



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:20 AM UTC

PDB ID : 5LZV / pdb_00005lzv
EMDB ID : EMD-4133
Title : Structure of the mammalian ribosomal termination complex with accommodated eRF1(AAQ) and ABCE1.
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.
Deposited on : 2016-10-02
Resolution : 3.35 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:

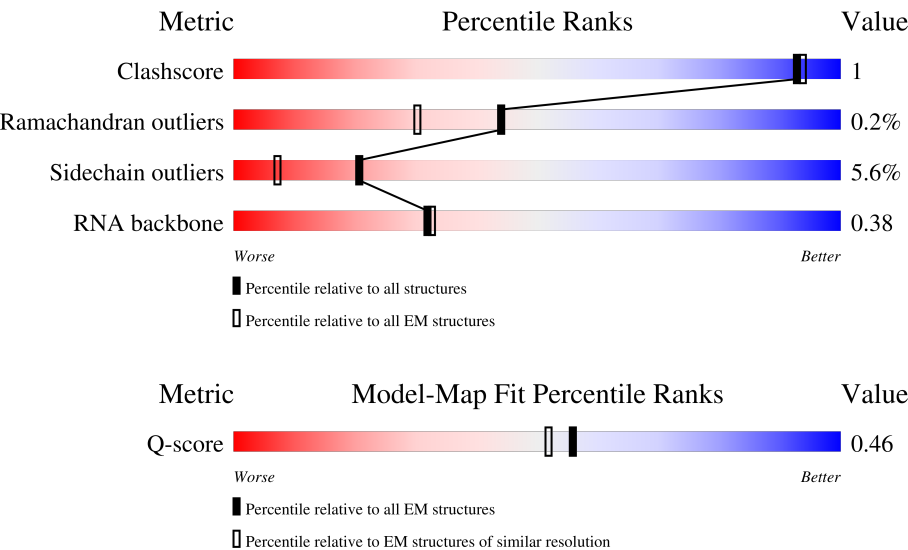
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.35 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.



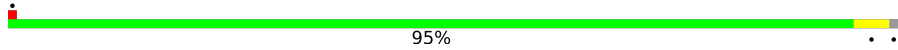
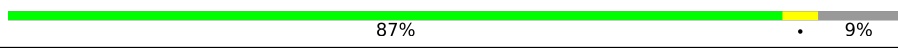
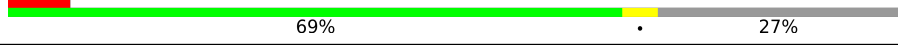
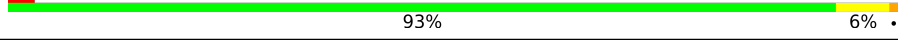
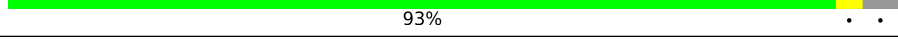
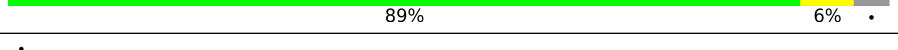
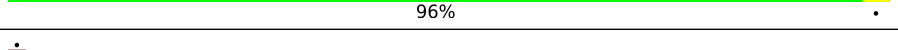
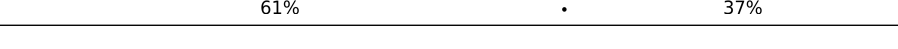
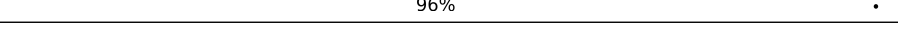
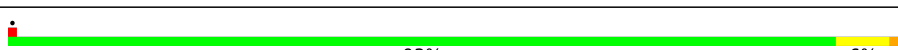
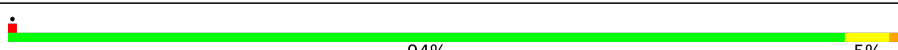
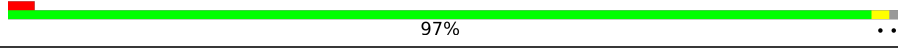
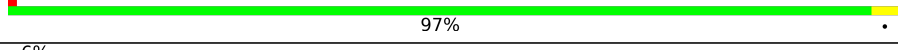
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14390 (2.85 - 3.85)

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

Mol	Chain	Length	Quality of chain
1	A	257	90% 6% . .
2	B	403	92% 5% .
3	C	425	81% 15%

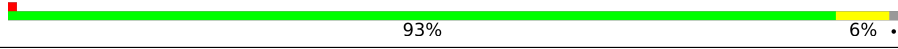
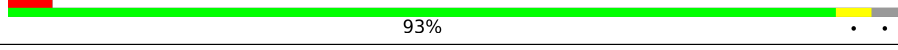
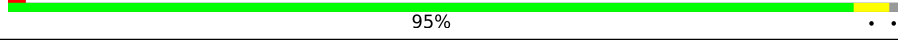
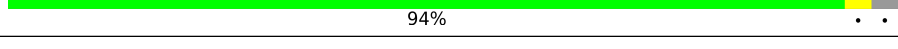
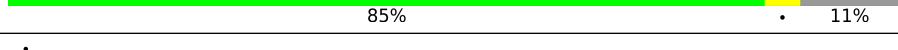
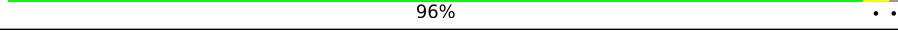
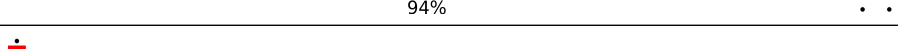
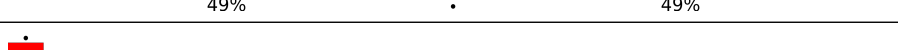
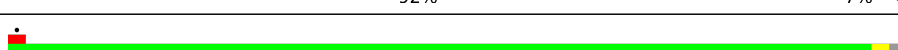
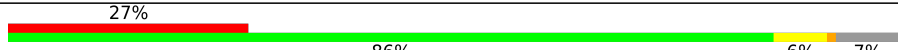
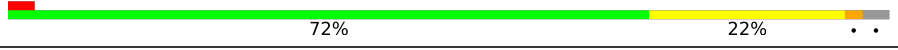
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Mol	Chain	Length	Quality of chain
4	D	297	
5	E	291	
6	F	247	
7	G	319	
8	H	192	
9	I	214	
10	J	178	
11	L	211	
12	M	218	
13	N	204	
14	O	203	
15	P	184	
16	Q	188	
17	R	196	
18	S	176	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	245	
28	c	115	

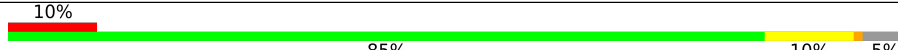
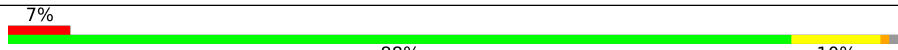
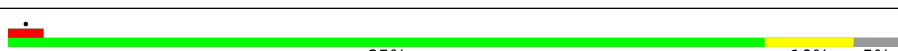
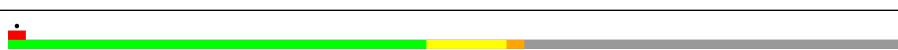
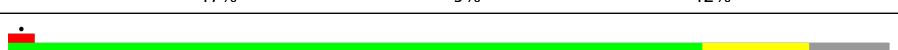
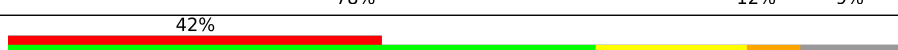
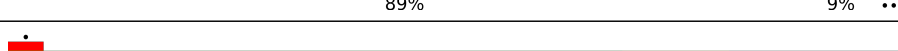
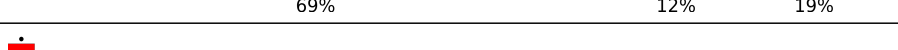
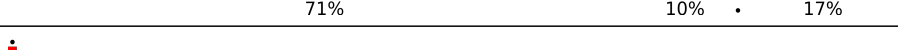
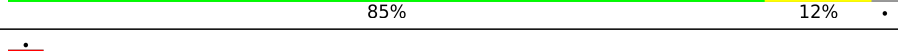
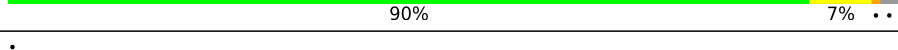
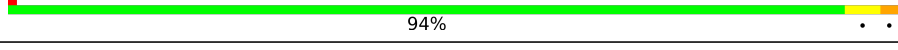
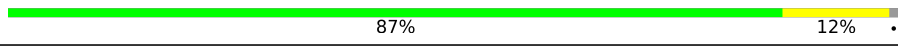
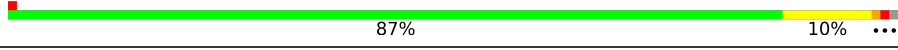
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Mol	Chain	Length	Quality of chain
29	d	125	
30	e	135	
31	f	110	
32	g	117	
33	h	123	
34	i	105	
35	j	97	
36	k	70	
37	l	51	
38	m	102	
39	n	25	
40	o	106	
41	p	92	
42	r	137	
43	s	318	
44	t	165	
45	1	15	
46	2	76	
47	3	75	
48	5	3543	
49	7	120	
50	8	156	
51	9	1869	
52	AA	295	
53	BB	264	

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Mol	Chain	Length	Quality of chain
54	CC	293	
55	DD	243	
56	EE	263	
57	FF	204	
58	GG	249	
59	HH	194	
60	II	208	
61	JJ	194	
62	KK	165	
63	LL	158	
64	MM	132	
65	NN	151	
66	OO	168	
67	PP	145	
68	QQ	146	
69	RR	135	
70	SS	152	
71	TT	145	
72	UU	119	
73	VV	83	
74	WW	130	
75	XX	143	
76	YY	130	
77	ZZ	125	
78	aa	115	

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Mol	Chain	Length	Quality of chain
79	bb	84	
80	cc	69	
81	dd	56	
82	ee	133	
83	ff	156	
84	gg	317	
85	hh	15	
86	ii	459	
87	jj	599	

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
89	ZN	ff	200	-	-	X	-
90	SF4	jj	601	-	-	X	-

2 Entry composition [i](#)

There are 90 unique types of molecules in this entry. The entry contains 223874 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 2 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	GLN	initiating methionine	UNP G1TL06

- Molecule 3 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 4 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	LYS	initiating methionine	UNP G1SYJ6

- Molecule 5 is a protein called eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 6 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	61	ARG	GLY	conflict	UNP G1TUB1
F	93	ARG	GLY	conflict	UNP G1TUB1
F	131	MET	VAL	conflict	UNP G1TUB1
F	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 7 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 8 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 9 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 10 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 11 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 12 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 13 is a protein called eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 14 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 15 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 16 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 17 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 18 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 19 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 20 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 21 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 22 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 23 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 24 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 25 is a protein called eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 26 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1	MET	GLN	conflict	UNP G1SNY0

- Molecule 27 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 28 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 29 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 30 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 31 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 32 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	117	LYS	-	insertion	UNP G1U945

- Molecule 33 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 34 is a protein called eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 35 is a protein called eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 36 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 37 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 38 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 39 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 40 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 41 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 42 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 43 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 44 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 45 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	15	Total	C	N	O	S	0	0
			125	82	20	22	1		

- Molecule 46 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 47 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 48 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	3543	Total	C	N	O	P	0	0
			75972	33833	13910	24686	3543		

- Molecule 49 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 50 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 51 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	1698	Total	C	N	O	P	0	0
			36249	16180	6508	11864	1697		

- Molecule 52 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AA	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 53 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BB	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 54 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	CC	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 55 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	DD	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 56 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	EE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 57 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	FF	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 58 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	GG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 59 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	HH	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 60 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	II	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
II	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 61 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	JJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 62 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	KK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 63 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	LL	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 64 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	MM	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 65 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	NN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 66 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	OO	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 67 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	PP	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 68 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	QQ	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 69 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	RR	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 70 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SS	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 71 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	TT	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
TT	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 72 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	UU	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 73 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	VV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 74 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	WW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 75 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	XX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 76 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	YY	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 77 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	ZZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 78 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	aa	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 79 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	bb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 80 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	cc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 81 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	dd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 82 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	ee	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 83 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	ff	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 84 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	gg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 85 is a RNA chain called mRNA (UGA stop codon).

Mol	Chain	Residues	Atoms					AltConf	Trace
85	hh	15	Total	C	N	O	P	0	0
			317	142	54	106	15		

- Molecule 86 is a protein called eRF1(AAQ).

Mol	Chain	Residues	Atoms					AltConf	Trace
86	ii	419	Total	C	N	O	S	0	0
			3309	2106	562	629	12		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	-21	MET	-	initiating methionine	UNP P62495
ii	-20	ARG	-	expression tag	UNP P62495
ii	-19	GLY	-	expression tag	UNP P62495
ii	-18	SER	-	expression tag	UNP P62495
ii	-17	HIS	-	expression tag	UNP P62495
ii	-16	HIS	-	expression tag	UNP P62495
ii	-15	HIS	-	expression tag	UNP P62495
ii	-14	HIS	-	expression tag	UNP P62495
ii	-13	HIS	-	expression tag	UNP P62495
ii	-12	HIS	-	expression tag	UNP P62495
ii	-11	GLY	-	expression tag	UNP P62495
ii	-10	MET	-	expression tag	UNP P62495
ii	-9	ALA	-	expression tag	UNP P62495
ii	-8	SER	-	expression tag	UNP P62495
ii	-7	GLU	-	expression tag	UNP P62495
ii	-6	ASN	-	expression tag	UNP P62495
ii	-5	LEU	-	expression tag	UNP P62495
ii	-4	TYR	-	expression tag	UNP P62495
ii	-3	PHE	-	expression tag	UNP P62495

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Chain	Residue	Modelled	Actual	Comment	Reference
ii	-2	GLN	-	expression tag	UNP P62495
ii	-1	GLY	-	expression tag	UNP P62495
ii	0	SER	-	expression tag	UNP P62495
ii	183	ALA	GLY	conflict	UNP P62495
ii	184	ALA	GLY	conflict	UNP P62495

- Molecule 87 is a protein called ABCE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	577	Total	C	N	O	S	0	0
			4555	2914	780	830	31		

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	B	1	Total	Mg	0
			1	1	
88	I	1	Total	Mg	0
			1	1	
88	L	1	Total	Mg	0
			1	1	
88	P	1	Total	Mg	0
			1	1	
88	Q	1	Total	Mg	0
			1	1	
88	V	1	Total	Mg	0
			1	1	
88	a	2	Total	Mg	0
			2	2	
88	e	1	Total	Mg	0
			1	1	
88	g	1	Total	Mg	0
			1	1	
88	j	1	Total	Mg	0
			1	1	
88	5	197	Total	Mg	0
			197	197	
88	7	7	Total	Mg	0
			7	7	
88	8	5	Total	Mg	0
			5	5	
88	9	79	Total	Mg	0
			79	79	

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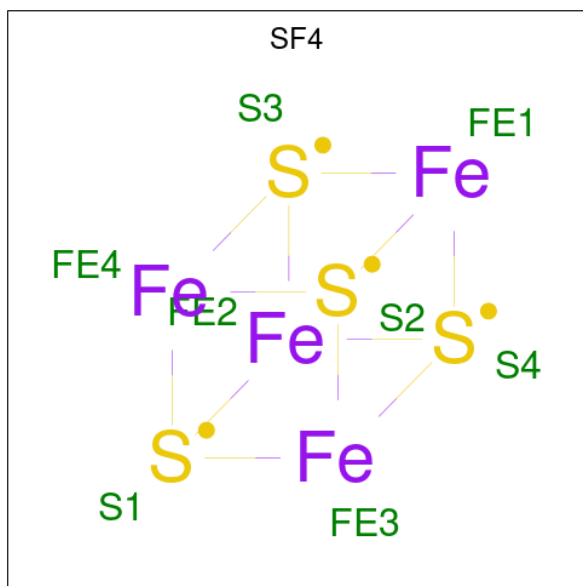
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Mol	Chain	Residues	Atoms		AltConf
88	hh	1	Total	Mg	0
			1	1	

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
89	g	1	Total	Zn	0
			1	1	
89	j	1	Total	Zn	0
			1	1	
89	m	1	Total	Zn	0
			1	1	
89	o	1	Total	Zn	0
			1	1	
89	p	1	Total	Zn	0
			1	1	
89	aa	1	Total	Zn	0
			1	1	
89	dd	1	Total	Zn	0
			1	1	
89	ff	1	Total	Zn	0
			1	1	

- Molecule 90 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
90	jj	1	Total 8	Fe 4	S 4	0
90	jj	1	Total 8	Fe 4	S 4	0

3 Residue-property plots [i](#)

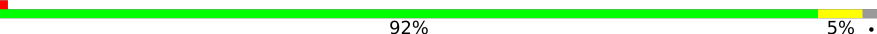
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

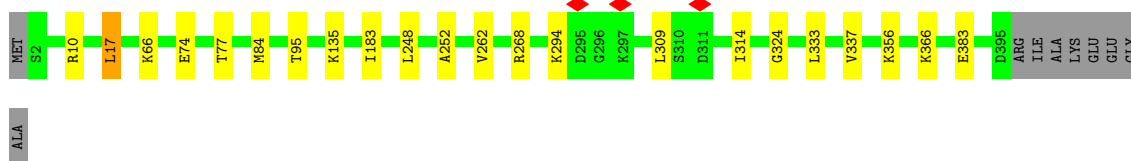
• Molecule 1: uL2

Chain A:  90% 6% . .



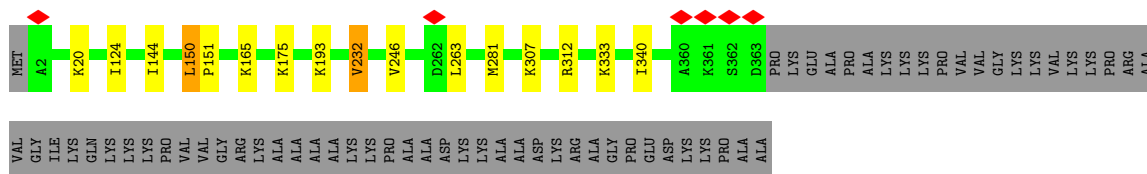
• Molecule 2: uL3

Chain B:  92% 5% .

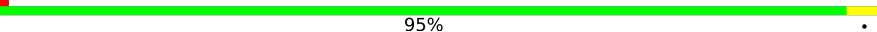


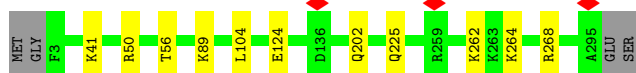
• Molecule 3: uL4

Chain C:  81% 15% .



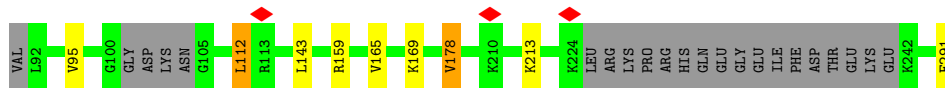
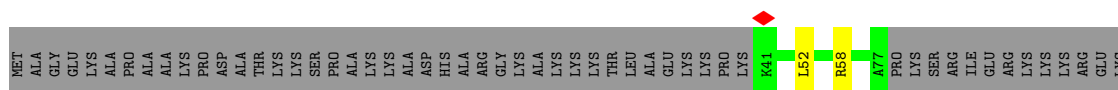
• Molecule 4: uL18

Chain D:  95% . .



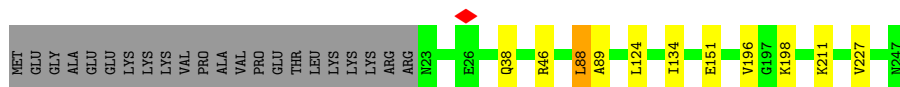
• Molecule 5: eL6

Chain E:  70% 26% . .



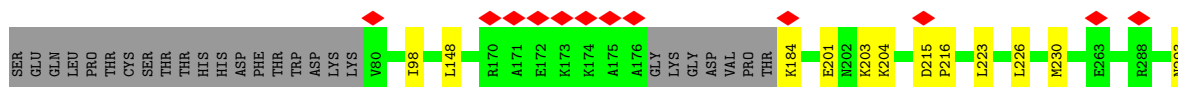
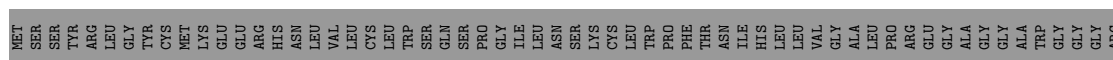
• Molecule 6: uL30

Chain F: 87% 9%



• Molecule 7: eL8

Chain G: 7% 69% 27%



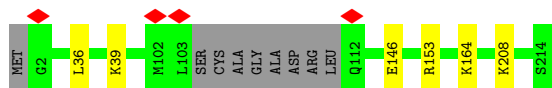
• Molecule 8: uL6

Chain H: 93% 6%



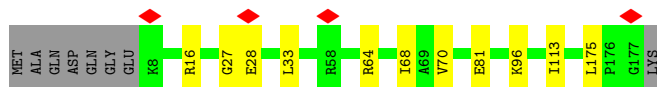
• Molecule 9: uL16

Chain I: 93% 6%

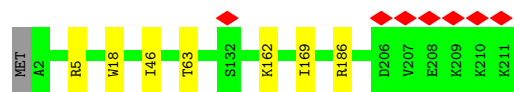


• Molecule 10: uL5

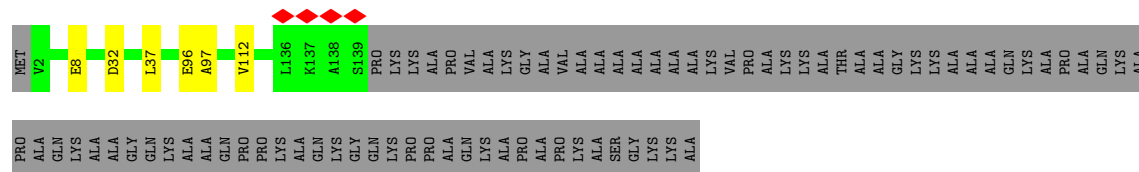
Chain J: 89% 6%



- Molecule 11: eL13



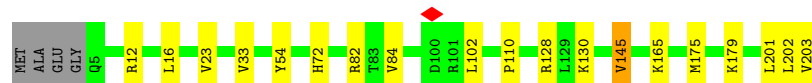
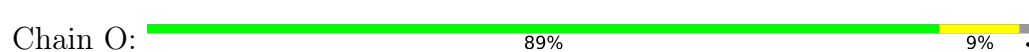
- Molecule 12: eL14



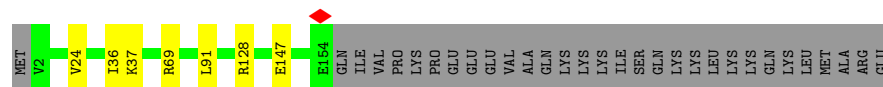
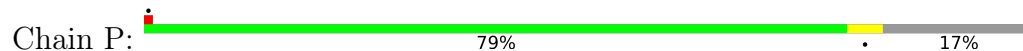
- Molecule 13: eL15



- Molecule 14: uL13



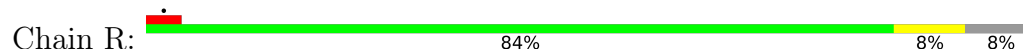
- Molecule 15: uL22



- Molecule 16: eL18



- Molecule 17: eL19

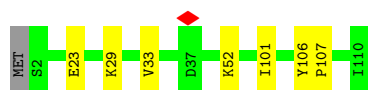


Chain e:  87% 7% 5%



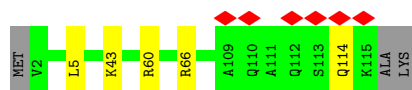
- Molecule 31: eL33

Chain f:  93% 6%



- Molecule 32: eL34

Chain g:  5% 93%



- Molecule 33: uL29

Chain h:  95%



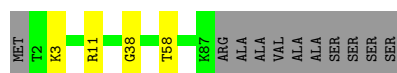
- Molecule 34: eL36

Chain i:  94%



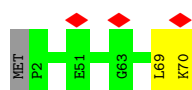
- Molecule 35: eL37

Chain j:  85% 11%

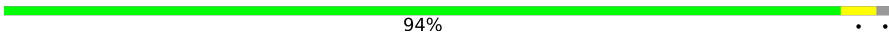
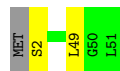


- Molecule 36: eL38

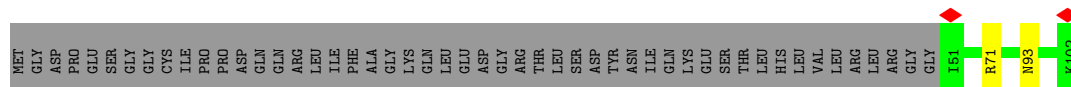
Chain k:  96%



• Molecule 37: eL39

Chain l:  94% ..

• Molecule 38: eL40

Chain m:  49% . 49%

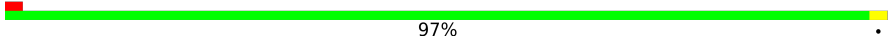
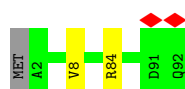
• Molecule 39: eL41

Chain n:  84% 16%

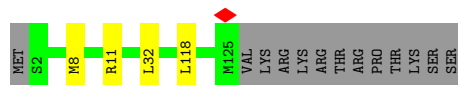
• Molecule 40: eL42

Chain o:  92% 7% .

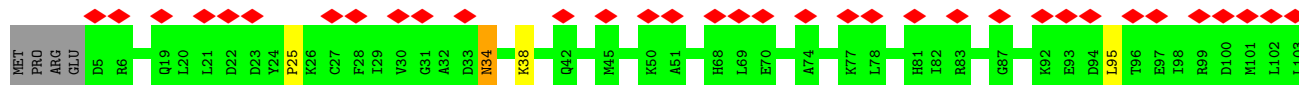
• Molecule 41: eL43

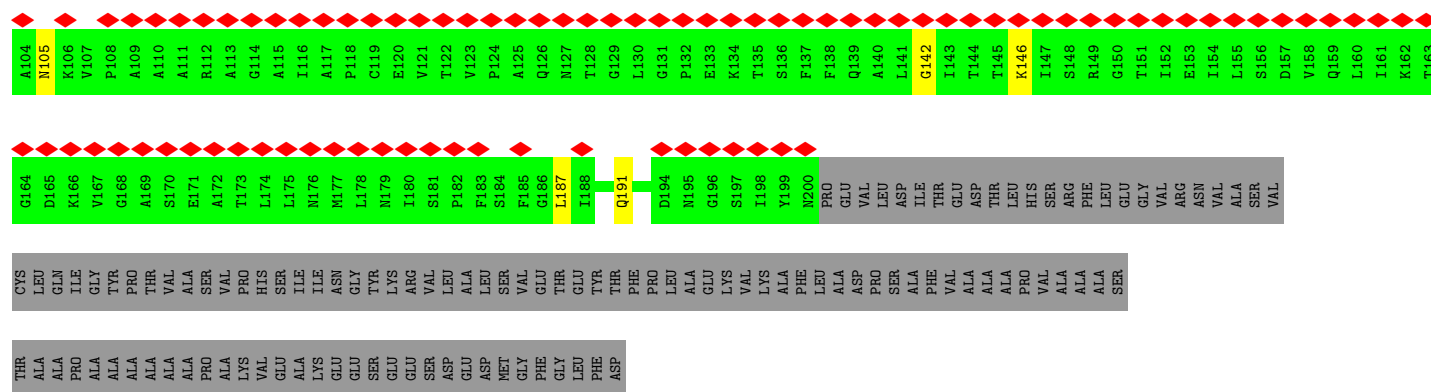
Chain p:  97% ..

• Molecule 42: eL28

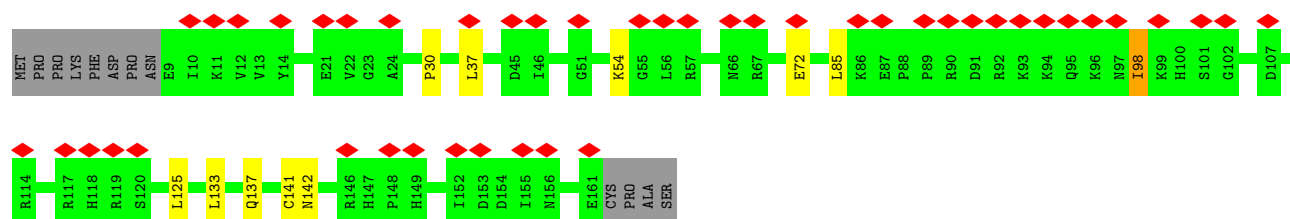
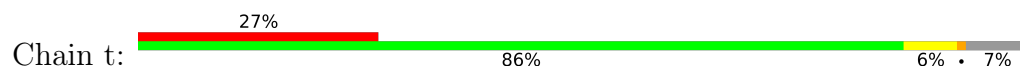
Chain r:  88% . 9%

• Molecule 43: uL10

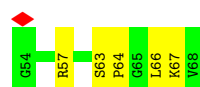
Chain s:  38% 59% . 38%



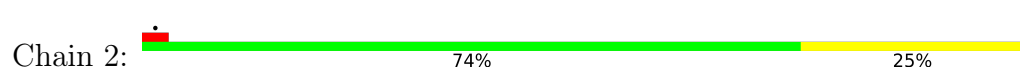
• Molecule 44: uL11



• Molecule 45: Nascent chain



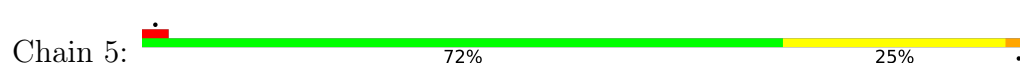
• Molecule 46: P-site tRNA

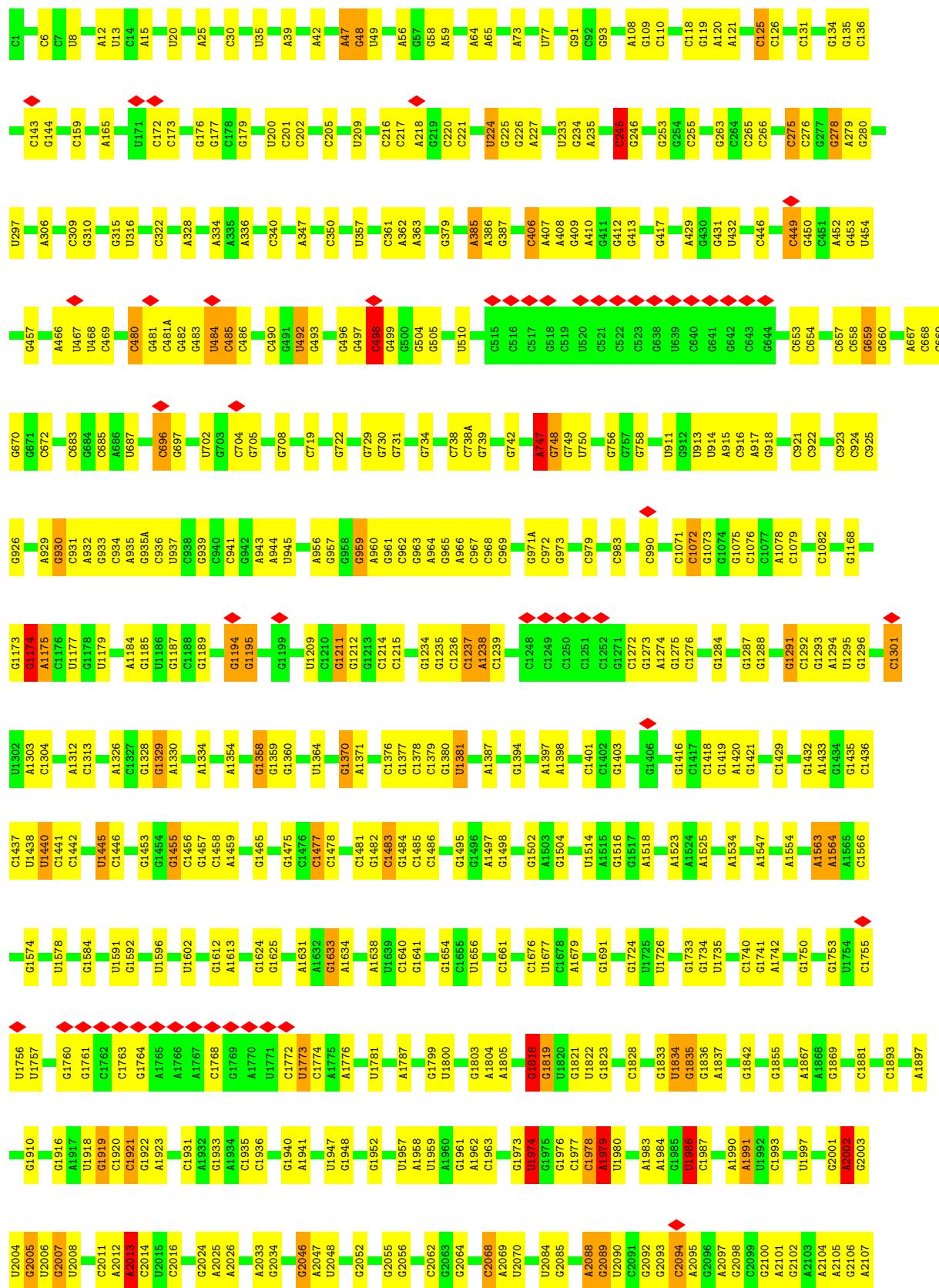


• Molecule 47: E-site tRNA

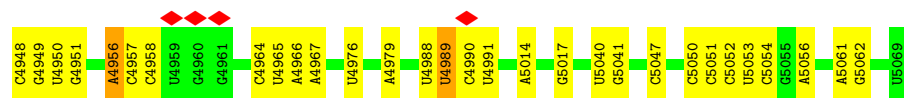


• Molecule 48: 28S ribosomal RNA

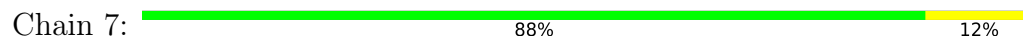




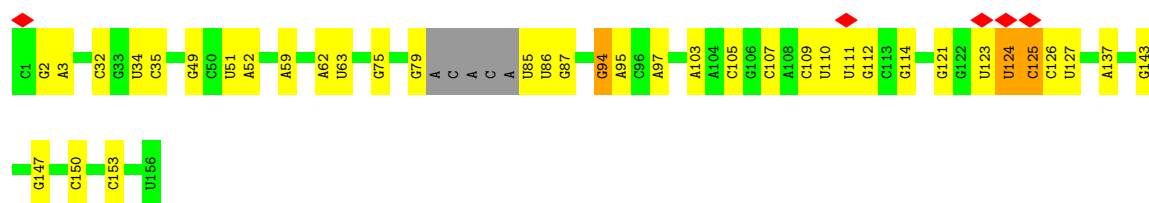
G4870	C4670	G4514	G4373	G4222	U4068	G3811	A3662	C2797	C2669	A2512	G2399	G2108
G4871	C4671	G4515	G4374	G4223	U4069	C3812	A3663	A2798	C2670	A2513	G2407	A2109
G4872	C4672	C4519	G4375	G4224	U4070	C3813	C3673	A2806	G2673	A2514	U2408	G2110
G4873	G4672	G4520	C4376	G4225	U4075	U3814	G3674	A2807	G2674	G2521	U2409	U2111
G4874	C4673	G4521	C4377	U4222	G4084	C3815	C3675	C2814	A2676	A2529	G2414	G2259
G4875	C4674	G4522	C4378	U4223	G4085	U3816	C3685	C2815	G2677	U2530	U2415	G2260
G4876	C4675	G4523	C4379	U4224	G4086	C3817	C3686	C2816	G2678	G2416	A2417	G2261
G4877	C4676	G4524	C4380	U4225	G4087	U3818	C3687	U2819	G2679	A2537	G2417	G2262
U4882	C4677	G4525	C4381	U4226	G4088	U3819	C3688	U2820	G2680	G2418	G2417	G2263
C4883	C4678	G4526	C4382	U4227	G4089	U3820	C3689	U2821	G2681	G2419	G2417	G2264
C4884	C4679	G4527	C4383	U4228	G4090	U3821	C3690	U2822	G2682	G2420	G2417	G2265
C4885	C4680	G4528	C4384	U4229	G4091	U3822	C3691	U2823	G2683	G2421	G2417	G2266
C4886	C4681	G4529	C4385	U4230	G4092	U3823	C3692	U2824	G2684	G2422	G2417	G2267
C4887	C4682	G4530	C4386	U4231	G4093	U3824	C3693	U2825	G2685	G2423	G2417	G2268
C4888	C4683	G4531	C4387	U4232	G4094	U3825	C3694	U2826	G2686	G2424	G2417	G2269
C4889	C4684	G4532	C4388	U4233	G4095	U3826	C3695	U2827	G2687	G2425	G2417	G2270
C4890	C4685	G4533	C4389	U4234	G4096	U3827	C3696	U2828	G2688	G2426	G2417	G2271
C4891	C4686	G4534	C4390	U4235	G4097	U3828	C3697	U2829	G2689	G2427	G2417	G2272
C4892	C4687	G4535	C4391	U4236	G4098	U3829	C3698	U2830	G2690	G2428	G2417	G2273
C4893	C4688	G4536	C4392	U4237	G4099	U3830	C3699	U2831	G2691	G2429	G2417	G2274
C4894	C4689	G4537	C4393	U4238	G4100	U3831	C3700	U2832	G2692	G2430	G2417	G2275
C4895	C4690	G4538	C4394	U4239	G4101	U3832	C3701	U2833	G2693	G2431	G2417	G2276
C4896	C4691	G4539	C4395	U4240	G4102	U3833	C3702	U2834	G2694	G2432	G2417	G2277
C4897	C4692	G4540	C4396	U4241	G4103	U3834	C3703	U2835	G2695	G2433	G2417	G2278
C4898	C4693	G4541	C4397	U4242	G4104	U3835	C3704	U2836	G2696	G2434	G2417	G2279
C4899	C4694	G4542	C4398	U4243	G4105	U3836	C3705	U2837	G2697	G2435	G2417	G2280
C4900	C4695	G4543	C4399	U4244	G4106	U3837	C3706	U2838	G2698	G2436	G2417	G2281
C4901	C4696	G4544	C4400	U4245	G4107	U3838	C3707	U2839	G2699	G2437	G2417	G2282
C4902	C4697	G4545	C4401	U4246	G4108	U3839	C3708	U2840	G2700	G2438	G2417	G2283
C4903	C4698	G4546	C4402	U4247	G4109	U3840	C3709	U2841	G2701	G2439	G2417	G2284
C4904	C4699	G4547	C4403	U4248	G4110	U3841	C3710	U2842	G2702	G2440	G2417	G2285
C4905	C4700	G4548	C4404	U4249	G4111	U3842	C3711	U2843	G2703	G2441	G2417	G2286
C4906	C4701	G4549	C4405	U4250	G4112	U3843	C3712	U2844	G2704	G2442	G2417	G2287
C4907	C4702	G4550	C4406	U4251	G4113	U3844	C3713	U2845	G2705	G2443	G2417	G2288
C4908	C4703	G4551	C4407	U4252	G4114	U3845	C3714	U2846	G2706	G2444	G2417	G2289
C4909	C4704	G4552	C4408	U4253	G4115	U3846	C3715	U2847	G2707	G2445	G2417	G2290
C4910	C4705	G4553	C4409	U4254	G4116	U3847	C3716	U2848	G2708	G2446	G2417	G2291
C4911	C4706	G4554	C4410	U4255	G4117	U3848	C3717	U2849	G2709	G2447	G2417	G2292
C4912	C4707	G4555	C4411	U4256	G4118	U3849	C3718	U2850	G2710	G2448	G2417	G2293
C4913	C4708	G4556	C4412	U4257	G4119	U3850	C3719	U2851	G2711	G2449	G2417	G2294
C4914	C4709	G4557	C4413	U4258	G4120	U3851	C3720	U2852	G2712	G2450	G2417	G2295
C4915	C4710	G4558	C4414	U4259	G4121	U3852	C3721	U2853	G2713	G2451	G2417	G2296
C4916	C4711	G4559	C4415	U4260	G4122	U3853	C3722	U2854	G2714	G2452	G2417	G2297
C4917	C4712	G4560	C4416	U4261	G4123	U3854	C3723	U2855	G2715	G2453	G2417	G2298
C4918	C4713	G4561	C4417	U4262	G4124	U3855	C3724	U2856	G2716	G2454	G2417	G2299
C4919	C4714	G4562	C4418	U4263	G4125	U3856	C3725	U2857	G2717	G2455	G2417	G2300
C4920	C4715	G4563	C4419	U4264	G4126	U3857	C3726	U2858	G2718	G2456	G2417	G2301
C4921	C4716	G4564	C4420	U4265	G4127	U3858	C3727	U2859	G2719	G2457	G2417	G2302
C4922	C4717	G4565	C4421	U4266	G4128	U3859	C3728	U2860	G2720	G2458	G2417	G2303
C4923	C4718	G4566	C4422	U4267	G4129	U3860	C3729	U2861	G2721	G2459	G2417	G2304
C4924	C4719	G4567	C4423	U4268	G4130	U3861	C3730	U2862	G2722	G2460	G2417	G2305
C4925	C4720	G4568	C4424	U4269	G4131	U3862	C3731	U2863	G2723	G2461	G2417	G2306
C4926	C4721	G4569	C4425	U4270	G4132	U3863	C3732	U2864	G2724	G2462	G2417	G2307
C4927	C4722	G4570	C4426	U4271	G4133	U3864	C3733	U2865	G2725	G2463	G2417	G2308
C4928	C4723	G4571	C4427	U4272	G4134	U3865	C3734	U2866	G2726	G2464	G2417	G2309
C4929	C4724	G4572	C4428	U4273	G4135	U3866	C3735	U2867	G2727	G2465	G2417	G2310
C4930	C4725	G4573	C4429	U4274	G4136	U3867	C3736	U2868	G2728	G2466	G2417	G2311
C4931	C4726	G4574	C4430	U4275	G4137	U3868	C3737	U2869	G2729	G2467	G2417	G2312
C4932	C4727	G4575	C4431	U4276	G4138	U3869	C3738	U2870	G2730	G2468	G2417	G2313
C4933	C4728	G4576	C4432	U4277	G4139	U3870	C3739	U2871	G2731	G2469	G2417	G2314
C4934	C4729	G4577	C4433	U4278	G4140	U3871	C3740	U2872	G2732	G2470	G2417	G2315
C4935	C4730	G4578	C4434	U4279	G4141	U3872	C3741	U2873	G2733	G2471	G2417	G2316
C4936	C4731	G4579	C4435	U4280	G4142	U3873	C3742	U2874	G2734	G2472	G2417	G2317
C4937	C4732	G4580	C4436	U4281	G4143	U3874	C3743	U2875	G2735	G2473	G2417	G2318
C4938	C4733	G4581	C4437	U4282	G4144	U3875	C3744	U2876	G2736	G2474	G2417	G2319
C4939	C4734	G4582	C4438	U4283	G4145	U3876	C3745	U2877	G2737	G2475	G2417	G2320
C4940	C4735	G4583	C4439	U4284	G4146	U3877	C3746	U2878	G2738	G2476	G2417	G2321
C4941	C4736	G4584	C4440	U4285	G4147	U3878	C3747	U2879	G2739	G2477	G2417	G2322
C4942	C4737	G4585	C4441	U4286	G4148	U3879	C3748	U2880	G2740	G2478	G2417	G2323
C4943	C4738	G4586	C4442	U4287	G4149	U3880	C3749	U2881	G2741	G2479	G2417	G2324
C4944	C4739	G4587	C4443	U4288	G4150	U3881	C3750	U2882	G2742	G2480	G2417	G2325
C4945	C4740	G4588	C4444	U4289	G4151	U3882	C3751	U2883	G2743	G2481	G2417	G2326
C4946	C4741	G4589	C4445	U4290	G4152	U3883	C3752	U2884	G2744	G2482	G2417	G2327
C4947	C4742	G4590	C4446	U4291	G4153	U3884	C3753	U2885	G2745	G2483	G2417	G2328
C4948	C4743	G4591	C4447	U4292	G4154	U3885	C3754	U2886	G2746	G2484	G2417	G2329
C4949	C4744	G4592	C4448	U4293	G4155	U3886	C3755	U2887	G2747	G2485	G2417	G2330
C4950	C4745	G4593	C4449	U4294	G4156	U3887	C3756	U2888	G2748	G2486	G2417	G2331
C4951	C4746	G4594	C4450	U4295	G4157	U3888	C3757	U2889	G2749	G2487	G2417	G2332
C4952	C4747	G4595	C4451	U4296	G4158	U3889	C3758	U2890	G2750	G2488	G2417	G2333
C4953	C4748	G4596	C4452	U4297	G4159	U3890	C3759	U2891	G2751	G2489	G2417	G2334
C4954	C4749	G4597	C4453	U4298	G4160	U3891	C3760	U2892	G2752	G2490	G2417	G2335
C4955	C4750	G4598	C4454	U4299	G4161	U3892	C3761	U2893	G2753	G2491	G2417	G2336
C4956	C4751	G4599	C4455	U4300	G4162	U3893	C3762	U2894	G2754	G2492	G2417	G2337
C4957	C4752	G4600	C4456	U4301	G4163	U3894	C3763	U2895	G2755	G2493	G2417	G2338
C4958	C4753	G4601	C4457	U4302	G4164	U3895	C3764	U2896	G2756	G2494	G2417	G2339
C4959	C4754	G4602	C4458	U4303	G4165	U3896	C3765	U2897	G2757	G2495	G2417	G2340
C4960	C4755	G4603	C4459	U4304	G4166	U3897	C3766	U2898	G2758	G2496	G2417	G2341
C4961	C4756	G4604	C4460	U4305	G4167	U3898	C3767	U2899	G2759	G2497	G2417	G2342
C4962	C4757	G4605	C4461	U4306	G4168	U3899	C3768	U2900	G2760	G2498	G2417	G2343
C4963	C4758	G4606	C4462	U4307	G4169	U3900	C3769	U2901	G2761	G2499	G2417	G2344
C4964	C4759	G4607	C4463	U4308	G4170	U3901	C3770	U2902	G2762	G2500	G2417	G2345
C4965	C4760	G4608	C4464	U4309	G4171	U3902	C3771	U2903	G2763	G2501	G2417	G2346
C4966	C4761	G4609	C4465	U4310	G4172	U3903	C3772	U2904	G2764	G2502	G2417	G2347
C4967	C4762	G4610	C4466	U4311	G4173	U3904	C3773	U2905	G2765	G2503	G2417	G2348
C4968	C4763	G4611	C4467	U4312	G4174	U3905	C3774	U2906	G2766	G2504	G2417	G2349
C4969	C4764	G4612	C4468	U4313	G4175	U3906	C3775	U2907	G2767	G2505	G2417	G2350
C4970	C4765	G4613	C4469	U4314	G4176	U3907	C3776	U2908	G2768	G2506	G2417	G2351
C4971	C4766	G4614	C4470	U4315	G4177	U3908	C3777	U2909	G2769	G2507	G2417	G2352
C4972	C4767	G4615	C4471	U4316	G4178	U3909	C3778	U2910	G2770	G2508	G2417	G2353
C4973	C4768	G4616	C4472	U4317	G4179	U3910	C3779	U2911	G2771	G2509	G2417	



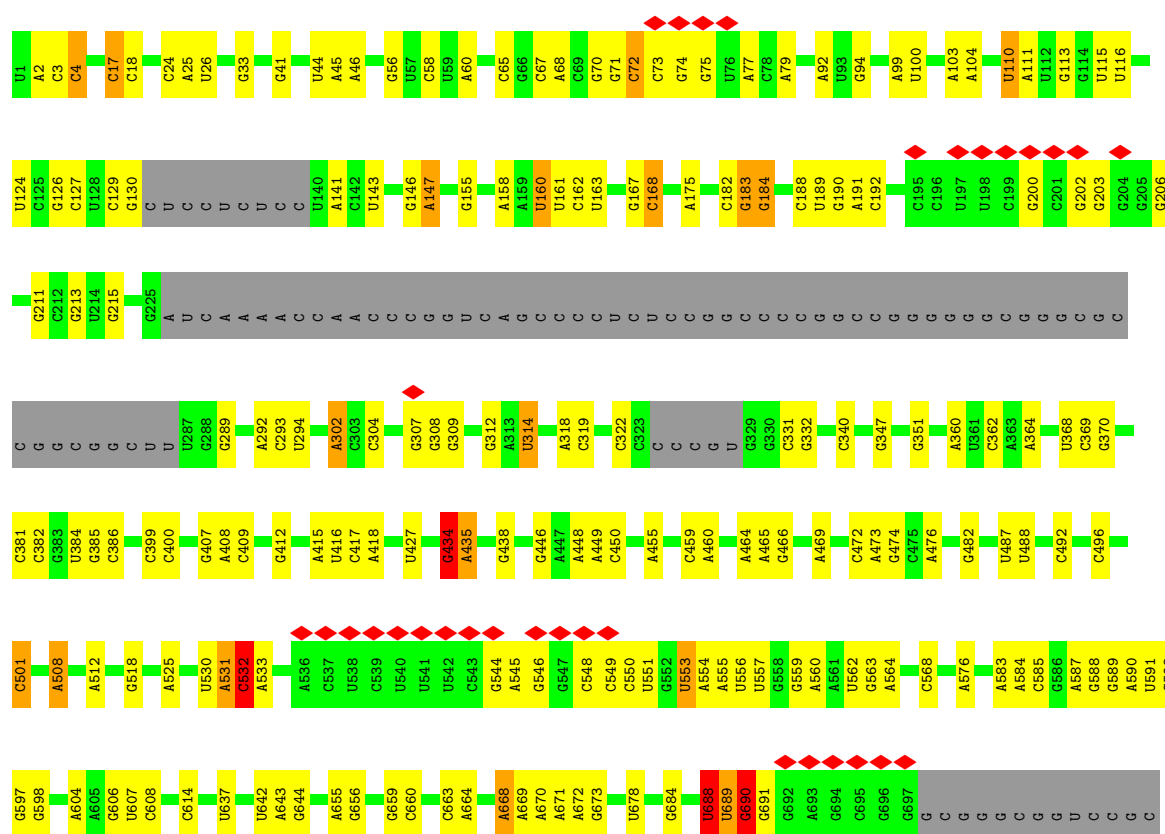
• Molecule 49: 5S ribosomal RNA



• Molecule 50: 5.8S ribosomal RNA



• Molecule 51: 18S ribosomal RNA



TRP
SER
ALA
ALA
PRO
THR
ALA
GLN
GLU
THR
TRP
VAL
GLY
THR
THR
THR
GLU
TRP
SER

• Molecule 53: eS1

Chain BB:  70% 9% 19%

MET
ALA
VAL
GLY
LYS
ASN
LYS
ARG
LEU
THR
LYS
GLY
LYS
LYS
GLY
ALA
LYS
LYS
V21
M38
T52
I57
K63
L71
L74
R82
I87
H101
L105
M113
V125
Y133
L134
Q157
M172
E175
L181
K182
E183
V184
V185

M186
I189
D191
D209
R213
L218
L225
L231
H232
G233
GLY
SER
SER
SER
GLY
LYS
ALA
THR
GLY
ASP
GLY
THR
GLY
ALA
LYS
VAL
GLY
ARG
ALA
ASP
GLY
TYR
GLY
PRO
PRO
VAL
GLN
GLU
SER
VAL

• Molecule 54: uS5

Chain CC:  66% 9% 25%

MET
ALA
ASP
ASP
ALA
GLY
ALA
ALA
GLY
GLY
PRO
PRO
ASP
GLY
PRO
GLY
PRO
ILE
GLY
GLY
GLY
GLY
PHE
PHE
ARG
GLY
GLY
PHE
GLY
SER
GLY
VAL
ARG
GLY
GLY
ARG
GLY
ARG
GLY
ARG
GLY
ARG
GLY
ALA
ARG
GLY
GLY
LYS
ALA
GLU
ASP
K58
M73

L78
I88
I94
D95
K114
R117
R121
I130
V137
A158
I162
V165
R166
R167
C188
V191
L192
I196
V209
L213
D220
Y223
T230
L233
F236
T240
I244
T252
F261
T278
ARG
VAL
SER
VAL

GLN
ARG
THR
GLN
ALA
PRO
ALA
VAL
ALA
THR
THR

• Molecule 55: uS3

Chain DD:  6% 84% 9% 6%

M1
A2
V3
F11
L21
E28
E31
T44
E47
I48
L51
R54
L59
R64
T70
A71
V72
L86
T93
R106
Y120
M127
E128
K132
V137
L142
R143
L156
D162
P163
L190
I198
D215
E216
I217
L218

I223
S224
E225
Q226
K227
G228
GLY
LYS
PRO
GLU
PRO
PRO
PRO
ALA
MET
PRO
GLN
PRO
VAL
PRO
THR
ALA

• Molecule 56: eS4

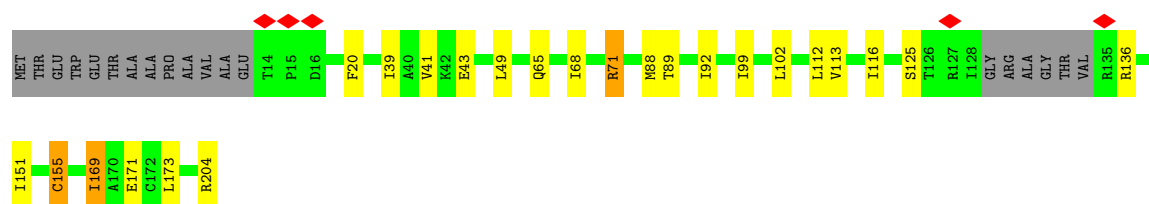
Chain EE:  86% 13% 6%

MET
A2
R3
H17
H18
H19
L23
P31
S32
L38
L42
P43
L44
R51
M66
I72
R77
T105
K106
G107
R108
K122
K125
G132
T133
I136
P137
H138
L139
I147
P150
K155
T159
I162
D163
T166
D176
C181

F205
L222
N232
L238
L246
Q260
S261
S262
G263

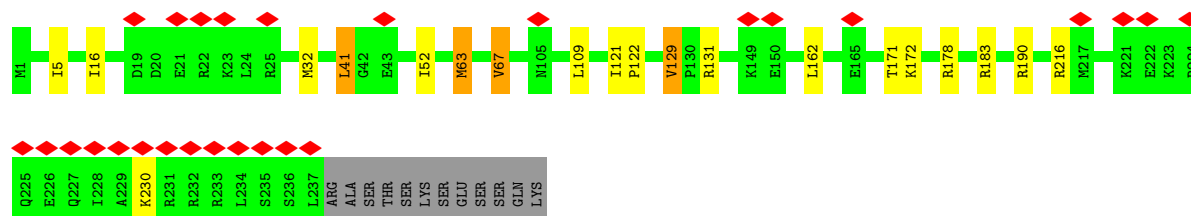
• Molecule 57: uS7

Chain FF:  79% 10% 9%



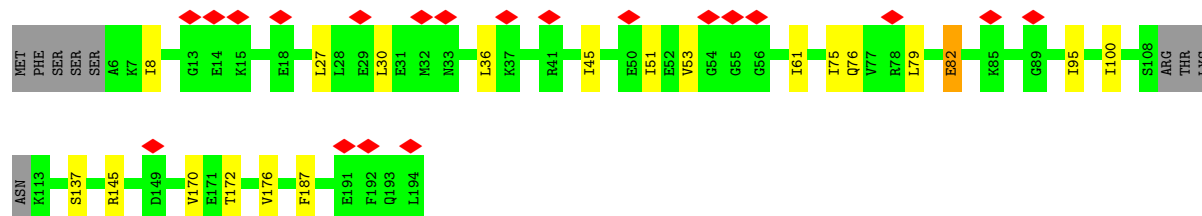
• Molecule 58: eS6

Chain GG:  11% 87% 6% 5%



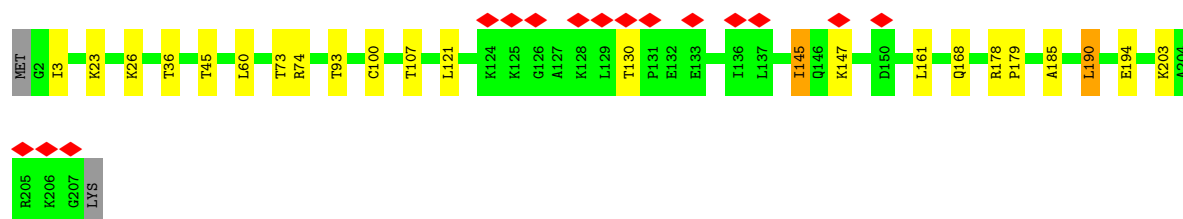
• Molecule 59: eS7

Chain HH:  10% 85% 10% 5%



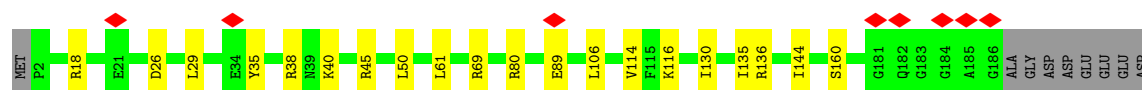
• Molecule 60: eS8

Chain II:  7% 88% 10% 5%

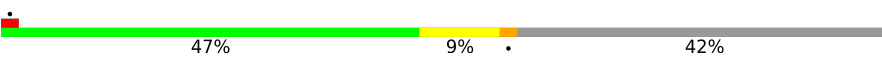


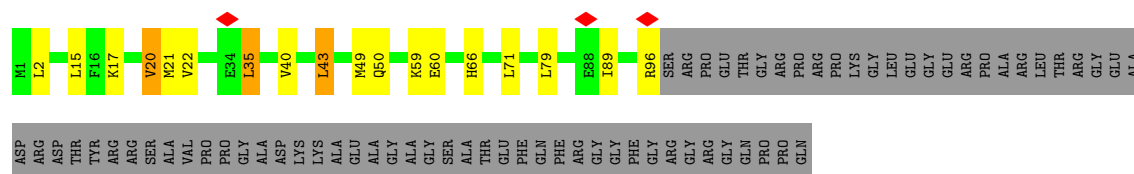
• Molecule 61: uS4

Chain JJ:  85% 10% 5%



• Molecule 62: eS10

Chain KK: 



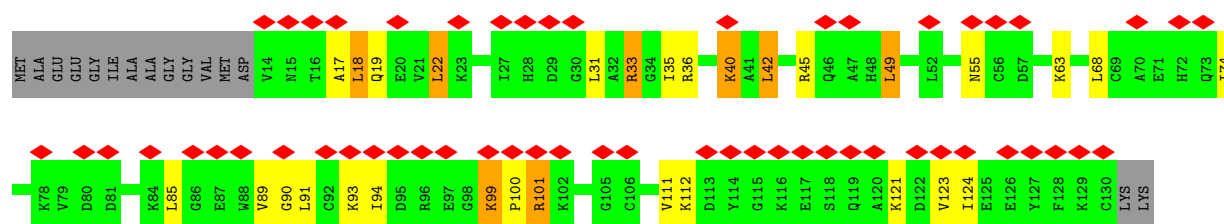
• Molecule 63: uS17

Chain LL: 



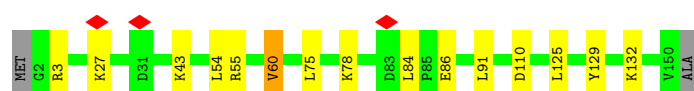
• Molecule 64: eS12

Chain MM: 



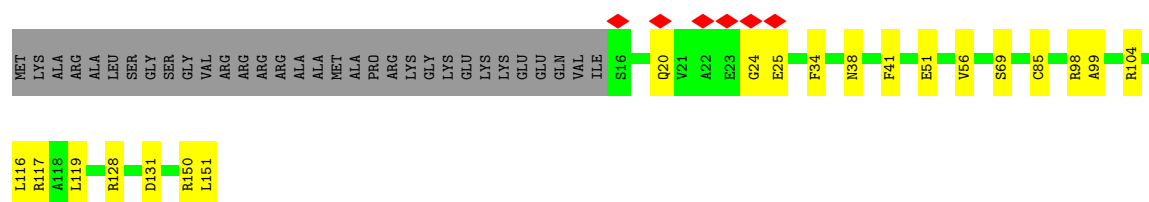
• Molecule 65: uS15

Chain NN: 



• Molecule 66: uS11

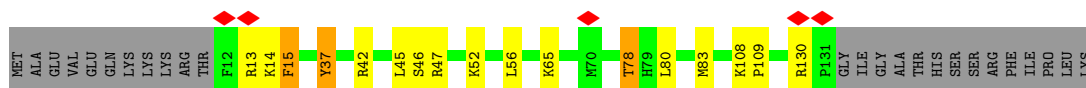
Chain OO: 



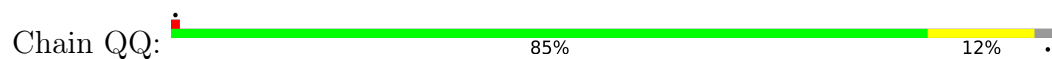
• Molecule 67: uS19

Chain PP: 

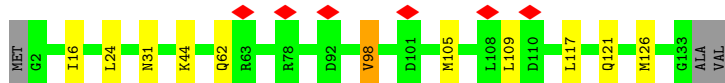




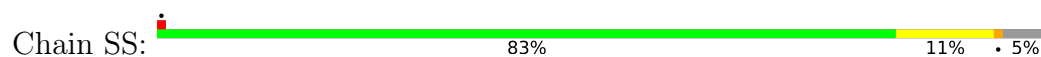
- Molecule 68: uS9



- Molecule 69: eS17



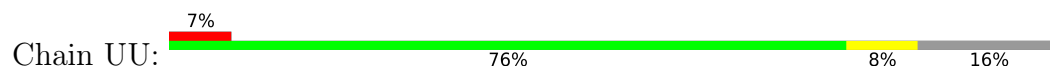
- Molecule 70: uS13



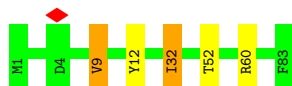
- Molecule 71: eS19



- Molecule 72: uS10



- Molecule 73: eS21



- Molecule 74: uS8

Chain WW:  87% 12% .



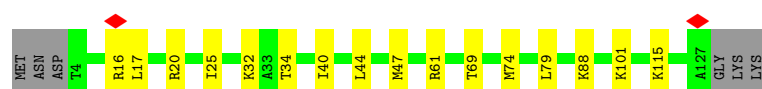
- Molecule 75: uS12

Chain XX:  87% 10% ...



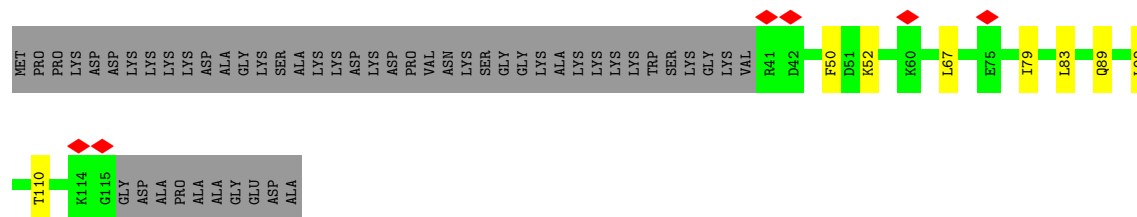
- Molecule 76: eS24

Chain YY:  83% 12% 5%



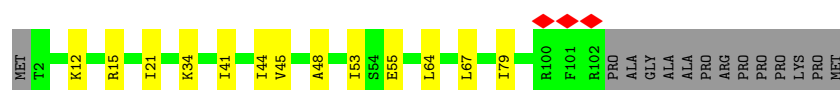
- Molecule 77: eS25

Chain ZZ:  5% 54% 6% 40%

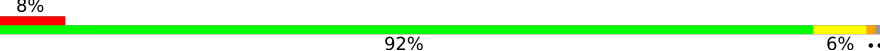


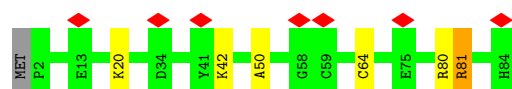
- Molecule 78: eS26

Chain aa:  77% 11% 12%



- Molecule 79: eS27

Chain bb:  8% 92% 6% ..

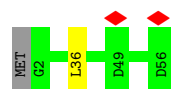


- Molecule 80: eS28

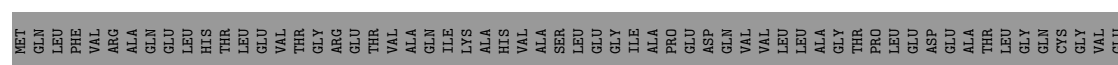
Chain cc:  7% 81% 9% 10%



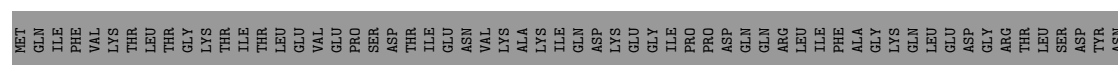
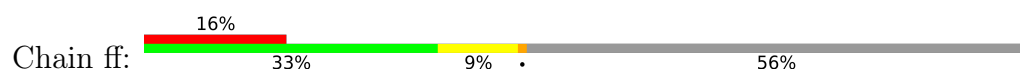
- Molecule 81: uS14



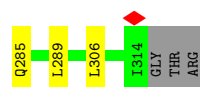
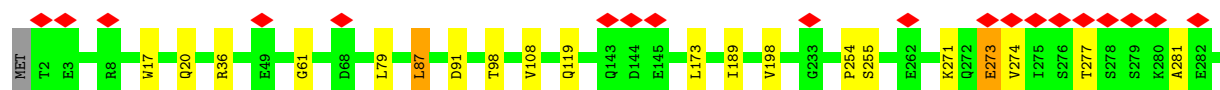
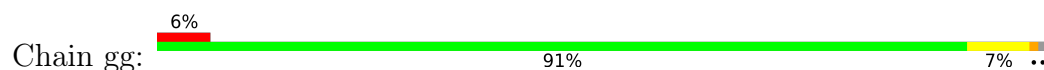
- Molecule 82: eS30



- Molecule 83: eS31



- Molecule 84: RACK1

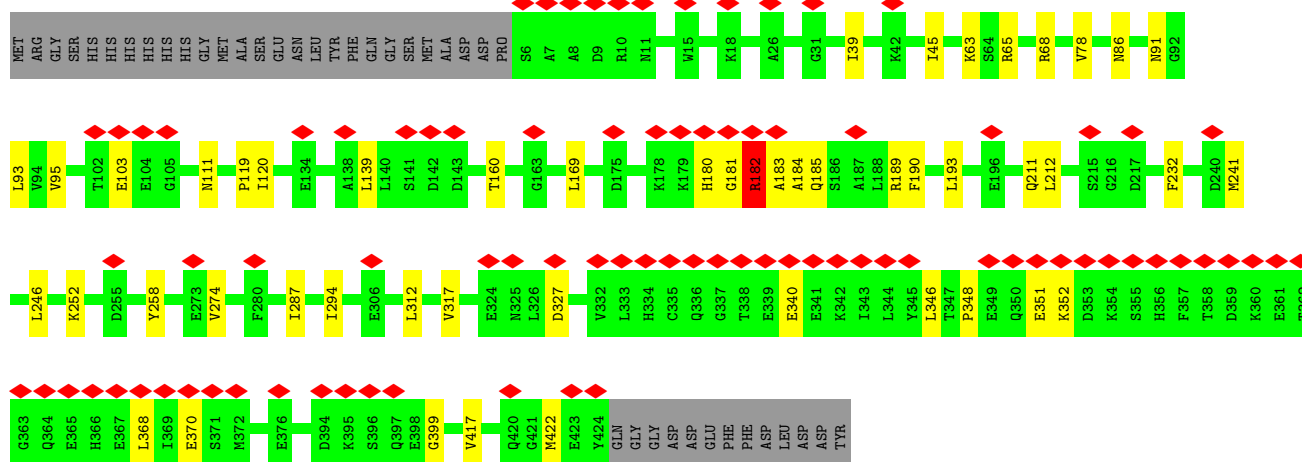
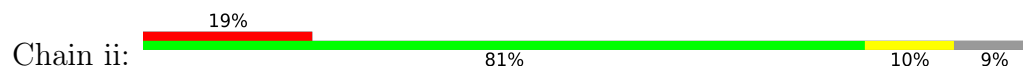


- Molecule 85: mRNA (UGA stop codon)

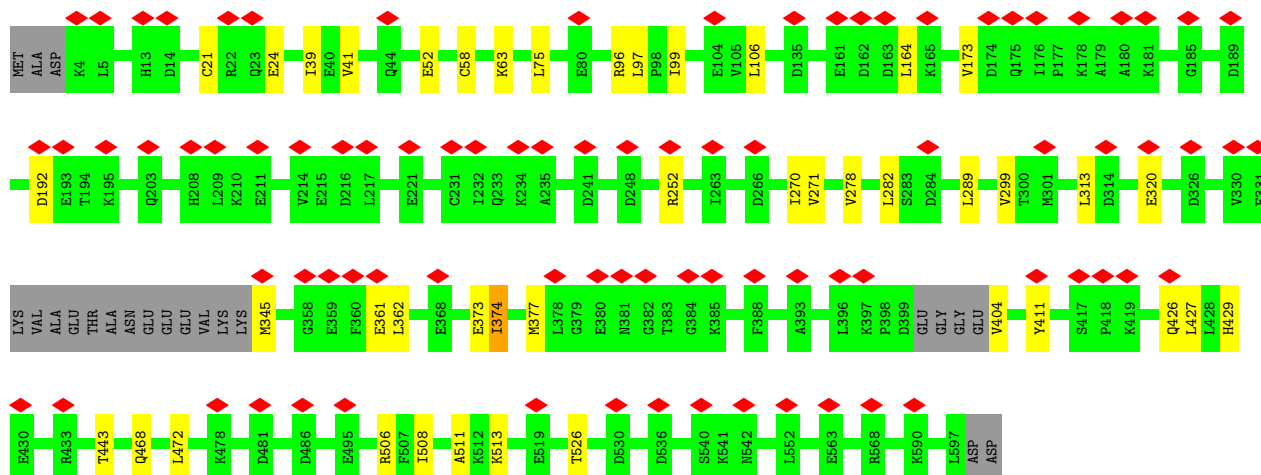
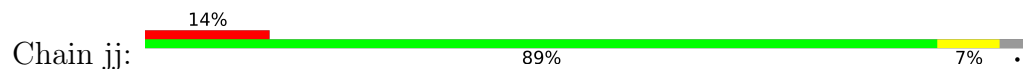




• Molecule 86: eRF1(AAQ)



• Molecule 87: ABCe1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80571	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.749	Depositor
Minimum map value	-0.443	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3399999, 1.3399999, 1.3399999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/1936	0.74	0/2596
2	B	0.50	0/3240	0.70	0/4339
3	C	0.52	0/2937	0.76	0/3946
4	D	0.49	0/2437	0.77	0/3264
5	E	0.53	0/1762	0.73	0/2362
6	F	0.50	0/1911	0.77	0/2549
7	G	0.54	0/1910	0.81	0/2569
8	H	0.51	0/1535	0.72	0/2063
9	I	0.50	0/1702	0.74	0/2272
10	J	0.52	0/1385	0.76	0/1852
11	L	0.53	0/1733	0.81	0/2316
12	M	0.52	0/1158	0.81	0/1547
13	N	0.50	0/1746	0.78	0/2338
14	O	0.53	0/1662	0.82	1/2222 (0.0%)
15	P	0.49	0/1268	0.75	1/1700 (0.1%)
16	Q	0.52	0/1539	0.76	0/2054
17	R	0.52	0/1524	0.82	0/2013
18	S	0.50	0/1501	0.73	1/2012 (0.0%)
19	T	0.51	0/1326	0.72	0/1770
20	U	0.52	0/823	0.70	0/1104
21	V	0.51	0/993	0.73	0/1332
22	W	0.50	0/873	0.79	0/1158
23	X	0.50	0/984	0.73	0/1323
24	Y	0.50	0/1132	0.74	0/1504
25	Z	0.51	0/1130	0.72	0/1507
26	a	0.47	0/1191	0.77	0/1590
27	b	0.49	0/861	0.84	0/1138
28	c	0.49	0/771	0.79	0/1034
29	d	0.52	0/903	0.72	0/1216
30	e	0.51	0/1071	0.75	0/1429
31	f	0.52	0/895	0.68	0/1198
32	g	0.52	0/916	0.78	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.51	0/1021	0.84	0/1348
34	i	0.50	0/841	0.79	0/1112
35	j	0.51	0/720	0.84	0/952
36	k	0.50	0/575	0.72	0/761
37	l	0.51	0/459	0.75	0/608
38	m	0.51	0/435	0.75	0/575
39	n	0.45	0/240	0.86	0/305
40	o	0.50	0/864	0.72	0/1140
41	p	0.50	0/718	0.79	0/953
42	r	0.53	0/1010	0.81	0/1354
43	s	0.55	0/1530	0.76	0/2064
44	t	0.58	0/1174	0.85	0/1582
45	1	0.53	0/129	1.01	2/173 (1.2%)
46	2	0.37	0/1805	0.69	0/2809
47	3	0.37	0/1777	0.70	0/2763
48	5	0.37	1/84974 (0.0%)	0.68	68/132512 (0.1%)
49	7	0.37	0/2858	0.63	0/4455
50	8	0.37	0/3581	0.66	2/5577 (0.0%)
51	9	0.37	1/40524 (0.0%)	0.72	31/63134 (0.0%)
52	AA	0.52	0/1747	0.83	0/2374
53	BB	0.51	1/1756 (0.1%)	0.87	0/2350
54	CC	0.51	0/1753	0.88	0/2369
55	DD	0.54	0/1796	0.86	0/2417
56	EE	0.54	0/2118	0.82	2/2849 (0.1%)
57	FF	0.52	0/1492	0.97	0/2005
58	GG	0.52	0/1946	0.85	1/2590 (0.0%)
59	HH	0.54	0/1510	0.85	0/2022
60	II	0.50	0/1715	0.82	0/2287
61	JJ	0.50	0/1550	0.93	0/2069
62	KK	0.52	0/834	0.88	0/1125
63	LL	0.48	0/1195	0.72	0/1597
64	MM	0.55	0/918	0.98	1/1233 (0.1%)
65	NN	0.51	0/1226	0.93	0/1649
66	OO	0.52	0/1029	0.91	1/1380 (0.1%)
67	PP	0.52	0/1017	0.92	0/1358
68	QQ	0.52	0/1146	0.82	0/1534
69	RR	0.51	0/1082	0.89	0/1452
70	SS	0.53	0/1208	0.90	0/1618
71	TT	0.53	0/1115	0.95	0/1493
72	UU	0.50	0/805	0.87	2/1081 (0.2%)
73	VV	0.53	0/643	0.87	1/860 (0.1%)
74	WW	0.50	0/1051	0.83	0/1406
75	XX	0.48	0/1116	0.83	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	YY	0.51	0/1028	0.84	0/1366
77	ZZ	0.53	0/604	0.91	0/810
78	aa	0.53	0/828	0.86	0/1109
79	bb	0.50	0/665	0.74	1/891 (0.1%)
80	cc	0.51	0/490	0.78	0/656
81	dd	0.52	0/470	0.76	0/623
82	ee	0.50	0/447	0.86	0/587
83	ff	0.49	0/567	0.75	0/753
84	gg	0.50	0/2493	0.72	2/3394 (0.1%)
85	hh	0.37	0/353	0.75	0/547
86	ii	0.52	0/3363	0.88	2/4523 (0.0%)
87	jj	0.51	0/4640	0.84	0/6264
All	All	0.44	3/239706 (0.0%)	0.74	119/350845 (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
48	5	0	4
56	EE	0	1
75	XX	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	1974	U	C2-N3	7.09	1.51	1.37
51	9	1412	C	O3'-P	-6.32	1.51	1.61
53	BB	189	ILE	CA-CB	5.02	1.57	1.54

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1835	A	C2'-C3'-O3'	11.25	126.38	109.50
51	9	1394	G	C2'-C3'-O3'	8.77	126.85	113.70
48	5	385	A	C4'-C3'-O3'	8.60	122.30	109.40
48	5	2474	G	C2'-C3'-O3'	8.39	122.08	109.50
48	5	2046	G	C2'-C3'-O3'	8.37	122.06	109.50
51	9	870	A	C4'-C3'-O3'	8.10	121.54	109.40
51	9	1664	A	C4'-C3'-O3'	7.93	121.29	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	2695	A	C2'-C3'-O3'	7.85	121.28	109.50
48	5	2068	C	C4'-C3'-O3'	7.85	121.17	109.40
48	5	2468	U	C4'-C3'-O3'	7.68	120.93	109.40
48	5	1979	A	C2'-C3'-O3'	7.64	125.16	113.70
51	9	688	U	C2'-C3'-O3'	7.54	120.81	109.50
48	5	498	C	C4'-C3'-O3'	7.52	120.68	109.40
48	5	1174	G	C2'-C3'-O3'	7.50	124.94	113.70
48	5	4942	C	C4'-C3'-O3'	7.19	120.18	109.40
48	5	48	G	C2'-C3'-O3'	7.13	120.19	109.50
48	5	1834	U	C2'-C3'-O3'	7.08	120.13	109.50
51	9	1115	U	C2'-C3'-O3'	7.05	120.08	109.50
14	O	110	PRO	N-CA-C	7.00	119.24	110.70
51	9	72	C	C4'-C3'-O3'	7.00	119.89	109.40
48	5	492	U	C2'-C3'-O3'	6.83	119.74	109.50
72	UU	93	SER	N-CA-C	6.81	114.13	108.07
50	8	124	U	C4'-C3'-O3'	6.71	119.46	109.40
48	5	449	C	C2'-C3'-O3'	6.65	119.47	109.50
48	5	47	A	C4'-C3'-O3'	6.63	119.35	109.40
51	9	874	G	C2'-C3'-O3'	6.62	123.63	113.70
48	5	1358	G	C4'-C3'-O3'	6.50	119.14	109.40
51	9	1646	C	C2'-C3'-O3'	6.42	123.33	113.70
48	5	696	C	C2'-C3'-O3'	6.39	119.09	109.50
48	5	4925	U	C2'-C3'-O3'	6.39	119.08	109.50
48	5	1445	U	C2'-C3'-O3'	6.38	123.28	113.70
48	5	1072	C	C2'-C3'-O3'	6.38	119.07	109.50
48	5	4699	U	C4'-C3'-O3'	6.23	118.75	109.40
48	5	1291	G	C2'-C3'-O3'	6.23	123.05	113.70
51	9	1061	U	C2'-C3'-O3'	-6.17	104.45	113.70
45	1	63	SER	CA-C-N	6.16	127.54	119.84
45	1	63	SER	C-N-CA	6.16	127.54	119.84
48	5	1477	C	C2'-C3'-O3'	6.14	122.91	113.70
48	5	406	C	C2'-C3'-O3'	6.12	122.89	113.70
51	9	1313	A	C4'-C3'-O3'	6.08	118.52	109.40
51	9	1253	A	C2'-C3'-O3'	6.08	118.61	109.50
51	9	752	G	C2'-C3'-O3'	6.03	118.54	109.50
51	9	887	U	C4'-C3'-O3'	-6.01	103.98	113.00
48	5	4232	U	C4'-C3'-O3'	6.00	118.39	109.40
48	5	2661	U	C2'-C3'-O3'	5.98	118.47	109.50
51	9	1520	G	C4'-C3'-O3'	5.96	121.94	113.00
64	MM	35	ILE	N-CA-C	5.96	116.14	110.42
48	5	1329	G	C2'-C3'-O3'	5.87	122.51	113.70
48	5	4075	U	C2'-C3'-O3'	5.84	118.26	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4947	U	C2'-C3'-O3'	5.81	122.41	113.70
48	5	2088	A	C2'-C3'-O3'	5.79	118.18	109.50
51	9	434	G	C2'-C3'-O3'	5.71	122.27	113.70
51	9	873	G	C2'-C3'-O3'	5.66	117.99	109.50
48	5	2089	G	C2'-C3'-O3'	5.64	117.96	109.50
48	5	3888	G	C2'-C3'-O3'	5.63	122.15	113.70
51	9	1395	C	C4'-C3'-O3'	5.63	121.44	113.00
51	9	1130	G	C4'-C3'-O3'	5.60	117.81	109.40
48	5	1370	G	C2'-C3'-O3'	5.59	117.89	109.50
56	EE	108	ARG	N-CA-C	5.59	117.91	110.53
51	9	160	U	C4'-C3'-O3'	5.58	117.76	109.40
48	5	3697	U	C3'-C2'-O2'	5.57	119.05	110.70
51	9	501	C	N1-C1'-C2'	5.56	120.34	112.00
48	5	1211	G	C2'-C3'-O3'	5.53	122.00	113.70
86	ii	370	GLU	N-CA-C	5.53	117.42	110.24
51	9	110	U	C2'-C3'-O3'	5.50	121.94	113.70
48	5	2089	G	C4'-C3'-O3'	5.48	117.62	109.40
48	5	245	C	C2'-C3'-O3'	5.45	121.88	113.70
48	5	3904	G	C4'-C3'-O3'	5.45	117.57	109.40
48	5	484	U	C4'-C3'-O3'	5.42	117.52	109.40
73	VV	9	VAL	N-CA-C	5.38	116.64	112.12
48	5	747	A	C4'-C3'-O3'	5.36	117.44	109.40
48	5	3625	G	C3'-C2'-O2'	5.33	118.69	110.70
51	9	1438	A	C4'-C3'-O3'	-5.32	105.02	113.00
56	EE	133	THR	N-CA-C	5.32	119.25	112.34
84	gg	273	GLU	N-CA-C	5.31	117.15	111.36
48	5	1818	G	C3'-C2'-O2'	5.29	118.64	110.70
48	5	4448	G	C4'-C3'-O3'	5.27	120.91	113.00
48	5	4232	U	C2'-C3'-O3'	5.26	117.39	109.50
15	P	37	LYS	N-CA-C	5.26	117.01	111.28
48	5	4170	A	C3'-C2'-O2'	5.25	118.58	110.70
48	5	1835	G	C2'-C3'-O3'	5.25	117.38	109.50
51	9	532	C	C2'-C3'-O3'	5.25	121.57	113.70
48	5	1455	G	C3'-C2'-O2'	5.23	118.54	110.70
48	5	959	G	C2'-C3'-O3'	5.22	117.34	109.50
48	5	930	G	C3'-C2'-O2'	5.22	118.53	110.70
48	5	480	C	C2'-C3'-O3'	5.22	121.53	113.70
48	5	2313	A	C4'-C3'-O3'	5.22	117.23	109.40
48	5	278	G	C4'-C3'-O3'	5.22	117.22	109.40
51	9	690	G	C2'-C3'-O3'	-5.20	105.91	113.70
72	UU	72	GLU	N-CA-C	5.19	117.64	107.57
51	9	1438	A	N9-C1'-C2'	5.18	119.76	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	24	C	C4'-C3'-O3'	-5.17	105.25	113.00
48	5	2313	A	C2'-C3'-O3'	5.16	117.24	109.50
79	bb	50	ALA	N-CA-C	5.16	116.98	111.36
66	OO	24	GLY	N-CA-C	5.15	118.91	112.73
48	5	485	C	C3'-C2'-O2'	5.15	118.42	110.70
48	5	275	C	C2'-C3'-O3'	5.15	121.42	113.70
51	9	1679	A	C4'-C3'-O3'	5.14	117.12	109.40
48	5	2265	G	C4'-C3'-O3'	5.14	117.11	109.40
48	5	1238	A	C3'-C2'-O2'	5.12	118.39	110.70
48	5	4119	C	C3'-C2'-O2'	5.12	118.38	110.70
48	5	2266	C	C4'-C3'-O3'	5.11	117.07	109.40
48	5	3603	G	C4'-C3'-O3'	-5.11	105.33	113.00
51	9	1532	C	C4'-C3'-O3'	-5.11	105.34	113.00
48	5	1921	C	C2'-C3'-O3'	5.10	117.15	109.50
51	9	553	U	C2'-C3'-O3'	5.07	121.31	113.70
48	5	125	C	C3'-C2'-O2'	5.06	118.29	110.70
48	5	4884	G	C3'-C2'-O2'	5.05	118.28	110.70
48	5	1440	U	C3'-C2'-O2'	5.05	118.27	110.70
58	GG	67	VAL	CB-CA-C	5.05	116.38	110.88
50	8	94	G	C2'-C3'-O3'	5.03	117.05	109.50
48	5	4124	G	C4'-C3'-O3'	5.03	116.95	109.40
18	S	34	ALA	N-CA-C	5.03	112.75	108.22
84	gg	274	VAL	N-CA-C	5.03	115.25	110.42
51	9	690	G	C4'-C3'-O3'	5.02	120.53	113.00
48	5	480	C	C3'-C2'-O2'	5.01	118.22	110.70
48	5	1633	G	C2'-C3'-O3'	-5.01	106.19	113.70
48	5	3603	G	C2'-C3'-O3'	5.01	121.21	113.70
86	ii	182	ARG	N-CA-C	5.01	121.46	110.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	5	1974	U	Sidechain
48	5	1986	U	Sidechain
48	5	2002	A	Sidechain
48	5	2013	A	Sidechain
56	EE	155	LYS	Peptide
75	XX	61	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1898	0	1993	5	0
2	B	3172	0	3310	4	0
3	C	2883	0	3053	2	0
4	D	2391	0	2424	1	0
5	E	1729	0	1887	3	0
6	F	1875	0	1995	3	0
7	G	1879	0	2027	3	0
8	H	1516	0	1597	1	0
9	I	1664	0	1712	0	0
10	J	1362	0	1399	3	0
11	L	1702	0	1820	2	0
12	M	1137	0	1211	3	0
13	N	1701	0	1749	2	0
14	O	1630	0	1778	8	0
15	P	1242	0	1274	0	0
16	Q	1515	0	1634	1	0
17	R	1508	0	1664	6	0
18	S	1462	0	1508	5	0
19	T	1298	0	1366	2	0
20	U	809	0	833	0	0
21	V	979	0	1039	2	0
22	W	860	0	903	2	0
23	X	967	0	1040	2	0
24	Y	1115	0	1205	1	0
25	Z	1107	0	1182	0	0
26	a	1162	0	1209	1	0
27	b	848	0	920	0	0
28	c	761	0	794	1	0
29	d	888	0	930	0	0
30	e	1053	0	1147	1	0
31	f	876	0	912	2	0
32	g	906	0	999	0	0
33	h	1013	0	1147	2	0
34	i	830	0	916	0	0
35	j	705	0	737	0	0
36	k	569	0	637	0	0
37	l	447	0	480	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	m	429	0	466	0	0
39	n	239	0	289	3	0
40	o	851	0	920	4	0
41	p	708	0	756	0	0
42	r	994	0	1051	0	0
43	s	1507	0	1564	1	0
44	t	1160	0	1218	4	0
45	1	125	0	117	2	0
46	2	1616	0	824	6	0
47	3	1593	0	811	6	0
48	5	75972	0	38391	148	0
49	7	2558	0	1296	0	0
50	8	3208	0	1629	1	0
51	9	36249	0	18316	163	0
52	AA	1710	0	1708	5	0
53	BB	1729	0	1803	12	0
54	CC	1716	0	1806	10	0
55	DD	1768	0	1866	8	0
56	EE	2076	0	2177	16	0
57	FF	1471	0	1522	12	0
58	GG	1923	0	2089	8	0
59	HH	1488	0	1582	5	0
60	II	1686	0	1772	9	0
61	JJ	1525	0	1640	7	0
62	KK	810	0	836	6	0
63	LL	1175	0	1249	5	0
64	MM	908	0	939	23	0
65	NN	1202	0	1289	4	0
66	OO	1016	0	1039	5	0
67	PP	997	0	1045	6	0
68	QQ	1128	0	1195	8	0
69	RR	1068	0	1121	3	0
70	SS	1190	0	1249	4	0
71	TT	1097	0	1132	5	0
72	UU	795	0	862	2	0
73	VV	636	0	637	3	0
74	WW	1034	0	1080	6	0
75	XX	1098	0	1167	7	0
76	YY	1011	0	1083	2	0
77	ZZ	598	0	656	5	0
78	aa	814	0	864	7	0
79	bb	651	0	672	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	cc	488	0	514	5	0
81	dd	459	0	451	0	0
82	ee	443	0	492	0	0
83	ff	555	0	566	18	0
84	gg	2436	0	2393	9	0
85	hh	317	0	161	1	0
86	ii	3309	0	3350	31	0
87	jj	4555	0	4691	16	0
88	5	197	0	0	0	0
88	7	7	0	0	0	0
88	8	5	0	0	0	0
88	9	79	0	0	0	0
88	B	1	0	0	0	0
88	I	1	0	0	0	0
88	L	1	0	0	0	0
88	P	1	0	0	0	0
88	Q	1	0	0	0	0
88	V	1	0	0	0	0
88	a	2	0	0	0	0
88	e	1	0	0	0	0
88	g	1	0	0	0	0
88	hh	1	0	0	0	0
88	j	1	0	0	0	0
89	aa	1	0	0	0	0
89	dd	1	0	0	0	0
89	ff	1	0	0	2	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	jj	16	0	0	3	0
All	All	223874	0	168777	552	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 1.

All (552) 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)
48:5:3914:U:O4	48:5:4378:A:N1	1.58	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1986:U:C2	48:5:2006:U:O4	1.82	1.32
51:9:1137:U:O4	51:9:1148:A:N1	1.70	1.24
48:5:1986:U:O2	48:5:2006:U:C4	1.91	1.23
48:5:1986:U:O2	48:5:2006:U:O4	1.57	1.20
48:5:2367:A:N1	48:5:2788:U:O4	1.73	1.19
51:9:1137:U:C4	51:9:1148:A:N1	2.12	1.17
48:5:1986:U:O4	48:5:2014:C:N4	1.83	1.11
48:5:2367:A:N6	48:5:2788:U:H3	1.51	1.08
51:9:1407:U:H2'	51:9:1408:U:C6	1.91	1.06
48:5:1986:U:H2'	48:5:2007:G:O6	1.56	1.02
48:5:77:U:O4	48:5:336:A:N1	1.99	0.96
64:MM:40:LYS:HE3	83:ff:130:VAL:HG22	1.49	0.95
51:9:1137:U:O4	51:9:1148:A:C2	2.20	0.94
48:5:3914:U:H3	48:5:4378:A:N6	1.66	0.92
51:9:872:A:N1	51:9:914:U:O4	2.05	0.89
51:9:885:U:O2'	51:9:886:A:O5'	1.89	0.88
83:ff:126:CYS:SG	83:ff:143:LYS:NZ	2.49	0.86
48:5:2367:A:H61	48:5:2788:U:H3	0.87	0.85
48:5:3810:C:N3	86:ii:258:TYR:OH	2.09	0.85
48:5:1986:U:O2	48:5:2006:U:C5	2.31	0.84
51:9:1407:U:O2'	51:9:1408:U:O4'	1.96	0.84
51:9:1137:U:O4	51:9:1148:A:C6	2.32	0.82
48:5:2367:A:N6	48:5:2788:U:N3	2.17	0.82
51:9:688:U:O2'	51:9:689:U:OP2	1.99	0.81
83:ff:144:CYS:SG	89:ff:200:ZN:ZN	1.68	0.81
48:5:3914:U:C4	48:5:4378:A:N1	2.48	0.80
48:5:3914:U:O4	48:5:4378:A:C2	2.35	0.80
48:5:2013:A:C2	48:5:2014:C:C2	2.70	0.79
48:5:3914:U:N3	48:5:4378:A:N6	2.27	0.79
53:BB:182:LYS:O	53:BB:186:ASN:ND2	2.15	0.78
51:9:872:A:N1	51:9:914:U:C4	2.52	0.78
48:5:1974:U:N3	48:5:2002:A:C6	2.52	0.78
64:MM:40:LYS:CE	83:ff:130:VAL:HG22	2.14	0.77
87:jj:21:CYS:HG	90:jj:601:SF4:FE2	0.99	0.77
51:9:530:U:H5''	51:9:530:U:H6	1.49	0.77
51:9:1137:U:C4	51:9:1148:A:C6	2.74	0.76
64:MM:101:ARG:HA	64:MM:101:ARG:CZ	2.16	0.75
48:5:3766:A:N1	51:9:1827:U:O2'	2.19	0.73
83:ff:144:CYS:HG	89:ff:200:ZN:ZN	0.98	0.72
87:jj:58:CYS:SG	90:jj:600:SF4:FE4	1.81	0.72
87:jj:21:CYS:SG	90:jj:601:SF4:FE2	1.80	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:EE:122:LYS:HG2	56:EE:162:ILE:HD11	1.73	0.71
51:9:1679:A:OP1	80:cc:20:ARG:NH2	2.23	0.71
48:5:2005:G:N2	48:5:2014:C:O2	2.17	0.71
51:9:1095:U:O4	51:9:1149:A:N1	2.24	0.70
48:5:2367:A:N1	48:5:2788:U:C4	2.60	0.69
51:9:530:U:H5''	51:9:530:U:C6	2.27	0.69
51:9:203:G:OP2	60:II:147:LYS:NZ	2.22	0.68
48:5:1986:U:C2'	48:5:2007:G:O6	2.39	0.68
51:9:1401:A:C2	51:9:1402:A:C6	2.83	0.68
56:EE:139:LEU:HD12	56:EE:150:PRO:HB3	1.76	0.67
56:EE:122:LYS:CG	56:EE:162:ILE:HD11	2.24	0.67
51:9:1137:U:N3	51:9:1148:A:N6	2.43	0.67
48:5:3810:C:C4	86:ii:258:TYR:OH	2.47	0.66
62:KK:15:LEU:HD22	62:KK:49:MET:HE1	1.78	0.66
48:5:4548:A:N1	86:ii:183:ALA:HB2	2.11	0.66
11:L:169:ILE:HD13	26:a:142:GLY:HA2	1.78	0.65
48:5:1974:U:N3	48:5:2002:A:N6	2.44	0.65
48:5:2007:G:C2	48:5:2013:A:N6	2.65	0.65
51:9:1091:C:HO2'	74:WW:2:VAL:N	1.96	0.64
57:FF:68:ILE:HD12	57:FF:112:LEU:HD22	1.80	0.64
48:5:1978:C:H3'	48:5:1979:A:H5''	1.79	0.63
48:5:2013:A:C2	48:5:2014:C:N1	2.66	0.63
51:9:1438:A:H2'	51:9:1439:A:C8	2.33	0.63
48:5:4744:A:N1	48:5:4956:A:N1	2.46	0.63
48:5:4213:A:N1	48:5:4218:U:O4	2.32	0.63
48:5:1974:U:O2	48:5:2002:A:N7	2.32	0.63
53:BB:189:ILE:HG22	53:BB:190:PRO:HD3	1.81	0.63
51:9:872:A:C6	51:9:914:U:O4	2.52	0.62
48:5:4723:A:H2'	48:5:4724:A:C8	2.34	0.62
51:9:1407:U:O2	51:9:1408:U:C2	2.53	0.62
86:ii:78:VAL:HG23	86:ii:95:VAL:HG11	1.82	0.62
64:MM:22:LEU:HD11	64:MM:89:VAL:HA	1.80	0.61
48:5:2409:U:C4	48:5:2783:A:N1	2.68	0.61
48:5:1986:U:N3	48:5:2013:A:N6	2.48	0.61
64:MM:17:ALA:C	64:MM:124:ILE:HD11	2.25	0.61
86:ii:327:ASP:HB3	86:ii:348:PRO:HG3	1.83	0.61
48:5:1986:U:C4	48:5:2013:A:N6	2.69	0.61
83:ff:130:VAL:HG11	83:ff:143:LYS:NZ	2.17	0.60
51:9:872:A:C6	51:9:914:U:C4	2.90	0.59
51:9:1412:C:H5''	51:9:1412:C:H6	1.66	0.59
54:CC:209:VAL:HG21	54:CC:233:LEU:CD1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1986:U:C4	48:5:2014:C:N4	2.70	0.59
86:ii:327:ASP:HB3	86:ii:348:PRO:CG	2.32	0.59
40:o:41:TYR:CD1	47:3:75:C:O2	2.56	0.58
48:5:3712:A:C2	51:9:970:G:C6	2.92	0.58
48:5:3629:A:C1'	51:9:1721:U:O2	2.51	0.58
48:5:3629:A:H4'	51:9:1721:U:O2	2.04	0.58
65:NN:125:LEU:HD22	65:NN:129:TYR:CE2	2.39	0.58
51:9:980:A:H2'	51:9:981:A:C8	2.39	0.58
67:PP:56:LEU:HD13	67:PP:78:THR:HG21	1.86	0.58
84:gg:87:LEU:HD21	84:gg:108:VAL:HG11	1.85	0.58
48:5:4699:U:N3	48:5:4701:A:N6	2.51	0.57
51:9:1546:G:H5'	68:QQ:18:THR:HG21	1.85	0.57
77:ZZ:79:ILE:HB	77:ZZ:83:LEU:HD12	1.86	0.57
55:DD:70:THR:HG22	55:DD:86:LEU:HD13	1.85	0.57
48:5:3629:A:C4'	51:9:1721:U:O2	2.52	0.57
48:5:1986:U:H2'	48:5:2007:G:C6	2.37	0.57
51:9:1149:A:N3	51:9:1149:A:H2'	2.20	0.57
12:M:97:ALA:HB2	14:O:203:VAL:HB	1.86	0.57
22:W:80:ARG:NH2	58:GG:129:VAL:O	2.38	0.57
51:9:1117:C:O2'	51:9:1118:C:O4'	2.23	0.57
51:9:1444:U:P	68:QQ:15:ARG:HH22	2.28	0.56
46:2:74:C:OP2	48:5:4548:A:H2'	2.04	0.56
51:9:1458:G:P	84:gg:281:ALA:HB2	2.45	0.56
46:2:16:C:O4'	46:2:16:C:O2	2.24	0.56
51:9:945:U:H2'	51:9:946:U:C6	2.40	0.56
48:5:77:U:N3	48:5:336:A:N6	2.44	0.56
48:5:2007:G:O2'	48:5:2012:A:N6	2.39	0.56
48:5:3712:A:C2	51:9:970:G:C5	2.94	0.56
69:RR:16:ILE:HG22	69:RR:24:LEU:HD11	1.88	0.56
48:5:1974:U:C4	48:5:2002:A:N6	2.73	0.56
28:c:20:LEU:HD21	65:NN:43:LYS:O	2.06	0.56
48:5:3810:C:O4'	48:5:3810:C:O2	2.23	0.56
61:JJ:136:ARG:HD3	61:JJ:160:SER:HA	1.87	0.56
51:9:830:A:N1	51:9:844:U:O4	2.40	0.55
83:ff:121:CYS:SG	83:ff:146:LEU:HD23	2.47	0.55
48:5:245:C:O4'	48:5:245:C:O2	2.24	0.55
51:9:183:G:O2'	51:9:184:G:O5'	2.21	0.55
64:MM:63:LYS:CD	83:ff:108:VAL:HG21	2.36	0.55
48:5:1483:C:O2	48:5:1483:C:O4'	2.23	0.55
48:5:2505:C:O2	48:5:2505:C:O4'	2.24	0.55
51:9:94:G:HO2'	51:9:508:A:HO2'	1.51	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4699:U:C4	48:5:4701:A:N6	2.75	0.55
48:5:1974:U:N3	48:5:2002:A:C5	2.73	0.55
51:9:501:C:H2'	51:9:501:C:O2	2.06	0.55
64:MM:33:ARG:NH2	64:MM:91:LEU:HD21	2.22	0.55
48:5:4548:A:C2	86:ii:182:ARG:HB2	2.42	0.55
61:JJ:35:TYR:CD2	61:JJ:106:LEU:HD23	2.42	0.55
80:cc:20:ARG:HG2	80:cc:20:ARG:HH11	1.72	0.54
76:YY:34:THR:HG23	76:YY:69:THR:HG21	1.89	0.54
48:5:3810:C:C4	86:ii:258:TYR:CZ	2.96	0.54
51:9:853:C:O4'	51:9:853:C:O2	2.26	0.54
51:9:1139:C:O4'	51:9:1139:C:O2	2.25	0.54
64:MM:22:LEU:HD21	64:MM:89:VAL:HG23	1.89	0.54
6:F:227:VAL:HA	18:S:39:VAL:HG12	1.90	0.54
39:n:21:ARG:HH22	51:9:1175:G:P	2.31	0.54
48:5:4887:C:C5'	48:5:4887:C:H6	2.21	0.54
56:EE:139:LEU:HD12	56:EE:150:PRO:CB	2.38	0.54
60:II:190:LEU:HD12	60:II:194:GLU:HB3	1.89	0.54
84:gg:254:PRO:HA	84:gg:285:GLN:HA	1.88	0.54
53:BB:82:ARG:NH1	53:BB:189:ILE:O	2.40	0.53
64:MM:63:LYS:HD2	83:ff:108:VAL:HG21	1.90	0.53
57:FF:92:ILE:HD13	57:FF:169:ILE:HG21	1.90	0.53
48:5:2627:C:O4'	48:5:2627:C:O2	2.25	0.53
51:9:92:A:O4'	56:EE:3:ARG:NH1	2.42	0.53
48:5:4723:A:C2	48:5:4724:A:C6	2.97	0.53
44:t:30:PRO:HA	86:ii:422:MET:HE3	1.89	0.53
51:9:1130:G:H2'	51:9:1130:G:N3	2.24	0.53
51:9:1315:U:O2	51:9:1315:U:O4'	2.27	0.53
75:XX:51:VAL:HG13	75:XX:70:VAL:CG1	2.39	0.53
39:n:4:LYS:HE2	51:9:1844:U:O4	2.09	0.53
51:9:1444:U:H2'	51:9:1445:U:C6	2.43	0.53
17:R:74:ARG:NH2	48:5:2891:U:OP2	2.42	0.53
51:9:1611:G:OP2	70:SS:121:ARG:NH1	2.39	0.53
57:FF:99:ILE:HG23	77:ZZ:67:LEU:HD21	1.90	0.53
51:9:455:A:O2'	51:9:1735:A:N3	2.40	0.53
48:5:4989:U:O2	48:5:4989:U:O4'	2.28	0.52
74:WW:6:VAL:HG13	74:WW:29:PRO:HB2	1.90	0.52
77:ZZ:50:PHE:CE2	77:ZZ:83:LEU:HD11	2.44	0.52
48:5:498:C:O2	48:5:498:C:O4'	2.27	0.52
56:EE:137:PRO:HB2	56:EE:150:PRO:HD2	1.90	0.52
51:9:501:C:O2	51:9:501:C:C2'	2.57	0.52
61:JJ:130:ILE:HG12	61:JJ:135:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:159:ARG:NH1	48:5:4940:C:OP1	2.42	0.52
54:CC:261:PHE:HB2	73:VV:52:THR:HG21	1.91	0.52
64:MM:101:ARG:HA	64:MM:101:ARG:NE	2.25	0.52
59:HH:61:ILE:HD11	59:HH:95:ILE:HD12	1.91	0.52
51:9:531:A:H3'	51:9:532:C:H5''	1.90	0.52
54:CC:209:VAL:HG21	54:CC:233:LEU:HD13	1.92	0.52
47:3:16:C:O2	47:3:16:C:O4'	2.24	0.52
51:9:1364:U:O4'	51:9:1364:U:O2	2.28	0.52
84:gg:277:THR:HB	84:gg:281:ALA:HB3	1.92	0.52
51:9:94:G:O2'	51:9:508:A:O2'	2.24	0.52
51:9:1137:U:H3	51:9:1148:A:N6	2.07	0.51
80:cc:14:VAL:HG13	80:cc:30:VAL:HG13	1.92	0.51
51:9:4:C:O2'	61:JJ:18:ARG:NH1	2.43	0.51
75:XX:84:PHE:HB2	75:XX:118:VAL:HG11	1.90	0.51
18:S:164:LYS:HB3	18:S:165:PRO:HD3	1.93	0.51
48:5:224:U:O2	48:5:224:U:O4'	2.28	0.51
48:5:1168:G:C2	48:5:1194:G:O6	2.63	0.51
51:9:17:C:O2'	51:9:1194:A:N1	2.40	0.51
37:l:2:SER:HB3	48:5:2407:G:O6	2.10	0.51
50:8:125:C:O2	50:8:125:C:O4'	2.28	0.51
87:jj:252:ARG:HD3	87:jj:278:VAL:HG21	1.93	0.51
48:5:4548:A:C2	86:ii:182:ARG:C	2.89	0.51
56:EE:44:LEU:HD13	56:EE:72:ILE:HD11	1.92	0.50
21:V:99:GLU:HB3	22:W:24:THR:HG23	1.92	0.50
48:5:2763:U:O2	48:5:2763:U:O4'	2.29	0.50
76:YY:25:ILE:HD11	76:YY:44:LEU:HD21	1.93	0.50
64:MM:49:LEU:HB3	64:MM:111:VAL:CG2	2.42	0.50
51:9:17:C:H2'	51:9:18:C:C6	2.47	0.50
66:OO:117:ARG:HE	78:aa:48:ALA:HB1	1.77	0.50
45:1:66:LEU:HD12	48:5:3908:A:C2	2.46	0.50
17:R:163:ARG:NH1	51:9:871:U:C4	2.79	0.50
48:5:2013:A:N3	48:5:2014:C:C6	2.80	0.50
51:9:1109:C:H42	69:RR:126:MET:HB3	1.76	0.50
48:5:1237:C:O2	48:5:1237:C:O4'	2.29	0.50
40:o:4:VAL:O	40:o:94:GLY:N	2.45	0.49
47:3:76:A:C2	48:5:4370:G:C6	2.99	0.49
48:5:1974:U:C2	48:5:2002:A:N7	2.80	0.49
48:5:2409:U:O4	48:5:2783:A:N1	2.46	0.49
51:9:823:U:O2	51:9:823:U:O4'	2.30	0.49
58:GG:32:MET:HE2	58:GG:63:MET:HG2	1.94	0.49
51:9:872:A:N6	51:9:914:U:C4	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1118:C:H2'	51:9:1119:A:C8	2.47	0.49
51:9:1863:A:H1'	78:aa:79:ILE:HD13	1.94	0.49
51:9:993:G:O6	78:aa:15:ARG:HG2	2.13	0.49
51:9:1130:G:HO2'	51:9:1131:G:C5'	2.26	0.49
62:KK:35:LEU:HD13	62:KK:40:VAL:HG21	1.95	0.49
69:RR:98:VAL:HG21	69:RR:117:LEU:HD22	1.94	0.48
86:ii:160:THR:HG23	86:ii:169:LEU:HD11	1.95	0.48
48:5:1986:U:C2	48:5:2006:U:C4	2.72	0.48
54:CC:88:ILE:HG21	54:CC:94:ILE:CD1	2.43	0.48
48:5:1174:G:C2'	48:5:1175:A:O5'	2.61	0.48
51:9:399:C:O2	63:LL:106:HIS:ND1	2.46	0.48
86:ii:312:LEU:HD13	86:ii:317:VAL:HG21	1.95	0.48
87:jj:271:VAL:HG21	87:jj:282:LEU:HD13	1.95	0.48
48:5:4548:A:H1'	86:ii:180:HIS:NE2	2.27	0.48
48:5:4548:A:H2	86:ii:182:ARG:C	2.21	0.48
67:PP:15:PHE:CE1	67:PP:109:PRO:HB3	2.48	0.48
83:ff:121:CYS:SG	83:ff:132:MET:HE3	2.53	0.48
48:5:1175:A:C2	48:5:1187:G:N7	2.82	0.48
51:9:302:A:H1'	60:II:73:THR:HG23	1.95	0.48
51:9:943:U:H2'	51:9:944:A:O4'	2.13	0.48
54:CC:130:ILE:HG22	54:CC:158:ALA:HB1	1.95	0.48
2:B:252:ALA:HB1	48:5:4524:G:N3	2.28	0.48
44:t:98:ILE:HG23	44:t:98:ILE:O	2.14	0.48
51:9:1438:A:C2	51:9:1439:A:C6	3.02	0.48
60:II:36:THR:HG21	60:II:179:PRO:HB2	1.94	0.48
51:9:1395:C:H2'	51:9:1396:A:N3	2.29	0.48
48:5:4548:A:C2	86:ii:181:GLY:O	2.67	0.48
48:5:4600:G:P	87:jj:506:ARG:HH22	2.37	0.48
51:9:302:A:H1'	60:II:73:THR:CG2	2.43	0.48
51:9:872:A:N6	51:9:914:U:C5	2.82	0.48
39:n:4:LYS:CE	51:9:1844:U:O4	2.62	0.48
61:JJ:114:VAL:HG21	61:JJ:135:ILE:CD1	2.44	0.48
66:OO:116:LEU:HD22	78:aa:53:ILE:HD11	1.95	0.48
74:WW:52:ILE:HG22	74:WW:61:ILE:HG12	1.96	0.48
31:f:29:LYS:NZ	48:5:1919:G:O6	2.45	0.47
48:5:4530:U:O3'	86:ii:182:ARG:O	2.32	0.47
51:9:690:G:O5'	51:9:690:G:H8	1.97	0.47
51:9:885:U:O2'	51:9:886:A:P	2.71	0.47
51:9:979:C:C4	51:9:980:A:N7	2.82	0.47
51:9:1546:G:C5'	68:QQ:18:THR:HG21	2.44	0.47
59:HH:27:LEU:HD13	59:HH:45:ILE:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:OO:98:ARG:NH1	66:OO:99:ALA:O	2.47	0.47
10:J:64:ARG:HD3	46:2:56:C:O4'	2.13	0.47
17:R:176:ARG:NH1	51:9:909:G:OP1	2.46	0.47
63:LL:101:ARG:HB2	75:XX:10:ALA:HB2	1.96	0.47
64:MM:36:ARG:CZ	64:MM:40:LYS:HZ1	2.28	0.47
48:5:4579:U:H2'	48:5:4580:U:C6	2.48	0.47
48:5:4724:A:C6	48:5:4725:C:C4	3.03	0.47
51:9:1129:G:C6	51:9:1130:G:O6	2.67	0.47
51:9:1551:U:O2	51:9:1551:U:O4'	2.31	0.47
64:MM:90:GLY:HA2	64:MM:93:LYS:HG3	1.94	0.47
8:H:105:ILE:CD1	8:H:136:VAL:HG23	2.45	0.47
48:5:1381:U:O2	48:5:1381:U:O4'	2.29	0.47
51:9:1520:G:H2'	51:9:1520:G:N3	2.30	0.47
54:CC:137:VAL:HG21	54:CC:244:ILE:HD12	1.97	0.47
61:JJ:130:ILE:CG1	61:JJ:135:ILE:HD11	2.45	0.47
14:O:72:HIS:N	48:5:4586:G:OP1	2.44	0.47
45:1:57:ARG:NH2	48:5:3862:A:O2'	2.47	0.47
48:5:4600:G:OP1	87:jj:506:ARG:NH2	2.41	0.47
51:9:1834:A:C2	51:9:1836:G:C4	3.03	0.47
57:FF:71:ARG:HG2	57:FF:151:ILE:HD13	1.96	0.47
57:FF:151:ILE:O	57:FF:155:CYS:HB2	2.15	0.47
64:MM:22:LEU:HD13	64:MM:22:LEU:C	2.40	0.47
10:J:27:GLY:HA2	10:J:68:ILE:HG23	1.95	0.47
48:5:2007:G:N3	48:5:2013:A:N6	2.62	0.47
48:5:4699:U:N3	48:5:4701:A:C6	2.83	0.47
51:9:944:A:C5	51:9:945:U:C5	3.03	0.47
63:LL:104:LYS:O	75:XX:11:ARG:NH2	2.48	0.47
74:WW:75:ILE:HD11	74:WW:93:LEU:HD11	1.97	0.47
1:A:101:VAL:HB	1:A:165:VAL:HG12	1.97	0.47
14:O:12:ARG:O	18:S:171:ARG:NH2	2.48	0.47
48:5:3712:A:N1	51:9:970:G:C6	2.83	0.47
51:9:1543:U:OP2	71:TT:62:ARG:NH1	2.48	0.47
10:J:33:LEU:HD21	10:J:70:VAL:HB	1.96	0.47
12:M:112:VAL:HG11	14:O:201:LEU:HD11	1.96	0.46
48:5:1194:G:C2	48:5:1195:G:H1'	2.51	0.46
51:9:1016:U:OP2	79:bb:20:LYS:NZ	2.46	0.46
51:9:1143:A:C2	51:9:1144:A:C2	3.03	0.46
5:E:95:VAL:CG2	5:E:112:LEU:HD21	2.45	0.46
48:5:1301:C:O2	48:5:1301:C:O4'	2.33	0.46
51:9:1351:G:O2'	51:9:1378:A:N1	2.43	0.46
68:QQ:49:TYR:O	68:QQ:53:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4942:C:H4'	48:5:4943:A:OP1	2.16	0.46
51:9:183:G:O2'	51:9:183:G:N3	2.48	0.46
51:9:1095:U:O2	51:9:1151:G:N2	2.49	0.46
48:5:77:U:C4	48:5:336:A:N1	2.80	0.46
48:5:1563:A:O2'	48:5:1564:A:O4'	2.34	0.46
51:9:1624:U:O2	51:9:1624:U:O4'	2.32	0.46
56:EE:19:MET:HE3	56:EE:108:ARG:HD3	1.96	0.46
51:9:1303:C:O2	51:9:1303:C:O4'	2.31	0.46
68:QQ:34:VAL:HG21	68:QQ:84:ILE:HD12	1.97	0.46
68:QQ:51:LEU:HD22	68:QQ:84:ILE:HD11	1.98	0.46
2:B:324:GLY:HA2	48:5:5051:C:H4'	1.96	0.46
48:5:4452:U:O2'	86:ii:185:GLN:HG3	2.15	0.46
51:9:1336:C:H2'	51:9:1337:C:O4'	2.16	0.46
71:TT:60:THR:HG23	71:TT:75:MET:HE2	1.98	0.46
18:S:164:LYS:HB3	18:S:165:PRO:CD	2.46	0.46
64:MM:19:GLN:HA	64:MM:19:GLN:NE2	2.30	0.46
60:II:60:LEU:HD23	60:II:185:ALA:HB2	1.98	0.46
1:A:207:VAL:HG12	48:5:3919:C:H5''	1.98	0.46
48:5:4602:A:OP1	87:jj:443:THR:HG21	2.16	0.46
51:9:1489:A:H4'	51:9:1490:G:OP2	2.16	0.46
64:MM:36:ARG:NH1	64:MM:40:LYS:HZ1	2.13	0.46
51:9:146:G:O2'	51:9:147:A:O5'	2.29	0.45
51:9:1834:A:H2'	51:9:1834:A:N3	2.31	0.45
52:AA:63:ARG:CG	52:AA:185:MET:HE1	2.46	0.45
43:s:34:ASN:ND2	43:s:34:ASN:O	2.50	0.45
51:9:1568:C:OP1	71:TT:96:SER:OG	2.32	0.45
53:BB:189:ILE:HB	53:BB:190:PRO:CD	2.47	0.45
59:HH:170:VAL:HG13	59:HH:187:PHE:HB2	1.99	0.45
64:MM:121:LYS:HA	64:MM:124:ILE:HD12	1.99	0.45
75:XX:81:ILE:CG2	75:XX:120:PHE:CD1	3.00	0.45
84:gg:255:SER:HB3	84:gg:271:LYS:HG2	1.98	0.45
87:jj:96:ARG:O	87:jj:299:VAL:HB	2.16	0.45
30:e:44:ARG:NH2	48:5:1312:A:O2'	2.49	0.45
46:2:53:G:C2	46:2:62:C:C2	3.05	0.45
48:5:77:U:O4	48:5:336:A:C2	2.69	0.45
48:5:4758:U:O2	48:5:4758:U:O4'	2.34	0.45
51:9:1401:A:C2	51:9:1402:A:N1	2.85	0.45
58:GG:162:LEU:HD11	58:GG:172:LYS:HB2	1.98	0.45
60:II:194:GLU:HA	63:LL:10:TYR:CE2	2.52	0.45
83:ff:130:VAL:HG21	83:ff:143:LYS:HE3	1.98	0.45
86:ii:120:ILE:HG22	86:ii:139:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:173:ARG:NH2	51:9:910:G:OP2	2.50	0.45
54:CC:94:ILE:HG13	54:CC:162:ILE:HD11	1.98	0.45
44:t:85:LEU:HD11	44:t:141:CYS:SG	2.57	0.45
51:9:846:G:H2'	56:EE:19:MET:HE2	1.98	0.45
51:9:953:C:H2'	51:9:954:U:O4'	2.16	0.45
51:9:1531:A:H2'	51:9:1532:C:C6	2.51	0.45
51:9:1407:U:H2'	51:9:1408:U:H6	1.66	0.45
57:FF:102:LEU:HD22	77:ZZ:110:THR:HG21	1.98	0.45
87:jj:374:ILE:HG12	87:jj:508:ILE:HD13	1.98	0.45
24:Y:55:VAL:HG13	24:Y:104:VAL:HG13	1.99	0.45
47:3:76:A:C6	48:5:4370:G:C5	3.05	0.45
55:DD:72:VAL:HG23	62:KK:20:VAL:HG21	1.99	0.45
17:R:71:ARG:NH1	48:5:3605:C:OP2	2.50	0.45
51:9:183:G:N3	51:9:183:G:C2'	2.79	0.45
48:5:1990:A:H3'	48:5:1991:A:H5''	1.99	0.44
51:9:434:G:H2'	51:9:435:A:C8	2.52	0.44
19:T:80:VAL:HG21	48:5:4305:G:C6	2.52	0.44
59:HH:30:LEU:HD22	59:HH:82:GLU:HG2	1.99	0.44
83:ff:126:CYS:HB3	83:ff:143:LYS:CE	2.47	0.44
87:jj:106:LEU:HD22	87:jj:270:ILE:HG23	1.98	0.44
48:5:2007:G:N2	48:5:2013:A:H62	2.15	0.44
48:5:2007:G:H5''	48:5:2007:G:H8	1.82	0.44
53:BB:134:LEU:CD2	53:BB:218:LEU:HD12	2.47	0.44
48:5:921:C:O2'	48:5:922:C:C5'	2.65	0.44
86:ii:39:ILE:HD12	86:ii:93:LEU:HD23	2.00	0.44
48:5:4548:A:N7	86:ii:190:PHE:CE2	2.86	0.44
51:9:1458:G:OP2	84:gg:281:ALA:HB2	2.18	0.44
66:OO:34:PHE:HB3	66:OO:41:PHE:HB2	2.00	0.44
75:XX:81:ILE:HG21	75:XX:120:PHE:CD1	2.52	0.44
48:5:1974:U:O2	48:5:2002:A:C8	2.71	0.44
51:9:831:G:N2	51:9:844:U:O2	2.50	0.44
51:9:1518:C:O2	51:9:1518:C:O5'	2.35	0.44
48:5:921:C:O2'	48:5:922:C:H5'	2.18	0.44
48:5:4119:C:O2	48:5:4119:C:O4'	2.35	0.44
51:9:1207:G:C6	51:9:1837:G:C6	3.06	0.44
55:DD:21:LEU:HD21	55:DD:48:ILE:HD11	2.00	0.44
87:jj:99:ILE:N	87:jj:99:ILE:HD12	2.32	0.44
48:5:1973:G:C2	48:5:2002:A:N6	2.86	0.43
48:5:2367:A:C2	48:5:2788:U:O4	2.59	0.43
51:9:1458:G:OP1	84:gg:281:ALA:HB2	2.18	0.43
54:CC:191:VAL:HG11	54:CC:236:PHE:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:314:U:O2	51:9:314:U:H2'	2.18	0.43
66:OO:116:LEU:HD22	78:aa:53:ILE:CD1	2.48	0.43
80:cc:14:VAL:HG22	80:cc:30:VAL:HG11	2.00	0.43
87:jj:39:ILE:HG22	87:jj:41:VAL:HG23	1.99	0.43
46:2:33:U:OP2	68:QQ:146:ARG:NH2	2.52	0.43
48:5:4452:U:H2'	86:ii:184:ALA:HB1	1.99	0.43
48:5:4887:C:H6	48:5:4887:C:H5''	1.81	0.43
64:MM:19:GLN:HA	64:MM:19:GLN:HE21	1.83	0.43
83:ff:126:CYS:HB3	83:ff:143:LYS:HE2	2.00	0.43
48:5:1173:G:C6	48:5:1174:G:C6	3.07	0.43
48:5:3810:C:N4	86:ii:258:TYR:OH	2.52	0.43
51:9:407:G:H3'	51:9:408:A:C5'	2.47	0.43
51:9:1274:G:N7	62:KK:43:LEU:HD13	2.33	0.43
53:BB:189:ILE:CB	53:BB:190:PRO:CD	2.96	0.43
55:DD:162:ASP:N	55:DD:163:PRO:CD	2.81	0.43
62:KK:40:VAL:HG23	62:KK:40:VAL:O	2.18	0.43
64:MM:19:GLN:HE21	64:MM:19:GLN:CA	2.32	0.43
64:MM:42:LEU:HG	64:MM:74:ILE:HD13	2.00	0.43
1:A:207:VAL:HG12	48:5:3919:C:C5'	2.48	0.43
51:9:427:U:O2	51:9:427:U:O4'	2.34	0.43
48:5:496:G:C4	48:5:659:G:N2	2.87	0.43
51:9:92:A:C6	51:9:446:G:C6	3.06	0.43
51:9:1035:A:H2'	51:9:1036:A:O4'	2.17	0.43
56:EE:132:GLY:N	56:EE:136:ILE:O	2.51	0.43
57:FF:41:VAL:HG11	57:FF:113:VAL:HG21	2.00	0.43
18:S:161:ARG:HG3	18:S:161:ARG:O	2.19	0.43
23:X:82:THR:HG21	33:h:37:THR:HG22	2.00	0.43
53:BB:52:THR:HG23	53:BB:57:ILE:HA	2.00	0.43
83:ff:121:CYS:SG	83:ff:122:PRO:HD2	2.59	0.43
14:O:54:TYR:CD1	14:O:145:VAL:HG21	2.54	0.43
48:5:1773:U:C5	48:5:1774:C:C5	3.07	0.43
2:B:84:MET:HE1	2:B:183:ILE:HD11	2.01	0.43
51:9:584:A:C6	51:9:585:C:C4	3.07	0.43
51:9:846:G:OP2	56:EE:108:ARG:NH1	2.51	0.43
51:9:910:G:C2	51:9:911:C:C2	3.07	0.43
51:9:1089:G:C6	51:9:1090:C:C4	3.07	0.43
58:GG:5:ILE:HD12	58:GG:16:ILE:HD13	2.00	0.43
64:MM:18:LEU:N	64:MM:124:ILE:HD11	2.34	0.43
70:SS:43:VAL:HG21	70:SS:83:PHE:CZ	2.53	0.43
40:o:104:ILE:HG21	46:2:56:C:N4	2.34	0.43
48:5:2094:C:O2	48:5:2094:C:O4'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:CC:196:ILE:HB	54:CC:223:TYR:HB2	1.99	0.43
62:KK:71:LEU:HD21	62:KK:79:LEU:HD12	2.01	0.43
11:L:18:TRP:CE3	13:N:198:LEU:HD12	2.54	0.42
14:O:23:VAL:HG13	14:O:33:VAL:HG11	2.00	0.42
48:5:4942:C:H3'	48:5:4942:C:O2	2.19	0.42
51:9:488:U:O2	51:9:488:U:O4'	2.34	0.42
51:9:872:A:C2	51:9:914:U:O4	2.70	0.42
51:9:1395:C:H2'	51:9:1396:A:O4'	2.19	0.42
4:D:41:LYS:NZ	19:T:30:TYR:O	2.39	0.42
56:EE:125:LYS:HA	56:EE:159:THR:HG22	2.01	0.42
60:II:194:GLU:HG2	63:LL:10:TYR:CD1	2.54	0.42
84:gg:91:ASP:HB2	84:gg:98:THR:HG23	2.01	0.42
48:5:1773:U:C4	48:5:1774:C:C4	3.08	0.42
48:5:4423:U:O2	48:5:4423:U:O4'	2.38	0.42
51:9:1220:A:N6	51:9:1221:G:C6	2.88	0.42
56:EE:163:ASP:HB3	56:EE:166:THR:HG22	2.01	0.42
75:XX:61:GLN:HB3	75:XX:62:PRO:CD	2.48	0.42
7:G:317:LYS:HD2	53:BB:225:LEU:HB3	2.02	0.42
51:9:1120:U:H2'	51:9:1121:G:H8	1.85	0.42
51:9:1666:C:H2'	51:9:1667:U:O4'	2.19	0.42
53:BB:87:ILE:HG23	53:BB:101:HIS:CG	2.54	0.42
5:E:165:VAL:HG11	5:E:178:VAL:HG13	2.00	0.42
13:N:89:VAL:HG13	48:5:3928:A:H5'	2.01	0.42
21:V:26:ILE:HG22	21:V:101:ASN:HB3	2.00	0.42
83:ff:116:ARG:HD3	83:ff:120:GLU:OE2	2.19	0.42
87:jj:511:ALA:HB1	87:jj:513:LYS:HD2	2.02	0.42
52:AA:63:ARG:HG2	52:AA:185:MET:HE1	2.02	0.42
51:9:1293:A:N6	51:9:1294:G:C6	2.88	0.42
57:FF:20:PHE:CD1	57:FF:20:PHE:C	2.97	0.42
67:PP:37:TYR:OH	67:PP:45:LEU:HD11	2.20	0.42
6:F:89:ALA:HB2	6:F:124:LEU:HD21	2.01	0.42
14:O:84:VAL:HG11	14:O:102:LEU:HD22	2.01	0.42
40:o:41:TYR:CG	47:3:75:C:O2	2.72	0.42
51:9:962:A:N1	51:9:1055:A:O2'	2.53	0.42
51:9:1046:U:H2'	51:9:1047:C:O4'	2.20	0.42
51:9:1445:U:O4	51:9:1446:A:N6	2.53	0.42
51:9:1834:A:N3	51:9:1834:A:C2'	2.82	0.42
55:DD:21:LEU:CD2	55:DD:48:ILE:HD11	2.50	0.42
57:FF:116:ILE:HD12	57:FF:151:ILE:HG13	2.02	0.42
58:GG:52:ILE:HD11	58:GG:109:LEU:HD22	2.01	0.42
85:hh:54:U:O2	85:hh:54:U:C2'	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:79:PHE:CD1	33:h:36:VAL:HG21	2.55	0.42
51:9:168:C:OP1	58:GG:131:ARG:NH2	2.53	0.42
51:9:944:A:C2	51:9:983:A:C2	3.07	0.42
51:9:1488:C:O2'	51:9:1490:G:OP2	2.36	0.42
53:BB:189:ILE:HB	53:BB:190:PRO:HD2	2.02	0.42
59:HH:51:ILE:HD11	59:HH:176:VAL:HG22	2.02	0.42
3:C:150:LEU:HB3	3:C:151:PRO:HD3	2.01	0.42
47:3:10:G:N2	47:3:11:C:C2	2.88	0.42
51:9:885:U:HO2'	51:9:886:A:P	2.42	0.42
51:9:1535:U:H2'	51:9:1535:U:O2	2.19	0.42
51:9:1619:A:OP2	67:PP:47:ARG:NH1	2.49	0.42
53:BB:189:ILE:CG2	53:BB:190:PRO:HD3	2.49	0.42
55:DD:11:PHE:CE2	72:UU:84:ILE:HD11	2.55	0.42
55:DD:11:PHE:CZ	72:UU:84:ILE:HD11	2.55	0.42
56:EE:147:ILE:HD11	56:EE:162:ILE:CG2	2.50	0.42
57:FF:125:SER:OG	57:FF:136:ARG:NH2	2.53	0.42
78:aa:45:VAL:HG11	78:aa:53:ILE:HD13	2.01	0.41
7:G:98:ILE:HG21	48:5:4125:C:H4'	2.03	0.41
48:5:1563:A:N7	51:9:678:U:O4'	2.54	0.41
48:5:1973:G:N1	48:5:2002:A:N6	2.69	0.41
51:9:1438:A:C2	51:9:1439:A:C2	3.08	0.41
51:9:1719:A:N6	51:9:1814:G:O2'	2.53	0.41
52:AA:180:ARG:HG2	52:AA:195:TRP:CE3	2.55	0.41
48:5:3810:C:N3	86:ii:258:TYR:CZ	2.89	0.41
51:9:1228:A:H2'	51:9:1229:G:C8	2.55	0.41
3:C:232:VAL:HG12	3:C:263:LEU:CD1	2.50	0.41
48:5:4530:U:O2'	86:ii:183:ALA:C	2.63	0.41
51:9:190:G:H5''	60:II:145:ILE:CD1	2.49	0.41
56:EE:105:THR:HG23	56:EE:106:LYS:HD2	2.01	0.41
1:A:11:GLY:O	48:5:3675:G:N2	2.51	0.41
48:5:1174:G:H2'	48:5:1175:A:O5'	2.21	0.41
48:5:1818:G:O2'	48:5:1819:G:OP1	2.31	0.41
51:9:1374:C:H2'	51:9:1375:G:O4'	2.19	0.41
51:9:1412:C:H6	51:9:1412:C:C5'	2.33	0.41
86:ii:294:ILE:O	87:jj:63:LYS:NZ	2.53	0.41
2:B:77:THR:HG21	2:B:337:VAL:HG22	2.03	0.41
48:5:4305:G:N3	48:5:4305:G:C2'	2.84	0.41
51:9:688:U:HO2'	51:9:689:U:P	2.32	0.41
51:9:824:C:C2	61:JJ:144:ILE:HD13	2.56	0.41
51:9:1520:G:N3	51:9:1520:G:C2'	2.83	0.41
87:jj:426:GLN:HA	87:jj:429:HIS:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:29:LYS:CE	48:5:1919:G:O6	2.69	0.41
58:GG:121:ILE:HG13	58:GG:122:PRO:HD2	2.02	0.41
67:PP:15:PHE:CD1	67:PP:15:PHE:C	2.97	0.41
86:ii:252:LYS:HD2	86:ii:274:VAL:HG21	2.03	0.41
51:9:830:A:H2'	51:9:831:G:O4'	2.19	0.41
51:9:1409:A:H5'	51:9:1410:C:OP2	2.20	0.41
52:AA:145:ILE:HG12	52:AA:159:ILE:CG2	2.51	0.41
65:NN:54:LEU:HB3	65:NN:60:VAL:HG13	2.02	0.41
16:Q:78:LYS:HG2	16:Q:137:VAL:HG23	2.03	0.41
48:5:3629:A:H1'	51:9:1721:U:O2	2.19	0.41
51:9:1045:U:H2'	51:9:1046:U:O4'	2.21	0.41
51:9:1518:C:O2	51:9:1518:C:O4'	2.38	0.41
65:NN:91:LEU:HD12	65:NN:125:LEU:HD12	2.03	0.41
84:gg:173:LEU:HD22	84:gg:189:ILE:HG12	2.03	0.41
6:F:88:LEU:HD22	6:F:89:ALA:N	2.36	0.41
7:G:215:ASP:HB3	7:G:216:PRO:HD3	2.02	0.41
51:9:1674:G:N7	68:QQ:17:LYS:NZ	2.60	0.41
55:DD:48:ILE:HG23	55:DD:86:LEU:HD12	2.03	0.41
56:EE:31:PRO:HG2	56:EE:38:LEU:HD12	2.03	0.41
71:TT:39:LEU:HD11	71:TT:52:TRP:CZ3	2.55	0.41
78:aa:45:VAL:HG22	78:aa:64:LEU:HD13	2.03	0.41
48:5:4895:C:O2	48:5:4895:C:C2'	2.69	0.40
51:9:1286:G:OP1	83:ff:99:LYS:HG3	2.21	0.40
64:MM:33:ARG:HH22	64:MM:89:VAL:HG21	1.86	0.40
80:cc:20:ARG:HH11	80:cc:20:ARG:CG	2.32	0.40
86:ii:346:LEU:HD23	86:ii:351:GLU:HA	2.02	0.40
12:M:112:VAL:CG1	14:O:201:LEU:HD11	2.51	0.40
44:t:141:CYS:SG	44:t:142:ASN:N	2.93	0.40
48:5:2013:A:C2	48:5:2014:C:C6	3.09	0.40
48:5:4440:G:OP2	86:ii:189:ARG:HD3	2.21	0.40
51:9:668:A:N1	51:9:1143:A:C5	2.89	0.40
51:9:958:G:H2'	51:9:959:G:O4'	2.22	0.40
53:BB:133:TYR:CE2	53:BB:181:LEU:HD12	2.56	0.40
54:CC:261:PHE:CB	73:VV:52:THR:HG21	2.50	0.40
57:FF:39:ILE:HG23	57:FF:68:ILE:HG21	2.02	0.40
57:FF:99:ILE:HD13	57:FF:171:GLU:HA	2.03	0.40
74:WW:28:ARG:CB	74:WW:29:PRO:HD3	2.51	0.40
83:ff:130:VAL:HG11	83:ff:143:LYS:HZ1	1.86	0.40
1:A:234:LYS:HG2	1:A:238:ILE:HD12	2.03	0.40
17:R:163:ARG:NH1	51:9:871:U:C5	2.90	0.40
48:5:1563:A:C8	51:9:678:U:C4'	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:415:A:H2'	51:9:416:U:O4'	2.21	0.40
48:5:3723:A:C2	48:5:3724:A:C6	3.09	0.40
51:9:412:G:O2'	51:9:812:A:N6	2.54	0.40
64:MM:99:LYS:HD3	64:MM:100:PRO:HD2	2.03	0.40
71:TT:18:LEU:HB3	71:TT:58:ALA:HB1	2.02	0.40
74:WW:55:ASP:O	74:WW:57:ARG:N	2.55	0.40
83:ff:122:PRO:HD2	83:ff:146:LEU:HD23	2.03	0.40
86:ii:91:ASN:HA	86:ii:119:PRO:HA	2.03	0.40
86:ii:287:ILE:HD13	86:ii:399:GLY:HA2	2.03	0.40
48:5:747:A:H4'	48:5:748:G:OP1	2.22	0.40
48:5:4530:U:H4'	86:ii:182:ARG:HA	2.03	0.40
51:9:1439:A:C6	51:9:1440:C:C4	3.10	0.40
52:AA:163:CYS:SG	52:AA:174:MET:HE2	2.62	0.40
58:GG:41:LEU:C	58:GG:41:LEU:HD22	2.47	0.40
67:PP:52:LYS:HE3	67:PP:80:LEU:HD21	2.03	0.40
70:SS:3:LEU:HB3	77:ZZ:50:PHE:CD2	2.56	0.40
70:SS:15:VAL:HG22	70:SS:68:ILE:HD11	2.04	0.40
73:VV:32:ILE:HD12	73:VV:60:ARG:HD2	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	A	246/257 (96%)	224 (91%)	21 (8%)	1 (0%)	30	58
2	B	392/403 (97%)	365 (93%)	26 (7%)	1 (0%)	36	63
3	C	360/425 (85%)	339 (94%)	21 (6%)	0	100	100
4	D	291/297 (98%)	277 (95%)	14 (5%)	0	100	100
5	E	208/291 (72%)	193 (93%)	15 (7%)	0	100	100
6	F	223/247 (90%)	213 (96%)	9 (4%)	1 (0%)	30	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	229/319 (72%)	220 (96%)	9 (4%)	0	100	100
8	H	188/192 (98%)	177 (94%)	11 (6%)	0	100	100
9	I	201/214 (94%)	184 (92%)	17 (8%)	0	100	100
10	J	168/178 (94%)	160 (95%)	8 (5%)	0	100	100
11	L	208/211 (99%)	201 (97%)	7 (3%)	0	100	100
12	M	136/218 (62%)	128 (94%)	8 (6%)	0	100	100
13	N	201/204 (98%)	189 (94%)	12 (6%)	0	100	100
14	O	197/203 (97%)	184 (93%)	13 (7%)	0	100	100
15	P	151/184 (82%)	141 (93%)	10 (7%)	0	100	100
16	Q	185/188 (98%)	175 (95%)	10 (5%)	0	100	100
17	R	178/196 (91%)	173 (97%)	5 (3%)	0	100	100
18	S	174/176 (99%)	164 (94%)	10 (6%)	0	100	100
19	T	157/160 (98%)	150 (96%)	7 (4%)	0	100	100
20	U	97/128 (76%)	86 (89%)	11 (11%)	0	100	100
21	V	129/140 (92%)	115 (89%)	14 (11%)	0	100	100
22	W	102/157 (65%)	97 (95%)	5 (5%)	0	100	100
23	X	116/156 (74%)	107 (92%)	9 (8%)	0	100	100
24	Y	132/145 (91%)	123 (93%)	9 (7%)	0	100	100
25	Z	133/136 (98%)	127 (96%)	4 (3%)	2 (2%)	8	29
26	a	145/148 (98%)	135 (93%)	10 (7%)	0	100	100
27	b	100/245 (41%)	93 (93%)	5 (5%)	2 (2%)	6	24
28	c	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
29	d	105/125 (84%)	95 (90%)	10 (10%)	0	100	100
30	e	126/135 (93%)	118 (94%)	8 (6%)	0	100	100
31	f	107/110 (97%)	101 (94%)	4 (4%)	2 (2%)	6	25
32	g	112/117 (96%)	106 (95%)	6 (5%)	0	100	100
33	h	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
34	i	100/105 (95%)	94 (94%)	6 (6%)	0	100	100
35	j	84/97 (87%)	78 (93%)	5 (6%)	1 (1%)	10	33
36	k	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
37	l	48/51 (94%)	44 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	m	50/102 (49%)	47 (94%)	3 (6%)	0	100	100
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	102/106 (96%)	99 (97%)	3 (3%)	0	100	100
41	p	89/92 (97%)	82 (92%)	7 (8%)	0	100	100
42	r	122/137 (89%)	114 (93%)	7 (6%)	1 (1%)	16	44
43	s	194/318 (61%)	176 (91%)	16 (8%)	2 (1%)	12	38
44	t	151/165 (92%)	136 (90%)	13 (9%)	2 (1%)	9	32
45	l	13/15 (87%)	8 (62%)	4 (31%)	1 (8%)	1	5
52	AA	215/295 (73%)	201 (94%)	13 (6%)	1 (0%)	24	52
53	BB	211/264 (80%)	201 (95%)	9 (4%)	1 (0%)	24	52
54	CC	219/293 (75%)	209 (95%)	10 (5%)	0	100	100
55	DD	226/243 (93%)	214 (95%)	9 (4%)	3 (1%)	9	32
56	EE	260/263 (99%)	246 (95%)	14 (5%)	0	100	100
57	FF	181/204 (89%)	171 (94%)	10 (6%)	0	100	100
58	GG	235/249 (94%)	221 (94%)	14 (6%)	0	100	100
59	HH	181/194 (93%)	171 (94%)	10 (6%)	0	100	100
60	II	204/208 (98%)	195 (96%)	8 (4%)	1 (0%)	24	52
61	JJ	183/194 (94%)	176 (96%)	7 (4%)	0	100	100
62	KK	94/165 (57%)	88 (94%)	6 (6%)	0	100	100
63	LL	139/158 (88%)	127 (91%)	12 (9%)	0	100	100
64	MM	115/132 (87%)	104 (90%)	11 (10%)	0	100	100
65	NN	147/151 (97%)	140 (95%)	7 (5%)	0	100	100
66	OO	134/168 (80%)	122 (91%)	11 (8%)	1 (1%)	18	46
67	PP	118/145 (81%)	108 (92%)	10 (8%)	0	100	100
68	QQ	140/146 (96%)	131 (94%)	9 (6%)	0	100	100
69	RR	130/135 (96%)	120 (92%)	10 (8%)	0	100	100
70	SS	142/152 (93%)	135 (95%)	7 (5%)	0	100	100
71	TT	139/145 (96%)	132 (95%)	7 (5%)	0	100	100
72	UU	98/119 (82%)	91 (93%)	7 (7%)	0	100	100
73	VV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
74	WW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	XX	139/143 (97%)	130 (94%)	6 (4%)	3 (2%)	5	23
76	YY	122/130 (94%)	113 (93%)	9 (7%)	0	100	100
77	ZZ	73/125 (58%)	68 (93%)	5 (7%)	0	100	100
78	aa	99/115 (86%)	93 (94%)	6 (6%)	0	100	100
79	bb	81/84 (96%)	71 (88%)	9 (11%)	1 (1%)	10	33
80	cc	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
81	dd	53/56 (95%)	49 (92%)	4 (8%)	0	100	100
82	ee	53/133 (40%)	50 (94%)	3 (6%)	0	100	100
83	ff	66/156 (42%)	61 (92%)	5 (8%)	0	100	100
84	gg	311/317 (98%)	290 (93%)	20 (6%)	1 (0%)	36	63
86	ii	417/459 (91%)	404 (97%)	12 (3%)	1 (0%)	43	70
87	jj	571/599 (95%)	538 (94%)	32 (6%)	1 (0%)	43	70
All	All	12520/14448 (87%)	11763 (94%)	727 (6%)	30 (0%)	44	70

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
75	XX	62	PRO
86	ii	182	ARG
43	s	142	GLY
44	t	125	LEU
52	AA	159	ILE
66	OO	20	GLN
75	XX	61	GLN
1	A	234	LYS
25	Z	91	LEU
27	b	102	PRO
53	BB	225	LEU
55	DD	48	ILE
75	XX	86	PRO
2	B	17	LEU
31	f	106	TYR
44	t	54	LYS
25	Z	90	PRO
27	b	29	TYR
43	s	25	PRO
55	DD	44	THR
79	bb	81	ARG

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Mol	Chain	Res	Type
87	jj	24	GLU
42	r	11	ARG
55	DD	93	THR
84	gg	61	GLY
45	l	64	PRO
6	F	196	VAL
35	j	38	GLY
31	f	107	PRO
60	II	3	ILE

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	A	190/199 (96%)	178 (94%)	12 (6%)	16	43
2	B	342/348 (98%)	326 (95%)	16 (5%)	23	50
3	C	302/347 (87%)	288 (95%)	14 (5%)	24	50
4	D	247/250 (99%)	237 (96%)	10 (4%)	28	53
5	E	190/251 (76%)	182 (96%)	8 (4%)	26	52
6	F	196/215 (91%)	189 (96%)	7 (4%)	31	56
7	G	200/272 (74%)	190 (95%)	10 (5%)	22	49
8	H	169/171 (99%)	158 (94%)	11 (6%)	15	42
9	I	175/181 (97%)	169 (97%)	6 (3%)	32	58
10	J	143/149 (96%)	137 (96%)	6 (4%)	26	52
11	L	175/176 (99%)	170 (97%)	5 (3%)	37	60
12	M	117/161 (73%)	113 (97%)	4 (3%)	32	58
13	N	171/172 (99%)	164 (96%)	7 (4%)	27	53
14	O	171/173 (99%)	162 (95%)	9 (5%)	20	48
15	P	134/163 (82%)	128 (96%)	6 (4%)	24	51
16	Q	164/165 (99%)	159 (97%)	5 (3%)	36	60
17	R	159/175 (91%)	148 (93%)	11 (7%)	14	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	S	157/157 (100%)	150 (96%)	7 (4%)	24	51
19	T	139/140 (99%)	131 (94%)	8 (6%)	18	45
20	U	89/114 (78%)	88 (99%)	1 (1%)	65	73
21	V	101/107 (94%)	91 (90%)	10 (10%)	7	27
22	W	86/126 (68%)	86 (100%)	0	100	100
23	X	106/134 (79%)	101 (95%)	5 (5%)	23	50
24	Y	124/135 (92%)	120 (97%)	4 (3%)	34	58
25	Z	117/118 (99%)	116 (99%)	1 (1%)	70	75
26	a	119/120 (99%)	116 (98%)	3 (2%)	42	61
27	b	84/184 (46%)	81 (96%)	3 (4%)	31	56
28	c	84/98 (86%)	83 (99%)	1 (1%)	63	72
29	d	98/110 (89%)	93 (95%)	5 (5%)	21	48
30	e	114/121 (94%)	105 (92%)	9 (8%)	11	37
31	f	88/89 (99%)	84 (96%)	4 (4%)	24	51
32	g	98/100 (98%)	93 (95%)	5 (5%)	21	48
33	h	109/110 (99%)	106 (97%)	3 (3%)	38	60
34	i	86/89 (97%)	83 (96%)	3 (4%)	32	57
35	j	73/80 (91%)	70 (96%)	3 (4%)	27	53
36	k	64/65 (98%)	62 (97%)	2 (3%)	35	59
37	l	47/48 (98%)	46 (98%)	1 (2%)	47	64
38	m	48/90 (53%)	46 (96%)	2 (4%)	26	52
39	n	24/24 (100%)	22 (92%)	2 (8%)	10	35
40	o	92/94 (98%)	89 (97%)	3 (3%)	33	58
41	p	74/75 (99%)	72 (97%)	2 (3%)	39	60
42	r	108/121 (89%)	105 (97%)	3 (3%)	38	60
43	s	164/258 (64%)	157 (96%)	7 (4%)	26	52
44	t	126/137 (92%)	121 (96%)	5 (4%)	28	53
45	1	13/13 (100%)	12 (92%)	1 (8%)	12	37
52	AA	180/245 (74%)	164 (91%)	16 (9%)	9	31
53	BB	194/231 (84%)	175 (90%)	19 (10%)	7	27
54	CC	187/225 (83%)	173 (92%)	14 (8%)	12	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	DD	190/202 (94%)	174 (92%)	16 (8%)	10	34
56	EE	224/225 (100%)	209 (93%)	15 (7%)	15	41
57	FF	158/170 (93%)	148 (94%)	10 (6%)	16	43
58	GG	207/218 (95%)	197 (95%)	10 (5%)	23	49
59	HH	165/174 (95%)	154 (93%)	11 (7%)	15	41
60	II	178/180 (99%)	163 (92%)	15 (8%)	10	34
61	JJ	161/168 (96%)	150 (93%)	11 (7%)	14	41
62	KK	87/136 (64%)	74 (85%)	13 (15%)	3	12
63	LL	130/142 (92%)	115 (88%)	15 (12%)	5	20
64	MM	99/108 (92%)	83 (84%)	16 (16%)	2	10
65	NN	130/131 (99%)	120 (92%)	10 (8%)	12	37
66	OO	106/130 (82%)	94 (89%)	12 (11%)	5	20
67	PP	109/130 (84%)	98 (90%)	11 (10%)	7	26
68	QQ	117/121 (97%)	108 (92%)	9 (8%)	12	37
69	RR	119/121 (98%)	112 (94%)	7 (6%)	18	44
70	SS	125/132 (95%)	112 (90%)	13 (10%)	7	24
71	TT	111/115 (96%)	103 (93%)	8 (7%)	13	39
72	UU	92/107 (86%)	85 (92%)	7 (8%)	12	38
73	VV	67/67 (100%)	64 (96%)	3 (4%)	24	51
74	WW	112/113 (99%)	106 (95%)	6 (5%)	20	47
75	XX	113/115 (98%)	107 (95%)	6 (5%)	20	48
76	YY	107/112 (96%)	95 (89%)	12 (11%)	6	21
77	ZZ	66/103 (64%)	63 (96%)	3 (4%)	24	51
78	aa	88/98 (90%)	81 (92%)	7 (8%)	11	36
79	bb	75/76 (99%)	71 (95%)	4 (5%)	20	48
80	cc	55/62 (89%)	52 (94%)	3 (6%)	19	47
81	dd	48/49 (98%)	47 (98%)	1 (2%)	47	64
82	ee	46/106 (43%)	41 (89%)	5 (11%)	6	22
83	ff	61/140 (44%)	55 (90%)	6 (10%)	7	27
84	gg	272/275 (99%)	262 (96%)	10 (4%)	30	55
86	ii	361/394 (92%)	344 (95%)	17 (5%)	23	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
87	jj	509/526 (97%)	488 (96%)	21 (4%)	27	53
All	All	10926/12272 (89%)	10314 (94%)	612 (6%)	21	46

All (612) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	102	LEU
1	A	128	ARG
1	A	163	ARG
1	A	165	VAL
1	A	200	ARG
1	A	209	HIS
1	A	221	LYS
1	A	226	ARG
1	A	233	ARG
1	A	235	VAL
1	A	242	ARG
2	B	10	ARG
2	B	17	LEU
2	B	66	LYS
2	B	74	GLU
2	B	95	THR
2	B	135	LYS
2	B	248	LEU
2	B	262	VAL
2	B	268	ARG
2	B	294	LYS
2	B	309	LEU
2	B	314	ILE
2	B	333	LEU
2	B	356	LYS
2	B	366	LYS
2	B	383	GLU
3	C	20	LYS
3	C	124	ILE
3	C	144	ILE
3	C	150	LEU
3	C	165	LYS
3	C	175	LYS
3	C	193	LYS
3	C	232	VAL

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Mol	Chain	Res	Type
3	C	246	VAL
3	C	281	MET
3	C	307	LYS
3	C	312	ARG
3	C	333	LYS
3	C	340	ILE
4	D	50	ARG
4	D	56	THR
4	D	89	LYS
4	D	104	LEU
4	D	124	GLU
4	D	202	GLN
4	D	225	GLN
4	D	262	LYS
4	D	264	LYS
4	D	268	ARG
5	E	52	LEU
5	E	58	ARG
5	E	112	LEU
5	E	143	LEU
5	E	169	LYS
5	E	178	VAL
5	E	213	LYS
5	E	291	PHE
6	F	38	GLN
6	F	46	ARG
6	F	88	LEU
6	F	134	ILE
6	F	151	GLU
6	F	198	LYS
6	F	211	LYS
7	G	148	LEU
7	G	184	LYS
7	G	201	GLU
7	G	203	LYS
7	G	204	LYS
7	G	223	LEU
7	G	226	LEU
7	G	230	MET
7	G	293	ASN
7	G	312	LYS
8	H	1	MET

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Mol	Chain	Res	Type
8	H	20	LEU
8	H	23	ARG
8	H	52	LYS
8	H	59	LYS
8	H	66	GLU
8	H	105	ILE
8	H	106	GLN
8	H	128	MET
8	H	141	LYS
8	H	173	ARG
9	I	36	LEU
9	I	39	LYS
9	I	146	GLU
9	I	153	ARG
9	I	164	LYS
9	I	208	LYS
10	J	16	ARG
10	J	28	GLU
10	J	81	GLU
10	J	96	LYS
10	J	113	ILE
10	J	175	LEU
11	L	5	ARG
11	L	46	ILE
11	L	63	THR
11	L	162	LYS
11	L	186	ARG
12	M	8	GLU
12	M	32	ASP
12	M	37	LEU
12	M	96	GLU
13	N	9	GLU
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	87	HIS
13	N	89	VAL
13	N	197	THR
14	O	16	LEU
14	O	82	ARG
14	O	128	ARG
14	O	130	LYS

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Mol	Chain	Res	Type
14	O	145	VAL
14	O	165	LYS
14	O	175	MET
14	O	179	LYS
14	O	202	LEU
15	P	24	VAL
15	P	36	ILE
15	P	69	ARG
15	P	91	LEU
15	P	128	ARG
15	P	147	GLU
16	Q	3	VAL
16	Q	61	LEU
16	Q	91	ARG
16	Q	138	LEU
16	Q	143	ARG
17	R	6	LEU
17	R	8	LYS
17	R	36	ASN
17	R	50	ILE
17	R	82	LYS
17	R	89	MET
17	R	99	MET
17	R	103	ARG
17	R	113	LYS
17	R	138	LEU
17	R	178	GLN
18	S	7	LEU
18	S	9	GLU
18	S	70	LYS
18	S	149	LYS
18	S	159	LEU
18	S	164	LYS
18	S	174	THR
19	T	5	LYS
19	T	33	ILE
19	T	60	LYS
19	T	80	VAL
19	T	96	ILE
19	T	144	ASN
19	T	157	GLU
19	T	159	MET

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Mol	Chain	Res	Type
20	U	33	ILE
21	V	15	ARG
21	V	16	ILE
21	V	18	LEU
21	V	35	LYS
21	V	60	MET
21	V	69	LYS
21	V	91	LYS
21	V	99	GLU
21	V	109	LYS
21	V	123	LYS
23	X	39	LYS
23	X	53	ARG
23	X	59	LYS
23	X	63	LYS
23	X	111	GLN
24	Y	2	LYS
24	Y	8	THR
24	Y	72	GLN
24	Y	104	VAL
25	Z	33	THR
26	a	4	ARG
26	a	84	GLU
26	a	132	ARG
27	b	22	LYS
27	b	40	LEU
27	b	101	HIS
28	c	78	ASN
29	d	23	ARG
29	d	48	GLU
29	d	56	GLU
29	d	98	SER
29	d	102	LEU
30	e	9	LYS
30	e	11	LYS
30	e	21	ILE
30	e	22	ARG
30	e	64	LYS
30	e	78	LEU
30	e	86	GLU
30	e	106	LYS
30	e	128	ARG

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Mol	Chain	Res	Type
31	f	23	GLU
31	f	33	VAL
31	f	52	LYS
31	f	101	ILE
32	g	5	LEU
32	g	43	LYS
32	g	60	ARG
32	g	66	ARG
32	g	114	GLN
33	h	15	GLU
33	h	28	LEU
33	h	67	GLU
34	i	77	VAL
34	i	86	LYS
34	i	89	GLU
35	j	3	LYS
35	j	11	ARG
35	j	58	THR
36	k	69	LEU
36	k	70	LYS
37	l	49	LEU
38	m	71	ARG
38	m	93	ASN
39	n	1	MET
39	n	13	LEU
40	o	17	LYS
40	o	28	LYS
40	o	36	GLN
41	p	8	VAL
41	p	84	ARG
42	r	8	MET
42	r	32	LEU
42	r	118	LEU
43	s	34	ASN
43	s	38	LYS
43	s	95	LEU
43	s	105	ASN
43	s	146	LYS
43	s	187	LEU
43	s	191	GLN
44	t	37	LEU
44	t	72	GLU

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Mol	Chain	Res	Type
44	t	98	ILE
44	t	133	LEU
44	t	137	GLN
45	1	67	LYS
52	AA	5	LEU
52	AA	12	GLU
52	AA	25	LEU
52	AA	46	ILE
52	AA	50	ASN
52	AA	56	GLU
52	AA	58	LEU
52	AA	59	LEU
52	AA	60	LEU
52	AA	122	LEU
52	AA	124	VAL
52	AA	132	GLN
52	AA	136	GLU
52	AA	155	ARG
52	AA	178	LEU
52	AA	198	MET
53	BB	38	MET
53	BB	63	LYS
53	BB	71	LEU
53	BB	74	LEU
53	BB	82	ARG
53	BB	105	LEU
53	BB	113	MET
53	BB	125	VAL
53	BB	157	GLN
53	BB	172	MET
53	BB	175	GLU
53	BB	181	LEU
53	BB	182	LYS
53	BB	184	VAL
53	BB	191	ASP
53	BB	209	ASP
53	BB	213	ARG
53	BB	225	LEU
53	BB	231	LEU
54	CC	73	MET
54	CC	78	LEU
54	CC	114	LYS

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Mol	Chain	Res	Type
54	CC	117	ARG
54	CC	121	ARG
54	CC	137	VAL
54	CC	165	VAL
54	CC	167	ARG
54	CC	188	CYS
54	CC	192	LEU
54	CC	213	LEU
54	CC	230	THR
54	CC	240	THR
54	CC	252	THR
55	DD	28	GLU
55	DD	31	GLU
55	DD	51	LEU
55	DD	59	LEU
55	DD	64	ARG
55	DD	72	VAL
55	DD	106	ARG
55	DD	120	TYR
55	DD	127	MET
55	DD	137	VAL
55	DD	142	LEU
55	DD	156	LEU
55	DD	190	LEU
55	DD	198	ILE
55	DD	218	LEU
55	DD	223	ILE
56	EE	17	HIS
56	EE	23	LEU
56	EE	32	SER
56	EE	42	LEU
56	EE	51	ARG
56	EE	66	MET
56	EE	77	ARG
56	EE	139	LEU
56	EE	162	ILE
56	EE	181	CYS
56	EE	205	PHE
56	EE	222	LEU
56	EE	232	ASN
56	EE	238	LEU
56	EE	246	LEU

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Mol	Chain	Res	Type
57	FF	43	GLU
57	FF	49	LEU
57	FF	65	GLN
57	FF	71	ARG
57	FF	88	MET
57	FF	89	THR
57	FF	155	CYS
57	FF	169	ILE
57	FF	173	LEU
57	FF	204	ARG
58	GG	41	LEU
58	GG	63	MET
58	GG	67	VAL
58	GG	129	VAL
58	GG	171	THR
58	GG	178	ARG
58	GG	183	ARG
58	GG	190	ARG
58	GG	216	ARG
58	GG	230	LYS
59	HH	8	ILE
59	HH	36	LEU
59	HH	53	VAL
59	HH	75	ILE
59	HH	76	GLN
59	HH	79	LEU
59	HH	82	GLU
59	HH	100	ILE
59	HH	137	SER
59	HH	145	ARG
59	HH	172	THR
60	II	23	LYS
60	II	26	LYS
60	II	45	THR
60	II	74	ARG
60	II	93	THR
60	II	100	CYS
60	II	107	THR
60	II	121	LEU
60	II	130	THR
60	II	145	ILE
60	II	161	LEU

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Mol	Chain	Res	Type
60	II	168	GLN
60	II	178	ARG
60	II	190	LEU
60	II	203	LYS
61	JJ	26	ASP
61	JJ	29	LEU
61	JJ	38	ARG
61	JJ	40	LYS
61	JJ	45	ARG
61	JJ	50	LEU
61	JJ	61	LEU
61	JJ	69	ARG
61	JJ	80	ARG
61	JJ	89	GLU
61	JJ	116	LYS
62	KK	2	LEU
62	KK	17	LYS
62	KK	20	VAL
62	KK	21	MET
62	KK	22	VAL
62	KK	35	LEU
62	KK	43	LEU
62	KK	50	GLN
62	KK	59	LYS
62	KK	60	GLU
62	KK	66	HIS
62	KK	89	ILE
62	KK	96	ARG
63	LL	16	ILE
63	LL	20	LYS
63	LL	32	LYS
63	LL	40	ILE
63	LL	42	LEU
63	LL	49	GLU
63	LL	56	ILE
63	LL	69	ARG
63	LL	85	THR
63	LL	91	ASP
63	LL	111	VAL
63	LL	121	GLN
63	LL	126	VAL
63	LL	134	LEU

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Mol	Chain	Res	Type
63	LL	153	LYS
64	MM	18	LEU
64	MM	22	LEU
64	MM	31	LEU
64	MM	33	ARG
64	MM	40	LYS
64	MM	42	LEU
64	MM	45	ARG
64	MM	49	LEU
64	MM	55	ASN
64	MM	68	LEU
64	MM	85	LEU
64	MM	94	ILE
64	MM	99	LYS
64	MM	101	ARG
64	MM	112	LYS
64	MM	123	VAL
65	NN	3	ARG
65	NN	27	LYS
65	NN	55	ARG
65	NN	60	VAL
65	NN	75	LEU
65	NN	78	LYS
65	NN	84	LEU
65	NN	86	GLU
65	NN	110	ASP
65	NN	132	LYS
66	OO	25	GLU
66	OO	38	ASN
66	OO	51	GLU
66	OO	56	VAL
66	OO	69	SER
66	OO	85	CYS
66	OO	104	ARG
66	OO	119	LEU
66	OO	128	ARG
66	OO	131	ASP
66	OO	150	ARG
66	OO	151	LEU
67	PP	13	ARG
67	PP	14	LYS
67	PP	15	PHE

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Mol	Chain	Res	Type
67	PP	37	TYR
67	PP	42	ARG
67	PP	46	SER
67	PP	65	LYS
67	PP	78	THR
67	PP	83	MET
67	PP	108	LYS
67	PP	130	ARG
68	QQ	26	LYS
68	QQ	31	LEU
68	QQ	41	MET
68	QQ	47	LEU
68	QQ	60	LYS
68	QQ	67	ASP
68	QQ	81	ILE
68	QQ	90	LYS
68	QQ	140	ARG
69	RR	31	ASN
69	RR	44	LYS
69	RR	62	GLN
69	RR	98	VAL
69	RR	105	MET
69	RR	109	LEU
69	RR	121	GLN
70	SS	8	LYS
70	SS	14	ARG
70	SS	21	ASP
70	SS	36	VAL
70	SS	46	ARG
70	SS	52	LEU
70	SS	59	LEU
70	SS	63	GLU
70	SS	83	PHE
70	SS	86	ARG
70	SS	98	VAL
70	SS	110	ASP
70	SS	132	ARG
71	TT	39	LEU
71	TT	62	ARG
71	TT	90	SER
71	TT	108	GLU
71	TT	110	LEU

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Mol	Chain	Res	Type
71	TT	124	THR
71	TT	131	LEU
71	TT	142	LYS
72	UU	29	VAL
72	UU	39	LEU
72	UU	56	MET
72	UU	79	ARG
72	UU	88	LEU
72	UU	106	ILE
72	UU	111	GLU
73	VV	9	VAL
73	VV	12	TYR
73	VV	32	ILE
74	WW	23	ARG
74	WW	51	GLU
74	WW	92	ASN
74	WW	103	VAL
74	WW	104	LEU
74	WW	114	GLU
75	XX	7	LEU
75	XX	29	LYS
75	XX	64	SER
75	XX	67	ARG
75	XX	112	VAL
75	XX	115	ILE
76	YY	16	ARG
76	YY	17	LEU
76	YY	20	ARG
76	YY	32	LYS
76	YY	40	ILE
76	YY	47	MET
76	YY	61	ARG
76	YY	74	MET
76	YY	79	LEU
76	YY	88	LYS
76	YY	101	LYS
76	YY	115	LYS
77	ZZ	52	LYS
77	ZZ	89	GLN
77	ZZ	92	LEU
78	aa	12	LYS
78	aa	21	ILE

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Mol	Chain	Res	Type
78	aa	34	LYS
78	aa	41	ILE
78	aa	44	ILE
78	aa	55	GLU
78	aa	67	LEU
79	bb	42	LYS
79	bb	64	CYS
79	bb	80	ARG
79	bb	81	ARG
80	cc	26	GLN
80	cc	33	GLU
80	cc	40	ARG
81	dd	36	LEU
82	ee	97	LYS
82	ee	98	LYS
82	ee	99	LYS
82	ee	110	GLN
82	ee	124	LYS
83	ff	83	LYS
83	ff	94	LYS
83	ff	99	LYS
83	ff	121	CYS
83	ff	138	ARG
83	ff	140	TYR
84	gg	17	TRP
84	gg	20	GLN
84	gg	36	ARG
84	gg	79	LEU
84	gg	87	LEU
84	gg	119	GLN
84	gg	198	VAL
84	gg	273	GLU
84	gg	289	LEU
84	gg	306	LEU
86	ii	45	ILE
86	ii	63	LYS
86	ii	65	ARG
86	ii	68	ARG
86	ii	86	ASN
86	ii	103	GLU
86	ii	111	ASN
86	ii	193	LEU

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Mol	Chain	Res	Type
86	ii	211	GLN
86	ii	212	LEU
86	ii	232	PHE
86	ii	241	MET
86	ii	246	LEU
86	ii	340	GLU
86	ii	352	LYS
86	ii	368	LEU
86	ii	417	VAL
87	jj	52	GLU
87	jj	75	LEU
87	jj	97	LEU
87	jj	164	LEU
87	jj	173	VAL
87	jj	192	ASP
87	jj	289	LEU
87	jj	313	LEU
87	jj	320	GLU
87	jj	345	MET
87	jj	361	GLU
87	jj	362	LEU
87	jj	373	GLU
87	jj	374	ILE
87	jj	377	MET
87	jj	404	VAL
87	jj	411	TYR
87	jj	427	LEU
87	jj	468	GLN
87	jj	472	LEU
87	jj	526	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
2	B	121	ASN
2	B	236	HIS
2	B	271	GLN
3	C	119	GLN
3	C	203	GLN
3	C	310	HIS
4	D	81	HIS

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Mol	Chain	Res	Type
4	D	191	ASN
5	E	185	ASN
6	F	79	ASN
6	F	204	ASN
7	G	143	GLN
7	G	161	GLN
7	G	206	GLN
7	G	259	GLN
7	G	261	ASN
7	G	293	ASN
9	I	100	ASN
9	I	123	GLN
11	L	27	ASN
11	L	87	HIS
11	L	104	ASN
11	L	113	ASN
12	M	20	HIS
12	M	48	GLN
12	M	56	GLN
13	N	15	GLN
13	N	149	GLN
14	O	50	ASN
15	P	56	GLN
17	R	34	ASN
17	R	36	ASN
17	R	40	GLN
17	R	141	HIS
18	S	50	GLN
18	S	144	GLN
21	V	27	ASN
21	V	50	ASN
24	Y	18	HIS
24	Y	20	ASN
24	Y	56	GLN
24	Y	61	HIS
26	a	60	HIS
26	a	62	HIS
27	b	60	ASN
28	c	15	ASN
28	c	50	ASN
29	d	34	HIS
29	d	69	ASN

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Mol	Chain	Res	Type
29	d	121	ASN
31	f	24	HIS
31	f	99	HIS
32	g	18	ASN
33	h	65	GLN
33	h	107	GLN
33	h	108	GLN
34	i	80	HIS
35	j	28	HIS
37	l	20	ASN
37	l	38	ASN
40	o	19	GLN
41	p	72	ASN
42	r	12	ASN
42	r	23	GLN
42	r	36	ASN
42	r	70	GLN
43	s	34	ASN
43	s	68	HIS
43	s	179	ASN
44	t	65	GLN
44	t	115	GLN
44	t	137	GLN
44	t	142	ASN
52	AA	36	GLN
52	AA	111	GLN
53	BB	95	ASN
53	BB	179	ASN
54	CC	235	ASN
56	EE	17	HIS
56	EE	50	ASN
56	EE	98	ASN
56	EE	138	HIS
56	EE	188	ASN
58	GG	177	GLN
59	HH	39	GLN
59	HH	91	HIS
59	HH	97	GLN
59	HH	163	GLN
59	HH	186	ASN
59	HH	193	GLN
60	II	7	ASN

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Mol	Chain	Res	Type
60	II	64	ASN
61	JJ	124	HIS
61	JJ	143	ASN
61	JJ	156	HIS
62	KK	32	HIS
62	KK	44	HIS
62	KK	84	HIS
63	LL	100	ASN
63	LL	141	ASN
64	MM	55	ASN
65	NN	62	GLN
65	NN	69	ASN
66	OO	20	GLN
66	OO	32	HIS
66	OO	83	GLN
67	PP	114	HIS
68	QQ	24	HIS
68	QQ	86	GLN
69	RR	83	ASN
69	RR	121	GLN
70	SS	11	HIS
70	SS	73	ASN
71	TT	83	GLN
73	VV	47	ASN
76	YY	85	ASN
77	ZZ	46	ASN
78	aa	86	ASN
79	bb	51	GLN
79	bb	65	GLN
80	cc	29	GLN
80	cc	45	ASN
84	gg	222	ASN
86	ii	79	GLN
86	ii	80	GLN
86	ii	121	ASN
86	ii	170	HIS
86	ii	238	GLN
86	ii	265	ASN
86	ii	266	GLN
86	ii	277	ASN
86	ii	381	ASN
87	jj	95	HIS

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Mol	Chain	Res	Type
87	jj	233	GLN
87	jj	440	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	15 (20%)	0
47	3	72/75 (96%)	25 (34%)	2 (2%)
48	5	3518/3543 (99%)	908 (25%)	167 (4%)
49	7	119/120 (99%)	15 (12%)	1 (0%)
50	8	150/156 (96%)	36 (24%)	7 (4%)
51	9	1682/1869 (89%)	423 (25%)	63 (3%)
85	hh	14/15 (93%)	7 (50%)	0
All	All	5629/5854 (96%)	1429 (25%)	240 (4%)

All (1429) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	8	U
46	2	9	A
46	2	16	C
46	2	19	G
46	2	20	U
46	2	21	A
46	2	34	A
46	2	46	G
46	2	47	U
46	2	49	C
46	2	61	C
46	2	64	G
46	2	67	G
46	2	72	C
46	2	75	C
47	3	7	A
47	3	8	U
47	3	13	C
47	3	14	A
47	3	21	A
47	3	25	C
47	3	28	C
47	3	29	A

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Mol	Chain	Res	Type
47	3	34	U
47	3	35	U
47	3	36	U
47	3	40	C
47	3	42	G
47	3	47	U
47	3	49	C
47	3	53	G
47	3	58	A
47	3	60	U
47	3	61	C
47	3	63	C
47	3	65	G
47	3	72	C
47	3	74	C
47	3	75	C
47	3	76	A
48	5	6	C
48	5	8	U
48	5	12	A
48	5	13	U
48	5	15	A
48	5	25	A
48	5	30	C
48	5	35	U
48	5	39	A
48	5	42	A
48	5	48	G
48	5	49	U
48	5	56	A
48	5	58	G
48	5	59	A
48	5	64	A
48	5	65	A
48	5	73	A
48	5	91	G
48	5	93	G
48	5	108	A
48	5	109	G
48	5	110	C
48	5	118	C
48	5	119	G

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Mol	Chain	Res	Type
48	5	120	A
48	5	121	A
48	5	126	C
48	5	131	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	143	C
48	5	144	G
48	5	159	C
48	5	165	A
48	5	172	C
48	5	173	C
48	5	176	G
48	5	177	G
48	5	179	G
48	5	200	U
48	5	201	C
48	5	202	C
48	5	205	C
48	5	209	U
48	5	216	C
48	5	217	C
48	5	218	A
48	5	220	C
48	5	221	C
48	5	224	U
48	5	225	G
48	5	226	G
48	5	227	A
48	5	233	U
48	5	234	G
48	5	235	A
48	5	246	G
48	5	253	G
48	5	255	C
48	5	263	G
48	5	266	C
48	5	276	C
48	5	279	A
48	5	280	G
48	5	297	U

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Mol	Chain	Res	Type
48	5	306	A
48	5	309	C
48	5	310	G
48	5	315	G
48	5	316	U
48	5	322	C
48	5	328	A
48	5	334	A
48	5	340	C
48	5	347	A
48	5	350	C
48	5	357	U
48	5	361	C
48	5	362	A
48	5	363	A
48	5	379	G
48	5	386	A
48	5	387	G
48	5	407	A
48	5	409	G
48	5	410	A
48	5	412	G
48	5	413	G
48	5	429	A
48	5	431	G
48	5	432	U
48	5	446	C
48	5	449	C
48	5	450	G
48	5	452	A
48	5	453	G
48	5	454	U
48	5	457	G
48	5	466	A
48	5	467	U
48	5	468	U
48	5	469	C
48	5	481	G
48	5	481(A)	C
48	5	482	G
48	5	483	G
48	5	484	U

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Mol	Chain	Res	Type
48	5	485	C
48	5	486	C
48	5	490	C
48	5	492	U
48	5	493	G
48	5	497	G
48	5	498	C
48	5	499	G
48	5	505	G
48	5	510	U
48	5	653	C
48	5	654	C
48	5	657	C
48	5	658	C
48	5	659	G
48	5	660	G
48	5	667	A
48	5	668	C
48	5	669	C
48	5	670	G
48	5	672	C
48	5	683	C
48	5	685	C
48	5	687	U
48	5	696	C
48	5	697	G
48	5	702	U
48	5	704	C
48	5	705	G
48	5	708	G
48	5	719	C
48	5	722	G
48	5	729	G
48	5	730	G
48	5	731	G
48	5	734	G
48	5	738	C
48	5	738(A)	C
48	5	739	G
48	5	742	G
48	5	747	A
48	5	748	G

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Mol	Chain	Res	Type
48	5	749	G
48	5	750	U
48	5	756	G
48	5	758	G
48	5	911	U
48	5	913	U
48	5	914	U
48	5	917	A
48	5	918	G
48	5	923	C
48	5	924	C
48	5	925	C
48	5	926	G
48	5	929	A
48	5	930	G
48	5	931	C
48	5	932	A
48	5	933	G
48	5	934	C
48	5	935	A
48	5	935(A)	G
48	5	936	C
48	5	937	U
48	5	939	G
48	5	941	C
48	5	943	A
48	5	944	A
48	5	945	U
48	5	956	A
48	5	957	G
48	5	959	G
48	5	960	A
48	5	961	G
48	5	962	C
48	5	963	G
48	5	964	A
48	5	965	G
48	5	966	A
48	5	967	C
48	5	968	C
48	5	969	C
48	5	972	C

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Mol	Chain	Res	Type
48	5	973	G
48	5	979	C
48	5	983	C
48	5	990	C
48	5	1071	C
48	5	1072	C
48	5	1073	G
48	5	1075	G
48	5	1076	C
48	5	1078	A
48	5	1079	C
48	5	1082	C
48	5	1174	G
48	5	1175	A
48	5	1177	U
48	5	1179	U
48	5	1184	A
48	5	1185	G
48	5	1189	G
48	5	1194	G
48	5	1195	G
48	5	1211	G
48	5	1212	G
48	5	1214	C
48	5	1215	C
48	5	1234	G
48	5	1235	G
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1239	C
48	5	1272	C
48	5	1273	G
48	5	1274	A
48	5	1275	G
48	5	1276	C
48	5	1284	G
48	5	1287	G
48	5	1288	G
48	5	1292	C
48	5	1293	G
48	5	1295	U

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Mol	Chain	Res	Type
48	5	1296	G
48	5	1301	C
48	5	1303	A
48	5	1304	C
48	5	1313	C
48	5	1326	A
48	5	1328	G
48	5	1330	A
48	5	1334	A
48	5	1354	A
48	5	1359	G
48	5	1360	G
48	5	1364	U
48	5	1370	G
48	5	1371	A
48	5	1377	G
48	5	1378	C
48	5	1379	C
48	5	1380	G
48	5	1381	U
48	5	1387	A
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1401	C
48	5	1403	G
48	5	1416	G
48	5	1418	C
48	5	1419	G
48	5	1420	A
48	5	1421	G
48	5	1429	C
48	5	1432	G
48	5	1433	A
48	5	1435	G
48	5	1436	C
48	5	1437	C
48	5	1438	U
48	5	1440	U
48	5	1441	C
48	5	1442	C
48	5	1445	U

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Mol	Chain	Res	Type
48	5	1446	C
48	5	1453	G
48	5	1456	C
48	5	1457	G
48	5	1458	C
48	5	1459	A
48	5	1465	G
48	5	1475	G
48	5	1478	C
48	5	1481	C
48	5	1482	G
48	5	1483	C
48	5	1484	G
48	5	1486	C
48	5	1495	G
48	5	1497	A
48	5	1498	G
48	5	1502	G
48	5	1504	G
48	5	1514	U
48	5	1516	G
48	5	1518	A
48	5	1523	A
48	5	1525	A
48	5	1534	A
48	5	1547	A
48	5	1554	A
48	5	1563	A
48	5	1564	A
48	5	1566	C
48	5	1574	G
48	5	1578	U
48	5	1584	G
48	5	1591	U
48	5	1592	G
48	5	1596	U
48	5	1602	U
48	5	1612	G
48	5	1613	A
48	5	1624	G
48	5	1625	G
48	5	1631	A

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Mol	Chain	Res	Type
48	5	1633	G
48	5	1634	A
48	5	1638	A
48	5	1640	C
48	5	1641	G
48	5	1654	G
48	5	1656	U
48	5	1661	C
48	5	1676	C
48	5	1677	U
48	5	1679	A
48	5	1691	G
48	5	1724	G
48	5	1726	U
48	5	1733	G
48	5	1734	G
48	5	1735	U
48	5	1740	C
48	5	1741	G
48	5	1742	A
48	5	1750	G
48	5	1753	G
48	5	1755	C
48	5	1756	U
48	5	1757	U
48	5	1760	G
48	5	1761	G
48	5	1763	C
48	5	1764	G
48	5	1768	C
48	5	1772	C
48	5	1773	U
48	5	1776	A
48	5	1781	U
48	5	1787	A
48	5	1799	G
48	5	1800	U
48	5	1803	G
48	5	1804	A
48	5	1805	A
48	5	1819	G
48	5	1821	G

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Mol	Chain	Res	Type
48	5	1822	U
48	5	1823	G
48	5	1828	C
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1837	A
48	5	1842	G
48	5	1855	G
48	5	1867	A
48	5	1869	G
48	5	1881	C
48	5	1893	C
48	5	1897	A
48	5	1910	G
48	5	1916	G
48	5	1918	U
48	5	1919	G
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1923	A
48	5	1931	C
48	5	1933	G
48	5	1935	C
48	5	1936	C
48	5	1940	G
48	5	1941	A
48	5	1948	G
48	5	1952	G
48	5	1957	U
48	5	1958	A
48	5	1959	U
48	5	1961	G
48	5	1962	A
48	5	1963	C
48	5	1976	G
48	5	1977	C
48	5	1978	C
48	5	1979	A
48	5	1980	U

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Mol	Chain	Res	Type
48	5	1983	A
48	5	1984	A
48	5	1986	U
48	5	1987	C
48	5	1991	A
48	5	1993	C
48	5	1997	U
48	5	2001	G
48	5	2002	A
48	5	2003	G
48	5	2004	U
48	5	2005	G
48	5	2007	G
48	5	2008	U
48	5	2011	C
48	5	2013	A
48	5	2016	C
48	5	2024	G
48	5	2025	A
48	5	2026	A
48	5	2033	A
48	5	2034	G
48	5	2046	G
48	5	2047	A
48	5	2048	U
48	5	2052	G
48	5	2055	G
48	5	2056	G
48	5	2062	C
48	5	2064	G
48	5	2069	A
48	5	2070	U
48	5	2084	U
48	5	2085	G
48	5	2089	G
48	5	2090	U
48	5	2092	G
48	5	2093	G
48	5	2094	C
48	5	2095	A
48	5	2097	A
48	5	2098	G

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Mol	Chain	Res	Type
48	5	2100	G
48	5	2101	A
48	5	2102	G
48	5	2104	A
48	5	2105	A
48	5	2106	G
48	5	2107	A
48	5	2108	G
48	5	2110	G
48	5	2111	U
48	5	2259	G
48	5	2260	C
48	5	2262	G
48	5	2266	C
48	5	2267	U
48	5	2268	A
48	5	2269	C
48	5	2270	G
48	5	2275	G
48	5	2277	C
48	5	2278	G
48	5	2279	A
48	5	2289	C
48	5	2294	G
48	5	2300	A
48	5	2301	G
48	5	2313	A
48	5	2314	G
48	5	2316	G
48	5	2331	G
48	5	2333	G
48	5	2348	G
48	5	2351	C
48	5	2357	G
48	5	2364	G
48	5	2366	A
48	5	2370	A
48	5	2374	A
48	5	2380	G
48	5	2395	A
48	5	2396	A
48	5	2399	G

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Mol	Chain	Res	Type
48	5	2414	G
48	5	2416	G
48	5	2417	A
48	5	2421	G
48	5	2422	C
48	5	2424	G
48	5	2425	U
48	5	2428	A
48	5	2433	G
48	5	2441	C
48	5	2447	U
48	5	2450	G
48	5	2467	U
48	5	2468	U
48	5	2469	C
48	5	2471	G
48	5	2475	G
48	5	2479	G
48	5	2483	G
48	5	2485	U
48	5	2488	C
48	5	2489	C
48	5	2490	U
48	5	2491	C
48	5	2493	G
48	5	2495	U
48	5	2499	C
48	5	2503	G
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2509	C
48	5	2512	A
48	5	2513	A
48	5	2521	G
48	5	2529	A
48	5	2530	U
48	5	2537	A
48	5	2546	G
48	5	2547	G
48	5	2554	U
48	5	2555	G

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Mol	Chain	Res	Type
48	5	2564	G
48	5	2566	G
48	5	2571	C
48	5	2572	C
48	5	2575	U
48	5	2577	C
48	5	2583	C
48	5	2586	G
48	5	2587	A
48	5	2588	C
48	5	2601	A
48	5	2618	G
48	5	2620	G
48	5	2622	G
48	5	2623	A
48	5	2627	C
48	5	2638	G
48	5	2639	U
48	5	2640	G
48	5	2647	A
48	5	2658	G
48	5	2661	U
48	5	2662	G
48	5	2663	G
48	5	2669	C
48	5	2670	C
48	5	2673	G
48	5	2676	A
48	5	2680	G
48	5	2681	G
48	5	2686	G
48	5	2687	U
48	5	2688	G
48	5	2689	C
48	5	2695	A
48	5	2696	A
48	5	2707	U
48	5	2708	U
48	5	2709	C
48	5	2710	C
48	5	2711	G
48	5	2712	G

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Mol	Chain	Res	Type
48	5	2716	C
48	5	2719	C
48	5	2721	G
48	5	2725	A
48	5	2726	G
48	5	2740	U
48	5	2743	A
48	5	2751	G
48	5	2754	G
48	5	2760	G
48	5	2761	U
48	5	2763	U
48	5	2764	A
48	5	2769	U
48	5	2787	A
48	5	2788	U
48	5	2789	A
48	5	2790	U
48	5	2796	G
48	5	2798	A
48	5	2806	A
48	5	2807	A
48	5	2814	C
48	5	2819	U
48	5	2826	U
48	5	2827	G
48	5	2828	U
48	5	2829	U
48	5	2838	G
48	5	2839	U
48	5	2842	G
48	5	2855	G
48	5	2857	A
48	5	2862	G
48	5	2864	A
48	5	2875	C
48	5	2884	G
48	5	2896	G
48	5	2897	G
48	5	3598	C
48	5	3599	A
48	5	3604	A

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Mol	Chain	Res	Type
48	5	3605	C
48	5	3615	G
48	5	3625	G
48	5	3626	G
48	5	3630	A
48	5	3635	A
48	5	3644	U
48	5	3646	A
48	5	3662	A
48	5	3673	C
48	5	3674	G
48	5	3685	C
48	5	3692	A
48	5	3698	G
48	5	3711	A
48	5	3712	A
48	5	3719	A
48	5	3722	G
48	5	3729	U
48	5	3733	A
48	5	3737	A
48	5	3740	G
48	5	3748	A
48	5	3750	G
48	5	3753	G
48	5	3755	G
48	5	3756	A
48	5	3759	A
48	5	3760	A
48	5	3765	G
48	5	3773	U
48	5	3774	A
48	5	3776	G
48	5	3777	G
48	5	3778	U
48	5	3783	A
48	5	3784	A
48	5	3785	A
48	5	3786	U
48	5	3810	C
48	5	3811	G
48	5	3812	C

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Mol	Chain	Res	Type
48	5	3814	U
48	5	3817	A
48	5	3819	G
48	5	3831	U
48	5	3838	U
48	5	3839	G
48	5	3840	U
48	5	3851	U
48	5	3859	G
48	5	3867	A
48	5	3876	A
48	5	3877	A
48	5	3878	C
48	5	3879	G
48	5	3889	G
48	5	3897	G
48	5	3898	G
48	5	3901	A
48	5	3905	A
48	5	3906	A
48	5	3907	G
48	5	3908	A
48	5	3915	U
48	5	3916	G
48	5	3927	U
48	5	3939	G
48	5	3943	A
48	5	3946	G
48	5	4067	U
48	5	4069	U
48	5	4076	G
48	5	4084	G
48	5	4085	A
48	5	4086	G
48	5	4088	C
48	5	4099	G
48	5	4100	C
48	5	4116	C
48	5	4117	U
48	5	4118	U
48	5	4119	C
48	5	4120	U

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Mol	Chain	Res	Type
48	5	4121	G
48	5	4122	G
48	5	4125	C
48	5	4127	A
48	5	4150	G
48	5	4162	C
48	5	4163	U
48	5	4166	G
48	5	4171	C
48	5	4183	G
48	5	4184	G
48	5	4190	U
48	5	4191	G
48	5	4203	A
48	5	4212	A
48	5	4218	U
48	5	4222	G
48	5	4225	G
48	5	4229	U
48	5	4232	U
48	5	4233	A
48	5	4251	A
48	5	4255	A
48	5	4257	A
48	5	4258	C
48	5	4265	U
48	5	4267	G
48	5	4268	A
48	5	4271	A
48	5	4273	A
48	5	4281	A
48	5	4291	G
48	5	4297	G
48	5	4304	A
48	5	4305	G
48	5	4306	U
48	5	4314	C
48	5	4317	A
48	5	4318	C
48	5	4319	C
48	5	4326	G
48	5	4329	G

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Mol	Chain	Res	Type
48	5	4330	G
48	5	4336	A
48	5	4339	A
48	5	4349	C
48	5	4350	C
48	5	4354	U
48	5	4355	G
48	5	4373	G
48	5	4376	A
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4387	C
48	5	4393	G
48	5	4394	A
48	5	4395	U
48	5	4398	C
48	5	4401	G
48	5	4415	A
48	5	4419	U
48	5	4421	C
48	5	4422	A
48	5	4436	U
48	5	4437	U
48	5	4438	U
48	5	4440	G
48	5	4441	A
48	5	4444	C
48	5	4448	G
48	5	4449	A
48	5	4450	U
48	5	4453	C
48	5	4464	A
48	5	4471	U
48	5	4475	G
48	5	4476	C
48	5	4488	A
48	5	4495	G
48	5	4500	U
48	5	4510	A
48	5	4512	U
48	5	4513	A

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Mol	Chain	Res	Type
48	5	4515	G
48	5	4519	C
48	5	4520	G
48	5	4524	G
48	5	4527	G
48	5	4528	G
48	5	4548	A
48	5	4549	G
48	5	4560	C
48	5	4563	U
48	5	4567	G
48	5	4570	G
48	5	4573	G
48	5	4574	U
48	5	4575	G
48	5	4578	G
48	5	4581	G
48	5	4586	G
48	5	4590	A
48	5	4606	G
48	5	4618	G
48	5	4627	U
48	5	4636	U
48	5	4637	G
48	5	4650	G
48	5	4652	G
48	5	4656	A
48	5	4657	U
48	5	4660	G
48	5	4661	G
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4678	G
48	5	4687	A
48	5	4694	G
48	5	4699	U
48	5	4700	A
48	5	4701	A
48	5	4709	U
48	5	4712	C
48	5	4719	G

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Mol	Chain	Res	Type
48	5	4720	C
48	5	4721	G
48	5	4728	U
48	5	4736	C
48	5	4737	G
48	5	4745	G
48	5	4751	G
48	5	4754	G
48	5	4756	C
48	5	4757	C
48	5	4759	C
48	5	4761	G
48	5	4765	G
48	5	4771	C
48	5	4772	C
48	5	4868	G
48	5	4870	G
48	5	4871	C
48	5	4872	G
48	5	4873	G
48	5	4874	A
48	5	4875	G
48	5	4876	A
48	5	4877	G
48	5	4882	U
48	5	4883	C
48	5	4885	U
48	5	4887	C
48	5	4891	G
48	5	4895	C
48	5	4897	G
48	5	4904	G
48	5	4910	A
48	5	4912	G
48	5	4913	G
48	5	4914	G
48	5	4915	G
48	5	4918	C
48	5	4919	G
48	5	4921	C
48	5	4922	C
48	5	4924	C

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Mol	Chain	Res	Type
48	5	4925	U
48	5	4926	C
48	5	4927	G
48	5	4928	C
48	5	4931	G
48	5	4935	C
48	5	4936	G
48	5	4937	C
48	5	4940	C
48	5	4942	C
48	5	4943	A
48	5	4944	C
48	5	4945	G
48	5	4947	U
48	5	4948	C
48	5	4949	G
48	5	4950	U
48	5	4951	G
48	5	4956	A
48	5	4957	C
48	5	4958	C
48	5	4964	C
48	5	4965	U
48	5	4966	A
48	5	4967	A
48	5	4976	U
48	5	4979	A
48	5	4988	U
48	5	4989	U
48	5	4990	C
48	5	4991	U
48	5	5014	A
48	5	5017	G
48	5	5040	U
48	5	5041	G
48	5	5047	C
48	5	5050	C
48	5	5052	C
48	5	5053	U
48	5	5054	C
48	5	5056	A
48	5	5061	A

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Mol	Chain	Res	Type
48	5	5062	G
49	7	7	G
49	7	13	A
49	7	33	U
49	7	38	U
49	7	42	A
49	7	53	U
49	7	54	A
49	7	64	G
49	7	97	G
49	7	100	A
49	7	109	U
49	7	110	G
49	7	116	G
49	7	117	G
49	7	120	U
50	8	2	G
50	8	3	A
50	8	32	C
50	8	34	U
50	8	35	C
50	8	49	G
50	8	52	A
50	8	59	A
50	8	62	A
50	8	63	U
50	8	75	G
50	8	79	G
50	8	86	U
50	8	87	G
50	8	94	G
50	8	95	A
50	8	97	A
50	8	103	A
50	8	105	C
50	8	107	C
50	8	109	C
50	8	110	U
50	8	111	U
50	8	112	G
50	8	114	G
50	8	121	G

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Mol	Chain	Res	Type
50	8	123	U
50	8	124	U
50	8	125	C
50	8	126	C
50	8	127	U
50	8	137	A
50	8	143	G
50	8	147	G
50	8	150	C
50	8	153	C
51	9	2	A
51	9	3	C
51	9	4	C
51	9	17	C
51	9	25	A
51	9	26	U
51	9	33	G
51	9	41	G
51	9	44	U
51	9	45	A
51	9	46	A
51	9	56	G
51	9	58	C
51	9	60	A
51	9	65	C
51	9	67	C
51	9	68	A
51	9	70	G
51	9	71	G
51	9	73	C
51	9	74	G
51	9	75	G
51	9	77	A
51	9	79	A
51	9	99	A
51	9	100	U
51	9	103	A
51	9	104	A
51	9	110	U
51	9	111	A
51	9	113	G
51	9	115	U

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Mol	Chain	Res	Type
51	9	116	U
51	9	124	U
51	9	126	G
51	9	127	C
51	9	129	C
51	9	130	G
51	9	141	A
51	9	143	U
51	9	147	A
51	9	155	G
51	9	158	A
51	9	161	U
51	9	162	C
51	9	163	U
51	9	167	G
51	9	168	C
51	9	175	A
51	9	182	C
51	9	183	G
51	9	184	G
51	9	188	C
51	9	189	U
51	9	191	A
51	9	192	C
51	9	200	G
51	9	202	G
51	9	206	G
51	9	211	G
51	9	213	G
51	9	215	G
51	9	289	G
51	9	292	A
51	9	293	C
51	9	294	U
51	9	302	A
51	9	304	C
51	9	307	G
51	9	308	G
51	9	309	G
51	9	312	G
51	9	314	U
51	9	318	A

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Mol	Chain	Res	Type
51	9	319	C
51	9	322	C
51	9	331	C
51	9	332	G
51	9	340	C
51	9	347	G
51	9	351	G
51	9	360	A
51	9	362	C
51	9	364	A
51	9	368	U
51	9	370	G
51	9	381	C
51	9	382	C
51	9	384	U
51	9	385	G
51	9	386	C
51	9	400	C
51	9	409	C
51	9	417	C
51	9	418	A
51	9	435	A
51	9	438	G
51	9	448	A
51	9	449	A
51	9	450	C
51	9	459	C
51	9	460	A
51	9	464	A
51	9	465	A
51	9	466	G
51	9	469	A
51	9	472	C
51	9	473	A
51	9	474	G
51	9	476	A
51	9	482	G
51	9	487	U
51	9	492	C
51	9	496	C
51	9	508	A
51	9	512	A

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Mol	Chain	Res	Type
51	9	518	G
51	9	525	A
51	9	531	A
51	9	532	C
51	9	533	A
51	9	544	G
51	9	545	A
51	9	546	G
51	9	548	C
51	9	549	C
51	9	550	C
51	9	551	U
51	9	554	A
51	9	555	A
51	9	556	U
51	9	557	U
51	9	559	G
51	9	560	A
51	9	562	U
51	9	563	G
51	9	564	A
51	9	568	C
51	9	576	A
51	9	583	A
51	9	587	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U
51	9	592	C
51	9	597	G
51	9	598	G
51	9	604	A
51	9	606	G
51	9	607	U
51	9	608	C
51	9	614	C
51	9	637	U
51	9	643	A
51	9	644	G
51	9	655	A
51	9	659	G

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Mol	Chain	Res	Type
51	9	660	C
51	9	663	C
51	9	664	A
51	9	668	A
51	9	669	A
51	9	670	A
51	9	671	A
51	9	672	A
51	9	673	G
51	9	684	G
51	9	688	U
51	9	689	U
51	9	690	G
51	9	691	G
51	9	732	U
51	9	733	C
51	9	752	G
51	9	753	C
51	9	754	G
51	9	811	A
51	9	812	A
51	9	821	G
51	9	822	U
51	9	830	A
51	9	834	C
51	9	847	A
51	9	861	A
51	9	862	A
51	9	868	G
51	9	869	A
51	9	870	A
51	9	871	U
51	9	872	A
51	9	873	G
51	9	874	G
51	9	875	A
51	9	877	C
51	9	878	G
51	9	885	U
51	9	886	A
51	9	887	U
51	9	890	U

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Mol	Chain	Res	Type
51	9	892	U
51	9	902	G
51	9	913	A
51	9	914	U
51	9	920	A
51	9	930	C
51	9	933	G
51	9	934	G
51	9	943	U
51	9	955	A
51	9	971	G
51	9	985	G
51	9	989	C
51	9	990	A
51	9	992	A
51	9	999	G
51	9	1016	U
51	9	1017	U
51	9	1023	A
51	9	1041	G
51	9	1060	A
51	9	1061	U
51	9	1062	A
51	9	1067	C
51	9	1083	A
51	9	1085	C
51	9	1089	G
51	9	1096	G
51	9	1099	G
51	9	1100	A
51	9	1111	U
51	9	1114	U
51	9	1115	U
51	9	1116	C
51	9	1117	C
51	9	1118	C
51	9	1120	U
51	9	1121	G
51	9	1131	G
51	9	1132	C
51	9	1133	A
51	9	1138	C

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Mol	Chain	Res	Type
51	9	1139	C
51	9	1148	A
51	9	1149	A
51	9	1153	C
51	9	1154	U
51	9	1165	G
51	9	1166	G
51	9	1195	A
51	9	1207	G
51	9	1208	A
51	9	1211	G
51	9	1213	C
51	9	1215	C
51	9	1221	G
51	9	1223	A
51	9	1224	G
51	9	1240	A
51	9	1242	U
51	9	1248	U
51	9	1251	A
51	9	1253	A
51	9	1254	C
51	9	1256	G
51	9	1257	G
51	9	1259	A
51	9	1260	A
51	9	1265	A
51	9	1268	C
51	9	1270	G
51	9	1271	C
51	9	1274	G
51	9	1275	G
51	9	1281	G
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1287	A
51	9	1289	U
51	9	1291	A
51	9	1293	A
51	9	1298	G
51	9	1299	A

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Mol	Chain	Res	Type
51	9	1300	U
51	9	1301	A
51	9	1302	G
51	9	1307	U
51	9	1308	U
51	9	1313	A
51	9	1314	U
51	9	1316	C
51	9	1321	G
51	9	1330	G
51	9	1331	C
51	9	1342	U
51	9	1354	G
51	9	1369	A
51	9	1371	U
51	9	1372	U
51	9	1376	A
51	9	1378	A
51	9	1395	C
51	9	1396	A
51	9	1397	U
51	9	1398	G
51	9	1401	A
51	9	1402	A
51	9	1404	U
51	9	1406	G
51	9	1407	U
51	9	1410	C
51	9	1412	C
51	9	1413	G
51	9	1414	A
51	9	1424	G
51	9	1428	G
51	9	1439	A
51	9	1449	G
51	9	1454	A
51	9	1458	G
51	9	1459	G
51	9	1462	U
51	9	1463	U
51	9	1466	G
51	9	1473	G

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Mol	Chain	Res	Type
51	9	1476	A
51	9	1477	U
51	9	1478	U
51	9	1490	G
51	9	1494	U
51	9	1497	G
51	9	1498	A
51	9	1507	G
51	9	1509	U
51	9	1510	G
51	9	1521	C
51	9	1522	A
51	9	1531	A
51	9	1533	A
51	9	1536	G
51	9	1544	C
51	9	1545	A
51	9	1548	G
51	9	1552	G
51	9	1553	C
51	9	1555	U
51	9	1556	A
51	9	1557	C
51	9	1560	U
51	9	1570	G
51	9	1574	C
51	9	1575	G
51	9	1580	A
51	9	1581	C
51	9	1582	C
51	9	1585	U
51	9	1586	U
51	9	1587	G
51	9	1588	A
51	9	1589	A
51	9	1600	G
51	9	1601	A
51	9	1602	U
51	9	1604	G
51	9	1621	U
51	9	1623	A
51	9	1625	U

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Mol	Chain	Res	Type
51	9	1637	A
51	9	1638	G
51	9	1639	G
51	9	1641	A
51	9	1647	A
51	9	1648	G
51	9	1654	G
51	9	1664	A
51	9	1665	G
51	9	1671	G
51	9	1680	G
51	9	1682	C
51	9	1683	C
51	9	1686	G
51	9	1689	C
51	9	1695	A
51	9	1698	C
51	9	1699	A
51	9	1715	A
51	9	1721	U
51	9	1722	G
51	9	1726	G
51	9	1729	U
51	9	1730	U
51	9	1737	G
51	9	1750	C
51	9	1753	C
51	9	1756	C
51	9	1758	G
51	9	1760	G
51	9	1772	C
51	9	1783	C
51	9	1785	C
51	9	1800	A
51	9	1822	A
51	9	1823	A
51	9	1824	A
51	9	1825	A
51	9	1826	G
51	9	1829	G
51	9	1831	A
51	9	1835	A

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Mol	Chain	Res	Type
51	9	1836	G
51	9	1838	U
51	9	1849	G
51	9	1850	A
51	9	1851	A
51	9	1861	G
51	9	1862	G
51	9	1863	A
51	9	1865	C
51	9	1866	A
51	9	1867	U
51	9	1868	U
51	9	1869	A
85	hh	42	C
85	hh	43	A
85	hh	45	A
85	hh	46	G
85	hh	49	U
85	hh	52	G
85	hh	55	C

All (240) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	3	7	A
47	3	74	C
48	5	20	U
48	5	47	A
48	5	48	G
48	5	64	A
48	5	125	C
48	5	134	G
48	5	143	C
48	5	217	C
48	5	226	G
48	5	234	G
48	5	245	C
48	5	265	C
48	5	275	C
48	5	278	G
48	5	361	C
48	5	385	A

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Mol	Chain	Res	Type
48	5	387	G
48	5	406	C
48	5	408	A
48	5	409	G
48	5	417	G
48	5	449	C
48	5	466	A
48	5	480	C
48	5	481(A)	C
48	5	484	U
48	5	485	C
48	5	492	U
48	5	497	G
48	5	498	C
48	5	504	G
48	5	669	C
48	5	696	C
48	5	729	G
48	5	738(A)	C
48	5	747	A
48	5	748	G
48	5	749	G
48	5	915	A
48	5	916	C
48	5	924	C
48	5	930	G
48	5	933	G
48	5	935(A)	G
48	5	936	C
48	5	956	A
48	5	959	G
48	5	963	G
48	5	965	G
48	5	966	A
48	5	971(A)	G
48	5	1071	C
48	5	1072	C
48	5	1174	G
48	5	1209	U
48	5	1211	G
48	5	1214	C
48	5	1236	C

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Mol	Chain	Res	Type
48	5	1237	C
48	5	1238	A
48	5	1287	G
48	5	1291	G
48	5	1294	A
48	5	1295	U
48	5	1329	G
48	5	1358	G
48	5	1359	G
48	5	1370	G
48	5	1376	C
48	5	1378	C
48	5	1380	G
48	5	1420	A
48	5	1432	G
48	5	1440	U
48	5	1445	U
48	5	1455	G
48	5	1477	C
48	5	1481	C
48	5	1484	G
48	5	1485	C
48	5	1633	G
48	5	1733	G
48	5	1734	G
48	5	1740	C
48	5	1804	A
48	5	1818	G
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1919	G
48	5	1921	C
48	5	1935	C
48	5	1947	U
48	5	1979	A
48	5	1983	A
48	5	1986	U
48	5	2001	G
48	5	2046	G
48	5	2068	C
48	5	2088	A

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Mol	Chain	Res	Type
48	5	2089	G
48	5	2100	G
48	5	2265	G
48	5	2266	C
48	5	2278	G
48	5	2313	A
48	5	2398	U
48	5	2425	U
48	5	2428	A
48	5	2467	U
48	5	2468	U
48	5	2474	G
48	5	2490	U
48	5	2502	A
48	5	2529	A
48	5	2546	G
48	5	2587	A
48	5	2661	U
48	5	2695	A
48	5	2696	A
48	5	2754	G
48	5	2794	C
48	5	2806	A
48	5	3603	G
48	5	3625	G
48	5	3648	A
48	5	3673	C
48	5	3697	U
48	5	3710	G
48	5	3809	G
48	5	3876	A
48	5	3888	G
48	5	3904	G
48	5	4075	U
48	5	4076	G
48	5	4084	G
48	5	4116	C
48	5	4119	C
48	5	4121	G
48	5	4124	G
48	5	4162	C
48	5	4170	A

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Mol	Chain	Res	Type
48	5	4232	U
48	5	4254	G
48	5	4266	G
48	5	4348	A
48	5	4378	A
48	5	4448	G
48	5	4449	A
48	5	4463	U
48	5	4527	G
48	5	4572	U
48	5	4573	G
48	5	4656	A
48	5	4699	U
48	5	4719	G
48	5	4871	C
48	5	4872	G
48	5	4876	A
48	5	4884	G
48	5	4894	A
48	5	4925	U
48	5	4936	G
48	5	4942	C
48	5	4947	U
48	5	4949	G
48	5	4965	U
49	7	109	U
50	8	2	G
50	8	51	U
50	8	85	U
50	8	86	U
50	8	94	G
50	8	110	U
50	8	124	U
51	9	2	A
51	9	72	C
51	9	103	A
51	9	110	U
51	9	126	G
51	9	160	U
51	9	182	C
51	9	293	C
51	9	314	U

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Mol	Chain	Res	Type
51	9	369	C
51	9	434	G
51	9	448	A
51	9	465	A
51	9	473	A
51	9	531	A
51	9	532	C
51	9	553	U
51	9	555	A
51	9	559	G
51	9	563	G
51	9	591	U
51	9	642	U
51	9	656	G
51	9	670	A
51	9	688	U
51	9	690	G
51	9	752	G
51	9	821	G
51	9	861	A
51	9	868	G
51	9	869	A
51	9	870	A
51	9	872	A
51	9	874	G
51	9	885	U
51	9	1016	U
51	9	1114	U
51	9	1115	U
51	9	1120	U
51	9	1137	U
51	9	1165	G
51	9	1253	A
51	9	1264	C
51	9	1284	A
51	9	1286	G
51	9	1313	A
51	9	1330	G
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1489	A

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Mol	Chain	Res	Type
51	9	1520	G
51	9	1636	G
51	9	1637	A
51	9	1646	C
51	9	1664	A
51	9	1679	A
51	9	1721	U
51	9	1744	G
51	9	1824	A
51	9	1835	A
51	9	1867	U
51	9	1868	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 310 ligands modelled in this entry, 308 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
90	SF4	jj	600	87	0,12,12	-	-	-		
90	SF4	jj	601	87	0,12,12	-	-	-		

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
90	SF4	jj	600	87	-	-	0/6/5/5
90	SF4	jj	601	87	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	jj	600	SF4	1	0
90	jj	601	SF4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	5	29
51	9	7
47	3	2
46	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.35
1	5	1252:C	O3'	1271:G	P	35.93
1	5	1219:G	O3'	1233:G	P	23.06
1	5	3948:C	O3'	4065:G	P	19.73
1	5	1406(C):G	O3'	1411:C	P	18.70
1	5	990:C	O3'	1064:G	P	18.45
1	5	523:C	O3'	638:G	P	18.03

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	4138:C	O3'	4146:G	P	17.86
1	5	4101:C	O3'	4107:G	P	17.54
1	5	4777:C	O3'	4859:C	P	16.83
1	5	760:G	O3'	904:C	P	15.36
1	5	5022:U	O3'	5028:G	P	14.91
1	5	1696:C	O3'	1720:C	P	14.34
1	5	182:G	O3'	189:G	P	14.28
1	5	1364:U	O3'	1368:A	P	14.23
1	5	2901:G	O3'	3597:G	P	13.50
1	5	512:U	O3'	515:C	P	10.15
1	5	4729:A	O3'	4735:G	P	10.00
1	5	1180:C	O3'	1183:C	P	8.82
1	5	500:G	O3'	504:G	P	6.45
1	3	19:G	O3'	20:U	P	5.79
1	5	1100:U	O3'	1168:G	P	5.75
1	5	1239:C	O3'	1244:G	P	5.52
1	9	322:C	O3'	323:C	P	5.16
1	5	4740:G	O3'	4743:G	P	4.87
1	3	16:C	O3'	18:U	P	4.78
1	9	309:G	O3'	310:C	P	4.71
1	9	304:C	O3'	305:U	P	4.64
1	9	798:G	O3'	799:U	P	4.41
1	2	16:C	O3'	18:G	P	4.19
1	5	170:C	O3'	171:U	P	3.86
1	5	751:G	O3'	752:G	P	3.52
1	5	5020:G	O3'	5021:C	P	3.42
1	9	902:G	O3'	903:A	P	3.39
1	5	1438:U	O3'	1440:U	P	3.37
1	5	4899:G	O3'	4902:C	P	3.36
1	5	267:G	O3'	268:G	P	3.34
1	9	903:A	O3'	904:A	P	3.33
1	9	1295:A	O3'	1296:U	P	3.29

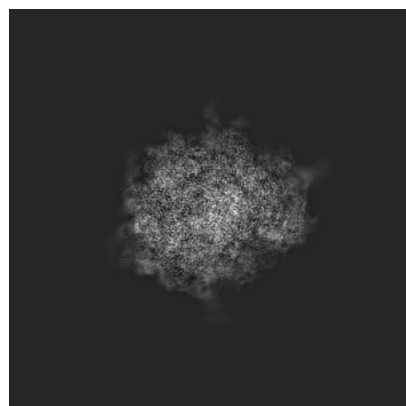
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4133. These allow visual inspection of the internal detail of the map and identification of artifacts.

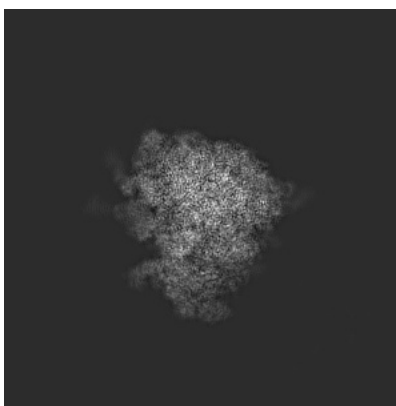
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

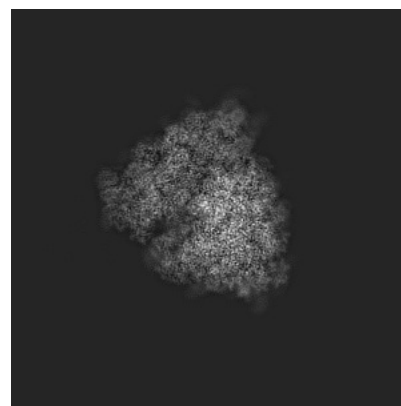
6.1.1 Primary map



X

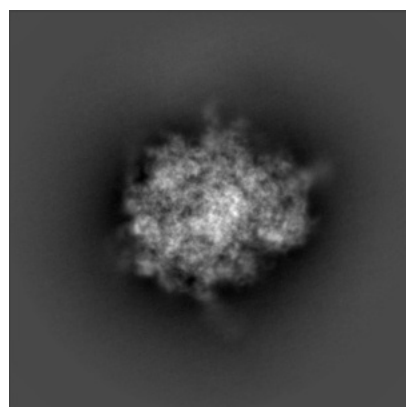


Y

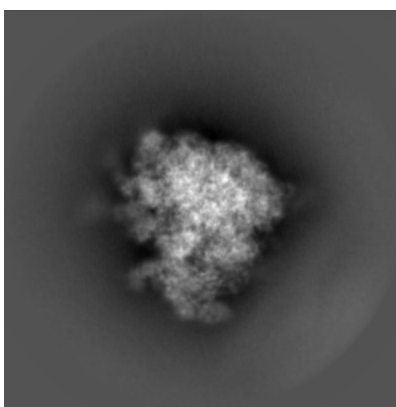


Z

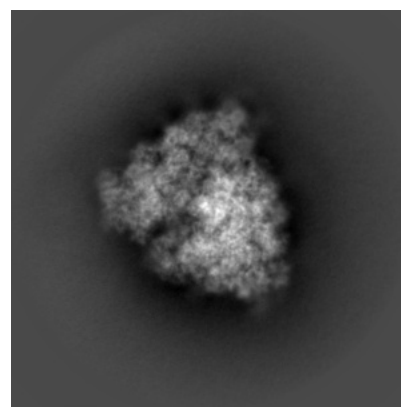
6.1.2 Raw map



X



Y



Z

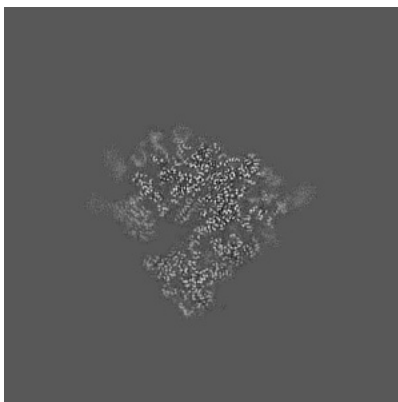
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

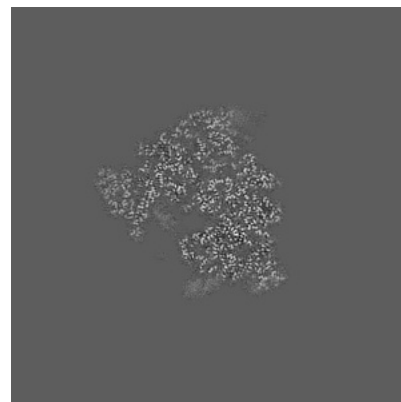
6.2.1 Primary map



X Index: 210

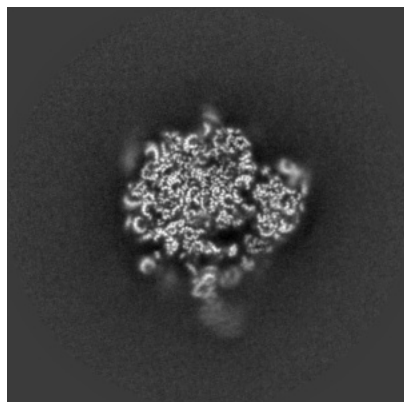


Y Index: 210

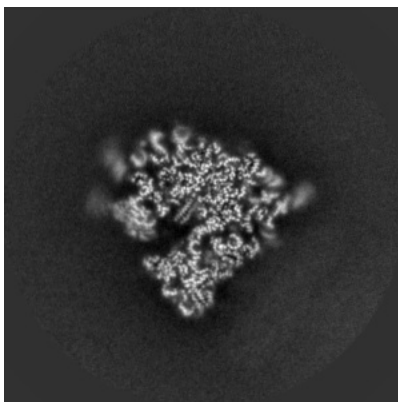


Z Index: 210

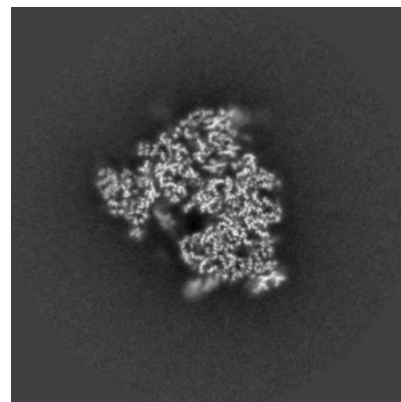
6.2.2 Raw map



X Index: 210



Y Index: 210

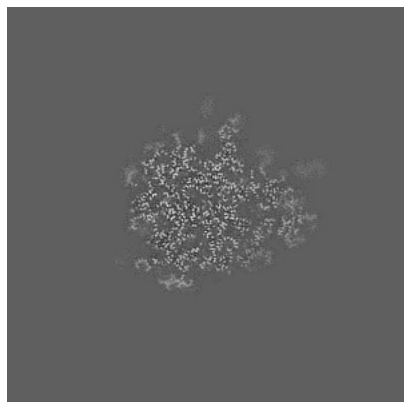


Z Index: 210

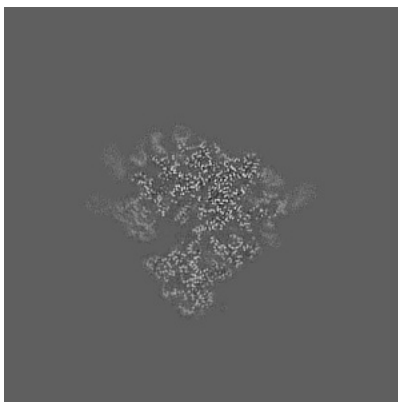
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

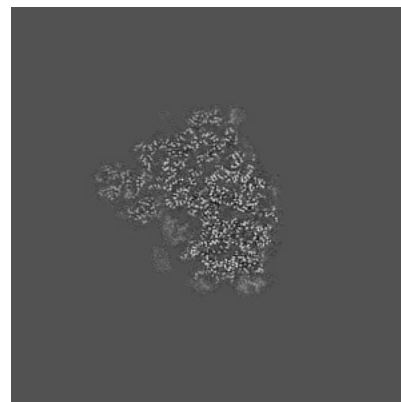
6.3.1 Primary map



X Index: 228

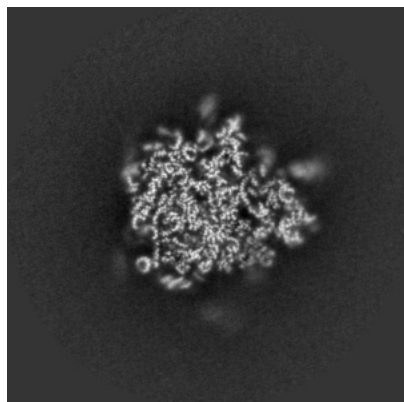


Y Index: 211

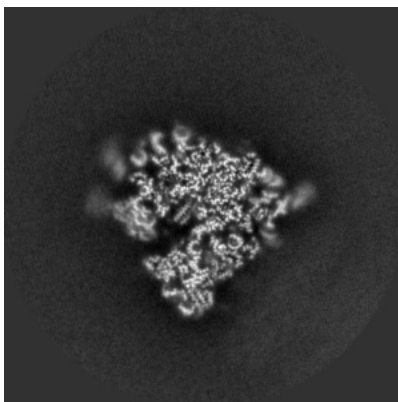


Z Index: 220

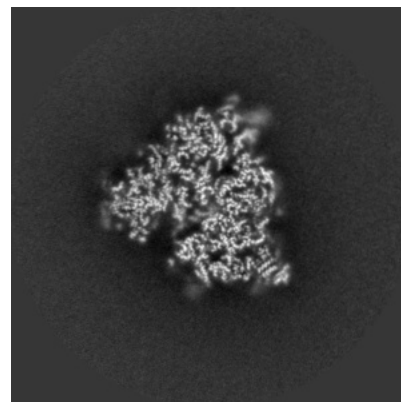
6.3.2 Raw map



X Index: 225



Y Index: 211

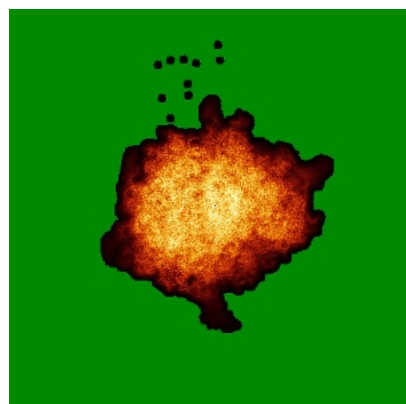


Z Index: 202

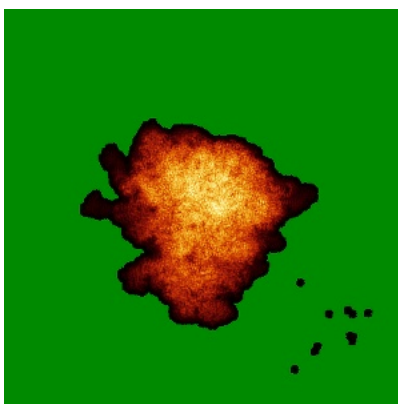
The images above show the largest variance slices of the map in three orthogonal directions.

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

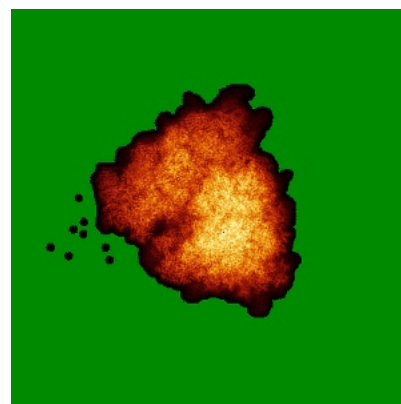
6.4.1 Primary map



X

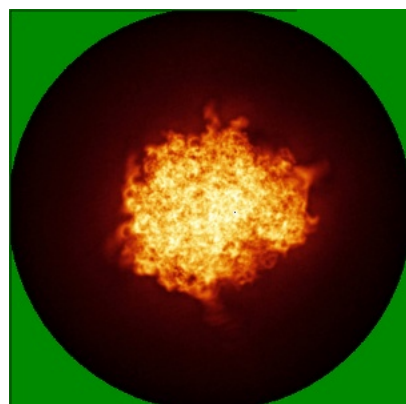


Y

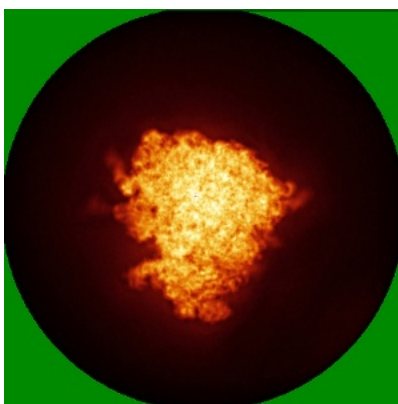


Z

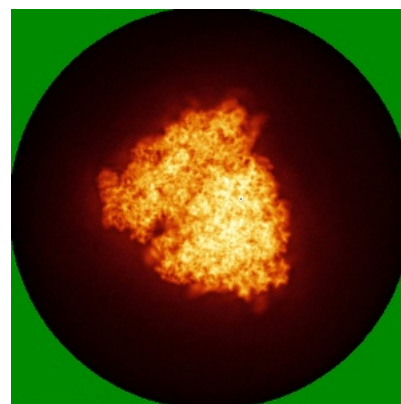
6.4.2 Raw map



X



Y

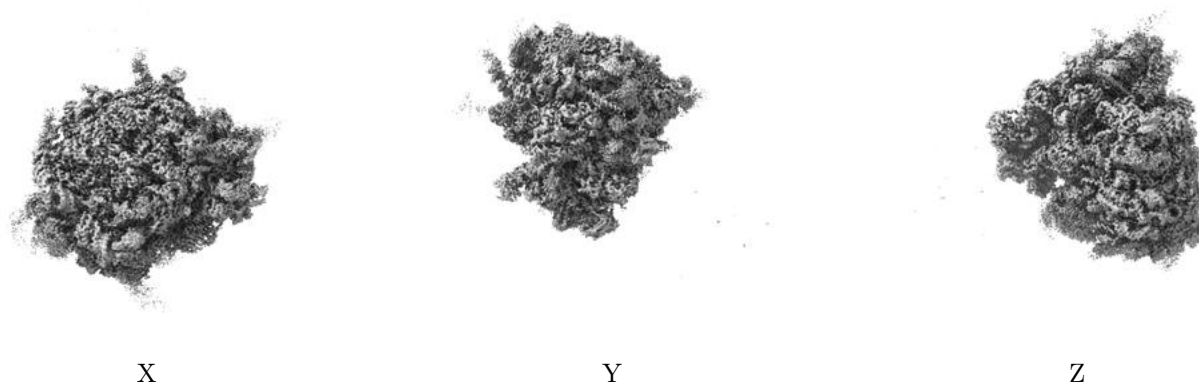


Z

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

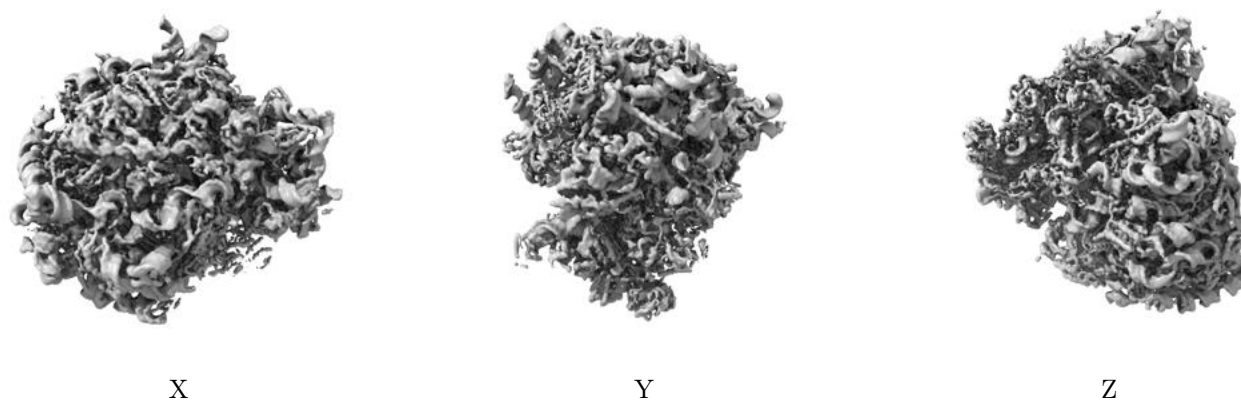
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

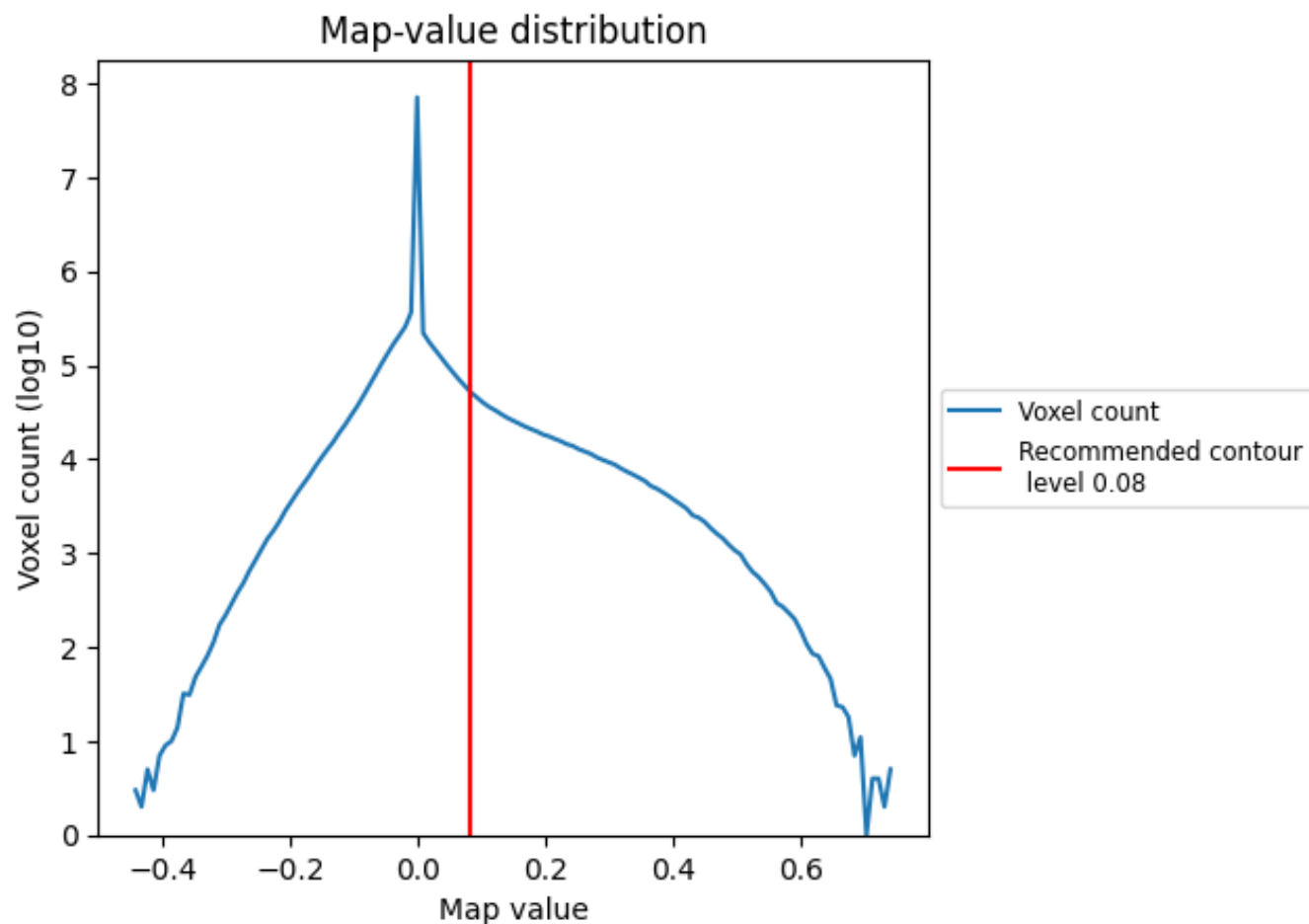
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

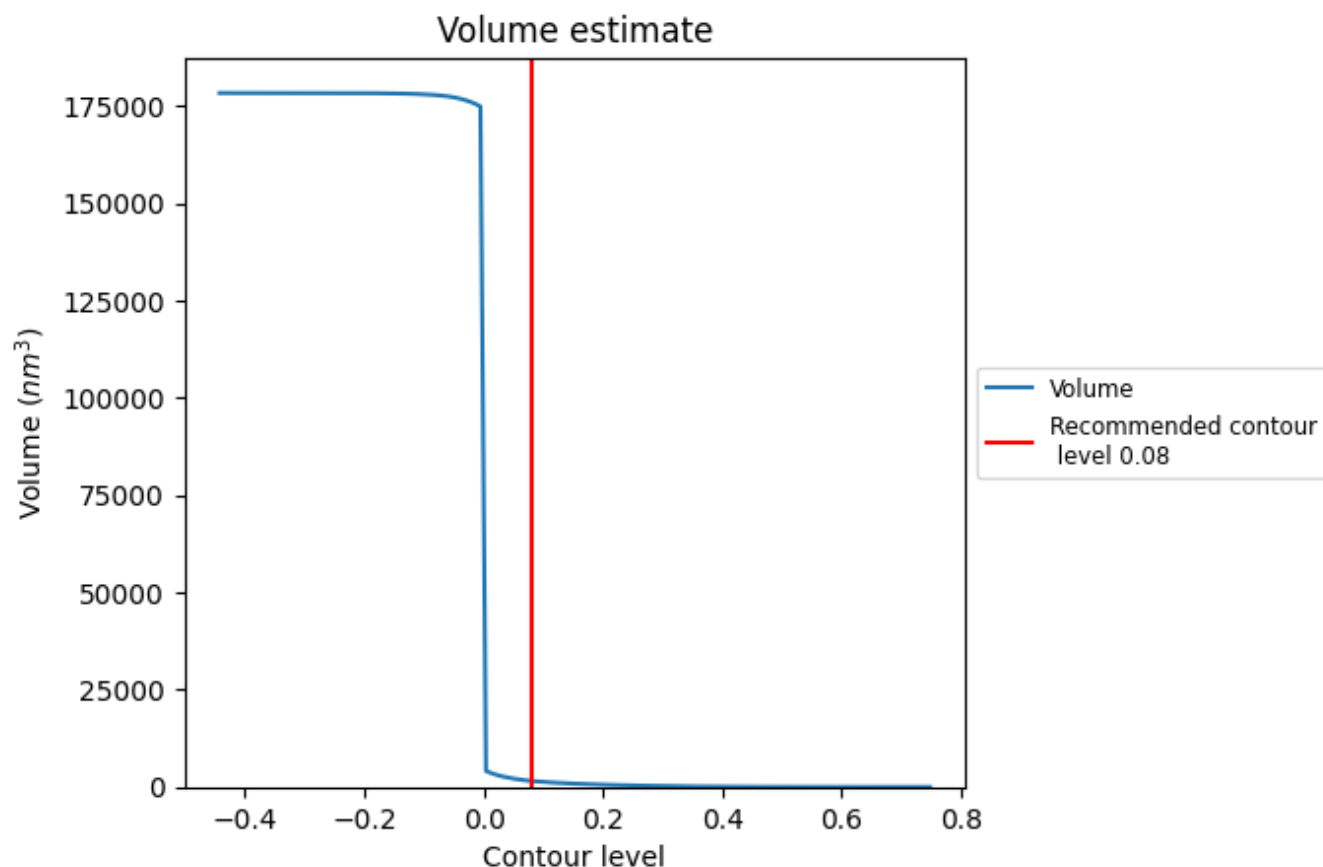
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

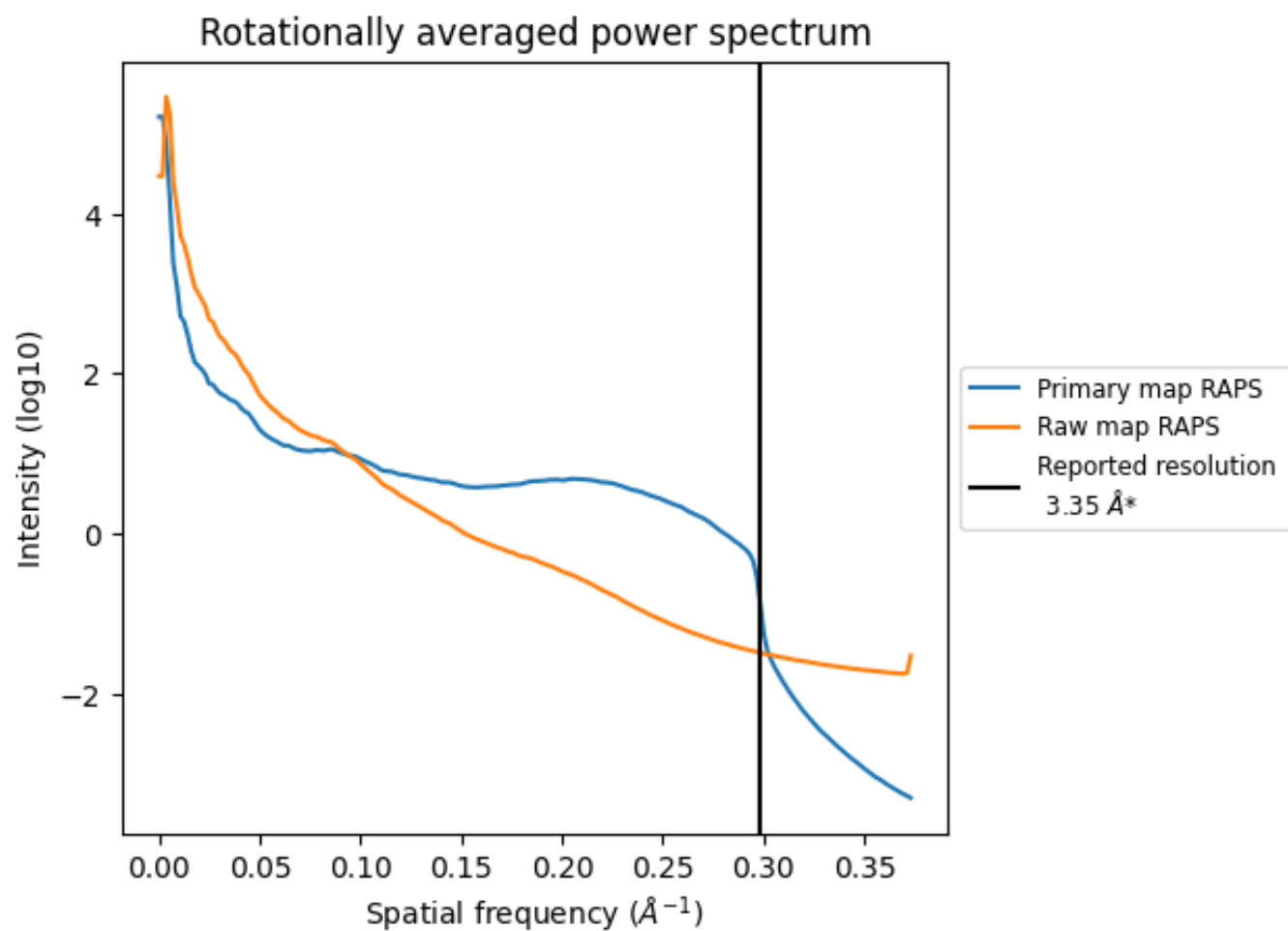
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1553 nm³; this corresponds to an approximate mass of 1402 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 ⓘ

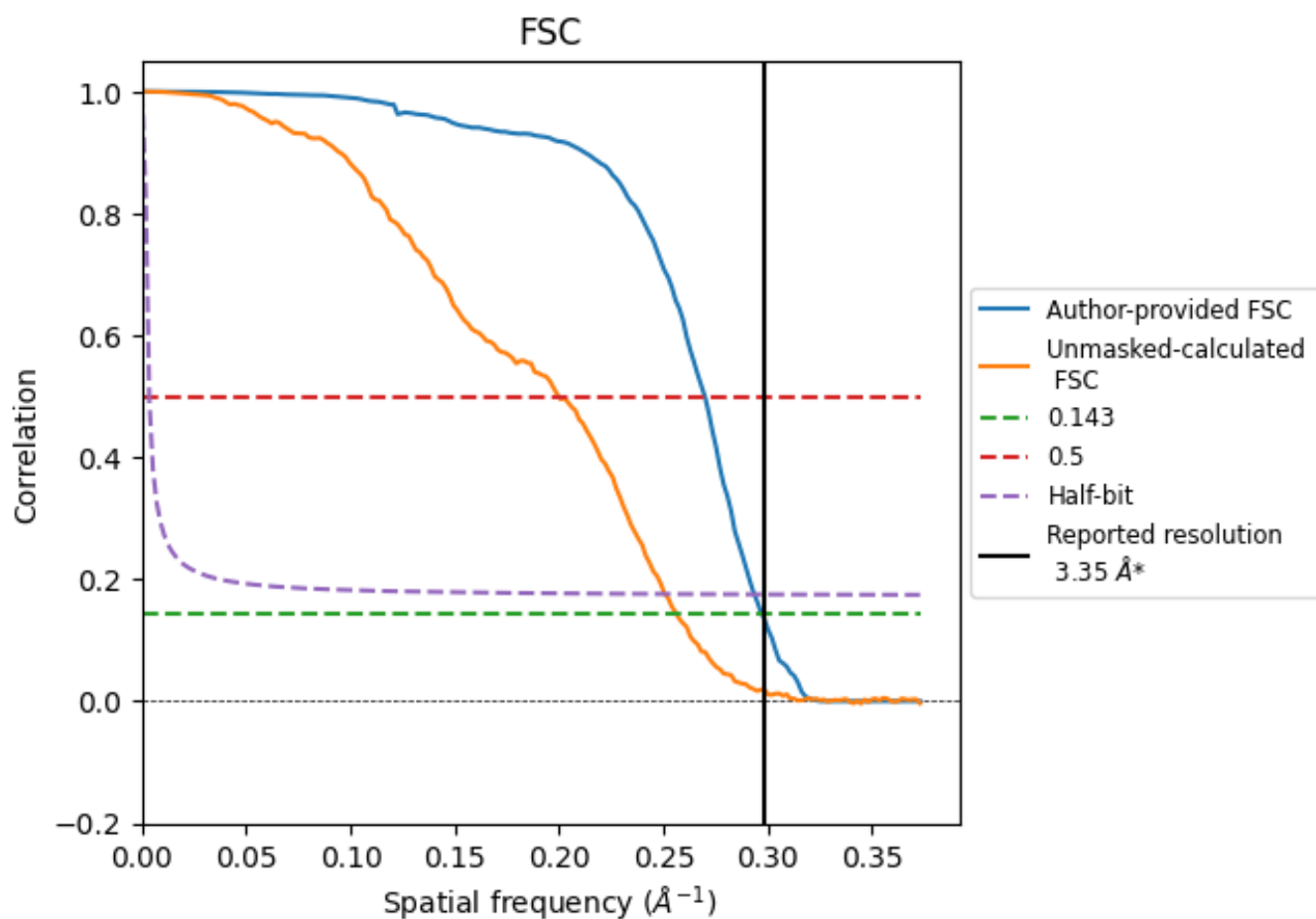


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.299 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

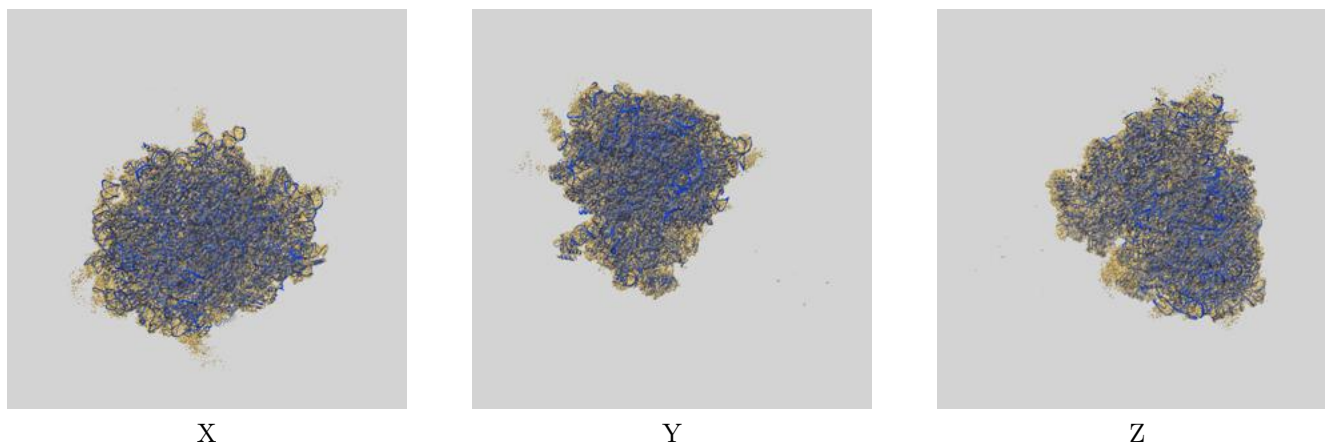
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.36	3.71	3.41
Unmasked-calculated*	3.90	5.01	3.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 3.35 by more than 10 %

9 Map-model fit [i](#)

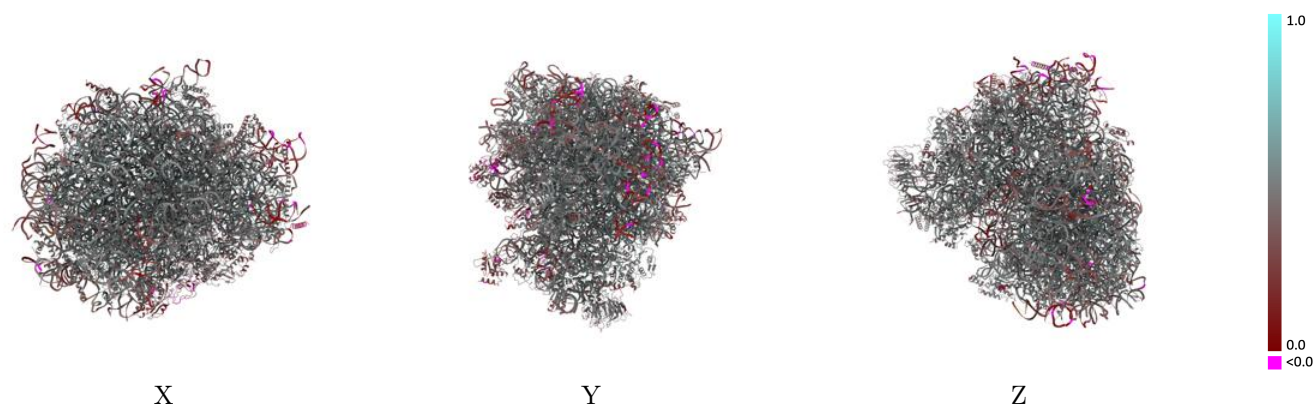
This section contains information regarding the fit between EMDB map EMD-4133 and PDB model 5LZV. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



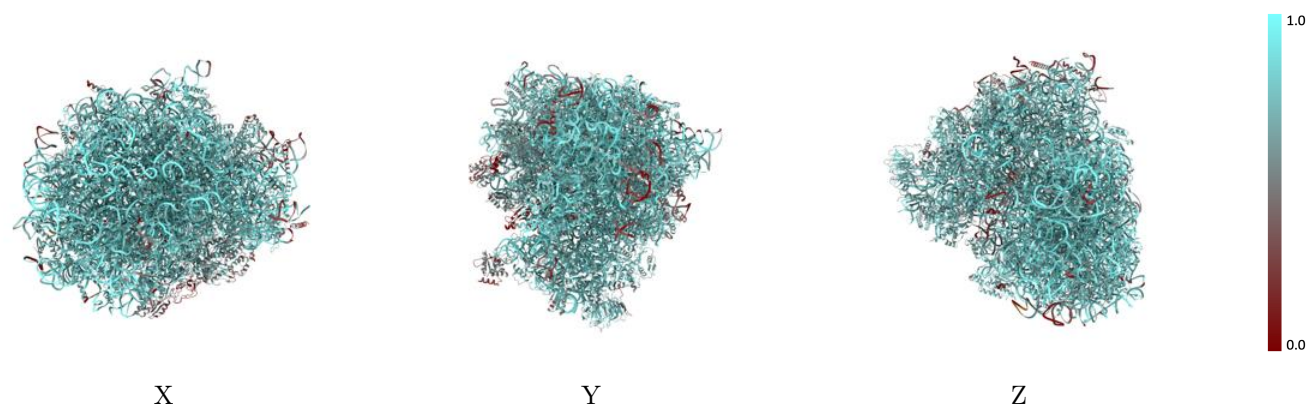
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



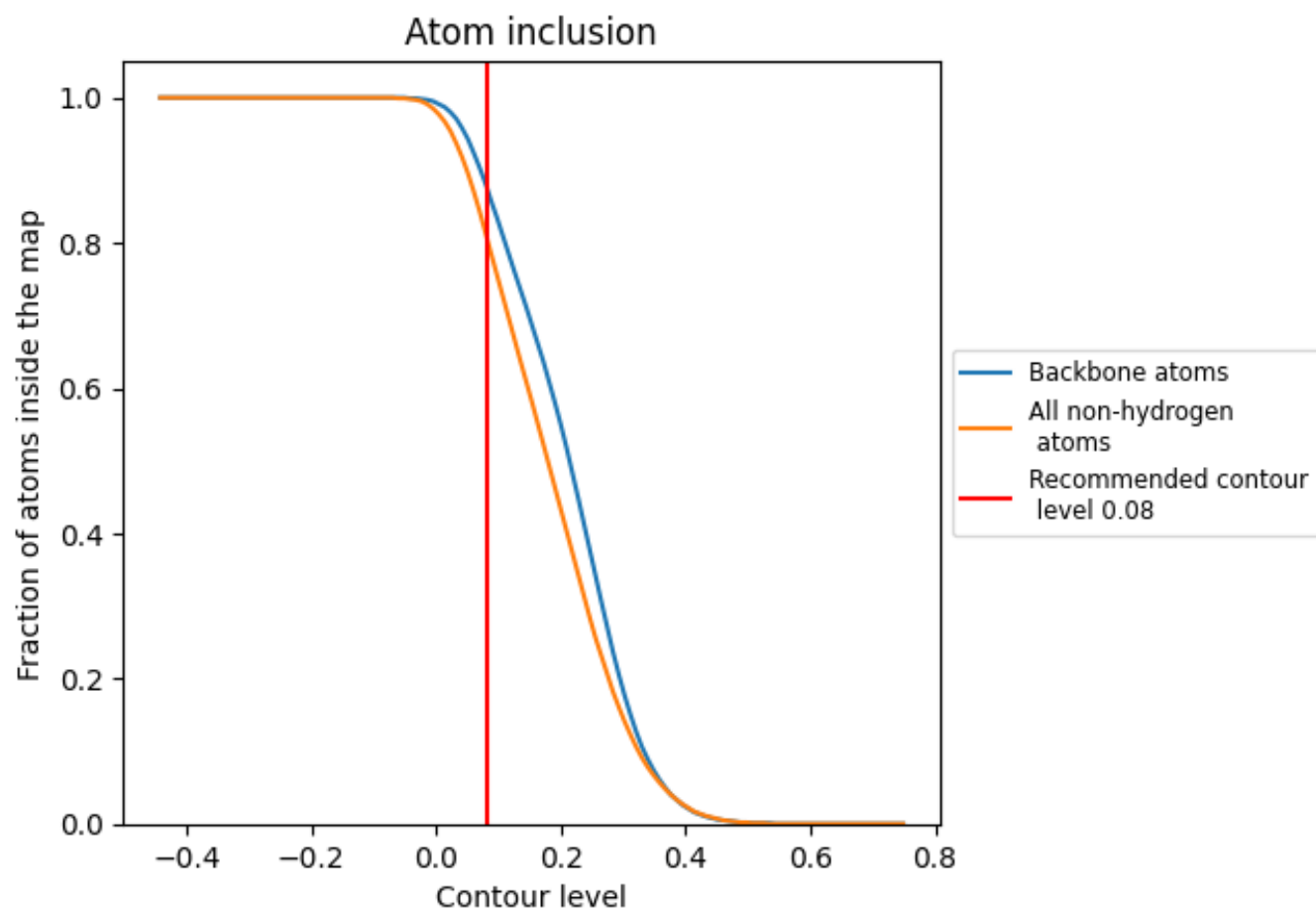
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8100	 0.4600
1	 0.6940	 0.4640
2	 0.8290	 0.4240
3	 0.5220	 0.2700
5	 0.8750	 0.4640
7	 0.9270	 0.4980
8	 0.8880	 0.4720
9	 0.8650	 0.4580
A	 0.8170	 0.5010
AA	 0.7620	 0.4790
B	 0.7970	 0.4860
BB	 0.7620	 0.4890
C	 0.8120	 0.4930
CC	 0.7630	 0.4860
D	 0.8020	 0.4710
DD	 0.6950	 0.4450
E	 0.7860	 0.4620
EE	 0.7690	 0.4830
F	 0.7970	 0.4930
FF	 0.7330	 0.4670
G	 0.7260	 0.4380
GG	 0.7000	 0.4270
H	 0.7680	 0.4710
HH	 0.6720	 0.4300
I	 0.7660	 0.4840
II	 0.7570	 0.4760
J	 0.7450	 0.4520
JJ	 0.7580	 0.4740
KK	 0.7370	 0.4460
L	 0.7710	 0.4640
LL	 0.7890	 0.4970
M	 0.7890	 0.4700
MM	 0.4080	 0.2890
N	 0.8440	 0.5100
NN	 0.7740	 0.4850



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Chain	Atom inclusion	Q-score
O	 0.7960	 0.4850
OO	 0.7740	 0.4920
P	 0.8060	 0.4980
PP	 0.7400	 0.4480
Q	 0.8230	 0.4930
QQ	 0.7670	 0.4780
R	 0.7500	 0.4510
RR	 0.7060	 0.4490
S	 0.8160	 0.4950
SS	 0.7670	 0.4670
T	 0.7930	 0.4810
TT	 0.7680	 0.4640
U	 0.7380	 0.4160
UU	 0.6850	 0.4390
V	 0.7650	 0.4880
VV	 0.7480	 0.4810
W	 0.6340	 0.3930
WW	 0.7930	 0.5020
X	 0.7520	 0.4580
XX	 0.7910	 0.5090
Y	 0.7980	 0.4760
YY	 0.7650	 0.4710
Z	 0.7950	 0.4630
ZZ	 0.7190	 0.4550
a	 0.8480	 0.5100
aa	 0.7940	 0.5010
b	 0.6850	 0.4250
bb	 0.7200	 0.4640
c	 0.7470	 0.4670
cc	 0.7150	 0.4700
d	 0.7780	 0.4710
dd	 0.8100	 0.5020
e	 0.8100	 0.5100
ee	 0.6880	 0.4560
f	 0.8350	 0.5020
ff	 0.5100	 0.3280
g	 0.7800	 0.4740
gg	 0.6960	 0.4420
h	 0.7710	 0.4740
hh	 0.7450	 0.4250
i	 0.7450	 0.4590
ii	 0.5650	 0.4080

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Chain	Atom inclusion	Q-score
j	 0.8440	 0.5030
jj	 0.5990	 0.4250
k	 0.7110	 0.4330
l	 0.8310	 0.4970
m	 0.8100	 0.4950
n	 0.7750	 0.4860
o	 0.7930	 0.4880
p	 0.7530	 0.4790
r	 0.8350	 0.5010
s	 0.3340	 0.2230
t	 0.4890	 0.3140