



Full wwPDB EM Validation Report ⓘ

Jul 31, 2025 – 04:51 PM EDT

PDB ID : 9E9C / pdb_00009e9c
EMDB ID : EMD-47791
Title : Mouse mitoribosome large subunit assembly intermediate bound to NSUN4, METRF4, GTPBP7, GTPBP10 and the MALSU1-L0R8F8-mt-ACP complex (without uL16m), State B1 (SAMC knock-out)
Authors : Singh, V.; Rorbach, J.; Freyer, C.; Amunts, A.; Wredenber, A.
Deposited on : 2024-11-08
Resolution : 3.62 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:

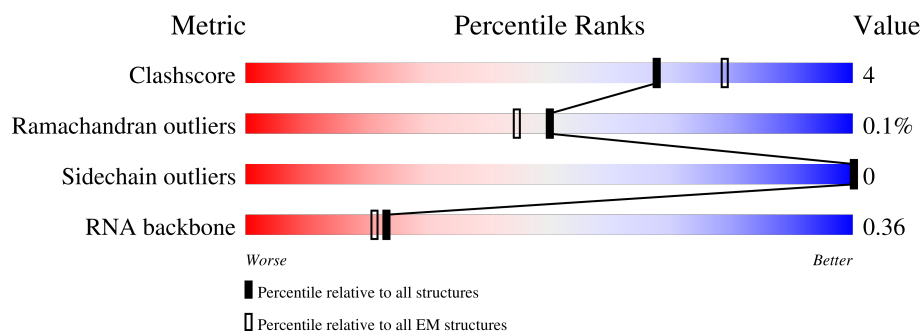
EMDB validation analysis : 0.0.1.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

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 3.62 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	1584	
2	B	68	
3	D	306	
4	E	348	
5	F	294	
6	H	265	
7	I	262	

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Mol	Chain	Length	Quality of chain
8	J	192	
9	K	178	
10	L	145	
11	M	295	
12	O	176	
13	P	180	
14	Q	292	
15	R	149	
16	S	209	
17	T	206	
18	U	146	
19	V	216	
20	W	148	
21	X	257	
22	Y	252	
23	Z	160	
24	x	381	
25	0	187	
26	1	65	
27	2	92	
28	3	188	
29	4	101	
30	6	380	
31	7	336	
32	b	159	

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Mol	Chain	Length	Quality of chain
33	c	308	
34	d	306	
35	e	283	
36	f	211	
37	g	166	
38	h	159	
39	i	128	
40	j	121	
41	k	118	
42	o	102	
43	p	206	
44	q	222	
45	r	196	
46	s	442	
47	u	228	
48	v	70	
49	w	156	
50	5	423	
51	8	206	
52	9	135	
53	a	142	
54	m	127	
55	z	326	
56	l	135	
57	y	346	

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Mol	Chain	Length	Quality of chain
58	t	366	<div><div></div><div>64%</div><div></div><div>73%</div><div></div><div>14%</div><div></div><div>12%</div></div>

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 198874 atoms, of which 92086 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 RNA chain called RNA (1428-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1427	Total	C	H	N	O	P	0	0
			45657	13623	15322	5466	9819	1427		

- Molecule 2 is a RNA chain called RNA (56-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	62	Total	C	H	N	O	P	0	0
			1993	595	667	244	425	62		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2m.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	227	Total	C	H	N	O	S	0	0
			3598	1105	1830	349	305	9		

- Molecule 4 is a protein called Large ribosomal subunit protein uL3m.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	308	Total	C	H	N	O	S	0	0
			4901	1577	2442	432	442	8		

- Molecule 5 is a protein called Large ribosomal subunit protein uL4m.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	250	Total	C	H	N	O	S	0	0
			4029	1286	2024	364	349	6		

- Molecule 6 is a protein called Large ribosomal subunit protein bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	95	Total	C	H	N	O	0	0
			1593	492	814	150	137		

- Molecule 7 is a protein called Large ribosomal subunit protein uL10m.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	139	Total	C	H	N	O	S	0	0
			2325	728	1205	202	184	6		

- Molecule 8 is a protein called Large ribosomal subunit protein uL11m.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	104	Total	C	H	N	O	S	0	0
			1598	500	823	135	138	2		

- Molecule 9 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	177	Total	C	H	N	O	S	0	0
			2893	927	1444	262	253	7		

- Molecule 10 is a protein called Large ribosomal subunit protein uL14m.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	115	Total	C	H	N	O	S	0	0
			1837	560	944	174	155	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL15m.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	M	287	Total	C	H	N	O	S	0	0
			4691	1475	2376	428	406	6		

- Molecule 12 is a protein called Large ribosomal subunit protein bL17m.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	O	153	Total	C	H	N	O	S	0	0
			2541	795	1282	240	219	5		

- Molecule 13 is a protein called Large ribosomal subunit protein uL18m.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	P	141	Total	C	H	N	O	S	0	0
			2302	725	1148	221	203	5		

- Molecule 14 is a protein called Large ribosomal subunit protein bL19m.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	Q	217	Total	C	H	N	O	S	0	0
			3612	1150	1822	309	322	9		

- Molecule 15 is a protein called Large ribosomal subunit protein bL20m.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	R	140	Total	C	H	N	O	S	0	0
			2385	738	1224	233	187	3		

- Molecule 16 is a protein called Large ribosomal subunit protein bL21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	S	159	Total	C	H	N	O	S	0	0
			2673	840	1372	233	226	2		

- Molecule 17 is a protein called Large ribosomal subunit protein uL22m.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	T	166	Total	C	H	N	O	S	0	0
			2771	871	1402	256	234	8		

- Molecule 18 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	U	127	Total	C	H	N	O	S	0	0
			2109	675	1057	196	178	3		

- Molecule 19 is a protein called Large ribosomal subunit protein uL24m.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	V	201	Total	C	H	N	O	S	0	0
			3295	1043	1643	305	298	6		

- Molecule 20 is a protein called Large ribosomal subunit protein bL27m.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	W	100	Total	C	H	N	O	S	0	0
			1602	515	808	141	135	3		

- Molecule 21 is a protein called Large ribosomal subunit protein bL28m.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	X	242	Total	C	H	N	O	S	0	0
			4072	1304	2051	358	355	4		

- Molecule 22 is a protein called Large ribosomal subunit protein uL29m.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	Y	176	Total	C	H	N	O	S	0	0
			3076	973	1553	290	255	5		

- Molecule 23 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Z	112	Total	C	H	N	O	S	0	0
			1868	583	957	168	157	3		

- Molecule 24 is a protein called 5-cytosine rRNA methyltransferase NSUN4.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	x	325	Total	C	H	N	O	S	1	0
			5110	1626	2546	448	473	17		

- Molecule 25 is a protein called Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	0	108	Total	C	H	N	O	S	0	0
			1789	546	908	174	155	6		

- Molecule 26 is a protein called Large ribosomal subunit protein bL33m.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	1	52	Total	C	H	N	O		0	0
			900	278	472	80	70			

- Molecule 27 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	2	46	Total	C	H	N	O	S	0	0
			787	235	407	86	58	1		

- Molecule 28 is a protein called Large ribosomal subunit protein bL35m.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	3	95	Total	C	H	N	O	S	0	0
			1695	528	872	164	127	4		

- Molecule 29 is a protein called Large ribosomal subunit protein bL36m.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	4	37	Total	C	H	N	O	S	0	0
			676	206	354	68	45	3		

- Molecule 30 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	6	312	Total	C	H	N	O	S	0	0
			5202	1713	2536	483	464	6		

- Molecule 31 is a protein called Large ribosomal subunit protein mL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	7	292	Total	C	H	N	O	S	0	0
			4757	1517	2378	409	438	15		

- Molecule 32 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	b	148	Total	C	H	N	O	S	0	0
			2376	731	1195	234	214	2		

- Molecule 33 is a protein called Large ribosomal subunit protein mL44.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	c	279	Total	C	H	N	O	S	0	0
			4502	1440	2256	389	409	8		

- Molecule 34 is a protein called Large ribosomal subunit protein mL45.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	d	246	Total	C	H	N	O	S	0	0
			4036	1303	2011	358	354	10		

- Molecule 35 is a protein called Large ribosomal subunit protein mL46.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	e	193	Total	C	H	N	O	S	0	0
			3174	1013	1598	278	279	6		

- Molecule 36 is a protein called Large ribosomal subunit protein mL48.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	f	101	Total	C	H	N	O	S	0	0
			1635	521	817	138	155	4		

- Molecule 37 is a protein called Large ribosomal subunit protein mL49.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	g	132	Total	C	H	N	O	S	0	0
			2184	709	1094	187	192	2		

- Molecule 38 is a protein called Large ribosomal subunit protein mL50.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	h	110	Total	C	H	N	O	S	0	0
			1739	552	867	156	160	4		

- Molecule 39 is a protein called Large ribosomal subunit protein mL51.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	i	97	Total	C	H	N	O	S	0	0
			1685	540	854	161	128	2		

- Molecule 40 is a protein called Large ribosomal subunit protein mL52.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	j	93	Total	C	H	N	O	S	0	0
			1512	467	768	145	130	2		

- Molecule 41 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	k	80	Total	C	H	N	O	S	0	0
			1268	393	639	114	117	5		

- Molecule 42 is a protein called Large ribosomal subunit protein mL63.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	o	78	Total	C	H	N	O	S	0	0
			1263	402	623	118	116	4		

- Molecule 43 is a protein called Large ribosomal subunit protein mL62.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	p	140	Total	C	H	N	O	S	0	0
			2324	721	1174	213	212	4		

- Molecule 44 is a protein called Large ribosomal subunit protein mL64.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	q	135	Total	C	H	N	O	S	0	0
			2253	703	1123	223	199	5		

- Molecule 45 is a protein called Large ribosomal subunit protein mL66.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	r	157	Total	C	H	N	O	S	0	0
			2604	812	1329	242	210	11		

- Molecule 46 is a protein called Large ribosomal subunit protein mL65.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	s	377	Total	C	H	N	O	S	0	0
			6103	1938	3058	555	540	12		

- Molecule 47 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	u	129	Total	C	H	N	O	S	0	0
			2105	679	1048	174	195	9		

- Molecule 48 is a protein called Predicted gene, 55359.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	v	69	Total	C	H	N	O	S	0	0
			1189	374	603	112	99	1		

- Molecule 49 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	w	79	Total	C	H	N	O	S	0	0
			1277	410	640	95	127	5		

- Molecule 50 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	5	394	Total	C	H	N	O	S	0	0
			6468	2081	3243	564	571	9		

- Molecule 51 is a protein called Large ribosomal subunit protein mL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	8	70	Total	C	H	N	O	S	0	0
			1163	368	574	102	117	2		

- Molecule 52 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	9	122	Total	C	H	N	O	S	0	0
			1973	635	990	167	179	2		

- Molecule 53 is a protein called Large ribosomal subunit protein mL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	a	103	Total	C	H	N	O	S	0	0
			1703	542	843	156	159	3		

- Molecule 54 is a protein called Large ribosomal subunit protein mL55.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	m	45	Total	C	H	N	O	S	0	0
			769	233	395	77	61	3		

- Molecule 55 is a protein called Mitochondrial ribosome-associated GTPase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	z	311	Total	C	H	N	O	S	0	0
			5002	1562	2547	444	433	16		

- Molecule 56 is a protein called Large ribosomal subunit protein mL54.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	l	64	Total	C	H	N	O	S	0	0
			1086	346	542	101	96	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
57	y	237	Total	C	H	N	O	S	0	0
			3938	1238	1995	345	351	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
58	t	321	Total	C	H	N	O	S	0	0
			5015	1569	2551	431	455	9		

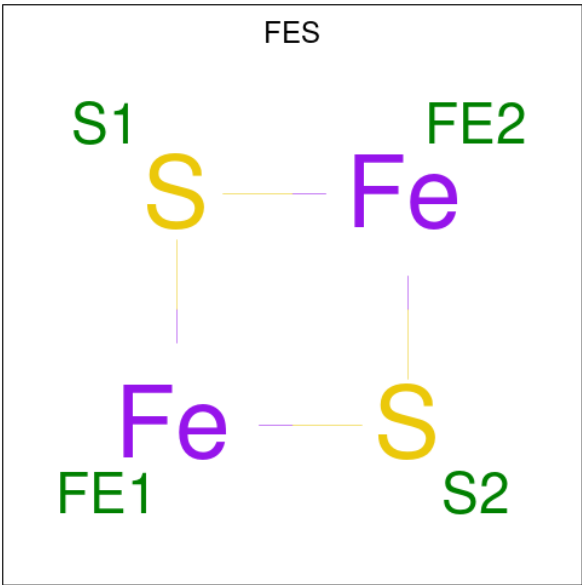
- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	A	92	Total	Mg	0
			92	92	
59	E	1	Total	Mg	0
			1	1	
59	M	1	Total	Mg	0
			1	1	
59	O	1	Total	Mg	0
			1	1	

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

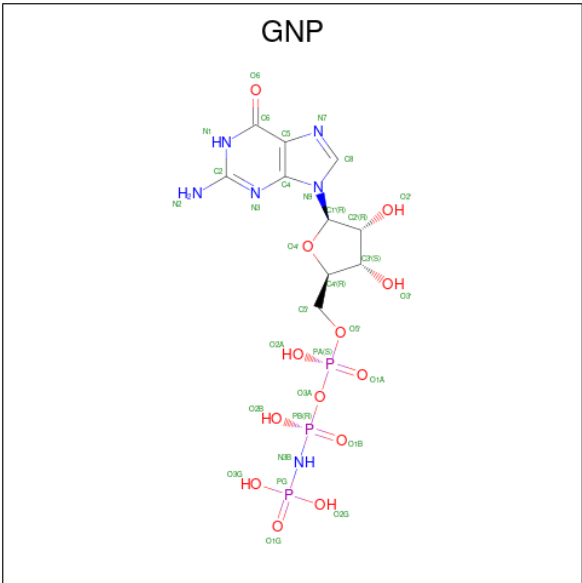
Mol	Chain	Residues	Atoms		AltConf
60	0	1	Total	Zn	0
			1	1	
60	4	1	Total	Zn	0
			1	1	

- Molecule 61 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
61	r	1	Total	Fe	S	0
			4	2	2	

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

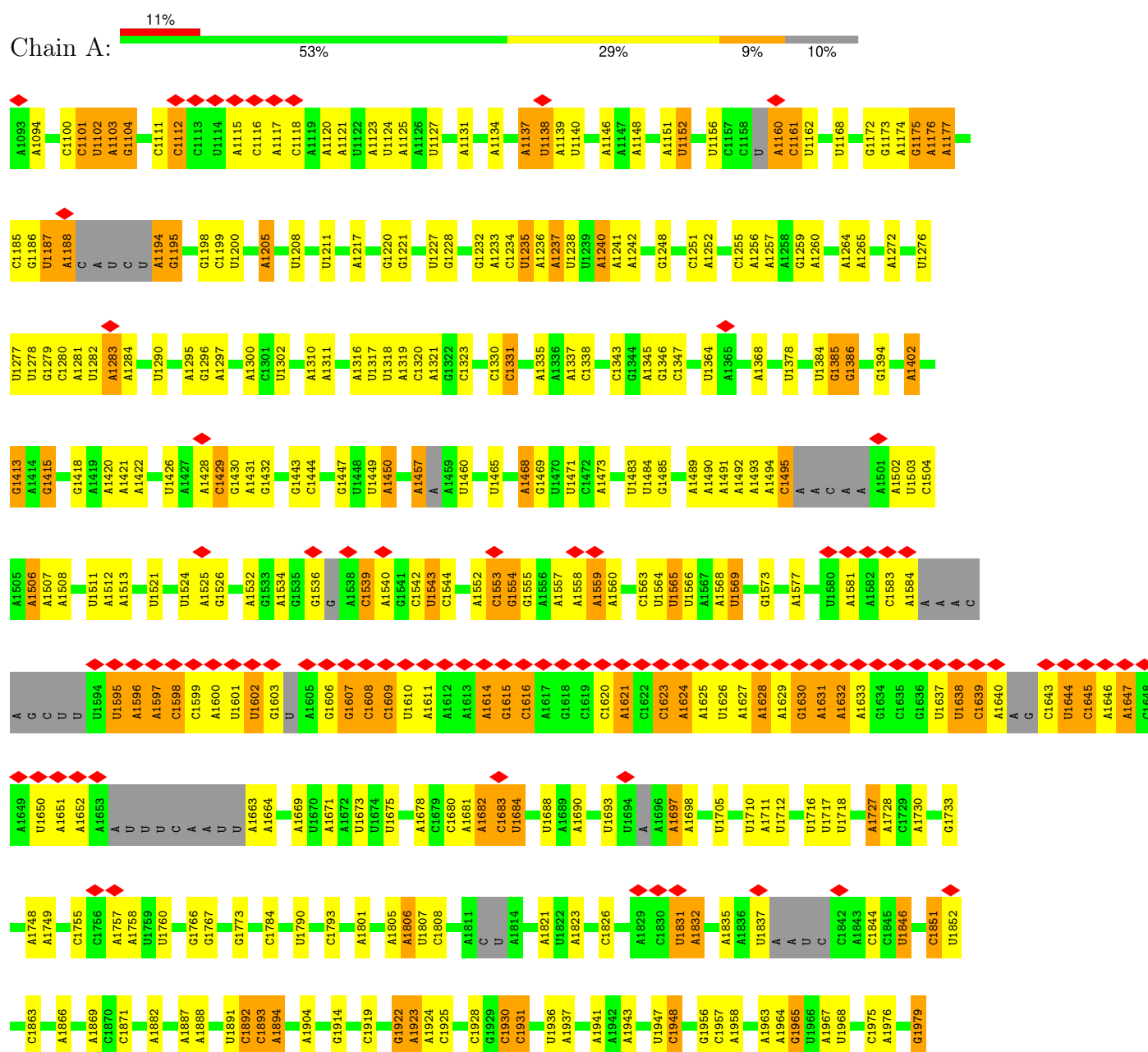


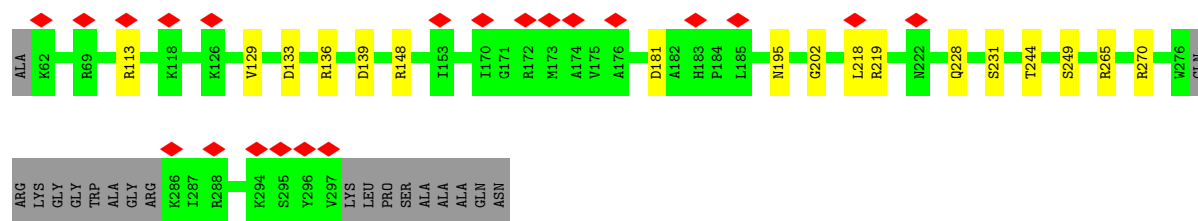
Mol	Chain	Residues	Atoms						AltConf
62	z	1	Total	C	H	N	O	P	0
			45	10	13	6	13	3	
62	t	1	Total	C	H	N	O	P	0
			45	10	13	6	13	3	

3 Residue-property plots

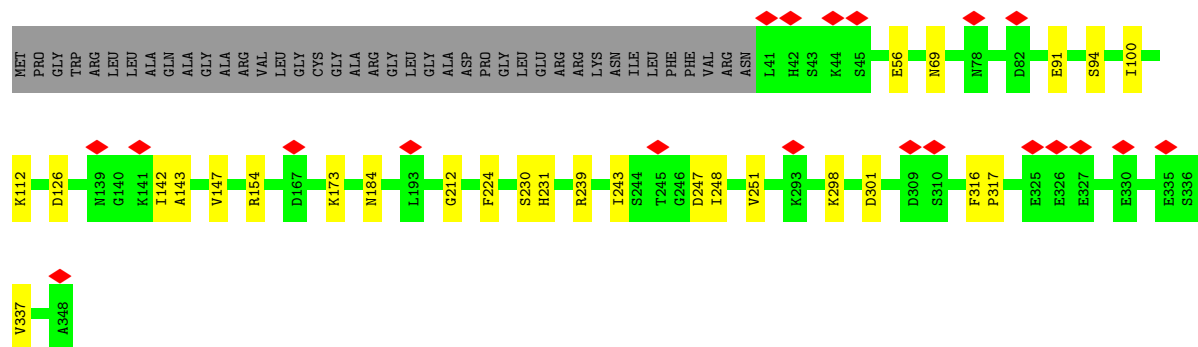
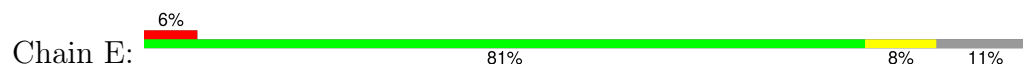
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: RNA (1428-MER)

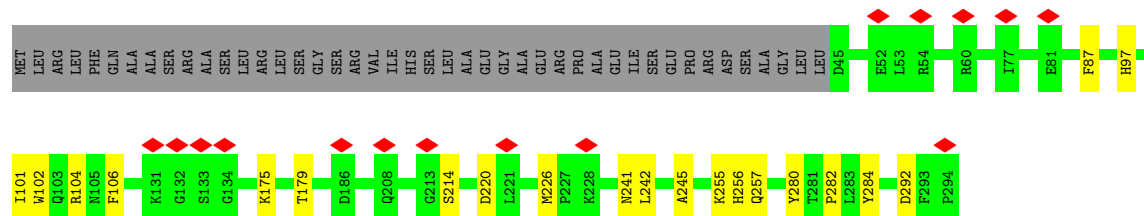
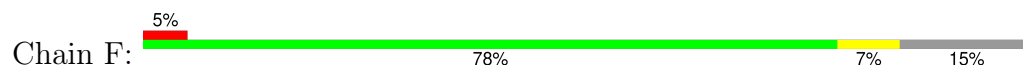




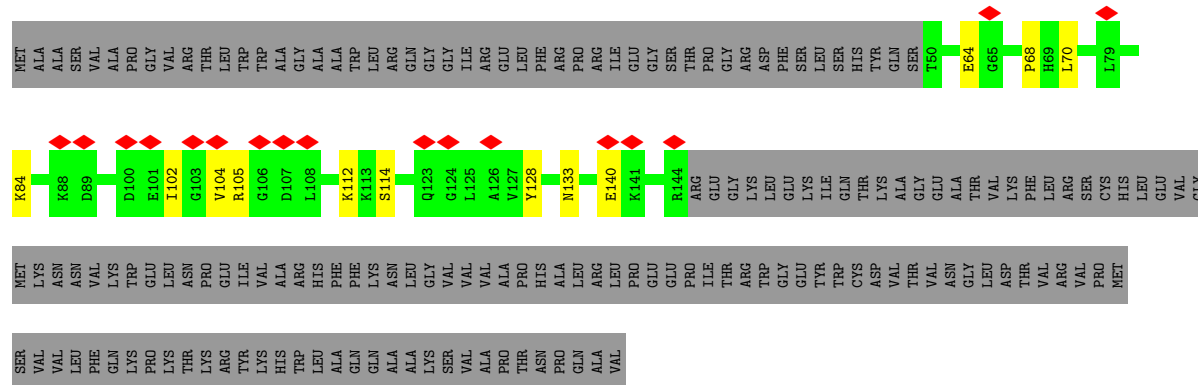
• Molecule 4: Large ribosomal subunit protein uL3m



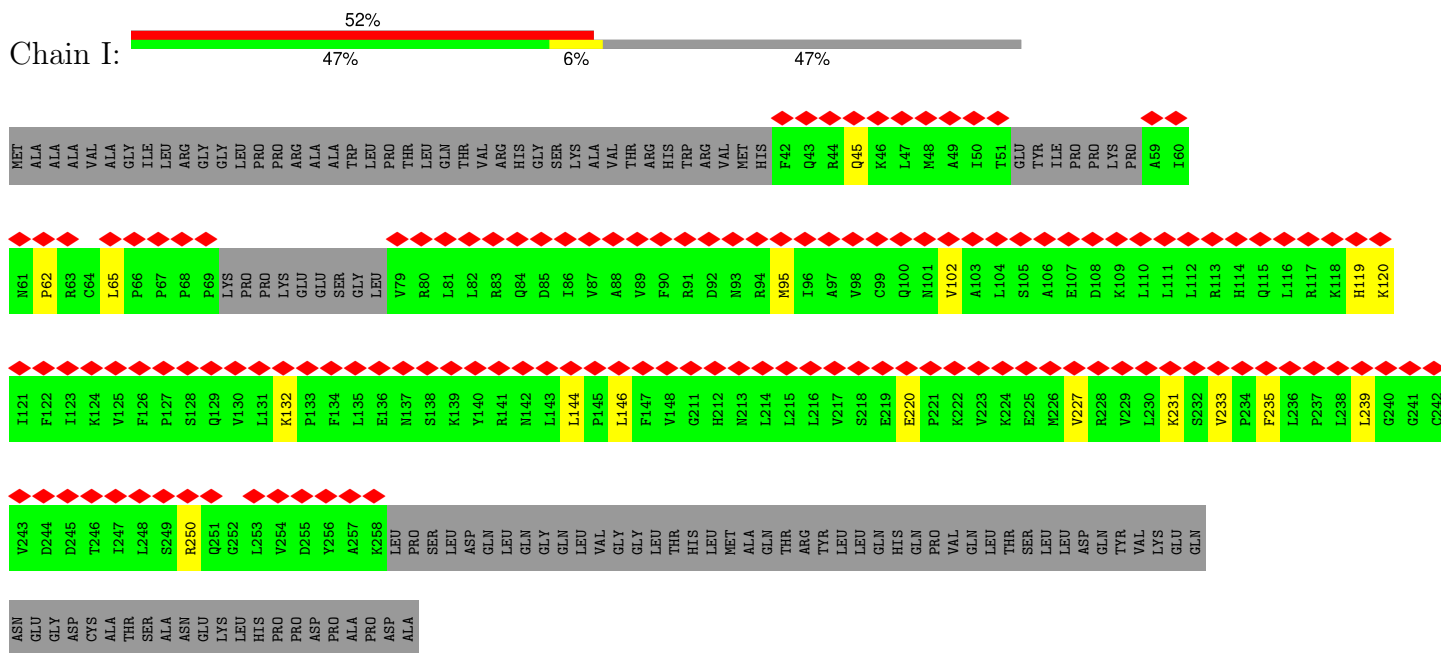
• Molecule 5: Large ribosomal subunit protein uL4m



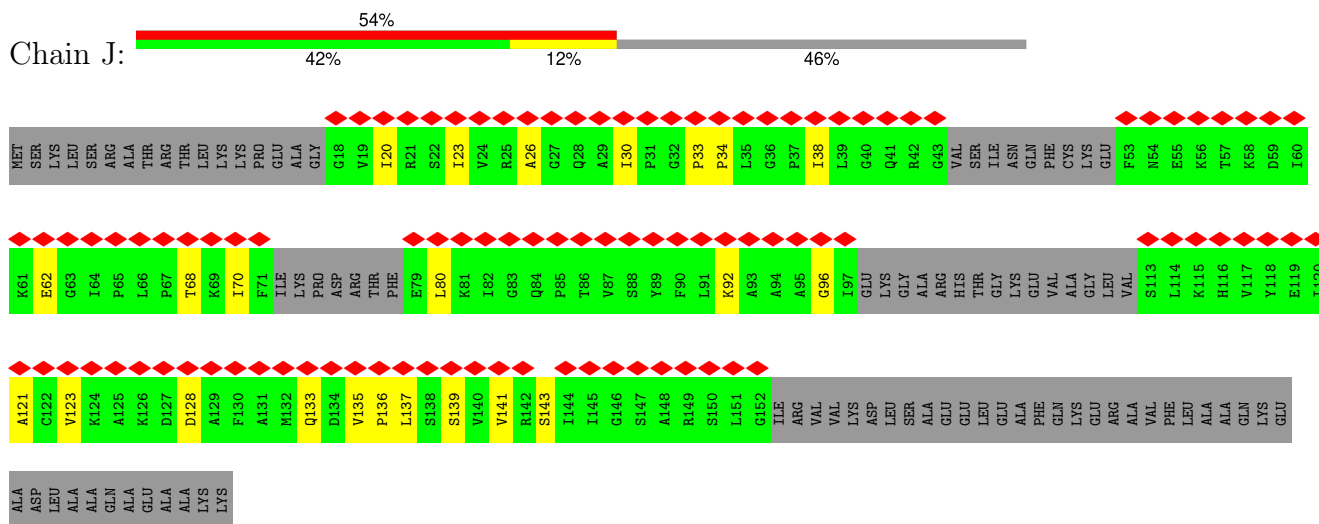
• Molecule 6: Large ribosomal subunit protein bL9m



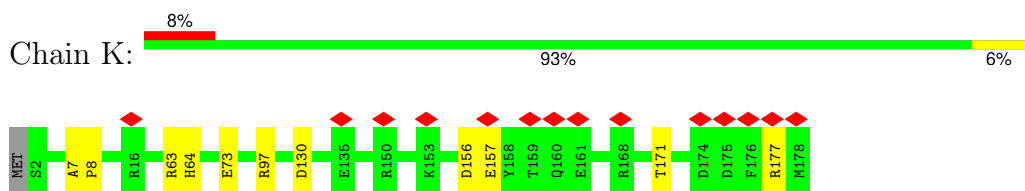
• Molecule 7: Large ribosomal subunit protein uL10m



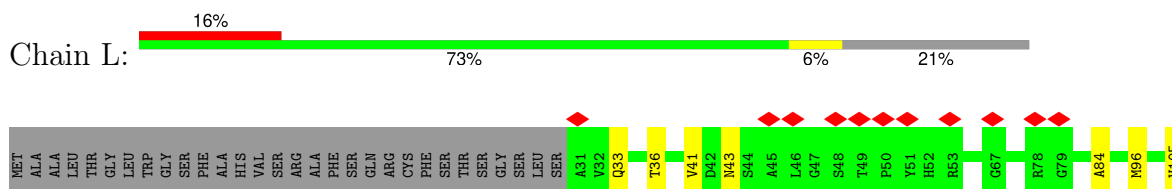
- Molecule 8: Large ribosomal subunit protein uL11m

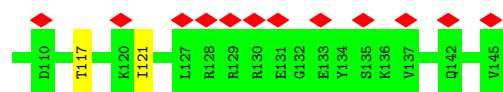


- Molecule 9: Large ribosomal subunit protein uL13m

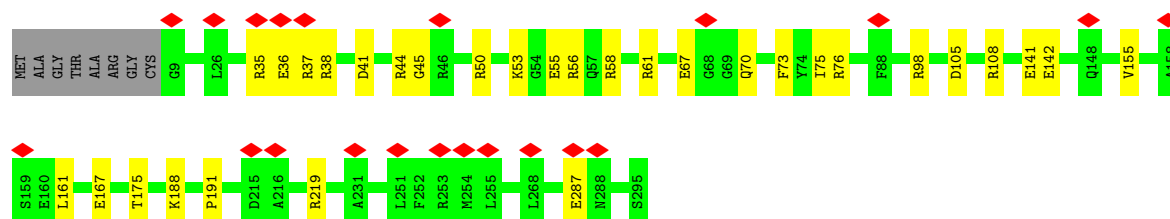
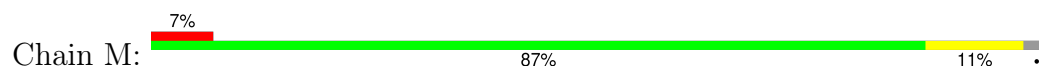


- Molecule 10: Large ribosomal subunit protein uL14m

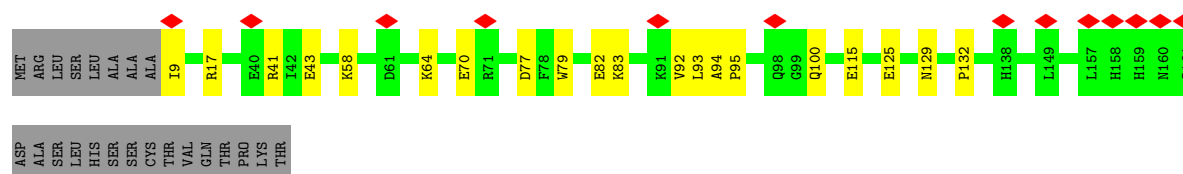
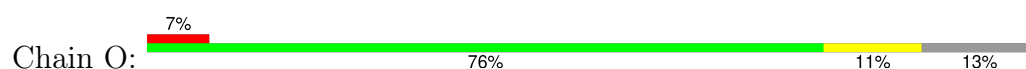




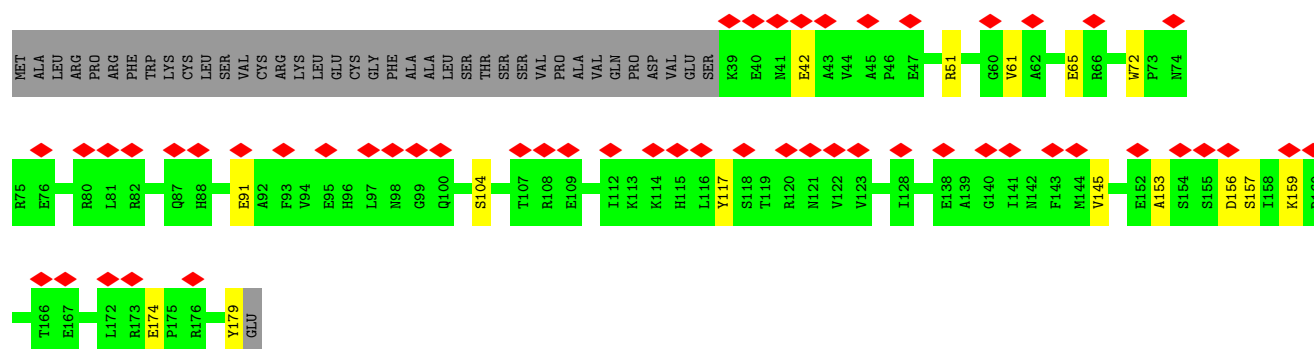
- Molecule 11: Large ribosomal subunit protein uL15m



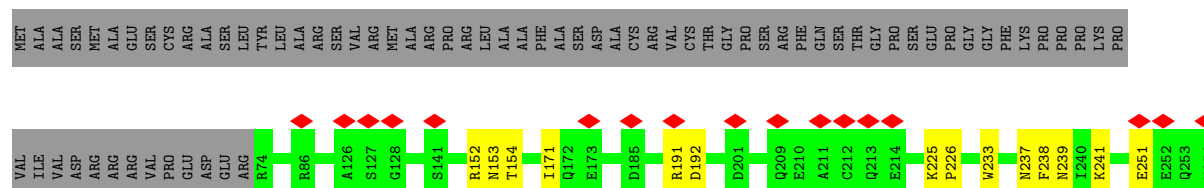
- Molecule 12: Large ribosomal subunit protein bL17m

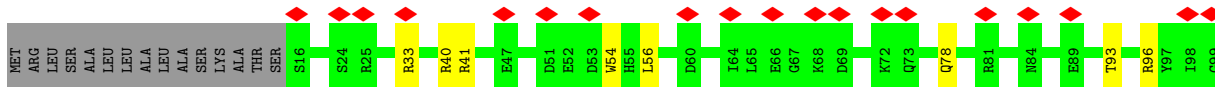


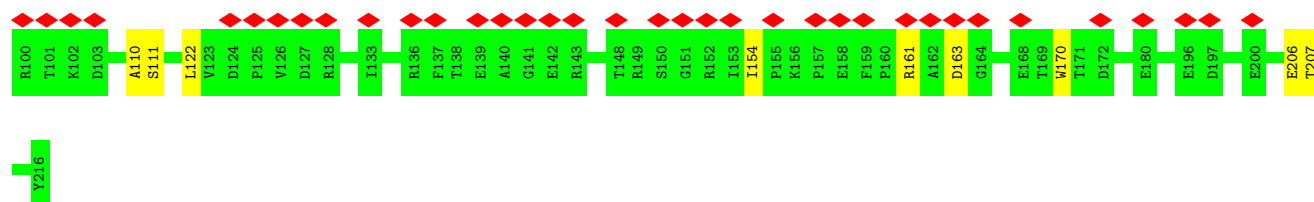
- Molecule 13: Large ribosomal subunit protein uL18m



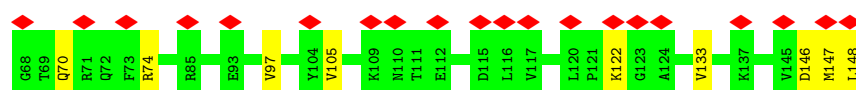
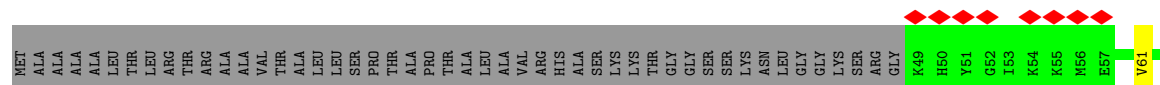
- Molecule 14: Large ribosomal subunit protein bL19m



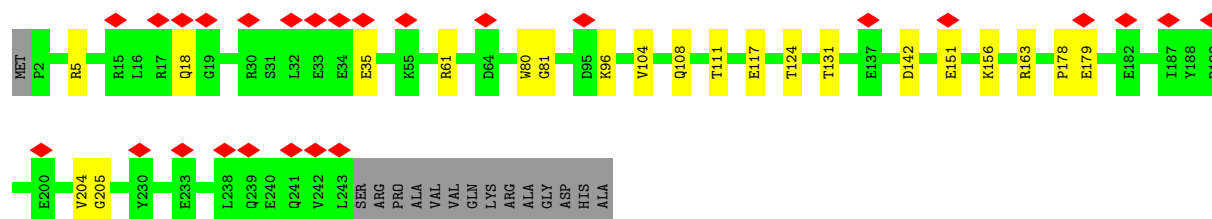
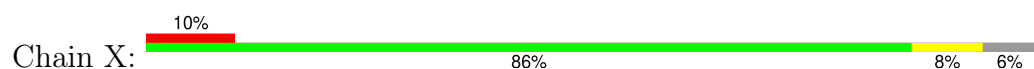




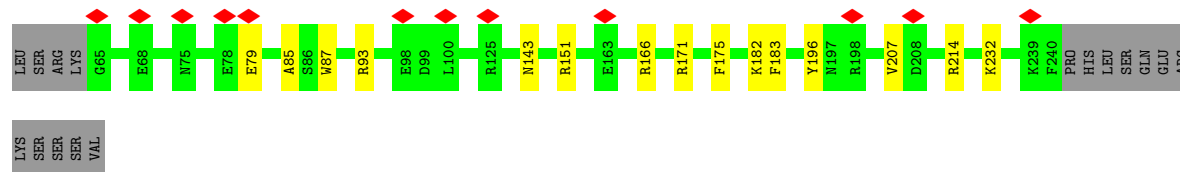
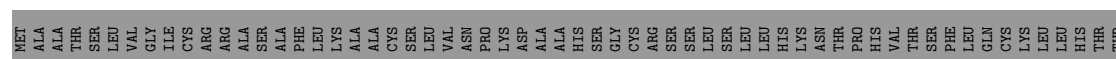
- Molecule 20: Large ribosomal subunit protein bL27m



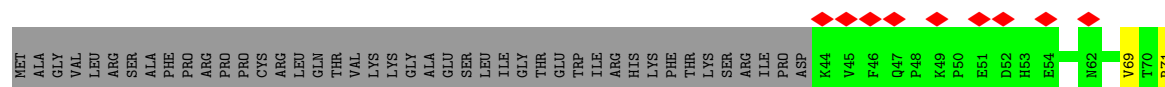
- Molecule 21: Large ribosomal subunit protein bL28m

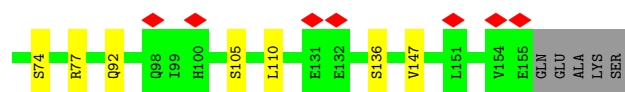


- Molecule 22: Large ribosomal subunit protein uL29m

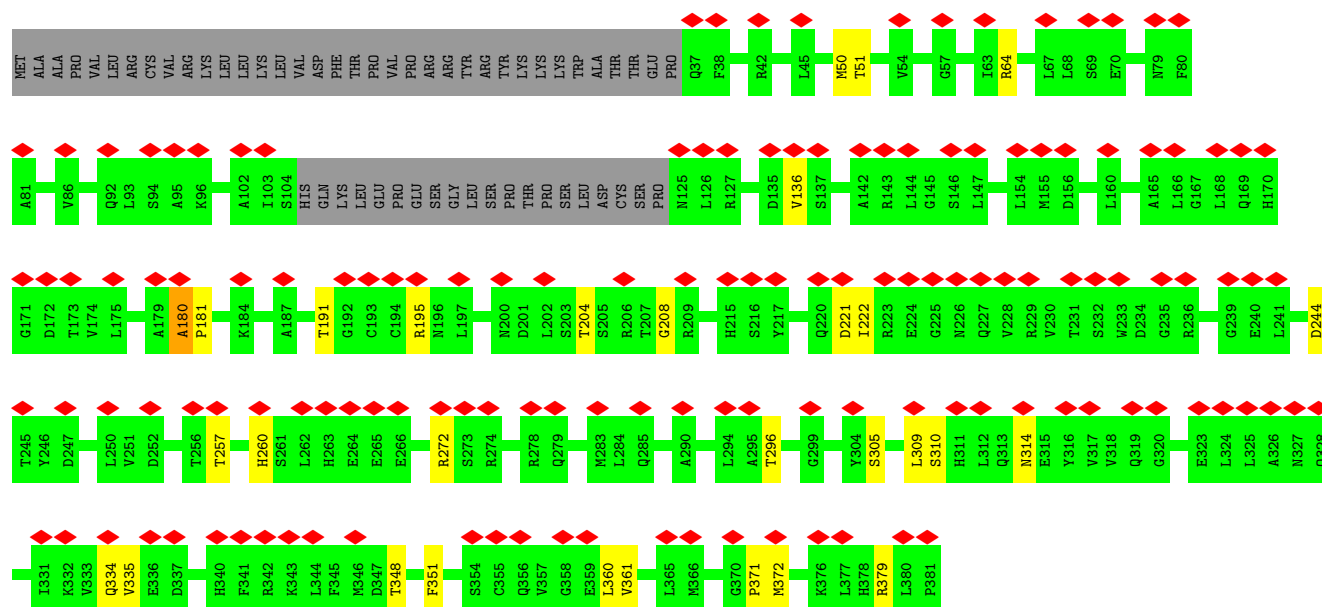
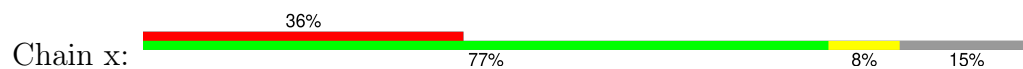


- Molecule 23: Large ribosomal subunit protein uL30m

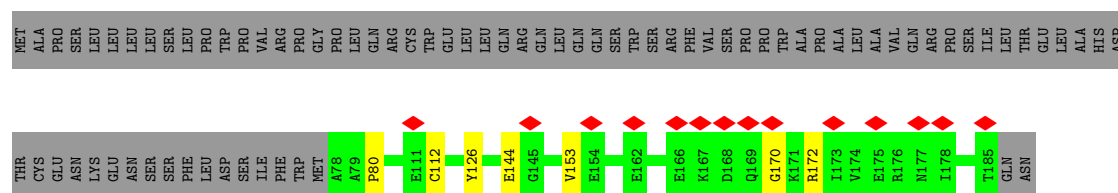




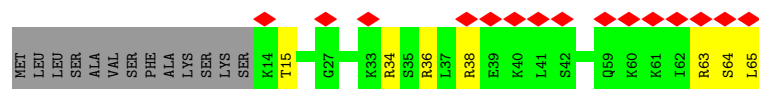
• Molecule 24: 5-cytosine rRNA methyltransferase NSUN4



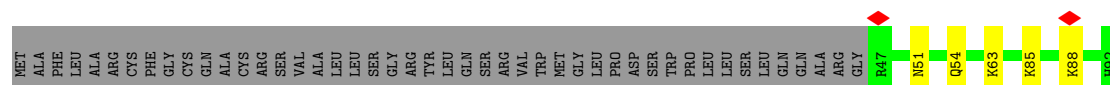
• Molecule 25: Large ribosomal subunit protein bL32m



• Molecule 26: Large ribosomal subunit protein bL33m

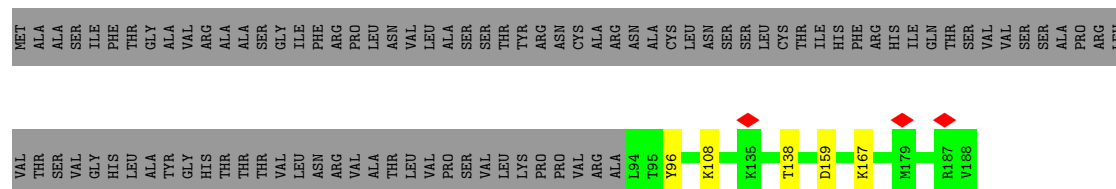


• Molecule 27: Large ribosomal subunit protein bL34m



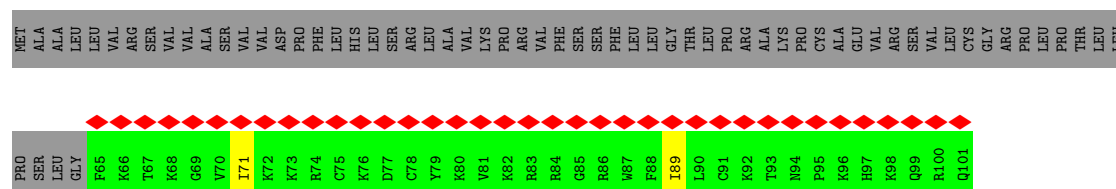
- Molecule 28: Large ribosomal subunit protein bL35m

Chain 3: 



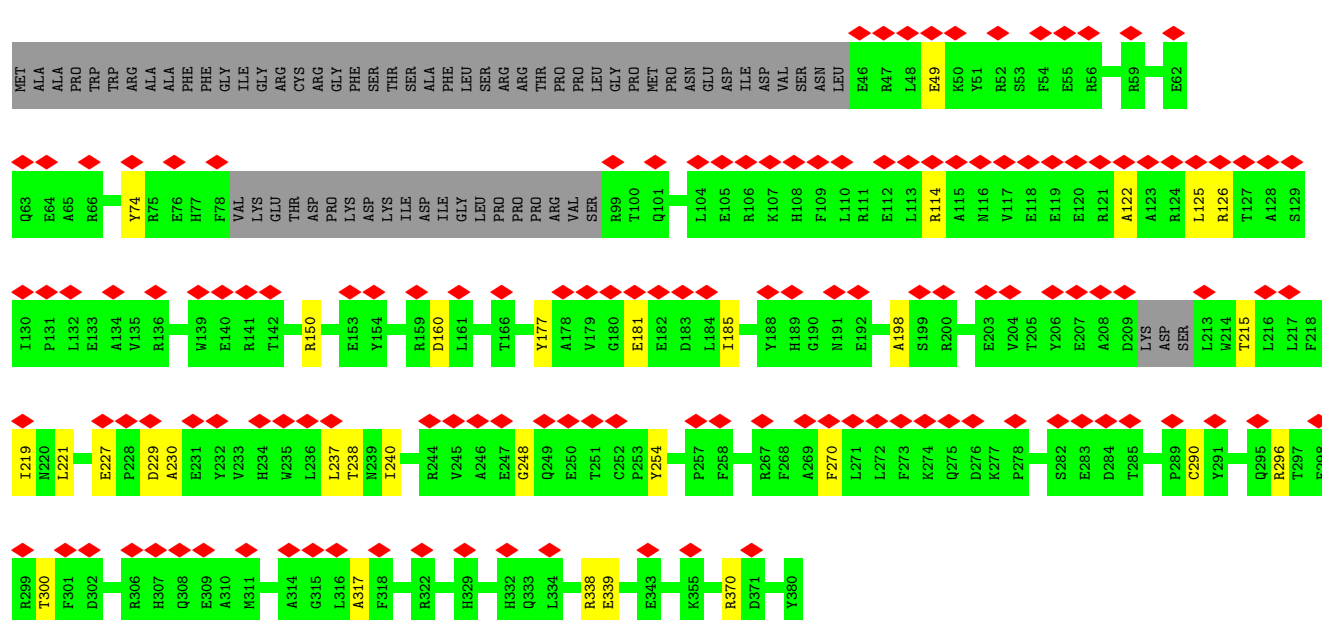
- Molecule 29: Large ribosomal subunit protein bL36m

Chain 4: 




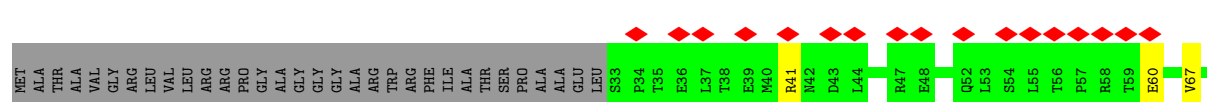
- Molecule 30: Large ribosomal subunit protein mL38

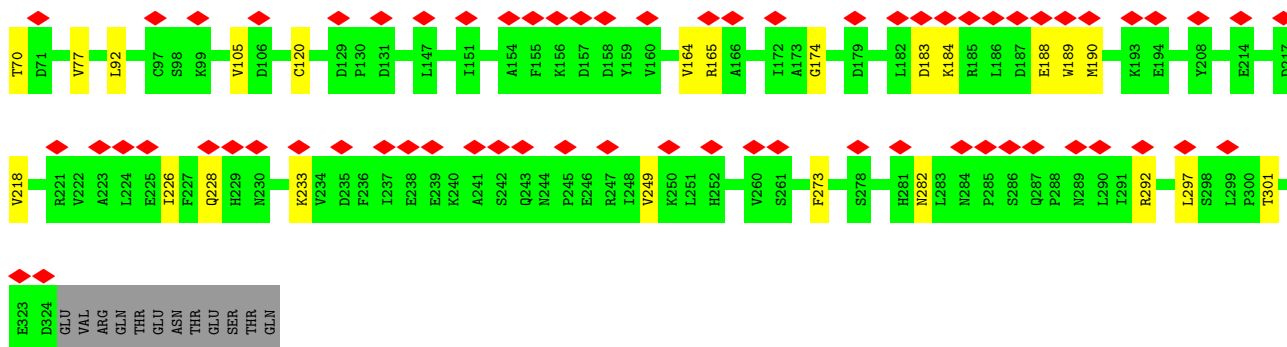
Chain 6: 



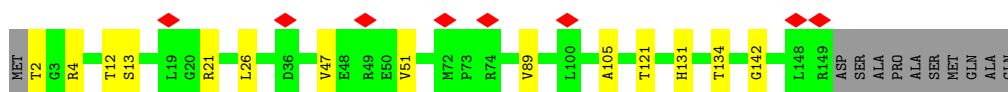
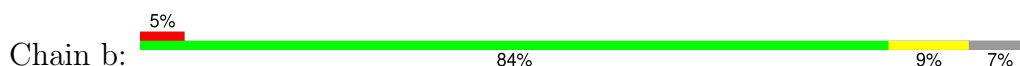
- Molecule 31: Large ribosomal subunit protein mL39

Chain 7: 

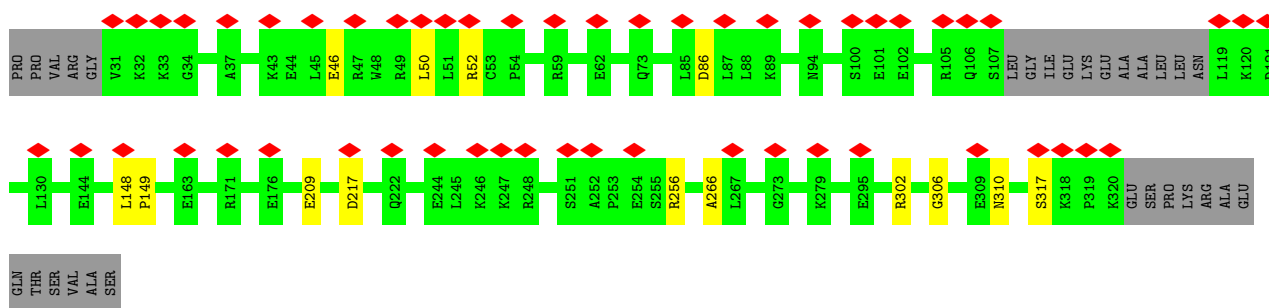
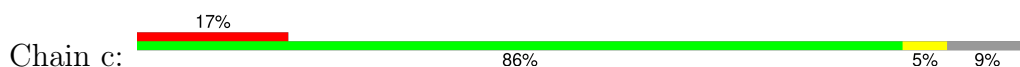




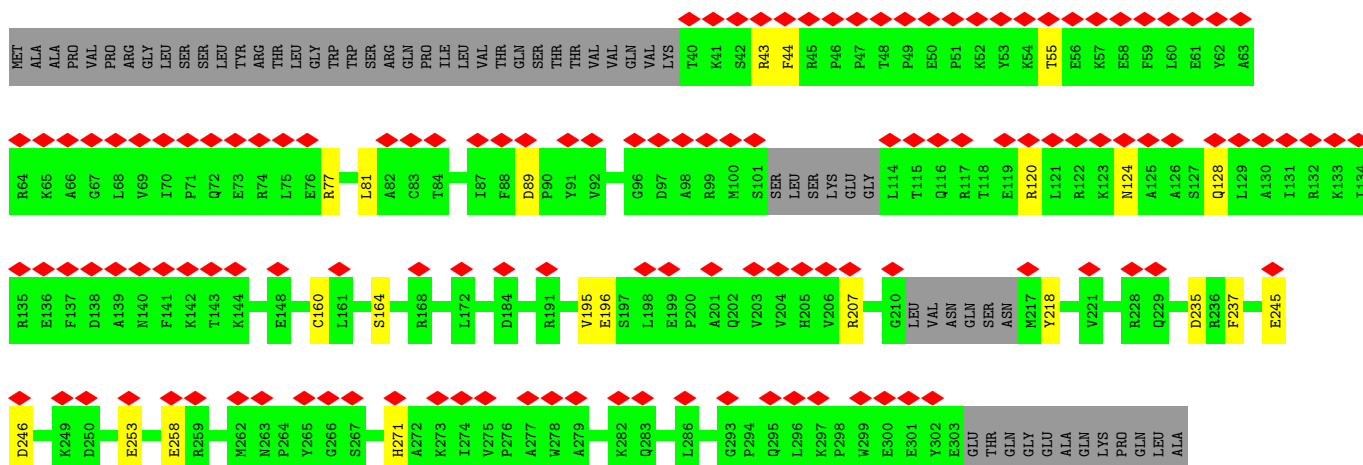
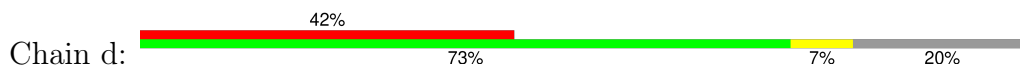
- Molecule 32: Large ribosomal subunit protein mL43



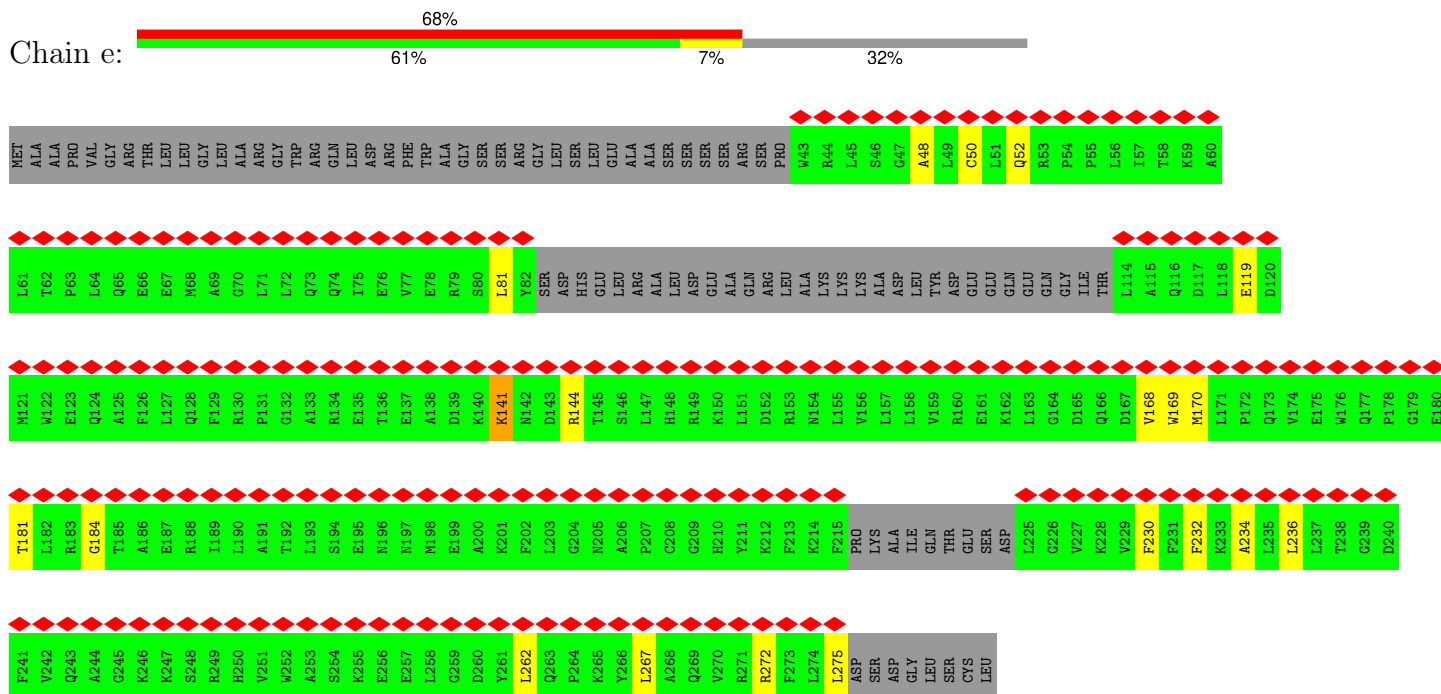
- Molecule 33: Large ribosomal subunit protein mL44



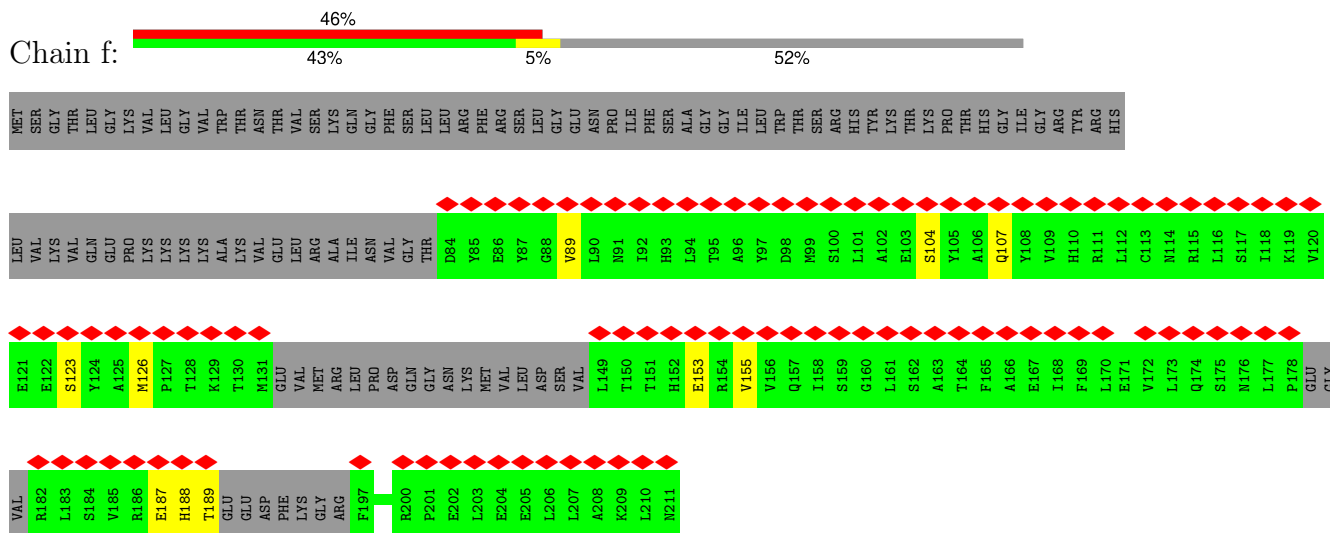
- Molecule 34: Large ribosomal subunit protein mL45



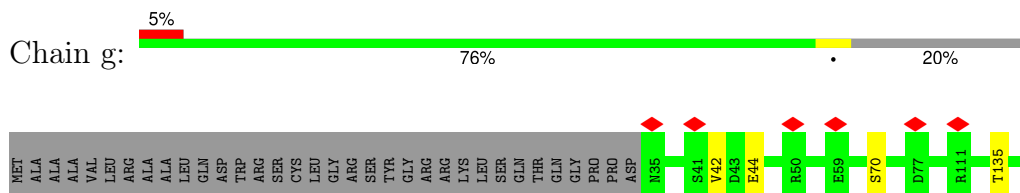
- Molecule 35: Large ribosomal subunit protein mL46



- Molecule 36: Large ribosomal subunit protein mL48

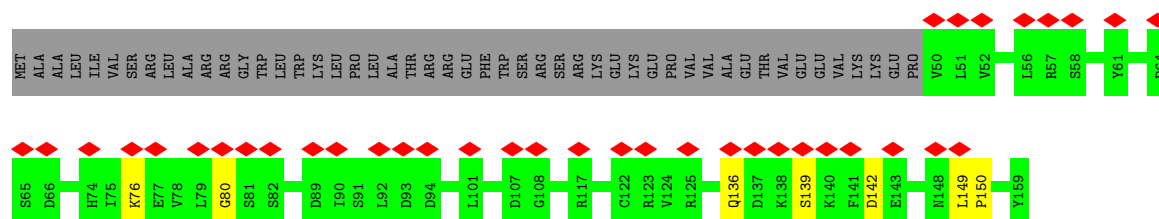


- Molecule 37: Large ribosomal subunit protein mL49

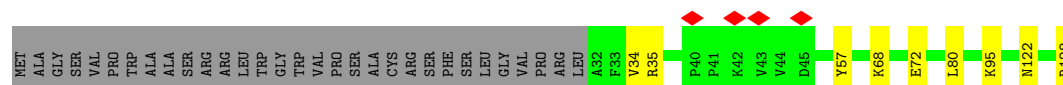


- Molecule 38: Large ribosomal subunit protein mL50

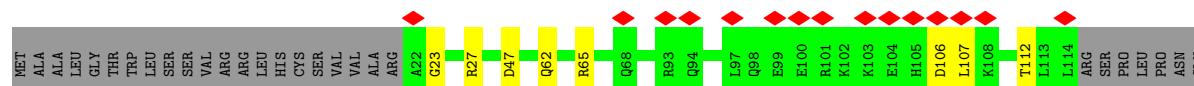




- Molecule 39: Large ribosomal subunit protein mL51



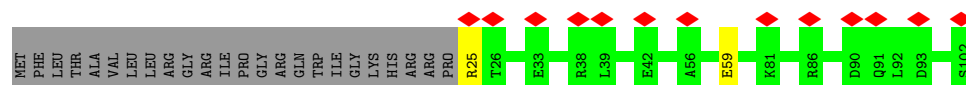
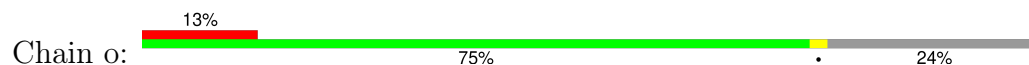
- Molecule 40: Large ribosomal subunit protein mL52



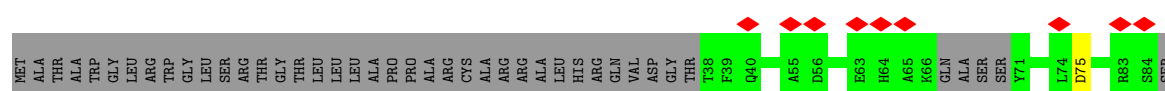
- Molecule 41: Large ribosomal subunit protein mL53

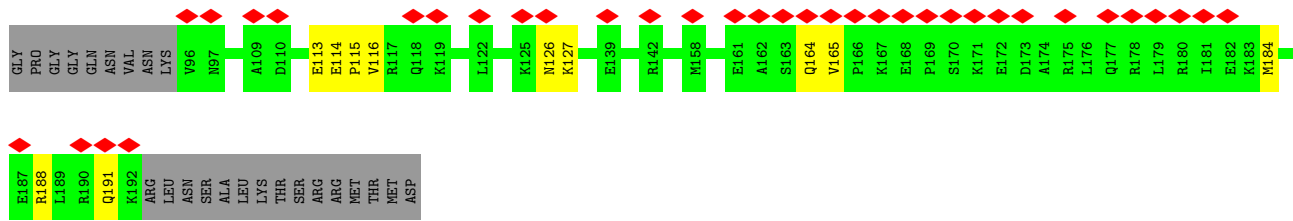


- Molecule 42: Large ribosomal subunit protein mL63

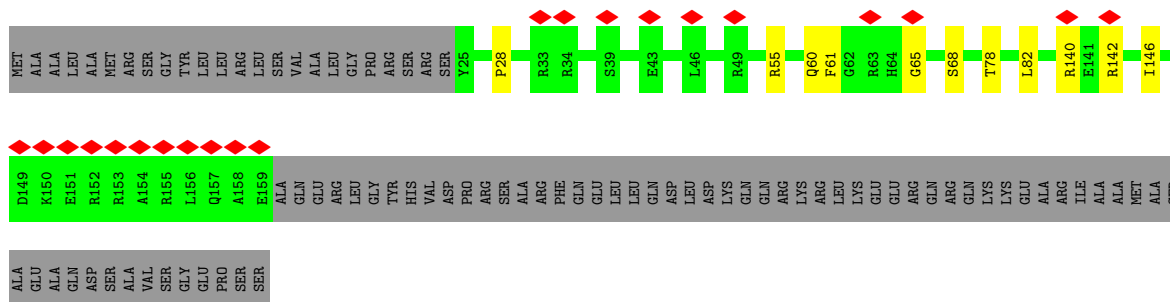


- Molecule 43: Large ribosomal subunit protein mL62

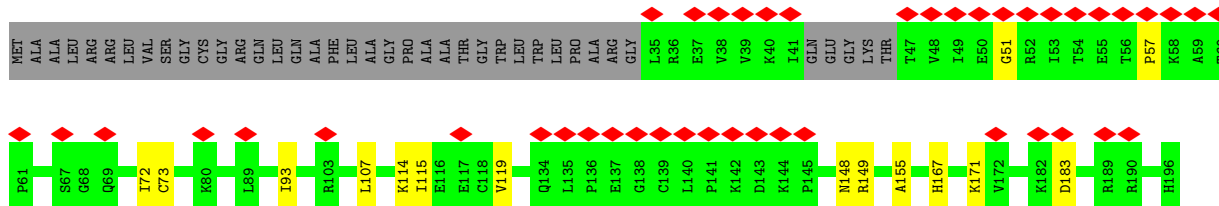




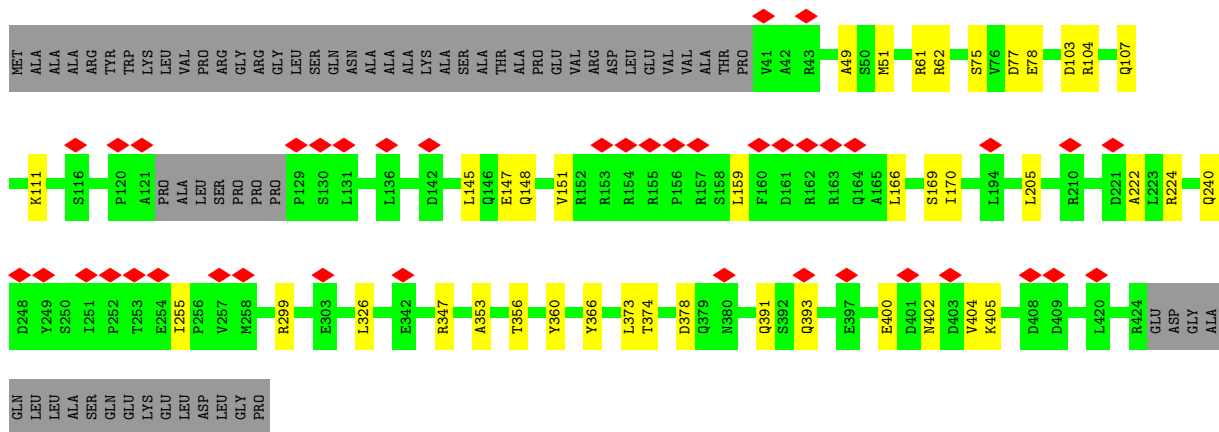
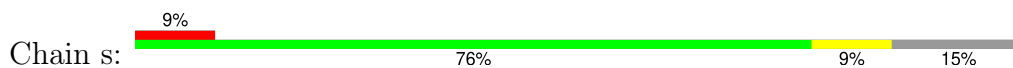
- Molecule 44: Large ribosomal subunit protein mL64



- Molecule 45: Large ribosomal subunit protein mL66



- Molecule 46: Large ribosomal subunit protein mL65



- Molecule 47: Mitochondrial assembly of ribosomal large subunit protein 1

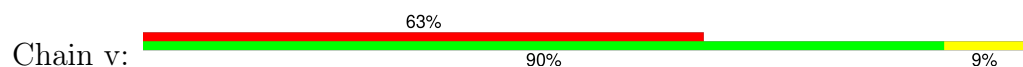


MET GLY PRO GLY TRP SER PRO ALA ARG ARG TRP PRO LEU TRP ARG ARG ALA VAL PHE GLN ILE GLY ALA PRO MET ALA SER VAL TRP PRO LEU ARG LEU ALA GLU TRP PRO ALA ARG PRO CYS THR LEU THR PRO SER THR ARG GLY HIS HIS

GLY PRO GLN PRO GLU TRP ARG THR ALA ASP ALA TRP LEU GLN PRO GLY ARG PRO ALA ASP HIS ILE GLY ALA K85 F86 L91 Q97 E98 N99 A100 R101 D102 I103 I106 R113 Y114 T115 F118 S125 H134 K138 R146 S147 D148 P149 Y150 V151 K152 K156

D159 D160 G167 S168 M169 V170 L173 M174 L175 L184 E185 K186 L187 W188 R191 D195 A198 A201 A202 E203 T204 L205 P206 E207 T210 L211 G212 L213 GLU ASP THR SER LEU THR PRO VAL GLU PHE LYS CYS LYS

- Molecule 48: Predicted gene, 55359



MET A2 P3 W4 E7 A8 C11 Y13 Y14 R14 L16 L17 R18 Q19 G20 R21 E22 L23 T26 D27 R28 D29 F30 Y31 F32 A33 S34 I35 R36 R37 E38 F39 R40 K41 N42 Q43 K44 L45 E46 N47 A50 R51 E52 K53 Q54 L55 E56 K57 G58 L59 V60 F61 L62 H63 S64

K65 L66 G67 L69 I70

- Molecule 49: Acyl carrier protein, mitochondrial

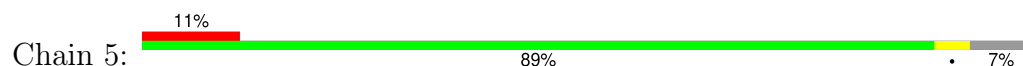


MET ALA SER ARG VAL LEU CYS ALA CYS VAL ARG LEU ARG PRO ALA ALA PHE LEU PRO ALA LEU ALA ARG ARG PRO THR LEU ALA LEU ALA ARG ARG PRO LEU SER THR LEU THR LEU CYS PRO GLU ILE ARG ARG PRO GLY ALA LEU GLN SER ALA LEU LEU ALA ALA VAL VAL PRO GLY THR

VAL THR HIS LEU CYS ARG GLN TYR ASP ALA PRO L74 T75 L76 D77 G78 I79 K80 D81 R82 V83 L84 Y85 V86 L87 R88 L89 Y90 D91 I93 I94 D94 P95 E96 K97 L98 S99 V100 M101 S102 H103 M105 K106 D107 L108 G109 L110 L113 D114 Q115 V116 I117 I118 I119 M120 A121

M122 E123 D124 E125 F126 F127 F128 E129 I130 P131 D132 I133 D134 A135 E136 K137 L138 M139 C140 P141 Q142 E143 I144 V145 D146 Y147 I148 A149 D150 K151 K152 ASP VAL TYR GLU

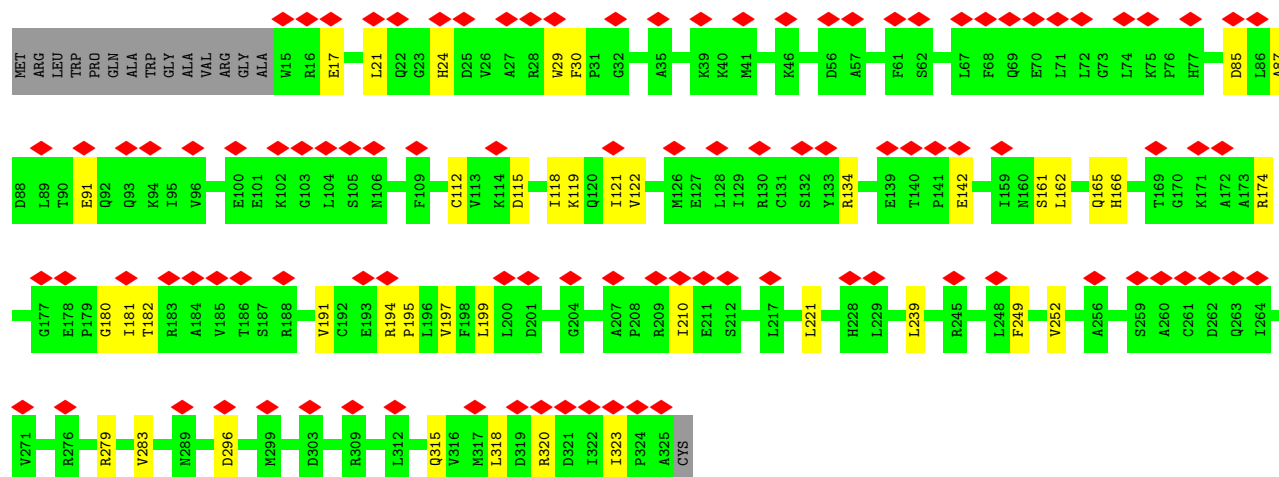
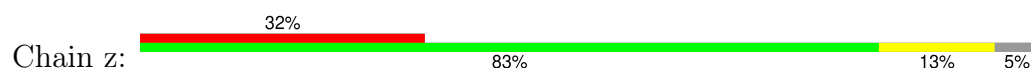
- Molecule 50: Large ribosomal subunit protein mL37



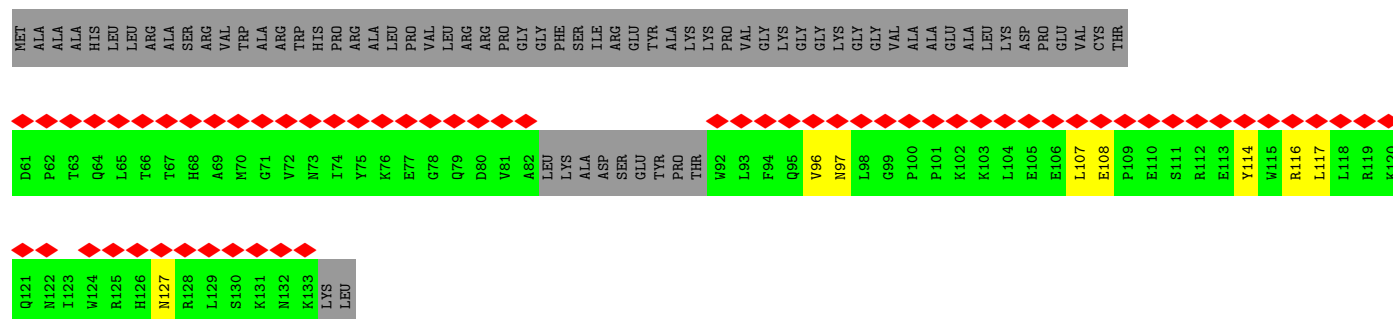
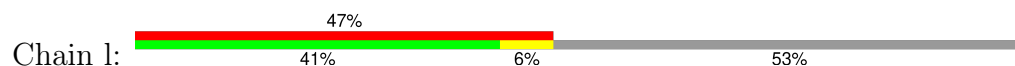
MET ALA LEU ALA SER GLY PRO ALA ARG ALA ARG ALA GLY SER GLY ARG LEU GLY GLY TYR THR PRO LYS ARG GLY A30 G34 S42 P43 R44 P45 L46 R72 R89 A90 H94 E102 R112 L113 L114 E115 G116 Q119 L128 L132

K135 Y140 D141 D142 P143 H146 E151 D169 K172 R173 E174 T175 Y176 C177 P178 K194 N206 L209 S226 S227 A240 E243 E254 T255 P261 C268 H269 V270 T277 N320 L327 L328 N331 T332 A333 K334 T347 D348 L355

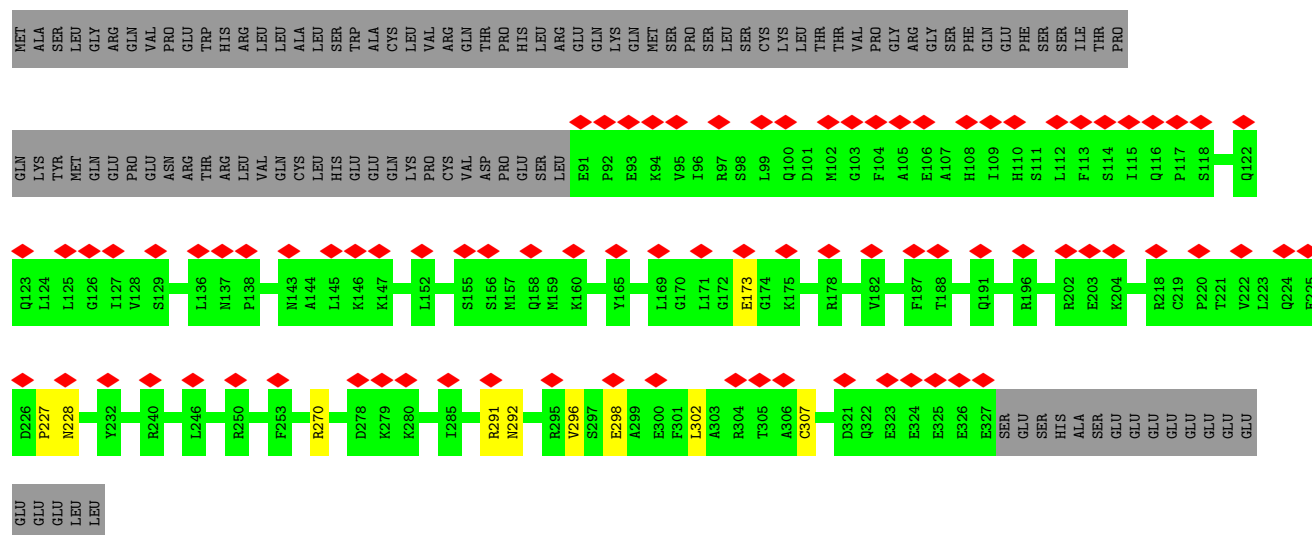
V374 D379 R389 I392 K395 V396 V397 V398 V401 R412 V423



• Molecule 56: Large ribosomal subunit protein mL54

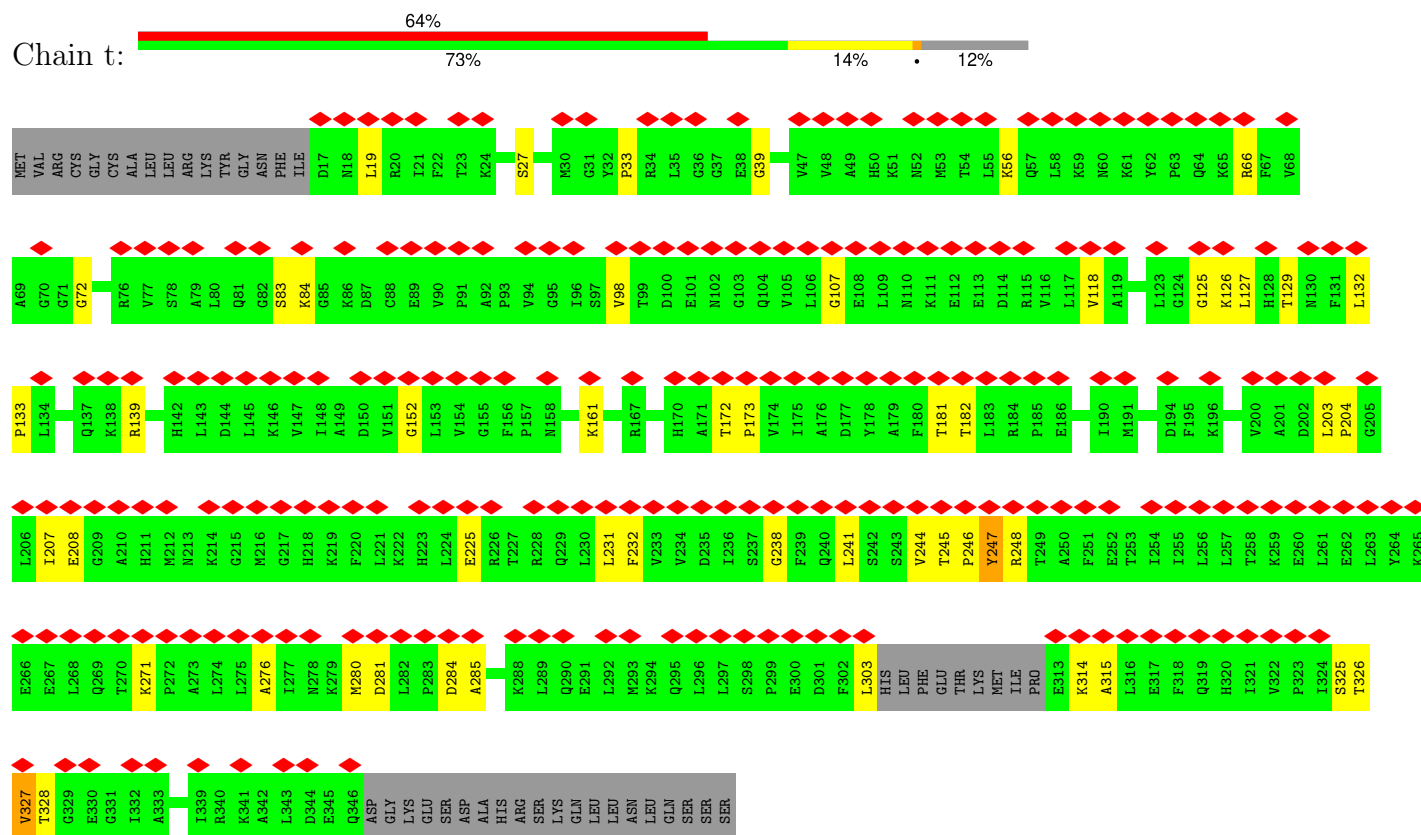


• Molecule 57: Transcription termination factor 4, mitochondrial



• Molecule 58: GTP-binding protein 10

Chain t:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6503	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.049	Depositor
Minimum map value	-0.019	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	457.2925, 457.2925, 457.2925	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.846838, 0.846838, 0.846838	Depositor

5 Model quality

5.1 Standard geometry

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

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	A	0.12	0/33941	0.24	0/52776
2	B	0.10	0/1483	0.23	0/2299
3	D	0.09	0/1802	0.24	0/2424
4	E	0.10	0/2535	0.24	0/3443
5	F	0.12	0/2061	0.25	0/2805
6	H	0.07	0/793	0.22	0/1066
7	I	0.08	0/1140	0.22	0/1538
8	J	0.09	0/786	0.25	0/1056
9	K	0.08	0/1491	0.21	0/2022
10	L	0.09	0/908	0.24	0/1224
11	M	0.11	0/2369	0.27	0/3197
12	O	0.09	0/1285	0.24	0/1732
13	P	0.07	0/1181	0.22	0/1600
14	Q	0.09	0/1832	0.23	0/2471
15	R	0.10	0/1182	0.21	0/1585
16	S	0.10	0/1328	0.26	0/1798
17	T	0.11	0/1402	0.27	0/1885
18	U	0.10	0/1080	0.24	0/1464
19	V	0.08	0/1695	0.22	0/2295
20	W	0.07	0/816	0.21	0/1105
21	X	0.08	0/2075	0.22	0/2806
22	Y	0.09	0/1561	0.20	0/2093
23	Z	0.07	0/935	0.22	0/1264
24	x	0.07	0/2620	0.20	0/3549
25	0	0.09	0/896	0.22	0/1200
26	1	0.07	0/434	0.20	0/578
27	2	0.12	0/387	0.25	0/514
28	3	0.10	0/843	0.25	0/1122
29	4	0.09	0/328	0.22	0/430
30	6	0.08	0/2759	0.21	0/3748
31	7	0.08	0/2436	0.21	0/3300
32	b	0.09	0/1203	0.24	0/1625

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.08	0/2297	0.21	0/3106
34	d	0.08	0/2083	0.24	0/2823
35	e	0.08	0/1608	0.21	0/2165
36	f	0.07	0/830	0.20	0/1119
37	g	0.09	0/1126	0.23	0/1533
38	h	0.07	0/894	0.19	0/1216
39	i	0.11	0/855	0.24	0/1147
40	j	0.08	0/759	0.22	0/1019
41	k	0.07	0/636	0.19	0/857
42	o	0.07	0/655	0.18	0/880
43	p	0.08	0/1168	0.20	0/1565
44	q	0.08	0/1161	0.20	0/1571
45	r	0.08	0/1309	0.24	0/1767
46	s	0.09	0/3118	0.23	0/4232
47	u	0.08	0/1081	0.21	0/1463
48	v	0.08	0/596	0.20	0/795
49	w	0.08	0/646	0.23	0/869
50	5	0.08	0/3317	0.24	0/4519
51	8	0.06	0/598	0.17	0/799
52	9	0.09	0/1009	0.22	0/1358
53	a	0.09	0/884	0.23	0/1197
54	m	0.07	0/380	0.20	0/510
55	z	0.08	0/2500	0.21	0/3380
56	l	0.07	0/557	0.20	0/751
57	y	0.06	0/1980	0.18	0/2667
58	t	0.09	0/2504	0.25	0/3369
All	All	0.10	0/112138	0.23	0/158691

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30335	15322	15349	213	0
2	B	1326	667	670	7	0
3	D	1768	1830	1830	13	0
4	E	2459	2442	2441	17	0
5	F	2005	2024	2024	16	0
6	H	779	814	814	8	0
7	I	1120	1205	1205	12	0
8	J	775	823	823	15	0
9	K	1449	1444	1444	9	0
10	L	893	944	944	5	0
11	M	2315	2376	2376	25	0
12	O	1259	1282	1282	14	0
13	P	1154	1148	1148	13	0
14	Q	1790	1822	1822	11	0
15	R	1161	1224	1224	5	0
16	S	1301	1372	1372	13	0
17	T	1369	1402	1402	12	0
18	U	1052	1057	1057	4	0
19	V	1652	1643	1643	13	0
20	W	794	808	808	8	0
21	X	2021	2051	2051	16	0
22	Y	1523	1553	1553	10	0
23	Z	911	957	957	6	0
24	x	2564	2546	2546	21	0
25	0	881	908	908	5	0
26	1	428	472	472	5	0
27	2	380	407	407	4	0
28	3	823	872	872	4	0
29	4	322	354	354	1	0
30	6	2666	2536	2536	23	0
31	7	2379	2378	2378	18	0
32	b	1181	1195	1195	13	0
33	c	2246	2256	2256	11	0
34	d	2025	2011	2011	14	0
35	e	1576	1598	1598	15	0
36	f	818	817	817	7	0
37	g	1090	1094	1094	6	0
38	h	872	867	867	4	0
39	i	831	854	854	7	0
40	j	744	768	768	5	0
41	k	629	639	639	8	0
42	o	640	623	623	2	0
43	p	1150	1174	1174	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	q	1130	1123	1123	7	0
45	r	1275	1329	1329	11	0
46	s	3045	3058	3057	23	0
47	u	1057	1048	1048	5	0
48	v	586	603	603	4	0
49	w	637	640	640	4	0
50	5	3225	3243	3243	12	0
51	8	589	574	574	6	0
52	9	983	990	990	2	0
53	a	860	843	843	8	0
54	m	374	395	395	4	0
55	z	2455	2547	2546	29	0
56	l	544	542	542	8	0
57	y	1943	1995	1995	7	0
58	t	2464	2551	2551	35	0
59	A	92	0	0	0	0
59	E	1	0	0	0	0
59	M	1	0	0	0	0
59	O	1	0	0	0	0
60	0	1	0	0	0	0
60	4	1	0	0	0	0
61	r	4	0	0	1	0
62	t	32	13	13	2	0
62	z	32	13	13	1	0
All	All	106788	92086	92113	673	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 (673) 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)
1:A:1936:U:OP2	1:A:1941:A:N6	2.10	0.85
3:D:139:ASP:OD1	3:D:249:SER:OG	1.94	0.85
1:A:1276:U:O2	1:A:1283:A:N6	2.09	0.84
1:A:1112:C:N4	21:X:18:GLN:OE1	2.11	0.83
16:S:58:THR:OG1	16:S:61:SER:OG	1.98	0.82
1:A:1615:G:O6	1:A:1643:C:N4	2.13	0.82
30:6:198:ALA:O	30:6:254:TYR:OH	1.99	0.80
35:e:275:LEU:HD13	51:8:139:MET:HE2	1.63	0.80
1:A:1489:A:O2'	1:A:1506:A:N7	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2524:G:N2	1:A:2527:A:OP2	2.17	0.77
1:A:1385:G:N2	17:T:158:PHE:O	2.17	0.77
16:S:143:ASP:OD2	33:c:310:ASN:ND2	2.19	0.76
1:A:2462:A:OP1	1:A:2574:A:O2'	2.04	0.74
1:A:1682:A:OP2	15:R:62:ARG:NH2	2.21	0.73
1:A:1608:C:O2'	1:A:1609:C:OP1	2.08	0.72
58:t:326:THR:O	58:t:328:THR:N	2.22	0.72
13:P:65:GLU:OE2	30:6:74:TYR:OH	2.06	0.71
1:A:1137:A:O2'	1:A:1138:U:OP1	2.09	0.71
1:A:1104:G:OP2	22:Y:232:LYS:NZ	2.24	0.70
1:A:1205:A:N6	1:A:1208:U:OP2	2.25	0.70
1:A:1102:U:O2'	1:A:1103:A:OP2	2.09	0.69
1:A:2233:U:O2'	6:H:84:LYS:NZ	2.25	0.69
24:x:244:ASP:OD1	24:x:379:ARG:NH1	2.24	0.69
1:A:1710:U:O2'	5:F:104:ARG:NH2	2.25	0.69
46:s:49:ALA:O	46:s:61:ARG:NE	2.25	0.69
17:T:63:ARG:NH1	34:d:237:PHE:O	2.26	0.69
17:T:127:ASN:ND2	34:d:235:ASP:OD2	2.26	0.68
1:A:2458:G:O3'	58:t:56:LYS:NZ	2.26	0.68
24:x:310:SER:O	24:x:314:ASN:ND2	2.26	0.67
1:A:1539:C:N4	1:A:2385:G:O2'	2.27	0.67
30:6:181:GLU:N	30:6:181:GLU:OE1	2.28	0.67
8:J:128:ASP:OD1	8:J:133:GLN:NE2	2.28	0.67
46:s:107:GLN:O	46:s:111:LYS:N	2.27	0.67
1:A:1564:U:O2'	1:A:1577:A:N3	2.28	0.67
1:A:2080:G:O2'	1:A:2082:G:OP2	2.05	0.66
1:A:1160:A:O2'	1:A:1161:C:OP1	2.11	0.66
31:7:228:GLN:OE1	31:7:228:GLN:N	2.28	0.66
58:t:152:GLY:O	58:t:231:LEU:N	2.27	0.66
1:A:1240:A:OP1	33:c:52:ARG:NH2	2.28	0.66
19:V:78:GLN:OE1	34:d:77:ARG:NH1	2.29	0.66
1:A:1242:A:N3	1:A:1290:U:O2'	2.29	0.65
1:A:1614:A:N6	1:A:1639:C:O2	2.28	0.65
1:A:2112:G:OP1	17:T:75:LYS:NZ	2.29	0.65
1:A:1628:A:OP2	56:l:116:ARG:NE	2.30	0.65
1:A:1965:G:OP1	3:D:136:ARG:NH2	2.30	0.65
35:e:275:LEU:CD1	51:8:139:MET:HE2	2.25	0.65
46:s:222:ALA:O	46:s:224:ARG:NH1	2.30	0.65
46:s:75:SER:OG	46:s:77:ASP:OD1	2.14	0.64
32:b:89:VAL:HG12	32:b:89:VAL:O	1.98	0.64
1:A:1806:A:O2'	46:s:299:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:z:134:ARG:NH2	55:z:142:GLU:O	2.31	0.63
55:z:180:GLY:N	62:z:401:GNP:O3G	2.32	0.63
34:d:258:GLU:OE2	34:d:271:HIS:ND1	2.31	0.63
9:K:63:ARG:NH1	9:K:130:ASP:OD2	2.32	0.62
35:e:52:GLN:N	35:e:234:ALA:O	2.32	0.62
1:A:1194:A:O2'	1:A:1195:G:OP1	2.16	0.62
6:H:68:PRO:O	6:H:70:LEU:HD12	2.00	0.62
55:z:279:ARG:NE	55:z:296:ASP:OD1	2.32	0.62
12:O:70:GLU:N	12:O:70:GLU:OE1	2.32	0.62
45:r:93:ILE:HD11	45:r:119:VAL:HG21	1.80	0.62
50:5:206:ASN:N	50:5:227:SER:O	2.32	0.62
4:E:69:ASN:OD1	4:E:154:ARG:NH1	2.32	0.62
1:A:1259:G:O6	32:b:4:ARG:NH1	2.33	0.62
1:A:1296:G:N7	11:M:50:ARG:NH1	2.48	0.61
1:A:1318:U:O2'	1:A:1323:C:OP1	2.18	0.61
1:A:2366:U:O2'	1:A:2368:C:OP1	2.18	0.61
27:2:51:ASN:O	27:2:54:GLN:NE2	2.33	0.61
12:O:79:TRP:NE1	14:Q:267:PHE:O	2.31	0.61
24:x:204:THR:O	24:x:208:GLY:N	2.34	0.61
32:b:21:ARG:NH2	33:c:217:ASP:OD2	2.33	0.61
38:h:136:GLN:N	38:h:136:GLN:OE1	2.32	0.61
43:p:184:MET:SD	43:p:188:ARG:NH2	2.74	0.61
49:w:80:LYS:HG3	49:w:145:VAL:HG11	1.81	0.61
1:A:2516:A:N6	1:A:2537:G:O2'	2.33	0.61
45:r:73:CYS:N	61:r:201:FES:S2	2.74	0.61
4:E:94:SER:OG	4:E:184:ASN:ND2	2.34	0.60
12:O:41:ARG:NH2	12:O:132:PRO:O	2.33	0.60
33:c:302:ARG:O	33:c:306:GLY:N	2.35	0.60
7:I:45:GLN:NE2	42:o:25:ARG:O	2.35	0.60
3:D:113:ARG:O	3:D:148:ARG:NH2	2.34	0.59
3:D:219:ARG:NH2	57:y:173:GLU:OE2	2.35	0.59
58:t:208:GLU:OE2	58:t:248:ARG:NH1	2.35	0.59
1:A:1265:A:OP1	32:b:4:ARG:NH2	2.35	0.59
31:7:218:VAL:O	31:7:249:VAL:N	2.33	0.59
1:A:1121:A:N3	1:A:1127:U:O2'	2.35	0.59
1:A:1152:U:O2'	21:X:96:LYS:O	2.14	0.59
40:j:62:GLN:OE1	40:j:65:ARG:NH1	2.35	0.59
1:A:1471:U:OP2	11:M:61:ARG:NH2	2.35	0.59
22:Y:93:ARG:O	22:Y:151:ARG:NH2	2.35	0.59
1:A:2263:G:O2'	1:A:2332:U:O4	2.11	0.58
58:t:118:VAL:O	58:t:139:ARG:NH1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1174:A:OP2	1:A:2337:C:O2'	2.21	0.58
1:A:1638:U:H3'	1:A:1639:C:H5''	1.85	0.58
4:E:126:ASP:O	4:E:173:LYS:NZ	2.36	0.58
1:A:1469:G:O2'	11:M:55:GLU:OE1	2.20	0.58
1:A:1630:G:N3	56:l:127:ASN:ND2	2.51	0.58
1:A:2328:C:O2'	1:A:2329:U:O4'	2.20	0.58
26:1:34:ARG:NH1	26:1:38:ARG:O	2.35	0.58
21:X:151:GLU:OE1	21:X:151:GLU:N	2.36	0.58
55:z:91:GLU:N	55:z:91:GLU:OE1	2.36	0.58
1:A:1160:A:O2'	1:A:1161:C:P	2.61	0.57
8:J:70:ILE:HD13	8:J:80:LEU:HG	1.85	0.57
6:H:112:LYS:O	6:H:114:SER:N	2.37	0.57
1:A:2116:U:O2'	25:0:80:PRO:O	2.16	0.57
11:M:61:ARG:O	39:i:128:ARG:NH2	2.36	0.57
14:Q:251:GLU:OE1	14:Q:251:GLU:N	2.36	0.57
22:Y:175:PHE:O	22:Y:214:ARG:NH2	2.37	0.57
23:Z:105:SER:OG	42:o:59:GLU:OE2	2.13	0.57
30:6:290:CYS:SG	30:6:296:ARG:NH2	2.74	0.57
46:s:51:MET:O	46:s:62:ARG:NH1	2.35	0.57
1:A:1688:U:O2'	16:S:122:ASN:ND2	2.35	0.57
50:5:209:LEU:HD12	50:5:209:LEU:O	2.04	0.57
1:A:1431:A:OP2	1:A:2171:A:O2'	2.23	0.57
40:j:23:GLY:O	40:j:27:ARG:NH1	2.37	0.57
50:5:119:GLN:NE2	50:5:261:PRO:O	2.38	0.57
1:A:1597:A:O2'	1:A:1598:C:O5'	2.15	0.57
3:D:133:ASP:OD2	3:D:136:ARG:NH1	2.35	0.57
31:7:189:TRP:O	31:7:292:ARG:NH2	2.36	0.57
1:A:2130:A:O2'	1:A:2131:A:OP1	2.22	0.56
3:D:195:ASN:OD1	3:D:244:THR:HG23	2.04	0.56
23:Z:136:SER:OG	23:Z:147:VAL:O	2.22	0.56
26:1:36:ARG:NH2	26:1:64:SER:OG	2.38	0.56
16:S:131:ARG:NH2	33:c:317:SER:OG	2.38	0.56
20:W:146:ASP:OD1	20:W:147:MET:N	2.38	0.56
55:z:119:LYS:NZ	55:z:165:GLN:OE1	2.33	0.56
1:A:1680:C:OP1	15:R:99:ARG:NH2	2.37	0.56
15:R:33:GLY:O	15:R:36:ASN:ND2	2.39	0.56
31:7:190:MET:SD	31:7:282:ASN:ND2	2.78	0.56
46:s:147:GLU:OE2	46:s:170:ILE:HG23	2.06	0.56
1:A:1418:G:OP1	3:D:270:ARG:NH2	2.38	0.56
1:A:2358:G:O6	11:M:76:ARG:NH2	2.38	0.56
1:A:2615:U:O2'	9:K:97:ARG:NH2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:z:112:CYS:SG	55:z:161:SER:OG	2.64	0.56
58:t:98:VAL:N	58:t:107:GLY:O	2.36	0.56
6:H:128:TYR:O	6:H:133:ASN:ND2	2.39	0.56
25:0:112:CYS:O	31:7:70:THR:OG1	2.23	0.56
13:P:145:VAL:HG23	13:P:174:GLU:OE1	2.06	0.55
46:s:145:LEU:HD11	46:s:402:ASN:HA	1.88	0.55
1:A:2505:G:O2'	1:A:2508:C:OP2	2.22	0.55
1:A:1846:U:O2'	50:5:270:VAL:O	2.24	0.55
1:A:1705:U:O4	11:M:35:ARG:NH2	2.39	0.55
9:K:171:THR:OG1	45:r:57:PRO:O	2.19	0.55
34:d:124:ASN:O	34:d:128:GLN:N	2.39	0.55
1:A:2659:C:H4'	1:A:2660:U:OP1	2.07	0.55
33:c:266:ALA:O	53:a:86:HIS:NE2	2.40	0.55
57:y:302:LEU:O	57:y:307:CYS:N	2.40	0.55
1:A:1628:A:O2'	1:A:1647:A:N3	2.38	0.55
1:A:2409:C:OP1	58:t:66:ARG:NH1	2.38	0.55
20:W:122:LYS:N	30:6:49:GLU:O	2.37	0.54
23:Z:71:ARG:NH2	23:Z:92:GLN:O	2.40	0.54
45:r:72:ILE:HG12	45:r:107:LEU:HD22	1.88	0.54
1:A:1101:C:O2'	1:A:1102:U:OP2	2.23	0.54
13:P:117:TYR:O	30:6:114:ARG:NH2	2.38	0.54
16:S:161:GLU:OE1	16:S:201:THR:OG1	2.25	0.54
30:6:227:GLU:OE1	30:6:230:ALA:N	2.40	0.54
1:A:1156:U:O3'	39:i:95:LYS:NZ	2.41	0.54
19:V:161:ARG:NH1	19:V:163:ASP:OD2	2.40	0.54
45:r:167:HIS:O	45:r:171:LYS:N	2.40	0.54
12:O:125:GLU:OE1	12:O:129:ASN:ND2	2.38	0.54
40:j:112:THR:HG22	40:j:112:THR:O	2.06	0.54
21:X:178:PRO:O	21:X:179:GLU:HG2	2.07	0.54
48:v:59:LEU:O	48:v:63:HIS:ND1	2.40	0.54
1:A:2057:G:O2'	1:A:2058:G:P	2.66	0.54
11:M:98:ARG:NH1	11:M:142:GLU:OE2	2.41	0.54
1:A:1185:C:OP2	44:q:55:ARG:NH2	2.40	0.54
1:A:2598:A:OP1	14:Q:271:ARG:NH2	2.39	0.54
31:7:183:ASP:OD1	31:7:184:LYS:N	2.41	0.54
13:P:153:ALA:O	13:P:159:LYS:NZ	2.35	0.53
18:U:22:THR:HG22	18:U:24:PHE:H	1.73	0.53
46:s:77:ASP:OD1	46:s:78:GLU:N	2.41	0.53
35:e:48:ALA:N	35:e:230:PHE:O	2.33	0.53
35:e:141:LYS:O	35:e:144:ARG:NH1	2.41	0.53
58:t:181:THR:O	58:t:182:THR:OG1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:41:ASP:O	11:M:45:GLY:N	2.42	0.53
1:A:2451:C:O2'	1:A:2556:U:OP1	2.22	0.53
49:w:80:LYS:CG	49:w:145:VAL:HG11	2.38	0.53
30:6:237:LEU:HB3	30:6:240:ILE:HD11	1.90	0.53
1:A:2182:U:O4	21:X:104:VAL:N	2.42	0.53
8:J:121:ALA:HB1	8:J:137:LEU:HD11	1.91	0.53
58:t:284:ASP:OD1	58:t:285:ALA:N	2.41	0.53
1:A:1602:U:O4'	1:A:1602:U:P	2.67	0.53
24:x:136:VAL:HG12	24:x:136:VAL:O	2.09	0.53
1:A:2057:G:O2'	1:A:2058:G:OP1	2.26	0.52
24:x:180:ALA:HB1	24:x:181:PRO:HD2	1.91	0.52
35:e:262:LEU:HD23	35:e:267:LEU:O	2.09	0.52
58:t:246:PRO:O	58:t:247:TYR:HB2	2.09	0.52
1:A:1760:U:O2'	12:O:82:GLU:OE2	2.27	0.52
7:I:62:PRO:HA	7:I:65:LEU:HD12	1.91	0.52
17:T:49:ASN:OD1	17:T:126:HIS:NE2	2.42	0.52
56:l:107:LEU:HD11	56:l:117:LEU:HD12	1.90	0.52
58:t:245:THR:HB	58:t:246:PRO:HD3	1.91	0.52
51:8:125:LYS:O	51:8:129:HIS:ND1	2.43	0.52
20:W:133:VAL:HG13	20:W:133:VAL:O	2.08	0.52
48:v:43:GLN:O	48:v:51:ARG:NH2	2.40	0.52
1:A:1281:A:N3	1:A:2130:A:N6	2.58	0.52
19:V:170:TRP:O	52:9:75:ARG:NH2	2.42	0.52
11:M:167:GLU:OE2	11:M:219:ARG:NH2	2.42	0.52
24:x:221:ASP:OD1	24:x:222:ILE:N	2.41	0.52
43:p:188:ARG:O	43:p:191:GLN:NE2	2.43	0.52
53:a:96:VAL:O	53:a:96:VAL:HG13	2.10	0.52
56:l:108:GLU:N	56:l:108:GLU:OE1	2.42	0.52
58:t:132:LEU:HB2	58:t:133:PRO:CD	2.39	0.52
1:A:1175:G:HO2'	1:A:1176:A:P	2.32	0.52
4:E:316:PHE:HB3	4:E:317:PRO:HD3	1.91	0.52
17:T:131:ARG:NH2	31:7:92:LEU:O	2.38	0.52
38:h:139:SER:N	38:h:142:ASP:OD2	2.42	0.52
1:A:1211:U:OP1	27:2:88:LYS:N	2.42	0.52
12:O:64:LYS:NZ	12:O:100:GLN:O	2.42	0.52
1:A:1175:G:O2'	1:A:1176:A:OP1	2.27	0.52
43:p:126:ASN:OD1	43:p:127:LYS:N	2.43	0.52
55:z:17:GLU:N	55:z:17:GLU:OE1	2.43	0.52
21:X:81:GLY:N	21:X:131:THR:OG1	2.42	0.51
58:t:326:THR:O	58:t:327:VAL:HG12	2.10	0.51
1:A:1237:A:H4'	1:A:1237:A:OP1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1627:A:OP1	1:A:1628:A:N6	2.43	0.51
12:O:77:ASP:OD1	12:O:83:LYS:NZ	2.38	0.51
13:P:51:ARG:NH1	30:6:160:ASP:OD1	2.43	0.51
50:5:177:CYS:SG	50:5:178:PRO:HD3	2.50	0.51
1:A:1595:U:O2'	1:A:1596:A:OP2	2.27	0.51
24:x:309:LEU:CD1	24:x:360:LEU:HD21	2.41	0.51
4:E:301:ASP:OD1	4:E:301:ASP:N	2.43	0.51
24:x:50:MET:HG3	24:x:51:THR:HG23	1.93	0.51
18:U:19:VAL:O	18:U:19:VAL:HG13	2.10	0.51
22:Y:166:ARG:NH2	22:Y:183:PHE:O	2.41	0.51
55:z:21:LEU:O	55:z:24:HIS:ND1	2.39	0.50
1:A:1621:A:N1	1:A:1631:A:H2'	2.26	0.50
9:K:177:ARG:NH2	41:k:85:GLU:OE2	2.40	0.50
31:7:164:VAL:HG13	31:7:165:ARG:H	1.76	0.50
39:i:57:TYR:OH	44:q:28:PRO:O	2.23	0.50
58:t:132:LEU:HB2	58:t:133:PRO:HD3	1.93	0.50
1:A:2158:G:O6	1:A:2159:A:N6	2.44	0.50
24:x:348:THR:O	24:x:348:THR:HG22	2.11	0.50
1:A:1468:A:N1	1:A:2373:G:O2'	2.41	0.50
1:A:2507:U:OP2	4:E:239:ARG:NH2	2.43	0.50
10:L:84:ALA:HB1	10:L:105:VAL:HG22	1.93	0.50
21:X:163:ARG:NH1	21:X:204:VAL:O	2.41	0.50
24:x:351:PHE:CE1	24:x:361:VAL:HG22	2.46	0.50
1:A:2088:A:O4'	55:z:279:ARG:NH1	2.45	0.50
14:Q:239:ASN:OD1	14:Q:241:LYS:NZ	2.45	0.50
41:k:64:VAL:N	41:k:76:MET:O	2.38	0.50
46:s:326:LEU:HD13	46:s:366:TYR:HB2	1.94	0.50
1:A:1450:A:OP1	16:S:185:ARG:NH2	2.45	0.49
1:A:1402:A:N3	3:D:265:ARG:NH1	2.59	0.49
41:k:81:LEU:HD21	45:r:51:GLY:H	1.76	0.49
47:u:212:GLY:C	47:u:213:LEU:HD23	2.37	0.49
57:y:291:ARG:NH2	57:y:292:ASN:OD1	2.45	0.49
1:A:1111:C:OP2	21:X:5:ARG:NH1	2.44	0.49
1:A:1251:C:OP2	53:a:126:GLY:N	2.43	0.49
55:z:323:ILE:HD12	55:z:323:ILE:H	1.77	0.49
46:s:148:GLN:HG2	46:s:166:LEU:HD21	1.93	0.49
1:A:1638:U:O5'	1:A:1639:C:OP2	2.31	0.49
1:A:1644:U:H4'	1:A:1645:C:OP1	2.12	0.49
1:A:2617:A:O2'	1:A:2618:A:OP2	2.26	0.49
4:E:112:LYS:NZ	4:E:337:VAL:O	2.45	0.49
16:S:136:LYS:NZ	40:j:47:ASP:OD1	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1773:G:N2	1:A:1863:C:O2'	2.45	0.49
8:J:20:ILE:HG12	8:J:38:ILE:HG21	1.95	0.49
33:c:209:GLU:OE1	33:c:209:GLU:N	2.45	0.49
2:B:48:G:H22	2:B:58:C:H42	1.60	0.49
8:J:23:ILE:HB	8:J:68:THR:HG22	1.95	0.49
19:V:54:TRP:NE1	19:V:56:LEU:O	2.45	0.49
44:q:61:PHE:O	44:q:65:GLY:N	2.44	0.49
34:d:120:ARG:O	34:d:124:ASN:N	2.46	0.49
1:A:1426:U:OP1	1:A:1429:C:N4	2.38	0.48
1:A:2302:U:C2'	1:A:2303:A:O5'	2.61	0.48
13:P:61:VAL:HG12	13:P:61:VAL:O	2.12	0.48
2:B:31:C:O2'	2:B:32:U:OP1	2.24	0.48
41:k:48:ASN:OD1	41:k:49:CYS:N	2.45	0.48
1:A:1217:A:N3	1:A:1343:C:O2'	2.42	0.48
1:A:2342:U:O2'	1:A:2343:A:OP1	2.27	0.48
22:Y:79:GLU:OE1	22:Y:79:GLU:N	2.38	0.48
1:A:1524:U:O4	11:M:56:ARG:NH2	2.40	0.48
7:I:95:MET:SD	7:I:95:MET:N	2.86	0.48
19:V:93:THR:HG22	19:V:110:ALA:HB1	1.94	0.48
57:y:292:ASN:O	57:y:296:VAL:HG22	2.13	0.48
6:H:64:GLU:OE1	21:X:61:ARG:NH2	2.45	0.48
4:E:100:ILE:HD12	4:E:147:VAL:O	2.13	0.48
1:A:2564:G:H1'	1:A:2565:U:OP2	2.13	0.48
58:t:246:PRO:HG2	58:t:248:ARG:NE	2.29	0.48
1:A:1194:A:HO2'	1:A:1195:G:P	2.37	0.48
1:A:1597:A:H1'	1:A:1598:C:O4'	2.14	0.48
1:A:2342:U:O2'	1:A:2343:A:P	2.72	0.48
5:F:282:PRO:HB2	5:F:284:TYR:O	2.14	0.47
13:P:104:SER:OG	30:6:150:ARG:NH2	2.47	0.47
36:f:188:HIS:O	36:f:189:THR:C	2.57	0.47
39:i:80:LEU:HD12	39:i:80:LEU:O	2.14	0.47
1:A:1335:A:N3	1:A:2371:U:O2'	2.42	0.47
1:A:1563:C:OP2	23:Z:77:ARG:NH1	2.43	0.47
13:P:72:TRP:O	20:W:105:VAL:HG23	2.14	0.47
26:l:15:THR:O	26:l:65:LEU:N	2.45	0.47
43:p:75:ASP:OD1	43:p:75:ASP:N	2.45	0.47
5:F:97:HIS:NE2	5:F:101:ILE:HD11	2.29	0.47
1:A:1137:A:O2'	1:A:1138:U:P	2.72	0.47
1:A:2256:U:O2'	24:x:272:ARG:NH1	2.47	0.47
34:d:81:LEU:O	34:d:218:TYR:OH	2.32	0.47
55:z:87:ALA:O	55:z:315:GLN:NE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:z:182:THR:O	55:z:182:THR:HG23	2.15	0.47
1:A:2396:U:H4'	1:A:2396:U:OP1	2.15	0.47
8:J:30:ILE:HD13	58:t:245:THR:HA	1.96	0.47
11:M:67:GLU:OE2	11:M:73:PHE:N	2.44	0.47
1:A:1235:U:H2'	34:d:55:THR:HG21	1.97	0.47
20:W:70:GLN:OE1	20:W:74:ARG:N	2.47	0.47
1:A:1168:U:OP2	28:3:108:LYS:NZ	2.44	0.47
1:A:1295:A:O2'	1:A:1331:C:O2	2.25	0.47
1:A:1413:G:OP1	1:A:1415:G:O2'	2.29	0.47
1:A:1728:A:OP2	15:R:17:ARG:NH2	2.44	0.47
1:A:2312:A:H4'	13:P:179:TYR:CD2	2.50	0.47
1:A:2653:C:OP2	4:E:298:LYS:NZ	2.38	0.47
4:E:243:ILE:CG2	4:E:251:VAL:HG13	2.45	0.47
5:F:175:LYS:O	5:F:179:THR:HG23	2.15	0.47
5:F:241:ASN:OD1	5:F:256:HIS:NE2	2.43	0.47
11:M:67:GLU:OE1	11:M:70:GLN:NE2	2.43	0.47
17:T:69:HIS:NE2	17:T:117:GLU:OE1	2.45	0.47
30:6:177:TYR:O	30:6:185:ILE:N	2.48	0.47
31:7:105:VAL:HG13	31:7:120:CYS:SG	2.55	0.47
37:g:154:ASP:OD1	37:g:154:ASP:N	2.47	0.47
46:s:374:THR:O	46:s:378:ASP:N	2.46	0.47
54:m:45:GLN:O	54:m:46:ALA:HB3	2.14	0.47
58:t:225:GLU:O	58:t:271:LYS:NZ	2.48	0.47
1:A:1228:G:O6	19:V:41:ARG:NH1	2.48	0.47
5:F:220:ASP:O	5:F:245:ALA:N	2.48	0.47
1:A:2332:U:H4'	1:A:2333:U:OP1	2.14	0.47
36:f:187:GLU:OE1	36:f:187:GLU:N	2.45	0.47
16:S:103:VAL:HG11	16:S:134:LEU:HD13	1.96	0.47
30:6:227:GLU:OE1	30:6:229:ASP:N	2.47	0.47
1:A:1727:A:OP2	11:M:38:ARG:NH2	2.48	0.46
1:A:1831:U:H2'	1:A:1832:A:O4'	2.14	0.46
58:t:281:ASP:OD1	58:t:281:ASP:N	2.48	0.46
1:A:2076:A:H4'	1:A:2077:A:OP1	2.15	0.46
24:x:136:VAL:O	24:x:136:VAL:CG1	2.63	0.46
36:f:104:SER:O	36:f:107:GLN:NE2	2.48	0.46
13:P:51:ARG:NH2	30:6:221:LEU:O	2.47	0.46
55:z:210:ILE:O	55:z:210:ILE:HG22	2.15	0.46
58:t:238:GLY:O	58:t:241:LEU:HD22	2.15	0.46
1:A:2073:G:H5''	1:A:2074:C:OP2	2.15	0.46
5:F:292:ASP:OD1	5:F:292:ASP:N	2.46	0.46
10:L:33:GLN:H	10:L:36:THR:HG21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:88:ILE:HD12	17:T:136:ILE:HD13	1.96	0.46
18:U:111:PHE:N	18:U:112:PRO:HD3	2.30	0.46
1:A:2482:G:N2	1:A:2485:C:O4'	2.47	0.46
8:J:33:PRO:N	8:J:34:PRO:CD	2.78	0.46
8:J:141:VAL:CG1	56:l:96:VAL:HG11	2.46	0.46
9:K:7:ALA:HB3	9:K:8:PRO:HD3	1.97	0.46
34:d:89:ASP:OD2	34:d:207:ARG:NE	2.49	0.46
46:s:404:VAL:HG23	46:s:404:VAL:O	2.15	0.46
53:a:53:ASP:OD1	53:a:54:GLY:N	2.49	0.46
3:D:218:LEU:HD11	3:D:228:GLN:HB2	1.97	0.46
22:Y:85:ALA:N	52:9:72:VAL:O	2.49	0.46
32:b:12:THR:HG22	32:b:13:SER:N	2.30	0.46
32:b:121:THR:O	53:a:141:ARG:NH1	2.46	0.46
55:z:221:LEU:HD13	55:z:239:LEU:HD11	1.98	0.46
1:A:2260:C:O2'	1:A:2356:C:OP2	2.33	0.46
1:A:2397:A:O2'	1:A:2410:G:N2	2.48	0.46
1:A:2480:U:H3'	1:A:2481:U:H5'	1.96	0.46
4:E:56:GLU:OE1	4:E:56:GLU:N	2.45	0.46
6:H:102:ILE:O	6:H:102:ILE:HG22	2.15	0.46
6:H:104:VAL:HG12	6:H:105:ARG:N	2.31	0.46
45:r:115:ILE:O	45:r:119:VAL:HG23	2.16	0.46
8:J:123:VAL:HG12	8:J:123:VAL:O	2.14	0.46
16:S:137:VAL:HG13	16:S:137:VAL:O	2.15	0.46
33:c:86:ASP:N	33:c:86:ASP:OD1	2.48	0.46
55:z:191:VAL:HG21	55:z:199:LEU:HD12	1.98	0.46
1:A:1447:G:N7	11:M:53:LYS:NZ	2.53	0.46
1:A:1681:A:H5''	1:A:1682:A:OP2	2.15	0.46
1:A:2441:C:H4'	4:E:224:PHE:CE2	2.50	0.46
30:6:240:ILE:HD13	30:6:248:GLY:HA3	1.97	0.46
53:a:61:HIS:ND1	53:a:61:HIS:O	2.49	0.46
9:K:73:GLU:N	9:K:73:GLU:OE1	2.49	0.46
15:R:122:ARG:NH2	16:S:76:GLU:OE2	2.49	0.46
19:V:93:THR:CG2	19:V:110:ALA:HB1	2.46	0.46
22:Y:171:ARG:NH1	22:Y:196:TYR:OH	2.44	0.46
24:x:64:ARG:NH1	57:y:270:ARG:O	2.48	0.46
40:j:106:ASP:CG	40:j:107:LEU:H	2.24	0.46
55:z:174:ARG:O	55:z:181:ILE:HG21	2.16	0.46
4:E:247:ASP:OD1	4:E:248:ILE:N	2.48	0.45
8:J:92:LYS:O	8:J:96:GLY:N	2.49	0.45
31:7:164:VAL:O	31:7:233:LYS:NZ	2.49	0.45
24:x:305:SER:OG	24:x:372:MET:SD	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:89:VAL:O	32:b:89:VAL:CG1	2.63	0.45
1:A:1893:C:O2'	1:A:1894:A:OP2	2.33	0.45
24:x:334:GLN:NE2	24:x:335:VAL:O	2.49	0.45
31:7:273:PHE:HB2	31:7:301:THR:HG22	1.99	0.45
50:5:177:CYS:N	50:5:178:PRO:CD	2.80	0.45
1:A:1194:A:O2'	1:A:1195:G:P	2.75	0.45
46:s:356:THR:OG1	46:s:360:TYR:O	2.29	0.45
49:w:79:ILE:CG2	49:w:145:VAL:HG13	2.46	0.45
56:l:107:LEU:HD13	56:l:114:TYR:HA	1.98	0.45
58:t:303:LEU:H	58:t:303:LEU:HD23	1.82	0.45
1:A:2122:U:O4'	1:A:2134:G:N2	2.49	0.45
32:b:26:LEU:HD22	32:b:105:ALA:HA	1.97	0.45
36:f:126:MET:SD	36:f:155:VAL:HG23	2.57	0.45
37:g:44:GLU:OE1	37:g:44:GLU:N	2.47	0.45
58:t:161:LYS:N	62:t:501:GNP:O1B	2.50	0.45
1:A:1120:A:OP2	22:Y:182:LYS:NZ	2.43	0.45
1:A:1386:G:N7	17:T:154:GLY:O	2.50	0.45
2:B:15:A:O2'	2:B:17:A:N6	2.43	0.45
33:c:148:LEU:HD12	33:c:149:PRO:HD2	1.97	0.45
38:h:76:LYS:O	38:h:80:GLY:N	2.48	0.45
58:t:27:SER:O	58:t:72:GLY:N	2.43	0.45
21:X:117:GLU:N	21:X:142:ASP:OD2	2.50	0.45
25:0:144:GLU:OE2	25:0:172:ARG:NH1	2.43	0.45
35:e:50:CYS:N	35:e:232:PHE:O	2.42	0.45
35:e:275:LEU:HD11	51:8:139:MET:HG2	1.99	0.45
1:A:1199:C:N4	1:A:1200:U:O4	2.50	0.45
50:5:277:THR:O	50:5:320:ASN:ND2	2.49	0.45
58:t:326:THR:OG1	62:t:501:GNP:O6	2.33	0.45
1:A:1790:U:O2'	1:A:2110:G:O2'	2.31	0.45
13:P:42:GLU:OE2	30:6:338:ARG:NH1	2.50	0.45
17:T:88:ILE:HD11	17:T:168:TYR:OH	2.16	0.45
44:q:60:GLN:O	44:q:68:SER:OG	2.34	0.45
46:s:240:GLN:OE1	46:s:347:ARG:NH1	2.46	0.45
1:A:1345:A:OP1	27:2:63:LYS:NZ	2.44	0.45
1:A:2559:U:O2	1:A:2580:G:N2	2.49	0.45
2:B:31:C:OP2	54:m:41:ARG:NH2	2.44	0.45
24:x:257:THR:HG23	24:x:257:THR:O	2.17	0.45
32:b:131:HIS:CE1	32:b:134:THR:HG23	2.52	0.45
1:A:2328:C:O2'	1:A:2329:U:OP1	2.35	0.44
7:I:102:VAL:HG21	7:I:235:PHE:HD2	1.82	0.44
24:x:309:LEU:HD13	24:x:360:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:d:43:ARG:HD3	34:d:44:PHE:H	1.82	0.44
34:d:160:CYS:O	34:d:164:SER:N	2.50	0.44
1:A:1712:U:OP1	5:F:255:LYS:NZ	2.50	0.44
1:A:1846:U:O2'	50:5:268:CYS:SG	2.73	0.44
12:O:58:LYS:NZ	14:Q:269:MET:O	2.41	0.44
43:p:164:GLN:NE2	43:p:165:VAL:O	2.50	0.44
50:5:175:THR:O	50:5:175:THR:HG22	2.17	0.44
1:A:1623:C:H2'	1:A:1624:A:H5'	2.00	0.44
11:M:105:ASP:OD2	37:g:70:SER:OG	2.28	0.44
24:x:296:THR:O	24:x:379:ARG:NH1	2.51	0.44
33:c:256:ARG:NH2	53:a:71:THR:O	2.45	0.44
48:v:43:GLN:N	48:v:43:GLN:OE1	2.51	0.44
1:A:1930:C:H2'	1:A:1931:C:H5'	2.00	0.44
1:A:2302:U:O2'	1:A:2303:A:P	2.75	0.44
11:M:287:GLU:OE1	11:M:287:GLU:N	2.46	0.44
13:P:91:GLU:OE1	13:P:91:GLU:N	2.50	0.44
34:d:195:VAL:HG12	34:d:196:GLU:N	2.33	0.44
55:z:194:ARG:HB3	55:z:195:PRO:HD3	2.00	0.44
1:A:1559:A:C8	1:A:1559:A:OP2	2.70	0.44
5:F:102:TRP:O	5:F:106:PHE:CD1	2.70	0.44
19:V:154:ILE:HG23	19:V:154:ILE:O	2.16	0.44
31:7:164:VAL:HG13	31:7:165:ARG:N	2.32	0.44
1:A:1553:C:O2'	1:A:1554:G:O5'	2.34	0.44
1:A:2290:A:H61	44:q:140:ARG:HG3	1.83	0.44
1:A:2191:U:O2	21:X:108:GLN:NE2	2.43	0.44
30:6:177:TYR:N	30:6:185:ILE:O	2.51	0.44
1:A:1172:G:N2	1:A:1175:G:H3'	2.33	0.44
1:A:2629:A:N3	1:A:2629:A:H2'	2.33	0.44
30:6:125:LEU:O	30:6:126:ARG:HG2	2.18	0.44
35:e:52:GLN:O	35:e:236:LEU:N	2.51	0.44
37:g:42:VAL:HG12	37:g:42:VAL:O	2.16	0.44
1:A:1615:G:H2'	1:A:1616:C:C6	2.53	0.44
1:A:1220:G:OP2	27:2:85:LYS:NZ	2.51	0.43
12:O:92:VAL:HG13	12:O:93:LEU:HD12	1.99	0.43
21:X:35:GLU:O	21:X:35:GLU:HG3	2.17	0.43
35:e:119:GLU:OE1	54:m:72:ARG:NH2	2.51	0.43
46:s:147:GLU:OE2	46:s:169:SER:HB2	2.18	0.43
46:s:326:LEU:HD21	46:s:353:ALA:HB2	1.99	0.43
51:8:135:ALA:HB1	51:8:139:MET:HE3	2.00	0.43
55:z:115:ASP:HA	55:z:118:ILE:HD12	2.00	0.43
1:A:1495:C:OP1	20:W:74:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2177:A:N3	1:A:2362:A:O2'	2.50	0.43
1:A:2480:U:H2'	1:A:2481:U:H5''	2.01	0.43
5:F:284:TYR:CE1	11:M:191:PRO:CG	3.02	0.43
46:s:103:ASP:OD1	46:s:104:ARG:N	2.51	0.43
58:t:172:THR:N	58:t:173:PRO:HD3	2.34	0.43
58:t:208:GLU:OE2	58:t:248:ARG:HG2	2.19	0.43
1:A:1232:G:OP2	19:V:33:ARG:NH2	2.51	0.43
14:Q:237:ASN:OD1	14:Q:238:PHE:N	2.51	0.43
17:T:84:LEU:HB3	17:T:111:ILE:HD12	2.00	0.43
31:7:41:ARG:NE	31:7:226:ILE:O	2.52	0.43
31:7:174:GLY:O	31:7:297:LEU:HD21	2.18	0.43
49:w:100:VAL:O	49:w:100:VAL:HG12	2.17	0.43
1:A:1457:A:N3	1:A:1457:A:H2'	2.33	0.43
1:A:1711:A:O4'	5:F:104:ARG:NH2	2.52	0.43
28:3:159:ASP:O	28:3:167:LYS:NZ	2.51	0.43
34:d:253:GLU:N	34:d:253:GLU:OE1	2.52	0.43
55:z:118:ILE:O	55:z:121:ILE:HG22	2.18	0.43
58:t:314:LYS:O	58:t:315:ALA:HB3	2.19	0.43
1:A:1174:A:H4'	1:A:1175:G:H5''	2.01	0.43
1:A:1608:C:O2'	1:A:1609:C:P	2.76	0.43
1:A:2461:G:O2'	1:A:2566:A:N1	2.49	0.43
47:u:212:GLY:O	47:u:213:LEU:C	2.61	0.43
1:A:2111:U:H2'	1:A:2112:G:O4'	2.19	0.43
5:F:87:PHE:C	5:F:179:THR:HG22	2.44	0.43
17:T:150:ILE:HG23	17:T:150:ILE:O	2.17	0.43
39:i:68:LYS:NZ	39:i:72:GLU:OE1	2.45	0.43
46:s:205:LEU:O	46:s:373:LEU:O	2.37	0.43
57:y:227:PRO:O	57:y:228:ASN:HB2	2.18	0.43
58:t:207:ILE:HG22	58:t:208:GLU:N	2.34	0.43
1:A:1543:U:H2'	1:A:1544:C:O4'	2.18	0.43
28:3:96:TYR:N	39:i:122:ASN:OD1	2.52	0.43
31:7:67:VAL:O	31:7:67:VAL:HG22	2.19	0.43
37:g:156:GLN:OE1	37:g:156:GLN:N	2.43	0.43
57:y:298:GLU:OE1	57:y:298:GLU:N	2.43	0.43
1:A:1208:U:O4'	19:V:40:ARG:NH2	2.52	0.43
1:A:2161:G:O2'	1:A:2162:A:H5'	2.18	0.43
1:A:1102:U:O2'	1:A:1103:A:P	2.76	0.43
1:A:1176:A:C5	1:A:1177:A:H1'	2.54	0.43
1:A:2293:A:OP1	28:3:138:THR:OG1	2.25	0.43
21:X:111:THR:HG23	21:X:111:THR:O	2.19	0.43
46:s:391:GLN:O	46:s:393:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1956:G:N7	3:D:231:SER:OG	2.51	0.42
1:A:2329:U:O4'	1:A:2329:U:OP1	2.37	0.42
2:B:50:A:H2'	2:B:51:A:C1'	2.49	0.42
14:Q:192:ASP:OD2	14:Q:233:TRP:NE1	2.38	0.42
45:r:114:LYS:NZ	45:r:183:ASP:OD2	2.51	0.42
56:l:96:VAL:HG12	56:l:97:ASN:N	2.33	0.42
58:t:39:GLY:N	58:t:125:GLY:O	2.52	0.42
58:t:83:SER:O	58:t:84:LYS:HB3	2.19	0.42
58:t:203:LEU:HB2	58:t:204:PRO:HD2	2.01	0.42
1:A:1595:U:O2'	1:A:1596:A:P	2.76	0.42
1:A:1607:G:O3'	8:J:92:LYS:NZ	2.47	0.42
13:P:156:ASP:OD1	13:P:157:SER:N	2.52	0.42
14:Q:225:LYS:HB2	14:Q:226:PRO:CD	2.49	0.42
6:H:105:ARG:NH1	6:H:140:GLU:OE1	2.52	0.42
7:I:102:VAL:HG21	7:I:235:PHE:CD2	2.55	0.42
20:W:61:VAL:HG21	20:W:97:VAL:HG23	2.00	0.42
22:Y:207:VAL:HG12	22:Y:207:VAL:O	2.20	0.42
30:6:122:ALA:O	30:6:126:ARG:N	2.53	0.42
43:p:113:GLU:O	43:p:116:VAL:HG12	2.20	0.42
50:5:401:VAL:HG23	50:5:401:VAL:O	2.20	0.42
55:z:249:PHE:O	55:z:252:VAL:HG22	2.19	0.42
1:A:1444:C:OP2	11:M:58:ARG:NH1	2.52	0.42
1:A:1947:U:H5''	1:A:1948:C:OP1	2.20	0.42
8:J:139:SER:O	8:J:143:SER:OG	2.28	0.42
30:6:219:ILE:HD13	30:6:300:THR:HG21	2.01	0.42
30:6:370:ARG:O	30:6:370:ARG:HG3	2.19	0.42
33:c:46:GLU:O	33:c:50:LEU:HG	2.19	0.42
35:e:181:THR:HG23	35:e:184:GLY:H	1.83	0.42
1:A:1187:U:H4'	1:A:1188:A:OP2	2.18	0.42
24:x:191:THR:O	24:x:195:ARG:NH1	2.53	0.42
41:k:77:ARG:O	41:k:81:LEU:HD23	2.19	0.42
44:q:78:THR:O	44:q:82:LEU:N	2.39	0.42
1:A:1615:G:O2'	1:A:1632:A:H5'	2.19	0.42
1:A:1630:G:C4	1:A:1632:A:H1'	2.55	0.42
1:A:1922:G:H2'	1:A:1923:A:H5''	2.01	0.42
12:O:9:ILE:O	12:O:9:ILE:HG22	2.19	0.42
20:W:148:LEU:O	30:6:339:GLU:N	2.52	0.42
32:b:142:GLY:N	53:a:70:HIS:O	2.51	0.42
58:t:33:PRO:HA	58:t:127:LEU:HD22	2.02	0.42
1:A:1175:G:O2'	1:A:1176:A:P	2.75	0.42
1:A:1697:A:H5'	16:S:180:LYS:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1979:G:H1	1:A:2073:G:H22	1.68	0.42
1:A:2102:U:OP2	12:O:17:ARG:NE	2.53	0.42
11:M:155:VAL:O	11:M:175:THR:HA	2.20	0.42
12:O:94:ALA:HB3	12:O:95:PRO:HD3	2.00	0.42
31:7:77:VAL:HG23	31:7:77:VAL:O	2.19	0.42
41:k:26:ASN:OD1	41:k:26:ASN:N	2.53	0.42
55:z:122:VAL:HG21	55:z:166:HIS:CE1	2.55	0.42
21:X:156:LYS:NZ	21:X:205:GLY:O	2.53	0.42
1:A:1137:A:HO2'	1:A:1138:U:P	2.40	0.42
1:A:1663:A:N3	1:A:2445:A:O2'	2.43	0.42
7:I:233:VAL:HG23	7:I:233:VAL:O	2.20	0.42
41:k:61:GLU:N	41:k:62:PRO:CD	2.83	0.42
1:A:1614:A:H5''	1:A:1616:C:OP2	2.20	0.42
1:A:2288:U:OP1	26:1:38:ARG:NH2	2.53	0.42
30:6:270:PHE:N	30:6:317:ALA:O	2.43	0.42
46:s:255:ILE:H	46:s:255:ILE:HD12	1.83	0.42
48:v:23:LEU:HD21	48:v:26:THR:HB	2.02	0.42
1:A:1602:U:C2'	1:A:1603:G:O5'	2.66	0.41
3:D:202:GLY:O	50:5:30:ALA:N	2.53	0.41
7:I:132:LYS:NZ	7:I:144:LEU:O	2.52	0.41
8:J:135:VAL:N	8:J:136:PRO:HD2	2.35	0.41
22:Y:87:TRP:O	22:Y:143:ASN:ND2	2.51	0.41
29:4:71:ILE:CG2	29:4:89:ILE:HD12	2.50	0.41
43:p:114:GLU:HB3	43:p:115:PRO:HD3	2.02	0.41
58:t:126:LYS:HB2	58:t:129:THR:HG22	2.02	0.41
1:A:1506:A:HO2'	1:A:1507:A:H8	1.64	0.41
1:A:1565:U:H5'	23:Z:74:SER:HB2	2.02	0.41
8:J:123:VAL:O	8:J:123:VAL:CG1	2.68	0.41
10:L:41:VAL:HG13	10:L:121:ILE:HD12	2.01	0.41
35:e:272:ARG:NH1	51:8:145:GLU:OE2	2.54	0.41
36:f:126:MET:HE2	36:f:153:GLU:HB2	2.01	0.41
47:u:98:GLU:OE2	47:u:100:ALA:HB2	2.20	0.41
1:A:1607:G:N2	1:A:1620:C:O2	2.53	0.41
1:A:1981:C:O2	1:A:2072:G:N2	2.53	0.41
1:A:2073:G:H3'	1:A:2074:C:H5''	2.02	0.41
4:E:142:ILE:HG22	4:E:143:ALA:N	2.35	0.41
7:I:146:LEU:HD12	7:I:239:LEU:HB3	2.01	0.41
7:I:227:VAL:O	7:I:231:LYS:N	2.45	0.41
34:d:245:GLU:HG2	34:d:246:ASP:H	1.85	0.41
1:A:2130:A:HO2'	1:A:2131:A:P	2.42	0.41
1:A:2515:C:H2'	1:A:2516:A:C5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:x:257:THR:OG1	24:x:260:HIS:HB3	2.20	0.41
32:b:12:THR:HG22	32:b:13:SER:O	2.19	0.41
58:t:232:PHE:O	58:t:276:ALA:N	2.47	0.41
1:A:1568:A:O2'	1:A:1569:U:P	2.78	0.41
1:A:1646:A:H3'	1:A:1647:A:H5''	2.02	0.41
1:A:2161:G:O4'	1:A:2161:G:OP1	2.38	0.41
3:D:181:ASP:OD1	3:D:181:ASP:O	2.37	0.41
21:X:124:THR:HG23	21:X:124:THR:O	2.19	0.41
55:z:174:ARG:NH2	55:z:181:ILE:O	2.53	0.41
55:z:195:PRO:HB2	55:z:197:VAL:HG23	2.02	0.41
1:A:1891:U:H2'	1:A:1892:C:O4'	2.20	0.41
31:7:60:GLU:OE1	31:7:60:GLU:N	2.53	0.41
46:s:400:GLU:HG2	46:s:405:LYS:HD2	2.03	0.41
55:z:221:LEU:HD23	55:z:318:LEU:HD21	2.02	0.41
1:A:1616:C:OP1	1:A:1631:A:O2'	2.39	0.41
1:A:2666:A:OP2	4:E:212:GLY:N	2.52	0.41
8:J:26:ALA:HB3	8:J:62:GLU:HA	2.03	0.41
30:6:215:THR:HG22	30:6:238:THR:HA	2.02	0.41
55:z:29:TRP:O	55:z:30:PHE:C	2.64	0.41
55:z:162:LEU:HB3	55:z:191:VAL:HG13	2.03	0.41
2:B:33:G:N2	36:f:123:SER:O	2.51	0.41
5:F:214:SER:N	5:F:257:GLN:OE1	2.52	0.41
11:M:37:ARG:HB3	11:M:44:ARG:HD3	2.02	0.41
31:7:188:GLU:OE1	31:7:188:GLU:N	2.53	0.41
32:b:47:VAL:O	32:b:51:VAL:HG12	2.21	0.41
36:f:89:VAL:O	36:f:89:VAL:HG23	2.19	0.41
44:q:142:ARG:O	44:q:146:ILE:HG13	2.20	0.41
50:5:355:LEU:HD11	50:5:374:VAL:CG2	2.50	0.41
55:z:283:VAL:O	55:z:283:VAL:HG13	2.20	0.41
58:t:19:LEU:H	58:t:19:LEU:HD23	1.86	0.41
1:A:1614:A:H4'	1:A:1615:G:OP2	2.21	0.41
1:A:1630:G:N2	56:l:127:ASN:OD1	2.50	0.41
1:A:1683:C:H1'	1:A:1684:U:P	2.61	0.41
1:A:1851:C:O2	46:s:159:LEU:HD13	2.21	0.41
1:A:1930:C:C2'	1:A:1931:C:H5'	2.50	0.41
5:F:226:MET:SD	5:F:242:LEU:HD21	2.61	0.41
5:F:280:TYR:OH	11:M:108:ARG:NE	2.53	0.41
10:L:96:MET:HE1	14:Q:171:ILE:HD11	2.02	0.41
11:M:75:ILE:O	11:M:75:ILE:HG22	2.21	0.41
14:Q:152:ARG:HH12	14:Q:191:ARG:N	2.19	0.41
16:S:174:ILE:HD12	32:b:2:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:26:ILE:CG2	18:U:44:ILE:HG22	2.51	0.41
19:V:96:ARG:NE	19:V:111:SER:OG	2.46	0.41
21:X:80:TRP:CD1	21:X:80:TRP:N	2.88	0.41
25:O:153:VAL:HG21	25:O:170:GLY:O	2.21	0.41
47:u:115:THR:HG21	47:u:170:VAL:HG22	2.01	0.41
55:z:85:ASP:OD1	55:z:85:ASP:N	2.54	0.41
58:t:280:MET:HG2	58:t:325:SER:HB2	2.03	0.41
1:A:1821:A:C2	3:D:129:VAL:HG11	2.56	0.41
1:A:2350:G:OP1	26:1:63:ARG:NH1	2.54	0.41
4:E:91:GLU:N	4:E:91:GLU:OE1	2.54	0.41
7:I:250:ARG:HE	41:k:55:VAL:HG11	1.85	0.41
10:L:43:ASN:ND2	10:L:117:THR:OG1	2.46	0.41
39:i:34:VAL:HG12	39:i:35:ARG:N	2.36	0.41
47:u:188:TRP:O	47:u:191:ARG:NE	2.52	0.41
55:z:320:ARG:HA	55:z:323:ILE:CD1	2.51	0.41
1:A:1607:G:H2'	1:A:1608:C:H5'	2.03	0.40
1:A:1683:C:C1'	1:A:1684:U:P	3.09	0.40
1:A:2337:C:H2'	1:A:2338:C:O4'	2.22	0.40
2:B:7:G:N2	2:B:60:C:N3	2.68	0.40
7:I:220:GLU:N	7:I:220:GLU:OE1	2.54	0.40
9:K:156:ASP:OD1	9:K:157:GLU:N	2.54	0.40
11:M:35:ARG:NH1	11:M:36:GLU:O	2.54	0.40
12:O:115:GLU:O	12:O:115:GLU:HG2	2.20	0.40
14:Q:153:ASN:OD1	14:Q:154:THR:N	2.50	0.40
16:S:103:VAL:HG11	16:S:134:LEU:CD1	2.51	0.40
37:g:135:THR:HG23	37:g:135:THR:O	2.22	0.40
1:A:2334:G:O2'	1:A:2353:C:N4	2.49	0.40
4:E:230:SER:O	4:E:231:HIS:HB2	2.22	0.40
5:F:284:TYR:OH	11:M:188:LYS:HA	2.21	0.40
9:K:73:GLU:OE2	45:r:149:ARG:NH2	2.53	0.40
12:O:43:GLU:OE2	25:O:126:TYR:OH	2.32	0.40
1:A:1644:U:O2'	1:A:1645:C:P	2.80	0.40
1:A:2635:A:O2'	45:r:155:ALA:N	2.40	0.40
9:K:64:HIS:O	45:r:148:ASN:ND2	2.52	0.40
11:M:141:GLU:HB2	11:M:161:LEU:HD23	2.03	0.40
19:V:122:LEU:HD21	19:V:154:ILE:HD13	2.03	0.40
19:V:206:GLU:OE1	19:V:207:THR:N	2.55	0.40
35:e:81:LEU:N	54:m:47:TYR:O	2.52	0.40
1:A:1928:C:O2'	1:A:1943:A:O4'	2.37	0.40
1:A:2089:A:H2'	1:A:2090:C:O4'	2.21	0.40
1:A:2570:A:H2'	1:A:2571:A:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2302:U:HO2'	1:A:2303:A:P	2.45	0.40
1:A:2325:U:H2'	1:A:2326:A:H5''	2.04	0.40
7:I:119:HIS:O	7:I:120:LYS:HG2	2.21	0.40
23:Z:69:VAL:HG11	23:Z:110:LEU:HD11	2.02	0.40
24:x:309:LEU:HD21	24:x:371:PRO:HB3	2.04	0.40
35:e:168:VAL:HG12	35:e:169:TRP:N	2.35	0.40
35:e:170:MET:SD	35:e:267:LEU:HD11	2.62	0.40
38:h:149:LEU:HB3	38:h:150:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	223/306 (73%)	221 (99%)	2 (1%)	0	100	100
4	E	306/348 (88%)	297 (97%)	9 (3%)	0	100	100
5	F	248/294 (84%)	244 (98%)	4 (2%)	0	100	100
6	H	93/265 (35%)	87 (94%)	6 (6%)	0	100	100
7	I	133/262 (51%)	131 (98%)	2 (2%)	0	100	100
8	J	96/192 (50%)	95 (99%)	1 (1%)	0	100	100
9	K	175/178 (98%)	175 (100%)	0	0	100	100
10	L	113/145 (78%)	111 (98%)	2 (2%)	0	100	100
11	M	285/295 (97%)	277 (97%)	8 (3%)	0	100	100
12	O	151/176 (86%)	145 (96%)	6 (4%)	0	100	100
13	P	139/180 (77%)	139 (100%)	0	0	100	100
14	Q	215/292 (74%)	212 (99%)	3 (1%)	0	100	100
15	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	S	157/209 (75%)	149 (95%)	8 (5%)	0	100	100
17	T	164/206 (80%)	159 (97%)	5 (3%)	0	100	100
18	U	123/146 (84%)	121 (98%)	2 (2%)	0	100	100
19	V	199/216 (92%)	194 (98%)	5 (2%)	0	100	100
20	W	98/148 (66%)	95 (97%)	3 (3%)	0	100	100
21	X	240/257 (93%)	237 (99%)	3 (1%)	0	100	100
22	Y	174/252 (69%)	174 (100%)	0	0	100	100
23	Z	110/160 (69%)	109 (99%)	1 (1%)	0	100	100
24	x	322/381 (84%)	311 (97%)	10 (3%)	1 (0%)	37	67
25	0	106/187 (57%)	104 (98%)	2 (2%)	0	100	100
26	1	50/65 (77%)	50 (100%)	0	0	100	100
27	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
28	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
29	4	35/101 (35%)	35 (100%)	0	0	100	100
30	6	306/380 (80%)	303 (99%)	3 (1%)	0	100	100
31	7	290/336 (86%)	279 (96%)	11 (4%)	0	100	100
32	b	146/159 (92%)	143 (98%)	3 (2%)	0	100	100
33	c	275/308 (89%)	272 (99%)	3 (1%)	0	100	100
34	d	240/306 (78%)	234 (98%)	6 (2%)	0	100	100
35	e	187/283 (66%)	178 (95%)	8 (4%)	1 (0%)	25	59
36	f	93/211 (44%)	92 (99%)	1 (1%)	0	100	100
37	g	130/166 (78%)	128 (98%)	2 (2%)	0	100	100
38	h	108/159 (68%)	107 (99%)	1 (1%)	0	100	100
39	i	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
40	j	91/121 (75%)	87 (96%)	4 (4%)	0	100	100
41	k	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
42	o	76/102 (74%)	76 (100%)	0	0	100	100
43	p	134/206 (65%)	129 (96%)	5 (4%)	0	100	100
44	q	133/222 (60%)	133 (100%)	0	0	100	100
45	r	153/196 (78%)	153 (100%)	0	0	100	100
46	s	373/442 (84%)	363 (97%)	9 (2%)	1 (0%)	37	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	u	127/228 (56%)	124 (98%)	3 (2%)	0	100	100
48	v	67/70 (96%)	67 (100%)	0	0	100	100
49	w	77/156 (49%)	75 (97%)	2 (3%)	0	100	100
50	5	392/423 (93%)	386 (98%)	6 (2%)	0	100	100
51	8	68/206 (33%)	68 (100%)	0	0	100	100
52	9	120/135 (89%)	117 (98%)	3 (2%)	0	100	100
53	a	99/142 (70%)	95 (96%)	4 (4%)	0	100	100
54	m	43/127 (34%)	42 (98%)	1 (2%)	0	100	100
55	z	309/326 (95%)	301 (97%)	8 (3%)	0	100	100
56	l	60/135 (44%)	60 (100%)	0	0	100	100
57	y	235/346 (68%)	232 (99%)	3 (1%)	0	100	100
58	t	317/366 (87%)	297 (94%)	17 (5%)	3 (1%)	14	48
All	All	9050/12193 (74%)	8853 (98%)	191 (2%)	6 (0%)	50	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
46	s	151	VAL
58	t	244	VAL
35	e	141	LYS
24	x	180	ALA
58	t	247	TYR
58	t	327	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	186/246 (76%)	186 (100%)	0	100	100
4	E	270/298 (91%)	270 (100%)	0	100	100
5	F	216/250 (86%)	216 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	H	86/228 (38%)	86 (100%)	0	100	100
7	I	128/230 (56%)	128 (100%)	0	100	100
8	J	83/152 (55%)	83 (100%)	0	100	100
9	K	157/158 (99%)	157 (100%)	0	100	100
10	L	99/122 (81%)	99 (100%)	0	100	100
11	M	248/252 (98%)	248 (100%)	0	100	100
12	O	133/152 (88%)	133 (100%)	0	100	100
13	P	123/157 (78%)	123 (100%)	0	100	100
14	Q	197/258 (76%)	197 (100%)	0	100	100
15	R	119/128 (93%)	119 (100%)	0	100	100
16	S	145/180 (81%)	145 (100%)	0	100	100
17	T	147/180 (82%)	147 (100%)	0	100	100
18	U	114/133 (86%)	114 (100%)	0	100	100
19	V	179/190 (94%)	179 (100%)	0	100	100
20	W	84/116 (72%)	84 (100%)	0	100	100
21	X	219/230 (95%)	219 (100%)	0	100	100
22	Y	162/228 (71%)	162 (100%)	0	100	100
23	Z	105/146 (72%)	105 (100%)	0	100	100
24	x	283/334 (85%)	283 (100%)	0	100	100
25	0	97/170 (57%)	97 (100%)	0	100	100
26	1	49/60 (82%)	49 (100%)	0	100	100
27	2	40/77 (52%)	40 (100%)	0	100	100
28	3	88/165 (53%)	88 (100%)	0	100	100
29	4	35/90 (39%)	35 (100%)	0	100	100
30	6	277/335 (83%)	277 (100%)	0	100	100
31	7	269/301 (89%)	269 (100%)	0	100	100
32	b	130/138 (94%)	130 (100%)	0	100	100
33	c	243/266 (91%)	243 (100%)	0	100	100
34	d	217/272 (80%)	217 (100%)	0	100	100
35	e	166/238 (70%)	166 (100%)	0	100	100
36	f	91/185 (49%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	g	122/148 (82%)	122 (100%)	0	100	100
38	h	100/143 (70%)	100 (100%)	0	100	100
39	i	87/111 (78%)	87 (100%)	0	100	100
40	j	75/99 (76%)	75 (100%)	0	100	100
41	k	72/95 (76%)	72 (100%)	0	100	100
42	o	65/85 (76%)	65 (100%)	0	100	100
43	p	126/177 (71%)	126 (100%)	0	100	100
44	q	117/187 (63%)	117 (100%)	0	100	100
45	r	142/168 (84%)	142 (100%)	0	100	100
46	s	329/378 (87%)	329 (100%)	0	100	100
47	u	118/197 (60%)	118 (100%)	0	100	100
48	v	60/61 (98%)	60 (100%)	0	100	100
49	w	73/135 (54%)	73 (100%)	0	100	100
50	5	356/372 (96%)	356 (100%)	0	100	100
51	8	62/182 (34%)	62 (100%)	0	100	100
52	9	104/114 (91%)	104 (100%)	0	100	100
53	a	97/129 (75%)	97 (100%)	0	100	100
54	m	40/114 (35%)	40 (100%)	0	100	100
55	z	270/280 (96%)	270 (100%)	0	100	100
56	l	59/112 (53%)	59 (100%)	0	100	100
57	y	220/322 (68%)	220 (100%)	0	100	100
58	t	266/306 (87%)	266 (100%)	0	100	100
All	All	8145/10580 (77%)	8145 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	100	HIS
3	D	102	GLN
4	E	52	HIS
4	E	227	GLN
6	H	71	HIS

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Mol	Chain	Res	Type
6	H	85	HIS
7	I	119	HIS
9	K	74	GLN
10	L	59	HIS
11	M	83	ASN
12	O	98	GLN
12	O	138	HIS
13	P	89	HIS
17	T	119	GLN
18	U	27	GLN
21	X	4	HIS
21	X	76	GLN
21	X	177	HIS
22	Y	94	ASN
22	Y	181	HIS
23	Z	107	ASN
23	Z	120	GLN
24	x	215	HIS
24	x	287	GLN
24	x	313	GLN
24	x	328	GLN
26	1	31	ASN
29	4	99	GLN
30	6	77	HIS
30	6	292	GLN
30	6	307	HIS
32	b	16	HIS
32	b	27	GLN
33	c	73	GLN
33	c	139	GLN
34	d	80	HIS
34	d	176	HIS
34	d	260	HIS
35	e	73	GLN
36	f	110	HIS
37	g	63	HIS
38	h	111	HIS
39	i	59	ASN
41	k	80	HIS
44	q	38	HIS
45	r	167	HIS
46	s	393	GLN

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Mol	Chain	Res	Type
46	s	414	GLN
48	v	54	GLN
50	5	320	ASN
53	a	125	HIS
55	z	315	GLN
57	y	143	ASN
57	y	148	ASN
57	y	224	GLN
58	t	50	HIS
58	t	158	ASN
58	t	197	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1403/1584 (88%)	464 (33%)	24 (1%)
2	B	58/68 (85%)	23 (39%)	2 (3%)
All	All	1461/1652 (88%)	487 (33%)	26 (1%)

All (487) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1094	A
1	A	1100	C
1	A	1101	C
1	A	1102	U
1	A	1103	A
1	A	1104	G
1	A	1112	C
1	A	1115	A
1	A	1116	C
1	A	1117	A
1	A	1118	C
1	A	1123	A
1	A	1124	U
1	A	1125	A
1	A	1131	A
1	A	1134	A
1	A	1137	A
1	A	1138	U
1	A	1139	A

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Mol	Chain	Res	Type
1	A	1140	U
1	A	1146	A
1	A	1148	A
1	A	1151	A
1	A	1152	U
1	A	1161	C
1	A	1162	U
1	A	1173	G
1	A	1175	G
1	A	1176	A
1	A	1177	A
1	A	1186	G
1	A	1188	A
1	A	1195	G
1	A	1198	G
1	A	1205	A
1	A	1221	G
1	A	1227	U
1	A	1233	A
1	A	1234	C
1	A	1235	U
1	A	1236	A
1	A	1237	A
1	A	1238	U
1	A	1240	A
1	A	1241	A
1	A	1248	G
1	A	1252	A
1	A	1255	C
1	A	1256	A
1	A	1257	A
1	A	1260	A
1	A	1264	A
1	A	1272	A
1	A	1277	U
1	A	1278	U
1	A	1279	G
1	A	1280	C
1	A	1282	U
1	A	1283	A
1	A	1284	A
1	A	1297	A

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Mol	Chain	Res	Type
1	A	1300	A
1	A	1302	U
1	A	1310	A
1	A	1311	A
1	A	1316	A
1	A	1317	U
1	A	1319	A
1	A	1320	C
1	A	1321	A
1	A	1330	C
1	A	1331	C
1	A	1337	A
1	A	1338	C
1	A	1346	G
1	A	1347	C
1	A	1364	U
1	A	1368	A
1	A	1378	U
1	A	1384	U
1	A	1385	G
1	A	1386	G
1	A	1394	G
1	A	1402	A
1	A	1413	G
1	A	1415	G
1	A	1420	A
1	A	1421	A
1	A	1422	A
1	A	1428	A
1	A	1429	C
1	A	1430	G
1	A	1432	G
1	A	1443	G
1	A	1449	U
1	A	1450	A
1	A	1457	A
1	A	1460	U
1	A	1465	U
1	A	1468	A
1	A	1473	A
1	A	1483	U
1	A	1484	U

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Mol	Chain	Res	Type
1	A	1485	G
1	A	1490	A
1	A	1491	A
1	A	1492	A
1	A	1493	A
1	A	1494	A
1	A	1495	C
1	A	1502	A
1	A	1503	U
1	A	1504	C
1	A	1506	A
1	A	1508	A
1	A	1511	U
1	A	1512	A
1	A	1513	A
1	A	1521	U
1	A	1525	A
1	A	1526	G
1	A	1532	A
1	A	1534	A
1	A	1536	G
1	A	1539	C
1	A	1540	A
1	A	1542	C
1	A	1543	U
1	A	1552	A
1	A	1553	C
1	A	1554	G
1	A	1555	G
1	A	1557	A
1	A	1558	A
1	A	1559	A
1	A	1560	A
1	A	1565	U
1	A	1566	U
1	A	1569	U
1	A	1573	G
1	A	1581	A
1	A	1583	C
1	A	1584	A
1	A	1595	U
1	A	1596	A

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Mol	Chain	Res	Type
1	A	1598	C
1	A	1599	C
1	A	1600	A
1	A	1601	U
1	A	1602	U
1	A	1606	G
1	A	1607	G
1	A	1608	C
1	A	1609	C
1	A	1611	A
1	A	1614	A
1	A	1615	G
1	A	1616	C
1	A	1621	A
1	A	1623	C
1	A	1624	A
1	A	1625	A
1	A	1626	U
1	A	1628	A
1	A	1629	A
1	A	1630	G
1	A	1631	A
1	A	1632	A
1	A	1633	A
1	A	1637	U
1	A	1638	U
1	A	1639	C
1	A	1640	A
1	A	1645	C
1	A	1647	A
1	A	1650	U
1	A	1651	A
1	A	1652	A
1	A	1664	A
1	A	1669	A
1	A	1671	A
1	A	1673	U
1	A	1675	U
1	A	1678	A
1	A	1682	A
1	A	1683	C
1	A	1684	U

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Mol	Chain	Res	Type
1	A	1690	A
1	A	1693	U
1	A	1697	A
1	A	1698	A
1	A	1716	U
1	A	1717	U
1	A	1718	U
1	A	1727	A
1	A	1730	A
1	A	1733	G
1	A	1748	A
1	A	1749	A
1	A	1755	C
1	A	1757	A
1	A	1758	A
1	A	1766	G
1	A	1767	G
1	A	1784	C
1	A	1793	C
1	A	1801	A
1	A	1805	A
1	A	1806	A
1	A	1807	U
1	A	1808	C
1	A	1823	A
1	A	1826	C
1	A	1831	U
1	A	1832	A
1	A	1835	A
1	A	1837	U
1	A	1844	C
1	A	1846	U
1	A	1851	C
1	A	1852	U
1	A	1866	A
1	A	1869	A
1	A	1871	C
1	A	1882	A
1	A	1887	A
1	A	1888	A
1	A	1892	C
1	A	1894	A

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Mol	Chain	Res	Type
1	A	1904	A
1	A	1914	G
1	A	1919	C
1	A	1922	G
1	A	1923	A
1	A	1924	A
1	A	1925	C
1	A	1930	C
1	A	1931	C
1	A	1937	A
1	A	1948	C
1	A	1957	C
1	A	1958	A
1	A	1963	A
1	A	1964	A
1	A	1965	G
1	A	1968	U
1	A	1975	C
1	A	1976	A
1	A	1979	G
1	A	1983	G
1	A	1984	C
1	A	1985	C
1	A	1987	A
1	A	1988	G
1	A	1990	G
1	A	1991	A
1	A	2040	C
1	A	2048	C
1	A	2050	U
1	A	2057	G
1	A	2058	G
1	A	2059	G
1	A	2060	A
1	A	2063	A
1	A	2068	G
1	A	2069	A
1	A	2072	G
1	A	2073	G
1	A	2074	C
1	A	2075	U
1	A	2076	A

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Mol	Chain	Res	Type
1	A	2077	A
1	A	2082	G
1	A	2084	G
1	A	2085	U
1	A	2091	U
1	A	2093	U
1	A	2097	U
1	A	2120	C
1	A	2123	U
1	A	2128	U
1	A	2131	A
1	A	2132	G
1	A	2135	G
1	A	2136	C
1	A	2143	A
1	A	2145	A
1	A	2146	A
1	A	2155	C
1	A	2156	G
1	A	2158	G
1	A	2159	A
1	A	2160	A
1	A	2161	G
1	A	2162	A
1	A	2169	G
1	A	2170	G
1	A	2175	U
1	A	2176	A
1	A	2177	A
1	A	2182	U
1	A	2185	A
1	A	2186	A
1	A	2187	C
1	A	2188	U
1	A	2193	U
1	A	2195	U
1	A	2196	U
1	A	2229	A
1	A	2230	G
1	A	2231	U
1	A	2232	A
1	A	2239	U

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Mol	Chain	Res	Type
1	A	2240	G
1	A	2241	A
1	A	2247	C
1	A	2248	G
1	A	2251	U
1	A	2252	G
1	A	2253	G
1	A	2258	A
1	A	2259	C
1	A	2279	U
1	A	2282	G
1	A	2284	A
1	A	2285	U
1	A	2286	G
1	A	2289	U
1	A	2290	A
1	A	2291	U
1	A	2292	A
1	A	2293	A
1	A	2295	C
1	A	2297	A
1	A	2303	A
1	A	2308	U
1	A	2325	U
1	A	2326	A
1	A	2328	C
1	A	2329	U
1	A	2332	U
1	A	2333	U
1	A	2334	G
1	A	2339	A
1	A	2340	G
1	A	2341	A
1	A	2342	U
1	A	2343	A
1	A	2347	U
1	A	2351	A
1	A	2352	U
1	A	2354	A
1	A	2358	G
1	A	2359	A
1	A	2360	C

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Mol	Chain	Res	Type
1	A	2363	A
1	A	2364	G
1	A	2367	A
1	A	2368	C
1	A	2369	C
1	A	2373	G
1	A	2385	G
1	A	2386	C
1	A	2387	A
1	A	2389	U
1	A	2392	U
1	A	2396	U
1	A	2398	A
1	A	2399	G
1	A	2400	A
1	A	2401	G
1	A	2402	U
1	A	2403	U
1	A	2404	C
1	A	2405	A
1	A	2406	U
1	A	2407	A
1	A	2408	U
1	A	2413	A
1	A	2415	U
1	A	2418	G
1	A	2419	G
1	A	2422	U
1	A	2424	A
1	A	2428	C
1	A	2431	C
1	A	2432	G
1	A	2437	G
1	A	2442	A
1	A	2447	A
1	A	2458	G
1	A	2462	A
1	A	2468	U
1	A	2478	G
1	A	2480	U
1	A	2481	U
1	A	2482	G

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Mol	Chain	Res	Type
1	A	2486	A
1	A	2487	A
1	A	2489	G
1	A	2493	A
1	A	2495	A
1	A	2496	G
1	A	2498	C
1	A	2501	A
1	A	2502	C
1	A	2505	G
1	A	2509	U
1	A	2511	A
1	A	2515	C
1	A	2516	A
1	A	2520	C
1	A	2521	G
1	A	2523	A
1	A	2531	A
1	A	2532	G
1	A	2533	G
1	A	2537	G
1	A	2538	U
1	A	2539	U
1	A	2542	U
1	A	2544	U
1	A	2550	U
1	A	2551	A
1	A	2552	C
1	A	2558	C
1	A	2564	G
1	A	2565	U
1	A	2570	A
1	A	2573	G
1	A	2575	C
1	A	2577	A
1	A	2578	G
1	A	2582	A
1	A	2598	A
1	A	2600	A
1	A	2601	U
1	A	2605	C
1	A	2614	C

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Mol	Chain	Res	Type
1	A	2615	U
1	A	2617	A
1	A	2618	A
1	A	2619	U
1	A	2621	U
1	A	2625	A
1	A	2627	U
1	A	2628	A
1	A	2629	A
1	A	2630	A
1	A	2631	A
1	A	2635	A
1	A	2636	A
1	A	2640	A
1	A	2647	U
1	A	2648	A
1	A	2651	U
1	A	2655	C
1	A	2656	C
1	A	2657	C
1	A	2659	C
1	A	2660	U
1	A	2665	U
1	A	2666	A
1	A	2676	A
2	B	3	U
2	B	5	A
2	B	6	U
2	B	7	G
2	B	8	U
2	B	9	A
2	B	14	A
2	B	16	U
2	B	21	A
2	B	32	U
2	B	33	G
2	B	44	G
2	B	45	A
2	B	46	U
2	B	47	G
2	B	48	G
2	B	51	A

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Mol	Chain	Res	Type
2	B	52	U
2	B	53	U
2	B	58	C
2	B	60	C
2	B	63	A
2	B	66	C

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1137	A
1	A	1160	A
1	A	1175	G
1	A	1187	U
1	A	1194	A
1	A	1428	A
1	A	1492	A
1	A	1597	A
1	A	1608	C
1	A	1610	U
1	A	1614	A
1	A	1644	U
1	A	1683	C
1	A	1893	C
1	A	1967	A
1	A	2056	A
1	A	2057	G
1	A	2076	A
1	A	2302	U
1	A	2332	U
1	A	2342	U
1	A	2485	C
1	A	2564	G
1	A	2659	C
2	B	31	C
2	B	52	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 100 ligands modelled in this entry, 97 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
62	GNP	z	401	-	29,34,34	1.24	4 (13%)	33,54,54	2.06	5 (15%)
61	FES	r	201	45,7	0,4,4	-	-	-		
62	GNP	t	501	-	29,34,34	1.25	4 (13%)	33,54,54	2.08	5 (15%)

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
62	GNP	z	401	-	-	6/14/38/38	0/3/3/3
61	FES	r	201	45,7	-	-	0/1/1/1
62	GNP	t	501	-	-	8/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	t	501	GNP	PG-O1G	3.44	1.51	1.46
62	t	501	GNP	PB-O2B	-3.26	1.48	1.56
62	z	401	GNP	PG-O1G	3.25	1.51	1.46
62	z	401	GNP	PB-O2B	-3.17	1.48	1.56
62	z	401	GNP	PG-O3G	-2.12	1.51	1.56
62	z	401	GNP	PG-O2G	-2.08	1.51	1.56
62	t	501	GNP	PG-O3G	-2.02	1.51	1.56
62	t	501	GNP	PG-O2G	-2.00	1.51	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	t	501	GNP	C5-C6-N1	-7.56	113.31	123.42
62	z	401	GNP	C5-C6-N1	-7.56	113.32	123.42
62	t	501	GNP	C2-N1-C6	6.70	125.27	115.96
62	z	401	GNP	C2-N1-C6	6.66	125.22	115.96
62	t	501	GNP	N3-C2-N1	-3.05	123.33	127.21
62	z	401	GNP	C2-N3-C4	-3.04	112.21	115.48
62	z	401	GNP	N3-C2-N1	-2.99	123.40	127.21
62	t	501	GNP	C2-N3-C4	-2.97	112.29	115.48
62	z	401	GNP	C4-C5-C6	-2.24	117.81	121.23
62	t	501	GNP	C4-C5-C6	-2.23	117.82	121.23

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	z	401	GNP	PG-N3B-PB-O1B
62	z	401	GNP	PA-O3A-PB-O2B
62	t	501	GNP	PB-N3B-PG-O1G
62	t	501	GNP	PG-N3B-PB-O1B
62	t	501	GNP	PG-N3B-PB-O3A
62	t	501	GNP	C5'-O5'-PA-O3A
62	t	501	GNP	C5'-O5'-PA-O2A
62	t	501	GNP	O4'-C4'-C5'-O5'
62	t	501	GNP	C3'-C4'-C5'-O5'
62	z	401	GNP	C3'-C4'-C5'-O5'
62	t	501	GNP	C4'-C5'-O5'-PA
62	z	401	GNP	C5'-O5'-PA-O1A
62	z	401	GNP	C4'-C5'-O5'-PA
62	z	401	GNP	PA-O3A-PB-O1B

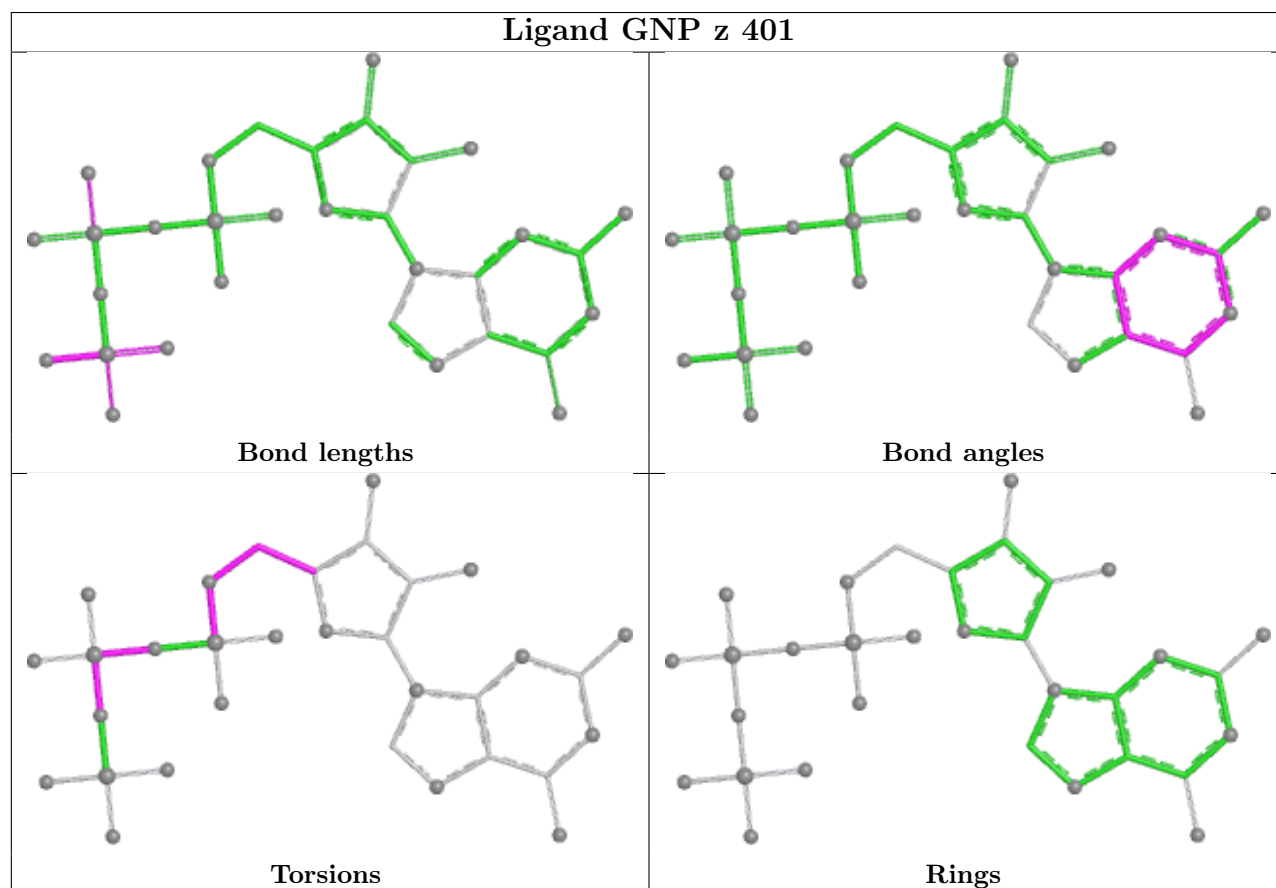
There are no ring outliers.

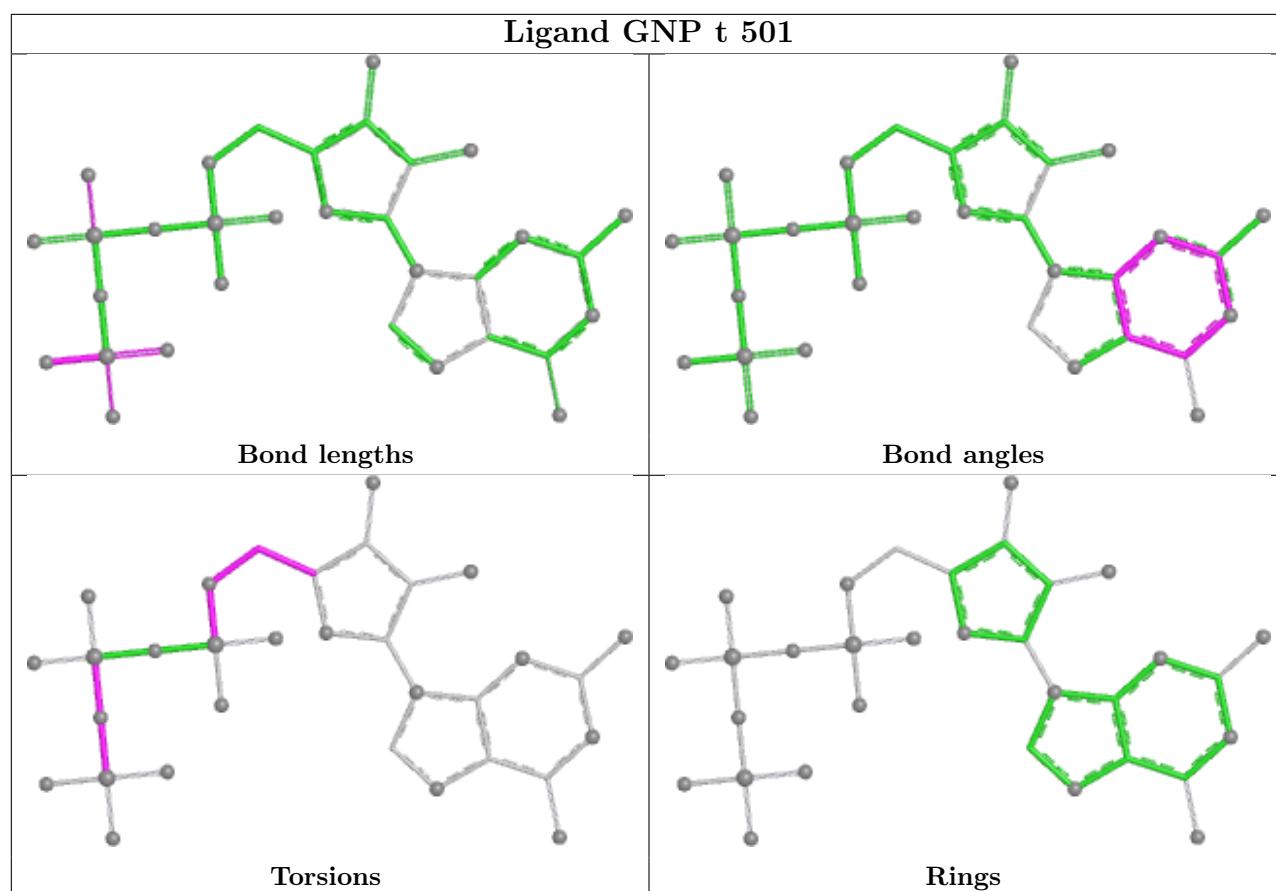
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	z	401	GNP	1	0
61	r	201	FES	1	0
62	t	501	GNP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

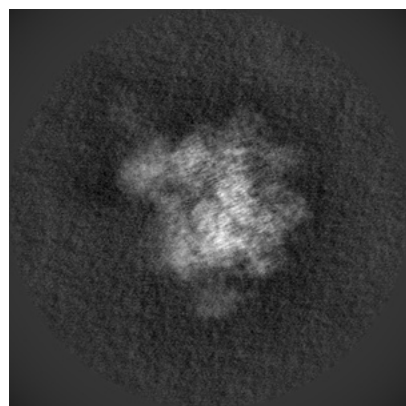
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47791. These allow visual inspection of the internal detail of the map and identification of artifacts.

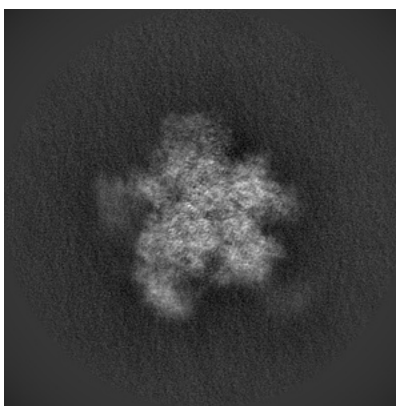
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

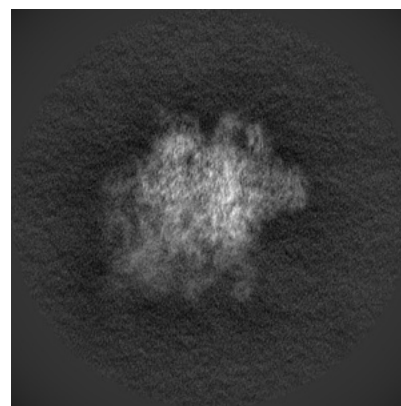
6.1.1 Primary map



X

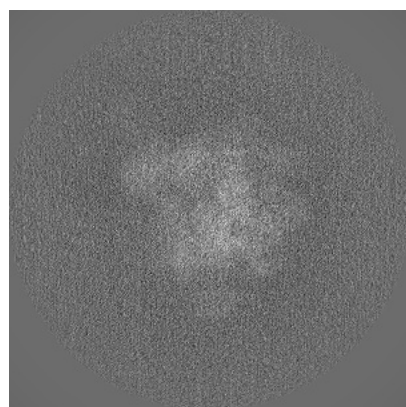


Y

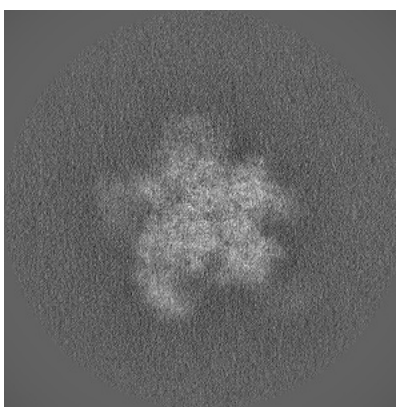


Z

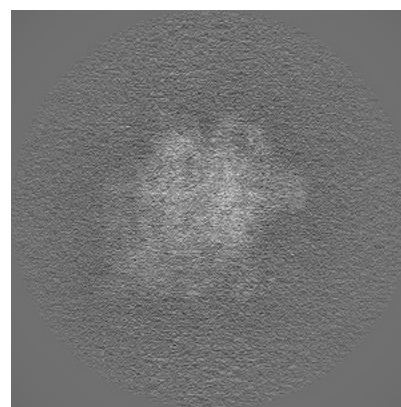
6.1.2 Raw map



X



Y

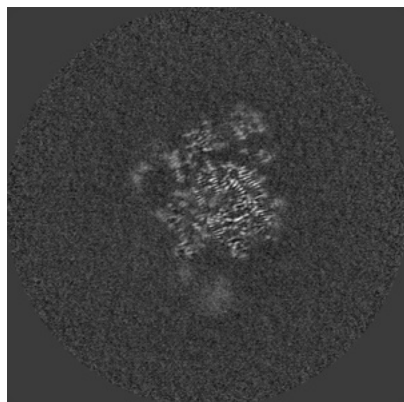


Z

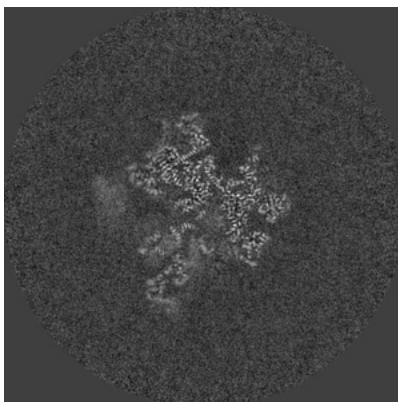
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

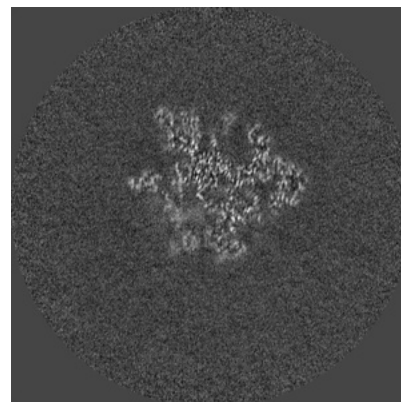
6.2.1 Primary map



X Index: 270

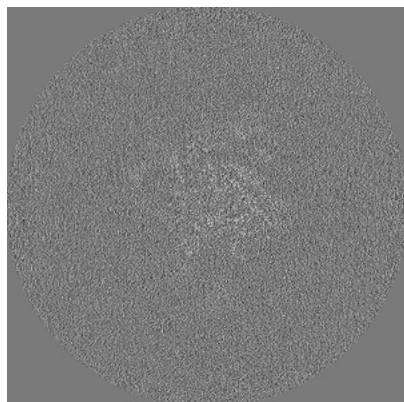


Y Index: 270

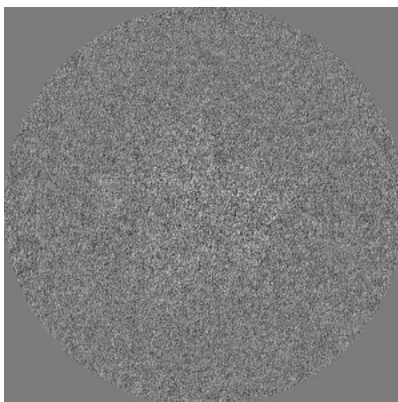


Z Index: 270

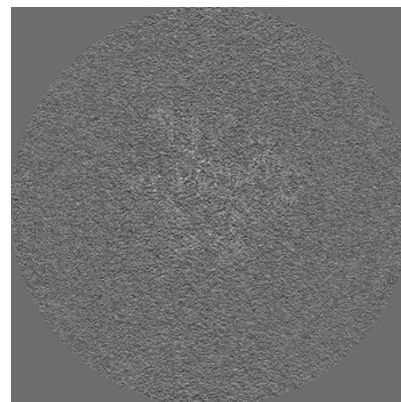
6.2.2 Raw map



X Index: 270



Y Index: 270

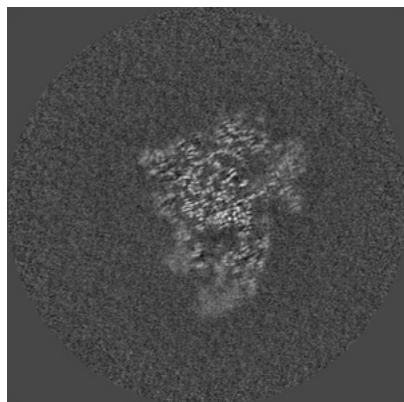


Z Index: 270

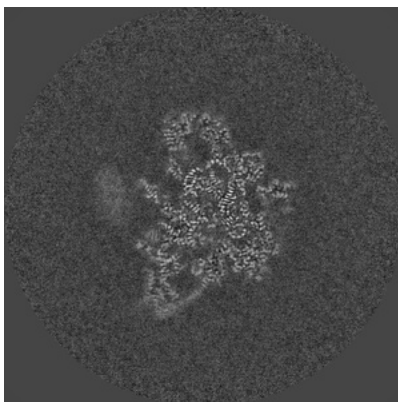
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

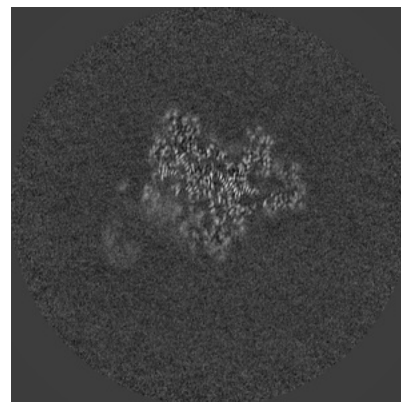
6.3.1 Primary map



X Index: 296

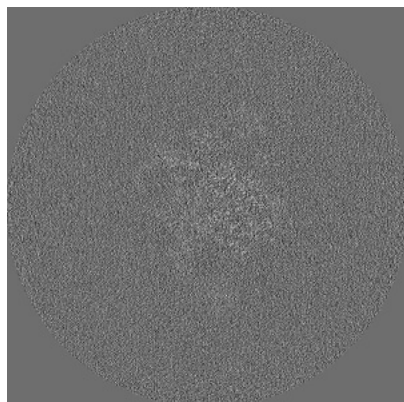


Y Index: 296

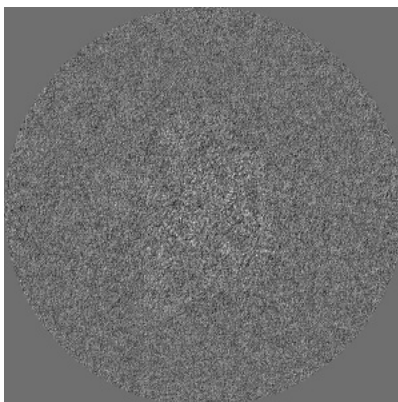


Z Index: 254

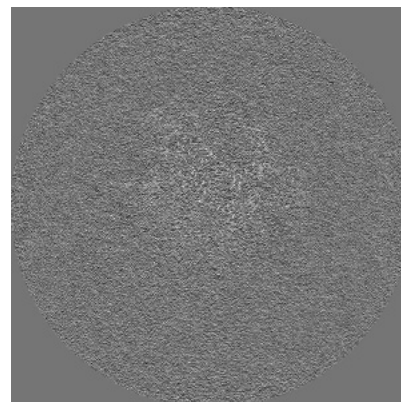
6.3.2 Raw map



X Index: 272



Y Index: 296

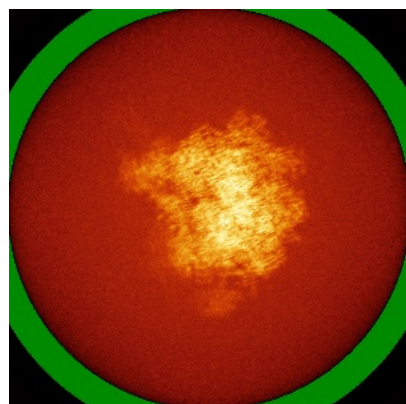


Z Index: 264

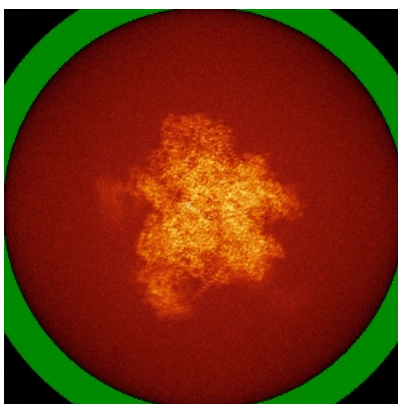
The images above show the largest variance slices of the map in three orthogonal directions.

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

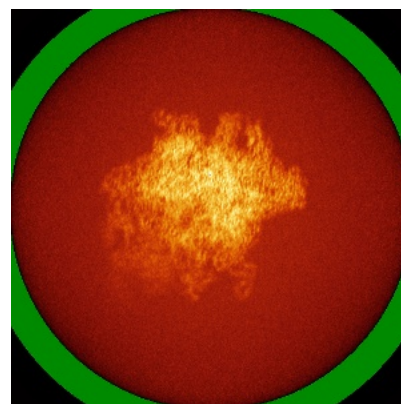
6.4.1 Primary map



X

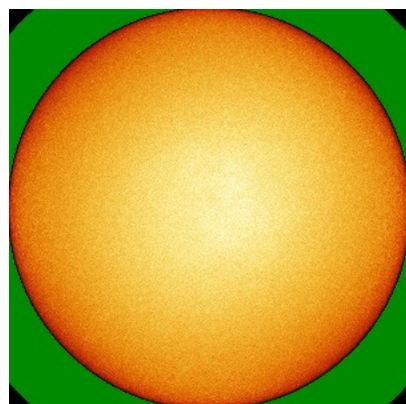


Y

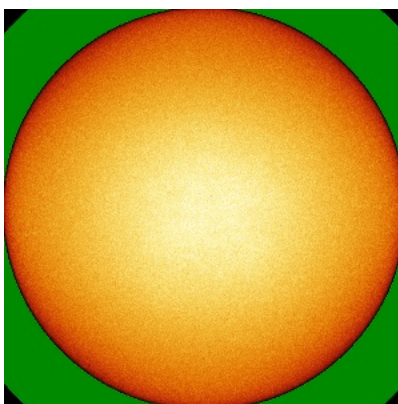


Z

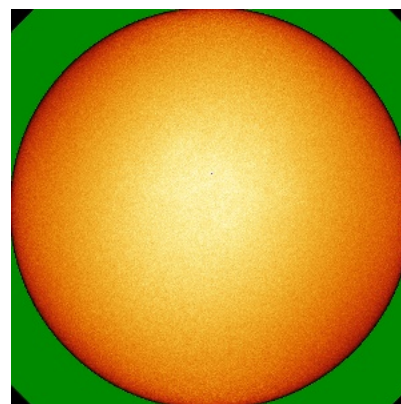
6.4.2 Raw map



X



Y

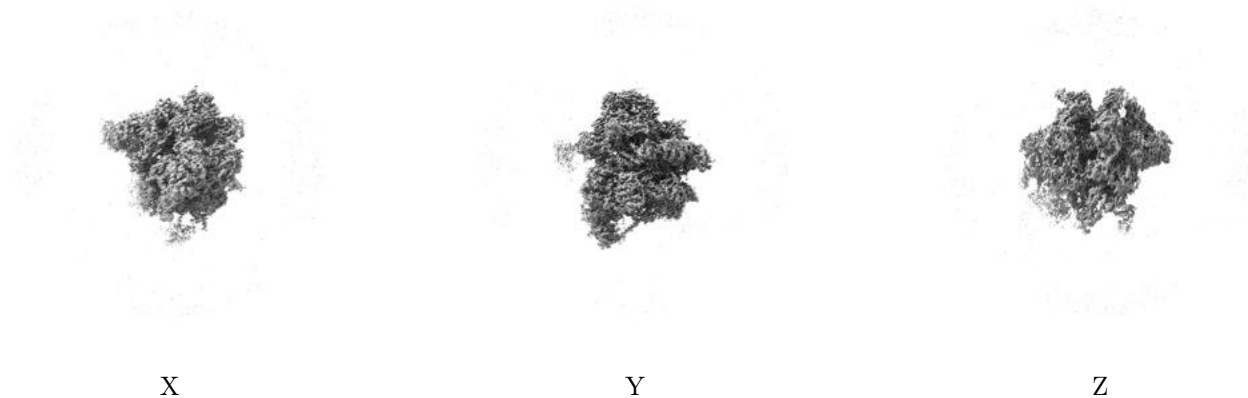


Z

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.

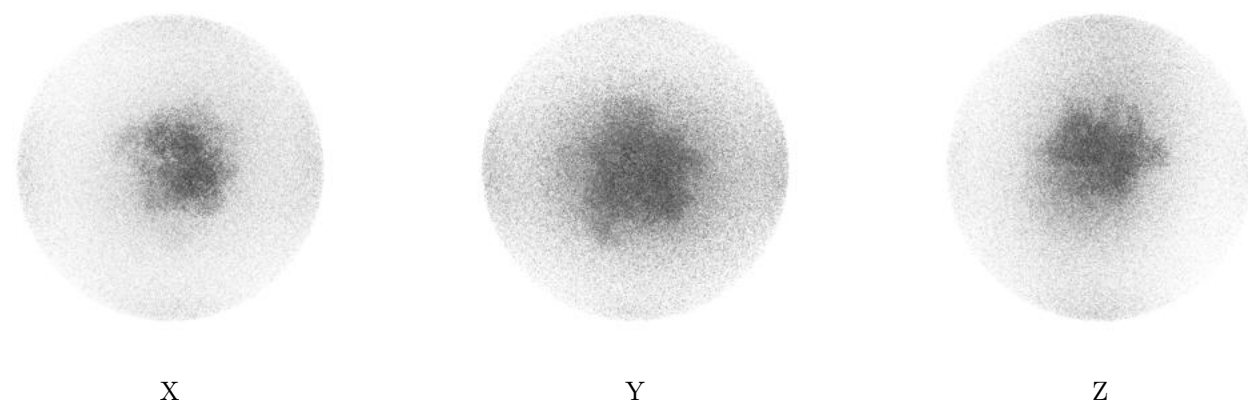
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

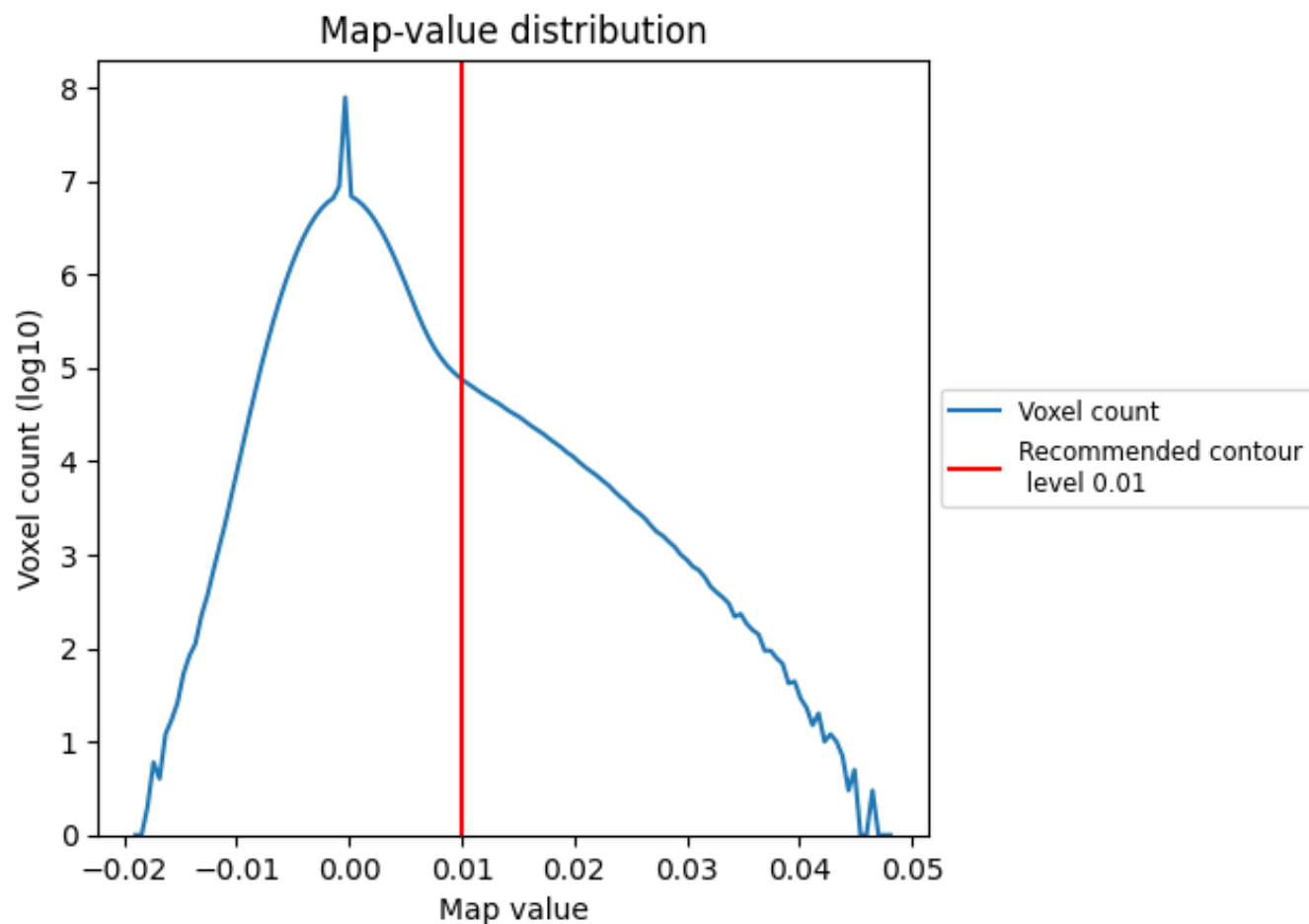
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

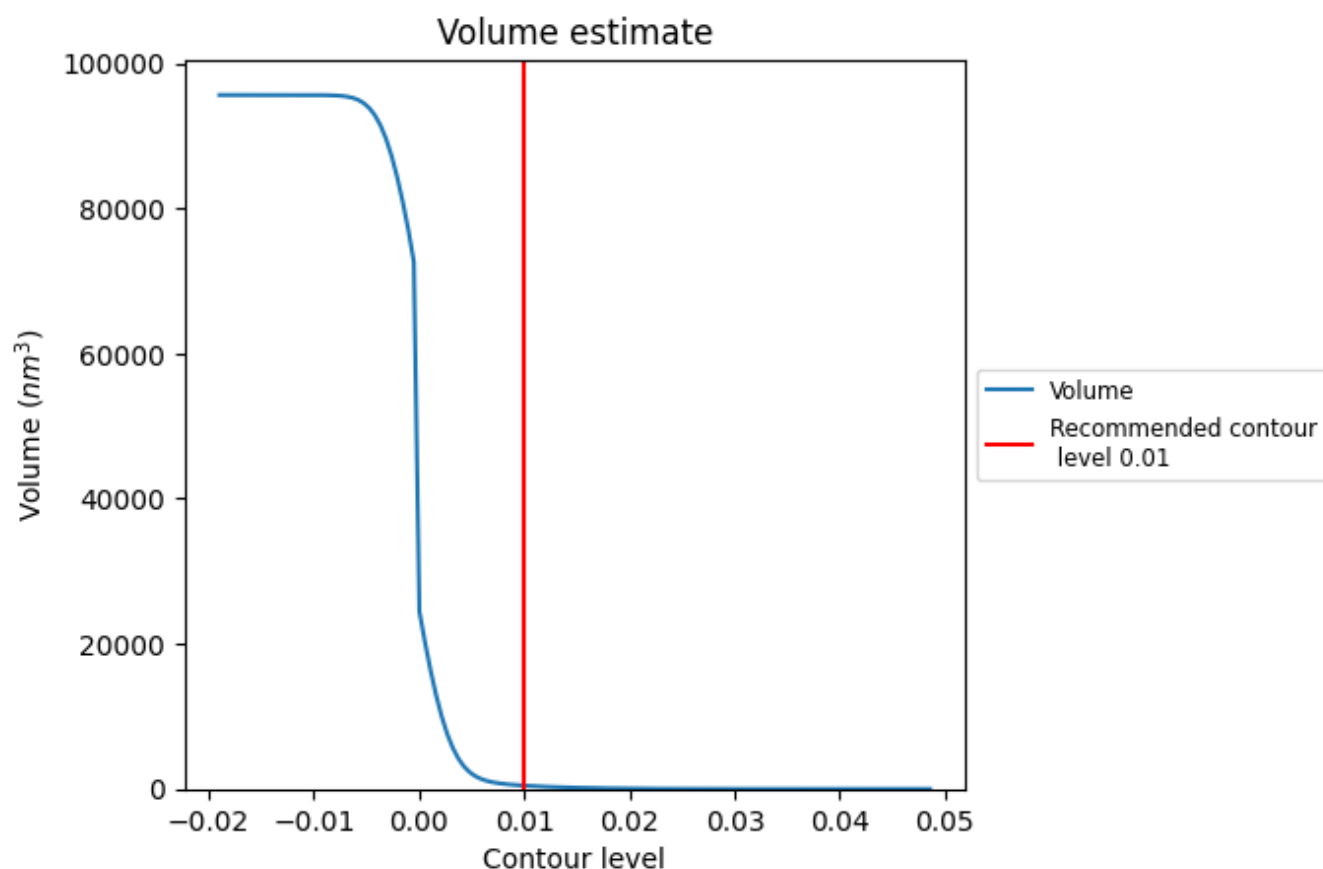
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

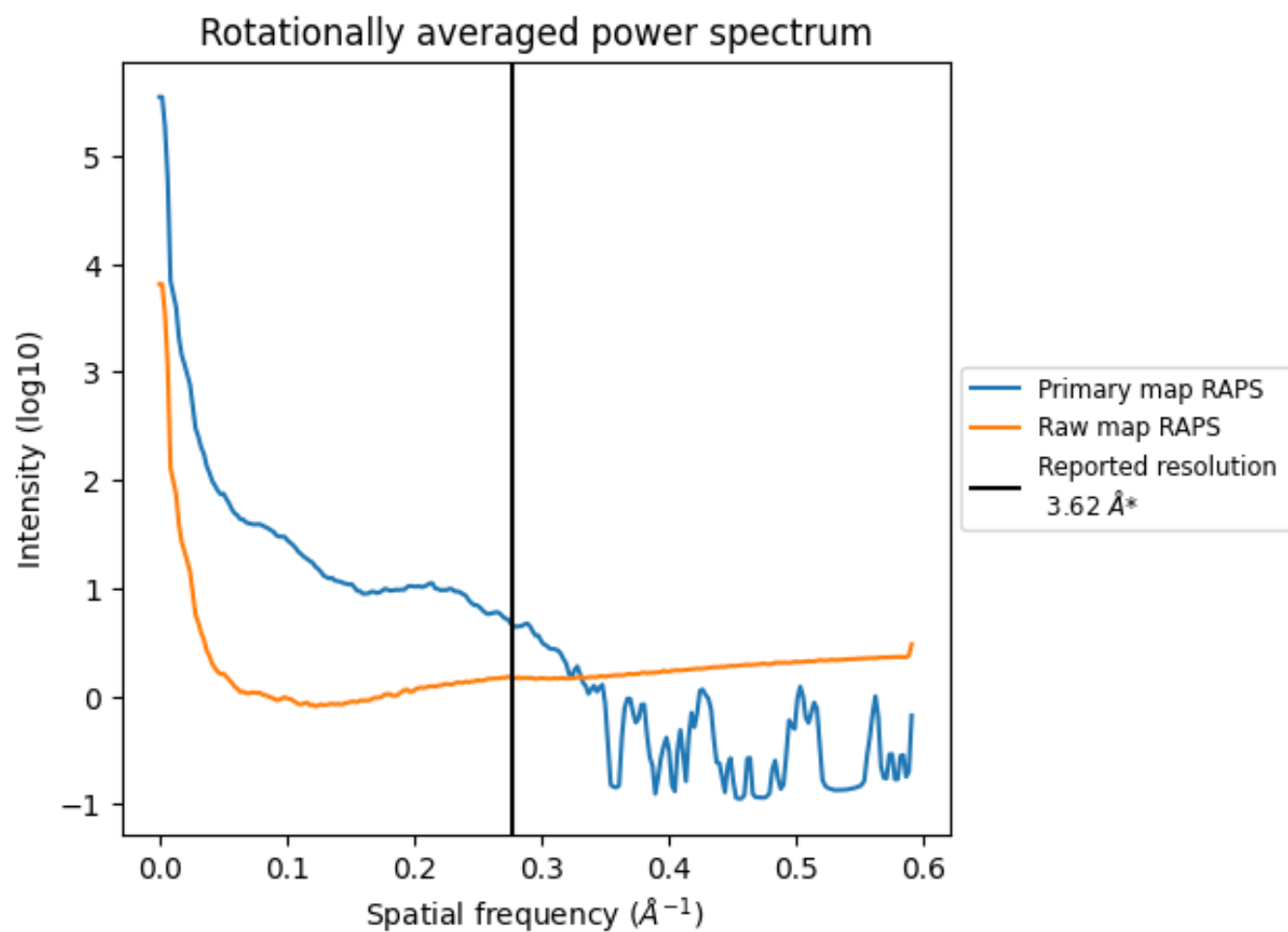
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 463 nm³; this corresponds to an approximate mass of 418 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 ⓘ

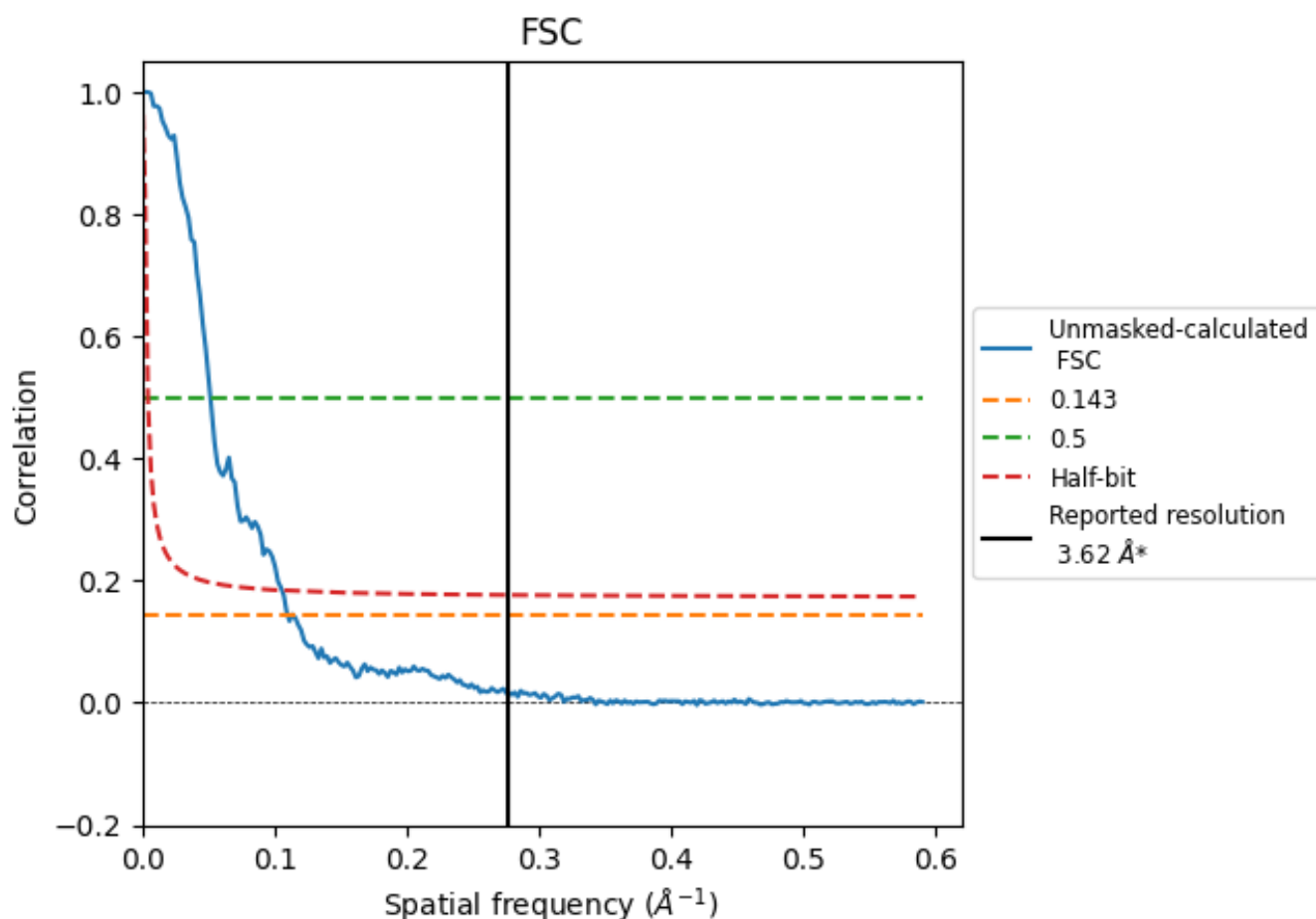


*Reported resolution corresponds to spatial frequency of 0.276 \AA^{-1}

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 0.276 \AA^{-1}

8.2 Resolution estimates [i](#)

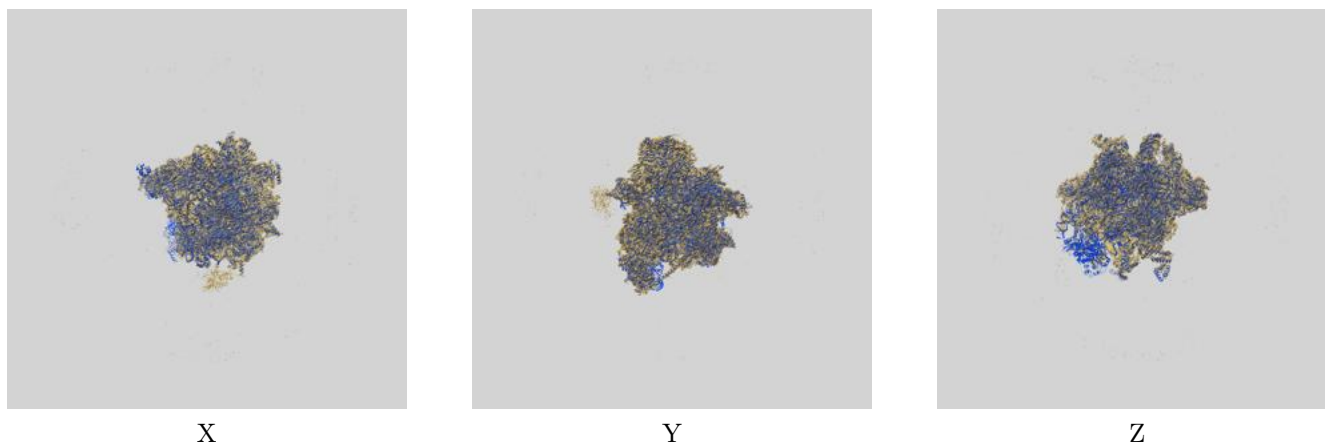
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.07	19.38	9.45

*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 9.07 differs from the reported value 3.62 by more than 10 %

9 Map-model fit [i](#)

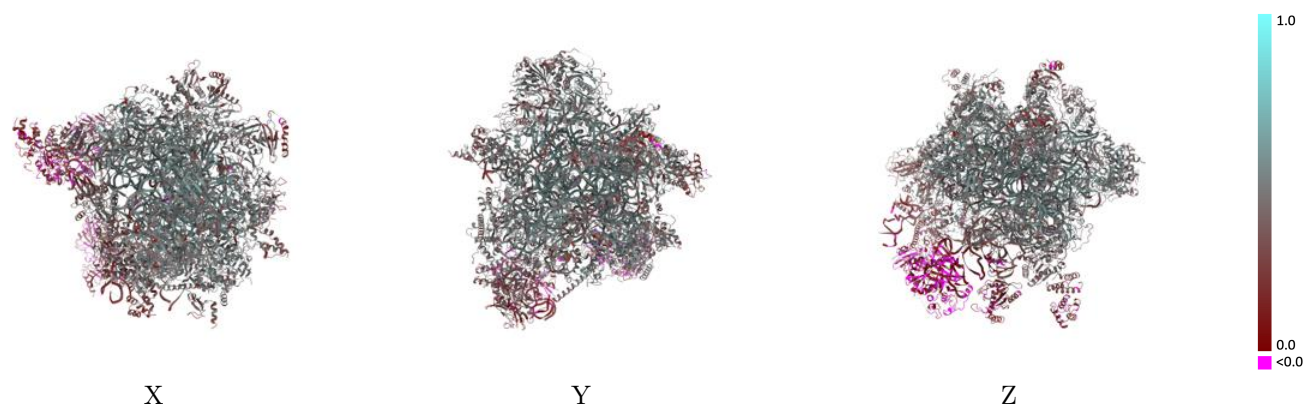
This section contains information regarding the fit between EMDB map EMD-47791 and PDB model 9E9C. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



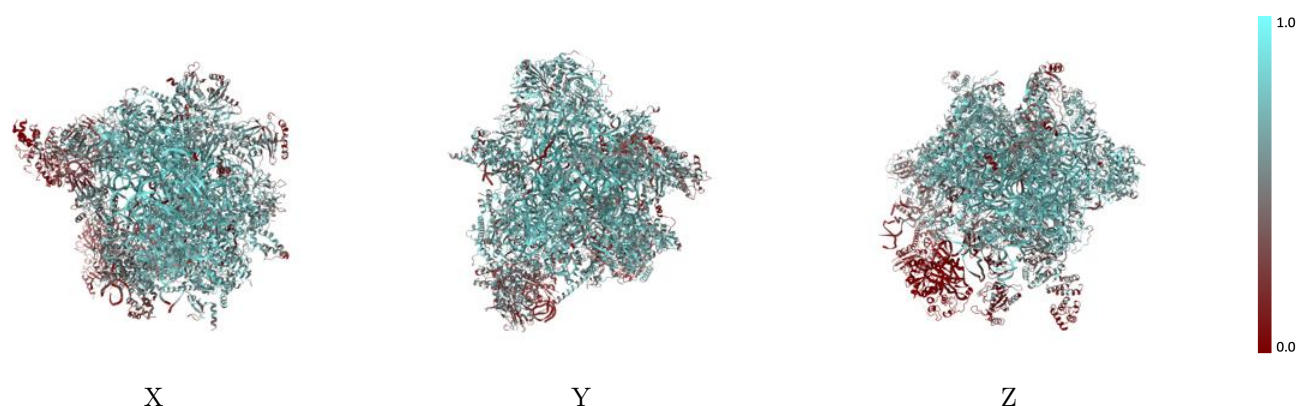
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



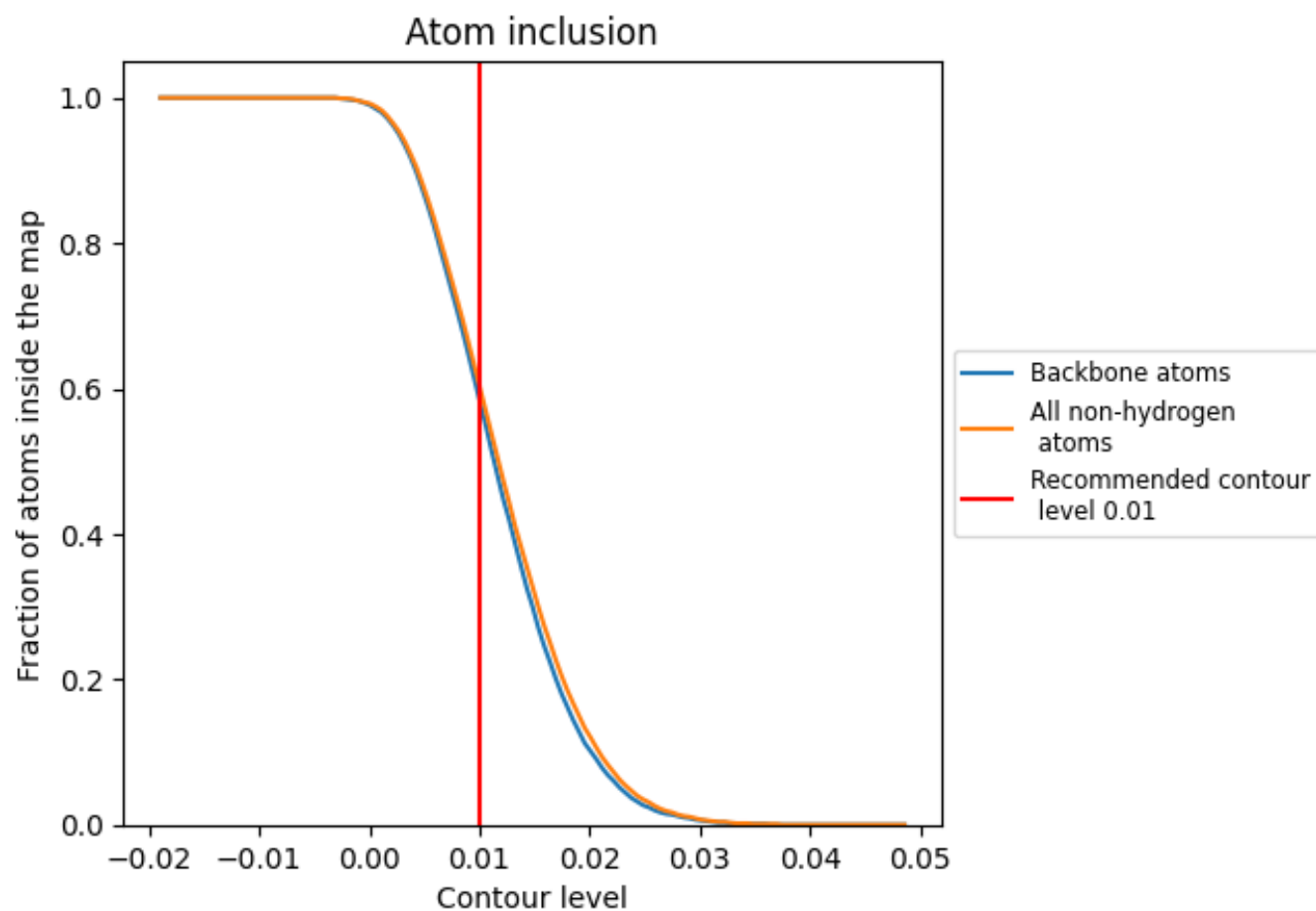
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 60% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6040	 0.4190
0	 0.6520	 0.4880
1	 0.5370	 0.4380
2	 0.8230	 0.5660
3	 0.7890	 0.5550
4	 0.0100	 0.2560
5	 0.6430	 0.4600
6	 0.4620	 0.3270
7	 0.5340	 0.4030
8	 0.1030	 0.1450
9	 0.6290	 0.4630
A	 0.7540	 0.4670
B	 0.2770	 0.1390
D	 0.6610	 0.4900
E	 0.6930	 0.4920
F	 0.7130	 0.5000
H	 0.6050	 0.4380
I	 0.0200	 0.0920
J	 0.0140	 -0.0050
K	 0.7040	 0.5110
L	 0.5900	 0.4800
M	 0.7000	 0.5020
O	 0.7000	 0.5050
P	 0.4950	 0.3470
Q	 0.6590	 0.4850
R	 0.7200	 0.5160
S	 0.6250	 0.4720
T	 0.7040	 0.5270
U	 0.6940	 0.5130
V	 0.5560	 0.4180
W	 0.5820	 0.4450
X	 0.6650	 0.4770
Y	 0.7040	 0.5010
Z	 0.6080	 0.4790
a	 0.5230	 0.4690



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.7140	 0.5100
c	 0.6000	 0.4450
d	 0.3890	 0.3520
e	 0.0120	 0.0510
f	 0.0910	 0.1530
g	 0.6900	 0.4960
h	 0.5090	 0.3860
i	 0.7520	 0.5560
j	 0.6410	 0.4600
k	 0.0330	 0.0780
l	 0.0110	 0.0290
m	 0.0430	 0.1140
o	 0.6080	 0.4630
p	 0.5020	 0.3670
q	 0.6060	 0.3870
r	 0.5570	 0.4120
s	 0.6600	 0.4830
t	 0.2620	 0.1700
u	 0.5010	 0.4040
v	 0.3610	 0.2780
w	 0.0850	 0.1480
x	 0.4530	 0.3650
y	 0.4870	 0.3740
z	 0.4900	 0.4030