



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 11:51 AM UTC

PDB ID : 3JCN / pdb_00003jcn
EMDB ID : EMD-3285
Title : Structures of ribosome-bound initiation factor 2 reveal the mechanism of sub-unit association: Initiation Complex I
Authors : Sprink, T.; Ramrath, D.J.F.; Yamamoto, H.; Yamamoto, K.; Loerke, J.; Ismer, J.; Hildebrand, P.W.; Scheerer, P.; Buerger, J.; Mielke, T.; Spahn, C.M.T.
Deposited on : 2016-01-04
Resolution : 4.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

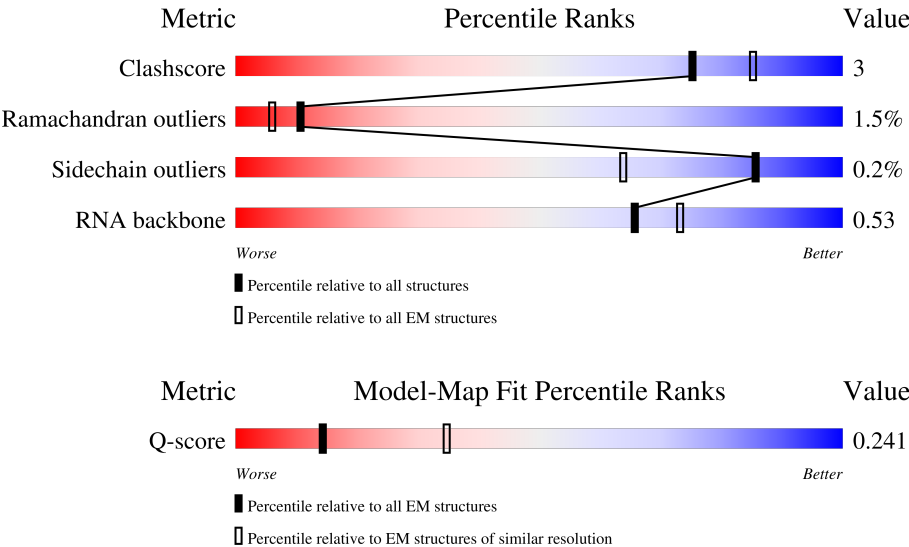
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2407 (4.10 - 5.10)

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

Mol	Chain	Length	Quality of chain
1	0	57	23% 96% ..
2	1	55	65% 87% 9%
3	2	46	11% 96% .

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Mol	Chain	Length	Quality of chain
4	3	65	17% 94% 5% .
5	4	38	18% 97% .
6	A	2904	6% 85% 14% .
7	B	120	. 87% 12% ..
8	C	273	25% 94% 5% .
9	D	209	26% 94% 6%
10	E	201	38% 96% .
11	F	179	53% 92% 7% .
12	G	177	36% 97% ..
13	H	149	27% 21% 7% .. 70%
14	I	142	96% 92% 8% .
15	J	142	22% 93% 6% .
16	K	123	41% 89% 10% ..
17	L	144	42% 93% 6% .
18	M	136	32% 92% 8%
19	N	127	13% 89% 6% 6%
20	O	117	32% 93% 6% .
21	P	115	33% 97% ..
22	Q	118	14% 97% ..
23	R	103	17% 99% .
24	S	110	12% 99% .
25	T	100	24% 88% 5% 7%
26	U	104	29% 91% 7% .
27	V	94	32% 100%
28	W	85	25% 86% 11%

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Mol	Chain	Length	Quality of chain
29	X	78	
30	Y	63	
31	Z	59	
32	a	1542	
33	b	890	
34	c	233	
35	d	241	
36	f	159	
37	g	206	
38	h	179	
39	i	135	
40	j	130	
41	k	130	
42	l	129	
43	m	102	
44	n	118	
45	o	124	
46	p	89	
47	q	101	
48	r	84	
49	s	82	
50	t	92	
51	u	75	
52	v	77	
53	w	71	

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Mol	Chain	Length	Quality of chain
54	x	87	
55	z	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	4SU	v	8	-	-	X	-
56	GNP	b	901	-	-	X	-
57	FME	v	101	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 147293 atoms, of which 1 is hydrogen and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		

- Molecule 7 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	119	Total	C	N	O	P	0	0
			2546	1135	466	827	118		

- Molecule 8 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 9 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 10 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 11 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 12 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 13 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	44	Total	C	N	O	S	0	0
			328	210	59	58	1		

- Molecule 14 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 15 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 16 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 17 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 18 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 19 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 20 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 21 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 22 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 23 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 24 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 25 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 26 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 27 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	76	Total	C	N	O	S	0	0
			575	356	117	101	1		

- Molecule 29 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 30 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 31 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 33 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	509	Total	C	N	O	S	0	0
			3847	2409	675	748	15		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	150	Total	C	N	O	S	0	0
			1106	687	211	202	6		

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	u	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 52 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	v	77	Total	C	N	O	P	S	0	0
			1643	733	297	535	77	1		

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

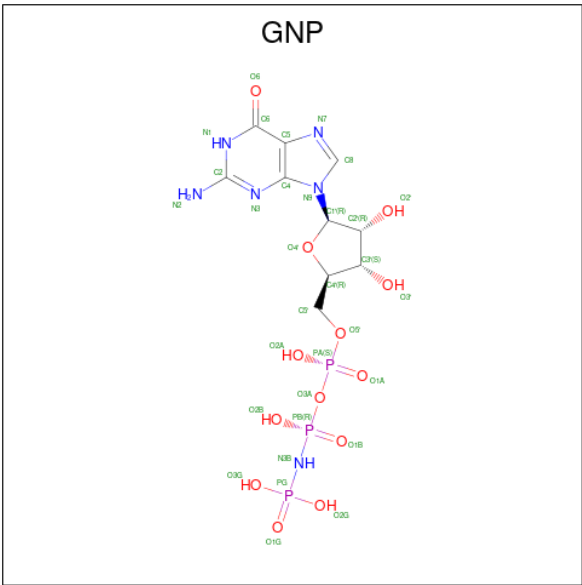
- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 55 is a RNA chain called messenger RNA.

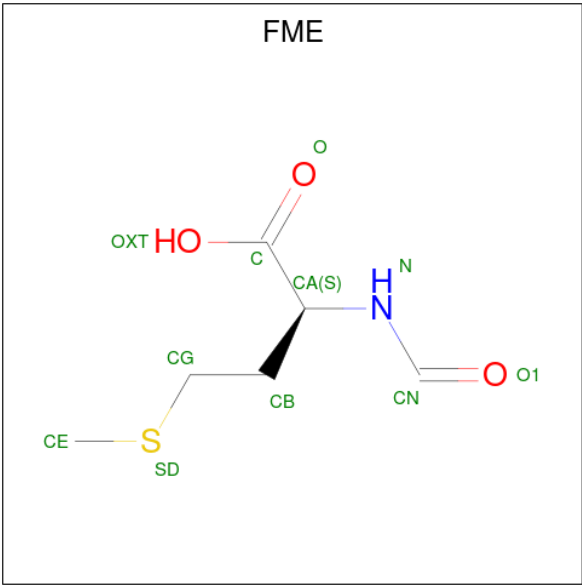
Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	6	Total	C	N	O	P	0	0
			129	58	24	41	6		

- Molecule 56 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
56	b	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 57 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).

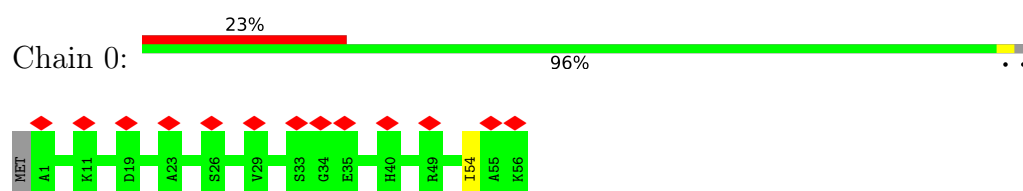


Mol	Chain	Residues	Atoms						AltConf
57	v	1	Total	C	H	N	O	S	0
			10	6	1	1	1	1	

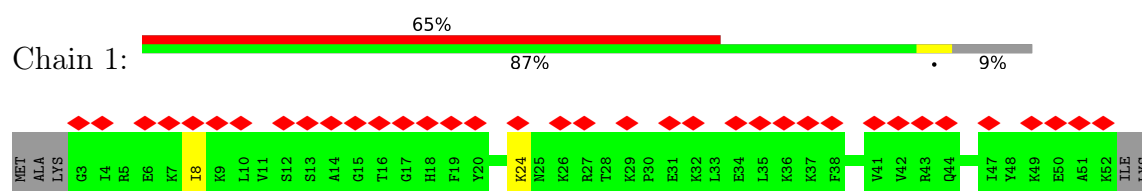
3 Residue-property plots [i](#)

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.

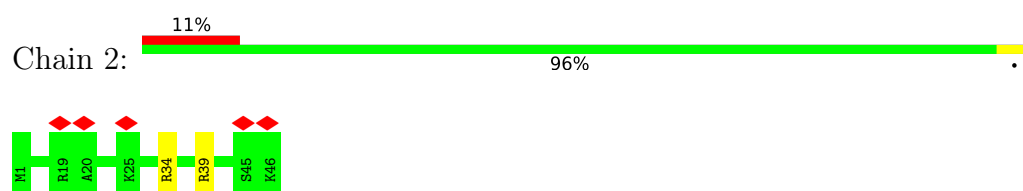
- Molecule 1: 50S ribosomal protein L32



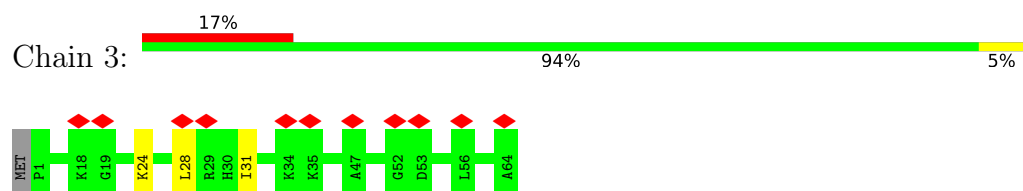
- Molecule 2: 50S ribosomal protein L33



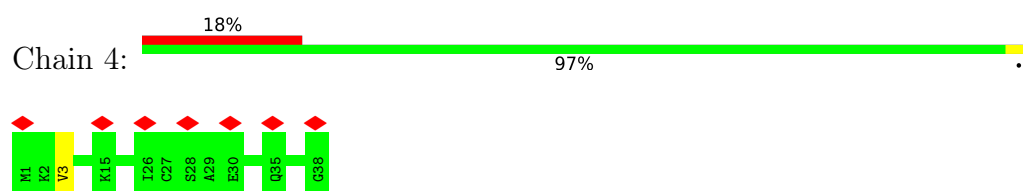
- Molecule 3: 50S ribosomal protein L34



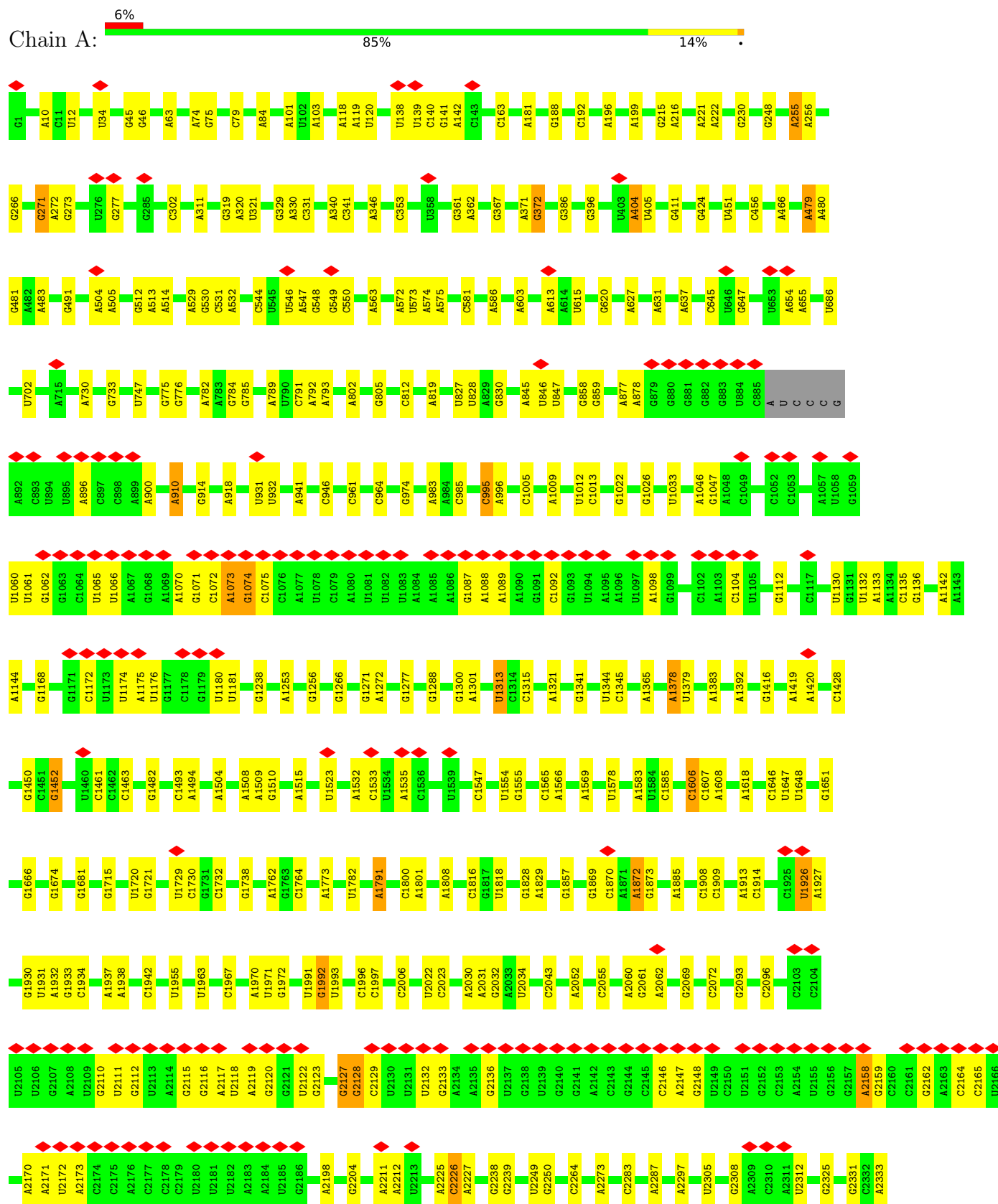
- Molecule 4: 50S ribosomal protein L35

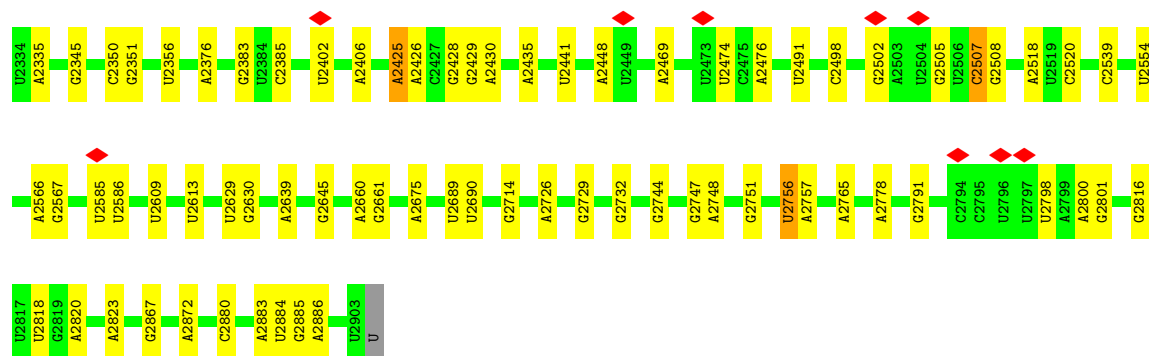


- Molecule 5: 50S ribosomal protein L36



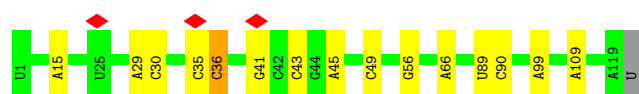
• Molecule 6: 23S ribosomal RNA





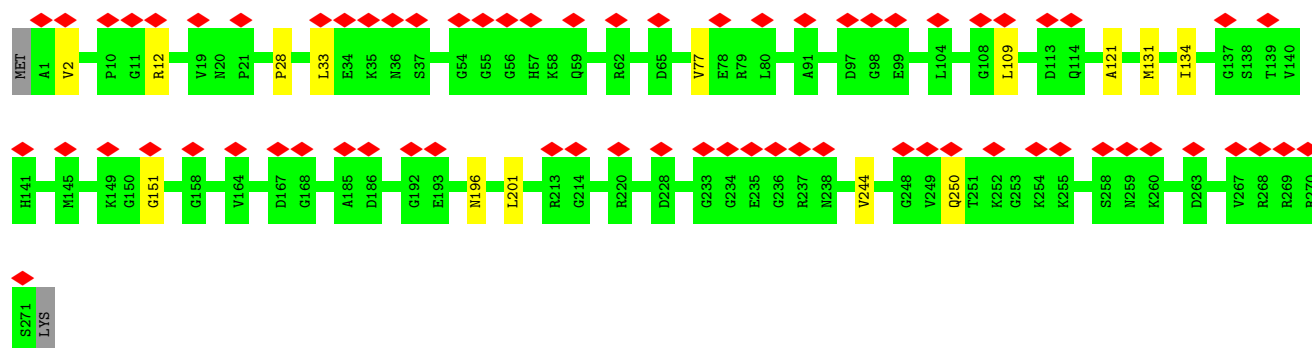
• Molecule 7: 5S ribosomal RNA

Chain B: 87% 12% ..



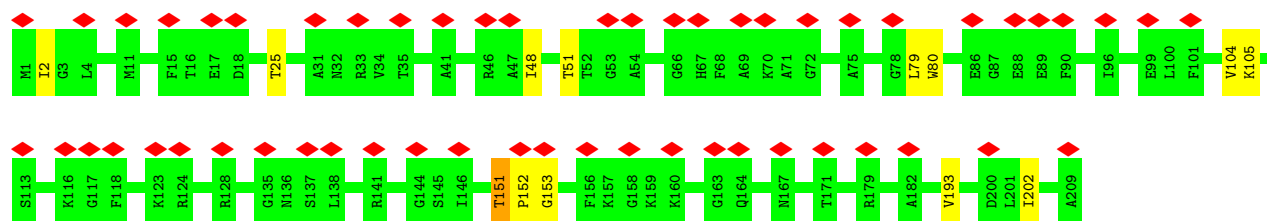
• Molecule 8: 50S ribosomal protein L2

Chain C: 25% 94% 5% .



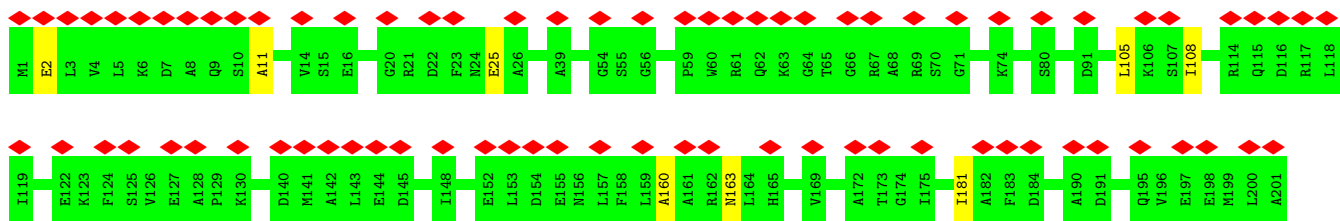
• Molecule 9: 50S ribosomal protein L3

Chain D: 26% 94% 6%

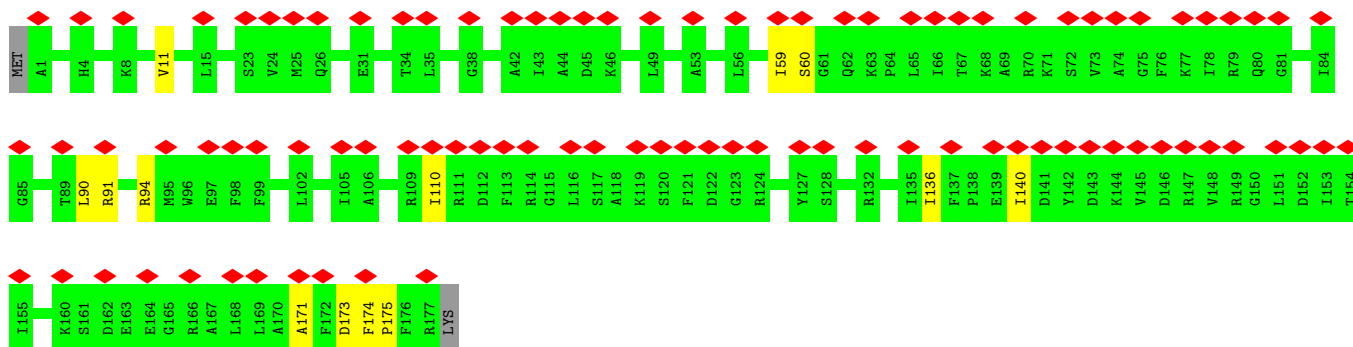
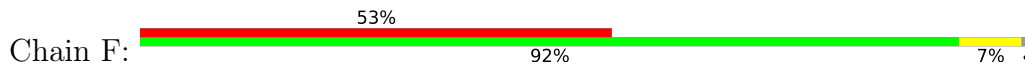


• Molecule 10: 50S ribosomal protein L4

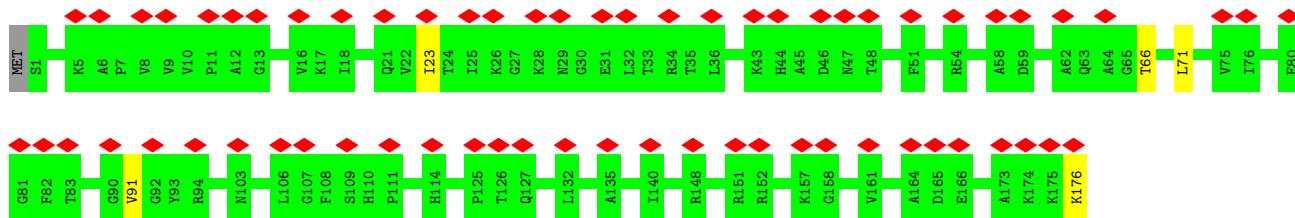
Chain E: 38% 96% .



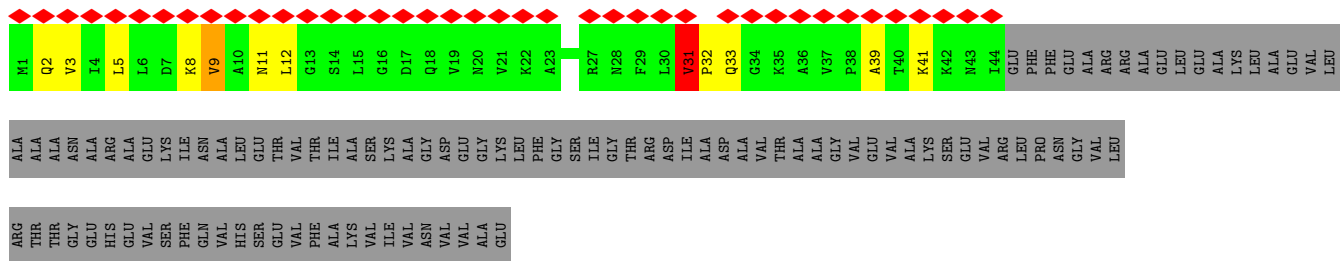
• Molecule 11: 50S ribosomal protein L5



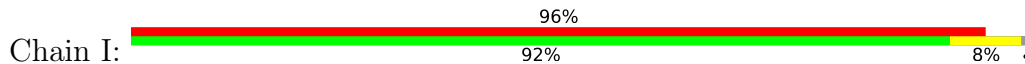
• Molecule 12: 50S ribosomal protein L6

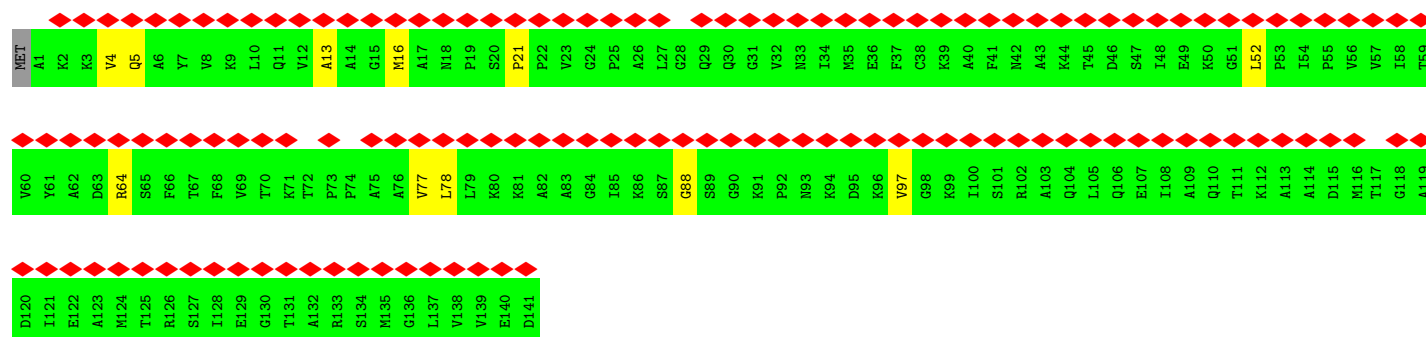


• Molecule 13: 50S ribosomal protein L9

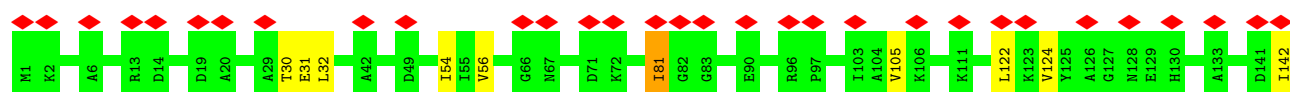


• Molecule 14: 50S ribosomal protein L11

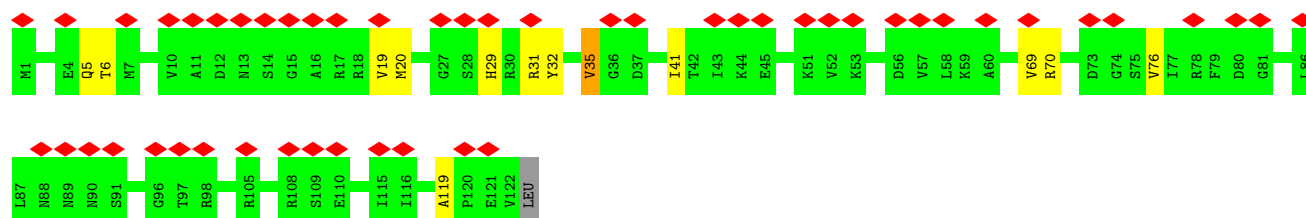
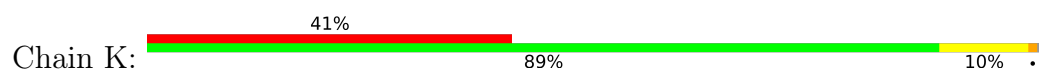




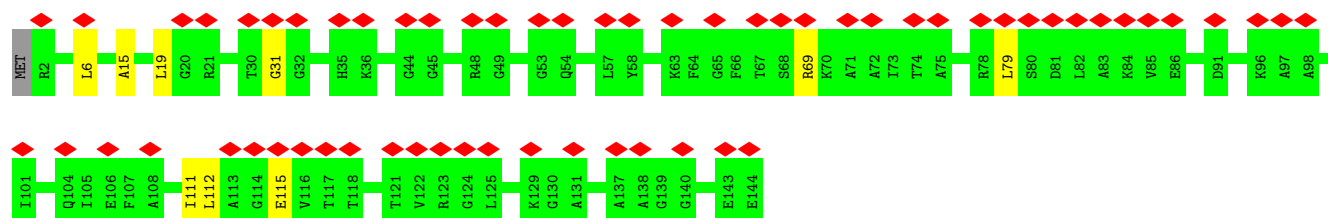
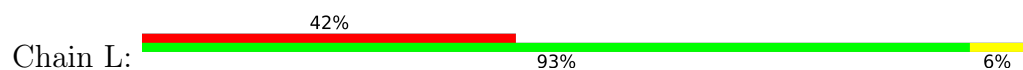
• Molecule 15: 50S ribosomal protein L13



• Molecule 16: 50S ribosomal protein L14

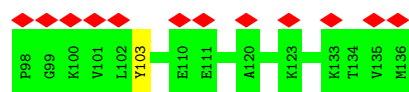


• Molecule 17: 50S ribosomal protein L15

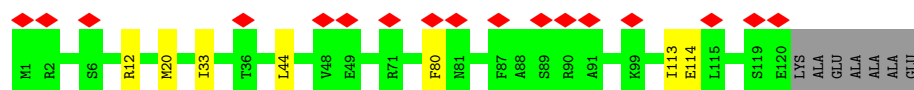
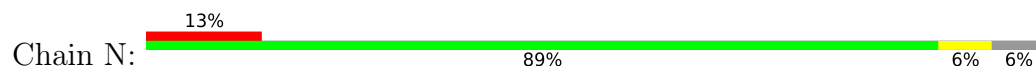


• Molecule 18: 50S ribosomal protein L16

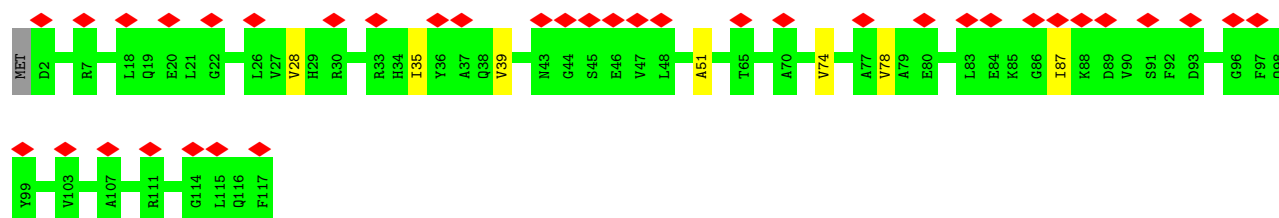




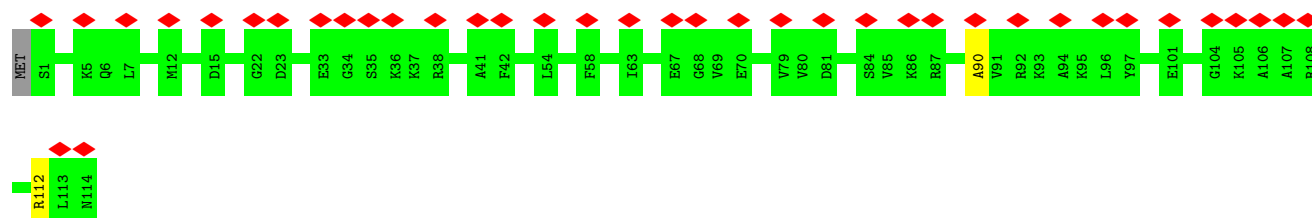
- Molecule 19: 50S ribosomal protein L17



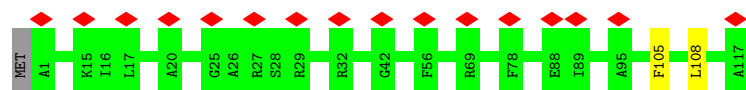
- Molecule 20: 50S ribosomal protein L18



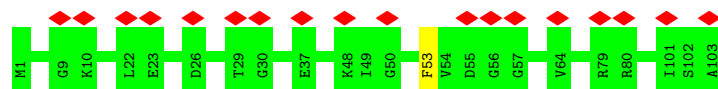
- Molecule 21: 50S ribosomal protein L19



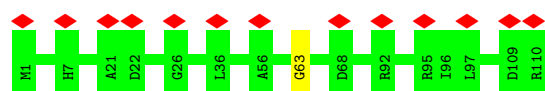
- Molecule 22: 50S ribosomal protein L20



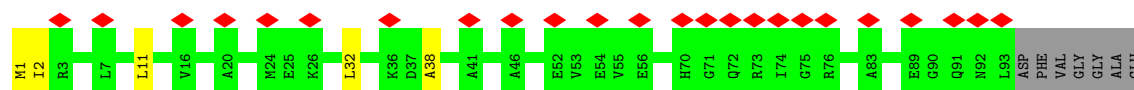
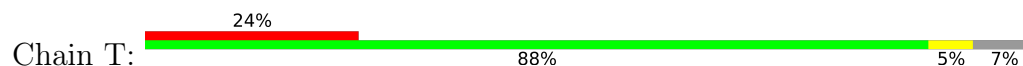
- Molecule 23: 50S ribosomal protein L21



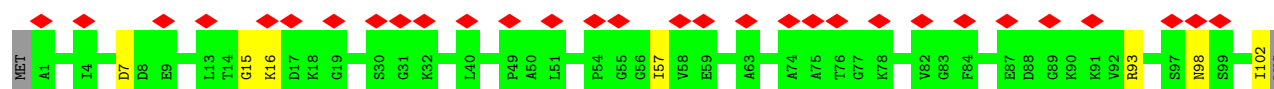
- Molecule 24: 50S ribosomal protein L22



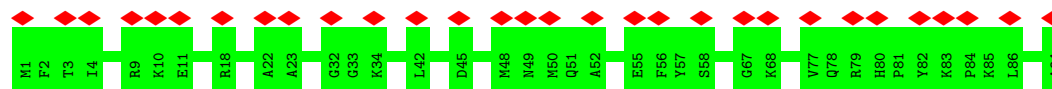
- Molecule 25: 50S ribosomal protein L23



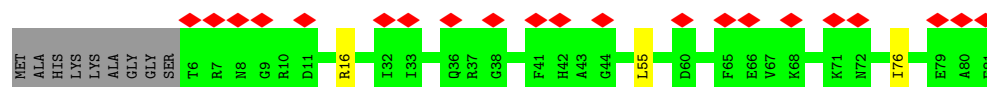
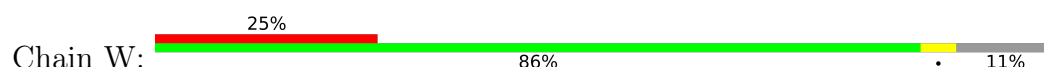
- Molecule 26: 50S ribosomal protein L24



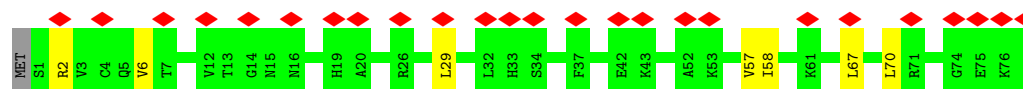
- Molecule 27: 50S ribosomal protein L25



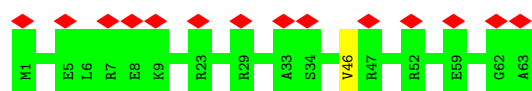
- Molecule 28: 50S ribosomal protein L27



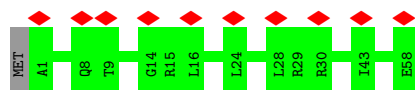
- Molecule 29: 50S ribosomal protein L28



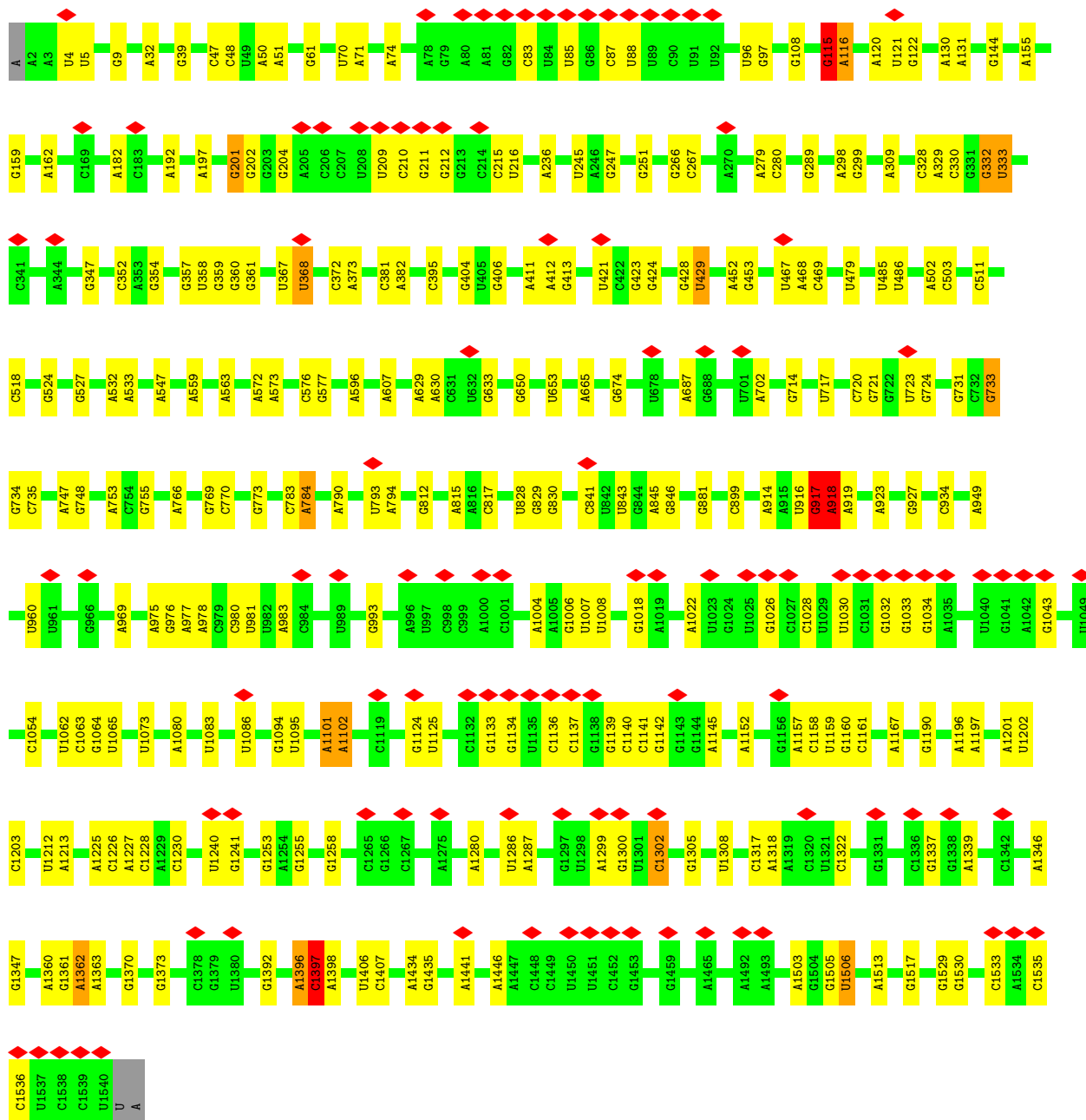
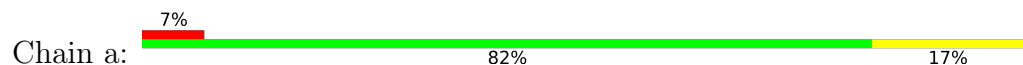
- Molecule 30: 50S ribosomal protein L29



- Molecule 31: 50S ribosomal protein L30



- Molecule 32: 16S ribosomal RNA



- Molecule 33: Translation initiation factor IF-2

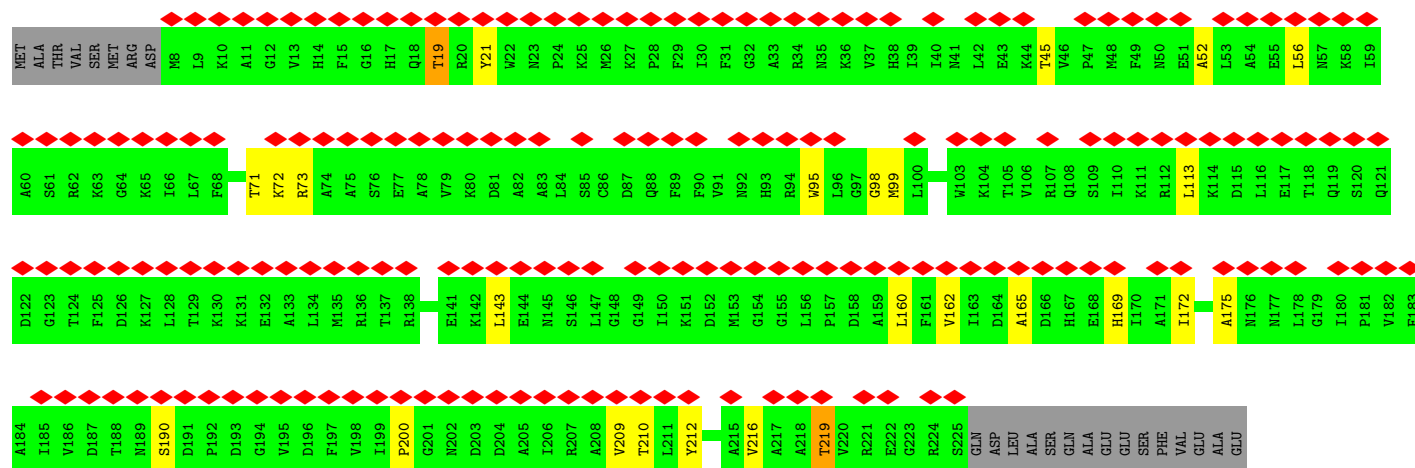


Chain c: 



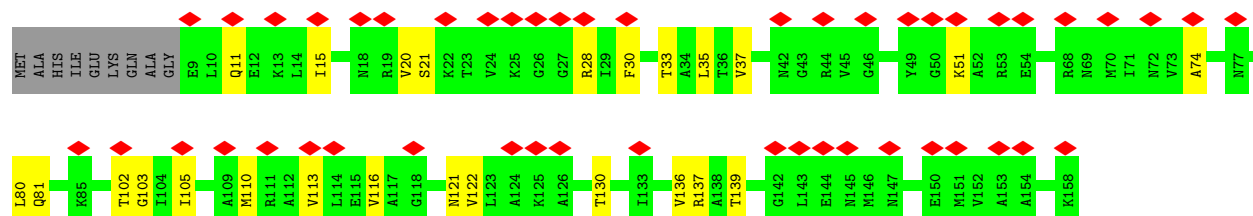
- Molecule 35: 30S ribosomal protein S2

Chain d: 

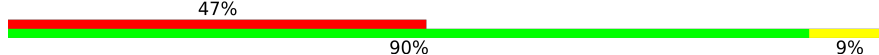


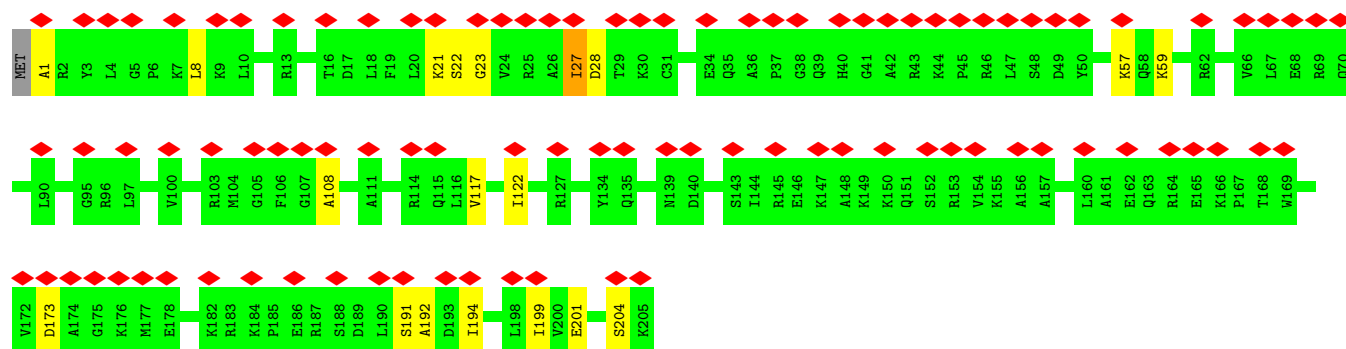
- Molecule 36: 30S ribosomal protein S5

Chain f: 

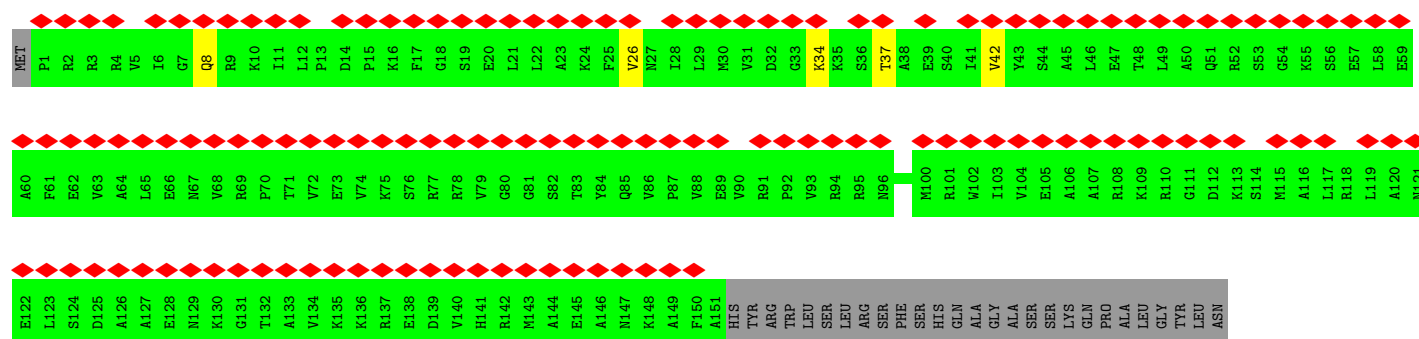
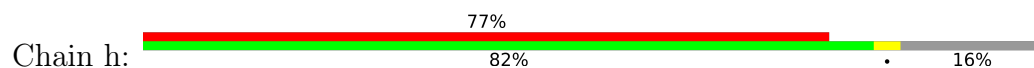


- Molecule 37: 30S ribosomal protein S4

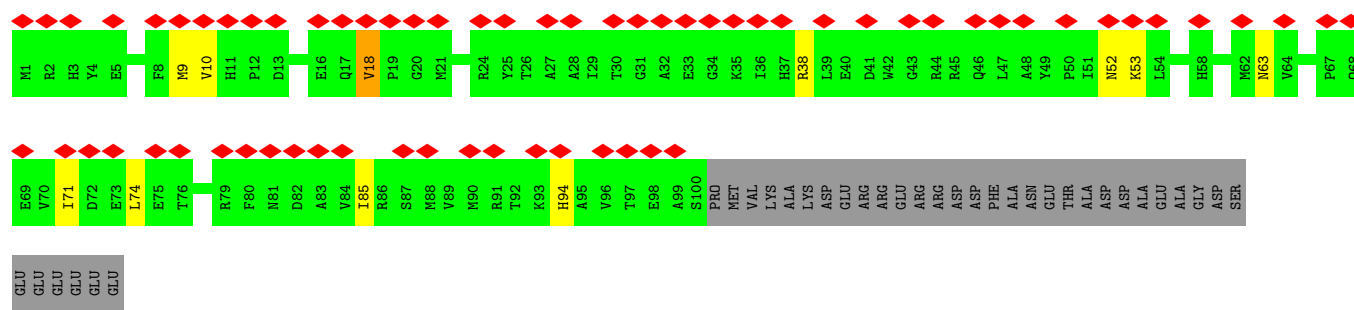
Chain g: 



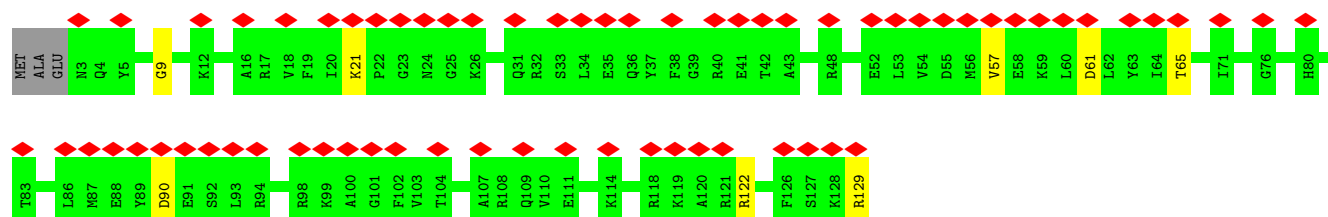
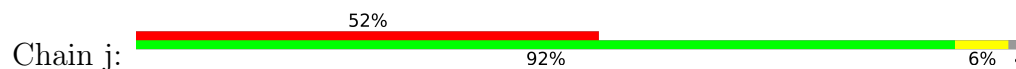
• Molecule 38: 30S ribosomal protein S7



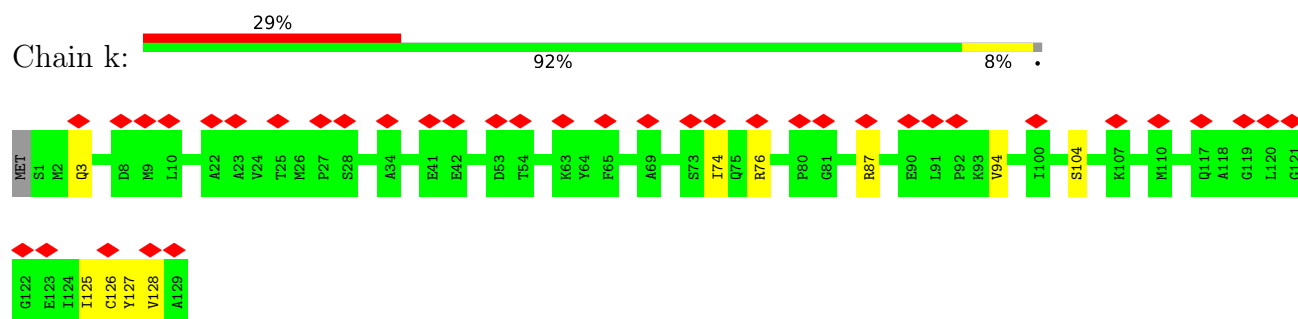
• Molecule 39: 30S ribosomal protein S6



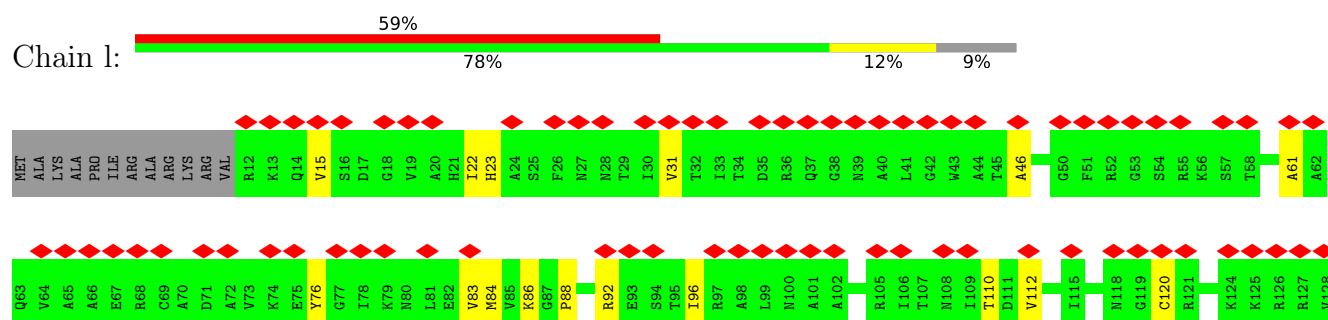
• Molecule 40: 30S ribosomal protein S9



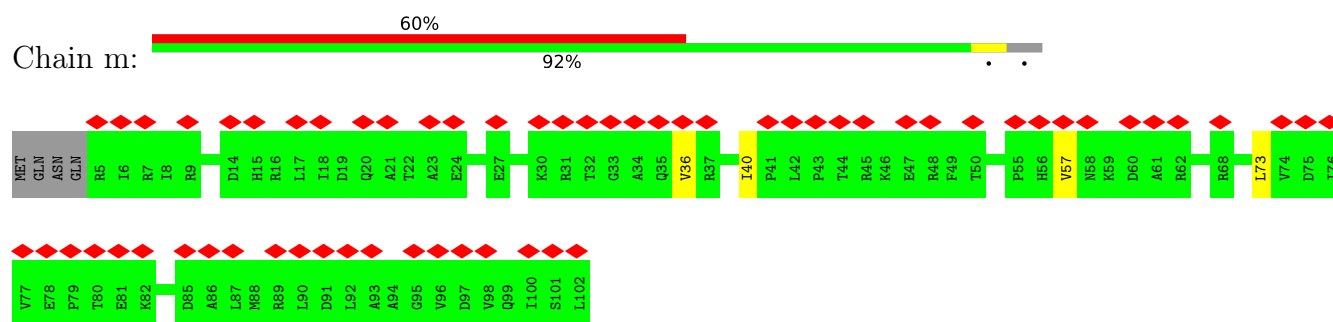
- Molecule 41: 30S ribosomal protein S8



- Molecule 42: 30S ribosomal protein S11



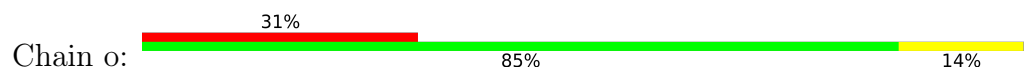
- Molecule 43: 30S ribosomal protein S10

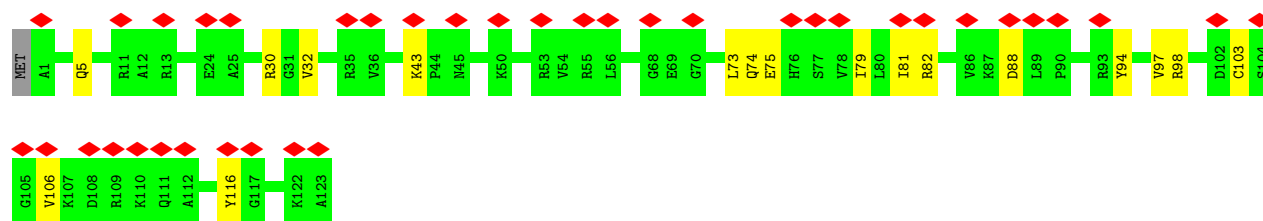


- Molecule 44: 30S ribosomal protein S13

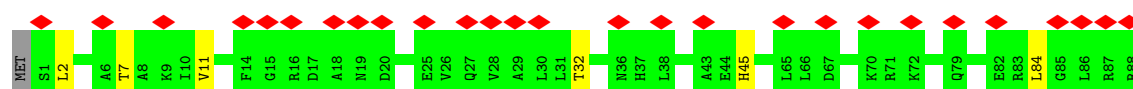
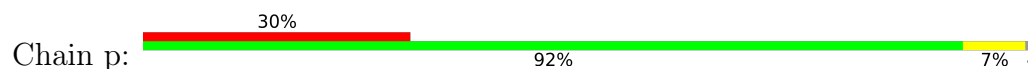


- Molecule 45: 30S ribosomal protein S12

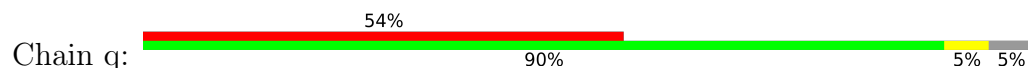




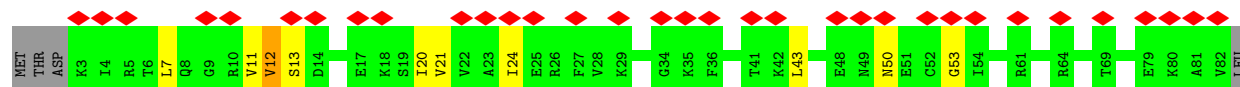
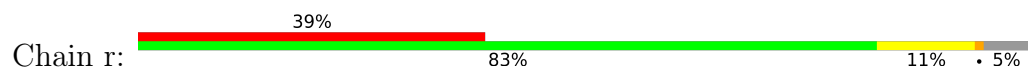
- Molecule 46: 30S ribosomal protein S15



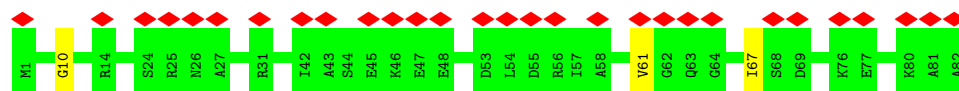
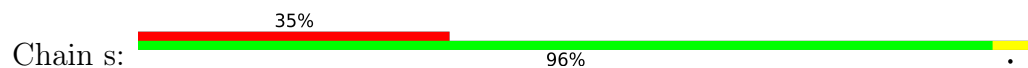
- Molecule 47: 30S ribosomal protein S14



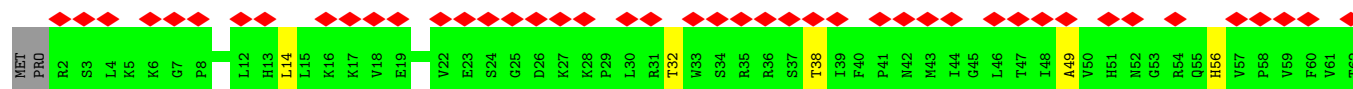
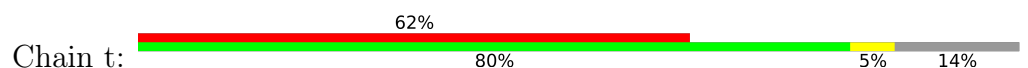
- Molecule 48: 30S ribosomal protein S17

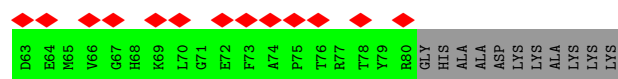


- Molecule 49: 30S ribosomal protein S16

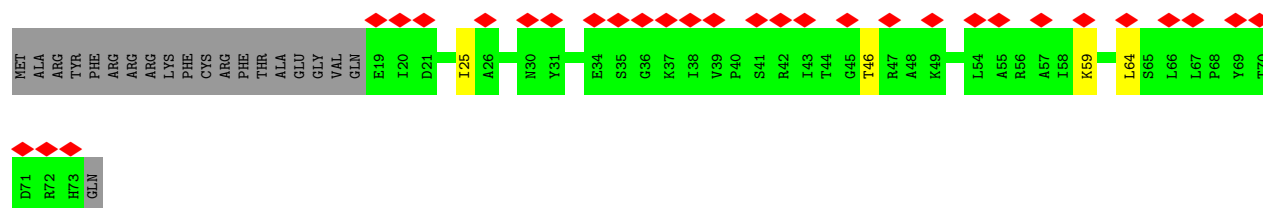


- Molecule 50: 30S ribosomal protein S19

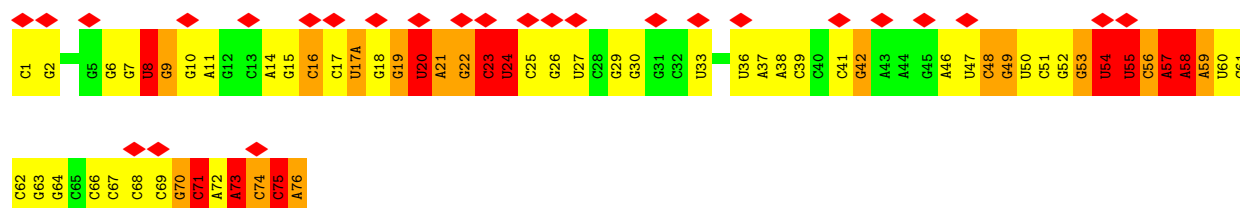
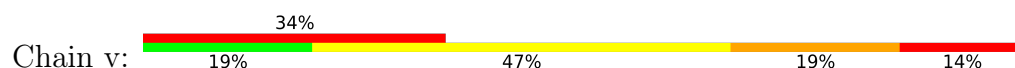




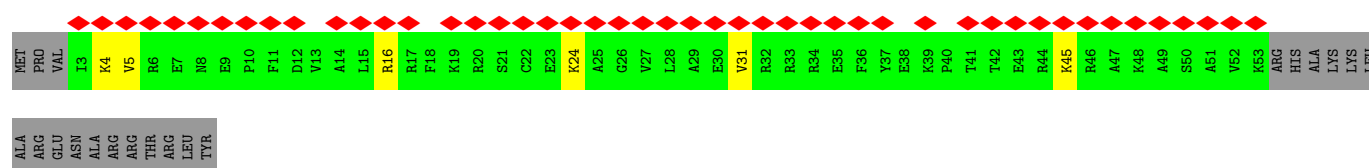
• Molecule 51: 30S ribosomal protein S18



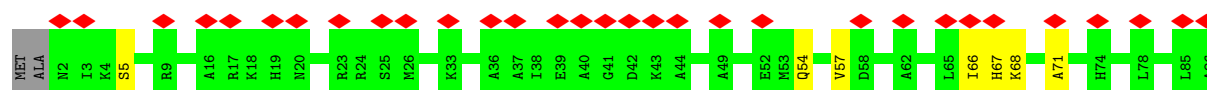
• Molecule 52: tRNA



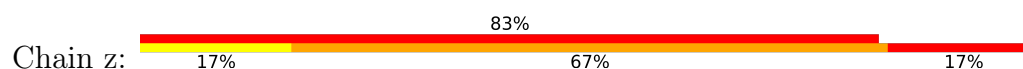
• Molecule 53: 30S ribosomal protein S21



• Molecule 54: 30S ribosomal protein S20



• Molecule 55: messenger RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14872	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	CTFFIND4	Depositor
Microscope	FEI POLARA 300, FEI POLARA 300	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20, 20	Depositor
Minimum defocus (nm)	640, 190	Depositor
Maximum defocus (nm)	7180, 7570	Depositor
Magnification	39000, 39000	Depositor
Image detector	GATAN K2 (4k x 4k), GATAN K2 (4k x 4k)	Depositor
Maximum map value	10.248	Depositor
Minimum map value	-4.187	Depositor
Average map value	0.072	Depositor
Map value standard deviation	0.559	Depositor
Recommended contour level	1.8	Depositor
Map size ($\text{\AA}$)	369.0, 369.0, 369.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.23, 1.23, 1.23	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FME, 4SU, H2U, GNP, 5MU, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.65	0/450	0.86	0/599
2	1	0.66	0/416	0.75	0/554
3	2	0.65	0/380	1.03	0/498
4	3	0.68	0/513	0.96	0/676
5	4	0.67	0/303	0.82	0/397
6	A	0.37	0/69659	0.67	12/108672 (0.0%)
7	B	0.37	0/2847	0.65	0/4440
8	C	0.70	0/2121	0.87	0/2852
9	D	0.70	0/1586	0.85	0/2134
10	E	0.67	0/1571	0.91	0/2113
11	F	0.72	0/1434	0.95	2/1926 (0.1%)
12	G	0.70	0/1343	0.83	0/1816
13	H	0.87	0/331	1.12	2/446 (0.4%)
14	I	0.79	0/1046	0.97	1/1410 (0.1%)
15	J	0.67	0/1152	0.89	0/1551
16	K	0.69	0/947	0.80	0/1268
17	L	0.72	0/1054	0.95	0/1403
18	M	0.65	0/1093	0.86	0/1460
19	N	0.69	0/973	0.98	0/1301
20	O	0.70	0/902	0.96	0/1209
21	P	0.69	0/929	0.87	0/1242
22	Q	0.68	0/960	1.03	0/1278
23	R	0.64	0/829	0.78	0/1107
24	S	0.66	0/864	0.89	1/1156 (0.1%)
25	T	0.66	0/744	0.88	0/994
26	U	0.68	0/787	0.87	1/1051 (0.1%)
27	V	0.66	0/766	0.79	0/1025
28	W	0.61	0/582	0.74	0/769
29	X	0.65	0/635	0.84	0/848
30	Y	0.71	0/510	1.03	0/677
31	Z	0.69	0/453	0.90	0/605
32	a	0.37	0/36966	0.67	10/57666 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.33	0/3895	0.81	8/5264 (0.2%)
34	c	0.71	0/1651	0.89	0/2225
35	d	0.79	0/1735	0.94	0/2338
36	f	0.74	0/1119	0.92	0/1504
37	g	0.73	0/1665	0.94	0/2227
38	h	0.71	0/1195	0.93	0/1602
39	i	0.77	1/835 (0.1%)	0.93	1/1128 (0.1%)
40	j	0.75	0/1034	0.91	0/1375
41	k	0.68	0/989	0.88	0/1326
42	l	0.72	0/893	0.87	0/1205
43	m	0.75	0/797	0.86	0/1077
44	n	0.75	0/892	1.02	0/1193
45	o	0.71	0/969	0.85	0/1300
46	p	0.70	0/722	0.98	0/964
47	q	0.70	0/785	0.90	0/1043
48	r	0.76	0/657	0.87	0/881
49	s	0.69	0/659	0.83	0/884
50	t	0.72	0/652	0.82	0/877
51	u	0.77	0/462	0.94	0/621
52	v	0.27	0/1746	0.74	11/2721 (0.4%)
53	w	0.78	0/430	0.95	0/570
54	x	0.70	0/671	0.98	0/888
55	z	1.20	1/144 (0.7%)	2.85	21/222 (9.5%)
All	All	0.49	2/159743 (0.0%)	0.74	70/238578 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	z	17	U	O3'-P	-6.88	1.50	1.61
39	i	18	VAL	CA-CB	5.74	1.57	1.54

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	z	14	A	C2'-C3'-O3'	13.38	133.78	113.70
55	z	15	U	O5'-P-OP2	-11.62	73.13	108.00
55	z	15	U	O5'-P-OP1	11.03	141.08	108.00
52	v	23	C	C2'-C3'-O3'	-10.61	97.78	113.70
55	z	13	A	C4'-C3'-O3'	-10.60	97.10	113.00
55	z	16	A	C2'-C3'-O3'	9.95	128.63	113.70
55	z	14	A	P-O3'-C3'	-9.84	105.44	120.20
55	z	15	U	C4'-C3'-O3'	-9.70	94.85	109.40
55	z	14	A	N9-C1'-C2'	9.05	125.58	112.00
6	A	2425	A	C4'-C3'-O3'	8.41	122.01	109.40
55	z	16	A	C4'-C3'-O3'	-8.34	100.49	113.00
52	v	71	C	C4'-C3'-O3'	8.13	125.20	113.00
32	a	115	G	C4'-C3'-O3'	8.01	121.42	109.40
52	v	71	C	C1'-C2'-O2'	-7.90	96.55	108.40
33	b	399	HIS	N-CA-C	-7.89	97.77	110.32
6	A	404	A	C4'-C3'-O3'	7.83	121.14	109.40
33	b	453	SER	N-CA-C	7.77	119.83	111.36
32	a	733	G	C4'-C3'-O3'	7.70	120.95	109.40
52	v	58	A	C2'-C3'-O3'	-7.63	98.06	109.50
33	b	576	LYS	N-CA-C	7.52	119.55	111.36
32	a	917	G	N9-C1'-C2'	-7.28	101.08	112.00
52	v	24	U	C1'-C2'-O2'	-7.18	97.63	108.40
55	z	14	A	P-O5'-C5'	-7.01	110.39	120.90
52	v	75	C	N1-C1'-C2'	-6.82	101.76	112.00
6	A	1378	A	C4'-C3'-O3'	6.73	119.50	109.40
55	z	15	U	OP1-P-OP2	-6.71	99.49	119.60
32	a	1201	A	C4'-C3'-O3'	6.68	119.43	109.40
32	a	1101	A	C2'-C3'-O3'	6.58	119.37	109.50
55	z	16	A	C5'-C4'-C3'	6.53	125.80	116.00
55	z	15	U	N1-C1'-C2'	6.51	123.76	114.00
33	b	795	ILE	N-CA-C	-6.37	104.82	111.58
55	z	15	U	P-O5'-C5'	-6.34	111.40	120.90
6	A	479	A	C4'-C3'-O3'	6.33	118.90	109.40
13	H	31	VAL	CA-C-N	-6.33	113.43	120.14
13	H	31	VAL	C-N-CA	-6.33	113.43	120.14
33	b	450	ALA	N-CA-C	6.31	118.16	111.28
33	b	588	GLU	N-CA-C	-6.31	98.95	109.24
55	z	14	A	O4'-C4'-C3'	6.30	110.30	104.00
6	A	1606	C	C2'-C3'-O3'	6.24	123.06	113.70
32	a	917	G	C4'-C3'-O3'	6.24	122.36	113.00
55	z	14	A	O5'-C5'-C4'	-6.24	102.14	111.50
6	A	271	G	C2'-C3'-O3'	6.18	118.77	109.50
55	z	13	A	P-O3'-C3'	-5.98	111.23	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	995	C	C2'-C3'-O3'	5.94	118.41	109.50
55	z	16	A	C1'-C2'-O2'	5.92	117.27	108.40
52	v	75	C	C4'-C3'-O3'	5.86	121.80	113.00
6	A	2756	U	C4'-C3'-O3'	5.81	118.12	109.40
52	v	57	A	C2'-C3'-O3'	-5.80	105.00	113.70
14	I	21	PRO	N-CA-C	5.76	117.72	110.70
32	a	1397	C	C2'-C3'-O3'	-5.71	100.93	109.50
52	v	24	U	C2'-C3'-O3'	-5.70	105.16	113.70
32	a	428	G	C4'-C3'-O3'	5.58	117.77	109.40
11	F	174	PHE	CA-C-N	5.52	126.74	119.84
11	F	174	PHE	C-N-CA	5.52	126.74	119.84
52	v	71	C	N1-C1'-C2'	-5.50	103.76	112.00
24	S	63	GLY	N-CA-C	5.48	120.49	114.40
6	A	2127	G	C2'-C3'-O3'	5.47	121.91	113.70
32	a	918	A	C2'-C3'-O3'	-5.47	105.50	113.70
39	i	52	ASN	N-CA-C	5.40	117.77	111.02
55	z	13	A	C1'-C2'-O2'	5.39	116.49	108.40
33	b	836	VAL	N-CA-C	5.33	116.03	107.98
55	z	15	U	O5'-C5'-C4'	-5.33	103.71	111.70
6	A	2158	A	C4'-C3'-O3'	5.32	117.39	109.40
55	z	17	U	P-O3'-C3'	5.32	128.18	120.20
6	A	1313	U	N1-C1'-C2'	5.25	119.87	112.00
6	A	1565	C	C2'-C3'-O3'	5.24	117.36	109.50
32	a	96	U	C3'-C2'-O2'	5.18	118.48	110.70
52	v	73	A	C2'-C3'-O3'	-5.17	105.94	113.70
33	b	401	ASP	N-CA-C	5.16	121.78	110.80
26	U	15	GLY	N-CA-C	5.16	119.18	112.68

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	H	11	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	444	0	461	0	0
2	1	409	0	440	1	0
3	2	377	0	418	2	0
4	3	504	0	574	2	0
5	4	302	0	343	1	0
6	A	62195	0	31280	53	0
7	B	2546	0	1292	3	0
8	C	2082	0	2157	6	0
9	D	1565	0	1616	8	0
10	E	1552	0	1619	7	0
11	F	1410	0	1447	7	0
12	G	1323	0	1374	9	0
13	H	328	0	357	3	0
14	I	1032	0	1088	4	0
15	J	1129	0	1162	6	0
16	K	938	0	1012	8	0
17	L	1045	0	1117	3	0
18	M	1074	0	1157	8	0
19	N	960	0	1000	4	0
20	O	892	0	923	4	0
21	P	917	0	965	2	0
22	Q	947	0	1022	1	0
23	R	816	0	839	0	0
24	S	857	0	922	0	0
25	T	738	0	807	2	0
26	U	779	0	834	2	0
27	V	753	0	780	0	0
28	W	575	0	589	2	0
29	X	625	0	655	4	0
30	Y	509	0	543	0	0
31	Z	449	0	491	0	0
32	a	33015	0	16617	97	0
33	b	3847	0	3909	303	0
34	c	1624	0	1699	7	0
35	d	1704	0	1732	11	0
36	f	1106	0	1148	14	0
37	g	1643	0	1710	13	0
38	h	1181	0	1240	2	0
39	i	817	0	808	5	0
40	j	1022	0	1070	2	0
41	k	979	0	1034	6	0
42	l	877	0	887	9	0
43	m	787	0	828	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	n	883	0	944	6	0
45	o	955	0	1019	13	0
46	p	714	0	737	3	0
47	q	774	0	827	4	0
48	r	648	0	691	6	0
49	s	649	0	666	1	0
50	t	637	0	665	2	0
51	u	455	0	478	2	0
52	v	1643	0	835	155	0
53	w	425	0	449	4	0
54	x	665	0	714	3	0
55	z	129	0	65	53	0
56	b	32	0	13	14	0
57	v	9	1	10	15	0
All	All	147292	1	100079	741	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 3.

All (741) 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)
33:b:848:PHE:H	57:v:101:FME:CN	1.36	1.36
33:b:812:ILE:HG12	52:v:76:A:C1'	1.60	1.32
33:b:788:PRO:CG	33:b:887:ARG:HG3	1.64	1.26
33:b:788:PRO:HG3	33:b:887:ARG:CG	1.65	1.24
55:z:16:A:H3'	55:z:17:U:C6	1.73	1.24
52:v:36:U:H3	55:z:16:A:N6	1.33	1.23
33:b:812:ILE:HG12	52:v:76:A:N9	1.50	1.23
33:b:531:VAL:HG11	33:b:544:LEU:HB2	1.20	1.17
33:b:804:PHE:HB2	33:b:812:ILE:CG2	1.73	1.17
33:b:540:GLY:HA2	33:b:541:ILE:HG22	1.25	1.16
33:b:812:ILE:CD1	52:v:76:A:C4	2.28	1.16
33:b:848:PHE:H	57:v:101:FME:HCN	1.10	1.16
55:z:16:A:H3'	55:z:17:U:H6	1.01	1.16
52:v:8:4SU:S4	52:v:14:A:N7	2.19	1.16
12:G:176:LYS:OXT	12:G:176:LYS:HD3	1.48	1.14
33:b:789:GLU:HA	33:b:884:GLU:HA	1.16	1.13
33:b:812:ILE:HD13	52:v:76:A:C4	1.86	1.11
52:v:21:A:N6	52:v:48:C:OP1	1.84	1.10
33:b:846:ARG:HB3	52:v:76:A:C2	1.87	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:499:LYS:HE2	56:b:901:GNP:C4	1.83	1.07
33:b:812:ILE:HG21	52:v:76:A:O4'	1.55	1.07
33:b:534:SER:CB	33:b:537:ALA:HB3	1.84	1.06
33:b:812:ILE:HD13	52:v:76:A:C5	1.90	1.06
12:G:91:VAL:HG23	33:b:504:GLU:HG3	1.06	1.05
33:b:591:LEU:HD12	33:b:620:ALA:HB3	1.36	1.05
33:b:848:PHE:N	57:v:101:FME:CN	2.19	1.04
33:b:848:PHE:N	57:v:101:FME:HCN	1.71	1.03
33:b:540:GLY:HA2	33:b:541:ILE:CG2	1.88	1.03
33:b:804:PHE:HB2	33:b:812:ILE:HG23	1.37	1.03
55:z:16:A:C4	55:z:17:U:C5	2.48	1.02
32:a:1506:U:OP2	55:z:13:A:P	2.18	1.01
32:a:1339:A:H1'	52:v:41:C:H1'	1.43	1.00
32:a:1506:U:OP2	55:z:13:A:OP1	1.80	0.99
52:v:22:G:C4	52:v:23:C:C5	2.51	0.98
33:b:403:GLY:HA2	56:b:901:GNP:O2A	1.64	0.98
33:b:812:ILE:HG12	52:v:76:A:H1'	1.48	0.96
32:a:368:U:C5	33:b:608:ALA:HB2	2.01	0.95
33:b:400:VAL:HA	56:b:901:GNP:O2G	1.67	0.95
52:v:74:C:C2'	52:v:75:C:H5'	1.96	0.94
55:z:16:A:C5	55:z:17:U:C5	2.55	0.94
33:b:727:GLY:HA2	33:b:748:VAL:HG23	1.49	0.94
55:z:16:A:C4	55:z:17:U:C6	2.56	0.93
33:b:812:ILE:CG1	52:v:76:A:N9	2.31	0.93
32:a:918:A:O2'	32:a:919:A:O4'	1.89	0.91
12:G:91:VAL:CG2	33:b:504:GLU:HG3	2.00	0.91
12:G:91:VAL:HG23	33:b:504:GLU:CG	2.00	0.90
32:a:359:G:H1'	33:b:576:LYS:HG3	1.54	0.89
33:b:789:GLU:CA	33:b:884:GLU:HA	2.02	0.89
33:b:860:GLU:HG3	57:v:101:FME:HE3	1.54	0.89
52:v:76:A:O2'	57:v:101:FME:O1	1.90	0.89
33:b:812:ILE:HD12	33:b:863:ILE:O	1.72	0.88
33:b:565:ALA:HB2	33:b:590:THR:CG2	2.02	0.88
33:b:531:VAL:HG21	33:b:544:LEU:HA	1.54	0.88
52:v:22:G:HO2'	52:v:23:C:H6	0.93	0.88
33:b:401:ASP:H	56:b:901:GNP:HNB3	1.21	0.88
52:v:71:C:O2'	52:v:72:A:H5'	1.73	0.87
32:a:1339:A:C1'	52:v:41:C:H1'	2.04	0.87
33:b:812:ILE:HD11	52:v:76:A:N3	1.88	0.87
33:b:728:ILE:HG13	33:b:748:VAL:HG21	1.56	0.87
32:a:916:U:C2'	32:a:917:G:H5'	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:11:A:N6	52:v:24:U:O4	2.08	0.86
52:v:36:U:N3	55:z:16:A:N6	2.11	0.86
52:v:36:U:H3	55:z:16:A:H61	0.90	0.86
52:v:74:C:H2'	52:v:75:C:H5'	1.57	0.86
55:z:16:A:C3'	55:z:17:U:H6	1.87	0.86
33:b:540:GLY:HA2	33:b:541:ILE:CB	2.05	0.84
33:b:531:VAL:HG11	33:b:544:LEU:CB	2.06	0.84
48:r:11:VAL:HG13	48:r:20:ILE:HD11	1.58	0.84
55:z:16:A:C5	55:z:17:U:C4	2.65	0.84
33:b:534:SER:OG	33:b:537:ALA:CB	2.25	0.83
33:b:812:ILE:HG12	52:v:76:A:C4	2.13	0.83
33:b:795:ILE:HG22	33:b:879:VAL:HG13	1.61	0.83
52:v:22:G:N3	52:v:23:C:C6	2.47	0.82
33:b:426:GLN:HE22	33:b:770:VAL:HB	1.44	0.82
55:z:16:A:N3	55:z:17:U:C6	2.47	0.82
52:v:8:4SU:H6	52:v:21:A:H2	1.45	0.81
33:b:786:LEU:HD12	33:b:887:ARG:HB3	1.61	0.81
33:b:812:ILE:CG1	52:v:76:A:C4	2.61	0.81
32:a:50:A:N6	33:b:753:SER:CB	2.44	0.81
33:b:789:GLU:HB2	33:b:883:ILE:O	1.81	0.80
33:b:589:GLY:HA3	33:b:622:PRO:N	1.97	0.80
33:b:795:ILE:CG2	33:b:879:VAL:HG13	2.11	0.80
55:z:16:A:N3	55:z:16:A:H2'	1.96	0.80
33:b:534:SER:HB3	33:b:537:ALA:HB3	1.61	0.80
52:v:69:C:C2'	52:v:70:G:H5'	2.12	0.80
52:v:74:C:O2'	52:v:75:C:H5'	1.82	0.79
55:z:16:A:C6	55:z:17:U:C4	2.71	0.79
52:v:37:A:H2	55:z:15:U:O2	1.66	0.78
33:b:537:ALA:HB3	33:b:539:THR:HG23	1.65	0.78
33:b:789:GLU:HA	33:b:884:GLU:CA	2.07	0.78
12:G:176:LYS:OXT	12:G:176:LYS:CD	2.30	0.77
33:b:613:LEU:HD12	33:b:614:GLY:N	1.99	0.77
55:z:16:A:C3'	55:z:17:U:C6	2.64	0.77
32:a:790:A:OP1	52:v:38:A:O2'	2.01	0.76
52:v:18:G:O2'	52:v:19:G:H5'	1.85	0.76
32:a:360:G:H5''	33:b:729:THR:HG22	1.67	0.76
55:z:16:A:OP2	55:z:17:U:O4	2.02	0.76
55:z:16:A:O2'	55:z:17:U:H5'	1.85	0.76
32:a:368:U:C4	33:b:608:ALA:HB2	2.21	0.76
33:b:565:ALA:HB2	33:b:590:THR:HG23	1.66	0.76
33:b:812:ILE:CD1	52:v:76:A:N3	2.46	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:358:U:H4'	33:b:579:GLY:HA3	1.68	0.75
52:v:8:4SU:H1'	52:v:21:A:C2	2.22	0.75
52:v:58:A:HO2'	52:v:60:U:H5	1.33	0.75
12:G:176:LYS:HD3	12:G:176:LYS:C	2.12	0.74
32:a:361:G:H5''	33:b:730:GLU:HB3	1.70	0.74
55:z:14:A:C2'	55:z:15:U:OP2	2.31	0.74
52:v:71:C:C2'	52:v:72:A:H5'	2.18	0.74
33:b:812:ILE:CG2	52:v:76:A:O4'	2.36	0.73
33:b:848:PHE:N	57:v:101:FME:O1	2.15	0.73
33:b:403:GLY:HA2	56:b:901:GNP:PA	2.28	0.73
52:v:20:H2U:H4'	52:v:21:A:OP2	1.87	0.73
32:a:1230:C:H5'	52:v:30:G:OP1	1.88	0.73
33:b:540:GLY:CA	33:b:541:ILE:HG22	2.13	0.73
52:v:8:4SU:H6	52:v:21:A:C2	2.23	0.72
33:b:550:LEU:C	33:b:550:LEU:HD23	2.14	0.72
32:a:918:A:H2'	32:a:919:A:C8	2.25	0.72
52:v:58:A:O2'	52:v:60:U:H5	1.72	0.72
18:M:78:LEU:N	33:b:858:GLY:O	2.15	0.72
33:b:812:ILE:CG1	52:v:76:A:C1'	2.55	0.71
32:a:358:U:H1'	33:b:577:GLY:O	1.89	0.71
32:a:1396:A:H5'	32:a:1397:C:OP1	1.90	0.71
33:b:847:ARG:HA	57:v:101:FME:CN	2.20	0.70
33:b:860:GLU:HG3	57:v:101:FME:CE	2.21	0.70
52:v:41:C:H3'	52:v:42:G:H5''	1.71	0.70
11:F:11:VAL:HG22	11:F:171:ALA:HB1	1.72	0.70
52:v:17:C:H2'	52:v:17(A):U:H5	1.55	0.70
38:h:26:VAL:HG12	38:h:42:VAL:HG21	1.72	0.70
33:b:812:ILE:HD12	33:b:863:ILE:C	2.15	0.70
55:z:16:A:H3'	55:z:17:U:C5	2.26	0.70
33:b:544:LEU:C	33:b:544:LEU:HD23	2.17	0.70
33:b:786:LEU:HB3	33:b:887:ARG:HD2	1.74	0.70
52:v:58:A:H1'	52:v:60:U:O4	1.92	0.69
33:b:534:SER:OG	33:b:537:ALA:HB3	1.85	0.69
52:v:70:G:H2'	52:v:71:C:C6	2.28	0.69
6:A:1926:U:O4'	52:v:71:C:OP1	2.11	0.69
33:b:716:VAL:HG21	33:b:786:LEU:HD21	1.74	0.69
33:b:533:VAL:HG12	33:b:541:ILE:H	1.57	0.68
33:b:796:GLY:O	33:b:879:VAL:HG12	1.93	0.68
6:A:2660:A:O3'	33:b:399:HIS:HE1	1.75	0.68
54:x:66:ILE:HG21	54:x:71:ALA:HB2	1.76	0.68
33:b:790:LEU:HD23	33:b:790:LEU:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:k:74:ILE:HD13	41:k:128:VAL:HG22	1.75	0.68
52:v:22:G:C4	52:v:23:C:C6	2.82	0.68
55:z:15:U:H6	55:z:15:U:OP1	1.74	0.68
52:v:20:H2U:O5'	52:v:21:A:OP2	2.12	0.68
33:b:797:LEU:HD23	33:b:798:ALA:N	2.08	0.68
33:b:738:ALA:CB	45:o:32:VAL:HG11	2.23	0.67
33:b:403:GLY:CA	56:b:901:GNP:O2A	2.40	0.67
32:a:916:U:H2'	32:a:917:G:H5'	1.75	0.67
33:b:540:GLY:CA	33:b:542:ASP:H	2.08	0.67
32:a:50:A:N6	33:b:753:SER:HB2	2.09	0.67
33:b:847:ARG:HA	57:v:101:FME:HCN	1.77	0.67
33:b:396:ILE:CG2	33:b:404:LYS:HG3	2.25	0.67
32:a:1339:A:C2	52:v:30:G:H1'	2.30	0.67
32:a:1339:A:O2'	52:v:41:C:H1'	1.95	0.66
33:b:565:ALA:HB2	33:b:590:THR:HG22	1.77	0.66
52:v:37:A:C2	55:z:15:U:O2	2.48	0.66
33:b:426:GLN:HE22	33:b:770:VAL:CB	2.06	0.66
33:b:569:VAL:HG22	33:b:584:VAL:HG22	1.78	0.66
33:b:396:ILE:HG22	33:b:404:LYS:HG3	1.77	0.66
33:b:804:PHE:CB	33:b:812:ILE:CG2	2.64	0.66
33:b:589:GLY:HA3	33:b:622:PRO:CD	2.25	0.65
55:z:16:A:C2	55:z:17:U:N1	2.64	0.65
33:b:533:VAL:HG12	33:b:541:ILE:N	2.12	0.65
33:b:786:LEU:HB2	33:b:887:ARG:HB2	1.79	0.65
33:b:404:LYS:HB3	56:b:901:GNP:O2B	1.97	0.65
33:b:855:VAL:HG11	33:b:861:CYS:CB	2.27	0.65
33:b:393:VAL:HG12	33:b:462:THR:HG22	1.79	0.65
52:v:22:G:O2'	52:v:23:C:O5'	2.15	0.64
32:a:361:G:H5''	33:b:730:GLU:CB	2.27	0.64
52:v:66:C:H2'	52:v:67:C:C6	2.32	0.64
52:v:69:C:O2'	52:v:70:G:H5'	1.96	0.64
32:a:714:G:N2	42:l:120:CYS:SG	2.70	0.64
33:b:468:VAL:HB	33:b:498:ASN:HD21	1.63	0.64
52:v:22:G:N3	52:v:23:C:C5	2.66	0.64
55:z:14:A:H2'	55:z:15:U:OP2	1.97	0.64
33:b:855:VAL:HG13	33:b:859:MET:HE3	1.79	0.64
52:v:22:G:C5	52:v:23:C:C5	2.86	0.64
52:v:67:C:H2'	52:v:68:C:C6	2.33	0.64
33:b:797:LEU:HD23	33:b:797:LEU:C	2.22	0.63
52:v:73:A:O2'	52:v:74:C:O4'	2.15	0.63
55:z:17:U:C6	55:z:17:U:OP2	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:847:ARG:CA	57:v:101:FME:HCN	2.28	0.63
32:a:50:A:H61	33:b:753:SER:CB	2.11	0.63
55:z:16:A:O5'	55:z:17:U:H5	1.81	0.63
52:v:51:C:H2'	52:v:52:G:C8	2.34	0.63
42:l:84:MET:HE3	42:l:112:VAL:HG11	1.80	0.62
33:b:534:SER:OG	33:b:537:ALA:HB2	1.99	0.62
52:v:8:4SU:H5''	52:v:8:4SU:O2	1.98	0.62
33:b:716:VAL:CG2	33:b:786:LEU:HD21	2.29	0.62
52:v:8:4SU:H1'	52:v:21:A:N1	2.14	0.62
33:b:738:ALA:HB2	45:o:32:VAL:HG11	1.81	0.62
49:s:61:VAL:HG22	49:s:67:ILE:HD11	1.81	0.62
52:v:8:4SU:C6	52:v:21:A:H2	2.13	0.62
6:A:574:A:N6	6:A:2034:U:OP1	2.33	0.62
32:a:50:A:C6	33:b:753:SER:HB3	2.35	0.62
52:v:8:4SU:O2	52:v:8:4SU:H3'	1.99	0.62
33:b:830:VAL:HG22	33:b:877:ILE:HG12	1.81	0.62
33:b:404:LYS:HE3	56:b:901:GNP:O3G	1.99	0.61
33:b:483:ILE:HD12	33:b:519:ILE:HG21	1.82	0.61
33:b:540:GLY:HA3	33:b:542:ASP:H	1.63	0.61
33:b:814:GLY:HA3	57:v:101:FME:SD	2.41	0.61
52:v:41:C:C3'	52:v:42:G:H5''	2.29	0.61
33:b:537:ALA:CB	33:b:539:THR:HG23	2.29	0.61
33:b:812:ILE:HD11	52:v:76:A:C2	2.35	0.61
32:a:790:A:OP1	52:v:39:C:H5'	2.00	0.61
33:b:611:ASN:O	33:b:612:GLU:HG2	2.00	0.61
33:b:847:ARG:C	57:v:101:FME:HCN	2.27	0.60
52:v:56:C:O2'	52:v:57:A:H5'	2.00	0.60
52:v:19:G:O2'	52:v:20:H2U:OP2	2.17	0.60
55:z:15:U:C6	55:z:15:U:P	2.95	0.60
33:b:855:VAL:HG13	33:b:859:MET:CE	2.32	0.59
33:b:471:ALA:HB3	33:b:505:ALA:HB1	1.84	0.59
32:a:916:U:O2'	32:a:917:G:H5'	2.00	0.59
32:a:50:A:C6	33:b:753:SER:CB	2.85	0.59
18:M:42:THR:HG22	18:M:93:VAL:HG12	1.84	0.59
20:O:39:VAL:HG11	20:O:87:ILE:HD12	1.85	0.59
44:n:76:ILE:HG22	44:n:80:MET:HE2	1.85	0.59
32:a:1339:A:H4'	52:v:41:C:H4'	1.84	0.59
33:b:855:VAL:HG11	33:b:861:CYS:HB3	1.82	0.59
6:A:514:A:N3	6:A:581:C:O2'	2.35	0.59
52:v:6:G:O2'	52:v:7:G:H5'	2.02	0.59
52:v:33:U:N3	52:v:36:U:OP2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:z:16:A:C2	55:z:17:U:C6	2.90	0.58
33:b:812:ILE:HB	52:v:76:A:C8	2.38	0.58
39:i:71:ILE:HD12	39:i:74:LEU:HD23	1.85	0.58
55:z:16:A:C2'	55:z:17:U:H5'	2.33	0.58
33:b:499:LYS:HE2	56:b:901:GNP:C5	2.33	0.58
52:v:17:C:H2'	52:v:17(A):U:C5	2.37	0.58
55:z:16:A:C2'	55:z:17:U:H6	2.15	0.58
52:v:69:C:H2'	52:v:70:G:H5'	1.84	0.58
33:b:448:HIS:HD2	33:b:772:TYR:OH	1.85	0.58
6:A:1073:A:H3'	6:A:1074:G:H5''	1.85	0.58
33:b:589:GLY:HA3	33:b:622:PRO:HD3	1.86	0.58
33:b:399:HIS:CB	33:b:402:HIS:HE1	2.17	0.58
55:z:13:A:C2	55:z:14:A:N6	2.72	0.58
33:b:731:THR:HB	45:o:30:ARG:HH22	1.69	0.58
52:v:56:C:H2'	52:v:57:A:C8	2.38	0.58
33:b:804:PHE:HB2	33:b:812:ILE:HG22	1.80	0.57
33:b:814:GLY:CA	57:v:101:FME:SD	2.92	0.57
33:b:746:PHE:O	33:b:747:ASN:OD1	2.22	0.57
50:t:14:LEU:HD13	50:t:32:THR:HG21	1.86	0.57
45:o:73:LEU:HD13	45:o:79:ILE:HD13	1.86	0.57
9:D:2:ILE:HD13	9:D:48:ILE:HD11	1.85	0.57
32:a:358:U:H4'	33:b:579:GLY:CA	2.33	0.57
33:b:586:VAL:HG23	33:b:622:PRO:HA	1.86	0.57
33:b:399:HIS:CD2	33:b:476:MET:CB	2.88	0.57
32:a:978:A:OP1	32:a:980:C:N4	2.38	0.57
34:c:67:ILE:HD12	34:c:100:ILE:HD11	1.86	0.57
55:z:15:U:OP1	55:z:15:U:C6	2.57	0.57
33:b:396:ILE:HG12	33:b:466:VAL:HB	1.86	0.56
33:b:499:LYS:HD3	56:b:901:GNP:C6	2.35	0.56
33:b:544:LEU:HD23	33:b:544:LEU:O	2.05	0.56
10:E:2:GLU:HB3	10:E:11:ALA:HB1	1.87	0.56
29:X:67:LEU:HD23	29:X:70:LEU:HD12	1.88	0.56
33:b:783:SER:OG	33:b:889:ILE:HG22	2.06	0.56
52:v:20:H2U:C4'	52:v:21:A:OP2	2.51	0.56
52:v:53:G:N1	52:v:61:C:N3	2.51	0.56
32:a:1506:U:OP2	55:z:13:A:OP2	2.24	0.56
33:b:748:VAL:HG22	33:b:749:ARG:N	2.21	0.56
33:b:815:CYS:SG	33:b:861:CYS:C	2.89	0.56
50:t:49:ALA:HB1	50:t:56:HIS:HB3	1.88	0.56
32:a:978:A:OP2	32:a:1362:A:N6	2.38	0.56
33:b:467:LEU:HB2	33:b:495:VAL:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:721:ILE:HG22	33:b:735:LEU:HD21	1.86	0.56
17:L:79:LEU:HD12	17:L:112:LEU:HD13	1.87	0.55
33:b:399:HIS:HB3	33:b:402:HIS:CE1	2.41	0.55
33:b:694:LYS:HG2	33:b:724:GLY:HA3	1.88	0.55
33:b:846:ARG:CB	52:v:76:A:C2	2.78	0.55
16:K:5:GLN:HA	16:K:20:MET:HE3	1.88	0.55
33:b:457:ARG:HH12	33:b:637:ALA:HB3	1.71	0.55
33:b:727:GLY:O	33:b:728:ILE:HG13	2.05	0.55
52:v:58:A:O2'	52:v:60:U:C5	2.51	0.55
33:b:567:GLY:HA2	33:b:587:ARG:HG3	1.88	0.55
33:b:786:LEU:HD13	33:b:887:ARG:HD3	1.88	0.55
52:v:57:A:O2'	52:v:58:A:O5'	2.20	0.55
15:J:32:LEU:HD22	15:J:54:ILE:HG21	1.89	0.55
33:b:397:MET:HE1	33:b:459:ALA:HB2	1.88	0.55
55:z:16:A:C2	55:z:17:U:C2	2.95	0.55
33:b:540:GLY:HA2	33:b:541:ILE:HB	1.88	0.55
33:b:591:LEU:HD12	33:b:620:ALA:CB	2.24	0.55
33:b:786:LEU:HD12	33:b:887:ARG:CB	2.35	0.55
33:b:589:GLY:N	33:b:622:PRO:HB3	2.22	0.54
33:b:613:LEU:HD12	33:b:613:LEU:C	2.32	0.54
33:b:673:LYS:HE3	45:o:74:GLN:HE22	1.72	0.54
42:l:110:THR:HG22	53:w:4:LYS:HB3	1.90	0.54
33:b:611:ASN:C	33:b:612:GLU:HG2	2.33	0.54
36:f:21:SER:OG	36:f:28:ARG:HG3	2.06	0.54
33:b:499:LYS:HE2	56:b:901:GNP:N3	2.21	0.54
33:b:830:VAL:O	33:b:836:VAL:HG23	2.08	0.54
43:m:40:ILE:HD12	43:m:73:LEU:HD22	1.90	0.54
33:b:499:LYS:HD2	56:b:901:GNP:C2	2.37	0.54
33:b:795:ILE:HG23	33:b:796:GLY:N	2.23	0.54
8:C:28:PRO:HG2	8:C:33:LEU:HD11	1.89	0.54
52:v:74:C:H2'	52:v:75:C:C5'	2.34	0.54
33:b:860:GLU:CG	57:v:101:FME:HE3	2.32	0.54
32:a:1302:C:C5	44:n:16:ILE:HD11	2.43	0.54
25:T:1:MET:HB3	25:T:2:ILE:HD12	1.90	0.53
33:b:531:VAL:CG1	33:b:544:LEU:HB2	2.14	0.53
19:N:44:LEU:HD23	19:N:113:ILE:HD13	1.91	0.53
33:b:566:SER:HB3	33:b:588:GLU:OE1	2.08	0.53
33:b:585:LEU:HD23	33:b:625:PRO:HB3	1.90	0.53
33:b:847:ARG:O	33:b:847:ARG:HG3	2.09	0.53
36:f:80:LEU:HD13	36:f:122:VAL:HG11	1.90	0.53
15:J:56:VAL:HB	15:J:124:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1339:A:O2'	52:v:41:C:C1'	2.57	0.53
33:b:812:ILE:CB	52:v:76:A:C8	2.92	0.53
8:C:2:VAL:HG11	8:C:201:LEU:HD23	1.91	0.53
33:b:812:ILE:HG23	33:b:812:ILE:O	2.08	0.53
33:b:882:ILE:HG13	33:b:882:ILE:O	2.07	0.53
13:H:31:VAL:HB	13:H:32:PRO:HD3	1.91	0.53
33:b:391:ALA:HB3	33:b:623:SER:HB2	1.91	0.53
33:b:399:HIS:CD2	33:b:476:MET:HB3	2.44	0.53
52:v:71:C:C2'	52:v:72:A:C5'	2.85	0.53
52:v:72:A:O2'	52:v:73:A:H5'	2.08	0.53
3:2:34:ARG:NH1	6:A:466:A:OP1	2.42	0.52
33:b:395:THR:HB	33:b:462:THR:HG21	1.90	0.52
52:v:51:C:H1'	52:v:64:G:N2	2.24	0.52
11:F:110:ILE:HG12	11:F:136:ILE:HG21	1.91	0.52
33:b:800:VAL:HG12	33:b:815:CYS:HB3	1.91	0.52
33:b:855:VAL:HG11	33:b:861:CYS:HB2	1.91	0.52
52:v:14:A:H2'	52:v:15:G:O4'	2.09	0.52
33:b:612:GLU:HG3	33:b:613:LEU:N	2.24	0.52
36:f:74:ALA:HB1	36:f:81:GLN:HE22	1.72	0.52
52:v:54:5MU:H71	52:v:55:PSU:O2	2.09	0.52
52:v:56:C:H2'	52:v:57:A:H8	1.73	0.52
6:A:2660:A:O3'	33:b:399:HIS:CE1	2.59	0.52
52:v:26:G:H2'	52:v:27:U:H5'	1.91	0.52
11:F:90:LEU:HD22	11:F:94:ARG:HB3	1.92	0.52
52:v:22:G:C2	52:v:23:C:C4	2.98	0.52
52:v:23:C:O2'	52:v:24:U:O5'	2.24	0.52
18:M:77:PRO:CB	33:b:816:MET:HE1	2.40	0.52
33:b:812:ILE:CG1	52:v:76:A:H1'	2.28	0.52
8:C:201:LEU:HD21	32:a:773:G:H4'	1.92	0.52
14:I:52:LEU:HD23	14:I:77:VAL:HG23	1.92	0.52
7:B:36:C:N4	7:B:49:C:O2	2.43	0.52
52:v:10:G:N2	52:v:26:G:H1'	2.25	0.52
33:b:816:MET:SD	33:b:860:GLU:HA	2.50	0.51
9:D:25:THR:HG21	9:D:193:VAL:HG22	1.92	0.51
32:a:923:A:N6	32:a:1392:G:O6	2.42	0.51
32:a:949:A:N7	44:n:104:ASN:ND2	2.57	0.51
13:H:5:LEU:HD13	13:H:9:VAL:HG11	1.92	0.51
32:a:1124:G:O2'	32:a:1145:A:N6	2.44	0.51
32:a:1339:A:H2	52:v:30:G:H1'	1.75	0.51
33:b:744:VAL:HG21	33:b:774:LEU:HD13	1.92	0.51
33:b:812:ILE:CD1	52:v:76:A:C2	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:1:C:OP2	52:v:2:G:H3'	2.11	0.51
52:v:49:G:N2	52:v:66:C:H1'	2.26	0.51
9:D:51:THR:HB	9:D:79:LEU:HD23	1.92	0.51
6:A:1926:U:OP1	52:v:70:G:H5''	2.09	0.51
52:v:22:G:C2	52:v:23:C:C5	2.99	0.51
3:2:34:ARG:HE	3:2:39:ARG:HD2	1.76	0.51
32:a:368:U:O4'	33:b:607:ARG:HD2	2.11	0.51
33:b:447:GLY:HA2	33:b:455:ARG:HD3	1.93	0.51
14:I:52:LEU:CD2	14:I:78:LEU:HD23	2.41	0.51
33:b:727:GLY:O	33:b:748:VAL:HG21	2.11	0.51
6:A:1313:U:O2	6:A:1313:U:H2'	2.11	0.50
19:N:12:ARG:NE	19:N:20:MET:HE1	2.25	0.50
55:z:16:A:N1	55:z:17:U:C2	2.78	0.50
52:v:59:A:H2'	52:v:60:U:O4'	2.10	0.50
32:a:1339:A:C2'	52:v:41:C:H1'	2.41	0.50
52:v:68:C:H2'	52:v:69:C:C6	2.46	0.50
26:U:93:ARG:HB2	26:U:102:ILE:HD12	1.93	0.50
6:A:79:C:O2'	6:A:346:A:N3	2.42	0.50
6:A:321:U:H5'	10:E:160:ALA:HB2	1.94	0.50
33:b:812:ILE:CD1	33:b:863:ILE:O	2.54	0.50
52:v:73:A:O2'	52:v:74:C:O5'	2.29	0.50
33:b:795:ILE:CG2	33:b:796:GLY:N	2.74	0.50
33:b:812:ILE:CG1	52:v:76:A:C8	2.94	0.50
52:v:51:C:H42	52:v:62:C:H42	1.60	0.50
33:b:812:ILE:HD13	52:v:76:A:C6	2.41	0.50
36:f:105:ILE:HD13	37:g:204:SER:HB3	1.93	0.50
37:g:8:LEU:HD11	37:g:21:LYS:HB2	1.93	0.50
40:j:21:LYS:HB2	40:j:61:ASP:HB2	1.94	0.50
18:M:53:MET:HE1	18:M:103:TYR:CG	2.47	0.50
36:f:113:VAL:HG11	36:f:139:THR:HG21	1.94	0.50
52:v:8:4SU:O2'	52:v:9:G:O5'	2.28	0.50
32:a:429:U:H5'	37:g:8:LEU:HD22	1.94	0.49
6:A:1681:G:O2'	6:A:1762:A:N3	2.46	0.49
33:b:778:VAL:HG23	33:b:779:LYS:N	2.27	0.49
33:b:797:LEU:C	33:b:797:LEU:CD2	2.85	0.49
33:b:399:HIS:CD2	33:b:476:MET:HB2	2.48	0.49
33:b:812:ILE:CD1	33:b:863:ILE:C	2.85	0.49
52:v:6:G:N2	52:v:67:C:O2	2.34	0.49
52:v:8:4SU:H1'	52:v:21:A:H2	1.74	0.49
32:a:368:U:H5	33:b:608:ALA:HB2	1.68	0.49
33:b:539:THR:O	33:b:541:ILE:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:727:GLY:CA	33:b:748:VAL:HG23	2.33	0.49
32:a:502:A:H2'	32:a:503:C:O4'	2.11	0.49
33:b:728:ILE:HG22	33:b:729:THR:N	2.27	0.49
41:k:104:SER:HB2	41:k:125:ILE:HD11	1.94	0.49
9:D:151:THR:O	9:D:152:PRO:C	2.56	0.49
32:a:358:U:H5'	33:b:607:ARG:NH1	2.27	0.49
32:a:1006:G:H2'	32:a:1007:U:C6	2.47	0.49
33:b:519:ILE:HG12	33:b:520:LEU:HD12	1.95	0.49
33:b:727:GLY:C	33:b:728:ILE:HG13	2.38	0.49
33:b:836:VAL:HG13	33:b:836:VAL:O	2.12	0.49
52:v:58:A:C6	52:v:61:C:H1'	2.47	0.49
33:b:612:GLU:HG3	33:b:613:LEU:H	1.77	0.49
33:b:789:GLU:CB	33:b:884:GLU:HA	2.43	0.49
33:b:795:ILE:CG2	33:b:879:VAL:CG1	2.88	0.49
52:v:8:4SU:HO2'	52:v:9:G:C5'	2.25	0.49
33:b:452:THR:HG23	33:b:453:SER:N	2.27	0.48
33:b:885:ILE:O	33:b:886:GLN:HB2	2.13	0.48
55:z:16:A:O5'	55:z:17:U:C5	2.62	0.48
33:b:399:HIS:HB3	33:b:402:HIS:HE1	1.78	0.48
42:l:22:ILE:HG22	42:l:31:VAL:HG13	1.95	0.48
6:A:2356:U:H4'	28:W:16:ARG:HG3	1.94	0.48
6:A:964:C:O2'	6:A:2273:A:N3	2.46	0.48
35:d:113:LEU:HD13	35:d:143:LEU:HD12	1.94	0.48
8:C:244:VAL:HG12	8:C:250:GLN:HA	1.94	0.48
32:a:452:A:H2'	32:a:453:G:O4'	2.14	0.48
32:a:236:A:H5''	48:r:43:LEU:HD21	1.96	0.48
33:b:611:ASN:O	33:b:612:GLU:CG	2.62	0.48
6:A:1450:G:N2	6:A:1452:G:O6	2.44	0.48
32:a:1339:A:HO2'	52:v:41:C:C1'	2.27	0.48
33:b:727:GLY:C	33:b:748:VAL:HG21	2.38	0.48
41:k:74:ILE:HD11	41:k:126:CYS:SG	2.54	0.48
52:v:18:G:O2'	52:v:19:G:C5'	2.57	0.48
6:A:1992:G:N2	6:A:1996:C:O2'	2.47	0.48
15:J:105:VAL:HG11	15:J:122:LEU:HD22	1.95	0.48
16:K:19:VAL:HB	16:K:41:ILE:HD13	1.95	0.48
52:v:71:C:H2'	52:v:72:A:C5'	2.44	0.48
7:B:43:C:O2	11:F:91:ARG:NH2	2.45	0.48
32:a:1506:U:P	55:z:13:A:OP1	2.70	0.48
33:b:789:GLU:HG3	33:b:789:GLU:O	2.12	0.48
6:A:1996:C:OP1	16:K:31:ARG:NE	2.47	0.47
14:I:52:LEU:HD21	14:I:78:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:25:THR:HG21	9:D:193:VAL:CG2	2.44	0.47
18:M:77:PRO:HG2	18:M:80:VAL:HG21	1.96	0.47
33:b:772:TYR:HA	33:b:775:ILE:HG22	1.96	0.47
33:b:540:GLY:CA	33:b:541:ILE:CB	2.85	0.47
33:b:812:ILE:HG12	52:v:76:A:O4'	2.12	0.47
52:v:54:5MU:C5	52:v:55:PSU:C2	3.01	0.47
32:a:358:U:O2'	33:b:576:LYS:O	2.33	0.47
33:b:544:LEU:C	33:b:544:LEU:CD2	2.85	0.47
52:v:8:4SU:H3'	52:v:8:4SU:C2	2.44	0.47
6:A:2661:G:H5''	33:b:400:VAL:CG1	2.44	0.47
17:L:19:LEU:HD13	17:L:31:GLY:HA3	1.97	0.47
32:a:783:C:H2'	32:a:784:A:H5'	1.96	0.47
32:a:50:A:N1	33:b:753:SER:HB3	2.30	0.47
37:g:8:LEU:HD21	37:g:21:LYS:HD2	1.96	0.47
52:v:22:G:C6	52:v:23:C:N4	2.82	0.47
4:3:31:ILE:HG22	4:3:31:ILE:O	2.15	0.47
6:A:483:A:C2	26:U:57:ILE:HD11	2.50	0.47
6:A:1666:G:H4'	16:K:6:THR:HG23	1.96	0.47
6:A:2645:G:OP1	6:A:2732:G:N2	2.46	0.47
6:A:2675:A:H4'	16:K:29:HIS:HB2	1.97	0.47
33:b:590:THR:O	33:b:591:LEU:HG	2.15	0.47
33:b:591:LEU:O	33:b:592:HIS:CG	2.68	0.47
33:b:795:ILE:HG23	33:b:879:VAL:HG13	1.93	0.47
52:v:8:4SU:S4	52:v:14:A:C8	3.02	0.47
54:x:57:VAL:HG12	54:x:71:ALA:HB1	1.96	0.47
33:b:396:ILE:HG21	33:b:404:LYS:HG3	1.96	0.47
33:b:786:LEU:CB	33:b:887:ARG:HB2	2.45	0.47
20:O:51:ALA:HB3	20:O:78:VAL:CG2	2.45	0.47
32:a:1203:C:C5'	47:q:1:ALA:HB2	2.45	0.47
8:C:131:MET:HG2	8:C:134:ILE:HD12	1.96	0.46
32:a:201:G:H2'	32:a:202:G:O4'	2.16	0.46
33:b:812:ILE:HG12	52:v:76:A:C8	2.41	0.46
39:i:38:ARG:HD3	39:i:63:ASN:HD22	1.80	0.46
55:z:13:A:H2'	55:z:14:A:N7	2.31	0.46
55:z:16:A:H2'	55:z:17:U:C6	2.50	0.46
10:E:108:ILE:HD11	10:E:181:ILE:CG1	2.45	0.46
11:F:60:SER:OG	11:F:90:LEU:HD21	2.15	0.46
32:a:1339:A:H1'	52:v:41:C:C1'	2.31	0.46
9:D:2:ILE:CD1	9:D:48:ILE:HD11	2.45	0.46
33:b:534:SER:CB	33:b:539:THR:HG23	2.46	0.46
55:z:16:A:H2'	55:z:17:U:H6	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:z:16:A:C6	55:z:17:U:N3	2.84	0.46
33:b:481:GLU:O	33:b:485:HIS:ND1	2.45	0.46
39:i:10:VAL:HG11	39:i:18:VAL:CG2	2.46	0.46
6:A:1315:C:O2'	6:A:1392:A:N3	2.44	0.46
33:b:804:PHE:C	33:b:812:ILE:HG22	2.40	0.46
36:f:15:ILE:HD11	36:f:37:VAL:HG23	1.97	0.46
52:v:22:G:C2	52:v:23:C:C6	3.04	0.46
12:G:23:ILE:HG21	12:G:71:LEU:HD21	1.98	0.46
13:H:2:GLN:HB2	13:H:39:ALA:HB2	1.97	0.46
32:a:629:A:H2'	32:a:630:A:O4'	2.16	0.46
33:b:788:PRO:HD2	33:b:886:GLN:HA	1.98	0.46
52:v:62:C:H2'	52:v:63:G:O4'	2.16	0.46
55:z:15:U:H6	55:z:15:U:P	2.36	0.46
6:A:192:C:O2'	6:A:802:A:N3	2.46	0.46
33:b:404:LYS:NZ	33:b:445:THR:O	2.46	0.46
33:b:526:GLY:O	33:b:527:GLU:HG2	2.15	0.46
34:c:9:ILE:HD12	47:q:98:LYS:HG3	1.97	0.46
52:v:22:G:N1	52:v:23:C:C4	2.84	0.46
33:b:403:GLY:C	56:b:901:GNP:O2A	2.59	0.46
33:b:728:ILE:C	33:b:729:THR:CG2	2.89	0.46
25:T:11:LEU:HD22	25:T:32:LEU:HD13	1.97	0.45
33:b:396:ILE:HD12	33:b:408:LEU:HD11	1.98	0.45
37:g:27:ILE:HG22	37:g:27:ILE:O	2.15	0.45
2:1:8:ILE:HD13	2:1:24:LYS:CD	2.47	0.45
6:A:2660:A:O2'	33:b:399:HIS:CE1	2.69	0.45
18:M:77:PRO:HB3	33:b:816:MET:CE	2.46	0.45
32:a:674:G:N2	32:a:717:U:O2	2.50	0.45
32:a:881:G:N7	45:o:5:GLN:NE2	2.64	0.45
33:b:496:ALA:HB2	33:b:544:LEU:HD12	1.97	0.45
55:z:16:A:C2'	55:z:17:U:C6	2.95	0.45
6:A:1869:G:O2'	6:A:1872:A:N6	2.49	0.45
15:J:31:GLU:HG2	15:J:142:ILE:HG23	1.99	0.45
52:v:66:C:H2'	52:v:67:C:H6	1.76	0.45
6:A:2747:G:O2'	12:G:66:THR:HG22	2.15	0.45
33:b:786:LEU:HD23	33:b:786:LEU:N	2.30	0.45
39:i:10:VAL:HG11	39:i:18:VAL:HG22	1.97	0.45
52:v:53:G:O2'	52:v:54:5MU:O5'	2.26	0.45
52:v:72:A:H2'	52:v:73:A:C8	2.50	0.45
6:A:2751:G:N2	6:A:2751:G:OP1	2.50	0.45
33:b:399:HIS:HB2	33:b:479:THR:HG23	1.99	0.45
52:v:18:G:H4'	52:v:60:U:O2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:430:ALA:HB2	33:b:443:LEU:HD13	1.98	0.45
35:d:209:VAL:HG23	35:d:210:THR:HG23	1.98	0.45
36:f:33:THR:HG22	36:f:51:LYS:HB3	1.99	0.45
35:d:162:VAL:HG21	35:d:172:ILE:HD11	1.98	0.45
37:g:117:VAL:HG22	37:g:122:ILE:HG13	1.99	0.45
52:v:16:C:H4'	52:v:60:U:O2'	2.17	0.45
55:z:15:U:H1'	55:z:16:A:C8	2.52	0.45
33:b:666:LEU:HD12	33:b:667:ALA:N	2.32	0.44
41:k:125:ILE:HG22	41:k:126:CYS:SG	2.57	0.44
52:v:22:G:C6	52:v:23:C:C4	3.05	0.44
6:A:340:A:H2'	6:A:341:C:O4'	2.17	0.44
10:E:105:LEU:HA	10:E:108:ILE:HG22	2.00	0.44
32:a:395:C:H5'	33:b:647:GLU:OE2	2.17	0.44
32:a:916:U:C3'	32:a:917:G:H5'	2.46	0.44
33:b:794:ILE:HA	33:b:880:PHE:HB3	2.00	0.44
35:d:160:LEU:HD22	35:d:175:ALA:HB2	1.99	0.44
11:F:59:ILE:CG1	11:F:140:ILE:HD11	2.47	0.44
32:a:368:U:O5'	33:b:607:ARG:HG2	2.16	0.44
33:b:838:TYR:CZ	33:b:839:GLU:O	2.71	0.44
52:v:54:5MU:C4	52:v:55:PSU:O2	2.70	0.44
32:a:1339:A:H4'	52:v:41:C:C4'	2.46	0.44
32:a:1406:U:H2'	32:a:1407:C:O4'	2.18	0.44
33:b:550:LEU:C	33:b:550:LEU:CD2	2.85	0.44
34:c:154:GLY:HA2	34:c:162:ALA:HB1	2.00	0.44
48:r:11:VAL:O	48:r:12:VAL:HG12	2.18	0.44
6:A:2006:C:O2'	6:A:2823:A:N3	2.51	0.44
39:i:9:MET:HE2	51:u:64:LEU:HD22	2.00	0.44
42:l:46:ALA:HB1	42:l:61:ALA:HB1	1.99	0.44
52:v:29:G:H1	52:v:41:C:H42	1.66	0.44
9:D:80:TRP:CD1	9:D:202:ILE:HD11	2.52	0.44
33:b:400:VAL:CA	56:b:901:GNP:O2G	2.54	0.44
33:b:456:ALA:HA	33:b:485:HIS:HD2	1.82	0.44
33:b:566:SER:O	33:b:587:ARG:N	2.50	0.44
42:l:110:THR:HG22	53:w:4:LYS:CB	2.48	0.44
52:v:24:U:H2'	52:v:25:C:H6	1.83	0.44
53:w:31:VAL:HG12	53:w:31:VAL:O	2.18	0.44
55:z:17:U:OP2	55:z:17:U:C2'	2.66	0.44
32:a:429:U:H3'	37:g:8:LEU:HD13	2.00	0.44
33:b:666:LEU:HD12	33:b:666:LEU:C	2.43	0.44
33:b:796:GLY:H	33:b:879:VAL:HG13	1.83	0.44
33:b:889:ILE:O	33:b:890:ALA:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:21:A:O2'	52:v:22:G:C8	2.70	0.44
6:A:1926:U:C1'	52:v:71:C:OP1	2.65	0.43
32:a:1064:G:O2'	32:a:1190:G:N2	2.51	0.43
32:a:1308:U:OP1	44:n:96:VAL:N	2.51	0.43
33:b:515:SER:OG	33:b:524:TRP:CH2	2.71	0.43
36:f:35:LEU:HD21	36:f:136:VAL:HG11	1.98	0.43
37:g:59:LYS:HD2	37:g:194:ILE:HG22	2.00	0.43
52:v:56:C:C6	52:v:56:C:OP1	2.70	0.43
55:z:15:U:O3'	55:z:16:A:C8	2.71	0.43
33:b:511:LYS:HG3	33:b:530:PHE:HE2	1.83	0.43
33:b:647:GLU:O	33:b:651:ARG:HG3	2.18	0.43
33:b:846:ARG:HA	33:b:851:ASP:HA	2.00	0.43
37:g:57:LYS:HA	37:g:199:ILE:HD12	2.00	0.43
38:h:34:LYS:HB3	38:h:37:THR:HG22	1.99	0.43
8:C:77:VAL:HG21	8:C:109:LEU:HD21	2.00	0.43
33:b:794:ILE:HA	33:b:880:PHE:CB	2.48	0.43
46:p:2:LEU:HD23	46:p:7:THR:HG22	2.01	0.43
6:A:1720:U:H2'	6:A:1721:G:O4'	2.19	0.43
33:b:575:ASP:OD1	33:b:576:LYS:N	2.52	0.43
33:b:578:ARG:HB3	33:b:629:LEU:HD11	2.01	0.43
33:b:856:ARG:H	33:b:859:MET:HE2	1.83	0.43
48:r:7:LEU:HD22	48:r:24:ILE:HD13	2.00	0.43
52:v:51:C:H1'	52:v:64:G:H22	1.83	0.43
52:v:51:C:H42	52:v:62:C:N4	2.16	0.43
5:4:3:VAL:HG21	6:A:2539:C:H5'	1.99	0.43
6:A:1996:C:N4	16:K:32:TYR:OH	2.51	0.43
6:A:2350:C:H2'	6:A:2351:G:O4'	2.17	0.43
32:a:1255:G:O2'	32:a:1258:G:N3	2.46	0.43
33:b:390:ARG:NH1	33:b:463:ASP:OD2	2.52	0.43
36:f:103:GLY:HA2	36:f:121:ASN:HA	2.00	0.43
16:K:70:ARG:HG2	16:K:76:VAL:HG22	2.01	0.43
28:W:55:LEU:CD1	28:W:76:ILE:HD12	2.48	0.43
32:a:735:C:H5'	51:u:59:LYS:HD3	2.01	0.43
32:a:766:A:OP2	32:a:812:G:N2	2.51	0.43
34:c:123:LEU:HD12	34:c:188:ALA:HB2	2.01	0.43
41:k:76:ARG:NH1	41:k:125:ILE:HG23	2.34	0.43
52:v:2:G:H2'	52:v:2:G:N3	2.33	0.43
33:b:399:HIS:CB	33:b:402:HIS:CE1	3.00	0.43
33:b:534:SER:C	33:b:536:LYS:H	2.26	0.43
34:c:117:ASP:HA	34:c:120:THR:HG22	2.00	0.43
52:v:22:G:O2'	52:v:23:C:P	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:192:A:N3	54:x:54:GLN:NE2	2.65	0.43
32:a:1203:C:H5'	47:q:1:ALA:HB2	1.99	0.43
45:o:81:ILE:HD11	45:o:94:TYR:CB	2.49	0.43
52:v:38:A:H2'	52:v:39:C:O4'	2.19	0.43
33:b:790:LEU:O	33:b:791:LYS:HD3	2.19	0.43
22:Q:105:PHE:HA	22:Q:108:LEU:HD12	2.00	0.43
32:a:368:U:O4	33:b:608:ALA:HB2	2.18	0.43
32:a:1347:G:O2'	32:a:1373:G:O6	2.34	0.43
33:b:390:ARG:HD3	33:b:559:ALA:HB2	2.01	0.43
46:p:32:THR:HG21	46:p:84:LEU:HD11	2.01	0.43
52:v:20:H2U:O2	52:v:20:H2U:H2'	2.19	0.43
6:A:1791:A:N6	6:A:1828:G:O2'	2.52	0.42
6:A:2800:A:H3'	6:A:2801:G:H5'	2.00	0.42
21:P:90:ALA:HB2	21:P:112:ARG:HA	2.00	0.42
32:a:359:G:H5''	33:b:574:LEU:HD11	1.99	0.42
32:a:1434:A:H2'	32:a:1435:G:O4'	2.19	0.42
33:b:386:ALA:HB3	33:b:560:VAL:HG23	2.01	0.42
33:b:493:VAL:HG11	33:b:519:ILE:HD11	2.01	0.42
33:b:644:VAL:HG21	33:b:650:ALA:HB2	2.01	0.42
45:o:82:ARG:HB3	45:o:97:VAL:HG22	2.00	0.42
52:v:41:C:C2'	52:v:42:G:H5''	2.49	0.42
32:a:1062:U:H2'	32:a:1063:C:C6	2.54	0.42
33:b:586:VAL:HG23	33:b:586:VAL:O	2.17	0.42
52:v:2:G:N3	52:v:2:G:C2'	2.82	0.42
32:a:769:G:H4'	32:a:1513:A:H4'	2.01	0.42
32:a:1360:A:H2'	32:a:1361:G:O4'	2.20	0.42
33:b:470:ALA:HB3	33:b:473:ASP:HB2	2.01	0.42
33:b:778:VAL:CG2	33:b:779:LYS:N	2.82	0.42
52:v:46:A:O2'	52:v:47:U:H5''	2.19	0.42
29:X:2:ARG:NH2	29:X:29:LEU:HD13	2.34	0.42
32:a:357:G:H4'	33:b:607:ARG:CD	2.49	0.42
33:b:436:GLU:HA	33:b:437:ASN:HA	1.74	0.42
33:b:451:PHE:N	33:b:451:PHE:CD1	2.86	0.42
33:b:495:VAL:HG11	33:b:520:LEU:HD11	2.01	0.42
33:b:506:ASP:HA	33:b:507:PRO:HD3	1.83	0.42
33:b:598:LEU:HD12	33:b:650:ALA:HB1	2.00	0.42
6:A:2226:C:H2'	6:A:2227:A:O4'	2.20	0.42
6:A:2660:A:HO2'	33:b:399:HIS:CE1	2.36	0.42
32:a:1080:A:C5'	36:f:20:VAL:HG11	2.49	0.42
33:b:477:PRO:HA	33:b:480:ILE:HG22	2.01	0.42
33:b:796:GLY:O	33:b:879:VAL:CG1	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:w:5:VAL:HG22	53:w:16:ARG:NH1	2.34	0.42
6:A:1932:A:H2'	6:A:1933:G:O4'	2.20	0.42
10:E:108:ILE:HD11	10:E:181:ILE:HG12	2.01	0.42
32:a:1083:U:O2'	32:a:1102:A:OP2	2.37	0.42
33:b:388:GLU:HG3	33:b:561:ARG:HG2	2.01	0.42
37:g:59:LYS:CD	37:g:194:ILE:HG22	2.50	0.42
6:A:319:G:H2'	6:A:320:A:O4'	2.19	0.42
6:A:1005:C:O2'	15:J:30:THR:HG21	2.20	0.42
6:A:255:A:H2'	6:A:256:A:O4'	2.20	0.42
6:A:910:A:N3	6:A:2264:C:O2'	2.45	0.42
42:l:15:VAL:HG12	42:l:76:TYR:HB3	2.02	0.42
6:A:1942:C:O2'	33:b:824:ARG:NH1	2.53	0.42
9:D:151:THR:O	9:D:153:GLY:N	2.52	0.42
32:a:115:G:H4'	32:a:116:A:O5'	2.20	0.42
35:d:45:THR:HG23	35:d:200:PRO:HD2	2.02	0.42
36:f:105:ILE:HG22	37:g:201:GLU:HA	2.02	0.42
4:3:24:LYS:HE2	4:3:28:LEU:HD23	2.02	0.42
33:b:838:TYR:CG	33:b:839:GLU:N	2.87	0.42
35:d:95:TRP:CD1	35:d:99:MET:HE3	2.55	0.42
44:n:4:ALA:HB2	44:n:56:ARG:HG3	2.01	0.42
55:z:15:U:H1'	55:z:16:A:H8	1.85	0.42
55:z:17:U:P	55:z:17:U:H3'	2.59	0.42
10:E:25:GLU:HA	17:L:6:LEU:HD22	2.02	0.41
32:a:298:A:H2'	32:a:299:G:O4'	2.20	0.41
33:b:396:ILE:HA	33:b:466:VAL:O	2.19	0.41
35:d:52:ALA:O	35:d:56:LEU:N	2.53	0.41
44:n:3:ILE:HD11	44:n:9:PRO:HD2	2.02	0.41
33:b:716:VAL:CG2	33:b:786:LEU:CD2	2.98	0.41
55:z:15:U:P	55:z:15:U:O4'	2.79	0.41
55:z:16:A:N9	55:z:17:U:C5	2.88	0.41
6:A:1277:G:H5'	19:N:20:MET:HE2	2.02	0.41
32:a:332:G:H2'	32:a:333:U:H5'	2.03	0.41
33:b:399:HIS:CD2	33:b:478:GLN:HB3	2.55	0.41
33:b:774:LEU:O	33:b:778:VAL:HG13	2.20	0.41
35:d:71:THR:HG22	35:d:72:LYS:H	1.85	0.41
6:A:2128:G:H2'	6:A:2129:C:O4'	2.20	0.41
33:b:445:THR:OG1	33:b:446:PRO:HD2	2.19	0.41
33:b:589:GLY:H	33:b:622:PRO:HB3	1.85	0.41
33:b:748:VAL:CG2	33:b:749:ARG:N	2.81	0.41
32:a:981:U:OP1	47:q:5:MET:HE1	2.20	0.41
32:a:1339:A:C2	52:v:30:G:O2'	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:794:ILE:HA	33:b:880:PHE:HA	2.03	0.41
55:z:17:U:OP2	55:z:17:U:H2'	2.20	0.41
6:A:372:G:H2'	29:X:57:VAL:HG22	2.03	0.41
11:F:11:VAL:HG13	11:F:171:ALA:CB	2.50	0.41
42:l:23:HIS:HA	42:l:86:LYS:HB2	2.02	0.41
45:o:81:ILE:HD11	45:o:94:TYR:HB3	2.02	0.41
16:K:35:VAL:HG13	16:K:69:VAL:HG12	2.02	0.41
33:b:425:THR:O	33:b:446:PRO:HB3	2.21	0.41
33:b:545:LEU:HA	33:b:545:LEU:HD12	1.83	0.41
35:d:212:TYR:O	35:d:216:VAL:HG23	2.21	0.41
36:f:11:GLN:HG3	36:f:116:VAL:HG12	2.03	0.41
52:v:53:G:H2'	52:v:54:5MU:O4'	2.20	0.41
33:b:838:TYR:CE2	33:b:839:GLU:O	2.73	0.41
41:k:94:VAL:HG21	41:k:127:TYR:HB3	2.02	0.41
46:p:7:THR:O	46:p:11:VAL:HG23	2.20	0.41
52:v:73:A:O2'	52:v:74:C:P	2.78	0.41
6:A:2816:G:N3	6:A:2883:A:O2'	2.53	0.41
14:I:13:ALA:HB3	14:I:16:MET:HG2	2.02	0.41
18:M:77:PRO:HB3	33:b:816:MET:HE1	2.03	0.41
20:O:51:ALA:HB3	20:O:78:VAL:HG23	2.03	0.41
32:a:404:G:N7	37:g:1:ALA:N	2.68	0.41
32:a:770:C:O2'	32:a:899:C:N3	2.53	0.41
32:a:1225:A:H2'	32:a:1226:C:C5	2.56	0.41
33:b:676:ASN:ND2	33:b:678:PHE:O	2.53	0.41
33:b:706:ASP:O	33:b:710:LYS:HG3	2.21	0.41
33:b:727:GLY:C	33:b:748:VAL:CG2	2.94	0.41
35:d:165:ALA:HB3	35:d:190:SER:HB3	2.03	0.41
45:o:73:LEU:HD22	45:o:79:ILE:HG21	2.02	0.41
45:o:98:ARG:HB2	45:o:116:TYR:HA	2.03	0.41
45:o:106:VAL:HG23	45:o:116:TYR:HB3	2.01	0.41
18:M:50:ARG:HD3	18:M:65:ILE:HD11	2.02	0.41
29:X:6:VAL:HG21	29:X:58:ILE:HD11	2.03	0.41
32:a:215:C:H2'	32:a:216:U:O4'	2.20	0.41
33:b:540:GLY:CA	33:b:542:ASP:N	2.81	0.41
6:A:2507:C:H2'	6:A:2508:G:O4'	2.20	0.40
19:N:33:ILE:HD12	19:N:114:GLU:OE1	2.21	0.40
34:c:7:ASN:HD21	34:c:18:ASN:HD21	1.69	0.40
35:d:169:HIS:HA	35:d:172:ILE:HD12	2.02	0.40
36:f:30:PHE:O	36:f:30:PHE:CD1	2.74	0.40
45:o:73:LEU:HD11	45:o:103:CYS:SG	2.61	0.40
6:A:320:A:N3	10:E:163:ASN:ND2	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:29:A:H2'	7:B:30:C:O4'	2.21	0.40
32:a:1080:A:H5''	36:f:20:VAL:HG11	2.03	0.40
33:b:515:SER:OG	33:b:524:TRP:CZ3	2.70	0.40
33:b:824:ARG:HE	33:b:845:LEU:HB3	1.86	0.40
34:c:21:TRP:HB3	34:c:57:GLU:HA	2.03	0.40
48:r:11:VAL:HG11	48:r:53:GLY:C	2.46	0.40
52:v:47:U:C4	52:v:50:U:H5''	2.57	0.40
6:A:1933:G:H2'	6:A:1934:C:O4'	2.22	0.40
32:a:309:A:O2'	32:a:607:A:N1	2.54	0.40
32:a:747:A:H2'	32:a:748:G:O4'	2.20	0.40
37:g:23:GLY:HA2	37:g:108:ALA:HB1	2.04	0.40
40:j:129:ARG:HD2	52:v:33:U:OP2	2.22	0.40
55:z:16:A:C8	55:z:17:U:C5	3.10	0.40
6:A:877:A:O2'	6:A:900:A:N6	2.54	0.40
12:G:176:LYS:OXT	12:G:176:LYS:CG	2.69	0.40
20:O:35:ILE:HG23	20:O:74:VAL:HG11	2.04	0.40
33:b:719:LYS:HG3	33:b:721:ILE:HD11	2.04	0.40
33:b:885:ILE:O	33:b:886:GLN:CB	2.69	0.40
48:r:13:SER:HB3	48:r:21:VAL:HG12	2.03	0.40
52:v:23:C:O2'	52:v:24:U:P	2.78	0.40
15:J:31:GLU:CG	15:J:142:ILE:HD12	2.52	0.40
21:P:90:ALA:HB2	21:P:112:ARG:CA	2.52	0.40
32:a:381:C:H2'	32:a:382:A:O4'	2.21	0.40
33:b:728:ILE:CG2	33:b:729:THR:N	2.84	0.40
42:l:83:VAL:HG11	42:l:96:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	54/57 (95%)	51 (94%)	2 (4%)	1 (2%)	6 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	48/55 (87%)	44 (92%)	4 (8%)	0	100	100
3	2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
4	3	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
5	4	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	C	269/273 (98%)	248 (92%)	17 (6%)	4 (2%)	8	38
9	D	207/209 (99%)	189 (91%)	15 (7%)	3 (1%)	9	39
10	E	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
11	F	175/179 (98%)	161 (92%)	12 (7%)	2 (1%)	11	45
12	G	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
13	H	42/149 (28%)	29 (69%)	6 (14%)	7 (17%)	0	2
14	I	139/142 (98%)	113 (81%)	21 (15%)	5 (4%)	2	20
15	J	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	18	55
16	K	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	7	35
17	L	141/144 (98%)	118 (84%)	19 (14%)	4 (3%)	4	24
18	M	134/136 (98%)	125 (93%)	7 (5%)	2 (2%)	8	38
19	N	118/127 (93%)	110 (93%)	7 (6%)	1 (1%)	16	53
20	O	114/117 (97%)	106 (93%)	7 (6%)	1 (1%)	14	49
21	P	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
22	Q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
23	R	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	12	47
24	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
25	T	91/100 (91%)	84 (92%)	6 (7%)	1 (1%)	11	45
26	U	100/104 (96%)	90 (90%)	7 (7%)	3 (3%)	3	22
27	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
28	W	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
29	X	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
30	Y	61/63 (97%)	52 (85%)	8 (13%)	1 (2%)	7	37
31	Z	56/59 (95%)	56 (100%)	0	0	100	100
33	b	507/890 (57%)	488 (96%)	17 (3%)	2 (0%)	30	67
34	c	204/233 (88%)	181 (89%)	20 (10%)	3 (2%)	8	38
35	d	216/241 (90%)	189 (88%)	22 (10%)	5 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	f	148/159 (93%)	127 (86%)	18 (12%)	3 (2%)	6	31
37	g	203/206 (98%)	186 (92%)	11 (5%)	6 (3%)	3	22
38	h	149/179 (83%)	138 (93%)	10 (7%)	1 (1%)	18	55
39	i	98/135 (73%)	82 (84%)	13 (13%)	3 (3%)	3	22
40	j	125/130 (96%)	107 (86%)	14 (11%)	4 (3%)	3	21
41	k	127/130 (98%)	117 (92%)	8 (6%)	2 (2%)	7	37
42	l	115/129 (89%)	101 (88%)	12 (10%)	2 (2%)	7	35
43	m	96/102 (94%)	85 (88%)	9 (9%)	2 (2%)	5	30
44	n	112/118 (95%)	106 (95%)	5 (4%)	1 (1%)	14	49
45	o	121/124 (98%)	106 (88%)	12 (10%)	3 (2%)	4	26
46	p	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	42
47	q	92/101 (91%)	75 (82%)	15 (16%)	2 (2%)	5	29
48	r	78/84 (93%)	66 (85%)	10 (13%)	2 (3%)	4	26
49	s	80/82 (98%)	71 (89%)	8 (10%)	1 (1%)	9	41
50	t	77/92 (84%)	70 (91%)	7 (9%)	0	100	100
51	u	53/75 (71%)	50 (94%)	1 (2%)	2 (4%)	2	19
53	w	49/71 (69%)	40 (82%)	7 (14%)	2 (4%)	2	18
54	x	83/87 (95%)	79 (95%)	1 (1%)	3 (4%)	2	20
All	All	6020/6866 (88%)	5514 (92%)	417 (7%)	89 (2%)	11	38

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	C	121	ALA
9	D	151	THR
11	F	173	ASP
13	H	31	VAL
13	H	33	GLN
14	I	4	VAL
39	i	85	ILE
1	0	54	ILE
8	C	12	ARG
9	D	105	LYS
13	H	3	VAL
17	L	115	GLU
26	U	98	ASN

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Mol	Chain	Res	Type
34	c	16	PRO
35	d	19	THR
35	d	73	ARG
35	d	219	THR
36	f	110	MET
37	g	22	SER
37	g	28	ASP
37	g	173	ASP
37	g	192	ALA
40	j	57	VAL
43	m	57	VAL
48	r	12	VAL
48	r	50	ASN
51	u	46	THR
53	w	24	LYS
11	F	175	PRO
13	H	9	VAL
14	I	64	ARG
16	K	35	VAL
17	L	15	ALA
19	N	80	PHE
25	T	38	ALA
26	U	16	LYS
34	c	145	ALA
36	f	102	THR
39	i	53	LYS
41	k	3	GLN
45	o	75	GLU
47	q	21	ALA
54	x	5	SER
54	x	68	LYS
13	H	8	LYS
13	H	12	LEU
13	H	41	LYS
14	I	5	GLN
14	I	88	GLY
14	I	97	VAL
15	J	81	ILE
17	L	69	ARG
26	U	7	ASP
33	b	886	GLN
36	f	137	ARG

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Mol	Chain	Res	Type
38	h	8	GLN
39	i	94	HIS
40	j	9	GLY
40	j	90	ASP
40	j	122	ARG
41	k	87	ARG
42	l	92	ARG
44	n	4	ALA
46	p	45	HIS
47	q	81	ARG
8	C	196	ASN
9	D	104	VAL
18	M	58	LYS
33	b	788	PRO
43	m	36	VAL
53	w	45	LYS
8	C	151	GLY
17	L	111	ILE
20	O	28	VAL
23	R	53	PHE
35	d	21	TYR
37	g	191	SER
45	o	88	ASP
54	x	67	HIS
18	M	69	PRO
34	c	65	VAL
45	o	43	LYS
51	u	25	ILE
30	Y	46	VAL
35	d	98	GLY
37	g	27	ILE
49	s	10	GLY
16	K	119	ALA
42	l	88	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/48 (98%)	47 (100%)	0	100	100
2	1	45/49 (92%)	45 (100%)	0	100	100
3	2	38/38 (100%)	38 (100%)	0	100	100
4	3	51/52 (98%)	51 (100%)	0	100	100
5	4	34/34 (100%)	34 (100%)	0	100	100
8	C	216/218 (99%)	216 (100%)	0	100	100
9	D	164/164 (100%)	164 (100%)	0	100	100
10	E	165/165 (100%)	165 (100%)	0	100	100
11	F	148/150 (99%)	148 (100%)	0	100	100
12	G	137/138 (99%)	137 (100%)	0	100	100
13	H	35/114 (31%)	35 (100%)	0	100	100
14	I	109/110 (99%)	109 (100%)	0	100	100
15	J	116/116 (100%)	115 (99%)	1 (1%)	70	76
16	K	103/104 (99%)	103 (100%)	0	100	100
17	L	102/103 (99%)	102 (100%)	0	100	100
18	M	109/109 (100%)	109 (100%)	0	100	100
19	N	100/103 (97%)	100 (100%)	0	100	100
20	O	86/87 (99%)	86 (100%)	0	100	100
21	P	99/100 (99%)	99 (100%)	0	100	100
22	Q	89/90 (99%)	89 (100%)	0	100	100
23	R	84/84 (100%)	84 (100%)	0	100	100
24	S	93/93 (100%)	93 (100%)	0	100	100
25	T	80/84 (95%)	80 (100%)	0	100	100
26	U	83/85 (98%)	83 (100%)	0	100	100
27	V	78/78 (100%)	78 (100%)	0	100	100
28	W	56/63 (89%)	56 (100%)	0	100	100
29	X	67/68 (98%)	67 (100%)	0	100	100
30	Y	55/55 (100%)	55 (100%)	0	100	100
31	Z	48/49 (98%)	48 (100%)	0	100	100
33	b	409/713 (57%)	406 (99%)	3 (1%)	76	79
34	c	170/190 (90%)	170 (100%)	0	100	100
35	d	180/199 (90%)	178 (99%)	2 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	f	113/119 (95%)	112 (99%)	1 (1%)	70	76
37	g	172/173 (99%)	172 (100%)	0	100	100
38	h	124/147 (84%)	124 (100%)	0	100	100
39	i	87/116 (75%)	87 (100%)	0	100	100
40	j	105/107 (98%)	104 (99%)	1 (1%)	68	76
41	k	104/105 (99%)	104 (100%)	0	100	100
42	l	90/99 (91%)	90 (100%)	0	100	100
43	m	86/90 (96%)	86 (100%)	0	100	100
44	n	92/96 (96%)	92 (100%)	0	100	100
45	o	103/104 (99%)	103 (100%)	0	100	100
46	p	76/77 (99%)	76 (100%)	0	100	100
47	q	79/84 (94%)	79 (100%)	0	100	100
48	r	74/78 (95%)	74 (100%)	0	100	100
49	s	65/65 (100%)	65 (100%)	0	100	100
50	t	70/79 (89%)	69 (99%)	1 (1%)	59	71
51	u	48/65 (74%)	48 (100%)	0	100	100
53	w	44/61 (72%)	44 (100%)	0	100	100
54	x	65/66 (98%)	65 (100%)	0	100	100
All	All	4993/5584 (89%)	4984 (100%)	9 (0%)	85	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	J	81	ILE
33	b	541	ILE
33	b	790	LEU
33	b	861	CYS
35	d	19	THR
35	d	219	THR
36	f	130	THR
40	j	65	THR
50	t	38	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	25	ASN
5	4	13	ASN
5	4	35	GLN
8	C	14	HIS
8	C	142	ASN
8	C	152	GLN
8	C	250	GLN
10	E	41	GLN
10	E	62	GLN
10	E	90	GLN
10	E	163	ASN
10	E	195	GLN
11	F	20	ASN
11	F	26	GLN
12	G	72	ASN
14	I	104	GLN
15	J	58	ASN
15	J	77	HIS
15	J	80	HIS
17	L	104	GLN
20	O	98	GLN
21	P	40	GLN
21	P	55	HIS
21	P	65	ASN
22	Q	58	GLN
23	R	11	GLN
23	R	12	HIS
23	R	91	GLN
24	S	57	ASN
24	S	102	HIS
26	U	73	ASN
27	V	24	ASN
27	V	87	GLN
30	Y	39	GLN
30	Y	58	ASN
33	b	399	HIS
33	b	402	HIS
33	b	426	GLN
33	b	437	ASN
33	b	448	HIS
33	b	484	GLN
33	b	498	ASN
33	b	551	GLN

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Mol	Chain	Res	Type
33	b	853	ASN
33	b	886	GLN
34	c	5	HIS
34	c	7	ASN
34	c	175	HIS
35	d	14	HIS
35	d	35	ASN
35	d	38	HIS
36	f	72	ASN
36	f	76	ASN
36	f	81	GLN
36	f	96	GLN
37	g	125	ASN
37	g	151	GLN
38	h	147	ASN
39	i	11	HIS
39	i	52	ASN
39	i	63	ASN
40	j	31	GLN
40	j	36	GLN
41	k	15	ASN
41	k	37	ASN
41	k	66	GLN
41	k	75	GLN
42	l	27	ASN
44	n	51	GLN
45	o	74	GLN
45	o	76	HIS
46	p	34	GLN
46	p	37	HIS
47	q	49	GLN
51	u	53	GLN
54	x	20	ASN
54	x	51	ASN
54	x	77	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	a	1538/1542 (99%)	198 (12%)	0
52	v	76/77 (98%)	26 (34%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	z	5/6 (83%)	2 (40%)	0
6	A	2895/2904 (99%)	368 (12%)	20 (0%)
7	B	118/120 (98%)	11 (9%)	0
All	All	4632/4649 (99%)	605 (13%)	20 (0%)

All (605) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	10	A
6	A	12	U
6	A	34	U
6	A	45	G
6	A	46	G
6	A	63	A
6	A	74	A
6	A	75	G
6	A	84	A
6	A	101	A
6	A	103	A
6	A	118	A
6	A	119	A
6	A	120	U
6	A	138	U
6	A	139	U
6	A	140	C
6	A	141	G
6	A	142	A
6	A	163	C
6	A	181	A
6	A	188	G
6	A	196	A
6	A	199	A
6	A	215	G
6	A	216	A
6	A	221	A
6	A	222	A
6	A	230	G
6	A	248	G
6	A	255	A
6	A	266	G
6	A	271	G
6	A	272	A

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Mol	Chain	Res	Type
6	A	273	G
6	A	277	G
6	A	302	C
6	A	311	A
6	A	329	G
6	A	330	A
6	A	331	C
6	A	353	C
6	A	361	G
6	A	362	A
6	A	367	G
6	A	371	A
6	A	372	G
6	A	386	G
6	A	396	G
6	A	405	U
6	A	411	G
6	A	424	G
6	A	451	U
6	A	456	C
6	A	480	A
6	A	481	G
6	A	491	G
6	A	504	A
6	A	505	A
6	A	512	G
6	A	513	A
6	A	529	A
6	A	530	G
6	A	531	C
6	A	532	A
6	A	544	C
6	A	546	U
6	A	547	A
6	A	548	G
6	A	549	G
6	A	550	C
6	A	563	A
6	A	572	A
6	A	573	U
6	A	575	A
6	A	586	A

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Mol	Chain	Res	Type
6	A	603	A
6	A	613	A
6	A	615	U
6	A	627	A
6	A	631	A
6	A	637	A
6	A	645	C
6	A	647	G
6	A	654	A
6	A	655	A
6	A	686	U
6	A	702	U
6	A	730	A
6	A	747	U
6	A	775	G
6	A	776	G
6	A	782	A
6	A	784	G
6	A	785	G
6	A	789	A
6	A	791	C
6	A	792	A
6	A	793	A
6	A	805	G
6	A	812	C
6	A	819	A
6	A	827	U
6	A	828	U
6	A	830	G
6	A	845	A
6	A	846	U
6	A	847	U
6	A	858	G
6	A	859	G
6	A	878	A
6	A	896	A
6	A	910	A
6	A	914	G
6	A	931	U
6	A	932	U
6	A	941	A
6	A	946	C

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Mol	Chain	Res	Type
6	A	961	C
6	A	974	G
6	A	983	A
6	A	985	C
6	A	995	C
6	A	996	A
6	A	1009	A
6	A	1012	U
6	A	1013	C
6	A	1022	G
6	A	1026	G
6	A	1033	U
6	A	1046	A
6	A	1047	G
6	A	1060	U
6	A	1061	U
6	A	1062	G
6	A	1065	U
6	A	1066	U
6	A	1070	A
6	A	1071	G
6	A	1072	C
6	A	1073	A
6	A	1074	G
6	A	1075	C
6	A	1087	G
6	A	1088	A
6	A	1089	A
6	A	1092	C
6	A	1098	A
6	A	1104	C
6	A	1112	G
6	A	1130	U
6	A	1132	U
6	A	1133	A
6	A	1135	C
6	A	1136	G
6	A	1142	A
6	A	1144	A
6	A	1168	G
6	A	1172	C
6	A	1174	U

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Mol	Chain	Res	Type
6	A	1175	A
6	A	1176	U
6	A	1180	U
6	A	1181	U
6	A	1238	G
6	A	1253	A
6	A	1256	G
6	A	1266	G
6	A	1271	G
6	A	1272	A
6	A	1300	G
6	A	1301	A
6	A	1321	A
6	A	1341	G
6	A	1345	C
6	A	1365	A
6	A	1378	A
6	A	1379	U
6	A	1383	A
6	A	1416	G
6	A	1419	A
6	A	1420	A
6	A	1428	C
6	A	1452	G
6	A	1461	C
6	A	1463	C
6	A	1482	G
6	A	1493	C
6	A	1494	A
6	A	1504	A
6	A	1508	A
6	A	1509	A
6	A	1510	G
6	A	1515	A
6	A	1523	U
6	A	1532	A
6	A	1533	C
6	A	1535	A
6	A	1547	C
6	A	1554	U
6	A	1555	G
6	A	1566	A

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Mol	Chain	Res	Type
6	A	1569	A
6	A	1578	U
6	A	1583	A
6	A	1585	C
6	A	1607	C
6	A	1608	A
6	A	1618	A
6	A	1646	C
6	A	1647	U
6	A	1648	U
6	A	1651	G
6	A	1674	G
6	A	1715	G
6	A	1729	U
6	A	1730	C
6	A	1732	C
6	A	1738	G
6	A	1764	C
6	A	1773	A
6	A	1782	U
6	A	1791	A
6	A	1800	C
6	A	1801	A
6	A	1808	A
6	A	1816	C
6	A	1829	A
6	A	1870	C
6	A	1872	A
6	A	1873	G
6	A	1885	A
6	A	1908	C
6	A	1909	C
6	A	1913	A
6	A	1914	C
6	A	1926	U
6	A	1927	A
6	A	1930	G
6	A	1931	U
6	A	1937	A
6	A	1938	A
6	A	1955	U
6	A	1963	U

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Mol	Chain	Res	Type
6	A	1967	C
6	A	1970	A
6	A	1971	U
6	A	1972	G
6	A	1991	U
6	A	1992	G
6	A	1993	U
6	A	1997	C
6	A	2022	U
6	A	2023	C
6	A	2030	A
6	A	2031	A
6	A	2032	G
6	A	2043	C
6	A	2052	A
6	A	2055	C
6	A	2060	A
6	A	2061	G
6	A	2062	A
6	A	2069	G
6	A	2072	C
6	A	2093	G
6	A	2096	C
6	A	2110	G
6	A	2111	U
6	A	2112	G
6	A	2115	G
6	A	2116	G
6	A	2117	A
6	A	2118	U
6	A	2119	A
6	A	2120	G
6	A	2122	U
6	A	2123	G
6	A	2128	G
6	A	2132	U
6	A	2133	G
6	A	2136	G
6	A	2146	C
6	A	2147	A
6	A	2148	G
6	A	2158	A

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Mol	Chain	Res	Type
6	A	2159	G
6	A	2162	G
6	A	2164	C
6	A	2165	C
6	A	2170	A
6	A	2171	A
6	A	2172	U
6	A	2173	A
6	A	2198	A
6	A	2204	G
6	A	2211	A
6	A	2212	A
6	A	2225	A
6	A	2226	C
6	A	2238	G
6	A	2239	G
6	A	2249	U
6	A	2250	G
6	A	2283	C
6	A	2287	A
6	A	2297	A
6	A	2305	U
6	A	2308	G
6	A	2312	U
6	A	2325	G
6	A	2331	G
6	A	2333	A
6	A	2335	A
6	A	2345	G
6	A	2376	A
6	A	2383	G
6	A	2385	C
6	A	2402	U
6	A	2406	A
6	A	2425	A
6	A	2426	A
6	A	2428	G
6	A	2429	G
6	A	2430	A
6	A	2435	A
6	A	2441	U
6	A	2448	A

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Mol	Chain	Res	Type
6	A	2469	A
6	A	2474	U
6	A	2476	A
6	A	2491	U
6	A	2498	C
6	A	2502	G
6	A	2505	G
6	A	2507	C
6	A	2518	A
6	A	2520	C
6	A	2554	U
6	A	2566	A
6	A	2567	G
6	A	2585	U
6	A	2586	U
6	A	2609	U
6	A	2613	U
6	A	2629	U
6	A	2630	G
6	A	2639	A
6	A	2689	U
6	A	2690	U
6	A	2714	G
6	A	2726	A
6	A	2729	G
6	A	2744	G
6	A	2748	A
6	A	2757	A
6	A	2765	A
6	A	2778	A
6	A	2791	G
6	A	2798	U
6	A	2818	U
6	A	2820	A
6	A	2867	G
6	A	2872	A
6	A	2880	C
6	A	2884	U
6	A	2885	G
6	A	2886	A
7	B	15	A
7	B	35	C

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Mol	Chain	Res	Type
7	B	36	C
7	B	41	G
7	B	45	A
7	B	56	G
7	B	66	A
7	B	89	U
7	B	90	C
7	B	99	A
7	B	109	A
32	a	4	U
32	a	5	U
32	a	9	G
32	a	32	A
32	a	39	G
32	a	47	C
32	a	48	C
32	a	51	A
32	a	61	G
32	a	70	U
32	a	71	A
32	a	74	A
32	a	83	C
32	a	85	U
32	a	87	C
32	a	88	U
32	a	97	G
32	a	108	G
32	a	115	G
32	a	116	A
32	a	120	A
32	a	121	U
32	a	122	G
32	a	130	A
32	a	131	A
32	a	144	G
32	a	155	A
32	a	159	G
32	a	162	A
32	a	182	A
32	a	197	A
32	a	201	G
32	a	204	G

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Mol	Chain	Res	Type
32	a	209	U
32	a	210	C
32	a	211	G
32	a	212	G
32	a	245	U
32	a	247	G
32	a	251	G
32	a	266	G
32	a	267	C
32	a	279	A
32	a	280	C
32	a	289	G
32	a	328	C
32	a	329	A
32	a	330	C
32	a	332	G
32	a	333	U
32	a	347	G
32	a	352	C
32	a	354	G
32	a	367	U
32	a	368	U
32	a	372	C
32	a	373	A
32	a	406	G
32	a	411	A
32	a	412	A
32	a	413	G
32	a	421	U
32	a	423	G
32	a	424	G
32	a	429	U
32	a	467	U
32	a	468	A
32	a	469	C
32	a	479	U
32	a	485	U
32	a	486	U
32	a	511	C
32	a	518	C
32	a	524	G
32	a	527	G

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Mol	Chain	Res	Type
32	a	532	A
32	a	533	A
32	a	547	A
32	a	559	A
32	a	563	A
32	a	572	A
32	a	573	A
32	a	576	C
32	a	577	G
32	a	596	A
32	a	633	G
32	a	650	G
32	a	653	U
32	a	665	A
32	a	687	A
32	a	702	A
32	a	720	C
32	a	721	G
32	a	723	U
32	a	724	G
32	a	731	G
32	a	733	G
32	a	734	G
32	a	753	A
32	a	755	G
32	a	784	A
32	a	793	U
32	a	794	A
32	a	815	A
32	a	817	C
32	a	828	U
32	a	829	G
32	a	830	G
32	a	841	C
32	a	843	U
32	a	845	A
32	a	846	G
32	a	914	A
32	a	917	G
32	a	918	A
32	a	927	G
32	a	934	C

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Mol	Chain	Res	Type
32	a	960	U
32	a	969	A
32	a	975	A
32	a	976	G
32	a	977	A
32	a	983	A
32	a	993	G
32	a	1004	A
32	a	1008	U
32	a	1018	G
32	a	1022	A
32	a	1026	G
32	a	1028	C
32	a	1030	U
32	a	1032	G
32	a	1033	G
32	a	1034	G
32	a	1043	G
32	a	1054	C
32	a	1065	U
32	a	1073	U
32	a	1086	U
32	a	1094	G
32	a	1095	U
32	a	1101	A
32	a	1102	A
32	a	1125	U
32	a	1133	G
32	a	1134	G
32	a	1136	C
32	a	1137	C
32	a	1139	G
32	a	1140	C
32	a	1141	C
32	a	1142	G
32	a	1152	A
32	a	1157	A
32	a	1158	C
32	a	1159	U
32	a	1160	G
32	a	1161	C
32	a	1167	A

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Mol	Chain	Res	Type
32	a	1196	A
32	a	1197	A
32	a	1202	U
32	a	1212	U
32	a	1213	A
32	a	1227	A
32	a	1228	C
32	a	1240	U
32	a	1241	G
32	a	1253	G
32	a	1280	A
32	a	1286	U
32	a	1287	A
32	a	1299	A
32	a	1300	G
32	a	1302	C
32	a	1305	G
32	a	1317	C
32	a	1318	A
32	a	1322	C
32	a	1337	G
32	a	1346	A
32	a	1362	A
32	a	1363	A
32	a	1370	G
32	a	1396	A
32	a	1397	C
32	a	1398	A
32	a	1441	A
32	a	1446	A
32	a	1503	A
32	a	1505	G
32	a	1506	U
32	a	1517	G
32	a	1529	G
32	a	1530	G
32	a	1533	C
32	a	1535	C
32	a	1536	C
52	v	8	4SU
52	v	9	G
52	v	16	C

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Mol	Chain	Res	Type
52	v	17(A)	U
52	v	19	G
52	v	20	H2U
52	v	21	A
52	v	22	G
52	v	23	C
52	v	24	U
52	v	42	G
52	v	48	C
52	v	49	G
52	v	53	G
52	v	54	5MU
52	v	55	PSU
52	v	56	C
52	v	57	A
52	v	58	A
52	v	59	A
52	v	70	G
52	v	71	C
52	v	73	A
52	v	74	C
52	v	75	C
52	v	76	A
55	z	17	U
55	z	18	G

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	271	G
6	A	404	A
6	A	479	A
6	A	512	G
6	A	620	G
6	A	733	G
6	A	918	A
6	A	995	C
6	A	1061	U
6	A	1180	U
6	A	1288	G
6	A	1344	U
6	A	1378	A

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Mol	Chain	Res	Type
6	A	1606	C
6	A	1818	U
6	A	1857	G
6	A	2127	G
6	A	2249	U
6	A	2425	A
6	A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
52	4SU	v	8	52	18,21,22	1.96	5 (27%)	25,30,33	2.61	11 (44%)
52	PSU	v	55	52	18,21,22	1.34	2 (11%)	21,30,33	2.20	5 (23%)
52	5MU	v	54	52	19,22,23	1.42	6 (31%)	27,32,35	2.18	7 (25%)
52	H2U	v	20	52	18,21,22	0.81	0	19,30,33	1.01	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	4SU	v	8	52	-	3/7/25/26	0/2/2/2
52	PSU	v	55	52	-	1/7/25/26	0/2/2/2
52	5MU	v	54	52	-	2/7/25/26	0/2/2/2
52	H2U	v	20	52	-	2/7/38/39	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	v	8	4SU	C4-S4	-4.93	1.60	1.68
52	v	8	4SU	C4-N3	-3.91	1.33	1.37
52	v	55	PSU	C6-C5	3.46	1.39	1.35
52	v	54	5MU	C6-C5	2.77	1.39	1.34
52	v	8	4SU	C5-C4	-2.59	1.39	1.42
52	v	55	PSU	C4-N3	-2.59	1.34	1.38
52	v	54	5MU	C4-N3	-2.55	1.34	1.38
52	v	54	5MU	C4-C5	2.48	1.48	1.44
52	v	8	4SU	C2-N1	2.48	1.42	1.38
52	v	8	4SU	C2-N3	-2.48	1.33	1.38
52	v	54	5MU	C6-N1	-2.22	1.34	1.38
52	v	54	5MU	C2-N1	2.12	1.41	1.38
52	v	54	5MU	C2-N3	-2.05	1.34	1.38

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	v	8	4SU	C4-N3-C2	-6.67	120.92	127.31
52	v	55	PSU	N1-C2-N3	6.34	121.85	115.17
52	v	8	4SU	C5-C4-N3	5.58	119.94	114.75
52	v	54	5MU	C4-N3-C2	-5.11	120.64	127.34
52	v	54	5MU	N3-C2-N1	4.98	121.38	114.89
52	v	8	4SU	N3-C2-N1	4.55	120.81	114.89
52	v	54	5MU	C5-C4-N3	4.32	119.08	115.32
52	v	55	PSU	C4-N3-C2	-4.17	120.63	126.37
52	v	54	5MU	O4-C4-C5	-3.92	120.44	124.92
52	v	8	4SU	C5-C4-S4	-3.74	120.03	124.31
52	v	54	5MU	C5-C6-N1	-3.64	119.36	123.31
52	v	55	PSU	O2-C2-N1	-3.54	119.14	122.79
52	v	55	PSU	C3'-C2'-C1'	3.48	105.80	101.69
52	v	8	4SU	O3'-C3'-C4'	3.27	120.48	111.08
52	v	8	4SU	O3'-C3'-C2'	2.75	120.62	111.82
52	v	8	4SU	O4'-C4'-C3'	-2.68	99.84	105.15
52	v	54	5MU	O2-C2-N1	-2.67	119.32	122.80
52	v	8	4SU	C3'-C2'-C1'	-2.62	96.51	101.46
52	v	8	4SU	C1'-N1-C2	2.51	122.10	117.59
52	v	54	5MU	C3'-C2'-C1'	2.40	106.00	101.46
52	v	20	H2U	C3'-C2'-C1'	2.34	105.89	101.46
52	v	8	4SU	O2-C2-N3	-2.32	117.20	121.49
52	v	55	PSU	C5-C6-N1	-2.14	119.16	122.14
52	v	8	4SU	O4'-C1'-N1	2.05	113.01	108.36

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	v	8	4SU	O4'-C1'-N1-C2
52	v	8	4SU	O4'-C1'-N1-C6
52	v	20	H2U	O4'-C1'-N1-C6
52	v	54	5MU	O4'-C1'-N1-C6
52	v	20	H2U	O4'-C1'-N1-C2
52	v	54	5MU	O4'-C1'-N1-C2
52	v	8	4SU	O4'-C4'-C5'-O5'
52	v	55	PSU	O4'-C1'-C5-C6

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	v	8	4SU	13	0
52	v	55	PSU	3	0
52	v	54	5MU	5	0
52	v	20	H2U	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	FME	v	101	52	8,8,10	0.42	0	7,8,11	0.97	0
56	GNP	b	901	-	34,34,34	3.02	8 (23%)	47,54,54	1.81	7 (14%)

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
57	FME	v	101	52	-	0/7/7/11	-
56	GNP	b	901	-	-	3/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	b	901	GNP	PG-O1G	10.11	1.61	1.46
56	b	901	GNP	PB-O1B	10.07	1.61	1.46
56	b	901	GNP	PG-N3B	4.64	1.75	1.63
56	b	901	GNP	PB-N3B	4.56	1.75	1.63
56	b	901	GNP	C5-C4	3.19	1.47	1.38
56	b	901	GNP	PB-O2B	-3.17	1.48	1.56
56	b	901	GNP	PG-O3G	-3.14	1.48	1.56
56	b	901	GNP	C6-N1	-2.43	1.34	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	b	901	GNP	C5-C4-N3	-6.21	118.51	128.39
56	b	901	GNP	C2-N3-C4	5.11	121.10	112.30
56	b	901	GNP	N9-C4-N3	4.58	135.11	125.95
56	b	901	GNP	C6-C5-N7	3.24	136.19	130.29
56	b	901	GNP	C4-C5-N7	-2.62	106.52	110.67
56	b	901	GNP	C3'-C2'-C1'	2.38	105.96	101.46
56	b	901	GNP	O6-C6-C5	-2.10	120.99	126.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

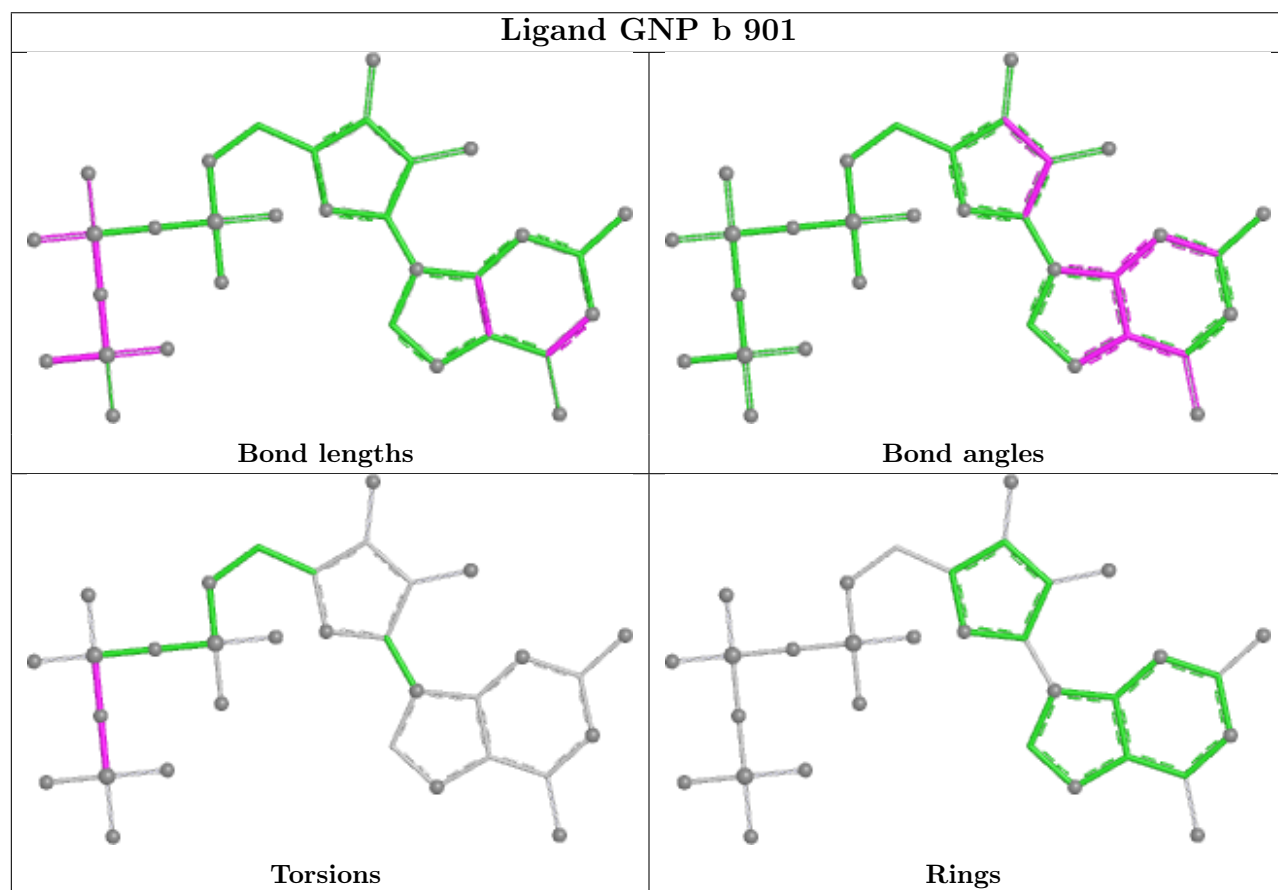
Mol	Chain	Res	Type	Atoms
56	b	901	GNP	PB-N3B-PG-O1G
56	b	901	GNP	PG-N3B-PB-O1B
56	b	901	GNP	PG-N3B-PB-O3A

There are no ring outliers.

2 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	v	101	FME	15	0
56	b	901	GNP	14	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 ⓘ

There are no chain breaks in this entry.

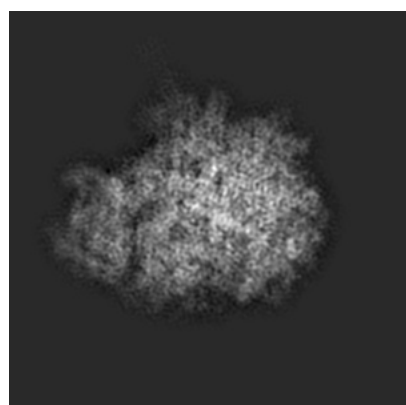
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3285. These allow visual inspection of the internal detail of the map and identification of artifacts.

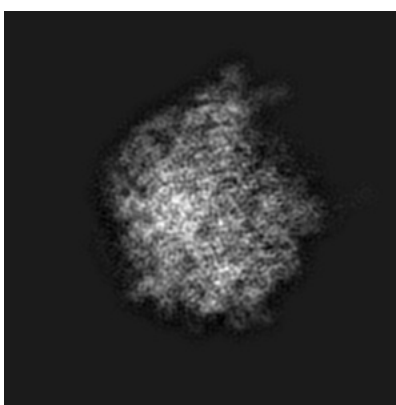
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

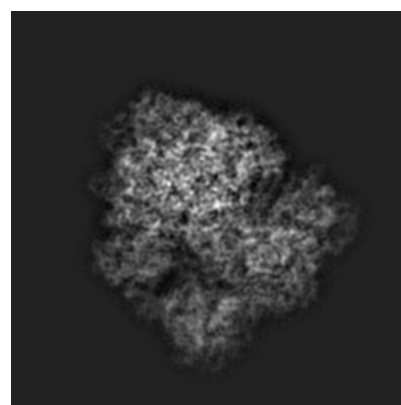
6.1.1 Primary map



X



Y

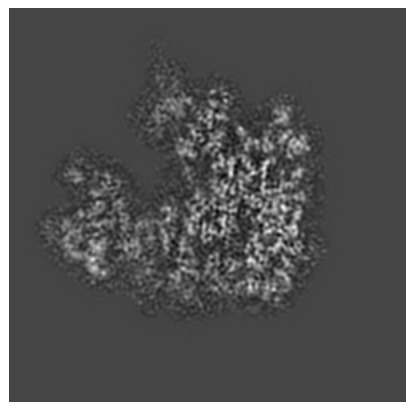


Z

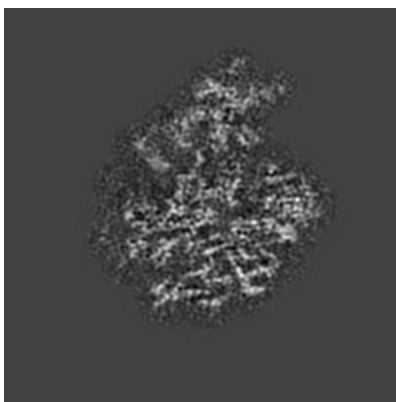
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

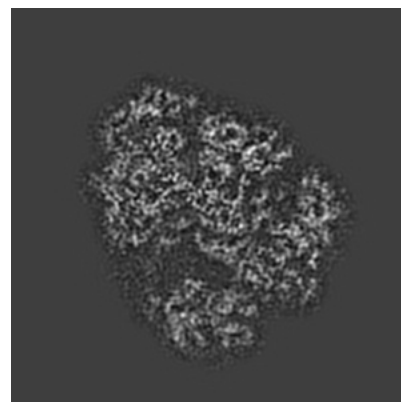
6.2.1 Primary map



X Index: 150



Y Index: 150

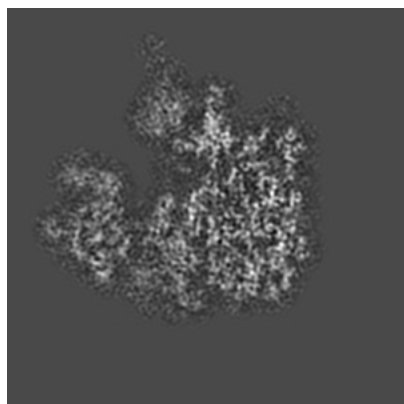


Z Index: 150

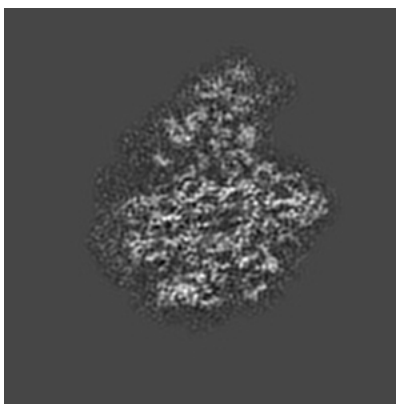
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

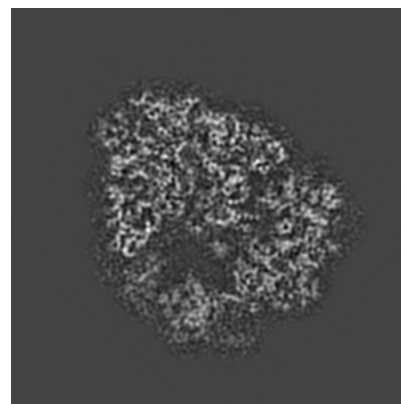
6.3.1 Primary map



X Index: 155



Y Index: 153

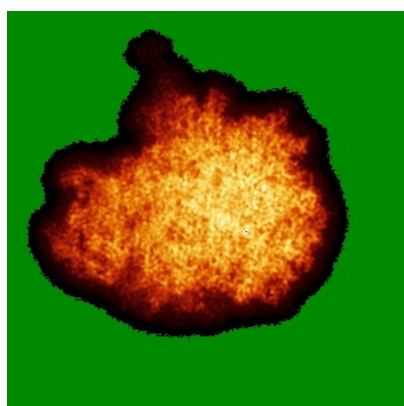


Z Index: 157

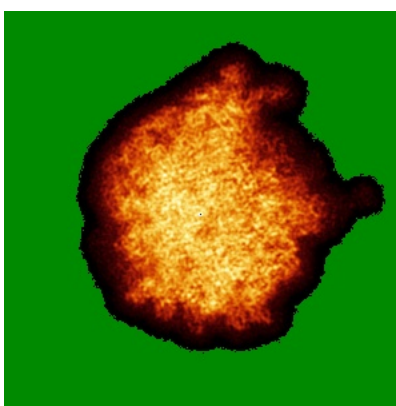
The images above show the largest variance slices of the map in three orthogonal directions.

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

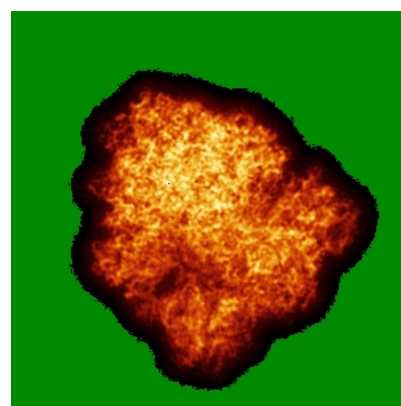
6.4.1 Primary map



X



Y

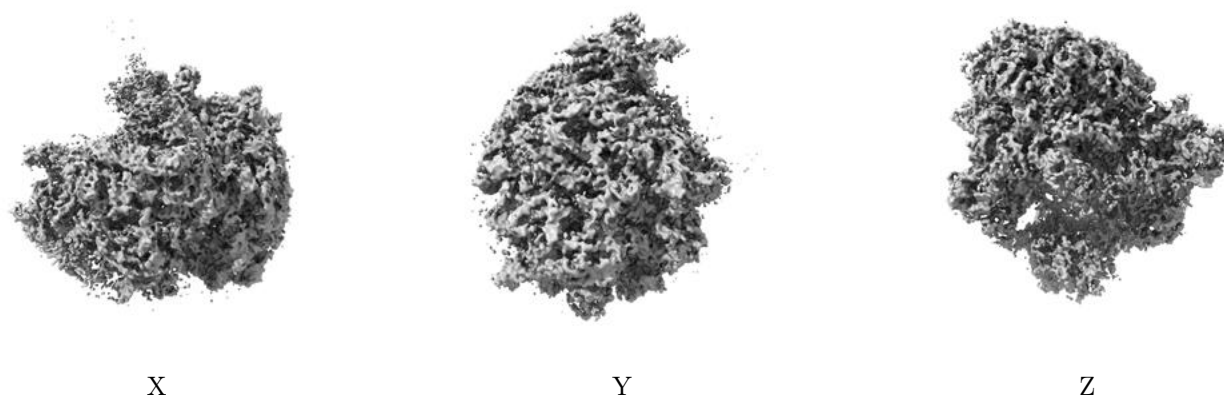


Z

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 1.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

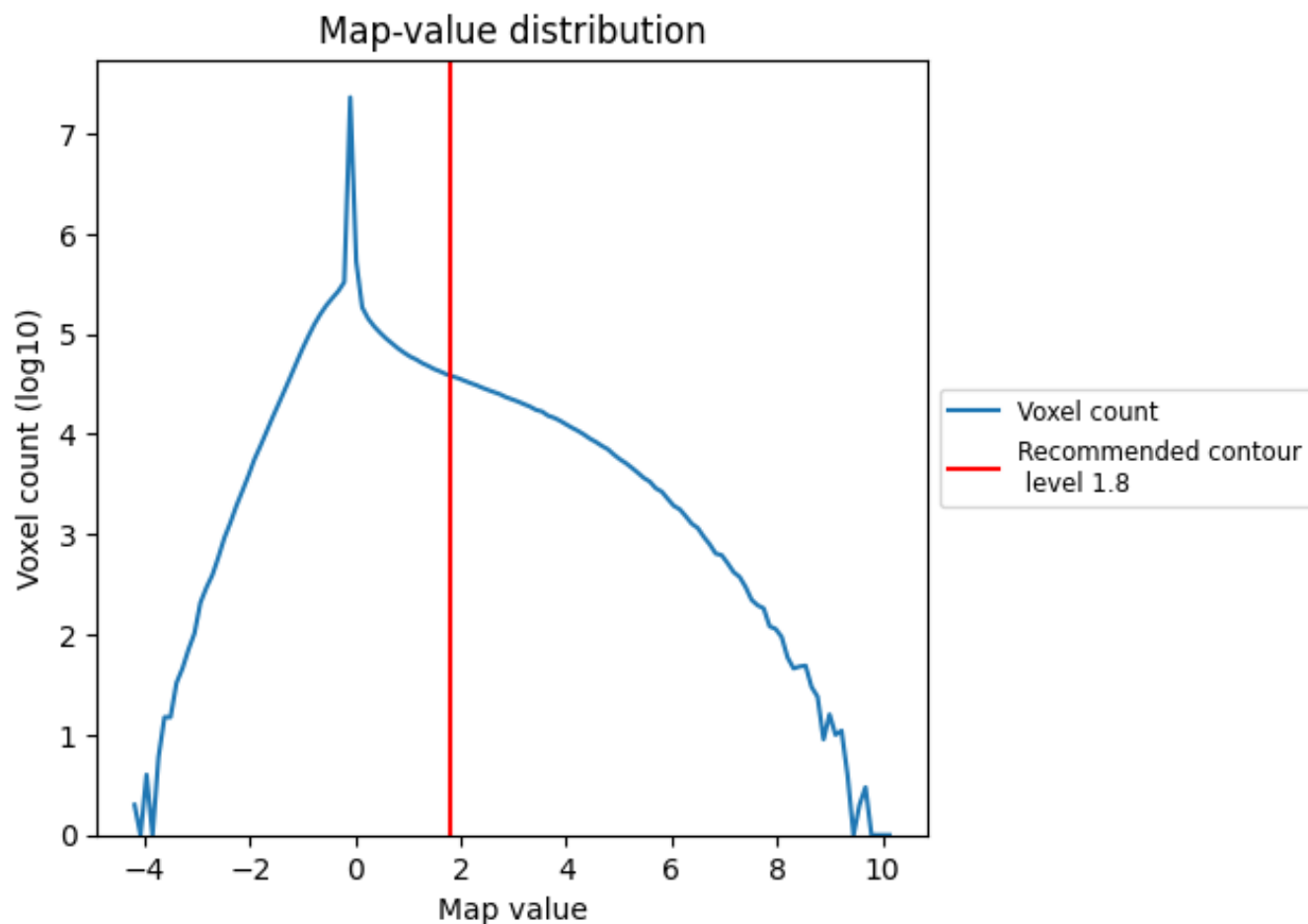
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

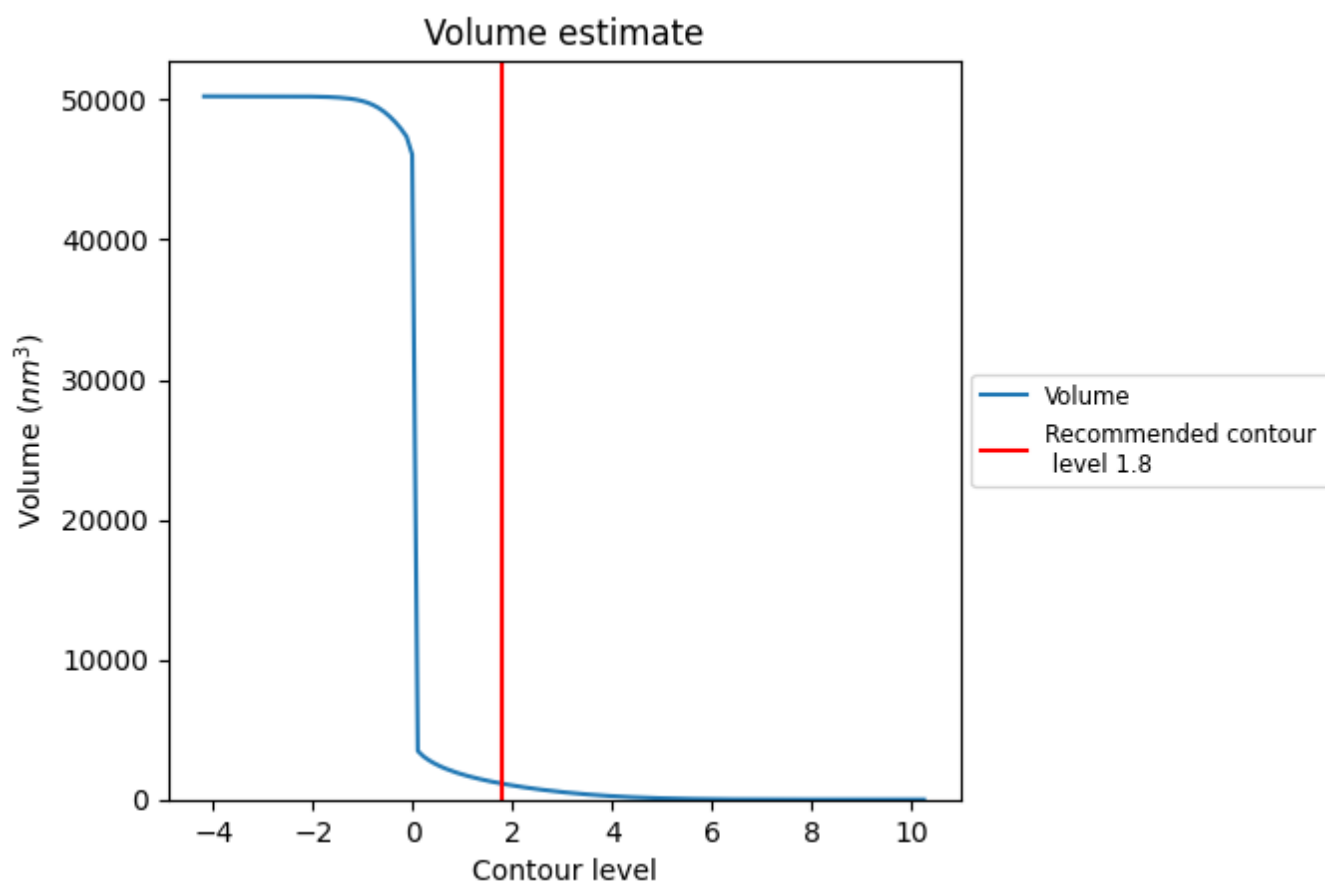
This section contains the results of statistical analysis of the map.

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.

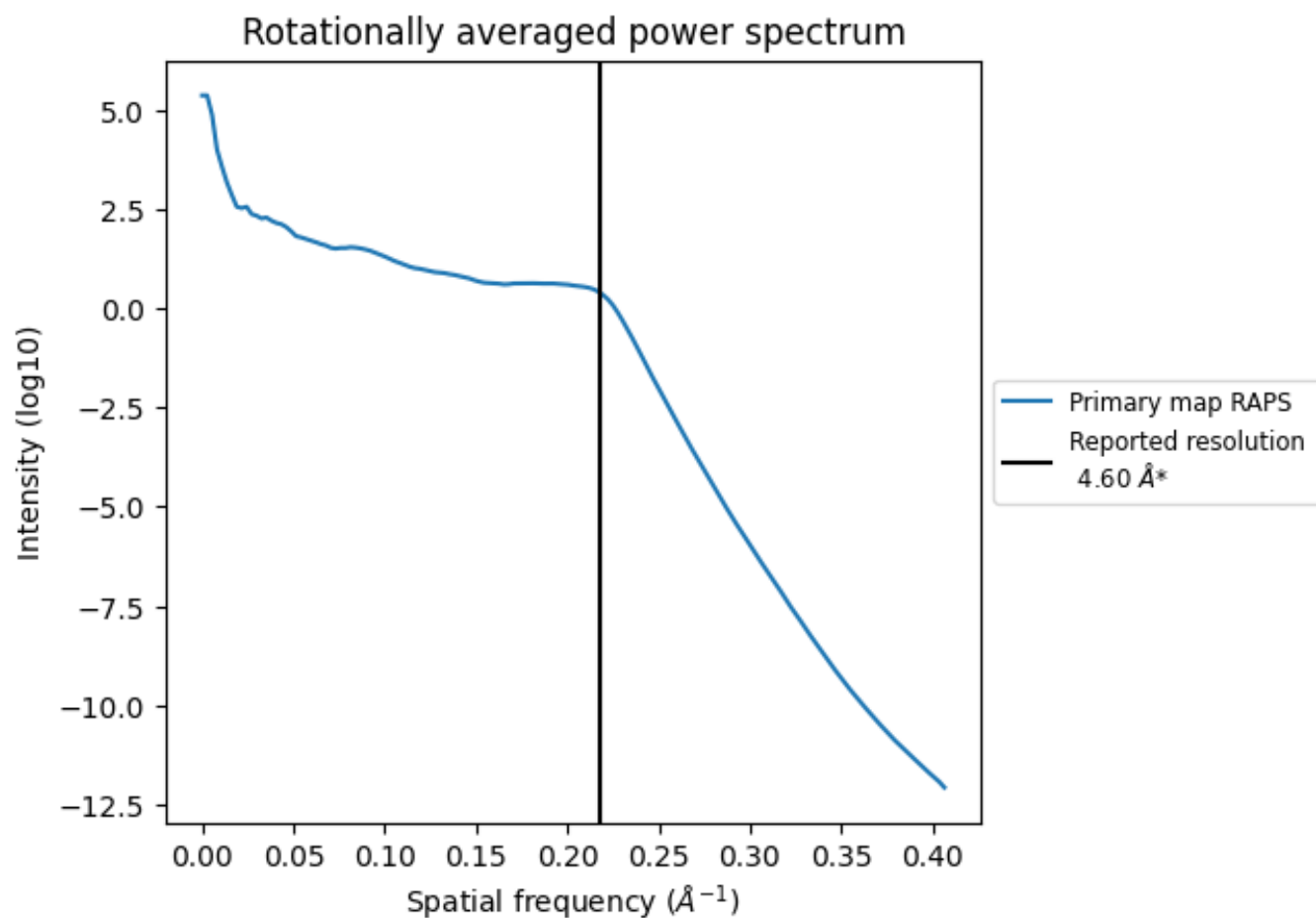
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1130 nm³; this corresponds to an approximate mass of 1021 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 0.217 Å⁻¹

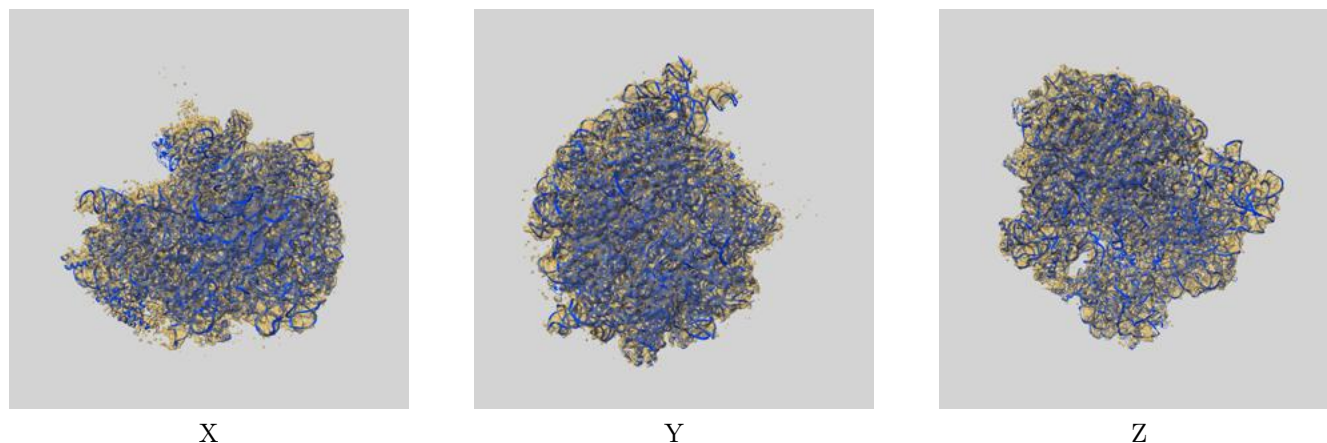
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

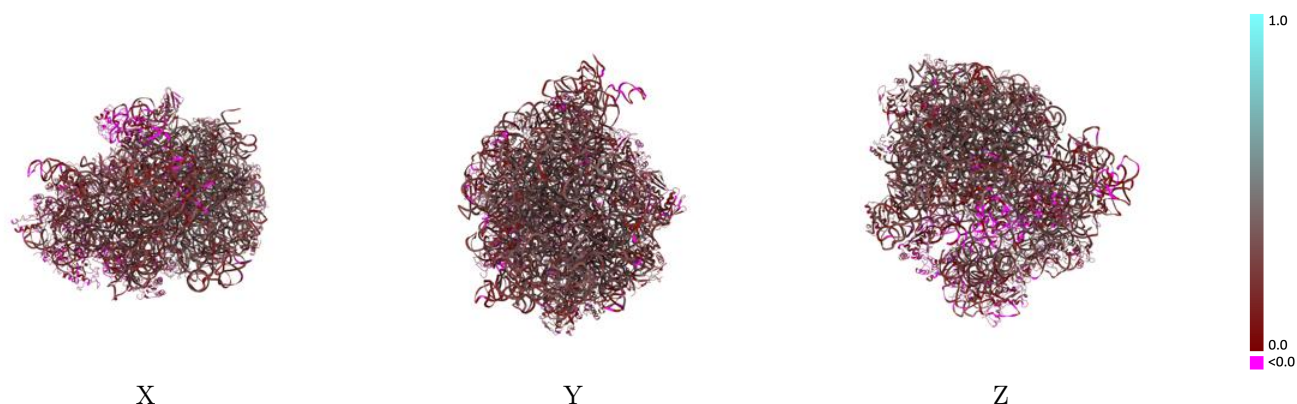
This section contains information regarding the fit between EMDB map EMD-3285 and PDB model 3JCN. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



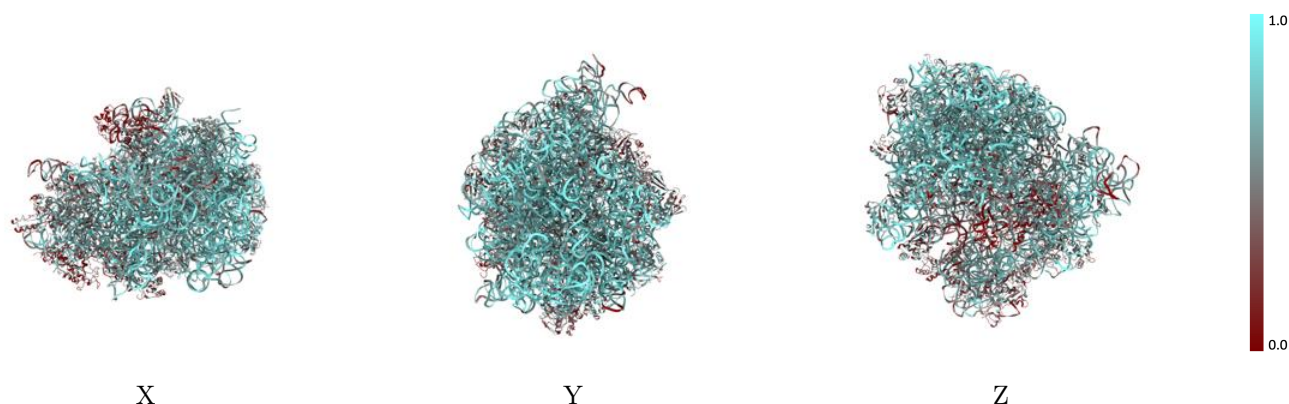
The images above show the 3D surface view of the map at the recommended contour level 1.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



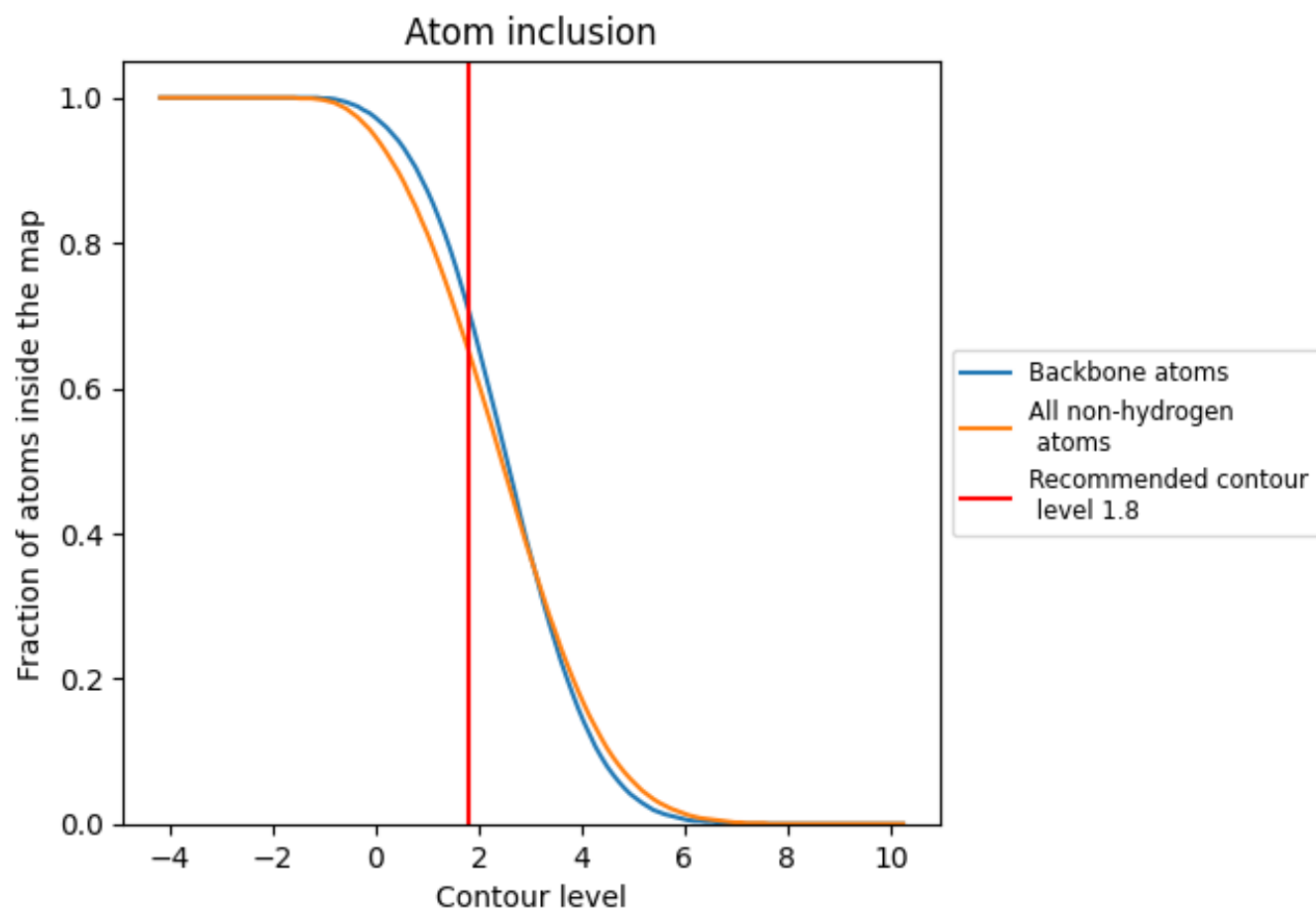
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 65% 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 (1.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6520	 0.2410
0	 0.5630	 0.2620
1	 0.2990	 0.1950
2	 0.6590	 0.2710
3	 0.6010	 0.2880
4	 0.5750	 0.2640
A	 0.7770	 0.2830
B	 0.7800	 0.2620
C	 0.5300	 0.2610
D	 0.5530	 0.2700
E	 0.4590	 0.2260
F	 0.3900	 0.1140
G	 0.4810	 0.1760
H	 0.1390	 0.1330
I	 0.0340	 -0.0270
J	 0.5720	 0.2690
K	 0.4410	 0.2500
L	 0.4740	 0.2390
M	 0.4960	 0.2600
N	 0.5990	 0.2510
O	 0.5050	 0.1950
P	 0.4900	 0.2330
Q	 0.5900	 0.2330
R	 0.5920	 0.2610
S	 0.6070	 0.2730
T	 0.5640	 0.2500
U	 0.5070	 0.2140
V	 0.4960	 0.2490
W	 0.5400	 0.2810
X	 0.4990	 0.2370
Y	 0.5390	 0.1690
Z	 0.5680	 0.2680
a	 0.7250	 0.2370
b	 0.3320	 0.1590
c	 0.3950	 0.1570



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Chain	Atom inclusion	Q-score
d	 0.1710	 0.1090
f	 0.5040	 0.2190
g	 0.4360	 0.1950
h	 0.1040	 0.0530
i	 0.2910	 0.1300
j	 0.3850	 0.1260
k	 0.5190	 0.2110
l	 0.3280	 0.1090
m	 0.3240	 0.1220
n	 0.2980	 0.1000
o	 0.5170	 0.2370
p	 0.5170	 0.1850
q	 0.3890	 0.1430
r	 0.4870	 0.2000
s	 0.5280	 0.2140
t	 0.2900	 0.1240
u	 0.3950	 0.1810
v	 0.4920	 0.1490
w	 0.1650	 0.0850
x	 0.4850	 0.1470
z	 0.2170	 0.1360