG:NH1	2.38	0.57
17:I:89:VAL:O	17:I:93:ASN:ND2	2.37	0.57
27:S:70:VAL:O	27:S:73:THR:OG1	2.19	0.57
21:M:203:ARG:NH2	21:M:261:ASP:O	2.38	0.57
24:P:112:LYS:O	24:P:115:LEU:N	2.38	0.57
6:5:104:CYS:SG	6:5:105:TYR:N	2.77	0.57
25:Q:279:GLU:OE1	25:Q:283:TRP:NE1	2.38	0.57
10:9:24:LYS:O	11:A:4099:C:N4	2.38	0.56
21:M:123:ASN:ND2	41:g:51:LEU:O	2.38	0.56
41:g:120:LEU:HD22	41:g:147:LEU:HD11	1.87	0.56
39:e:175:GLN:N	39:e:175:GLN:OE1	2.38	0.56
11:A:3832:A:N1	11:A:4590:A:O2'	2.32	0.56
11:A:3940:G:H22	11:A:3958:A:H62	1.52	0.56
15:F:129:PRO:N	15:F:129:PRO:C	2.60	0.56
4:3:168:ARG:NH2	4:3:170:ASN:OD1	2.38	0.56
11:A:4232:C:O2	11:A:4414:U:O2'	2.11	0.56
15:F:83:HIS:ND1	15:F:85:ASP:OD1	2.39	0.56
25:Q:121:THR:HG1	25:Q:131:SER:HG	1.51	0.56
10:9:127:LEU:O	10:9:134:ASN:ND2	2.38	0.56
11:A:3716:G:OP2	28:T:160:GLY:N	2.39	0.56
15:F:86:VAL:HG13	15:F:87:PHE:CD2	2.41	0.56
21:M:148:PHE:O	21:M:170:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:b:34:SER:OG	36:b:36:ASP:O	2.23	0.56
7:6:374:GLU:OE2	49:p:145:ARG:NH1	2.40	0.55
15:F:231:VAL:HG21	50:q:26:ARG:HH11	1.72	0.55
11:A:4824:C:O2'	14:E:233:GLN:OE1	2.24	0.55
22:N:222:ASN:OD1	22:N:226:ILE:N	2.39	0.55
39:e:264:LEU:O	39:e:273:ARG:NH2	2.40	0.55
23:O:23:GLU:O	23:O:27:HIS:ND1	2.40	0.55
30:V:131:THR:OG1	30:V:148:THR:HG22	2.07	0.55
11:A:3931:G:N3	18:J:150:SER:OG	2.40	0.55
3:2:70:LEU:O	33:Y:198:ARG:NH2	2.40	0.55
31:W:70:GLN:OE1	31:W:74:ARG:N	2.39	0.55
11:A:4260:C:O2	11:A:4853:G:O2'	2.20	0.55
11:A:4684:A:O2'	11:A:4845:C:OP1	2.18	0.55
17:I:107:GLU:N	17:I:107:GLU:OE1	2.38	0.55
52:s:80:LEU:O	52:s:84:THR:OG1	2.17	0.55
26:R:122:ARG:NH2	26:R:126:GLU:OE2	2.39	0.55
30:V:136:ARG:O	30:V:143:ARG:NH2	2.39	0.55
8:7:155:GLU:OE2	8:7:156:ARG:NH1	2.40	0.55
11:A:3998:C:OP2	19:K:71:LYS:NZ	2.37	0.54
28:T:95:ARG:NH2	28:T:145:SER:O	2.41	0.54
41:g:140:VAL:HG12	41:g:147:LEU:CD2	2.36	0.54
1:0:86:THR:OG1	11:A:4442:C:OP1	2.12	0.54
28:T:80:ILE:HD11	28:T:87:MET:HE2	1.88	0.54
11:A:3523:C:OP2	43:i:75:ARG:NH2	2.39	0.54
52:s:66:TRP:O	52:s:69:THR:OG1	2.18	0.54
10:9:26:GLY:O	10:9:31:ARG:NH1	2.41	0.54
11:A:3458:U:O4	33:Y:193:ARG:NH2	2.40	0.54
15:F:262:THR:O	15:F:265:THR:OG1	2.21	0.54
19:K:3:SER:O	37:c:302:ARG:NH2	2.41	0.54
25:Q:100:LEU:CD1	25:Q:286:ILE:HG22	2.37	0.54
16:H:58:ARG:NH1	16:H:77:HIS:O	2.41	0.54
16:H:99:THR:OG1	16:H:128:LEU:O	2.25	0.54
28:T:154:LYS:O	28:T:155:ARG:NE	2.37	0.54
30:V:54:TRP:NE1	30:V:56:LEU:O	2.40	0.54
11:A:4214:U:OP1	23:O:16:ARG:NH1	2.41	0.53
30:V:47:GLU:OE2	30:V:118:ARG:NH2	2.41	0.53
37:c:60:ARG:NH2	37:c:64:PRO:O	2.41	0.53
6:5:303:ARG:NH2	11:A:4153:A:OP2	2.40	0.53
23:O:64:LYS:NZ	23:O:97:TYR:O	2.39	0.53
50:q:111:GLU:OE1	50:q:115:ARG:NH1	2.41	0.53
11:A:4513:A:O2'	32:X:112:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:h:115:SER:O	42:h:118:HIS:NE2	2.42	0.53
11:A:4952:A:OP2	11:A:4953:G:O2'	2.16	0.53
10:9:44:LEU:O	11:A:4137:C:O2'	2.26	0.53
14:E:106:MET:HG2	14:E:120:THR:HG22	1.91	0.53
6:5:51:GLU:OE1	6:5:51:GLU:N	2.42	0.53
15:F:185:ASP:OD1	42:h:115:SER:N	2.42	0.53
24:P:107:ARG:O	24:P:112:LYS:NZ	2.41	0.53
7:6:206:TYR:OH	7:6:242:GLY:O	2.16	0.53
21:M:231:GLU:N	21:M:231:GLU:OE1	2.41	0.53
44:j:63:GLN:OE1	44:j:66:ARG:NH1	2.42	0.53
7:6:364:ARG:NE	11:A:4617:A:OP2	2.38	0.53
14:E:131:LYS:N	14:E:146:SER:OG	2.42	0.53
10:9:72:PRO:O	33:Y:85:TRP:NE1	2.42	0.52
38:d:200:SER:N	38:d:209:TYR:O	2.42	0.52
1:0:136:GLU:OE1	1:0:177:ARG:NH2	2.42	0.52
8:7:78:VAL:HG12	38:d:282:ILE:HD11	1.91	0.52
11:A:4452:A:N3	11:A:4700:C:O2'	2.40	0.52
16:H:84:GLU:OE1	32:X:44:ARG:NH2	2.42	0.52
14:E:292:HIS:ND1	14:E:293:LYS:O	2.42	0.52
20:L:35:MET:N	20:L:57:CYS:O	2.42	0.52
22:N:134:LYS:NZ	22:N:141:GLY:O	2.27	0.52
26:R:51:VAL:HG21	27:S:174:PHE:HB3	1.91	0.52
40:f:104:GLU:OE2	40:f:155:ARG:NH2	2.43	0.52
11:A:4958:A:OP1	19:K:98:ARG:NH1	2.43	0.52
7:6:197:GLU:OE1	49:p:189:ARG:NH1	2.42	0.52
25:Q:262:GLN:OE1	25:Q:262:GLN:N	2.42	0.52
11:A:3651:A:O2'	41:g:98:LYS:O	2.17	0.52
11:A:4132:A:N6	52:s:272:PRO:O	2.41	0.52
29:U:99:LEU:HD13	29:U:103:GLN:HB2	1.92	0.52
8:7:257:ILE:N	8:7:260:PHE:O	2.41	0.52
11:A:3868:A:OP2	22:N:67:LYS:NZ	2.33	0.52
24:P:59:SER:OG	49:p:177:ARG:NH1	2.43	0.52
11:A:4473:A:O2'	14:E:245:THR:O	2.27	0.52
25:Q:119:VAL:HG22	25:Q:174:ILE:HG22	1.92	0.52
43:i:118:TYR:O	43:i:122:ASN:ND2	2.43	0.52
6:5:149:ASN:ND2	6:5:152:GLU:OE2	2.42	0.51
11:A:4357:U:OP2	11:A:4383:5MC:N4	2.42	0.51
11:A:4976:G:O2'	11:A:4978:A:OP2	2.17	0.51
32:X:144:TYR:O	32:X:148:ALA:N	2.42	0.51
6:5:266:HIS:ND1	11:A:4166:U:O2'	2.42	0.51
7:6:119:GLU:N	7:6:119:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:4587:C:OP2	11:A:4588:A:O2'	2.13	0.51
38:d:175:ASP:O	38:d:179:LYS:NZ	2.41	0.51
41:g:141:ASN:ND2	41:g:144:THR:OG1	2.43	0.51
7:6:89:ASP:N	7:6:89:ASP:OD1	2.43	0.51
6:5:347:THR:OG1	6:5:351:VAL:O	2.19	0.51
11:A:3785:A:O2'	11:A:3806:U:OP1	2.28	0.51
11:A:3948:C:OP2	46:l:120:ARG:NH2	2.41	0.51
11:A:4045:U:O2'	21:M:27:LEU:O	2.25	0.51
17:I:90:PHE:CB	17:I:96:ILE:HD11	2.41	0.51
7:6:208:ALA:O	7:6:243:ASN:N	2.43	0.51
11:A:3851:U:O2	11:A:4024:U:O2'	2.29	0.51
33:Y:96:GLU:OE1	33:Y:96:GLU:N	2.44	0.51
3:2:82:ARG:NH2	11:A:3548:A:OP1	2.44	0.51
7:6:64:GLU:OE2	7:6:69:HIS:NE2	2.44	0.51
7:6:214:TRP:CE3	7:6:272:LEU:HD21	2.46	0.51
11:A:4908:A:N6	11:A:4920:G:O2'	2.43	0.51
21:M:117:ASP:OD1	21:M:118:LEU:N	2.44	0.51
43:i:125:GLY:O	43:i:128:ARG:NH1	2.44	0.51
8:7:309:HIS:NE2	14:E:155:PHE:O	2.44	0.50
11:A:4014:U:O2'	27:S:118:ASN:ND2	2.45	0.50
11:A:3990:A:O2'	11:A:4760:G:N3	2.39	0.50
50:q:78:SER:OG	50:q:81:GLN:OE1	2.12	0.50
13:D:64:VAL:O	13:D:80:ARG:NH2	2.44	0.50
14:E:134:SER:HG	14:E:136:GLU:N	2.08	0.50
11:A:3511:A:OP1	43:i:118:TYR:OH	2.24	0.50
12:B:1644:G:O6	24:P:87:HIS:NE2	2.44	0.50
30:V:132:GLU:OE1	30:V:132:GLU:N	2.45	0.50
2:1:23:GLU:N	2:1:23:GLU:OE1	2.44	0.50
18:J:115:LYS:NZ	46:l:70:THR:O	2.45	0.50
6:5:144:ARG:O	6:5:194:LYS:NZ	2.42	0.50
16:H:117:SER:O	16:H:121:ASN:ND2	2.44	0.50
14:E:54:SER:N	23:O:146:ASN:OD1	2.44	0.50
17:I:90:PHE:HB2	17:I:96:ILE:HD11	1.93	0.50
11:A:3663:C:O2	11:A:3776:G:C2	2.56	0.50
11:A:4450:G:N1	11:A:4454:A:OP2	2.44	0.50
17:I:51:THR:O	22:N:250:ARG:NH1	2.44	0.50
32:X:19:GLY:O	32:X:22:SER:OG	2.24	0.50
33:Y:169:ARG:NH1	33:Y:194:TYR:OH	2.44	0.50
7:6:176:ALA:HB1	7:6:184:LEU:HD13	1.94	0.49
11:A:3504:A:OP1	32:X:55:LYS:NZ	2.41	0.49
11:A:3632:A:O2'	11:A:3848:A:O2'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:3665:A:N3	11:A:4688:U:O2'	2.43	0.49
32:X:3:LEU:HD13	43:i:98:VAL:HG21	1.94	0.49
49:p:81:CYS:SG	49:p:82:ARG:N	2.84	0.49
11:A:3610:C:O2'	27:S:177:ARG:NH2	2.45	0.49
11:A:4084:C:OP2	52:s:55:SER:OG	2.22	0.49
52:s:92:MET:SD	52:s:276:ARG:NE	2.81	0.49
11:A:4036:A:OP1	43:i:51:ARG:NE	2.44	0.49
11:A:4086:C:N4	52:s:52:THR:O	2.40	0.49
17:I:64:CYS:SG	17:I:65:LEU:N	2.85	0.49
19:K:104:VAL:HG21	19:K:127:LEU:HD22	1.95	0.49
7:6:29:THR:OG1	40:f:50:THR:O	2.26	0.49
7:6:40:ILE:CD1	40:f:62:LEU:HD11	2.42	0.49
9:8:177:HIS:N	39:e:58:VAL:O	2.45	0.49
11:A:3627:A:N7	43:i:120:HIS:NE2	2.60	0.49
11:A:3928:G:N2	18:J:143:SER:O	2.45	0.49
11:A:4440:A:OP1	26:R:34:ARG:NH2	2.46	0.49
15:F:86:VAL:O	15:F:179:THR:OG1	2.31	0.49
27:S:106:TRP:CG	27:S:114:ILE:HD11	2.48	0.49
33:Y:111:MET:O	33:Y:114:THR:OG1	2.28	0.49
6:5:246:GLU:O	6:5:249:LYS:NZ	2.46	0.49
11:A:3615:U:H4'	11:A:4747:G:N7	2.27	0.49
14:E:118:VAL:O	14:E:287:GLY:N	2.45	0.49
24:P:160:LEU:HD23	24:P:164:MET:HE1	1.95	0.48
17:I:76:ILE:HD11	46:l:118:TRP:CH2	2.47	0.48
19:K:6:ARG:NE	37:c:230:GLU:OE2	2.46	0.48
36:b:81:ASN:OD1	37:c:172:ASN:ND2	2.44	0.48
45:k:8:LEU:HD12	45:k:10:LEU:H	1.78	0.48
15:F:277:ASP:O	41:g:90:ARG:NH2	2.47	0.48
52:s:191:HIS:O	52:s:428:ARG:NH2	2.47	0.48
11:A:3432:A:OP2	28:T:151:GLN:NE2	2.46	0.48
11:A:4964:A:N1	14:E:165:TYR:OH	2.38	0.48
11:A:3752:A:O2'	11:A:3760:G:N7	2.39	0.48
11:A:4884:G:N2	11:A:4887:A:OP2	2.44	0.48
21:M:146:ASP:OD1	49:p:143:GLN:NE2	2.47	0.48
37:c:276:CYS:SG	37:c:281:ILE:HD11	2.54	0.48
16:H:108:ARG:NH1	16:H:143:GLU:OE2	2.45	0.48
37:c:238:MET:SD	37:c:238:MET:N	2.85	0.48
47:m:50:ARG:O	47:m:51:LEU:HD22	2.13	0.48
11:A:4554:G:O2'	16:H:85:ASP:OD2	2.26	0.48
33:Y:140:ASP:OD1	33:Y:141:ALA:N	2.47	0.48
8:7:269:ILE:HB	8:7:274:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:4200:U:O3'	52:s:85:LYS:NZ	2.44	0.48
11:A:4512:A:N3	32:X:108:GLN:NE2	2.61	0.48
37:c:227:GLU:OE1	37:c:228:LEU:N	2.47	0.48
45:k:49:CYS:SG	45:k:50:SER:N	2.86	0.48
3:2:79:ILE:HG23	3:2:90:LEU:HD23	1.95	0.47
11:A:3945:C:O3'	18:J:106:LYS:NZ	2.47	0.47
18:J:107:GLU:OE1	18:J:109:ALA:N	2.45	0.47
19:K:69:GLY:N	51:r:151:LEU:O	2.47	0.47
34:Z:77:ARG:O	34:Z:78:ARG:NE	2.47	0.47
3:2:58:ILE:O	3:2:62:ASN:ND2	2.48	0.47
11:A:3774:C:OP1	11:A:3798:G:H5'	2.15	0.47
11:A:3809:A:N3	41:g:104:ASN:ND2	2.62	0.47
11:A:4077:A:O3'	23:O:42:ILE:HD11	2.15	0.47
11:A:4500:U:O2	32:X:99:LYS:NZ	2.45	0.47
26:R:97:LEU:HD12	26:R:101:VAL:HG21	1.96	0.47
7:6:124:ARG:NH2	9:8:112:GLU:OE1	2.47	0.47
42:h:84:SER:OG	42:h:85:ASN:OD1	2.25	0.47
11:A:3953:A:OP1	46:l:119:ARG:NH2	2.48	0.47
11:A:3718:A:OP1	11:A:4189:C:N4	2.46	0.47
19:K:155:LEU:HD22	51:r:86:VAL:HG21	1.97	0.47
21:M:161:GLU:N	21:M:161:GLU:OE1	2.47	0.47
25:Q:227:LYS:O	25:Q:229:TRP:N	2.48	0.47
27:S:165:GLU:OE2	36:b:103:LYS:NZ	2.31	0.47
9:8:172:GLU:OE1	40:f:185:SER:OG	2.32	0.47
11:A:4372:U:O3'	20:L:53:ARG:NH1	2.48	0.47
11:A:4770:U:O4'	11:A:4930:G:N2	2.47	0.47
13:D:193:ILE:HD11	13:D:226:ILE:CD1	2.45	0.47
11:A:3641:G:N7	15:F:281:ARG:NH1	2.63	0.47
11:A:4488:A:C4	11:A:4689:A:C2	3.02	0.47
17:I:187:SER:OG	17:I:188:ARG:N	2.48	0.47
27:S:129:ARG:N	44:j:50:SER:O	2.45	0.47
30:V:216:TYR:OH	33:Y:186:ILE:O	2.25	0.47
38:d:147:GLU:OE2	38:d:163:LEU:HD13	2.15	0.47
6:5:343:GLN:NE2	6:5:417:LEU:O	2.48	0.47
11:A:3615:U:H4'	11:A:4747:G:C8	2.50	0.47
7:6:239:ASN:OD1	7:6:275:GLN:NE2	2.47	0.46
19:K:69:GLY:O	51:r:152:THR:HG22	2.15	0.46
7:6:270:PHE:N	7:6:317:SER:O	2.47	0.46
10:9:16:ASP:OD1	10:9:25:ARG:NH1	2.48	0.46
11:A:3595:C:OP1	36:b:4:ARG:NH2	2.46	0.46
11:A:3649:A:N6	21:M:128:THR:OG1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:h:97:LYS:NZ	42:h:120:MET:O	2.47	0.46
11:A:3642:G:N3	11:A:3653:C:O2'	2.48	0.46
32:X:76:GLN:NE2	32:X:154:CYS:O	2.48	0.46
37:c:170:ALA:HB3	37:c:191:LEU:HD21	1.97	0.46
11:A:4230:A:OP1	20:L:37:ARG:NH2	2.45	0.46
6:5:202:ILE:HD12	6:5:285:TYR:CE2	2.50	0.46
9:8:164:ARG:NH1	40:f:84:THR:O	2.49	0.46
13:D:124:GLU:N	13:D:163:ILE:O	2.47	0.46
21:M:183:SER:O	21:M:187:VAL:HG23	2.16	0.46
22:N:88:ALA:CB	22:N:159:LEU:HD12	2.45	0.46
50:q:147:GLN:OE1	50:q:150:LYS:NZ	2.49	0.46
2:1:42:THR:C	2:1:43:LEU:HD12	2.40	0.46
14:E:145:LEU:CD1	14:E:181:ILE:HG21	2.46	0.46
23:O:26:ILE:O	23:O:30:ARG:N	2.47	0.46
19:K:133:ILE:CG2	19:K:137:ILE:HG23	2.45	0.46
11:A:3430:C:OP1	28:T:50:LYS:N	2.49	0.46
11:A:3640:A:N6	11:A:3651:A:O4'	2.49	0.46
11:A:4269:C:O2'	13:D:257:ILE:O	2.33	0.46
11:A:4273:U:O2'	13:D:282:ALA:O	2.34	0.46
26:R:47:ILE:O	26:R:51:VAL:HG23	2.15	0.46
28:T:157:ARG:HB2	28:T:167:MET:HE2	1.98	0.46
39:e:43:SER:O	39:e:43:SER:OG	2.32	0.46
11:A:3642:G:O2'	11:A:3653:C:O2	2.34	0.46
52:s:59:ARG:O	52:s:63:ILE:HD12	2.17	0.46
22:N:97:LEU:HD12	22:N:105:MET:HE1	1.98	0.45
25:Q:253:GLN:O	25:Q:257:ALA:N	2.49	0.45
10:9:137:ARG:NE	29:U:21:ARG:O	2.47	0.45
21:M:153:ASN:ND2	21:M:256:LEU:O	2.50	0.45
32:X:83:GLU:OE2	32:X:128:THR:OG1	2.22	0.45
14:E:103:LYS:O	14:E:294:ASN:N	2.49	0.45
14:E:202:GLN:NE2	14:E:301:ASP:OD1	2.49	0.45
18:J:53:PHE:O	18:J:57:THR:OG1	2.18	0.45
19:K:176:TYR:CD1	51:r:104:ILE:HD13	2.51	0.45
11:A:4932:A:OP2	11:A:4944:C:N4	2.48	0.45
41:g:120:LEU:CD2	41:g:147:LEU:HD11	2.45	0.45
10:9:52:GLN:NE2	11:A:4175:C:OP1	2.50	0.45
11:A:3838:U:O2'	48:o:60:ARG:O	2.22	0.45
15:F:199:ASP:N	15:F:199:ASP:OD1	2.48	0.45
26:R:112:THR:HG23	27:S:142:THR:HG21	1.99	0.45
36:b:48:GLU:OE2	42:h:139:LYS:NZ	2.48	0.45
14:E:137:ASN:OD1	14:E:138:CYS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:W:121:PRO:CG	40:f:62:LEU:HD12	2.47	0.45
50:q:110:GLU:OE2	50:q:114:ARG:NH2	2.49	0.45
11:A:3772:A:H2'	11:A:3774:C:C4	2.52	0.45
11:A:3924:C:N4	11:A:3970:C:OP2	2.50	0.45
13:D:193:ILE:HD11	13:D:226:ILE:HD11	1.99	0.45
23:O:129:CYS:SG	23:O:130:LEU:N	2.90	0.45
26:R:57:ARG:HH12	27:S:171:ILE:HG22	1.81	0.45
52:s:181:VAL:O	52:s:185:VAL:HG22	2.17	0.45
11:A:4481:A:N7	15:F:137:ARG:HD3	2.32	0.45
11:A:4777:G:N2	11:A:4888:G:O2'	2.50	0.45
11:A:4905:C:O2'	14:E:106:MET:SD	2.75	0.45
22:N:36:VAL:HG21	46:l:124:GLN:HB3	1.99	0.45
42:h:90:SER:C	42:h:91:LEU:HD22	2.42	0.45
51:r:94:ARG:N	51:r:98:GLY:O	2.50	0.45
30:V:197:GLU:OE1	33:Y:95:ASN:ND2	2.49	0.44
11:A:4413:G:N2	11:A:4417:C:O2'	2.50	0.44
15:F:225:GLU:OE1	15:F:225:GLU:N	2.46	0.44
23:O:94:ALA:HB3	23:O:95:PRO:HD3	1.99	0.44
11:A:3641:G:OP2	21:M:100:ARG:NH2	2.49	0.44
20:L:101:ASP:OD2	25:Q:152:ARG:NH2	2.47	0.44
11:A:4127:A:OP1	33:Y:117:GLN:NE2	2.50	0.44
37:c:101:GLU:OE1	37:c:105:ARG:NH1	2.51	0.44
41:g:140:VAL:HG12	41:g:147:LEU:HD23	1.99	0.44
6:5:50:TYR:OH	6:5:72:ARG:O	2.22	0.44
6:5:80:ARG:NH2	6:5:82:TYR:OH	2.50	0.44
9:8:173:LYS:NZ	40:f:175:GLN:OE1	2.49	0.44
11:A:3774:C:OP2	21:M:55:GLY:HA2	2.17	0.44
13:D:118:LYS:NZ	13:D:120:GLY:O	2.50	0.44
30:V:20:ARG:NH1	30:V:42:ARG:O	2.50	0.44
15:F:102:TRP:NE1	15:F:163:TYR:O	2.49	0.44
34:Z:90:GLY:C	34:Z:91:LEU:HD22	2.42	0.44
44:j:50:SER:OG	44:j:55:ARG:O	2.36	0.44
11:A:4923:U:O2'	14:E:269:TYR:O	2.29	0.44
12:B:1625:A:N7	24:P:86:GLN:NE2	2.65	0.44
1:0:144:GLN:OE1	1:0:175:ILE:HG22	2.17	0.44
11:A:3913:A:N7	51:r:173:ARG:NH2	2.63	0.44
20:L:40:VAL:HG11	20:L:47:GLY:CA	2.48	0.44
36:b:27:GLN:NE2	37:c:177:GLN:OE1	2.51	0.44
11:A:3566:A:O2'	11:A:3568:A:OP1	2.17	0.43
11:A:3764:C:O3'	15:F:125:ARG:NH2	2.51	0.43
22:N:85:GLY:O	22:N:192:ARG:NH2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:25:ARG:O	23:O:29:LEU:HD13	2.18	0.43
31:W:108:PRO:HA	31:W:114:VAL:HG21	1.99	0.43
11:A:4488:A:N3	11:A:4689:A:H2	2.15	0.43
11:A:4479:G:O5'	11:A:4479:G:H8	2.01	0.43
39:e:84:TYR:HE2	39:e:89:LEU:HD11	1.83	0.43
11:A:3570:C:N4	43:i:36:LEU:HD23	2.32	0.43
17:I:128:ASN:ND2	17:I:149:GLY:O	2.51	0.43
9:8:105:GLU:C	9:8:106:LEU:HD12	2.44	0.43
41:g:137:VAL:HG11	48:o:80:SER:HA	2.00	0.43
11:A:4209:A:N7	11:A:4210:A:N6	2.66	0.43
11:A:4303:U:O2'	11:A:4391:A:OP2	2.25	0.43
25:Q:118:ARG:NH2	25:Q:204:MET:O	2.52	0.43
8:7:262:ASP:OD1	8:7:263:VAL:N	2.52	0.43
11:A:3577:U:OP1	28:T:95:ARG:NH1	2.51	0.43
11:A:4488:A:N1	11:A:4689:A:C6	2.86	0.43
18:J:113:THR:OG1	18:J:116:HIS:ND1	2.48	0.43
21:M:270:ALA:HB1	21:M:271:PRO:HD2	2.01	0.43
25:Q:268:ASP:OD1	25:Q:269:MET:N	2.51	0.43
6:5:409:GLU:OE1	6:5:409:GLU:N	2.48	0.43
21:M:187:VAL:HG22	21:M:265:ILE:HG23	2.00	0.43
21:M:238:ARG:O	49:p:155:ARG:NH2	2.48	0.43
26:R:87:ILE:HD12	44:j:23:ALA:CB	2.49	0.43
35:a:103:LEU:HD23	35:a:103:LEU:H	1.83	0.43
6:5:201:ARG:NH1	6:5:418:TYR:O	2.52	0.43
11:A:4611:A:N1	11:A:4636:G:O2'	2.49	0.43
21:M:289:ASN:OD1	21:M:290:LEU:N	2.51	0.43
11:A:4083:U:OP1	52:s:57:ALA:N	2.47	0.43
8:7:82:ASN:O	8:7:86:SER:OG	2.36	0.42
11:A:3607:C:O2'	11:A:3609:G:N7	2.41	0.42
17:I:47:LEU:HD11	22:N:218:ILE:HD12	2.01	0.42
22:N:170:GLU:OE1	22:N:170:GLU:N	2.52	0.42
10:9:124:GLU:OE1	10:9:125:GLY:N	2.51	0.42
11:A:3779:U:O4	21:M:41:ARG:NH2	2.51	0.42
12:B:1630:A:OP1	47:m:42:ARG:NE	2.52	0.42
34:Z:51:GLU:OE1	34:Z:51:GLU:N	2.51	0.42
52:s:178:ASP:OD2	52:s:203:ARG:NH1	2.52	0.42
26:R:40:ARG:O	26:R:44:ARG:NE	2.44	0.42
32:X:110:PHE:N	32:X:127:VAL:O	2.53	0.42
11:A:3602:A:OP2	26:R:48:ARG:NH1	2.52	0.42
19:K:133:ILE:HG22	19:K:137:ILE:HG23	2.01	0.42
17:I:82:LEU:HD13	17:I:130:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:172:VAL:HG12	22:N:176:LEU:CD1	2.50	0.42
32:X:23:ARG:NH1	32:X:219:GLU:OE1	2.52	0.42
46:l:112:PRO:O	46:l:118:TRP:NE1	2.53	0.42
52:s:208:PHE:HE1	52:s:341:MET:HE3	1.83	0.42
52:s:306:LEU:HD13	52:s:323:VAL:HG21	2.01	0.42
11:A:4215:A:N3	23:O:17:ARG:NH2	2.67	0.42
15:F:191:ASP:OD1	15:F:192:SER:N	2.52	0.42
22:N:172:VAL:HG13	22:N:175:PHE:CZ	2.54	0.42
32:X:8:VAL:HG21	33:Y:210:ARG:CZ	2.50	0.42
45:k:9:GLY:C	45:k:10:LEU:HD23	2.44	0.42
11:A:3587:A:N3	26:R:52:LYS:NZ	2.68	0.42
11:A:4416:U:OP1	14:E:225:LYS:NZ	2.36	0.42
19:K:7:ALA:HB3	19:K:8:PRO:HD3	2.01	0.42
11:A:3539:A:OP1	29:U:83:ARG:NH1	2.53	0.42
12:B:1635:C:OP1	40:f:108:GLN:NE2	2.51	0.42
22:N:96:TYR:C	22:N:97:LEU:HD22	2.45	0.42
32:X:163:ARG:NH2	32:X:205:GLY:O	2.53	0.42
33:Y:110:ASN:O	33:Y:114:THR:HG23	2.20	0.42
51:r:99:MET:HE2	51:r:116:GLU:CB	2.49	0.42
22:N:68:ASN:O	22:N:129:LYS:NZ	2.49	0.42
38:d:157:HIS:O	38:d:161:HIS:ND1	2.53	0.42
6:5:384:GLN:NE2	11:A:4153:A:O2'	2.51	0.42
7:6:360:ARG:NH1	11:A:4628:G:N7	2.68	0.42
11:A:4099:C:O2'	29:U:74:HIS:NE2	2.53	0.42
13:D:216:LEU:HD23	13:D:216:LEU:H	1.84	0.42
23:O:59:LEU:HD21	23:O:89:LEU:HD11	2.02	0.42
27:S:122:LEU:HD21	44:j:49:TRP:CH2	2.55	0.42
39:e:142:GLU:OE1	39:e:151:ARG:NH2	2.52	0.42
39:e:203:LYS:N	39:e:237:LEU:O	2.52	0.42
11:A:3563:A:OP2	30:V:94:HIS:NE2	2.53	0.41
18:J:117:VAL:HG13	18:J:144:ILE:HD11	2.00	0.41
33:Y:91:ARG:NH1	33:Y:148:GLU:OE1	2.50	0.41
7:6:225:LEU:HD13	24:P:43:VAL:HG23	2.02	0.41
11:A:3992:C:O2'	11:A:4446:C:O2'	2.36	0.41
11:A:4488:A:C6	11:A:4689:A:C2	3.08	0.41
22:N:89:ILE:HD12	22:N:161:VAL:HG22	2.02	0.41
27:S:131:GLU:N	27:S:131:GLU:OE1	2.53	0.41
29:U:103:GLN:OE1	29:U:103:GLN:N	2.53	0.41
41:g:156:GLU:OE1	41:g:156:GLU:N	2.52	0.41
52:s:249:GLU:HA	52:s:356:VAL:HG21	2.02	0.41
6:5:393:LYS:O	6:5:396:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:S:106:TRP:CD2	27:S:114:ILE:HD11	2.55	0.41
8:7:99:TYR:O	8:7:103:SER:N	2.50	0.41
9:8:109:GLU:OE1	9:8:109:GLU:N	2.52	0.41
11:A:4339:A:O2'	11:A:4341:C:N4	2.54	0.41
11:A:4736:U:O2'	11:A:4815:C:OP1	2.30	0.41
41:g:88:ARG:O	41:g:112:LYS:NZ	2.52	0.41
10:9:134:ASN:OD1	10:9:135:PHE:N	2.53	0.41
11:A:4230:A:N3	11:A:4232:C:N4	2.68	0.41
15:F:84:PRO:O	15:F:88:ALA:N	2.53	0.41
22:N:87:PHE:O	22:N:163:MET:N	2.52	0.41
22:N:88:ALA:HB1	22:N:159:LEU:HD12	2.02	0.41
22:N:171:GLU:HB3	46:l:132:LEU:HD23	2.02	0.41
28:T:93:LEU:O	28:T:97:MET:HE3	2.21	0.41
52:s:74:GLU:OE1	52:s:74:GLU:N	2.53	0.41
51:r:66:PRO:O	51:r:67:SER:OG	2.33	0.41
11:A:3839:U:OP1	48:o:64:ALA:N	2.53	0.41
11:A:4057:U:O5'	11:A:4057:U:H6	2.04	0.41
23:O:107:MET:O	23:O:108:LEU:HD22	2.20	0.41
29:U:99:LEU:HD12	29:U:100:ALA:O	2.21	0.41
31:W:121:PRO:HG3	40:f:62:LEU:HD12	2.02	0.41
45:k:80:HIS:O	51:r:36:ARG:NH1	2.54	0.41
51:r:149:ARG:CG	51:r:152:THR:HG21	2.49	0.41
11:A:3992:C:O2'	11:A:3993:C:OP2	2.37	0.41
11:A:4836:C:N4	11:A:4837:G:O6	2.53	0.41
30:V:45:VAL:HG23	30:V:45:VAL:O	2.20	0.41
52:s:294:TYR:OH	52:s:353:ARG:NH2	2.54	0.41
11:A:3622:A:OP1	26:R:17:ARG:NH1	2.54	0.41
11:A:4287:U:HO2'	13:D:206:TYR:C	2.29	0.41
28:T:52:GLU:OE1	28:T:52:GLU:N	2.54	0.41
37:c:82:ASN:N	37:c:82:ASN:OD1	2.53	0.41
51:r:176:VAL:N	51:r:194:LEU:O	2.52	0.41
22:N:36:VAL:HG21	46:l:124:GLN:CB	2.51	0.41
1:0:86:THR:O	1:0:90:ASN:ND2	2.53	0.40
7:6:166:THR:OG1	7:6:167:PHE:N	2.54	0.40
11:A:3940:G:H22	11:A:3958:A:N6	2.19	0.40
11:A:4433:G:O2'	28:T:167:MET:SD	2.79	0.40
13:D:194:ASN:OD1	13:D:243:THR:HG23	2.22	0.40
29:U:26:ILE:HD13	29:U:56:TYR:CE2	2.55	0.40
11:A:3993:C:O2'	51:r:165:LYS:N	2.50	0.40
21:M:185:ASP:OD1	21:M:186:ILE:N	2.55	0.40
11:A:3570:C:O2'	37:c:48:GLN:OE1	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:3590:A:N6	11:A:3595:C:OP2	2.54	0.40
21:M:211:VAL:HG21	50:q:99:MET:HG2	2.02	0.40
7:6:265:ILE:HD13	24:P:57:LEU:HD13	2.03	0.40
8:7:144:ARG:NE	8:7:171:GLU:OE2	2.55	0.40
8:7:316:LEU:HD22	23:O:148:LEU:HD23	2.04	0.40
29:U:144:ARG:NH1	38:d:276:ILE:HD11	2.36	0.40
38:d:151:CYS:O	38:d:155:SER:N	2.54	0.40
41:g:91:MET:SD	41:g:91:MET:N	2.95	0.40
8:7:281:SER:OG	8:7:282:ALA:N	2.54	0.40
14:E:119:VAL:HG23	14:E:285:VAL:C	2.47	0.40
21:M:238:ARG:NH1	49:p:70:ASP:OD1	2.55	0.40
45:k:65:ASP:OD2	45:k:66:VAL:N	2.54	0.40
47:m:50:ARG:NH2	47:m:52:TYR:OH	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	106/188 (56%)	104 (98%)	2 (2%)	0	100	100
2	1	51/65 (78%)	51 (100%)	0	0	100	100
3	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
5	4	35/103 (34%)	33 (94%)	2 (6%)	0	100	100
6	5	385/423 (91%)	366 (95%)	19 (5%)	0	100	100
7	6	346/380 (91%)	326 (94%)	20 (6%)	0	100	100
8	7	283/338 (84%)	264 (93%)	19 (7%)	0	100	100
9	8	103/206 (50%)	98 (95%)	5 (5%)	0	100	100
10	9	122/137 (89%)	116 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	D	234/305 (77%)	219 (94%)	13 (6%)	2 (1%)	14	47
14	E	300/348 (86%)	288 (96%)	12 (4%)	0	100	100
15	F	248/311 (80%)	233 (94%)	15 (6%)	0	100	100
16	H	93/267 (35%)	90 (97%)	3 (3%)	0	100	100
17	I	165/261 (63%)	156 (94%)	9 (6%)	0	100	100
18	J	168/192 (88%)	158 (94%)	10 (6%)	0	100	100
19	K	175/178 (98%)	169 (97%)	6 (3%)	0	100	100
20	L	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
21	M	285/296 (96%)	266 (93%)	19 (7%)	0	100	100
22	N	219/251 (87%)	209 (95%)	10 (5%)	0	100	100
23	O	150/175 (86%)	150 (100%)	0	0	100	100
24	P	139/179 (78%)	133 (96%)	6 (4%)	0	100	100
25	Q	217/292 (74%)	211 (97%)	6 (3%)	0	100	100
26	R	138/149 (93%)	133 (96%)	5 (4%)	0	100	100
27	S	158/205 (77%)	155 (98%)	3 (2%)	0	100	100
28	T	164/212 (77%)	160 (98%)	4 (2%)	0	100	100
29	U	137/153 (90%)	133 (97%)	4 (3%)	0	100	100
30	V	198/216 (92%)	190 (96%)	8 (4%)	0	100	100
31	W	109/148 (74%)	105 (96%)	4 (4%)	0	100	100
32	X	241/256 (94%)	238 (99%)	3 (1%)	0	100	100
33	Y	176/250 (70%)	172 (98%)	4 (2%)	0	100	100
34	Z	118/161 (73%)	112 (95%)	6 (5%)	0	100	100
35	a	79/142 (56%)	76 (96%)	3 (4%)	0	100	100
36	b	146/215 (68%)	136 (93%)	10 (7%)	0	100	100
37	c	271/332 (82%)	262 (97%)	9 (3%)	0	100	100
38	d	206/306 (67%)	201 (98%)	5 (2%)	0	100	100
39	e	211/279 (76%)	205 (97%)	6 (3%)	0	100	100
40	f	119/212 (56%)	116 (98%)	3 (2%)	0	100	100
41	g	129/166 (78%)	125 (97%)	4 (3%)	0	100	100
42	h	105/158 (66%)	103 (98%)	2 (2%)	0	100	100
43	i	95/128 (74%)	91 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	j	84/123 (68%)	83 (99%)	1 (1%)	0	100	100
45	k	93/112 (83%)	91 (98%)	2 (2%)	0	100	100
46	l	78/138 (56%)	76 (97%)	2 (3%)	0	100	100
47	m	58/128 (45%)	54 (93%)	4 (7%)	0	100	100
48	o	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
49	p	119/206 (58%)	118 (99%)	1 (1%)	0	100	100
50	q	128/222 (58%)	128 (100%)	0	0	100	100
51	r	145/196 (74%)	138 (95%)	7 (5%)	0	100	100
52	s	366/439 (83%)	356 (97%)	10 (3%)	0	100	100
53	C	2/8 (25%)	0	0	2 (100%)	0	0
All	All	8039/10682 (75%)	7727 (96%)	308 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
53	C	2	THR
53	C	4	PRO
13	D	207	ILE
13	D	208	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	97/164 (59%)	97 (100%)	0	100	100
2	1	50/60 (83%)	50 (100%)	0	100	100
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	353 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	6	313/332 (94%)	313 (100%)	0	100	100
8	7	267/303 (88%)	267 (100%)	0	100	100
9	8	97/190 (51%)	97 (100%)	0	100	100
10	9	104/112 (93%)	104 (100%)	0	100	100
13	D	190/245 (78%)	190 (100%)	0	100	100
14	E	259/290 (89%)	259 (100%)	0	100	100
15	F	217/262 (83%)	217 (100%)	0	100	100
16	H	86/228 (38%)	86 (100%)	0	100	100
17	I	154/232 (66%)	154 (100%)	0	100	100
18	J	134/150 (89%)	134 (100%)	0	100	100
19	K	155/156 (99%)	155 (100%)	0	100	100
20	L	98/124 (79%)	98 (100%)	0	100	100
21	M	245/249 (98%)	245 (100%)	0	100	100
22	N	188/211 (89%)	188 (100%)	0	100	100
23	O	133/150 (89%)	133 (100%)	0	100	100
24	P	125/154 (81%)	125 (100%)	0	100	100
25	Q	201/256 (78%)	201 (100%)	0	100	100
26	R	118/126 (94%)	118 (100%)	0	100	100
27	S	145/180 (81%)	145 (100%)	0	100	100
28	T	146/182 (80%)	146 (100%)	0	100	100
29	U	126/135 (93%)	126 (100%)	0	100	100
30	V	180/191 (94%)	179 (99%)	1 (1%)	78	80
31	W	91/119 (76%)	91 (100%)	0	100	100
32	X	217/227 (96%)	217 (100%)	0	100	100
33	Y	161/223 (72%)	161 (100%)	0	100	100
34	Z	111/147 (76%)	111 (100%)	0	100	100
35	a	79/133 (59%)	79 (100%)	0	100	100
36	b	130/186 (70%)	130 (100%)	0	100	100
37	c	241/288 (84%)	241 (100%)	0	100	100
38	d	193/273 (71%)	193 (100%)	0	100	100
39	e	188/236 (80%)	188 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	f	113/188 (60%)	113 (100%)	0	100	100
41	g	121/148 (82%)	121 (100%)	0	100	100
42	h	103/148 (70%)	103 (100%)	0	100	100
43	i	86/110 (78%)	86 (100%)	0	100	100
44	j	68/97 (70%)	68 (100%)	0	100	100
45	k	80/90 (89%)	80 (100%)	0	100	100
46	l	75/116 (65%)	75 (100%)	0	100	100
47	m	54/113 (48%)	54 (100%)	0	100	100
48	o	80/87 (92%)	80 (100%)	0	100	100
49	p	117/181 (65%)	117 (100%)	0	100	100
50	q	111/178 (62%)	111 (100%)	0	100	100
51	r	139/169 (82%)	139 (100%)	0	100	100
52	s	326/381 (86%)	326 (100%)	0	100	100
53	C	2/2 (100%)	2 (100%)	0	100	100
All	All	7232/9217 (78%)	7231 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
30	V	119	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	106	ASN
3	2	57	ASN
3	2	62	ASN
6	5	183	ASN
8	7	82	ASN
9	8	158	HIS
10	9	113	ASN
13	D	156	ASN
13	D	158	GLN
13	D	205	GLN
17	I	45	GLN
17	I	193	ASN

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Mol	Chain	Res	Type
19	K	61	ASN
19	K	94	GLN
19	K	160	GLN
22	N	68	ASN
25	Q	132	GLN
27	S	118	ASN
28	T	105	GLN
29	U	84	ASN
32	X	237	GLN
33	Y	240	HIS
35	a	126	HIS
36	b	16	HIS
36	b	66	ASN
37	c	65	ASN
37	c	155	ASN
38	d	66	HIS
38	d	235	GLN
39	e	150	ASN
40	f	108	GLN
41	g	141	ASN
46	l	135	ASN
49	p	143	GLN
51	r	42	GLN
52	s	240	GLN
52	s	298	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1493/1558 (95%)	253 (16%)	3 (0%)
12	B	55/69 (79%)	9 (16%)	0
All	All	1548/1627 (95%)	262 (16%)	3 (0%)

All (262) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	3443	C
11	A	3447	C
11	A	3450	A
11	A	3451	C
11	A	3453	C

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Mol	Chain	Res	Type
11	A	3457	C
11	A	3458	U
11	A	3462	U
11	A	3465	C
11	A	3466	A
11	A	3467	G
11	A	3468	A
11	A	3470	A
11	A	3471	A
11	A	3473	C
11	A	3482	A
11	A	3485	A
11	A	3491	C
11	A	3494	A
11	A	3495	A
11	A	3499	A
11	A	3503	U
11	A	3506	G
11	A	3520	A
11	A	3521	A
11	A	3522	C
11	A	3523	C
11	A	3528	G
11	A	3541	U
11	A	3549	G
11	A	3562	A
11	A	3563	A
11	A	3567	U
11	A	3568	A
11	A	3569	A
11	A	3572	A
11	A	3575	C
11	A	3579	A
11	A	3581	A
11	A	3585	C
11	A	3586	A
11	A	3587	A
11	A	3590	A
11	A	3594	A
11	A	3602	A
11	A	3611	A
11	A	3612	U

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Mol	Chain	Res	Type
11	A	3614	A
11	A	3627	A
11	A	3630	U
11	A	3636	U
11	A	3640	A
11	A	3645	A
11	A	3651	A
11	A	3660	C
11	A	3661	C
11	A	3665	A
11	A	3676	G
11	A	3677	C
11	A	3698	A
11	A	3716	G
11	A	3732	A
11	A	3743	G
11	A	3750	C
11	A	3751	A
11	A	3752	A
11	A	3759	C
11	A	3760	G
11	A	3761	A
11	A	3773	G
11	A	3780	G
11	A	3788	U
11	A	3794	C
11	A	3795	U
11	A	3797	A
11	A	3813	U
11	A	3818	A
11	A	3825	C
11	A	3837	C
11	A	3850	C
11	A	3857	U
11	A	3863	G
11	A	3869	C
11	A	3871	G
11	A	3883	C
11	A	3884	U
11	A	3893	A
11	A	3917	U
11	A	3926	U

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Mol	Chain	Res	Type
11	A	3927	A
11	A	3934	C
11	A	3936	A
11	A	3938	A
11	A	3939	A
11	A	3940	G
11	A	3953	A
11	A	3954	A
11	A	3956	A
11	A	3958	A
11	A	3995	A
11	A	3999	A
11	A	4001	A
11	A	4002	U
11	A	4003	A
11	A	4009	A
11	A	4020	C
11	A	4021	C
11	A	4041	C
11	A	4042	C
11	A	4043	U
11	A	4055	A
11	A	4058	G
11	A	4074	U
11	A	4080	C
11	A	4090	C
11	A	4103	G
11	A	4115	C
11	A	4119	C
11	A	4132	A
11	A	4133	C
11	A	4139	A
11	A	4148	A
11	A	4165	U
11	A	4172	C
11	A	4173	C
11	A	4204	A
11	A	4209	A
11	A	4216	A
11	A	4236	G
11	A	4243	U
11	A	4251	C

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Mol	Chain	Res	Type
11	A	4259	C
11	A	4261	A
11	A	4263	A
11	A	4278	C
11	A	4281	C
11	A	4285	A
11	A	4288	A
11	A	4298	C
11	A	4315	C
11	A	4316	A
11	A	4317	U
11	A	4328	C
11	A	4333	U
11	A	4334	A
11	A	4335	C
11	A	4336	C
11	A	4337	C
11	A	4339	A
11	A	4350	G
11	A	4352	U
11	A	4359	A
11	A	4376	U
11	A	4384	U
11	A	4385	G
11	A	4386	U
11	A	4388	U
11	A	4391	A
11	A	4393	G
11	A	4412	U
11	A	4413	G
11	A	4414	U
11	A	4417	C
11	A	4418	U
11	A	4441	C
11	A	4444	G
11	A	4452	A
11	A	4454	A
11	A	4464	A
11	A	4473	A
11	A	4476	C
11	A	4477	G
11	A	4481	A

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Mol	Chain	Res	Type
11	A	4482	G
11	A	4483	A
11	A	4490	G
11	A	4491	G
11	A	4498	A
11	A	4516	G
11	A	4546	C
11	A	4547	C
11	A	4568	G
11	A	4590	A
11	A	4591	A
11	A	4605	C
11	A	4612	U
11	A	4617	A
11	A	4622	U
11	A	4623	C
11	A	4627	A
11	A	4629	U
11	A	4637	A
11	A	4651	A
11	A	4664	C
11	A	4668	A
11	A	4671	A
11	A	4674	G
11	A	4675	G
11	A	4676	A
11	A	4677	A
11	A	4679	A
11	A	4686	C
11	A	4690	G
11	A	4693	A
11	A	4697	C
11	A	4714	A
11	A	4720	C
11	A	4721	A
11	A	4743	C
11	A	4747	G
11	A	4748	2MA
11	A	4749	U
11	A	4750	G
11	A	4758	A
11	A	4763	A

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Mol	Chain	Res	Type
11	A	4765	C
11	A	4779	C
11	A	4799	U
11	A	4807	U
11	A	4811	A
11	A	4812	G
11	A	4825	U
11	A	4827	A
11	A	4829	U
11	A	4830	U
11	A	4847	A
11	A	4848	G
11	A	4854	U
11	A	4855	U
11	A	4858	U
11	A	4879	U
11	A	4881	U
11	A	4907	U
11	A	4908	A
11	A	4911	U
11	A	4914	C
11	A	4915	A
11	A	4919	C
11	A	4926	C
11	A	4929	C
11	A	4934	A
11	A	4938	U
11	A	4941	C
11	A	4946	C
11	A	4947	A
11	A	4951	U
11	A	4965	C
11	A	4966	A
11	A	4967	C
11	A	4969	C
11	A	4974	A
11	A	4975	A
11	A	4976	G
12	B	1608	G
12	B	1611	G
12	B	1615	A
12	B	1618	A

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Mol	Chain	Res	Type
12	B	1619	C
12	B	1620	A
12	B	1621	A
12	B	1646	U
12	B	1659	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	3824	C
11	A	4316	A
11	A	4332	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
53	004	C	7	53	9,10,11	1.01	1 (11%)	9,12,14	1.53	2 (22%)
53	DBB	C	3	53	4,5,6	0.52	0	1,5,7	0.07	0
53	MHV	C	6	53	7,9,10	0.37	0	8,11,13	1.54	1 (12%)
11	2MA	A	4748	55,11	22,25,26	1.50	5 (22%)	32,37,40	2.32	9 (28%)
11	2MU	A	4797	11	20,23,24	8.12	15 (75%)	27,33,36	3.15	10 (37%)
11	5MU	A	4360	11	19,22,23	5.02	7 (36%)	27,32,35	3.62	10 (37%)
53	MHU	C	5	53	14,15,16	0.57	0	18,19,21	1.47	3 (16%)
11	5MC	A	4383	11	19,22,23	3.92	8 (42%)	26,32,35	0.98	2 (7%)
53	MHW	C	1	53	9,9,10	0.75	0	10,11,13	2.63	2 (20%)

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
53	004	C	7	53	-	0/4/6/8	0/1/1/1
53	DBB	C	3	53	-	2/3/4/6	-
53	MHV	C	6	53	-	0/1/12/14	0/1/1/1
11	2MA	A	4748	55,11	-	4/7/25/26	0/3/3/3
11	2MU	A	4797	11	-	0/9/27/28	0/2/2/2
11	5MU	A	4360	11	-	0/7/25/26	0/2/2/2
53	MHU	C	5	53	-	6/9/12/14	0/1/1/1
11	5MC	A	4383	11	-	0/7/25/26	0/2/2/2
53	MHW	C	1	53	-	2/2/2/4	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	4797	2MU	C4-C5	22.25	1.81	1.44
11	A	4797	2MU	C6-N1	16.83	1.66	1.38
11	A	4360	5MU	C6-N1	11.92	1.58	1.38
11	A	4797	2MU	C6-C5	-11.91	1.15	1.34
11	A	4360	5MU	C2-N1	10.59	1.55	1.38
11	A	4797	2MU	C4-N3	-10.48	1.19	1.38
11	A	4360	5MU	C4-C5	10.32	1.61	1.44
11	A	4383	5MC	C6-C5	9.27	1.49	1.34
11	A	4797	2MU	C3'-C2'	-8.83	1.33	1.53
11	A	4360	5MU	C4-N3	-7.27	1.25	1.38
11	A	4383	5MC	C5-C4	6.93	1.49	1.44
11	A	4797	2MU	O4'-C1'	6.88	1.57	1.42
11	A	4360	5MU	C6-C5	6.87	1.45	1.34
11	A	4383	5MC	C4-N3	6.77	1.45	1.34
11	A	4383	5MC	C2-N3	6.43	1.49	1.36
11	A	4797	2MU	O4'-C4'	-5.85	1.32	1.45
11	A	4797	2MU	C1'-N1	-5.45	1.32	1.47
11	A	4383	5MC	C6-N1	4.86	1.46	1.38
11	A	4797	2MU	C2-N1	4.62	1.45	1.38
11	A	4797	2MU	C2-N3	4.56	1.45	1.38
11	A	4383	5MC	C2-N1	4.41	1.49	1.40
11	A	4383	5MC	C4-N4	4.39	1.45	1.34
11	A	4748	2MA	C5-C4	4.37	1.46	1.39
11	A	4797	2MU	C3'-C4'	4.14	1.63	1.53
11	A	4797	2MU	C5M-C5	3.57	1.59	1.50
11	A	4797	2MU	O2-C2	-3.55	1.16	1.23
11	A	4360	5MU	O2-C2	-3.04	1.17	1.23
53	C	7	004	CB-CA	-2.68	1.49	1.52
11	A	4748	2MA	C5-C6	2.63	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	4383	5MC	O2-C2	-2.59	1.18	1.23
11	A	4360	5MU	C2-N3	2.56	1.42	1.38
11	A	4797	2MU	O2'-C2'	2.54	1.48	1.42
11	A	4748	2MA	C8-N7	2.44	1.36	1.31
11	A	4797	2MU	O4-C4	-2.34	1.19	1.23
11	A	4748	2MA	C5-N7	-2.30	1.34	1.39
11	A	4748	2MA	C4-N9	-2.26	1.33	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	4360	5MU	C5-C4-N3	12.21	125.94	115.32
11	A	4797	2MU	C5-C4-N3	9.23	123.34	115.32
11	A	4360	5MU	C5-C6-N1	-8.53	114.05	123.31
11	A	4748	2MA	C5-C4-N3	-7.48	119.30	127.18
53	C	1	MHW	O-C-CA	-7.45	115.02	124.37
11	A	4797	2MU	C5-C6-N1	-6.64	116.09	123.31
11	A	4797	2MU	C4-N3-C2	-5.89	119.62	127.34
11	A	4748	2MA	N3-C4-N9	5.74	134.28	126.99
11	A	4360	5MU	O4-C4-C5	-5.12	119.06	124.92
11	A	4360	5MU	C4-N3-C2	-4.83	121.01	127.34
11	A	4360	5MU	N3-C2-N1	4.72	121.03	114.89
11	A	4360	5MU	C5M-C5-C4	4.51	123.60	118.78
53	C	5	MHU	CB-CA-N	-4.38	104.03	110.48
11	A	4797	2MU	C5M-C5-C6	-4.32	117.00	122.85
11	A	4797	2MU	N3-C2-N1	4.27	120.45	114.89
11	A	4797	2MU	C5M-C5-C4	3.83	122.87	118.78
11	A	4360	5MU	C5M-C5-C6	-3.81	117.69	122.85
11	A	4748	2MA	C4-C5-N7	-3.59	106.48	110.58
53	C	6	MHV	CB-CA-N	-3.55	105.17	112.50
11	A	4797	2MU	O4-C4-C5	-3.46	120.96	124.92
53	C	7	004	CG1-CB-CA	3.22	125.64	120.64
11	A	4748	2MA	C4-N9-C8	3.17	109.07	105.74
53	C	7	004	CG2-CB-CA	-3.16	115.73	120.64
11	A	4748	2MA	N6-C6-N1	3.11	121.22	117.03
11	A	4383	5MC	C5-C6-N1	-2.92	120.14	123.31
53	C	1	MHW	CE-N-CA	2.73	121.39	116.83
11	A	4360	5MU	O4-C4-N3	-2.72	115.00	120.11
11	A	4748	2MA	C2-N1-C6	2.70	122.25	118.10
53	C	5	MHU	O-C-CA	-2.70	117.83	124.77
11	A	4748	2MA	C5-N7-C8	2.69	107.68	103.45
11	A	4797	2MU	C6-C5-C4	2.57	120.14	118.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	4748	2MA	N9-C8-N7	-2.52	110.36	113.94
11	A	4360	5MU	O2-C2-N1	-2.52	119.52	122.80
11	A	4797	2MU	O4-C4-N3	-2.35	115.69	120.11
53	C	5	MHU	CM-N-CA	2.35	120.73	113.70
11	A	4748	2MA	C6-C5-N7	2.33	136.59	132.09
11	A	4797	2MU	C1'-N1-C2	2.22	121.58	117.59
11	A	4383	5MC	CM5-C5-C6	-2.20	119.87	122.85
11	A	4360	5MU	C6-N1-C2	-2.05	119.27	121.30

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	C	1	MHW	O-C-CA-N
53	C	1	MHW	O-C-CA-CB
53	C	3	DBB	N-CA-CB-CG
53	C	3	DBB	C-CA-CB-CG
53	C	5	MHU	CE1-CZ-NZ-CZ2
53	C	5	MHU	CE2-CZ-NZ-CZ1
53	C	5	MHU	CE1-CZ-NZ-CZ1
53	C	5	MHU	CE2-CZ-NZ-CZ2
11	A	4748	2MA	O4'-C1'-N9-C4
11	A	4748	2MA	O4'-C4'-C5'-O5'
11	A	4748	2MA	C3'-C4'-C5'-O5'
11	A	4748	2MA	O4'-C1'-N9-C8
53	C	5	MHU	C-CA-CB-CG
53	C	5	MHU	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	4748	2MA	1	0
11	A	4797	2MU	1	0
11	A	4383	5MC	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 138 ligands modelled in this entry, 137 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
56	H8T	A	5129	-	38,40,40	5.01	21 (55%)	46,55,55	3.05	20 (43%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	H8T	A	5129	-	-	17/48/48/48	0/2/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	A	5129	H8T	C28-C29	13.33	1.62	1.32
56	A	5129	H8T	C4-C3	10.73	1.60	1.37
56	A	5129	H8T	C4-N5	9.82	1.55	1.39
56	A	5129	H8T	C26-N25	8.73	1.52	1.34
56	A	5129	H8T	C22-C23	8.61	1.55	1.32
56	A	5129	H8T	C13-C10	8.47	1.60	1.50
56	A	5129	H8T	C19-C20	8.17	1.56	1.34
56	A	5129	H8T	O36-C37	7.82	1.51	1.34
56	A	5129	H8T	C17-C19	5.83	1.57	1.50
56	A	5129	H8T	C16-C14	5.32	1.58	1.51
56	A	5129	H8T	C28-C26	4.88	1.58	1.48
56	A	5129	H8T	C8-C6	4.42	1.56	1.49
56	A	5129	H8T	C1-N5	4.36	1.46	1.40
56	A	5129	H8T	C22-C20	4.18	1.54	1.46
56	A	5129	H8T	C1-C37	4.02	1.60	1.48
56	A	5129	H8T	C10-N9	3.15	1.32	1.29
56	A	5129	H8T	C8-N9	3.14	1.45	1.38
56	A	5129	H8T	C12-C8	2.95	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	A	5129	H8T	O18-C17	-2.71	1.39	1.43
56	A	5129	H8T	O7-C6	-2.28	1.18	1.23
56	A	5129	H8T	O27-C26	-2.01	1.20	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	A	5129	H8T	O11-C10-C13	7.99	125.08	117.70
56	A	5129	H8T	O36-C37-C1	6.62	120.17	110.77
56	A	5129	H8T	C8-C6-N5	-6.21	112.42	119.70
56	A	5129	H8T	C12-C8-N9	5.74	113.42	109.15
56	A	5129	H8T	C3-C2-C1	5.57	112.17	107.29
56	A	5129	H8T	O11-C12-C8	-5.20	104.28	108.12
56	A	5129	H8T	C24-N25-C26	-5.13	113.85	122.17
56	A	5129	H8T	C2-C1-N5	4.66	110.62	107.19
56	A	5129	H8T	C37-C1-N5	-4.45	117.66	123.23
56	A	5129	H8T	O11-C10-N9	-3.96	109.80	114.09
56	A	5129	H8T	O7-C6-C8	3.39	123.91	118.65
56	A	5129	H8T	C23-C22-C20	-3.26	120.97	125.89
56	A	5129	H8T	O36-C32-C30	3.23	112.46	107.12
56	A	5129	H8T	C3-C4-N5	-2.66	104.79	107.88
56	A	5129	H8T	O38-C37-C1	-2.64	117.52	124.34
56	A	5129	H8T	C4-C3-C2	-2.51	104.51	107.10
56	A	5129	H8T	C17-C16-C14	-2.26	109.17	113.90
56	A	5129	H8T	C4-N5-C1	-2.25	107.19	108.70
56	A	5129	H8T	C12-C8-C6	-2.23	123.41	127.60
56	A	5129	H8T	O7-C6-N5	2.23	123.66	120.46

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	A	5129	H8T	C2-C1-C37-O36
56	A	5129	H8T	C2-C1-C37-O38
56	A	5129	H8T	C19-C20-C22-C23
56	A	5129	H8T	C29-C30-C32-C33
56	A	5129	H8T	C31-C30-C32-C33
56	A	5129	H8T	N5-C6-C8-C12
56	A	5129	H8T	C21-C20-C22-C23
56	A	5129	H8T	N5-C1-C37-O38
56	A	5129	H8T	N5-C1-C37-O36
56	A	5129	H8T	C28-C29-C30-C31

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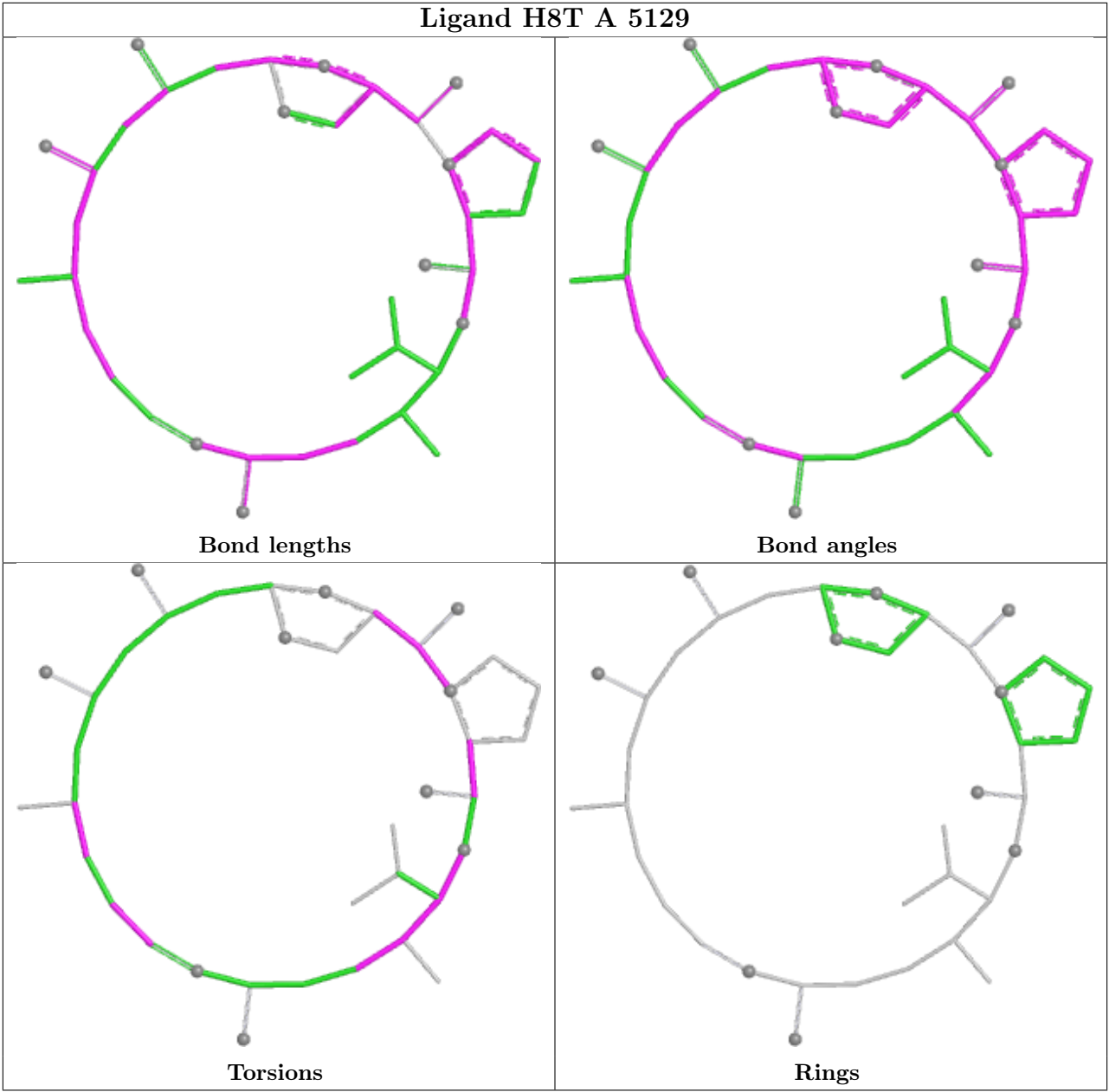
Mol	Chain	Res	Type	Atoms
56	A	5129	H8T	O7-C6-C8-C12
56	A	5129	H8T	O7-C6-N5-C1
56	A	5129	H8T	C22-C23-C24-N25
56	A	5129	H8T	C29-C30-C32-O36
56	A	5129	H8T	C31-C30-C32-O36
56	A	5129	H8T	N5-C6-C8-N9
56	A	5129	H8T	C30-C32-O36-C37

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	A	5129	H8T	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	7	3
6	5	3

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Mol	Chain	Number of breaks
7	6	3
51	r	2
38	d	2
14	E	1
5	4	1
12	B	1
42	h	1
24	P	1
30	V	1
11	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	285:ASN	C	286:LEU	N	6.23
1	7	158:PHE	C	159:LYS	N	5.66
1	r	134:ARG	C	135:LEU	N	5.51
1	E	135:LYS	C	136:GLU	N	4.66
1	5	365:ASP	C	366:CYS	N	4.59
1	r	41:THR	C	42:GLN	N	4.40
1	4	102:GLN	C	103:MET	N	3.84
1	B	1616:A	O3'	1617:C	P	3.73
1	h	78:PHE	C	79:GLY	N	3.34
1	6	209:GLU	C	210:GLU	N	3.29
1	6	79:GLY	C	80:GLU	N	3.19
1	5	392:ILE	C	393:LYS	N	3.18
1	7	185:LEU	C	186:ASP	N	3.16
1	P	114:HIS	C	115:LEU	N	3.16
1	5	141:ASP	C	142:ASP	N	3.14
1	6	282:SER	C	283:GLU	N	3.14
1	V	158:GLU	C	159:PHE	N	3.14
1	d	199:CYS	C	200:SER	N	3.14
1	d	252:LEU	C	253:THR	N	3.12
1	A	4748:2MA	O3'	4749:U	P	1.76

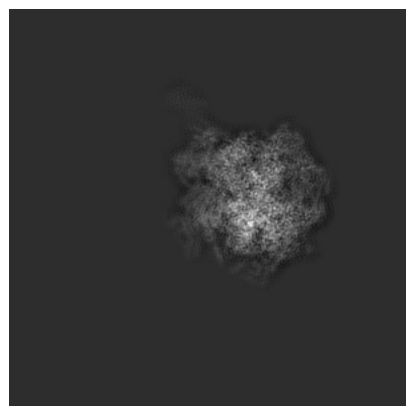
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4434. These allow visual inspection of the internal detail of the map and identification of artifacts.

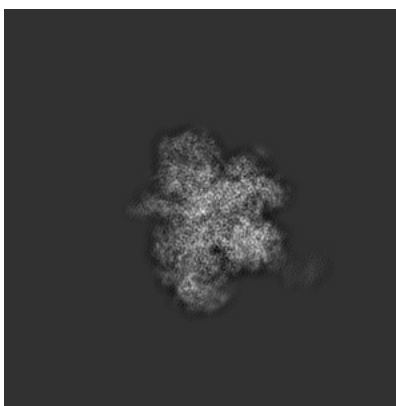
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

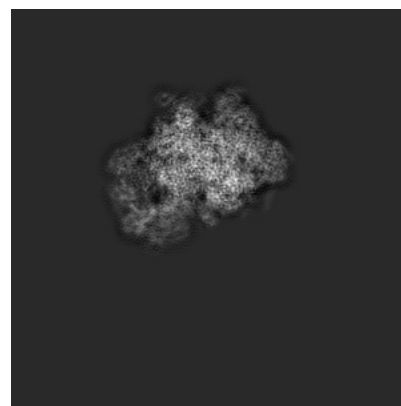
6.1.1 Primary map



X

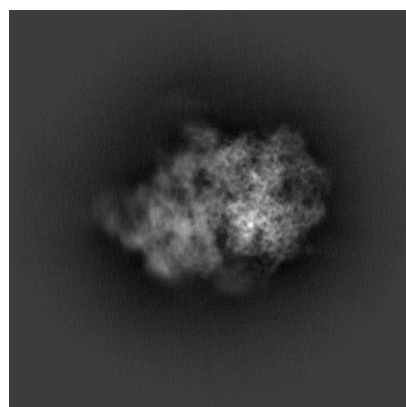


Y

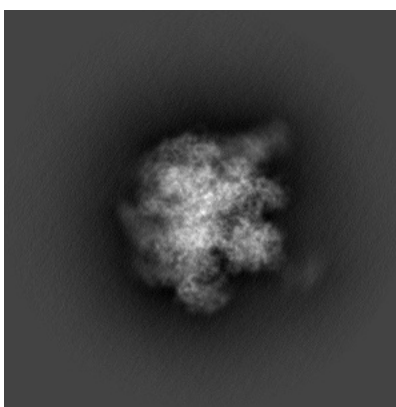


Z

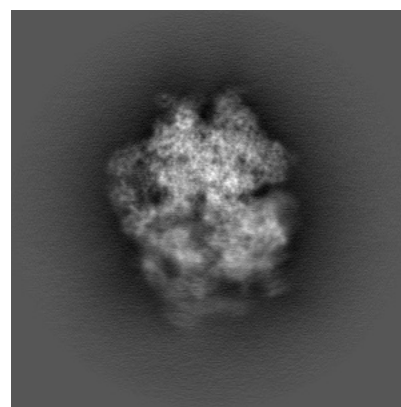
6.1.2 Raw map



X



Y

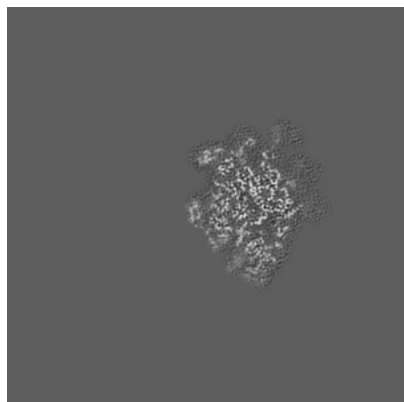


Z

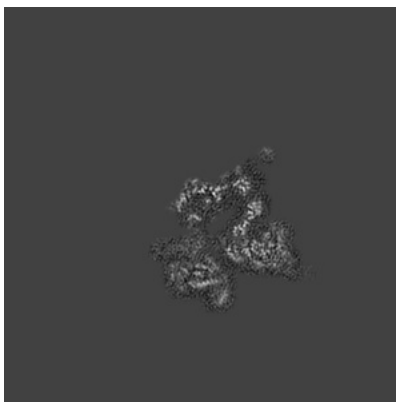
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

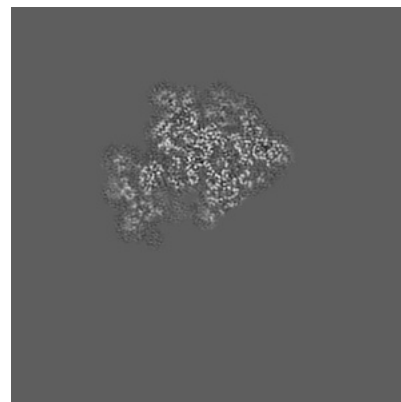
6.2.1 Primary map



X Index: 250

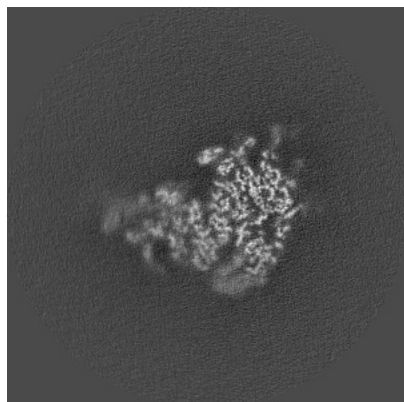


Y Index: 250

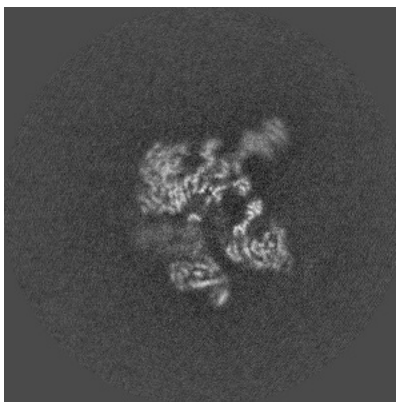


Z Index: 250

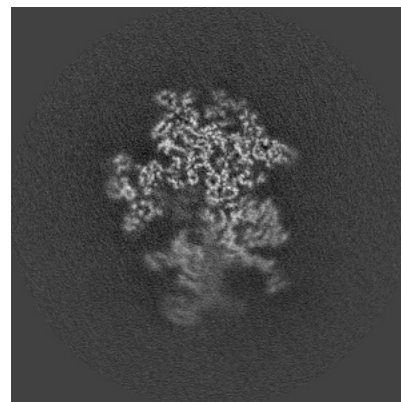
6.2.2 Raw map



X Index: 250



Y Index: 250

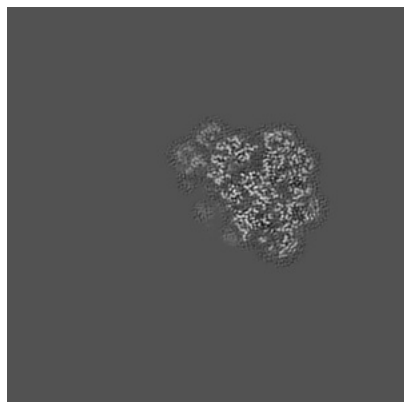


Z Index: 250

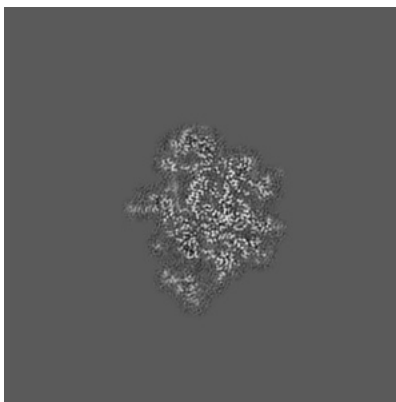
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

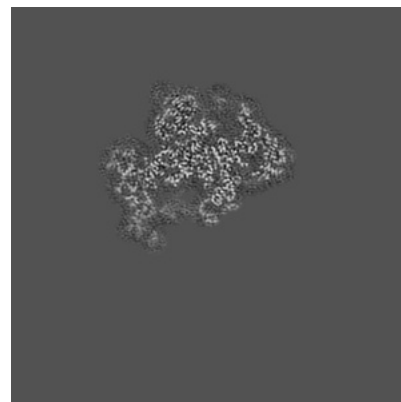
6.3.1 Primary map



X Index: 214

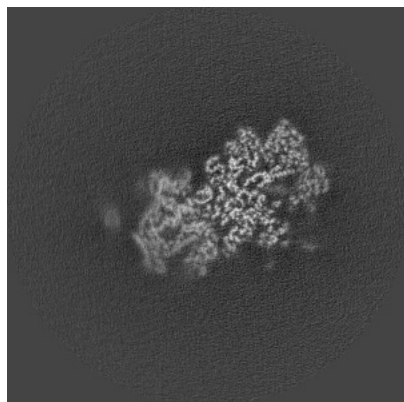


Y Index: 318

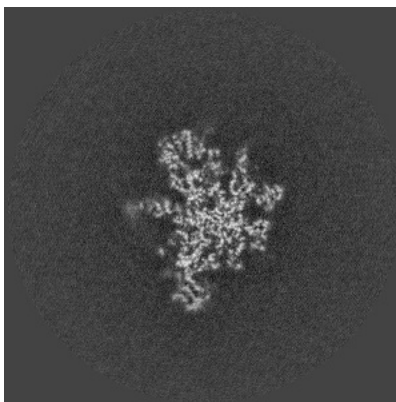


Z Index: 239

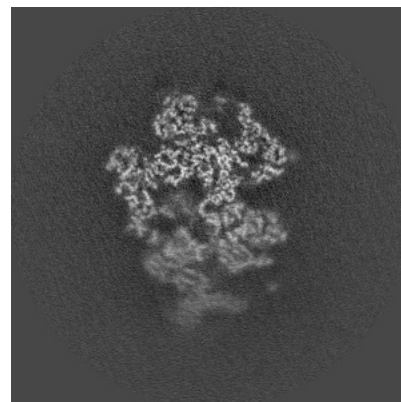
6.3.2 Raw map



X Index: 273



Y Index: 303

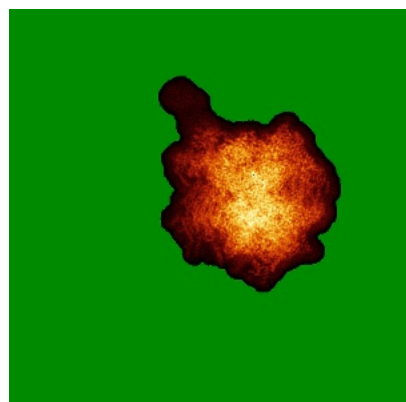


Z Index: 238

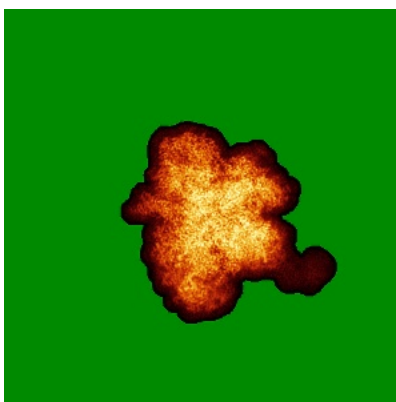
The images above show the largest variance slices of the map in three orthogonal directions.

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

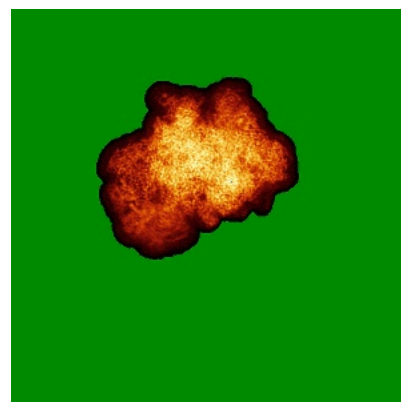
6.4.1 Primary map



X

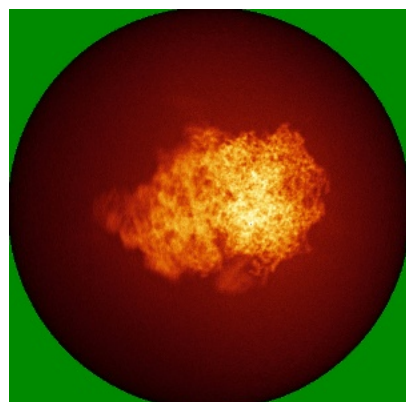


Y

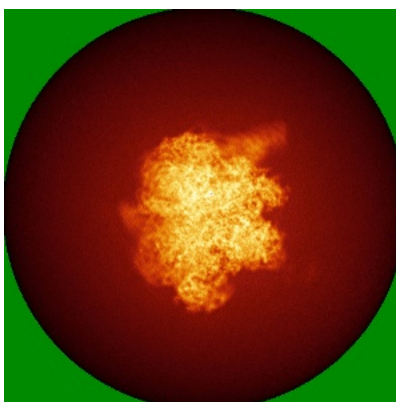


Z

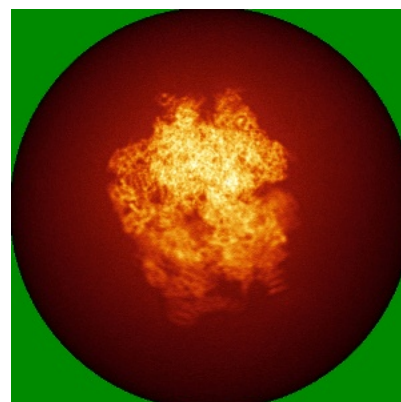
6.4.2 Raw map



X



Y

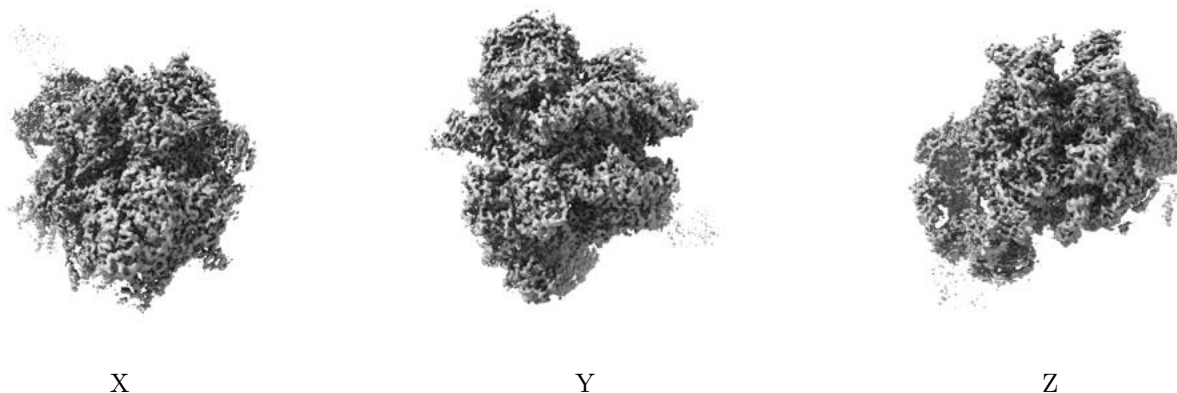


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

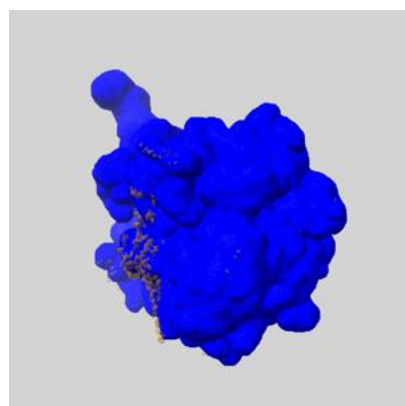
6.6 Mask visualisation [i](#)

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

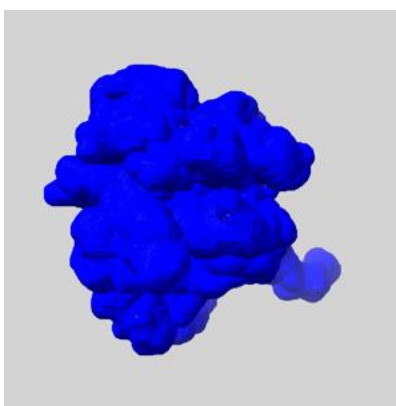
A mask typically either:

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

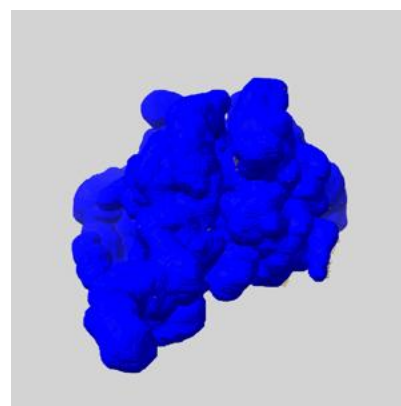
6.6.1 emd_4434_msk_1.map [i](#)



X



Y

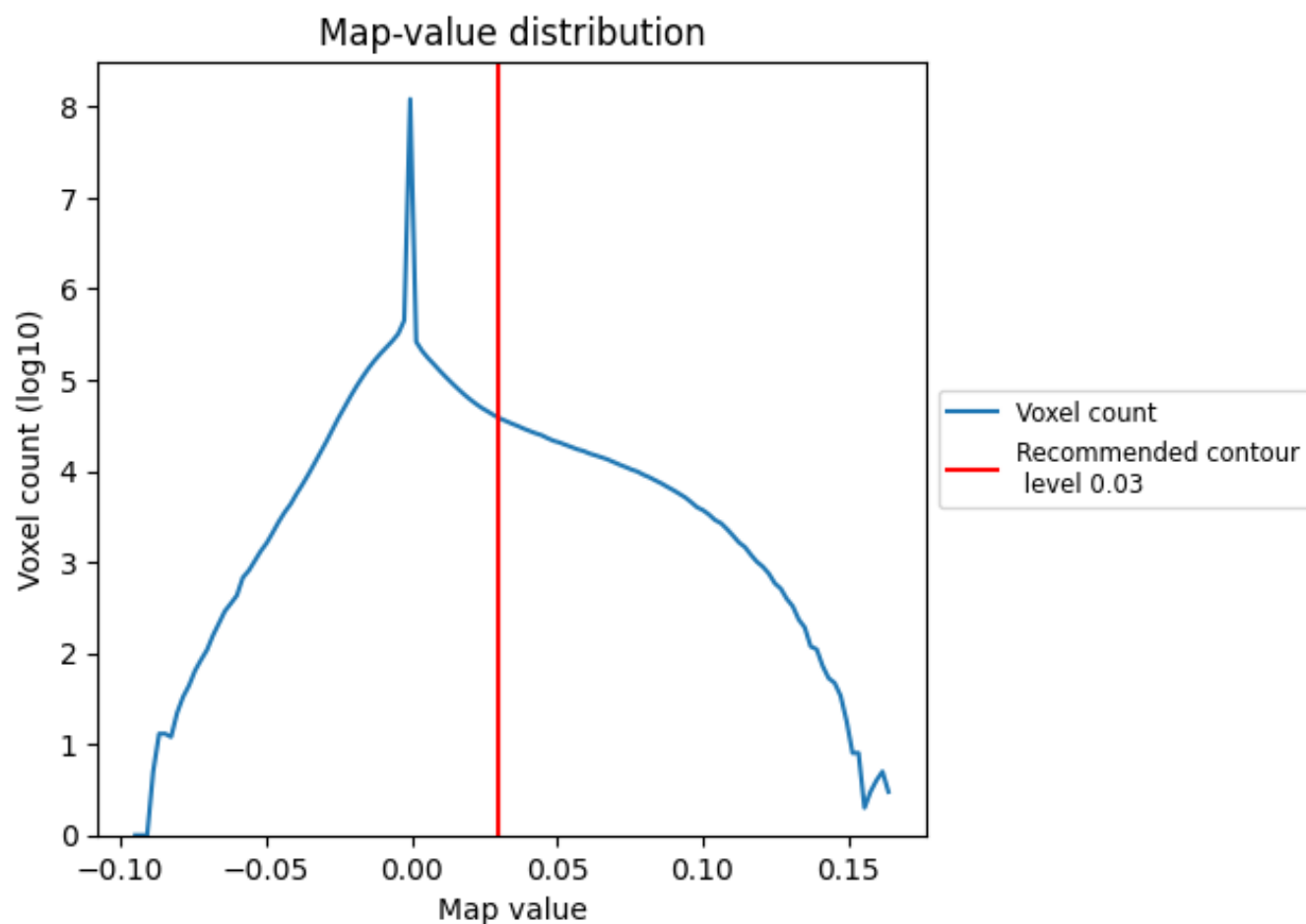


Z

7 Map analysis [i](#)

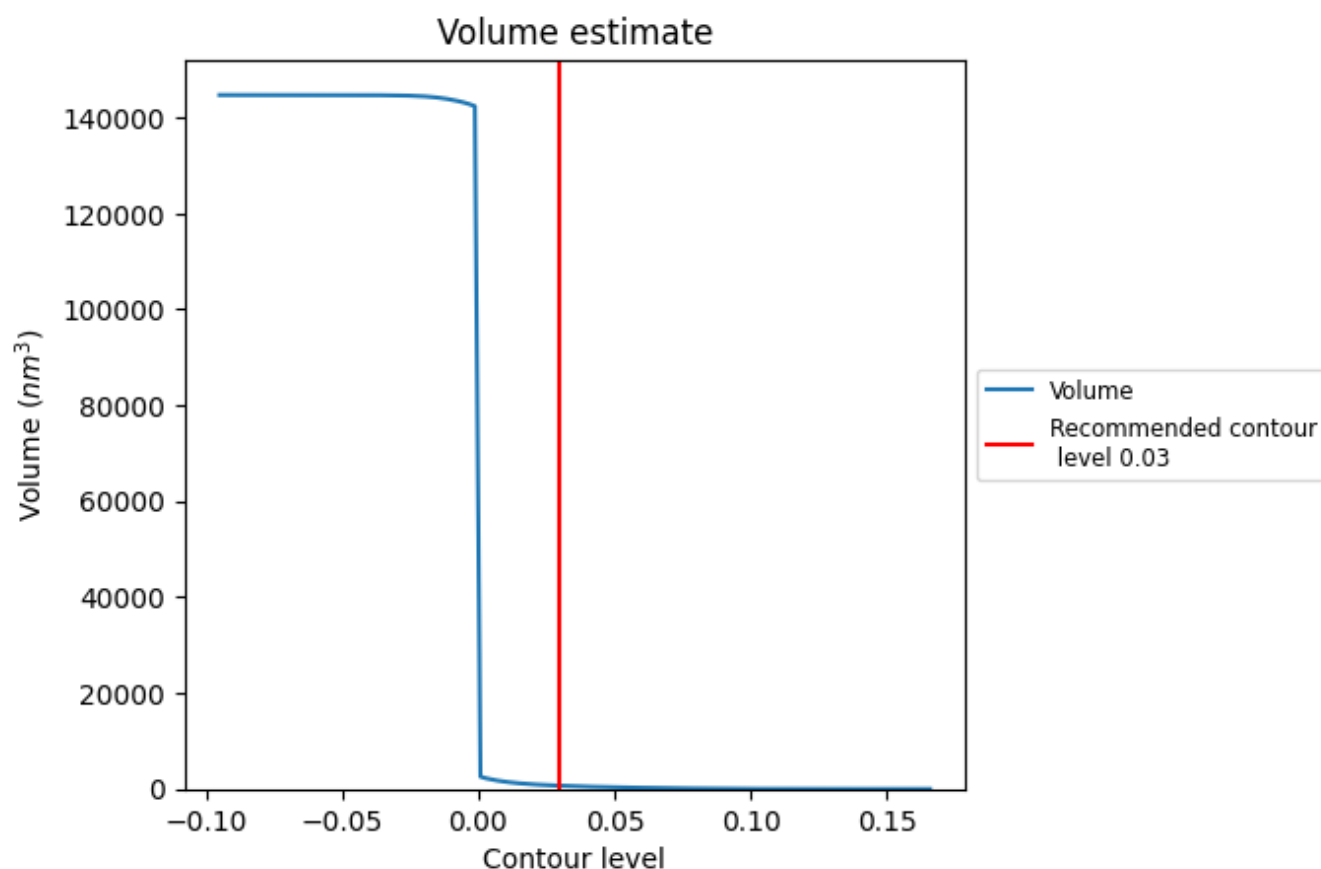
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

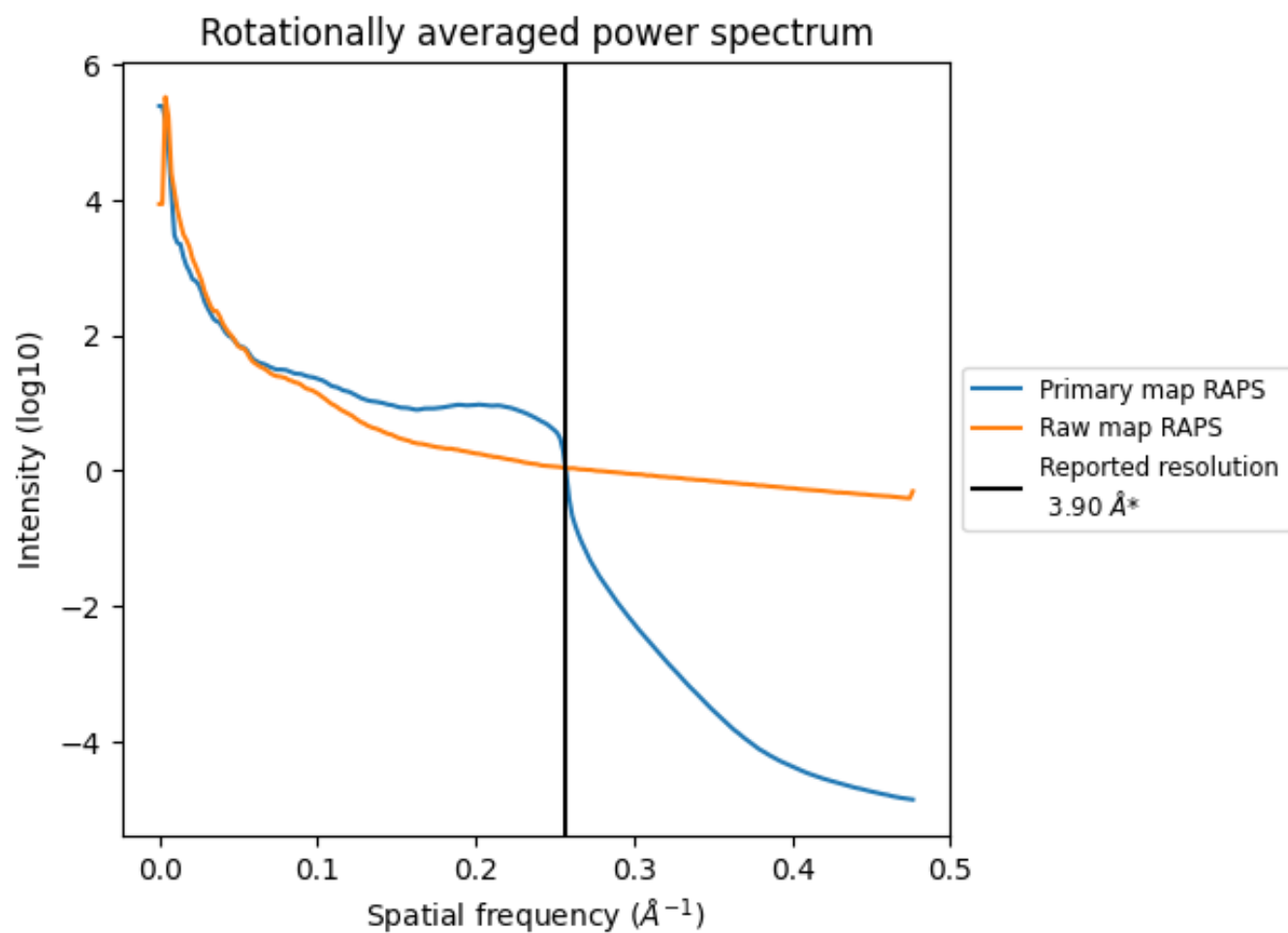
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 684 nm³; this corresponds to an approximate mass of 618 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 ⓘ

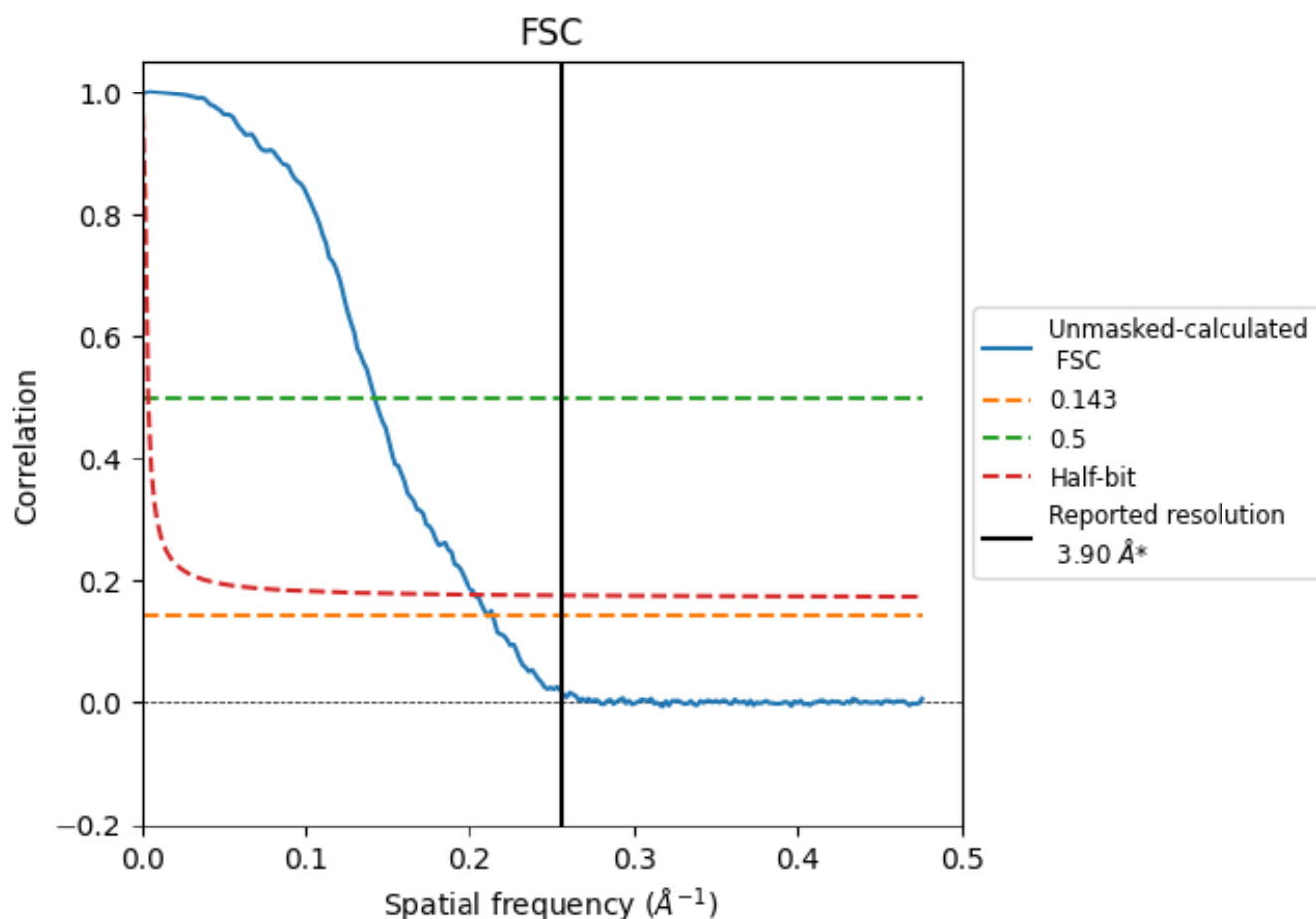


*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

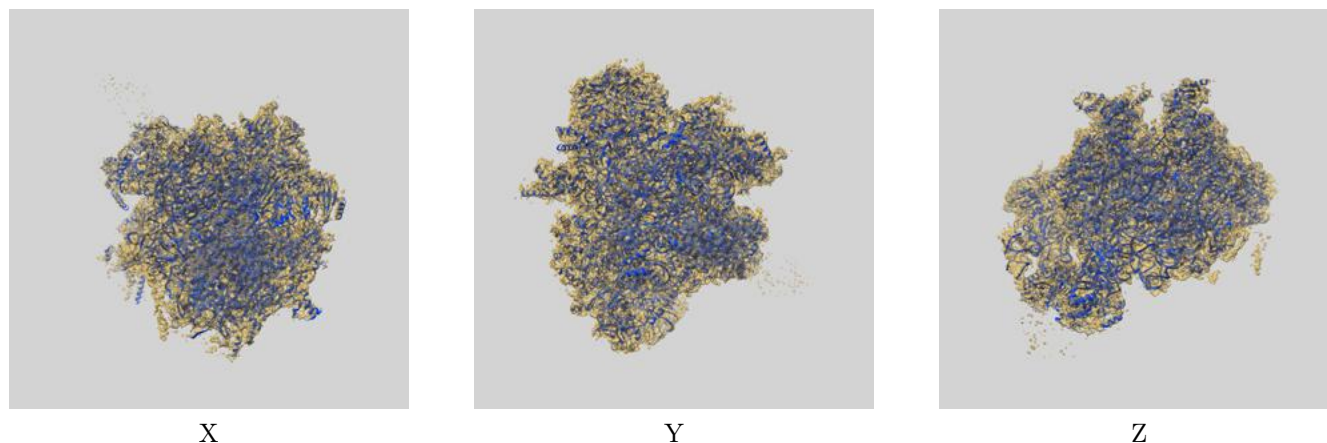
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.73	7.05	4.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.73 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

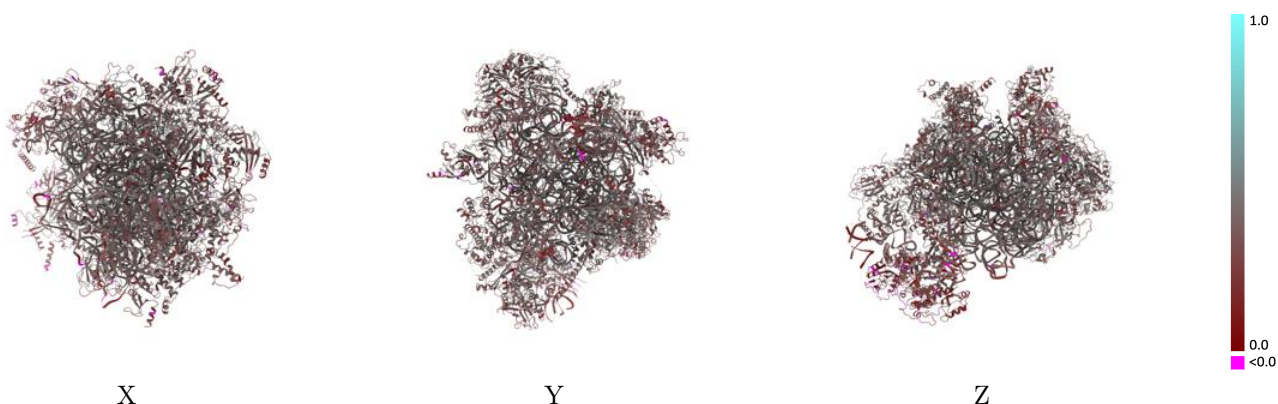
This section contains information regarding the fit between EMDB map EMD-4434 and PDB model 6I9R. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



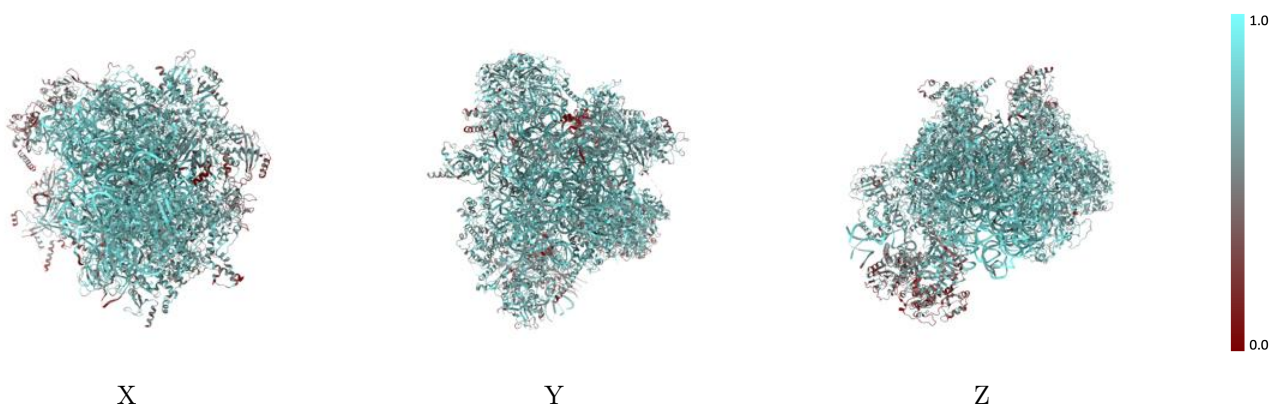
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



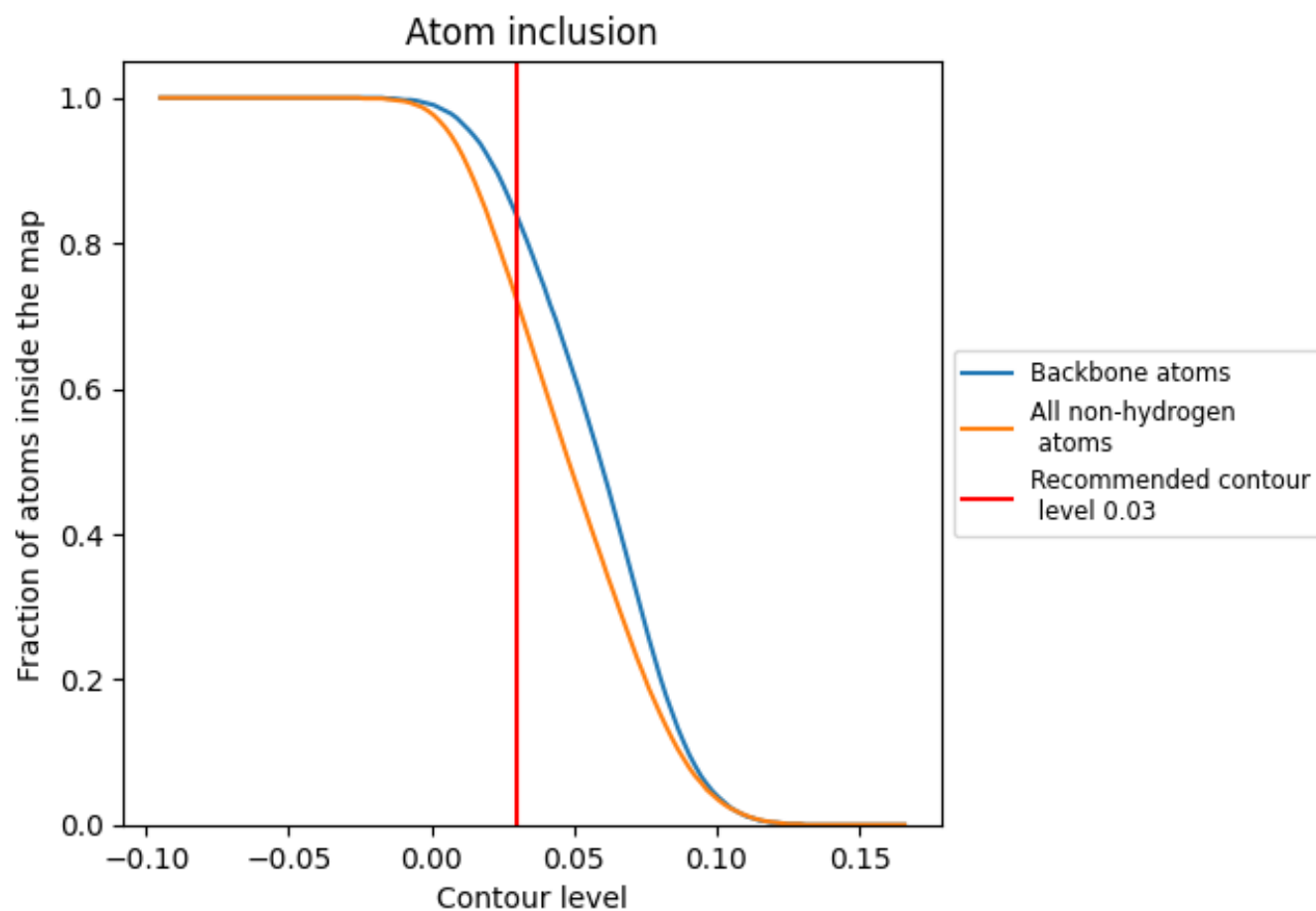
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7210	 0.3740
0	 0.7020	 0.3730
1	 0.6570	 0.3550
2	 0.7470	 0.3870
3	 0.7470	 0.4220
4	 0.7640	 0.4080
5	 0.7050	 0.3770
6	 0.6620	 0.3390
7	 0.6550	 0.3480
8	 0.5010	 0.2580
9	 0.6300	 0.3660
A	 0.8450	 0.4040
B	 0.7950	 0.2910
C	 0.5480	 0.3270
D	 0.7290	 0.4020
E	 0.7200	 0.4010
F	 0.7160	 0.3950
H	 0.6400	 0.3610
I	 0.4980	 0.2820
J	 0.3430	 0.2230
K	 0.7400	 0.4100
L	 0.7490	 0.4170
M	 0.6960	 0.3790
N	 0.7190	 0.4020
O	 0.7250	 0.3860
P	 0.6890	 0.3610
Q	 0.6980	 0.3710
R	 0.7240	 0.3970
S	 0.7150	 0.4010
T	 0.7130	 0.3980
U	 0.6680	 0.3800
V	 0.5210	 0.3460
W	 0.7470	 0.4280
X	 0.6680	 0.3760
Y	 0.7150	 0.3890



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Chain	Atom inclusion	Q-score
Z	 0.7410	 0.4020
a	 0.6840	 0.3550
b	 0.7310	 0.4010
c	 0.6900	 0.3650
d	 0.4820	 0.3210
e	 0.4350	 0.2040
f	 0.5830	 0.3060
g	 0.6920	 0.3670
h	 0.5320	 0.3390
i	 0.7210	 0.3890
j	 0.7100	 0.3910
k	 0.5220	 0.2910
l	 0.4150	 0.2450
m	 0.4640	 0.2120
o	 0.7420	 0.3940
p	 0.6330	 0.3460
q	 0.5710	 0.3440
r	 0.6800	 0.3460
s	 0.7230	 0.3850