Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 02:45 am GMT

PDB ID	:	6ZVJ
EMDB ID	:	EMD-11458
Title	:	Structure of a human ABCE1-bound 43S pre-initiation complex - State II
Authors	:	Kratzat, H.; Mackens-Kiani, T.; Ameismeier, A.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on	:	2020-07-24
Resolution	:	3.80 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:

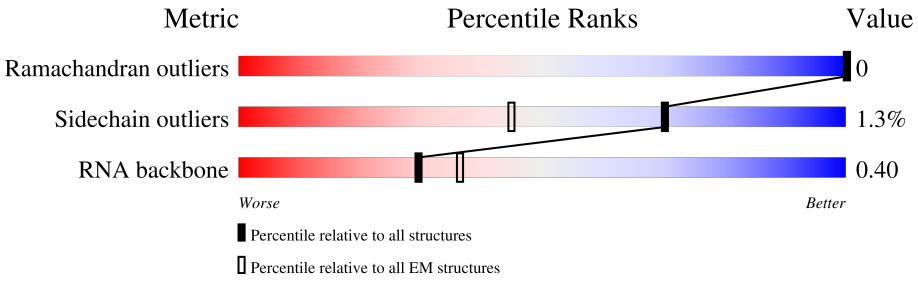
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	216	97%
2	p	211	99%
3	d	216	97%
4	Q	101	7% 100%
5	q	255	98%
6	W	24	25% 100%
7	r	222	99%
8	s	181	7% 94%

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Mol	Chain	Length	Quality of chain
9	t	205	97%
10	c	180	99%
11	n	144	93% 6%
12	m	149	99%
13	i	125	100%
14	y	82	98%
15	f	129	98%
16	j	139	98%
17	z	122	98%
18	R	82	5% 99%
19	T	44	5% 98%
20	2	1720	48% 42% 9%
21	w	130	8% 95%
22	g	138	7% 98%
23	b	224	18% 99%
24	e	189	16% 96%
25	u	95	35% 98%
26	v	116	50% 95%
27	o	119	50% 98%
28	k	140	33% 98%
29	x	141	16% 98%
30	h	98	16% 99%
31	P	70	31% 99%
32	S	61	36% 98%
33	l	54	6% 96%

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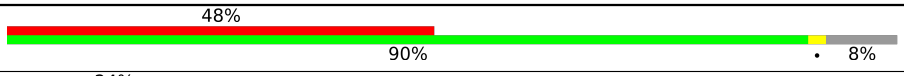
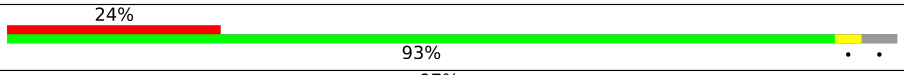
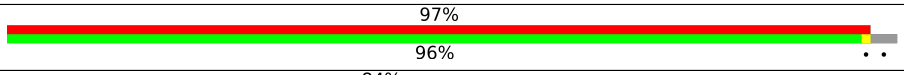
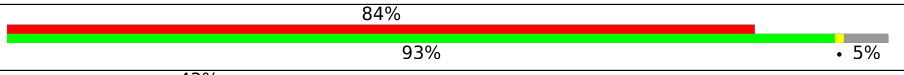
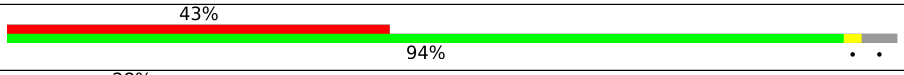
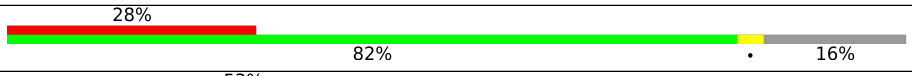
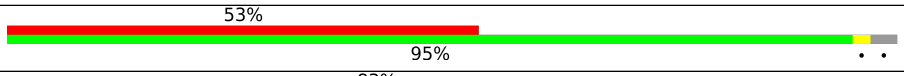
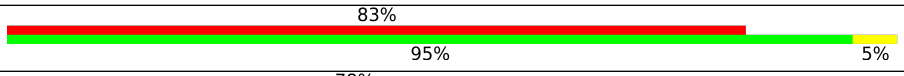
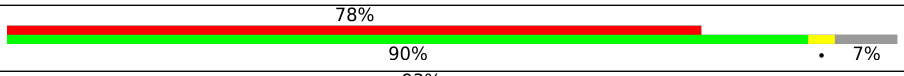
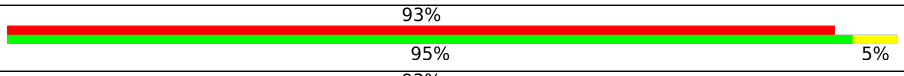
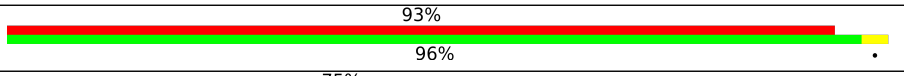
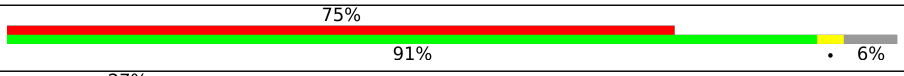
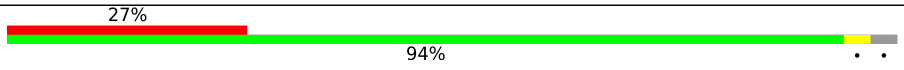
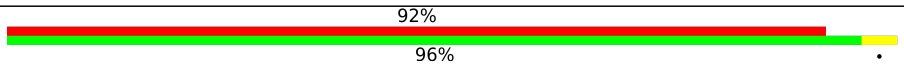
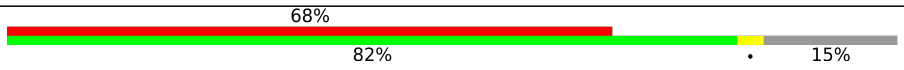
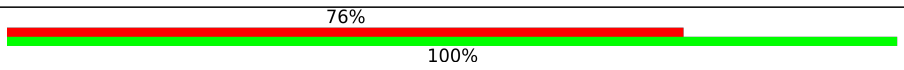
Mol	Chain	Length	Quality of chain
34	U	62	
35	V	309	
36	I	316	
37	B	566	
38	A	722	
39	C	743	
40	E	429	
41	F	269	
42	H	318	
43	K	217	
44	L	372	
45	M	362	
46	1	595	
47	N	91	
48	D	527	
49	Y	78	
50	G	258	
50	J	258	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 115020 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 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	216	1706	1083	299	316	8	0	0

- Molecule 2 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	p	211	1716	1088	307	307	14	0	0

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	d	216	1675	1085	287	293	10	0	0

- Molecule 4 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	Q	101	815	507	170	133	5	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	q	255	2032	1299	377	348	8	0	0

- Molecule 6 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	W	24	231	139	62	27	3	0	0

- Molecule 7 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	r	222	Total	C	N	O	S	0	0
			1795	1123	357	309	6		

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	s	173	Total	C	N	O	S	0	0
			1400	898	256	245	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
s	8	ILE	GLY	conflict	UNP P62081
s	9	VAL	GLU	conflict	UNP P62081
s	12	ASN	ASP	conflict	UNP P62081

- Molecule 9 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	t	199	Total	C	N	O	S	0	0
			1639	1027	322	285	5		

- Molecule 10 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	180	Total	C	N	O	S	0	0
			1500	955	300	243	2		

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	n	135	Total	C	N	O	S	0	0
			1120	715	211	188	6		

- Molecule 12 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	149	Total	C	N	O	S	0	0
			1203	770	228	204	1		

- Molecule 13 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	i	125	Total	C	N	O	S	0	0
			940	574	187	173	6		

- Molecule 14 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	y	82	Total	C	N	O	S	0	0
			626	384	116	121	5		

- Molecule 15 is a protein called 40S ribosomal protein S15a.

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

- Molecule 16 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	j	139	Total	C	N	O	S	0	0
			1081	682	214	182	3		

- Molecule 17 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	z	122	Total	C	N	O	S	0	0
			1000	633	196	166	5		

- Molecule 18 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	82	Total	C	N	O	S	0	0
			641	402	118	114	7		

- Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	44	Total	C	N	O	S	0	0
			355	216	81	57	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	54	GLY	VAL	conflict	UNP P62861
T	56	ASN	THR	conflict	UNP P62861
T	57	ALA	PHE	conflict	UNP P62861
T	58	ASN	GLY	conflict	UNP P62861

- Molecule 20 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	1720	Total	C	N	O	P	0	0
			36700	16391	6600	11998	1711		

- Molecule 21 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	w	128	Total	C	N	O	S	0	0
			1011	641	182	184	4		

- Molecule 22 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	138	Total	C	N	O	S	0	0
			1100	699	208	190	3		

- Molecule 23 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	224	Total	C	N	O	S	0	0
			1746	1112	314	313	7		

- Molecule 24 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 25 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	u	95	Total	C	N	O	S	0	0
			800	524	139	131	6		

- Molecule 26 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	v	111	Total	C	N	O	S	0	0
			862	544	151	160	7		

- Molecule 27 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	o	119	Total	C	N	O	S	0	0
			980	623	183	167	7		

- Molecule 28 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	k	140	Total	C	N	O	S	0	0
			1163	731	234	197	1		

- Molecule 29 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	x	141	Total	C	N	O	S	0	0
			1095	685	210	197	3		

- Molecule 30 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	98	Total	C	N	O	S	0	0
			781	489	148	140	4		

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	P	70	Total	C	N	O	S	0	0
			558	358	101	98	1		

- Molecule 32 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	61	Total	C	N	O	S	0	0
			480	292	95	91	2		

- Molecule 33 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	54	Total	C	N	O	S	0	0
			451	282	93	71	5		

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	U	57	Total	C	N	O	S	0	0
			466	295	89	75	7		

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	V	296	Total	C	N	O	S	0	0
			2315	1464	404	435	12		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	I	305	Total	C	N	O	0	0
			1497	887	305	305		

- Molecule 37 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B	536	Total	C	N	O	S	0	0
			2966	1801	580	580	5		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A	692	Total	C	N	O	S	0	0
			5384	3378	980	1004	22		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	C	625	Total	C	N	O	S	0	0
			5073	3205	899	934	35		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	130	MET	-	insertion	UNP B4DVU3
C	131	ASN	HIS	conflict	UNP B4DVU3
C	132	LYS	ASP	conflict	UNP B4DVU3
C	133	ASN	ARG	conflict	UNP B4DVU3
C	134	ASN	LYS	conflict	UNP B4DVU3
C	135	ALA	SER	conflict	UNP B4DVU3
C	137	ALA	ARG	conflict	UNP B4DVU3
C	?	-	ASP	deletion	UNP B4DVU3
C	?	-	GLU	deletion	UNP B4DVU3
C	?	-	GLU	deletion	UNP B4DVU3
C	?	-	GLU	deletion	UNP B4DVU3
C	?	-	GLU	deletion	UNP B4DVU3
C	?	-	ASP	deletion	UNP B4DVU3
C	?	-	ASN	deletion	UNP B4DVU3
C	?	-	GLU	deletion	UNP B4DVU3
C	?	-	GLY	deletion	UNP B4DVU3
C	?	-	GLY	deletion	UNP B4DVU3
C	?	-	GLU	deletion	UNP B4DVU3
C	?	-	TRP	deletion	UNP B4DVU3
C	?	-	GLU	deletion	UNP B4DVU3
C	?	-	ARG	deletion	UNP B4DVU3
C	?	-	VAL	deletion	UNP B4DVU3
C	?	-	ARG	deletion	UNP B4DVU3
C	?	-	GLY	deletion	UNP B4DVU3
C	?	-	GLY	deletion	UNP B4DVU3
C	?	-	VAL	deletion	UNP B4DVU3
C	139	SER	PRO	conflict	UNP B4DVU3
C	140	THR	LEU	conflict	UNP B4DVU3
C	141	LEU	VAL	conflict	UNP B4DVU3
C	142	ARG	LYS	conflict	UNP B4DVU3
C	143	GLN	GLU	conflict	UNP B4DVU3
C	145	ILE	PRO	conflict	UNP B4DVU3
C	146	ARG	LYS	conflict	UNP B4DVU3
C	147	LYS	MET	conflict	UNP B4DVU3
C	148	TYR	PHE	conflict	UNP B4DVU3
C	149	ASN	ALA	conflict	UNP B4DVU3

- Molecule 40 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	E	416	Total	C	N	O	S	0	0
			3437	2202	585	630	20		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	F	269	Total	C	N	O	S	0	0
			2090	1317	356	405	12		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	H	295	Total	C	N	O	S	0	0
			2413	1532	417	449	15		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	K	217	Total	C	N	O	S	0	0
			1750	1116	288	334	12		

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L	372	Total	C	N	O	S	0	0
			3112	2011	520	564	17		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	M	340	Total	C	N	O	S	0	0
			2718	1734	459	508	17		

- Molecule 46 is a protein called ATP-binding cassette sub-family E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1	576	Total	C	N	O	S	0	0
			4542	2899	779	836	28		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	N	91	Total	C	N	O	S	0	0
			728	460	131	135	2		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	D	447	Total	C	N	O	S	0	0
			3618	2279	625	692	22		

- Molecule 49 is a protein called RNA recognition motif (unknown).

Mol	Chain	Residues	Atoms				AltConf	Trace
49	Y	78	Total	C	N	O	0	0
			390	234	78	78		

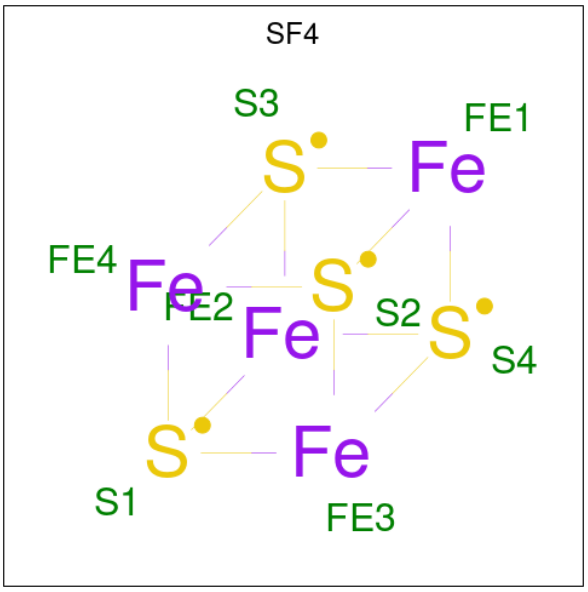
- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit J.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	G	70	Total	C	N	O	0	0
			348	208	70	70		
50	J	73	Total	C	N	O	0	0
			363	217	73	73		

- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

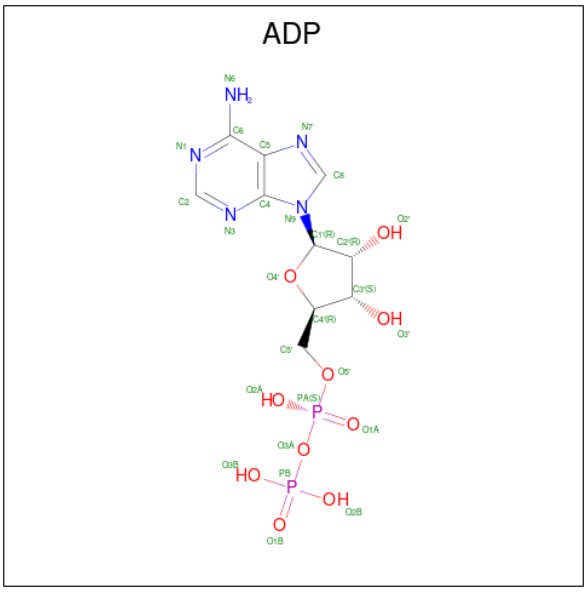
Mol	Chain	Residues	Atoms		AltConf
51	Q	1	Total	Zn	0
			1	1	
51	l	1	Total	Zn	0
			1	1	
51	U	1	Total	Zn	0
			1	1	

- Molecule 52 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
52	1	1	Total	Fe	S	0
			16	8	8	
52	1	1	Total	Fe	S	0
			16	8	8	

- Molecule 53 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

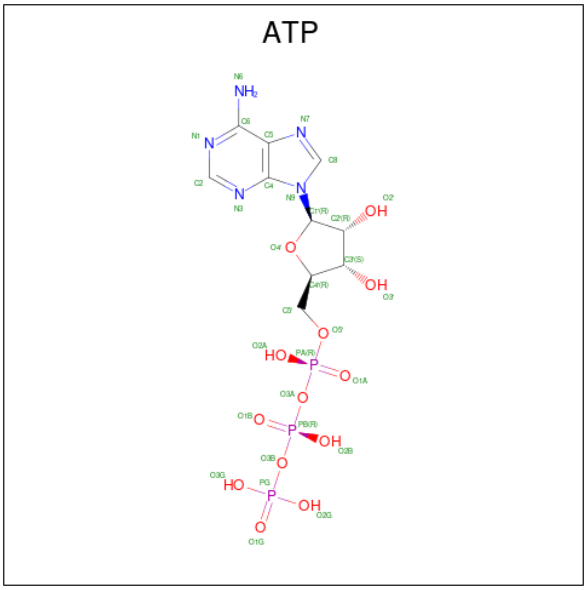


Mol	Chain	Residues	Atoms					AltConf
53	1	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	1	2	Total	Mg	0
			2	2	

- Molecule 55 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



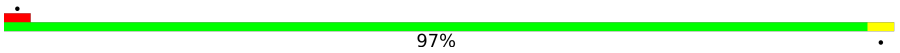
Mol	Chain	Residues	Atoms					AltConf
55	1	1	Total	C	N	O	P	0
			31	10	5	13	3	

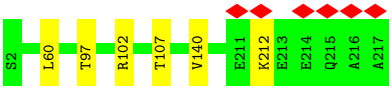
3 Residue-property plots (i)

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: 40S ribosomal protein SA

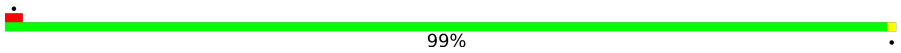
Chain a:

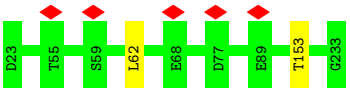




• Molecule 2: 40S ribosomal protein S3a

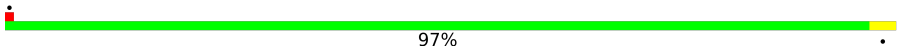
Chain p:

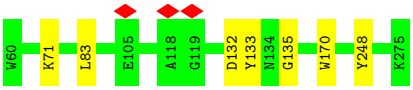




• Molecule 3: 40S ribosomal protein S2

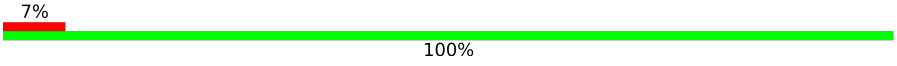
Chain d:

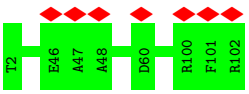




• Molecule 4: 40S ribosomal protein S26

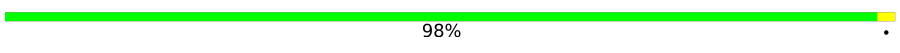
Chain Q:

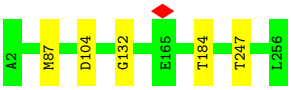




• Molecule 5: 40S ribosomal protein S4, X isoform

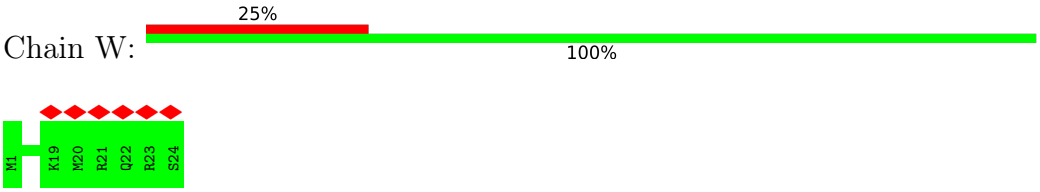
Chain q:





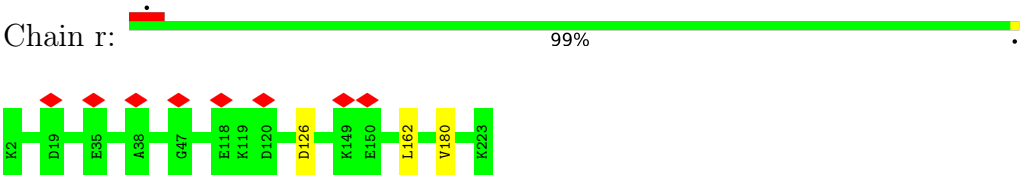
• Molecule 6: 60S ribosomal protein L41

Chain W:



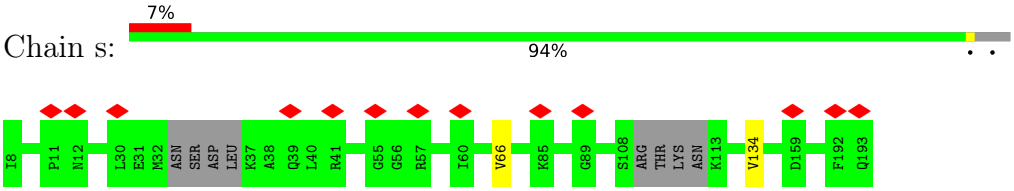
• Molecule 7: 40S ribosomal protein S6

Chain r:



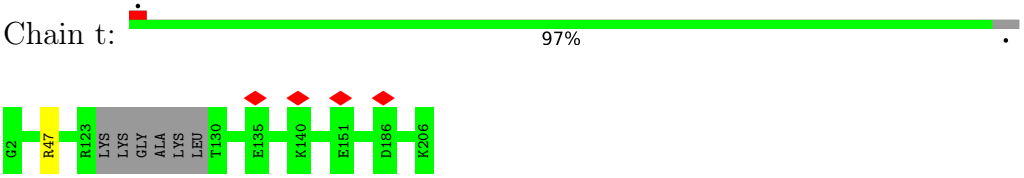
• Molecule 8: 40S ribosomal protein S7

Chain s:



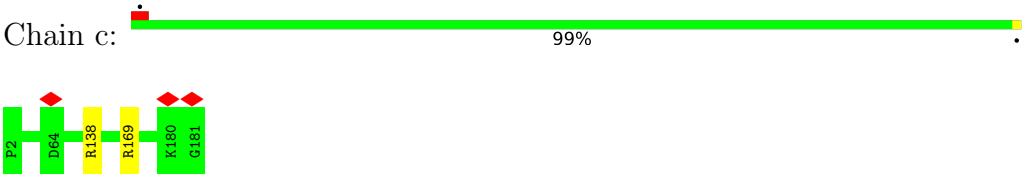
• Molecule 9: 40S ribosomal protein S8

Chain t:



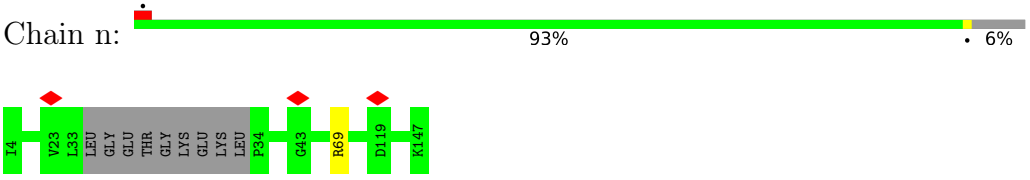
• Molecule 10: 40S ribosomal protein S9

Chain c:



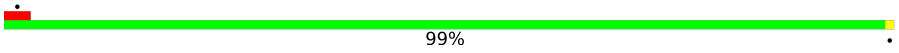
• Molecule 11: 40S ribosomal protein S11

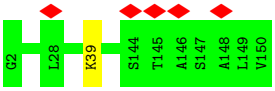
Chain n:



• Molecule 12: 40S ribosomal protein S13

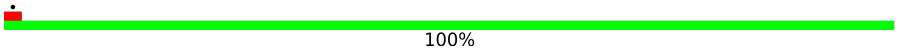
Chain m:

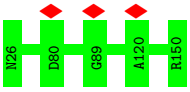




• Molecule 13: 40S ribosomal protein S14

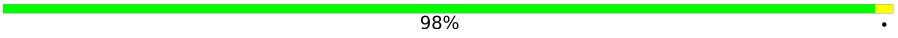
Chain i:

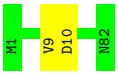




• Molecule 14: 40S ribosomal protein S21

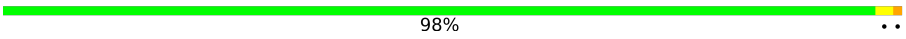
Chain y:

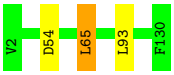




• Molecule 15: 40S ribosomal protein S15a

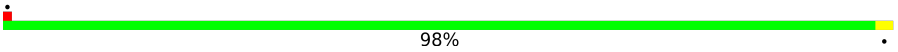
Chain f:

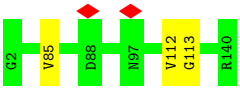




• Molecule 16: 40S ribosomal protein S23

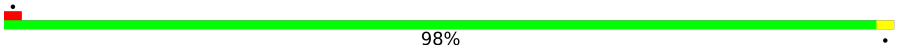
Chain j:

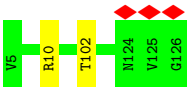




• Molecule 17: 40S ribosomal protein S24

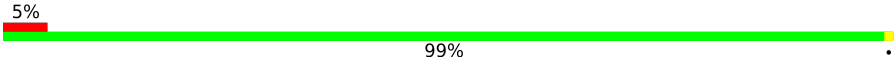
Chain z:

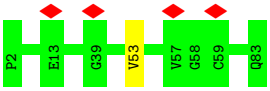




• Molecule 18: 40S ribosomal protein S27

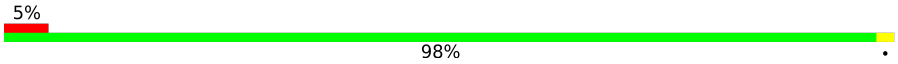
Chain R:

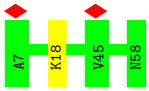




• Molecule 19: 40S ribosomal protein S30

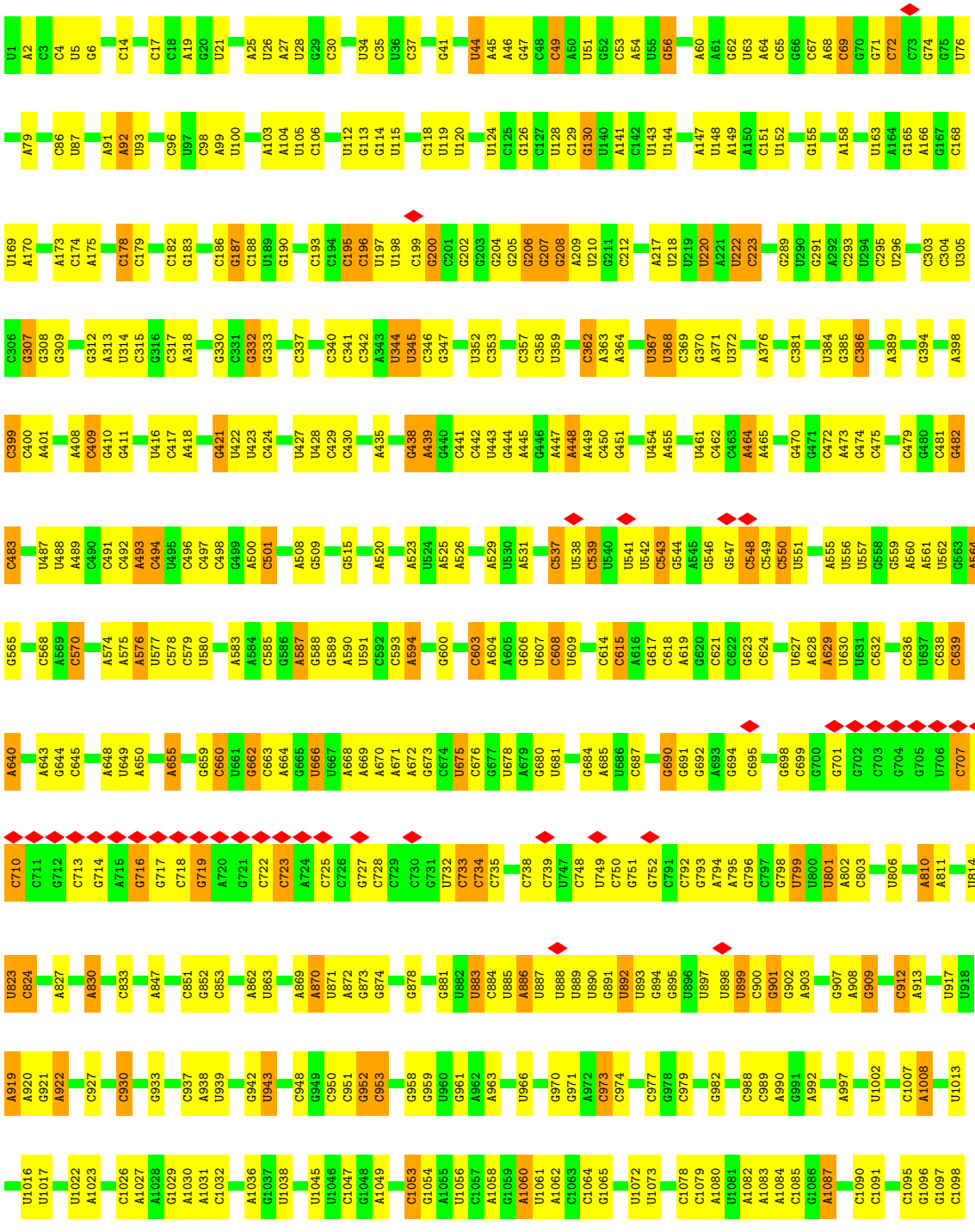
Chain T:

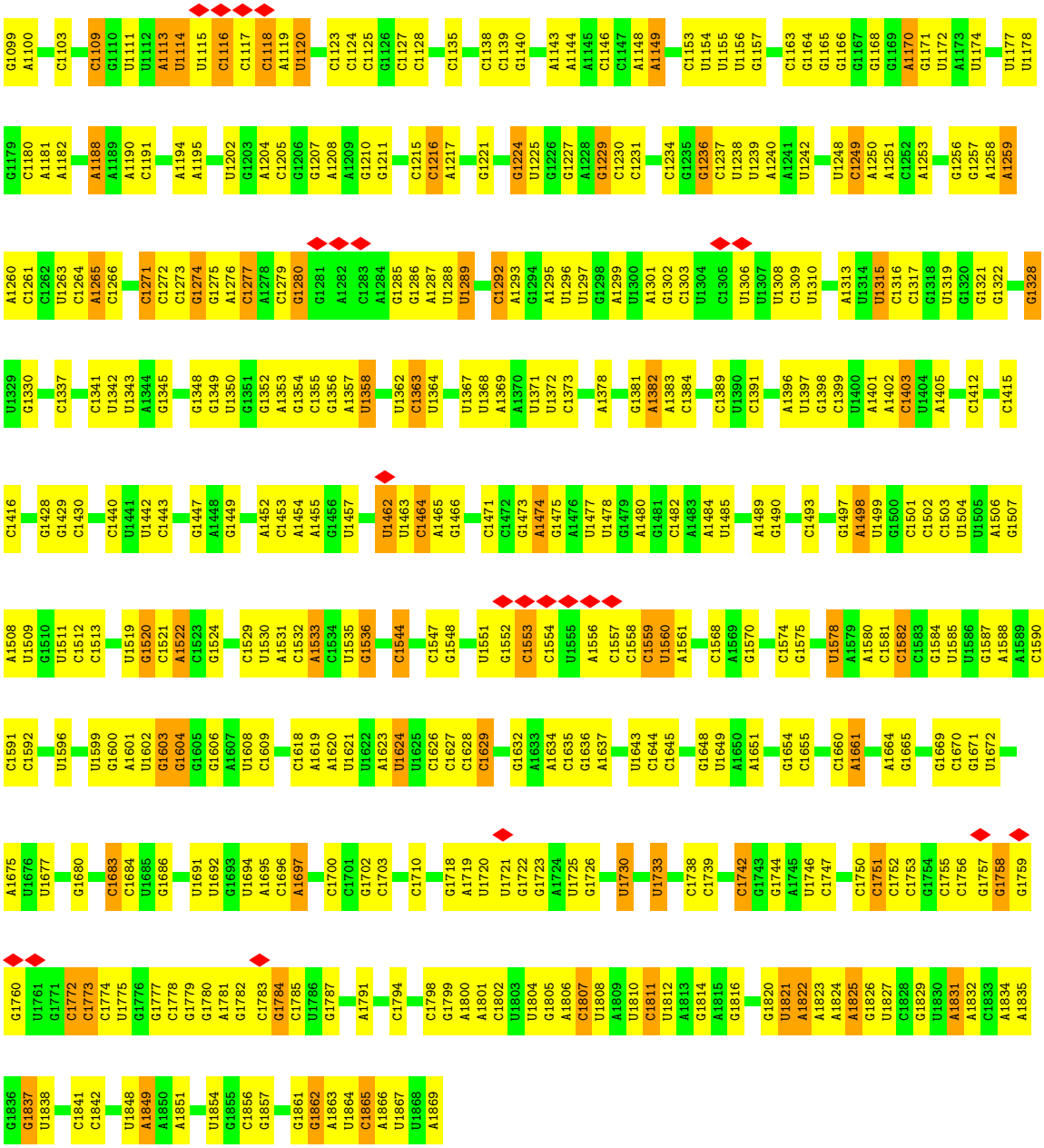




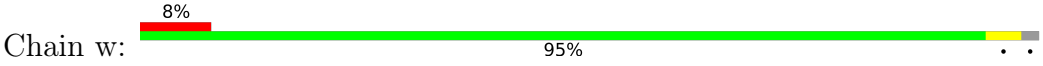
• Molecule 20: 18S ribosomal RNA

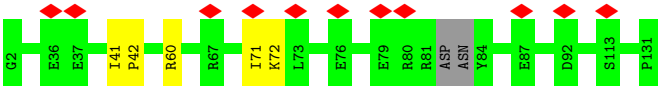
Chain 2:



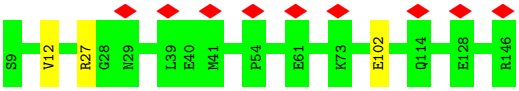


• Molecule 21: 40S ribosomal protein S17



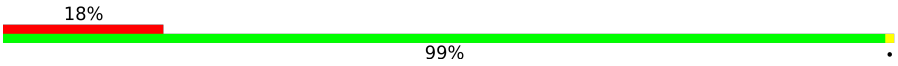


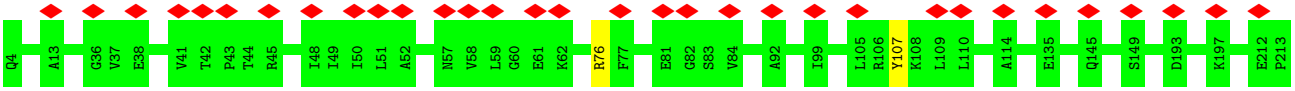
• Molecule 22: 40S ribosomal protein S16

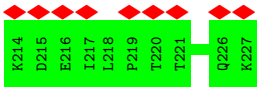


• Molecule 23: 40S ribosomal protein S3

Chain b:

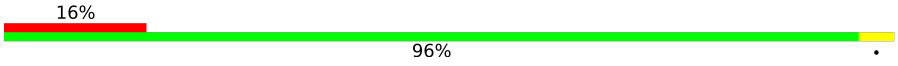


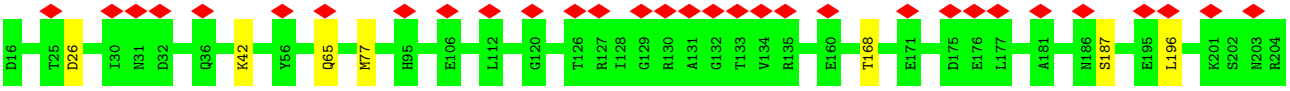




• Molecule 24: 40S ribosomal protein S5

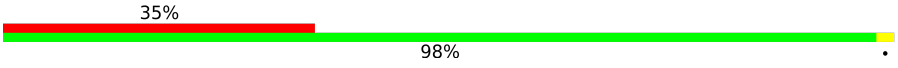
Chain e:

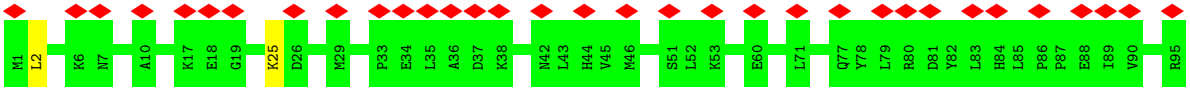




• Molecule 25: 40S ribosomal protein S10

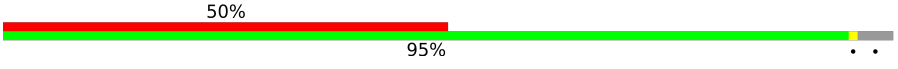
Chain u:

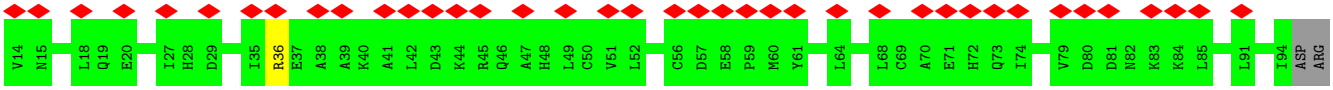


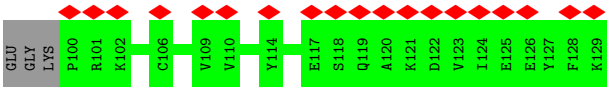


• Molecule 26: 40S ribosomal protein S12

Chain v:

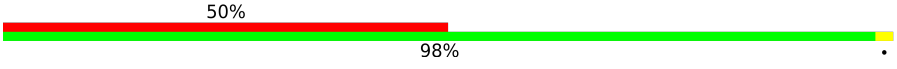


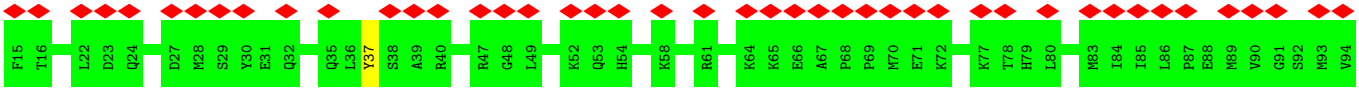


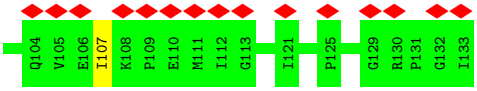


• Molecule 27: 40S ribosomal protein S15

Chain o:

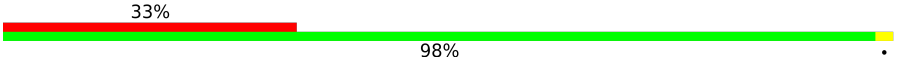


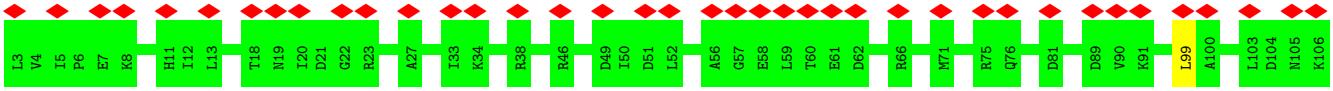


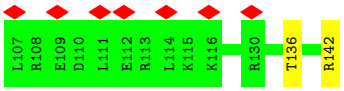


• Molecule 28: 40S ribosomal protein S18

Chain k:

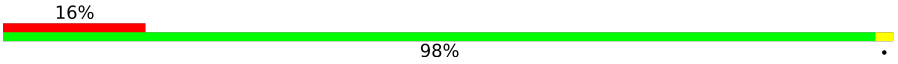


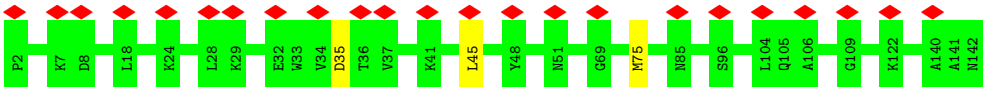




• Molecule 29: 40S ribosomal protein S19

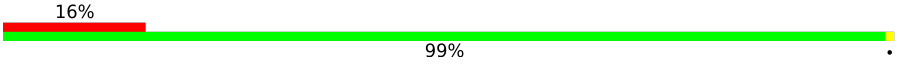
Chain x:

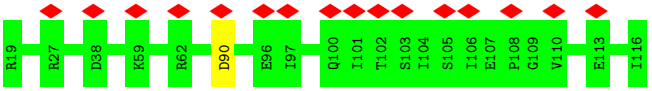




• Molecule 30: 40S ribosomal protein S20

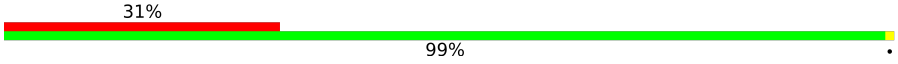
Chain h:

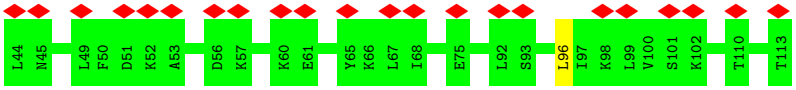




• Molecule 31: 40S ribosomal protein S25

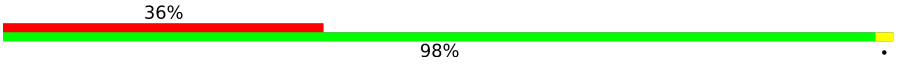
Chain P:

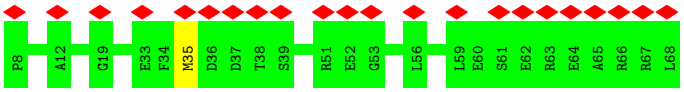




• Molecule 32: 40S ribosomal protein S28

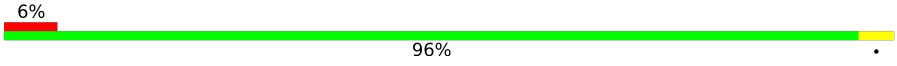
Chain S:

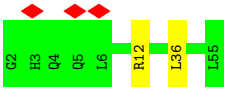




• Molecule 33: 40S ribosomal protein S29

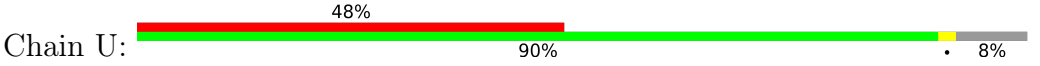
Chain l:

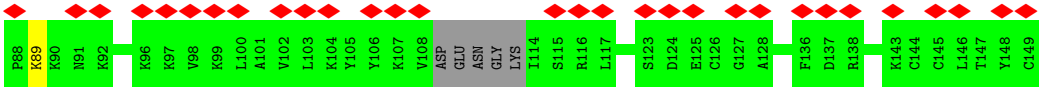




• Molecule 34: Ubiquitin-40S ribosomal protein S27a

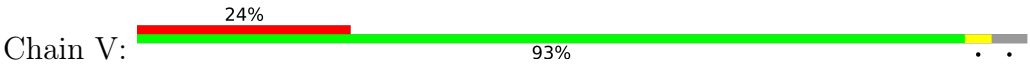
Chain U:

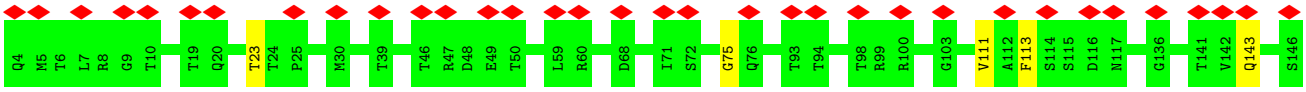


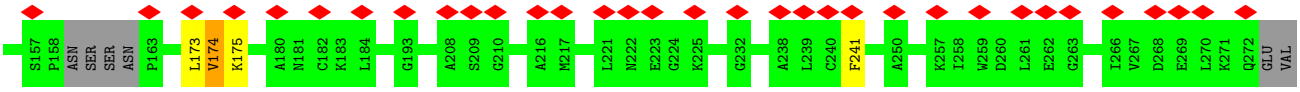


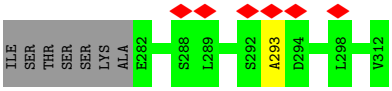
• Molecule 35: Receptor of activated protein C kinase 1

Chain V:



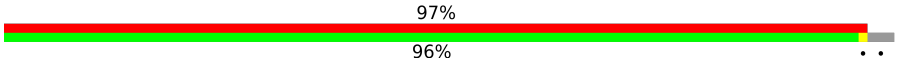


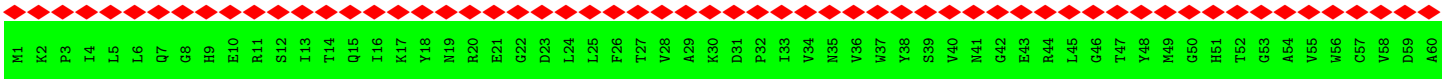


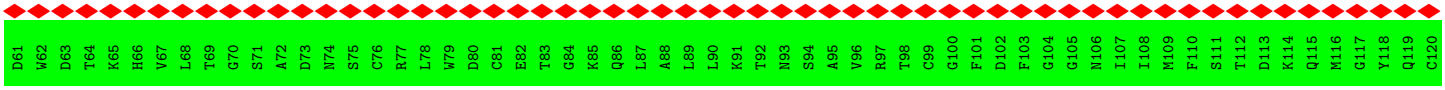


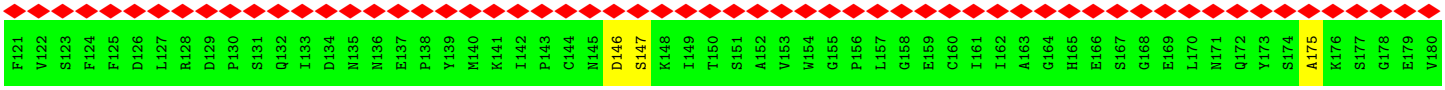
• Molecule 36: Eukaryotic translation initiation factor 3 subunit I

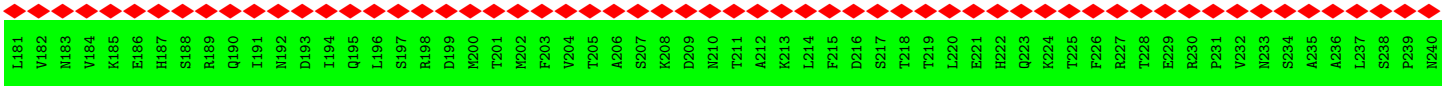
Chain I:

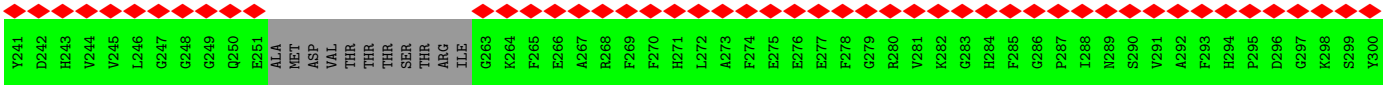








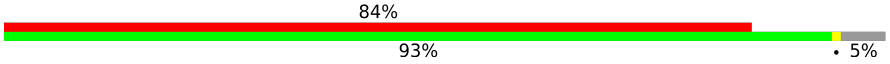




S301 S302 G303 G304 E305 D306 G307 Y308 V309 R310 I311 H312 Y313 F314 D315 P316

• Molecule 37: Eukaryotic translation initiation factor 3 subunit B

Chain B:



A180 D181 G182 I183 D184 S185 V186 I187 V188 V189 D190 N191 V192 P193 Q194 V195 G196 P197 D198 R199 L200 E201 K202 L203 K204 N205 V206 I207 H208 K209 I210 F211 S212 K213 F214 G215 K216 I217 T218 N219 D220 F221 Y222 P223 E224 E225 D226 G227 K228 T229 K230 G231 Y232 I233 F234 L235 E236 Y237 A238 S239

P240 A241 H242 A243 V244 D245 A246 V247 K248 N249 A250 D251 G252 Y253 K254 L255 D256 K257 Q258 H259 T260 F261 R262 V263 N264 L265 PHE THR ASP PHE ASP LYS TYR MET THR ILE SER ASP GLU TRP ASP ILE PRO GLU LYS GLN PRO PHE LYS D289 L290 G291 N292 L293 R294 Y295 W296 L297 E298 E299

A300 E301 C302 R303 D304 Q305 Y306 S307 V308 I309 F310 E311 S312 G313 D314 R315 T316 S317 I318 N321 D322 V323 K324 D325 P326 V327 S328 I329 E330 E331 R332 A333 R334 W335 T336 E337 T338 Y339 V340 R341 W342 S343 P344 K345 G346 T347 Y348 L349 A350 T351 F352 H353 Q354 R355 G356 I357 A358 L359 W360

G361 G362 E363 K364 F365 K366 Q367 I368 Q369 R370 F371 S372 H373 Q374 G375 V376 Q377 L378 I379 D380 F381 S382 P383 C384 E385 R386 V389 T390 F391 S392 P393 L394 M395 D396 T397 Q398 D399 D400 P401 Q402 A403 I404 I405 I406 W407 D408 I409 L410 T411 G412 H413 K414 K415 R416 G417 F418 H419 C420 E421

S422 S423 A424 H425 W426 P427 ILE F429 K430 W431 S432 H433 D434 G435 K436 F437 F438 A439 R440 M441 T442 L443 D444 T445 L446 S447 I448 Y449 E450 T451 P452 S453 M454 G455 L456 L457 D458 K459 K460 S461 L462 K463 I464 S465 G466 I467 K468 D469 F470 S471 W472 G475 G476 N477 I478 I479 A480 P484

E485 D486 K487 D488 T494 L495 M496 Q497 L498 P499 T500 R501 Q502 E503 I504 R505 V506 R507 N508 L509 F510 N511 V512 V513 K516 L517 H518 W519 Q520 K521 D524 Y525 L526 C527 V528 K529 V530 D531 R532 K535 G536 T537 Q538 G539 V540 V541 T542 N543 F544 E545 I546 F547 R548 N549 R550 E551

K552 Q553 V554 P555 V556 D557 V558 V559 E560 M561 K562 E563 T564 I565 I566 A567 F568 A569 W570 N573 G574 S575 K576 F577 A578 V579 L580 H581 G582 E583 A584 P585 R586 I587 S588 V589 S590 F591 Y592 H593 V594 K595 N596 N597 G598 K599 I600 E601 L602 I603 K604 M605 F606 D607 K608 Q609 Q610 A611 N612

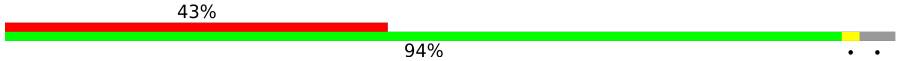
T613 I614 F615 W616 S617 P618 Q619 G620 Q621 F622 V623 V624 L625 A626 G627 L628 R629 S630 M631 N632 G633 A634 L635 A636 F637 V638 D639 T640 S641 D642 C643 T644 V645 M646 N647 I648 A649 E650 H651 Y652 M653 A654 S655 D656 V657 E658 W659 D660 P661 T662 G663 R664 Y665 V666 V667 T668 S669 V670 S671 W672

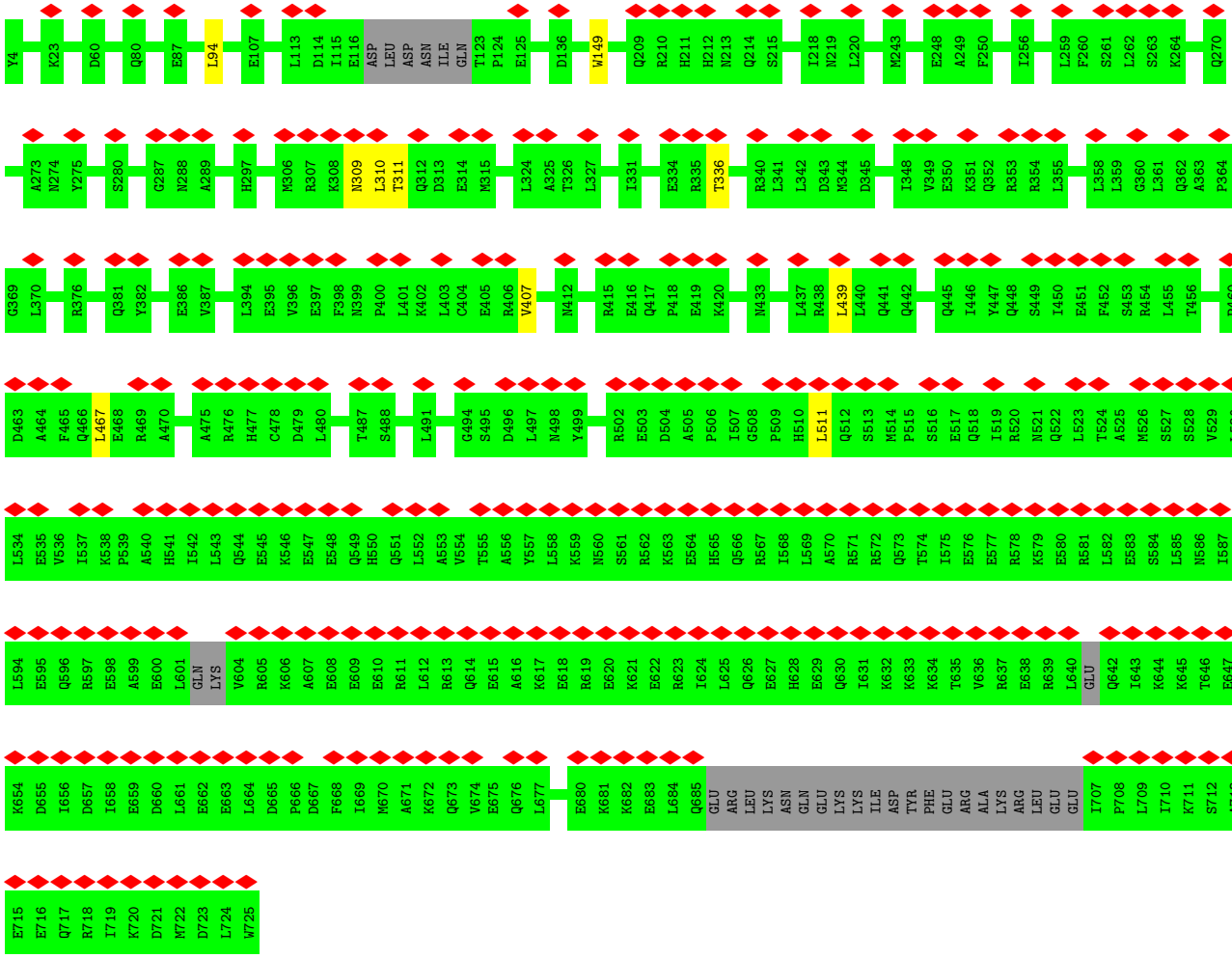
W673 S674 H675 K676 V677 D678 N679 A680 Y681 W682 L683 W684 T685 F686 Q687 G688 R689 L690 L691 Q692 K693 N694 N695 K696 D697 R698 F699 C700 Q701 L702 L703 W704 R705 P706 R707 P708 P709 T710 L711 L712 S713 Q714 E715 Q716 I717 K718 Q719 I720 K721 K722 ASP LEU LYS LYS TYR SER K729 I730 F731 E732

Q733 K734 D735 R736 L737 S738 Q739 S740 K741 A742 S743 K744 E745

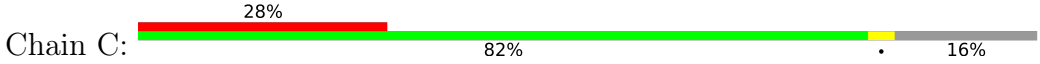
• Molecule 38: Eukaryotic translation initiation factor 3 subunit A

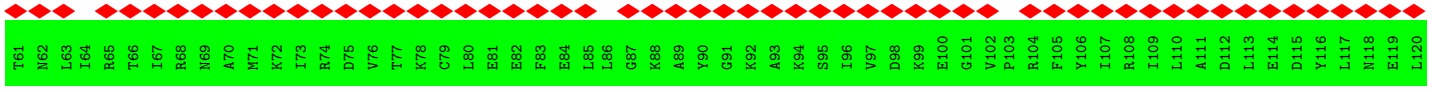
Chain A:

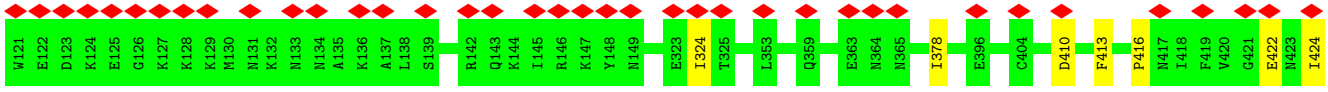


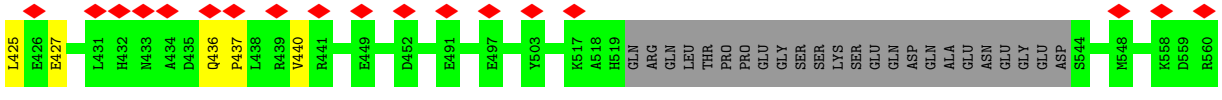


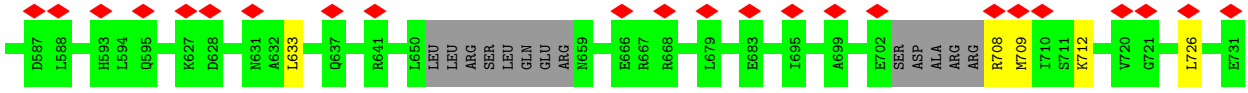
• Molecule 39: Eukaryotic translation initiation factor 3 subunit C

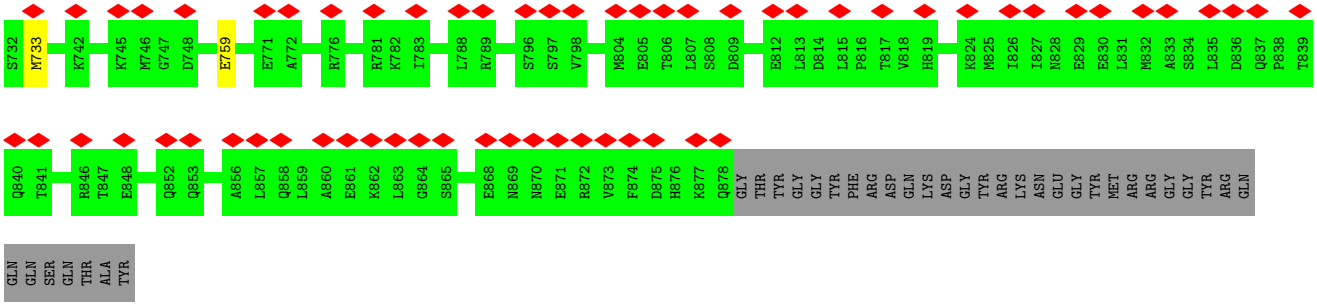




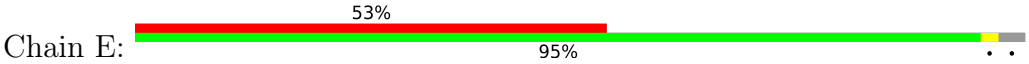


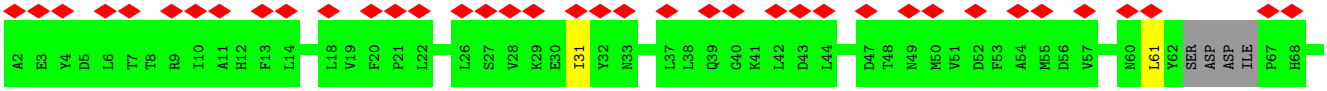


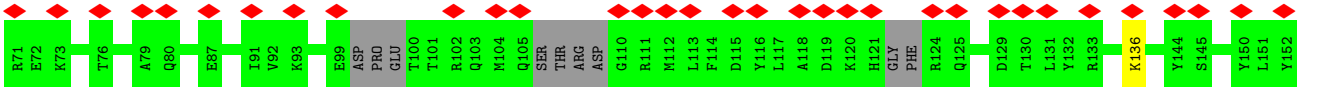


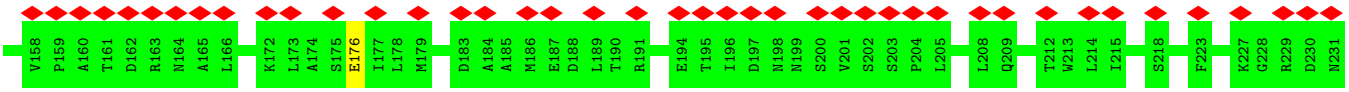


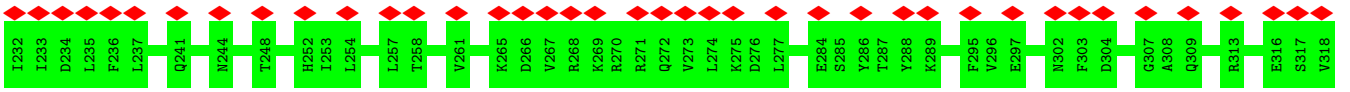
• Molecule 40: Eukaryotic translation initiation factor 3 subunit E

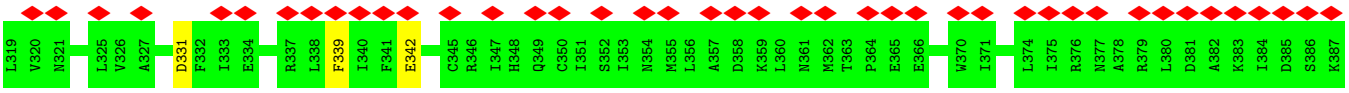


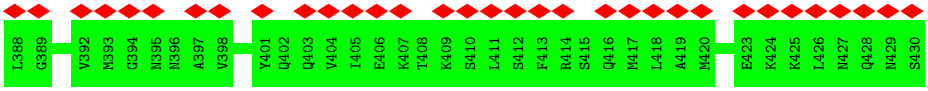




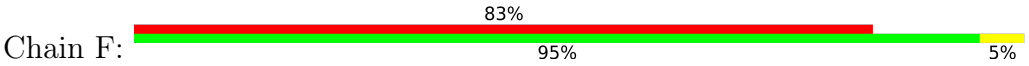


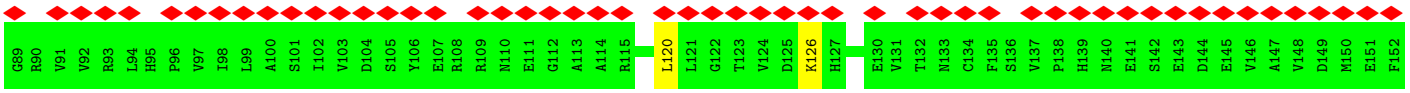


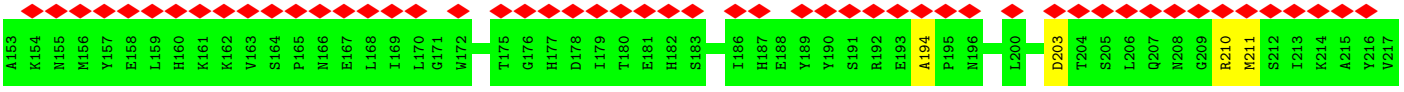


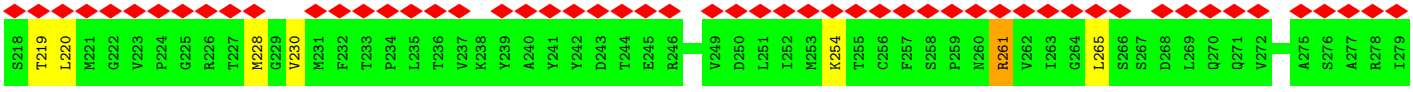


• Molecule 41: Eukaryotic translation initiation factor 3 subunit F

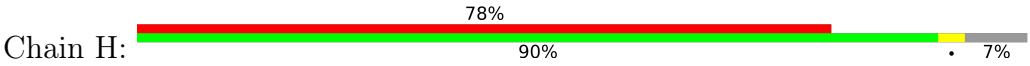


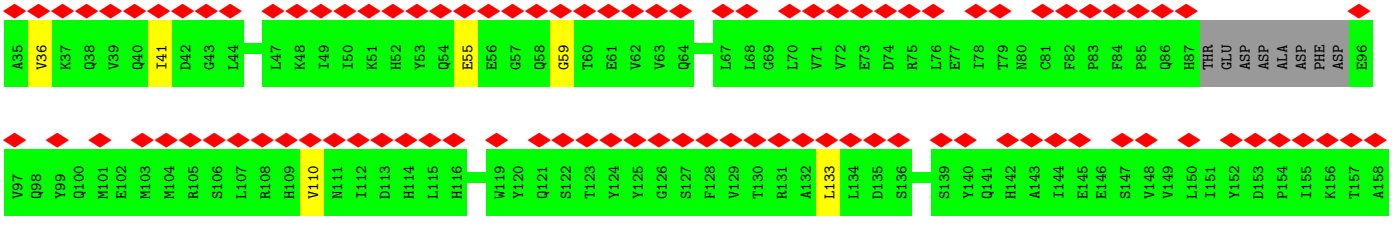




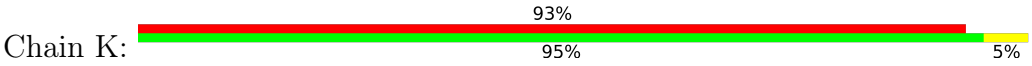


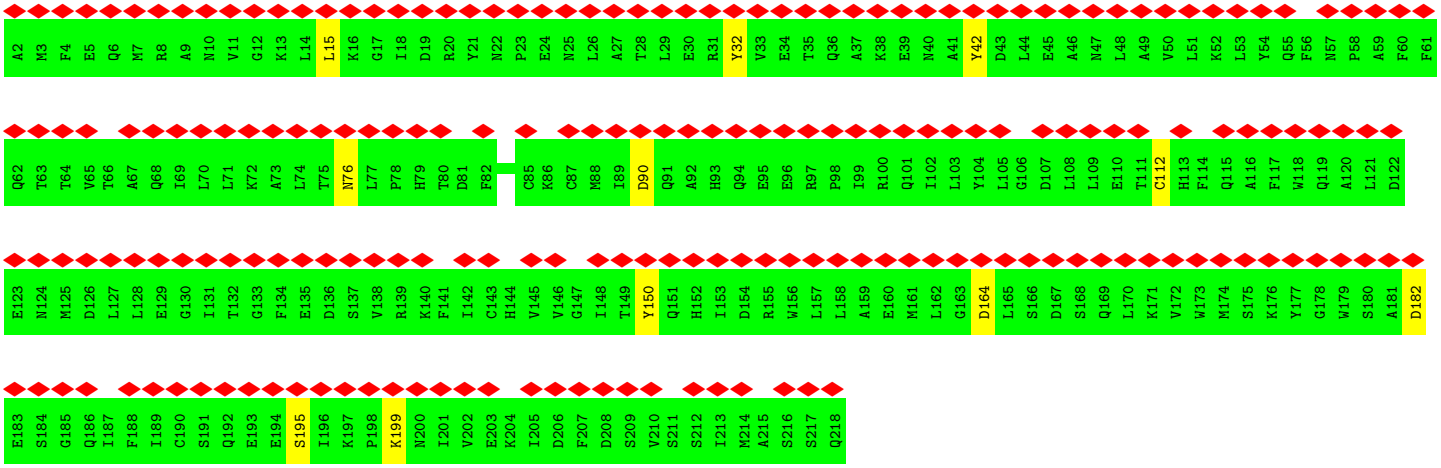
• Molecule 42: Eukaryotic translation initiation factor 3 subunit H





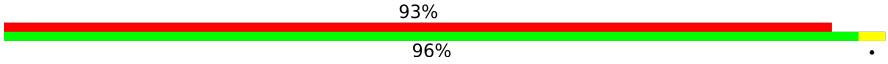
• Molecule 43: Eukaryotic translation initiation factor 3 subunit K

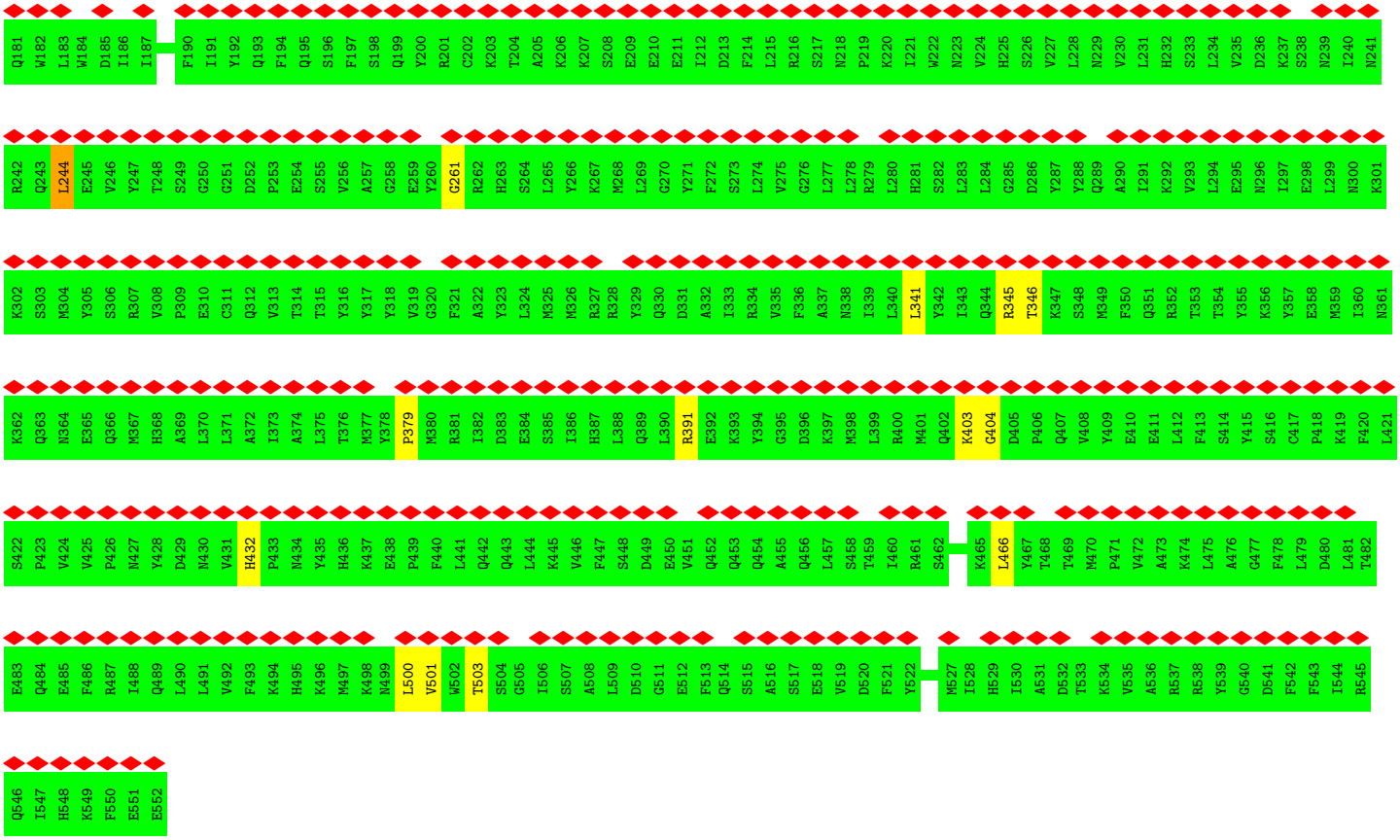




• Molecule 44: Eukaryotic translation initiation factor 3 subunit L

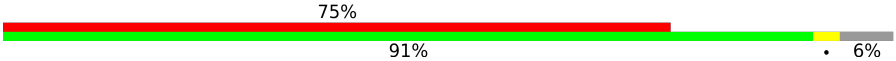
Chain L:

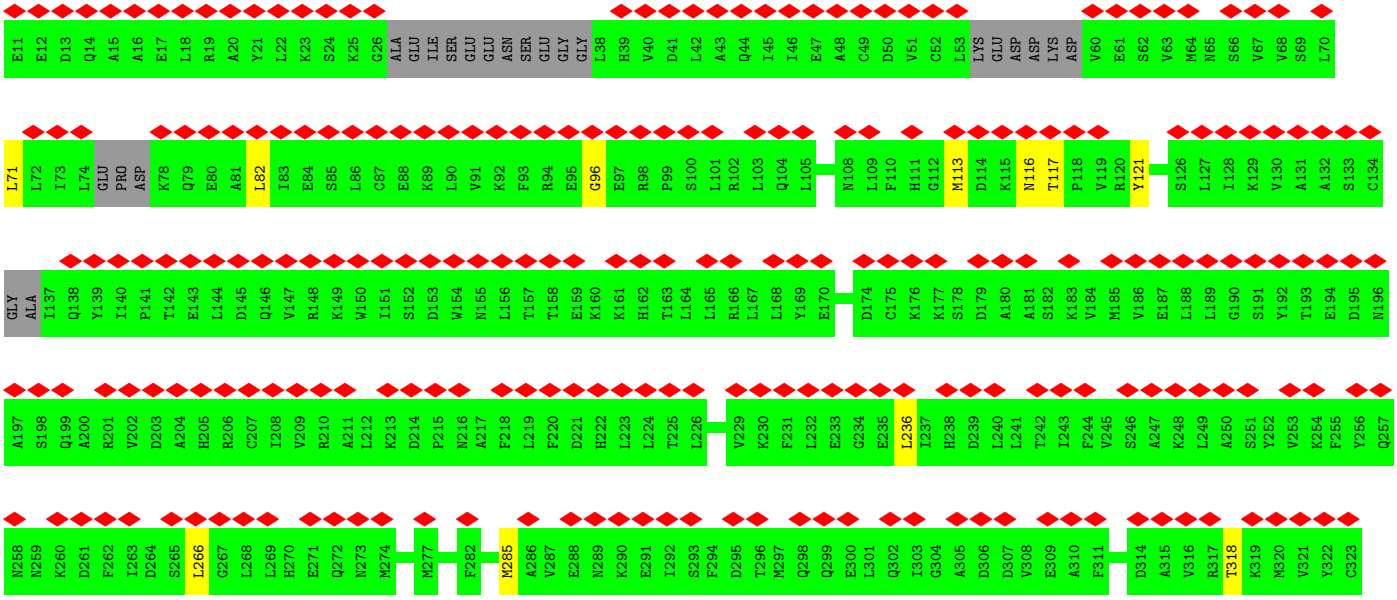


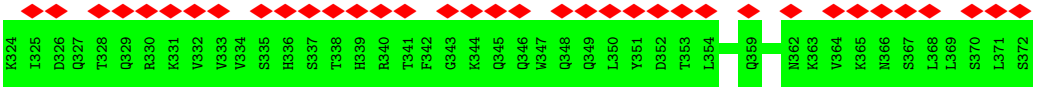


• Molecule 45: Eukaryotic translation initiation factor 3 subunit M

Chain M:

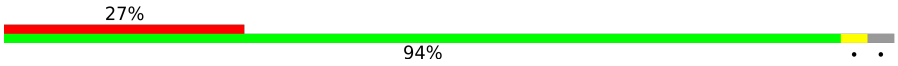


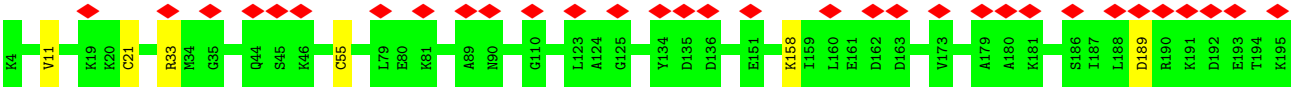


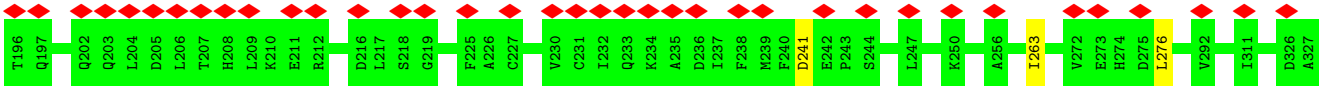


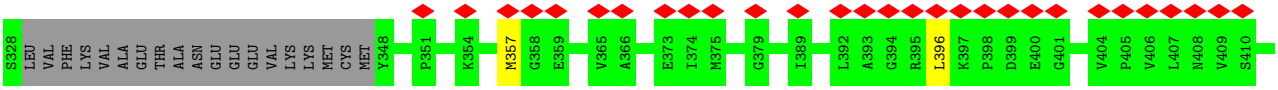
• Molecule 46: ATP-binding cassette sub-family E member 1

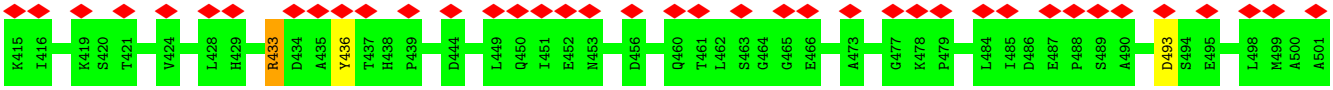
Chain 1:

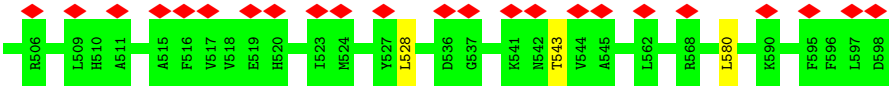






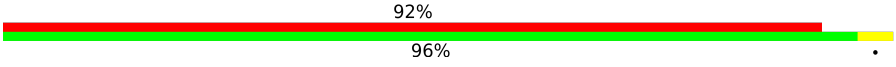


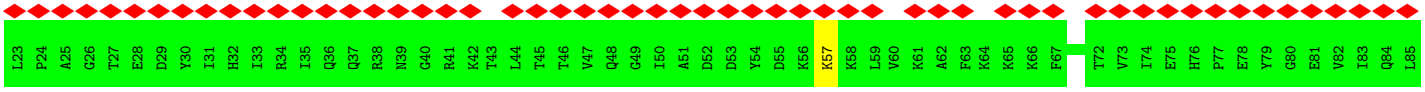


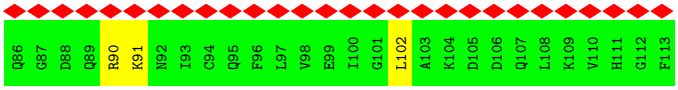


• Molecule 47: Eukaryotic translation initiation factor 1

Chain N:

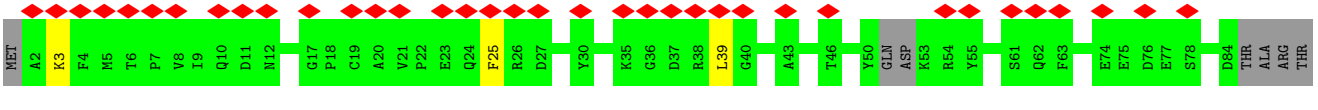


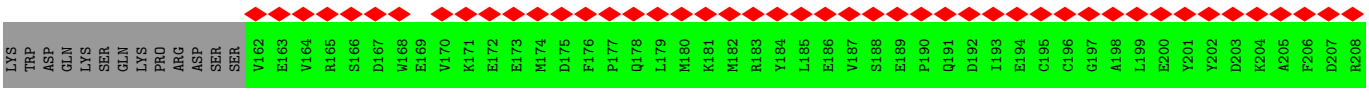


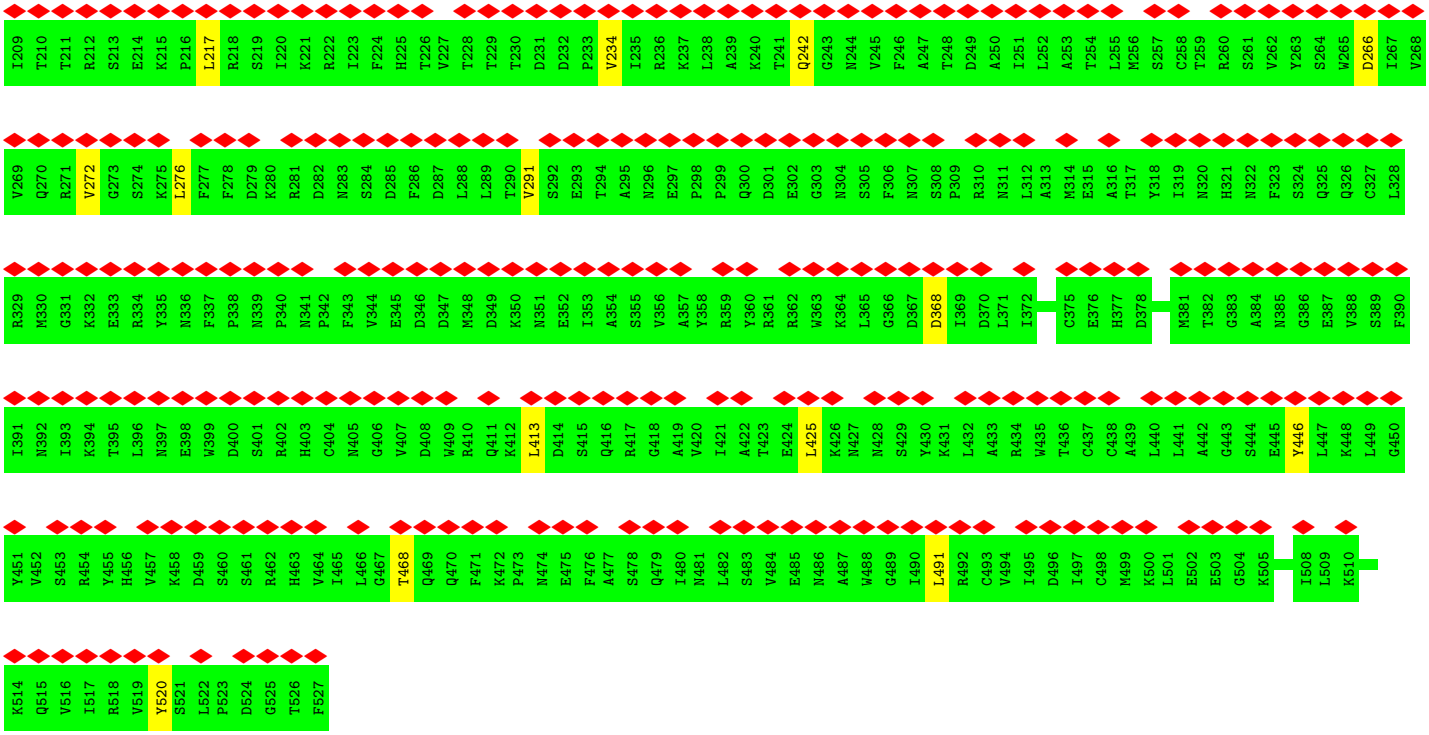


• Molecule 48: Eukaryotic translation initiation factor 3 subunit D

Chain D:





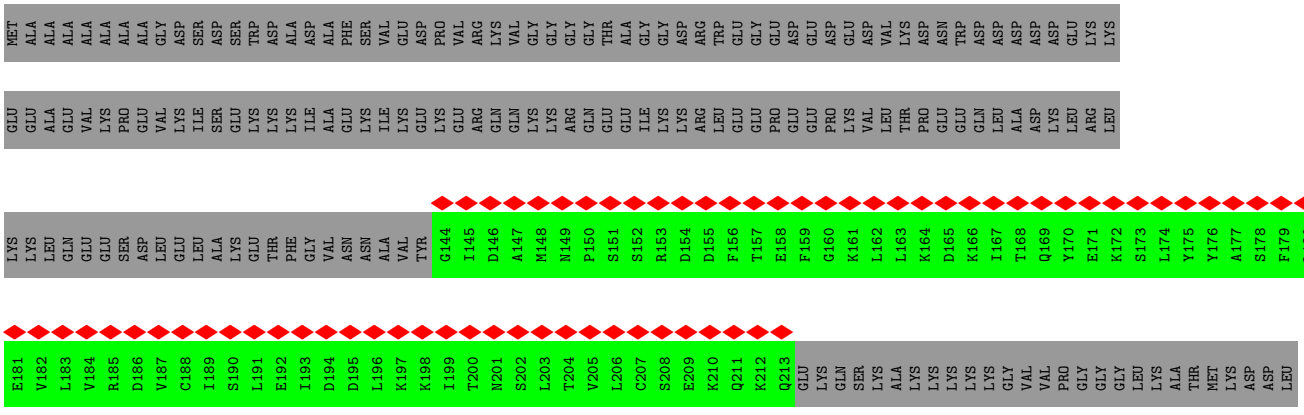


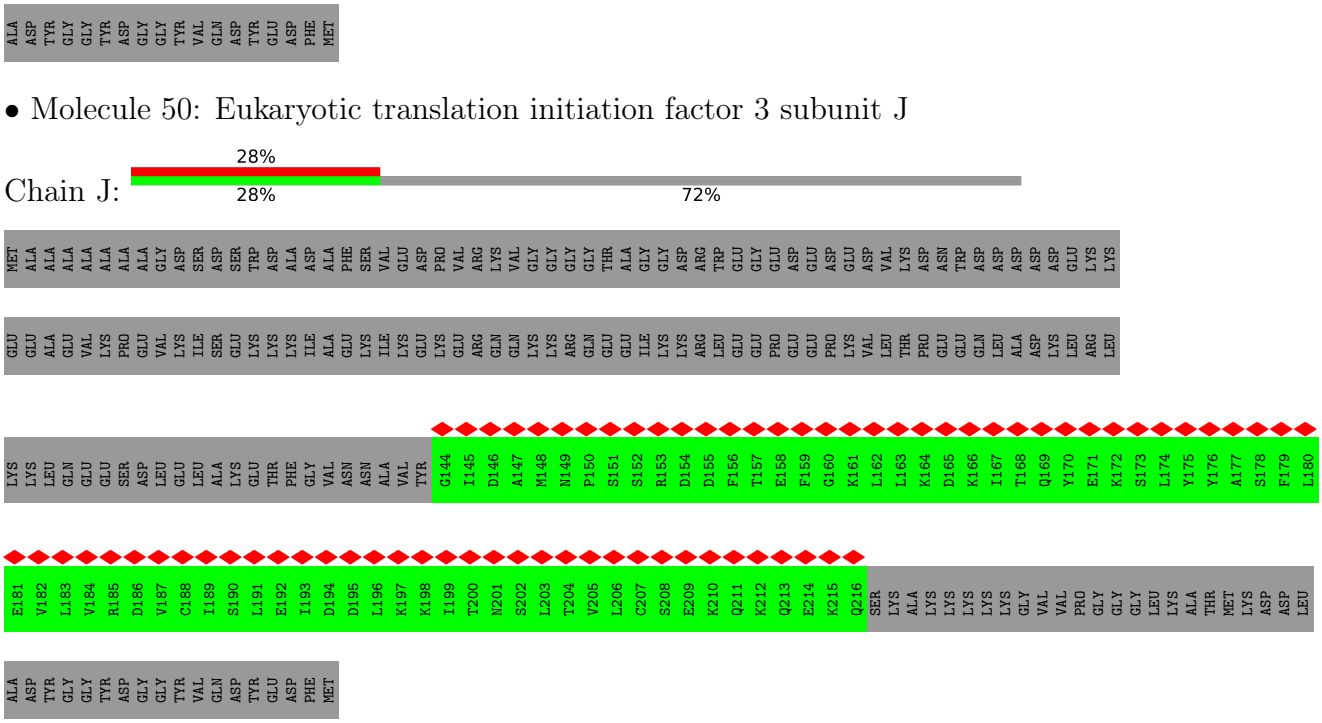
• Molecule 49: RNA recognition motif (unknown)

Chain Y:

• Molecule 50: Eukaryotic translation initiation factor 3 subunit J

Chain G:




ALA ASP TYR GLY GLY TYR ASP GLY GLY TYR VAL GLN ASP TYR GLU ASP PHE MET
• Molecule 50: Eukaryotic translation initiation factor 3 subunit J
Chain J:
28%
28%
72%
MET ALA ALA ALA ALA ALA ALA GLY ASP SER ASP SER TRP ASP ALA ASP ALA PHE SER VAL GLU ASP PRO VAL ARG LYS VAL GLY GLY GLY GLY THR ALA GLY GLY ASP ARG TRP GLU GLY GLU ASP GLU ASP GLU ASP VAL LYS ASP ASN TRP ASP ASP ASP ASP ASP GLU LYS LYS
GLU GLU ALA GLU VAL LYS PRO GLU VAL LYS ILE SER GLU LYS LYS LYS ILE ALA GLU LYS ILE LYS GLU LYS GLU ARG GLN GLN GLN LYS LYS ARG GLN GLU GLU ILE LYS LYS ARG LEU GLU GLU PRO GLU GLU PRO LYS VAL LEU THR PRO GLU GLU GLN LEU ALA ASP LYS LEU ARG LEU
LYS LYS LEU GLN GLU GLU SER ASP LEU GLU LEU ALA LYS GLU THR PHE GLY VAL ASN ASN ALA VAL TYR G144 I145 D146 A147 M148 N149 P150 S151 S152 R153 D154 D155 F156 T157 E158 F159 G160 K161 L162 L163 K164 D165 K166 I167 T168 Q169 Y170 E171 K172 S173 L174 Y175 Y176 A177 S178 F179 L180
E181 V182 L183 V184 R185 D186 V187 C188 I189 S190 L191 E192 I193 D194 D195 L196 K197 K198 I199 T200 N201 S202 L203 T204 V205 L206 C207 S208 E209 K210 Q211 K212 Q213 E214 K215 Q216 SER LYS ALA LYS LYS LYS LYS GLY VAL VAL PRO GLY GLY GLY LEU LYS ALA THR MET LYS ASP ASP LEU
ALA ASP TYR GLY GLY TYR ASP GLY GLY TYR VAL GLN ASP TYR GLU ASP PHE MET

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5231	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 ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.033	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	423.6, 423.6, 423.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.59	0/1743	0.72	1/2367 (0.0%)
2	p	0.53	0/1743	0.71	1/2330 (0.0%)
3	d	0.62	0/1711	0.79	2/2310 (0.1%)
4	Q	0.66	0/829	0.74	0/1109
5	q	0.59	0/2074	0.74	1/2791 (0.0%)
6	W	0.49	0/232	0.58	0/294
7	r	0.48	0/1818	0.69	0/2421
8	s	0.54	0/1419	0.73	0/1895
9	t	0.55	0/1667	0.66	0/2223
10	c	0.57	0/1525	0.74	2/2035 (0.1%)
11	n	0.67	0/1140	0.66	0/1524
12	m	0.51	0/1227	0.67	0/1649
13	i	0.51	0/952	0.72	0/1275
14	y	0.57	0/632	0.65	0/844
15	f	0.63	1/1051 (0.1%)	0.76	1/1406 (0.1%)
16	j	0.58	0/1098	0.72	1/1464 (0.1%)
17	z	0.53	0/1017	0.67	0/1349
18	R	0.57	0/654	0.74	0/876
19	T	0.53	0/357	0.63	0/466
20	2	1.12	24/41041 (0.1%)	1.67	1229/63969 (1.9%)
21	w	0.50	0/1024	0.75	0/1377
22	g	0.44	0/1117	0.72	0/1494
23	b	0.44	0/1774	0.70	0/2387
24	e	0.43	0/1516	0.73	1/2037 (0.0%)
25	u	0.41	0/824	0.72	1/1111 (0.1%)
26	v	0.39	0/871	0.75	0/1168
27	o	0.43	0/999	0.73	1/1336 (0.1%)
28	k	0.39	0/1181	0.70	0/1581
29	x	0.40	0/1114	0.68	1/1493 (0.1%)
30	h	0.42	0/790	0.72	0/1059
31	P	0.38	0/564	0.74	1/758 (0.1%)
32	S	0.41	0/482	0.70	0/643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	l	0.46	0/462	0.75	1/612 (0.2%)
34	U	0.43	0/475	0.70	0/626
35	V	0.43	0/2370	0.80	2/3221 (0.1%)
36	I	0.25	0/1495	0.52	0/2073
37	B	0.32	0/2981	0.64	0/4115
38	A	0.39	1/5468 (0.0%)	0.67	5/7401 (0.1%)
39	C	0.42	0/5157	0.72	3/6946 (0.0%)
40	E	0.39	0/3503	0.70	1/4728 (0.0%)
41	F	0.37	0/2126	0.72	3/2890 (0.1%)
42	H	0.41	0/2458	0.76	3/3313 (0.1%)
43	K	0.38	0/1785	0.75	4/2414 (0.2%)
44	L	0.41	0/3188	0.83	6/4299 (0.1%)
45	M	0.37	0/2757	0.71	2/3717 (0.1%)
46	1	0.44	1/4627 (0.0%)	0.74	4/6247 (0.1%)
47	N	0.40	0/739	0.77	1/989 (0.1%)
48	D	0.42	0/3700	0.74	5/5001 (0.1%)
49	Y	0.31	0/389	0.59	0/543
50	G	0.23	0/347	0.31	0/483
50	J	0.23	0/362	0.31	0/504
All	All	0.75	27/120575 (0.0%)	1.17	1283/171163 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	d	0	2
5	q	0	3
8	s	0	1
15	f	0	2
17	z	0	2
21	w	0	3
24	e	0	3
28	k	0	1
32	S	0	1
33	l	0	1
35	V	0	6
36	I	0	3
37	B	0	7
39	C	0	7
40	E	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	F	0	6
42	H	0	4
43	K	0	5
44	L	0	5
45	M	0	5
46	1	0	5
48	D	0	3
All	All	0	77

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	1100	A	N9-C4	-8.44	1.32	1.37
46	1	21	CYS	CB-SG	-6.79	1.70	1.82
15	f	93	LEU	C-N	-6.13	1.20	1.34
20	2	447	A	N9-C4	-6.13	1.34	1.37
20	2	640	A	N7-C5	-6.09	1.35	1.39
20	2	1084	A	N7-C5	-6.09	1.35	1.39
20	2	119	U	N3-C4	-6.05	1.33	1.38
20	2	862	A	N7-C5	-5.72	1.35	1.39
20	2	1140	G	N7-C5	-5.63	1.35	1.39
20	2	1099	G	N9-C4	-5.62	1.33	1.38
20	2	640	A	N9-C8	-5.61	1.33	1.37
20	2	659	G	C6-N1	-5.60	1.35	1.39
20	2	173	A	N7-C5	-5.51	1.35	1.39
20	2	594	A	N9-C4	-5.48	1.34	1.37
20	2	959	G	N7-C5	-5.45	1.35	1.39
20	2	1204	A	N7-C5	-5.39	1.36	1.39
20	2	1144	A	N7-C5	-5.36	1.36	1.39
20	2	1865	C	N3-C4	-5.36	1.30	1.33
20	2	491	C	N1-C6	-5.29	1.33	1.37
20	2	1697	A	N9-C4	-5.21	1.34	1.37
20	2	345	U	N1-C6	-5.21	1.33	1.38
38	A	149	TRP	CB-CG	-5.20	1.40	1.50
20	2	1345	G	N7-C5	-5.08	1.36	1.39
20	2	119	U	C2-N3	-5.07	1.34	1.37
20	2	98	C	N1-C6	-5.05	1.34	1.37
20	2	629	A	N9-C4	-5.04	1.34	1.37
20	2	1031	A	N9-C4	-5.01	1.34	1.37

All (1283) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	1773	C	N1-C2-O2	16.15	128.59	118.90
20	2	1865	C	N3-C2-O2	-15.40	111.12	121.90
20	2	501	C	N1-C2-O2	15.07	127.94	118.90
20	2	1016	U	N3-C2-O2	-15.05	111.67	122.20
20	2	1865	C	C6-N1-C2	-14.94	114.32	120.30
20	2	639	C	C6-N1-C2	-14.56	114.47	120.30
20	2	1139	C	N1-C2-O2	14.44	127.56	118.90
20	2	501	C	C2-N1-C1'	14.18	134.40	118.80
20	2	119	U	N3-C2-O2	-13.96	112.43	122.20
20	2	1016	U	N1-C2-O2	13.56	132.29	122.80
20	2	1557	C	N1-C2-O2	13.18	126.81	118.90
20	2	1865	C	N1-C2-O2	13.04	126.72	118.90
20	2	863	U	N3-C2-O2	-12.80	113.24	122.20
20	2	1315	U	N3-C2-O2	-12.72	113.30	122.20
20	2	1775	U	C2-N1-C1'	12.52	132.72	117.70
20	2	1139	C	N3-C2-O2	-12.41	113.21	121.90
20	2	501	C	N3-C2-O2	-12.37	113.24	121.90
20	2	1821	U	N3-C2-O2	-12.23	113.64	122.20
20	2	494	C	N1-C2-O2	12.15	126.19	118.90
20	2	570	C	C6-N1-C2	-12.13	115.45	120.30
20	2	218	U	N3-C2-O2	-12.10	113.73	122.20
20	2	1557	C	C2-N1-C1'	12.10	132.11	118.80
20	2	1118	C	N1-C2-O2	11.86	126.02	118.90
20	2	422	U	N3-C2-O2	-11.78	113.95	122.20
20	2	303	C	C6-N1-C2	-11.76	115.60	120.30
20	2	1773	C	C2-N1-C1'	11.71	131.69	118.80
20	2	639	C	C5-C6-N1	11.71	126.85	121.00
20	2	1773	C	N3-C2-O2	-11.64	113.75	121.90
20	2	1016	U	C2-N1-C1'	11.62	131.65	117.70
20	2	1123	C	N1-C2-O2	11.62	125.87	118.90
20	2	1453	C	C2-N1-C1'	11.53	131.49	118.80
20	2	632	C	C6-N1-C2	-11.50	115.70	120.30
20	2	1266	C	C6-N1-C2	-11.43	115.73	120.30
20	2	501	C	C6-N1-C2	-11.42	115.73	120.30
20	2	196	C	C6-N1-C2	-11.40	115.74	120.30
20	2	1775	U	N1-C2-O2	11.36	130.75	122.80
20	2	1389	C	N1-C2-O2	11.32	125.69	118.90
20	2	632	C	C5-C6-N1	11.24	126.62	121.00
20	2	1315	U	N1-C2-O2	11.17	130.62	122.80
20	2	1261	C	N1-C2-O2	11.11	125.56	118.90
20	2	1118	C	N3-C2-O2	-11.05	114.16	121.90
20	2	853	C	C2-N1-C1'	11.05	130.96	118.80
20	2	1775	U	N3-C2-O2	-11.03	114.48	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	35	C	C6-N1-C2	-11.02	115.89	120.30
20	2	570	C	C5-C6-N1	11.00	126.50	121.00
20	2	1821	U	N1-C2-O2	10.95	130.47	122.80
20	2	1742	C	C6-N1-C2	-10.94	115.93	120.30
20	2	119	U	N1-C2-O2	10.93	130.45	122.80
20	2	494	C	N3-C2-O2	-10.90	114.27	121.90
20	2	30	C	C6-N1-C2	-10.85	115.96	120.30
20	2	1389	C	C6-N1-C2	-10.69	116.02	120.30
20	2	951	C	C2-N1-C1'	10.69	130.56	118.80
20	2	1316	C	N1-C2-O2	10.69	125.31	118.90
20	2	853	C	C6-N1-C2	-10.68	116.03	120.30
20	2	977	C	N1-C2-O2	10.68	125.31	118.90
20	2	823	U	N3-C2-O2	-10.66	114.74	122.20
20	2	1078	C	C6-N1-C2	-10.56	116.08	120.30
20	2	1822	A	N7-C8-N9	10.56	119.08	113.80
20	2	953	C	N3-C2-O2	-10.48	114.56	121.90
20	2	1453	C	N1-C2-O2	10.44	125.17	118.90
20	2	953	C	N1-C2-O2	10.42	125.15	118.90
20	2	1822	A	C8-N9-C4	-10.39	101.64	105.80
20	2	494	C	C6-N1-C2	-10.39	116.14	120.30
48	D	413	LEU	CA-CB-CG	10.39	139.19	115.30
20	2	708	C	C5-C6-N1	10.28	126.14	121.00
20	2	1655	C	C6-N1-C2	-10.28	116.19	120.30
20	2	550	C	C6-N1-C2	-10.24	116.20	120.30
20	2	1742	C	N1-C2-O2	10.23	125.04	118.90
20	2	1618	C	N1-C2-O2	10.18	125.00	118.90
20	2	603	C	N1-C2-O2	10.17	125.00	118.90
20	2	1315	U	C2-N1-C1'	10.17	129.90	117.70
20	2	570	C	N1-C2-O2	10.14	124.99	118.90
20	2	409	C	C6-N1-C2	-10.08	116.27	120.30
20	2	853	C	N3-C2-O2	-10.04	114.87	121.90
20	2	195	C	C6-N1-C2	-10.02	116.29	120.30
20	2	1078	C	C5-C6-N1	9.96	125.98	121.00
20	2	578	C	C6-N1-C2	-9.93	116.33	120.30
20	2	1865	C	C2-N1-C1'	9.90	129.69	118.80
20	2	1485	U	N3-C2-O2	-9.79	115.35	122.20
20	2	853	C	N1-C2-O2	9.77	124.76	118.90
20	2	725	C	C6-N1-C2	-9.76	116.39	120.30
20	2	708	C	C6-N1-C2	-9.72	116.41	120.30
20	2	494	C	C2-N1-C1'	9.69	129.45	118.80
20	2	501	C	C5-C6-N1	9.65	125.82	121.00
20	2	1591	C	N1-C2-O2	9.64	124.69	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	1230	C	C5-C6-N1	9.63	125.82	121.00
20	2	953	C	C2-N1-C1'	9.63	129.39	118.80
20	2	37	C	C6-N1-C2	-9.60	116.46	120.30
20	2	977	C	N3-C2-O2	-9.56	115.21	121.90
20	2	1230	C	C6-N1-C2	-9.56	116.48	120.30
20	2	1462	U	N3-C2-O2	-9.53	115.53	122.20
20	2	1073	U	C2-N1-C1'	9.52	129.13	117.70
20	2	1389	C	C2-N1-C1'	9.50	129.25	118.80
20	2	422	U	C2-N1-C1'	9.49	129.08	117.70
20	2	1123	C	C5-C6-N1	9.46	125.73	121.00
20	2	1821	U	C2-N1-C1'	9.43	129.02	117.70
20	2	663	C	C6-N1-C2	-9.42	116.53	120.30
20	2	863	U	C2-N1-C1'	9.42	129.01	117.70
20	2	1557	C	N3-C2-O2	-9.41	115.31	121.90
20	2	53	C	C6-N1-C2	-9.40	116.54	120.30
20	2	1389	C	N3-C2-O2	-9.40	115.32	121.90
20	2	1503	C	N1-C2-O2	9.40	124.54	118.90
20	2	314	U	N3-C2-O2	-9.40	115.62	122.20
20	2	1618	C	C2-N1-C1'	9.39	129.13	118.80
20	2	1266	C	C5-C6-N1	9.38	125.69	121.00
20	2	863	U	N1-C2-O2	9.38	129.37	122.80
20	2	179	C	C6-N1-C2	-9.36	116.56	120.30
20	2	814	U	N3-C2-O2	-9.34	115.66	122.20
20	2	570	C	C2-N1-C1'	9.32	129.05	118.80
20	2	1655	C	C5-C6-N1	9.30	125.65	121.00
20	2	1261	C	N3-C2-O2	-9.27	115.41	121.90
20	2	1123	C	C6-N1-C2	-9.26	116.60	120.30
20	2	1742	C	C5-C6-N1	9.24	125.62	121.00
20	2	732	U	N3-C2-O2	-9.20	115.76	122.20
20	2	501	C	C6-N1-C1'	-9.18	109.78	120.80
20	2	636	C	C5-C6-N1	9.17	125.58	121.00
20	2	118	C	C6-N1-C2	-9.13	116.65	120.30
20	2	951	C	C6-N1-C2	-9.13	116.65	120.30
20	2	728	C	C6-N1-C2	-9.11	116.65	120.30
20	2	1864	U	N1-C2-O2	9.11	129.18	122.80
20	2	814	U	C2-N1-C1'	9.10	128.62	117.70
20	2	218	U	N1-C2-O2	9.09	129.16	122.80
20	2	1090	C	C6-N1-C2	-9.08	116.67	120.30
20	2	1864	U	N3-C2-O2	-9.08	115.84	122.20
20	2	977	C	C2-N1-C1'	9.08	128.79	118.80
20	2	1462	U	N1-C2-O2	9.07	129.15	122.80
20	2	1139	C	C2-N1-C1'	9.07	128.77	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	1389	C	C5-C6-N1	9.07	125.53	121.00
20	2	222	U	N3-C2-O2	-9.05	115.87	122.20
20	2	220	U	C2-N1-C1'	9.05	128.56	117.70
20	2	1864	U	C2-N1-C1'	9.01	128.51	117.70
20	2	314	U	N1-C2-O2	9.01	129.11	122.80
20	2	1811	C	C6-N1-C2	-9.01	116.70	120.30
20	2	179	C	C5-C6-N1	8.97	125.49	121.00
20	2	1292	C	C6-N1-C2	-8.96	116.72	120.30
20	2	168	C	N1-C2-O2	8.94	124.27	118.90
42	H	231	LEU	CA-CB-CG	8.94	135.86	115.30
20	2	1149	A	C2-N3-C4	8.94	115.07	110.60
20	2	1503	C	C6-N1-C2	-8.92	116.73	120.30
20	2	951	C	N1-C2-O2	8.91	124.25	118.90
20	2	1773	C	C6-N1-C2	-8.91	116.73	120.30
20	2	218	U	C2-N1-C1'	8.90	128.38	117.70
20	2	49	C	N1-C2-O2	8.87	124.22	118.90
20	2	1802	C	C6-N1-C2	-8.86	116.76	120.30
20	2	168	C	C6-N1-C2	-8.85	116.76	120.30
20	2	1591	C	C6-N1-C2	-8.85	116.76	120.30
20	2	30	C	C5-C6-N1	8.85	125.42	121.00
20	2	930	C	C6-N1-C2	-8.85	116.76	120.30
20	2	663	C	C5-C6-N1	8.85	125.42	121.00
20	2	222	U	N1-C2-O2	8.84	128.99	122.80
20	2	1205	C	C6-N1-C2	-8.83	116.77	120.30
20	2	1316	C	N3-C2-O2	-8.82	115.73	121.90
20	2	303	C	C5-C6-N1	8.81	125.40	121.00
20	2	441	C	C6-N1-C2	-8.80	116.78	120.30
20	2	1073	U	N3-C2-O2	-8.79	116.05	122.20
20	2	1742	C	N3-C2-O2	-8.76	115.77	121.90
20	2	1557	C	C6-N1-C1'	-8.75	110.30	120.80
20	2	151	C	C6-N1-C2	-8.75	116.80	120.30
20	2	1343	U	N3-C2-O2	-8.74	116.08	122.20
20	2	1471	C	N1-C2-O2	8.74	124.14	118.90
20	2	1773	C	C5-C6-N1	8.72	125.36	121.00
20	2	483	C	N1-C2-O2	8.70	124.12	118.90
20	2	732	U	C2-N1-C1'	8.70	128.14	117.70
20	2	1271	C	C6-N1-C2	-8.69	116.83	120.30
20	2	851	C	N1-C2-O2	8.68	124.11	118.90
20	2	1123	C	N3-C2-O2	-8.68	115.82	121.90
20	2	738	C	C5-C6-N1	8.68	125.34	121.00
20	2	1591	C	N3-C2-O2	-8.67	115.83	121.90
20	2	1520	G	C4-N9-C1'	8.65	137.74	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	974	C	C2-N1-C1'	8.63	128.29	118.80
20	2	1485	U	C2-N1-C1'	8.62	128.05	117.70
20	2	1271	C	N1-C2-O2	8.60	124.06	118.90
20	2	35	C	C5-C6-N1	8.60	125.30	121.00
20	2	1696	C	C6-N1-C2	-8.60	116.86	120.30
20	2	1279	C	C5-C6-N1	8.59	125.30	121.00
27	o	107	ILE	C-N-CA	8.54	143.04	121.70
20	2	1078	C	C2-N1-C1'	8.52	128.17	118.80
20	2	608	C	N1-C2-O2	8.51	124.01	118.90
20	2	1118	C	C6-N1-C2	-8.50	116.90	120.30
20	2	37	C	N1-C2-O2	8.49	123.99	118.90
20	2	948	C	C5-C6-N1	8.49	125.24	121.00
20	2	144	U	N3-C2-O2	-8.47	116.27	122.20
20	2	1205	C	C5-C6-N1	8.46	125.23	121.00
20	2	1453	C	C6-N1-C1'	-8.45	110.66	120.80
20	2	695	C	C6-N1-C2	-8.44	116.92	120.30
20	2	1277	C	C5-C6-N1	8.42	125.21	121.00
20	2	1849	A	N9-C4-C5	-8.42	102.43	105.80
20	2	4	C	C6-N1-C2	-8.41	116.94	120.30
20	2	738	C	C6-N1-C2	-8.39	116.94	120.30
20	2	422	U	N1-C2-O2	8.38	128.67	122.80
20	2	948	C	C6-N1-C2	-8.38	116.95	120.30
20	2	220	U	N3-C2-O2	-8.37	116.34	122.20
20	2	580	U	N3-C2-O2	-8.37	116.34	122.20
20	2	1618	C	N3-C2-O2	-8.36	116.05	121.90
20	2	1399	C	N1-C2-O2	8.34	123.90	118.90
20	2	1609	C	C6-N1-C2	-8.31	116.98	120.30
20	2	1118	C	C2-N1-C1'	8.30	127.94	118.80
20	2	148	U	N3-C2-O2	-8.30	116.39	122.20
20	2	577	U	N1-C2-O2	8.30	128.61	122.80
20	2	1696	C	C5-C6-N1	8.30	125.15	121.00
20	2	579	C	C6-N1-C2	-8.29	116.98	120.30
20	2	119	U	C2-N1-C1'	8.28	127.64	117.70
20	2	1442	U	N3-C2-O2	-8.28	116.41	122.20
20	2	1509	U	C2-N1-C1'	8.27	127.63	117.70
20	2	570	C	N3-C2-O2	-8.27	116.11	121.90
20	2	579	C	N1-C2-O2	8.27	123.86	118.90
20	2	1277	C	C6-N1-C2	-8.26	117.00	120.30
20	2	1609	C	C5-C6-N1	8.26	125.13	121.00
20	2	4	C	C5-C6-N1	8.25	125.13	121.00
20	2	37	C	N3-C2-O2	-8.25	116.13	121.90
20	2	1002	U	C5-C6-N1	8.25	126.82	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	959	G	N7-C8-N9	8.24	117.22	113.10
20	2	1279	C	C6-N1-C2	-8.23	117.01	120.30
20	2	557	U	C2-N1-C1'	8.23	127.57	117.70
20	2	345	U	C5-C6-N1	8.21	126.81	122.70
20	2	303	C	N1-C2-O2	8.20	123.82	118.90
20	2	49	C	N3-C2-O2	-8.18	116.17	121.90
20	2	636	C	C6-N1-C2	-8.18	117.03	120.30
20	2	303	C	N3-C2-O2	-8.17	116.18	121.90
20	2	429	C	C6-N1-C2	-8.16	117.04	120.30
20	2	120	U	N3-C2-O2	-8.15	116.49	122.20
20	2	862	A	N7-C8-N9	8.15	117.87	113.80
20	2	1135	C	C5-C6-N1	8.14	125.07	121.00
20	2	676	C	C6-N1-C2	-8.13	117.05	120.30
20	2	186	C	C5-C6-N1	8.07	125.03	121.00
20	2	1775	U	C5-C6-N1	8.06	126.73	122.70
20	2	723	C	C6-N1-C2	-8.06	117.08	120.30
20	2	734	C	N1-C2-O2	8.06	123.73	118.90
20	2	608	C	C2-N1-C1'	8.05	127.66	118.80
20	2	733	C	C6-N1-C2	-8.05	117.08	120.30
20	2	1520	G	N3-C4-C5	-8.05	124.58	128.60
20	2	1172	U	N3-C2-O2	-8.03	116.58	122.20
20	2	14	C	C5-C6-N1	8.02	125.01	121.00
20	2	1073	U	N1-C2-O2	8.01	128.40	122.80
20	2	49	C	C6-N1-C2	-8.00	117.10	120.30
20	2	603	C	N3-C2-O2	-8.00	116.30	121.90
20	2	193	C	C6-N1-C2	-8.00	117.10	120.30
20	2	1259	A	C2-N3-C4	7.99	114.59	110.60
20	2	1412	C	C6-N1-C2	-7.98	117.11	120.30
20	2	851	C	N3-C2-O2	-7.97	116.32	121.90
20	2	210	U	N3-C2-O2	-7.97	116.62	122.20
20	2	1511	U	C2-N1-C1'	7.97	127.26	117.70
20	2	1485	U	N1-C2-O2	7.96	128.37	122.80
20	2	732	U	N1-C2-O2	7.96	128.37	122.80
20	2	186	C	C6-N1-C2	-7.95	117.12	120.30
20	2	1358	U	N3-C2-O2	-7.94	116.64	122.20
20	2	118	C	N1-C2-O2	7.94	123.66	118.90
20	2	1315	U	C6-N1-C2	-7.92	116.25	121.00
20	2	1604	G	N3-C4-C5	-7.92	124.64	128.60
20	2	851	C	C2-N1-C1'	7.91	127.50	118.80
20	2	1292	C	N1-C2-O2	7.90	123.64	118.90
20	2	1750	C	C6-N1-C2	-7.89	117.14	120.30
20	2	1865	C	C5-C6-N1	7.89	124.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	814	U	N1-C2-O2	7.89	128.32	122.80
20	2	304	C	C6-N1-C2	-7.86	117.16	120.30
20	2	1100	A	N3-C4-C5	7.86	132.30	126.80
20	2	951	C	C5-C6-N1	7.85	124.92	121.00
20	2	537	C	N1-C2-O2	7.82	123.59	118.90
20	2	681	U	C5-C6-N1	7.82	126.61	122.70
20	2	1216	C	C6-N1-C2	-7.81	117.18	120.30
20	2	293	C	C2-N1-C1'	7.80	127.38	118.80
20	2	1649	U	C2-N1-C1'	7.79	127.05	117.70
20	2	1384	C	C6-N1-C2	-7.78	117.19	120.30
20	2	344	U	O4'-C1'-N1	7.78	114.42	108.20
20	2	1661	A	N7-C8-N9	7.77	117.69	113.80
20	2	1022	U	C2-N1-C1'	7.75	127.00	117.70
20	2	1462	U	C2-N1-C1'	7.75	127.00	117.70
43	K	164	ASP	CB-CG-OD1	7.75	125.28	118.30
20	2	892	U	C5-C6-N1	7.74	126.57	122.70
20	2	1238	U	N3-C2-O2	-7.74	116.78	122.20
20	2	1794	C	N1-C2-O2	7.73	123.54	118.90
20	2	959	G	C8-N9-C4	-7.73	103.31	106.40
44	L	466	LEU	CA-CB-CG	7.72	133.06	115.30
20	2	1773	C	C6-N1-C1'	-7.72	111.54	120.80
20	2	1628	C	N1-C2-O2	7.70	123.52	118.90
20	2	539	C	C5-C4-N4	-7.70	114.81	120.20
20	2	1453	C	C5-C6-N1	7.70	124.85	121.00
20	2	1343	U	N1-C2-O2	7.70	128.19	122.80
20	2	823	U	N1-C2-O2	7.69	128.19	122.80
20	2	708	C	N1-C2-O2	7.68	123.51	118.90
20	2	1503	C	C5-C6-N1	7.67	124.84	121.00
20	2	1775	U	C6-N1-C2	-7.67	116.40	121.00
20	2	578	C	C5-C6-N1	7.66	124.83	121.00
20	2	1453	C	N3-C2-O2	-7.65	116.54	121.90
20	2	824	C	N1-C2-O2	7.65	123.49	118.90
20	2	1172	U	N1-C2-O2	7.63	128.14	122.80
20	2	1289	U	N1-C2-O2	7.62	128.13	122.80
20	2	1095	C	C6-N1-C2	-7.62	117.25	120.30
20	2	1099	G	N3-C4-N9	-7.61	121.44	126.00
20	2	1204	A	N7-C8-N9	7.61	117.60	113.80
20	2	188	C	C6-N1-C2	-7.59	117.26	120.30
20	2	1775	U	C6-N1-C1'	-7.59	110.58	121.20
20	2	1649	U	N3-C2-O2	-7.58	116.89	122.20
20	2	675	U	N1-C2-O2	7.58	128.10	122.80
20	2	1367	U	C5-C6-N1	7.56	126.48	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	1683	C	N1-C2-O2	7.56	123.44	118.90
20	2	1091	C	N1-C2-O2	7.56	123.44	118.90
20	2	1337	C	C6-N1-C2	-7.56	117.28	120.30
20	2	210	U	N1-C2-O2	7.55	128.08	122.80
20	2	802	A	N1-C2-N3	-7.54	125.53	129.30
20	2	1535	U	C2-N1-C1'	7.54	126.75	117.70
20	2	953	C	C6-N1-C2	-7.53	117.29	120.30
20	2	1442	U	N1-C2-O2	7.53	128.07	122.80
20	2	1730	U	N3-C2-O2	-7.53	116.93	122.20
38	A	310	LEU	CA-CB-CG	7.53	132.61	115.30
20	2	196	C	C5-C6-N1	7.51	124.76	121.00
20	2	1204	A	C8-N9-C4	-7.51	102.80	105.80
20	2	429	C	N1-C2-O2	7.51	123.41	118.90
20	2	497	C	C6-N1-C2	-7.51	117.30	120.30
20	2	1349	G	N3-C4-C5	-7.49	124.86	128.60
20	2	708	C	C2-N1-C1'	7.47	127.02	118.80
20	2	1509	U	N3-C2-O2	-7.47	116.97	122.20
20	2	1842	C	C6-N1-C2	-7.47	117.31	120.30
20	2	723	C	N1-C2-O2	7.46	123.38	118.90
20	2	168	C	N3-C2-O2	-7.46	116.68	121.90
46	1	276	LEU	CA-CB-CG	7.45	132.44	115.30
20	2	37	C	C5-C6-N1	7.43	124.72	121.00
20	2	1509	U	N1-C2-O2	7.42	127.99	122.80
20	2	690	G	N3-C4-C5	-7.42	124.89	128.60
20	2	220	U	N1-C2-O2	7.40	127.98	122.80
20	2	675	U	N3-C2-O2	-7.40	117.02	122.20
20	2	1180	C	N1-C2-O2	7.39	123.34	118.90
20	2	1261	C	C6-N1-C2	-7.39	117.35	120.30
20	2	892	U	N3-C2-O2	-7.38	117.03	122.20
20	2	293	C	N1-C2-O2	7.38	123.33	118.90
20	2	1271	C	C5-C6-N1	7.37	124.69	121.00
20	2	1271	C	C2-N1-C1'	7.37	126.91	118.80
20	2	862	A	C5-N7-C8	-7.37	100.22	103.90
20	2	1364	U	N3-C2-O2	-7.36	117.05	122.20
20	2	579	C	N3-C2-O2	-7.36	116.75	121.90
20	2	685	A	O4'-C1'-N9	7.35	114.08	108.20
20	2	1730	U	N1-C2-O2	7.35	127.94	122.80
20	2	1016	U	C6-N1-C2	-7.35	116.59	121.00
20	2	1849	A	C4-C5-N7	7.34	114.37	110.70
20	2	725	C	C5-C6-N1	7.33	124.67	121.00
20	2	930	C	C5-C6-N1	7.33	124.67	121.00
20	2	340	C	N1-C2-O2	7.33	123.30	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	1520	G	C8-N9-C1'	-7.33	117.47	127.00
20	2	1503	C	N3-C2-O2	-7.32	116.78	121.90
20	2	892	U	C6-N1-C2	-7.32	116.61	121.00
20	2	442	C	C5-C6-N1	7.31	124.66	121.00
20	2	1047	C	C6-N1-C2	-7.31	117.38	120.30
20	2	1350	U	C5-C6-N1	7.30	126.35	122.70
20	2	1750	C	N1-C2-O2	7.30	123.28	118.90
20	2	1649	U	C5-C6-N1	7.29	126.34	122.70
2	p	62	LEU	CA-CB-CG	7.28	132.05	115.30
20	2	823	U	C2-N1-C1'	7.28	126.44	117.70
20	2	690	G	C4-N9-C1'	7.28	135.96	126.50
20	2	462	C	C6-N1-C2	-7.27	117.39	120.30
20	2	119	U	C5-C4-O4	7.26	130.26	125.90
20	2	1738	C	C6-N1-C2	-7.26	117.39	120.30
20	2	497	C	C5-C6-N1	7.26	124.63	121.00
20	2	1649	U	N1-C2-O2	7.26	127.88	122.80
20	2	734	C	C2-N1-C1'	7.26	126.78	118.80
20	2	429	C	C2-N1-C1'	7.24	126.77	118.80
20	2	799	U	C2-N1-C1'	7.24	126.39	117.70
20	2	119	U	C6-N1-C2	-7.23	116.66	121.00
20	2	649	U	N3-C2-O2	-7.22	117.14	122.20
20	2	899	U	C5-C6-N1	7.21	126.31	122.70
20	2	130	G	N3-C4-N9	7.21	130.32	126.00
20	2	151	C	C2-N1-C1'	7.21	126.73	118.80
20	2	1292	C	N3-C2-O2	-7.21	116.86	121.90
20	2	950	C	C6-N1-C2	-7.20	117.42	120.30
20	2	441	C	C5-C6-N1	7.20	124.60	121.00
20	2	615	C	C6-N1-C2	-7.19	117.42	120.30
20	2	51	U	C5-C6-N1	7.19	126.30	122.70
20	2	1316	C	C6-N1-C2	-7.19	117.42	120.30
20	2	1582	C	N1-C2-O2	7.18	123.21	118.90
20	2	1316	C	C2-N1-C1'	7.18	126.70	118.80
20	2	618	C	C5-C6-N1	7.18	124.59	121.00
20	2	738	C	N1-C2-O2	7.17	123.20	118.90
20	2	494	C	C5-C6-N1	7.17	124.58	121.00
20	2	1784	G	C4-N9-C1'	7.17	135.82	126.50
20	2	564	A	N7-C8-N9	7.17	117.38	113.80
20	2	498	C	C5-C6-N1	7.16	124.58	121.00
20	2	69	C	C6-N1-C2	-7.16	117.44	120.30
20	2	660	C	N1-C2-O2	7.15	123.19	118.90
20	2	748	C	C6-N1-C2	-7.15	117.44	120.30
20	2	105	U	N3-C2-O2	-7.14	117.20	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	1670	C	C6-N1-C2	-7.13	117.45	120.30
20	2	353	C	C5-C6-N1	7.12	124.56	121.00
20	2	537	C	C6-N1-C2	-7.12	117.45	120.30
20	2	168	C	C2-N1-C1'	7.11	126.62	118.80
20	2	1691	U	N3-C2-O2	-7.11	117.22	122.20
20	2	728	C	C2-N1-C1'	7.11	126.62	118.80
20	2	577	U	N3-C2-O2	-7.10	117.23	122.20
20	2	1811	C	C5-C6-N1	7.09	124.55	121.00
20	2	118	C	N3-C2-O2	-7.09	116.94	121.90
20	2	174	C	C6-N1-C2	-7.09	117.47	120.30
20	2	1002	U	N3-C2-O2	-7.08	117.25	122.20
20	2	148	U	N1-C2-O2	7.07	127.75	122.80
20	2	1511	U	N3-C2-O2	-7.06	117.26	122.20
20	2	1349	G	N3-C4-N9	7.06	130.24	126.00
20	2	676	C	N1-C2-O2	7.05	123.13	118.90
20	2	1007	C	C6-N1-C2	-7.05	117.48	120.30
20	2	367	U	P-O3'-C3'	7.04	128.15	119.70
20	2	1032	C	C6-N1-C2	-7.04	117.48	120.30
20	2	734	C	C6-N1-C2	-7.03	117.49	120.30
20	2	543	C	C6-N1-C2	-7.02	117.49	120.30
20	2	917	U	C5-C6-N1	7.02	126.21	122.70
20	2	830	A	C2-N3-C4	7.02	114.11	110.60
20	2	973	C	N1-C2-O2	7.00	123.10	118.90
20	2	409	C	C5-C6-N1	7.00	124.50	121.00
20	2	427	U	C2-N1-C1'	6.98	126.08	117.70
20	2	293	C	N3-C2-O2	-6.97	117.02	121.90
20	2	1841	C	C6-N1-C2	-6.97	117.51	120.30
20	2	580	U	N1-C2-O2	6.97	127.68	122.80
20	2	1471	C	C6-N1-C2	-6.97	117.51	120.30
20	2	1520	G	N3-C4-N9	6.96	130.18	126.00
20	2	1442	U	C5-C6-N1	6.96	126.18	122.70
20	2	824	C	C5-C6-N1	6.95	124.48	121.00
20	2	1261	C	C2-N1-C1'	6.94	126.44	118.80
20	2	579	C	C5-C6-N1	6.92	124.46	121.00
20	2	1053	C	C6-N1-C2	-6.92	117.53	120.30
20	2	1574	C	C5-C6-N1	6.92	124.46	121.00
20	2	681	U	C6-N1-C2	-6.91	116.85	121.00
20	2	1100	A	N3-C4-N9	-6.91	121.87	127.40
20	2	119	U	N3-C4-O4	-6.90	114.57	119.40
20	2	429	C	N3-C2-O2	-6.89	117.07	121.90
20	2	822	U	C2-N1-C1'	6.89	125.96	117.70
20	2	1053	C	C5-C6-N1	6.88	124.44	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	69	C	C2-N1-C1'	6.88	126.36	118.80
20	2	1535	U	N3-C2-O2	-6.87	117.39	122.20
20	2	959	G	C6-C5-N7	-6.86	126.28	130.40
20	2	1474	A	P-O3'-C3'	6.85	127.92	119.70
20	2	951	C	C6-N1-C1'	-6.84	112.59	120.80
20	2	1296	U	C5-C6-N1	6.83	126.12	122.70
20	2	462	C	C5-C6-N1	6.83	124.41	121.00
20	2	368	U	P-O3'-C3'	6.83	127.89	119.70
20	2	1364	U	N1-C2-O2	6.82	127.58	122.80
20	2	1784	G	N3-C4-N9	6.82	130.09	126.00
20	2	151	C	C5-C6-N1	6.81	124.41	121.00
20	2	1471	C	N3-C2-O2	-6.81	117.13	121.90
20	2	1644	C	C6-N1-C2	-6.81	117.58	120.30
20	2	723	C	N3-C2-O2	-6.80	117.14	121.90
20	2	718	C	C6-N1-C2	-6.80	117.58	120.30
20	2	1742	C	C2-N1-C1'	6.80	126.28	118.80
20	2	1442	U	C6-N1-C2	-6.79	116.93	121.00
20	2	732	U	C6-N1-C2	-6.78	116.93	121.00
20	2	1002	U	N1-C2-O2	6.78	127.55	122.80
20	2	1557	C	C6-N1-C2	-6.78	117.59	120.30
20	2	1227	G	N3-C4-N9	6.77	130.06	126.00
20	2	481	C	C6-N1-C2	-6.77	117.59	120.30
20	2	1047	C	C5-C6-N1	6.76	124.38	121.00
20	2	550	C	C5-C6-N1	6.76	124.38	121.00
20	2	952	G	O4'-C1'-N9	6.75	113.60	108.20
20	2	218	U	C6-N1-C2	-6.75	116.95	121.00
20	2	795	A	C2-N3-C4	6.75	113.97	110.60
20	2	930	C	C2-N1-C1'	6.75	126.22	118.80
20	2	1016	U	C6-N1-C1'	-6.75	111.75	121.20
20	2	423	U	N3-C2-O2	-6.75	117.48	122.20
20	2	1812	U	N3-C2-O2	-6.74	117.48	122.20
20	2	1440	C	N1-C2-O2	6.73	122.94	118.90
20	2	799	U	N1-C2-O2	6.73	127.51	122.80
20	2	632	C	C2-N1-C1'	6.72	126.20	118.80
20	2	734	C	N3-C2-O2	-6.72	117.20	121.90
35	V	174	VAL	C-N-CA	6.71	138.48	121.70
20	2	676	C	C5-C6-N1	6.71	124.36	121.00
20	2	1289	U	N3-C2-O2	-6.71	117.50	122.20
20	2	974	C	N1-C2-O2	6.71	122.92	118.90
20	2	892	U	N1-C2-O2	6.71	127.50	122.80
20	2	958	G	C4-N9-C1'	6.71	135.22	126.50
20	2	14	C	C6-N1-C2	-6.70	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	1271	C	N3-C2-O2	-6.70	117.21	121.90
20	2	799	U	N3-C2-O2	-6.70	117.51	122.20
20	2	1002	U	C6-N1-C2	-6.69	116.99	121.00
20	2	372	U	N3-C2-O2	-6.68	117.52	122.20
20	2	1822	A	C5-N7-C8	-6.68	100.56	103.90
20	2	982	G	C8-N9-C4	-6.66	103.73	106.40
20	2	1532	C	C2-N1-C1'	6.66	126.13	118.80
20	2	1670	C	C5-C6-N1	6.66	124.33	121.00
20	2	1590	C	N1-C2-O2	6.64	122.89	118.90
20	2	537	C	C5-C6-N1	6.64	124.32	121.00
20	2	206	G	C8-N9-C4	-6.63	103.75	106.40
20	2	429	C	C5-C6-N1	6.63	124.32	121.00
20	2	1216	C	C5-C6-N1	6.63	124.31	121.00
20	2	659	G	C4-N9-C1'	6.63	135.11	126.50
20	2	853	C	C5-C6-N1	6.63	124.31	121.00
20	2	1618	C	C6-N1-C1'	-6.62	112.85	120.80
20	2	594	A	N1-C2-N3	-6.61	125.99	129.30
20	2	1135	C	C6-N1-C2	-6.60	117.66	120.30
20	2	44	U	N3-C2-O2	-6.59	117.58	122.20
20	2	1296	U	N3-C2-O2	-6.59	117.58	122.20
20	2	1234	C	C6-N1-C2	-6.59	117.66	120.30
20	2	1146	C	C6-N1-C2	-6.59	117.66	120.30
20	2	169	U	N3-C2-O2	-6.59	117.59	122.20
20	2	1661	A	C8-N9-C4	-6.59	103.17	105.80
20	2	1849	A	N1-C6-N6	6.58	122.55	118.60
20	2	659	G	N3-C4-N9	6.58	129.95	126.00
20	2	1502	C	C6-N1-C2	-6.56	117.67	120.30
38	A	94	LEU	CA-CB-CG	-6.54	100.26	115.30
20	2	1399	C	C6-N1-C2	-6.54	117.69	120.30
20	2	973	C	C6-N1-C2	-6.54	117.69	120.30
20	2	719	G	N3-C4-N9	6.53	129.92	126.00
20	2	1827	U	N1-C2-O2	6.53	127.37	122.80
20	2	814	U	O4'-C1'-N1	6.53	113.42	108.20
20	2	1485	U	O4'-C1'-N1	6.53	113.42	108.20
20	2	1529	C	C6-N1-C2	-6.52	117.69	120.30
20	2	853	C	C6-N1-C1'	-6.52	112.97	120.80
20	2	217	A	C2-N3-C4	6.52	113.86	110.60
20	2	1310	U	N3-C2-O2	-6.51	117.64	122.20
20	2	1308	U	O4'-C1'-N1	6.51	113.41	108.20
20	2	1750	C	C2-N1-C1'	6.51	125.96	118.80
20	2	852	G	C4-N9-C1'	6.50	134.95	126.50
20	2	550	C	P-O3'-C3'	6.50	127.50	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	578	C	N1-C2-O2	6.49	122.80	118.90
20	2	1120	U	C5-C6-N1	6.49	125.94	122.70
20	2	1629	C	C5-C6-N1	6.49	124.25	121.00
20	2	498	C	C6-N1-C2	-6.49	117.71	120.30
20	2	537	C	C2-N1-C1'	6.49	125.93	118.80
20	2	1319	U	N1-C2-O2	6.48	127.33	122.80
20	2	1399	C	C5-C6-N1	6.48	124.24	121.00
20	2	922	A	N1-C2-N3	-6.47	126.06	129.30
20	2	1798	C	C6-N1-C2	-6.47	117.71	120.30
20	2	1274	G	N3-C4-C5	-6.47	125.36	128.60
20	2	1643	U	N1-C2-O2	6.47	127.33	122.80
20	2	1091	C	C6-N1-C2	-6.46	117.72	120.30
20	2	130	G	C4-N9-C1'	6.46	134.90	126.50
20	2	824	C	C6-N1-C2	-6.45	117.72	120.30
20	2	1462	U	C6-N1-C2	-6.45	117.13	121.00
20	2	482	G	C8-N9-C4	-6.45	103.82	106.40
20	2	63	U	N3-C2-O2	-6.44	117.69	122.20
20	2	1535	U	N1-C2-O2	6.44	127.31	122.80
47	N	102	LEU	CA-CB-CG	6.44	130.11	115.30
20	2	1124	C	C6-N1-C2	-6.43	117.73	120.30
20	2	144	U	N1-C2-O2	6.43	127.30	122.80
20	2	207	G	C4-N9-C1'	6.43	134.85	126.50
20	2	1802	C	C5-C6-N1	6.42	124.21	121.00
20	2	341	C	C6-N1-C2	-6.42	117.73	120.30
20	2	937	C	C5-C6-N1	6.42	124.21	121.00
20	2	1644	C	C5-C6-N1	6.42	124.21	121.00
20	2	639	C	N3-C2-O2	-6.42	117.41	121.90
20	2	618	C	O5'-P-OP1	-6.42	99.93	105.70
20	2	974	C	N3-C2-O2	-6.42	117.41	121.90
20	2	1146	C	C5-C6-N1	6.42	124.21	121.00
20	2	692	G	N9-C4-C5	-6.41	102.83	105.40
20	2	1750	C	C5-C6-N1	6.41	124.20	121.00
20	2	124	U	N3-C2-O2	-6.41	117.71	122.20
20	2	1784	G	C8-N9-C1'	-6.40	118.67	127.00
20	2	1604	G	N3-C4-N9	6.40	129.84	126.00
20	2	1733	U	N1-C2-O2	6.40	127.28	122.80
46	1	396	LEU	CA-CB-CG	6.40	130.02	115.30
20	2	863	U	C5-C4-O4	6.40	129.74	125.90
20	2	974	C	C6-N1-C2	-6.39	117.74	120.30
20	2	1292	C	C5-C6-N1	6.39	124.19	121.00
20	2	427	U	N3-C2-O2	-6.38	117.73	122.20
20	2	917	U	C6-N1-C2	-6.38	117.17	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	1670	C	C2-N1-C1'	6.37	125.81	118.80
20	2	37	C	C2-N1-C1'	6.37	125.81	118.80
20	2	977	C	C6-N1-C1'	-6.36	113.17	120.80
20	2	1811	C	N1-C2-O2	6.36	122.72	118.90
20	2	1675	A	N1-C2-N3	-6.36	126.12	129.30
20	2	206	G	N9-C4-C5	6.36	107.94	105.40
20	2	389	A	N1-C2-N3	-6.36	126.12	129.30
20	2	1139	C	C6-N1-C1'	-6.35	113.17	120.80
43	K	15	LEU	CA-CB-CG	6.35	129.91	115.30
20	2	56	G	C4-C5-N7	6.35	113.34	110.80
20	2	852	G	C6-C5-N7	-6.35	126.59	130.40
20	2	710	C	C6-N1-C2	-6.35	117.76	120.30
20	2	1503	C	C2-N1-C1'	6.35	125.78	118.80
20	2	1627	C	C5-C6-N1	6.35	124.17	121.00
20	2	1296	U	N1-C2-O2	6.34	127.24	122.80
20	2	1604	G	C2-N3-C4	6.34	115.07	111.90
20	2	1315	U	C5-C6-N1	6.34	125.87	122.70
20	2	394	G	C6-C5-N7	-6.33	126.60	130.40
20	2	130	G	N3-C4-C5	-6.33	125.43	128.60
20	2	1079	C	C5-C6-N1	6.33	124.17	121.00
20	2	1465	A	N7-C8-N9	6.33	116.97	113.80
20	2	814	U	C6-N1-C2	-6.33	117.20	121.00
20	2	1691	U	N1-C2-O2	6.33	127.23	122.80
20	2	795	A	P-O3'-C3'	6.32	127.28	119.70
20	2	1296	U	C2-N1-C1'	6.32	125.28	117.70
20	2	1343	U	C2-N1-C1'	6.32	125.28	117.70
20	2	803	C	N1-C2-O2	6.32	122.69	118.90
48	D	266	ASP	CB-CG-OD1	6.31	123.98	118.30
20	2	1604	G	C4-N9-C1'	6.30	134.69	126.50
20	2	1862	G	OP1-P-O3'	6.30	119.05	105.20
20	2	1091	C	N3-C2-O2	-6.29	117.49	121.90
20	2	106	C	C5-C6-N1	6.29	124.15	121.00
20	2	1811	C	C2-N3-C4	6.28	123.04	119.90
20	2	1180	C	C6-N1-C2	-6.28	117.79	120.30
20	2	1191	C	C6-N1-C2	-6.27	117.79	120.30
20	2	1008	A	N1-C2-N3	-6.27	126.17	129.30
20	2	900	C	C5-C6-N1	6.26	124.13	121.00
20	2	442	C	C6-N1-C2	-6.26	117.80	120.30
20	2	659	G	N1-C6-O6	-6.25	116.15	119.90
20	2	1188	A	N1-C2-N3	-6.25	126.18	129.30
20	2	1649	U	C6-N1-C2	-6.25	117.25	121.00
48	D	217	LEU	CA-CB-CG	6.24	129.66	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	208	G	C4-N9-C1'	6.24	134.61	126.50
20	2	1821	U	C6-N1-C2	-6.24	117.25	121.00
20	2	1864	U	C6-N1-C1'	-6.24	112.47	121.20
20	2	951	C	N3-C2-O2	-6.24	117.53	121.90
44	L	244	LEU	CA-CB-CG	6.24	129.64	115.30
20	2	342	C	N3-C2-O2	-6.23	117.54	121.90
20	2	953	C	C6-N1-C1'	-6.23	113.32	120.80
20	2	1099	G	N3-C4-C5	6.23	131.72	128.60
20	2	1807	C	P-O3'-C3'	6.23	127.18	119.70
20	2	178	C	C6-N1-C2	-6.23	117.81	120.30
20	2	473	A	N1-C2-N3	-6.23	126.19	129.30
20	2	900	C	C6-N1-C2	-6.23	117.81	120.30
20	2	1399	C	N3-C2-O2	-6.23	117.54	121.90
20	2	1672	U	N3-C2-O2	-6.22	117.84	122.20
20	2	1462	U	C5-C6-N1	6.22	125.81	122.70
20	2	1100	A	C2-N3-C4	-6.21	107.49	110.60
20	2	401	A	C2-N3-C4	6.21	113.71	110.60
20	2	1529	C	C5-C6-N1	6.21	124.10	121.00
20	2	937	C	C6-N1-C2	-6.20	117.82	120.30
20	2	1590	C	C6-N1-C2	-6.19	117.82	120.30
20	2	690	G	N3-C4-N9	6.19	129.71	126.00
20	2	1482	C	C5-C6-N1	6.19	124.09	121.00
20	2	659	G	C8-N9-C1'	-6.18	118.96	127.00
20	2	118	C	C5-C6-N1	6.18	124.09	121.00
20	2	1738	C	C5-C6-N1	6.18	124.09	121.00
20	2	1100	A	C4-C5-C6	-6.17	113.91	117.00
20	2	1165	G	N3-C4-N9	6.17	129.70	126.00
20	2	1090	C	C5-C6-N1	6.17	124.08	121.00
20	2	1367	U	C6-N1-C2	-6.16	117.30	121.00
20	2	1524	G	C4-N9-C1'	6.16	134.51	126.50
45	M	266	LEU	CA-CB-CG	6.16	129.47	115.30
20	2	1316	C	C5-C6-N1	6.16	124.08	121.00
20	2	1399	C	C2-N1-C1'	6.16	125.57	118.80
20	2	624	C	C5-C6-N1	6.15	124.08	121.00
20	2	680	G	N3-C4-C5	-6.15	125.52	128.60
20	2	1750	C	N3-C2-O2	-6.15	117.60	121.90
20	2	1363	C	N1-C2-O2	6.14	122.59	118.90
20	2	293	C	C6-N1-C2	-6.14	117.84	120.30
20	2	1310	U	N1-C2-O2	6.13	127.09	122.80
20	2	105	U	N1-C2-O2	6.13	127.09	122.80
20	2	645	C	C6-N1-C2	-6.13	117.85	120.30
20	2	1172	U	C2-N1-C1'	6.13	125.05	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	1628	C	C6-N1-C2	-6.13	117.85	120.30
20	2	1453	C	C6-N1-C2	-6.12	117.85	120.30
20	2	537	C	N3-C2-O2	-6.12	117.62	121.90
20	2	939	U	C5-C6-N1	6.12	125.76	122.70
20	2	917	U	C2-N1-C1'	6.11	125.04	117.70
20	2	1191	C	C5-C6-N1	6.10	124.05	121.00
20	2	1591	C	C5-C6-N1	6.10	124.05	121.00
20	2	1557	C	C5-C6-N1	6.10	124.05	121.00
20	2	1274	G	N3-C4-N9	6.09	129.65	126.00
20	2	1357	A	N1-C2-N3	-6.09	126.26	129.30
20	2	303	C	C2-N1-C1'	6.08	125.48	118.80
20	2	543	C	C5-C6-N1	6.08	124.04	121.00
20	2	493	A	C5-N7-C8	-6.07	100.86	103.90
20	2	725	C	N1-C2-O2	6.07	122.54	118.90
20	2	912	C	N3-C2-O2	-6.07	117.65	121.90
20	2	1128	C	C6-N1-C2	-6.07	117.87	120.30
20	2	1747	C	C6-N1-C2	-6.06	117.88	120.30
20	2	676	C	N3-C2-O2	-6.06	117.66	121.90
20	2	1511	U	O4'-C1'-N1	6.05	113.04	108.20
20	2	1412	C	C5-C6-N1	6.05	124.03	121.00
20	2	410	G	C4-C5-N7	6.05	113.22	110.80
20	2	1574	C	C6-N1-C2	-6.05	117.88	120.30
20	2	801	U	C5-C6-N1	6.05	125.72	122.70
20	2	833	C	C6-N1-C2	-6.04	117.88	120.30
20	2	1124	C	N1-C2-O2	6.04	122.52	118.90
20	2	49	C	C5-C6-N1	6.04	124.02	121.00
20	2	733	C	C5-C6-N1	6.04	124.02	121.00
20	2	919	A	N1-C2-N3	-6.04	126.28	129.30
20	2	1353	A	N9-C4-C5	-6.04	103.39	105.80
20	2	1591	C	C2-N1-C1'	6.04	125.44	118.80
20	2	1229	G	C8-N9-C4	-6.03	103.99	106.40
20	2	1710	C	N1-C2-O2	6.03	122.52	118.90
44	L	404	GLY	N-CA-C	6.03	128.16	113.10
20	2	222	U	C2-N1-C1'	6.02	124.93	117.70
20	2	1073	U	C6-N1-C1'	-6.02	112.77	121.20
20	2	422	U	C6-N1-C2	-6.01	117.39	121.00
20	2	1227	G	C4-N9-C1'	6.01	134.32	126.50
20	2	120	U	N1-C2-O2	6.01	127.01	122.80
20	2	1502	C	N1-C2-O2	6.01	122.50	118.90
20	2	594	A	C4-C5-C6	-6.00	114.00	117.00
20	2	1276	A	C2-N3-C4	6.00	113.60	110.60
20	2	1794	C	N3-C2-O2	-6.00	117.70	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	830	A	N1-C2-N3	-6.00	126.30	129.30
20	2	479	C	C6-N1-C2	-6.00	117.90	120.30
20	2	707	C	C5-C6-N1	5.99	124.00	121.00
20	2	475	C	C6-N1-C2	-5.99	117.90	120.30
20	2	564	A	C8-N9-C4	-5.99	103.40	105.80
20	2	579	C	C2-N1-C1'	5.99	125.39	118.80
20	2	1274	G	C4-N9-C1'	5.99	134.28	126.50
20	2	1303	C	C6-N1-C2	-5.99	117.91	120.30
20	2	342	C	N1-C2-O2	5.99	122.49	118.90
20	2	363	A	N1-C2-N3	-5.99	126.31	129.30
20	2	1103	C	C6-N1-C2	-5.99	117.91	120.30
20	2	675	U	C5-C6-N1	5.98	125.69	122.70
29	x	45	LEU	CA-CB-CG	5.98	129.06	115.30
20	2	28	U	C5-C6-N1	5.98	125.69	122.70
20	2	578	C	N3-C2-O2	-5.98	117.72	121.90
20	2	707	C	C6-N1-C2	-5.97	117.91	120.30
20	2	493	A	N7-C8-N9	5.97	116.78	113.80
20	2	1090	C	N3-C2-O2	-5.97	117.72	121.90
20	2	1249	C	C6-N1-C2	-5.97	117.91	120.30
20	2	352	U	N3-C2-O2	-5.97	118.02	122.20
20	2	632	C	N1-C2-O2	5.96	122.48	118.90
20	2	973	C	C5-C6-N1	5.96	123.98	121.00
20	2	1779	G	C8-N9-C4	-5.96	104.02	106.40
20	2	54	A	N1-C2-N3	-5.95	126.33	129.30
20	2	862	A	C8-N9-C4	-5.95	103.42	105.80
20	2	1603	G	N3-C4-C5	-5.94	125.63	128.60
20	2	1498	A	C8-N9-C4	-5.94	103.42	105.80
20	2	901	G	N3-C4-N9	-5.94	122.44	126.00
20	2	86	C	N1-C2-O2	5.93	122.46	118.90
20	2	1124	C	N3-C2-O2	-5.93	117.75	121.90
20	2	1149	A	C5-C6-N1	5.93	120.67	117.70
20	2	1635	C	C6-N1-C2	-5.93	117.93	120.30
20	2	1111	U	N3-C2-O2	-5.93	118.05	122.20
20	2	1457	U	N3-C2-O2	-5.93	118.05	122.20
20	2	1296	U	C6-N1-C2	-5.93	117.44	121.00
20	2	1627	C	C6-N1-C2	-5.92	117.93	120.30
20	2	1600	G	C4-N9-C1'	5.92	134.20	126.50
20	2	196	C	O4'-C1'-N1	5.92	112.94	108.20
20	2	640	A	N7-C8-N9	5.92	116.76	113.80
20	2	93	U	N3-C2-O2	-5.92	118.06	122.20
20	2	901	G	C8-N9-C1'	5.91	134.69	127.00
20	2	1672	U	N1-C2-O2	5.91	126.94	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	1533	A	C2-N3-C4	5.90	113.55	110.60
20	2	851	C	C6-N1-C2	-5.90	117.94	120.30
20	2	1177	U	N3-C2-O2	-5.89	118.07	122.20
20	2	577	U	C5-C6-N1	5.89	125.64	122.70
20	2	649	U	C6-N1-C2	-5.88	117.47	121.00
20	2	386	C	C6-N1-C2	-5.88	117.95	120.30
15	f	65	LEU	CA-CB-CG	5.87	128.80	115.30
20	2	489	A	C5-C6-N1	5.87	120.64	117.70
20	2	1628	C	C2-N1-C1'	5.87	125.26	118.80
20	2	659	G	N3-C4-C5	-5.87	125.67	128.60
20	2	1022	U	C6-N1-C1'	-5.87	112.99	121.20
20	2	608	C	C6-N1-C1'	-5.86	113.76	120.80
20	2	386	C	N1-C2-O2	5.86	122.41	118.90
20	2	1128	C	C5-C6-N1	5.86	123.93	121.00
20	2	56	G	C6-C5-N7	-5.84	126.89	130.40
20	2	1079	C	C2-N1-C1'	5.84	125.22	118.80
20	2	621	C	C5-C6-N1	5.84	123.92	121.00
20	2	608	C	N3-C2-O2	-5.84	117.81	121.90
20	2	359	U	N3-C2-O2	-5.84	118.11	122.20
20	2	1259	A	N1-C2-N3	-5.83	126.38	129.30
20	2	1236	G	N3-C4-N9	5.83	129.50	126.00
20	2	1524	G	C8-N9-C1'	-5.83	119.42	127.00
3	d	71	LYS	C-N-CA	5.83	136.27	121.70
20	2	307	G	O4'-C1'-N9	-5.82	103.54	108.20
20	2	862	A	C4-C5-N7	5.82	113.61	110.70
20	2	636	C	C2-N1-C1'	5.81	125.20	118.80
20	2	1812	U	C6-N1-C2	-5.81	117.51	121.00
20	2	222	U	C5-C6-N1	5.81	125.60	122.70
20	2	416	U	C6-N1-C2	-5.81	117.52	121.00
20	2	1692	U	C6-N1-C2	-5.81	117.52	121.00
20	2	806	U	C5-C6-N1	5.80	125.60	122.70
20	2	1234	C	C5-C6-N1	5.80	123.90	121.00
20	2	178	C	N1-C2-O2	5.79	122.38	118.90
20	2	719	G	C4-C5-N7	5.79	113.12	110.80
20	2	342	C	C6-N1-C2	-5.79	117.99	120.30
20	2	1831	A	C2-N3-C4	5.79	113.49	110.60
20	2	220	U	C6-N1-C1'	-5.78	113.10	121.20
20	2	1060	A	P-O3'-C3'	5.78	126.64	119.70
20	2	1471	C	C2-N1-C1'	5.78	125.16	118.80
20	2	708	C	C2-N3-C4	5.78	122.79	119.90
20	2	1319	U	N3-C2-O2	-5.78	118.15	122.20
20	2	728	C	C5-C6-N1	5.78	123.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	470	G	C8-N9-C1'	-5.77	119.50	127.00
20	2	943	U	C5-C6-N1	5.77	125.59	122.70
20	2	1047	C	C2-N1-C1'	5.77	125.15	118.80
20	2	1710	C	N3-C2-O2	-5.77	117.86	121.90
20	2	1784	G	N3-C4-C5	-5.77	125.71	128.60
20	2	208	G	C8-N9-C1'	-5.77	119.50	127.00
20	2	590	A	C2-N3-C4	5.77	113.48	110.60
20	2	1471	C	C5-C6-N1	5.77	123.88	121.00
20	2	690	G	C8-N9-C1'	-5.77	119.50	127.00
20	2	1099	G	C4-N9-C1'	-5.77	119.00	126.50
20	2	1180	C	N3-C2-O2	-5.76	117.86	121.90
20	2	814	U	C5-C6-N1	5.76	125.58	122.70
20	2	1849	A	N1-C2-N3	-5.76	126.42	129.30
20	2	1683	C	N3-C2-O2	-5.76	117.87	121.90
20	2	603	C	C2-N1-C1'	5.75	125.13	118.80
20	2	1536	G	C8-N9-C4	-5.75	104.10	106.40
20	2	1618	C	C6-N1-C2	-5.75	118.00	120.30
20	2	1827	U	N3-C2-O2	-5.75	118.18	122.20
20	2	1148	A	N1-C2-N3	-5.75	126.43	129.30
20	2	470	G	N3-C4-N9	5.75	129.45	126.00
20	2	179	C	N1-C2-O2	5.74	122.34	118.90
20	2	973	C	N3-C2-O2	-5.74	117.88	121.90
20	2	1180	C	C2-N1-C1'	5.74	125.11	118.80
20	2	1624	U	C5-C6-N1	5.73	125.57	122.70
20	2	168	C	C5-C6-N1	5.73	123.87	121.00
20	2	357	C	N1-C2-O2	5.73	122.34	118.90
20	2	863	U	C6-N1-C1'	-5.73	113.18	121.20
20	2	974	C	C6-N1-C1'	-5.72	113.93	120.80
20	2	939	U	C6-N1-C2	-5.72	117.57	121.00
20	2	1227	G	C8-N9-C1'	-5.72	119.56	127.00
20	2	1403	C	C6-N1-C2	-5.72	118.01	120.30
20	2	470	G	C6-C5-N7	-5.72	126.97	130.40
20	2	1127	C	N1-C2-O2	5.72	122.33	118.90
20	2	570	C	C2-N3-C4	5.71	122.76	119.90
20	2	1116	C	C6-N1-C2	-5.71	118.01	120.30
20	2	148	U	C2-N1-C1'	5.71	124.55	117.70
48	D	276	LEU	CA-CB-CG	5.71	128.44	115.30
20	2	72	C	N1-C2-O2	5.71	122.32	118.90
20	2	1123	C	C2-N1-C1'	5.70	125.07	118.80
20	2	1628	C	C5-C6-N1	5.70	123.85	121.00
40	E	61	LEU	CA-CB-CG	5.70	128.41	115.30
20	2	1319	U	C5-C6-N1	5.70	125.55	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	722	C	C6-N1-C2	-5.69	118.02	120.30
44	L	341	LEU	CA-CB-CG	5.69	128.39	115.30
20	2	91	A	C8-N9-C4	-5.69	103.53	105.80
20	2	694	G	N3-C4-N9	-5.69	122.59	126.00
20	2	1079	C	C6-N1-C2	-5.68	118.03	120.30
20	2	1165	G	C4-N9-C1'	5.68	133.89	126.50
20	2	806	U	C6-N1-C2	-5.68	117.59	121.00
20	2	1513	C	N3-C2-O2	-5.68	117.92	121.90
41	F	220	LEU	CA-CB-CG	5.68	128.37	115.30
20	2	1509	U	C5-C6-N1	5.68	125.54	122.70
20	2	1328	G	C4-N9-C1'	5.68	133.88	126.50
20	2	63	U	N1-C2-O2	5.68	126.77	122.80
20	2	852	G	N7-C8-N9	5.68	115.94	113.10
20	2	27	A	N1-C2-N3	-5.67	126.46	129.30
20	2	1509	U	C6-N1-C2	-5.67	117.59	121.00
20	2	341	C	C5-C6-N1	5.67	123.84	121.00
20	2	1645	C	C5-C6-N1	5.67	123.83	121.00
20	2	1782	G	C8-N9-C4	-5.67	104.13	106.40
20	2	207	G	C8-N9-C1'	-5.67	119.63	127.00
20	2	1072	U	N3-C2-O2	-5.67	118.23	122.20
20	2	1204	A	C5-N7-C8	-5.67	101.07	103.90
20	2	1091	C	C5-C6-N1	5.67	123.83	121.00
20	2	1373	C	C6-N1-C2	-5.66	118.03	120.30
42	H	233	LEU	CA-CB-CG	5.66	128.33	115.30
20	2	96	C	C6-N1-C2	-5.66	118.03	120.30
20	2	130	G	C8-N9-C1'	-5.66	119.64	127.00
20	2	1178	U	C6-N1-C2	-5.66	117.60	121.00
20	2	1368	U	N3-C2-O2	-5.66	118.24	122.20
20	2	1139	C	C6-N1-C2	-5.66	118.04	120.30
20	2	958	G	C8-N9-C4	-5.66	104.14	106.40
20	2	977	C	C6-N1-C2	-5.66	118.04	120.30
44	L	379	PRO	C-N-CA	5.65	135.83	121.70
20	2	912	C	N1-C2-O2	5.65	122.29	118.90
20	2	732	U	C5-C6-N1	5.65	125.52	122.70
20	2	195	C	C5-C6-N1	5.65	123.82	121.00
20	2	930	C	N1-C2-O2	5.65	122.29	118.90
20	2	1560	U	N3-C2-O2	-5.64	118.25	122.20
20	2	1751	C	N1-C2-O2	5.64	122.28	118.90
20	2	1356	G	N3-C4-C5	-5.64	125.78	128.60
20	2	1442	U	C2-N1-C1'	5.64	124.47	117.70
20	2	950	C	C5-C6-N1	5.63	123.82	121.00
20	2	1349	G	C4-N9-C1'	5.63	133.82	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	53	C	N3-C2-O2	-5.63	117.96	121.90
20	2	1553	C	C5-C6-N1	5.63	123.81	121.00
20	2	1570	G	C6-C5-N7	-5.63	127.02	130.40
20	2	1099	G	C8-N9-C1'	5.63	134.32	127.00
20	2	638	C	C6-N1-C2	-5.63	118.05	120.30
20	2	1582	C	N3-C2-O2	-5.63	117.96	121.90
20	2	1602	U	N3-C2-O2	-5.63	118.26	122.20
20	2	629	A	N1-C2-N3	-5.62	126.49	129.30
20	2	1225	U	N1-C2-O2	5.62	126.74	122.80
20	2	909	G	C4-N9-C1'	5.62	133.81	126.50
20	2	1643	U	N3-C2-O2	-5.62	118.26	122.20
20	2	206	G	N1-C6-O6	-5.62	116.53	119.90
20	2	1536	G	N3-C4-C5	-5.62	125.79	128.60
20	2	53	C	C5-C6-N1	5.62	123.81	121.00
20	2	398	A	N1-C2-N3	-5.61	126.49	129.30
20	2	1038	U	N3-C2-O2	-5.61	118.27	122.20
20	2	493	A	C4-C5-N7	5.61	113.50	110.70
20	2	624	C	C6-N1-C2	-5.61	118.06	120.30
20	2	1114	U	O4'-C1'-N1	5.61	112.69	108.20
20	2	1842	C	C5-C6-N1	5.60	123.80	121.00
20	2	958	G	N3-C4-C5	-5.60	125.80	128.60
20	2	1513	C	N1-C2-O2	5.59	122.26	118.90
20	2	21	U	N3-C2-O2	-5.59	118.29	122.20
20	2	1165	G	C8-N9-C1'	-5.58	119.74	127.00
20	2	1455	A	N1-C2-N3	-5.58	126.51	129.30
20	2	520	A	N1-C2-N3	-5.58	126.51	129.30
20	2	1602	U	C6-N1-C2	-5.58	117.65	121.00
20	2	304	C	C5-C6-N1	5.57	123.78	121.00
35	V	173	LEU	CA-CB-CG	5.57	128.11	115.30
44	L	244	LEU	CB-CG-CD2	-5.57	101.54	111.00
20	2	1384	C	C5-C6-N1	5.57	123.78	121.00
20	2	1692	U	C5-C6-N1	5.55	125.48	122.70
20	2	1773	C	C2-N3-C4	5.55	122.68	119.90
20	2	557	U	C5-C6-N1	5.55	125.47	122.70
20	2	917	U	N3-C2-O2	-5.55	118.31	122.20
20	2	337	C	C6-N1-C2	-5.55	118.08	120.30
20	2	1747	C	N1-C2-O2	5.55	122.23	118.90
20	2	1259	A	C5-C6-N1	5.54	120.47	117.70
20	2	1261	C	C5-C6-N1	5.54	123.77	121.00
20	2	1784	G	O4'-C1'-N9	5.54	112.64	108.20
3	d	83	LEU	CA-CB-CG	5.54	128.04	115.30
20	2	958	G	C6-C5-N7	-5.54	127.08	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	958	G	N3-C4-N9	5.54	129.32	126.00
20	2	430	C	C5-C6-N1	5.54	123.77	121.00
20	2	1119	A	O4'-C1'-N9	5.54	112.63	108.20
20	2	470	G	C4-N9-C1'	5.54	133.70	126.50
20	2	1578	U	C2-N1-C1'	5.54	124.34	117.70
20	2	1739	C	C5-C6-N1	5.54	123.77	121.00
20	2	92	A	N1-C6-N6	-5.53	115.28	118.60
20	2	1090	C	N1-C2-O2	5.53	122.22	118.90
20	2	51	U	C6-N1-C2	-5.53	117.68	121.00
20	2	959	G	C4-N9-C1'	5.53	133.69	126.50
20	2	1502	C	C5-C6-N1	5.53	123.76	121.00
39	C	410	ASP	CB-CG-OD1	5.53	123.27	118.30
20	2	217	A	N1-C2-N3	-5.52	126.54	129.30
20	2	483	C	N3-C2-O2	-5.52	118.03	121.90
20	2	1174	U	C6-N1-C2	-5.52	117.69	121.00
20	2	141	A	C4-C5-C6	-5.52	114.24	117.00
20	2	1608	U	C5-C6-N1	5.51	125.46	122.70
39	C	425	LEU	CA-CB-CG	5.51	127.98	115.30
20	2	438	G	C4-N9-C1'	5.51	133.66	126.50
20	2	443	U	C5-C6-N1	5.51	125.45	122.70
20	2	448	A	O4'-C1'-N9	5.51	112.61	108.20
20	2	1733	U	N3-C2-O2	-5.51	118.35	122.20
20	2	692	G	C4-C5-N7	5.50	113.00	110.80
20	2	1002	U	C2-N1-C1'	5.50	124.31	117.70
20	2	824	C	C2-N1-C1'	5.50	124.86	118.80
20	2	1164	G	C8-N9-C1'	-5.50	119.85	127.00
20	2	1182	A	C5-N7-C8	-5.50	101.15	103.90
20	2	562	U	N3-C2-O2	-5.50	118.35	122.20
20	2	1239	U	C5-C6-N1	5.50	125.45	122.70
20	2	87	U	C6-N1-C2	-5.50	117.70	121.00
20	2	824	C	N3-C2-O2	-5.50	118.05	121.90
20	2	1190	A	C8-N9-C4	-5.50	103.60	105.80
20	2	151	C	N1-C2-O2	5.49	122.19	118.90
20	2	1703	C	C6-N1-C2	-5.49	118.10	120.30
20	2	1609	C	N1-C2-O2	5.49	122.19	118.90
20	2	317	C	N1-C2-O2	5.49	122.19	118.90
20	2	422	U	C6-N1-C1'	-5.49	113.52	121.20
20	2	1350	U	C5-C4-O4	-5.49	122.61	125.90
20	2	1412	C	N3-C2-O2	-5.48	118.06	121.90
20	2	1482	C	C6-N1-C2	-5.48	118.11	120.30
20	2	1412	C	N1-C2-O2	5.48	122.19	118.90
20	2	1455	A	C2-N3-C4	5.48	113.34	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	1416	C	C6-N1-C2	-5.48	118.11	120.30
20	2	1802	C	N3-C2-O2	-5.48	118.06	121.90
20	2	619	A	C4-C5-N7	5.48	113.44	110.70
20	2	438	G	N3-C4-N9	5.48	129.28	126.00
38	A	439	LEU	CA-CB-CG	5.47	127.89	115.30
48	D	425	LEU	CA-CB-CG	5.47	127.89	115.30
20	2	585	C	N3-C2-O2	-5.47	118.07	121.90
20	2	666	U	C5-C6-N1	5.47	125.44	122.70
20	2	166	A	N1-C2-N3	-5.47	126.56	129.30
20	2	1590	C	N3-C2-O2	-5.47	118.07	121.90
20	2	44	U	N1-C2-O2	5.47	126.63	122.80
20	2	1013	U	C5-C6-N1	5.46	125.43	122.70
20	2	470	G	C4-C5-N7	5.46	112.98	110.80
20	2	852	G	C8-N9-C1'	-5.46	119.90	127.00
20	2	1485	U	C6-N1-C1'	-5.46	113.56	121.20
42	H	214	LEU	CB-CG-CD1	-5.46	101.72	111.00
20	2	367	U	OP1-P-O3'	5.46	117.21	105.20
20	2	332	G	P-O3'-C3'	5.45	126.24	119.70
20	2	1443	C	C5-C6-N1	5.45	123.73	121.00
25	u	25	LYS	CA-CB-CG	5.45	125.39	113.40
20	2	1259	A	N3-C4-N9	5.45	131.76	127.40
20	2	1802	C	N1-C2-O2	5.45	122.17	118.90
20	2	178	C	N3-C2-O2	-5.45	118.09	121.90
20	2	1356	G	N3-C4-N9	5.45	129.27	126.00
20	2	1065	G	C4-N9-C1'	5.44	133.57	126.50
20	2	578	C	C2-N1-C1'	5.44	124.78	118.80
41	F	120	LEU	CA-CB-CG	5.44	127.81	115.30
20	2	1474	A	C8-N9-C4	-5.44	103.62	105.80
20	2	183	G	C4-N9-C1'	5.43	133.56	126.50
20	2	728	C	N1-C2-O2	5.43	122.16	118.90
20	2	315	C	C5-C6-N1	5.43	123.71	121.00
20	2	491	C	N3-C4-C5	-5.43	119.73	121.90
41	F	261	ARG	CA-CB-CG	5.43	125.35	113.40
20	2	1719	A	N1-C2-N3	-5.43	126.59	129.30
20	2	1078	C	N1-C2-O2	5.42	122.16	118.90
20	2	1619	A	N1-C2-N3	-5.42	126.59	129.30
20	2	494	C	C6-N1-C1'	-5.42	114.29	120.80
20	2	662	G	OP1-P-O3'	5.42	117.13	105.20
20	2	205	G	N3-C2-N2	-5.41	116.11	119.90
20	2	1309	C	N1-C2-O2	5.41	122.15	118.90
20	2	1389	C	C2-N3-C4	5.41	122.61	119.90
46	1	433	ARG	CA-CB-CG	5.41	125.31	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	694	G	N3-C2-N2	-5.41	116.11	119.90
20	2	1062	A	O4'-C1'-N9	5.41	112.53	108.20
5	q	104	ASP	CB-CG-OD1	5.41	123.17	118.30
20	2	21	U	N1-C2-O2	5.41	126.58	122.80
20	2	1098	C	C6-N1-C2	-5.40	118.14	120.30
20	2	389	A	N9-C4-C5	-5.40	103.64	105.80
20	2	491	C	C6-N1-C2	-5.40	118.14	120.30
20	2	690	G	C8-N9-C4	-5.40	104.24	106.40
20	2	1578	U	N3-C2-O2	-5.40	118.42	122.20
20	2	1684	C	C6-N1-C2	-5.40	118.14	120.30
20	2	1758	G	C4-N9-C1'	5.40	133.52	126.50
20	2	1036	A	C2-N3-C4	5.39	113.30	110.60
20	2	1277	C	C2-N3-C4	5.39	122.60	119.90
20	2	318	A	N1-C2-N3	-5.39	126.60	129.30
20	2	1127	C	N3-C2-O2	-5.39	118.13	121.90
20	2	4	C	C2-N1-C1'	5.39	124.73	118.80
20	2	174	C	C5-C6-N1	5.38	123.69	121.00
20	2	399	C	C6-N1-C2	-5.38	118.15	120.30
20	2	974	C	C5-C6-N1	5.38	123.69	121.00
20	2	1348	G	N3-C4-N9	5.38	129.23	126.00
20	2	1628	C	N3-C2-O2	-5.38	118.14	121.90
20	2	441	C	C2-N1-C1'	5.38	124.71	118.80
20	2	72	C	N3-C2-O2	-5.37	118.14	121.90
20	2	1353	A	C4-C5-N7	5.37	113.39	110.70
20	2	1501	C	N1-C2-O2	5.37	122.12	118.90
20	2	577	U	C2-N1-C1'	5.37	124.14	117.70
20	2	1578	U	N1-C2-O2	5.37	126.56	122.80
20	2	1396	A	O4'-C1'-N9	5.36	112.49	108.20
20	2	358	C	N1-C2-O2	5.36	122.11	118.90
20	2	979	C	C5-C6-N1	5.36	123.68	121.00
20	2	17	C	C5-C6-N1	5.36	123.68	121.00
20	2	371	A	O5'-P-OP2	-5.36	100.88	105.70
10	c	138	ARG	CA-CB-CG	5.36	125.18	113.40
20	2	863	U	C6-N1-C2	-5.36	117.79	121.00
38	A	467	LEU	CB-CG-CD2	-5.36	101.90	111.00
20	2	118	C	C2-N1-C1'	5.35	124.69	118.80
20	2	966	U	N3-C2-O2	-5.35	118.45	122.20
20	2	496	C	C6-N1-C2	-5.35	118.16	120.30
20	2	587	A	N1-C2-N3	-5.35	126.62	129.30
20	2	1670	C	N1-C2-O2	5.35	122.11	118.90
20	2	670	A	N1-C6-N6	-5.35	115.39	118.60
20	2	951	C	C2-N3-C4	5.35	122.57	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	141	A	N1-C2-N3	-5.35	126.63	129.30
20	2	531	A	N1-C2-N3	-5.35	126.63	129.30
20	2	442	C	N1-C2-O2	5.34	122.11	118.90
20	2	1821	U	C6-N1-C1'	-5.34	113.72	121.20
20	2	1087	A	N1-C2-N3	-5.34	126.63	129.30
20	2	1391	C	C6-N1-C2	-5.34	118.16	120.30
20	2	1522	A	N1-C6-N6	-5.34	115.39	118.60
20	2	557	U	N3-C2-O2	-5.34	118.46	122.20
20	2	106	C	C6-N1-C2	-5.34	118.17	120.30
20	2	977	C	O4'-C1'-N1	5.34	112.47	108.20
20	2	1205	C	N1-C2-O2	5.34	122.10	118.90
20	2	557	U	C6-N1-C2	-5.33	117.80	121.00
20	2	942	G	C8-N9-C4	-5.33	104.27	106.40
20	2	1811	C	N3-C2-O2	-5.33	118.17	121.90
20	2	1831	A	N1-C2-N3	-5.33	126.63	129.30
20	2	974	C	O4'-C1'-N1	5.33	112.46	108.20
20	2	802	A	C2-N3-C4	5.33	113.27	110.60
20	2	130	G	C2-N3-C4	5.33	114.56	111.90
20	2	421	G	C6-C5-N7	-5.33	127.20	130.40
20	2	853	C	O4'-C1'-N1	5.32	112.46	108.20
20	2	1600	G	C8-N9-C1'	-5.32	120.08	127.00
20	2	165	G	C4-N9-C1'	5.32	133.41	126.50
20	2	416	U	C5-C6-N1	5.32	125.36	122.70
20	2	575	A	N1-C2-N3	-5.32	126.64	129.30
20	2	1111	U	C6-N1-C2	-5.32	117.81	121.00
20	2	1604	G	C8-N9-C4	-5.32	104.27	106.40
20	2	725	C	N3-C2-O2	-5.32	118.18	121.90
20	2	909	G	C8-N9-C1'	-5.32	120.09	127.00
20	2	927	C	C6-N1-C2	-5.31	118.17	120.30
20	2	690	G	C2-N3-C4	5.31	114.56	111.90
20	2	862	A	C4-N9-C1'	5.31	135.86	126.30
20	2	909	G	N3-C4-N9	5.31	129.19	126.00
20	2	1603	G	N3-C4-N9	5.31	129.19	126.00
33	l	36	LEU	CA-CB-CG	5.31	127.51	115.30
20	2	421	G	C4-N9-C1'	5.30	133.39	126.50
20	2	1217	A	N1-C2-N3	-5.30	126.65	129.30
20	2	1292	C	P-O3'-C3'	5.30	126.06	119.70
20	2	664	A	C4-C5-C6	-5.30	114.35	117.00
20	2	719	G	N9-C4-C5	-5.30	103.28	105.40
20	2	883	U	C5-C6-N1	5.30	125.35	122.70
20	2	1236	G	C4-N9-C1'	5.30	133.39	126.50
20	2	1383	A	N1-C2-N3	-5.30	126.65	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	424	C	N1-C2-O2	5.29	122.08	118.90
20	2	515	G	C6-C5-N7	-5.29	127.22	130.40
20	2	1443	C	C6-N1-C2	-5.29	118.18	120.30
20	2	296	U	N3-C2-O2	-5.29	118.50	122.20
20	2	1553	C	C6-N1-C2	-5.29	118.18	120.30
20	2	386	C	C2-N1-C1'	5.29	124.62	118.80
20	2	1511	U	N1-C2-O2	5.29	126.50	122.80
20	2	1315	U	C6-N1-C1'	-5.29	113.80	121.20
20	2	444	G	C4-C5-N7	5.29	112.91	110.80
20	2	1825	A	C2-N3-C4	5.29	113.24	110.60
20	2	223	C	C5-C6-N1	5.28	123.64	121.00
39	C	436	GLN	CA-CB-CG	5.28	125.02	113.40
20	2	376	A	C2-N3-C4	5.28	113.24	110.60
20	2	1772	C	C6-N1-C2	-5.28	118.19	120.30
46	1	580	LEU	CA-CB-CG	5.28	127.43	115.30
20	2	165	G	N3-C4-C5	-5.27	125.96	128.60
20	2	222	U	C6-N1-C2	-5.27	117.84	121.00
20	2	603	C	C6-N1-C2	-5.27	118.19	120.30
20	2	748	C	C5-C6-N1	5.27	123.64	121.00
20	2	1746	U	N1-C2-O2	5.27	126.49	122.80
20	2	330	G	N3-C4-N9	5.26	129.16	126.00
20	2	470	G	N9-C4-C5	-5.26	103.29	105.40
20	2	939	U	N3-C2-O2	-5.26	118.52	122.20
20	2	1072	U	N1-C2-O2	5.26	126.49	122.80
20	2	1382	A	C4-C5-N7	5.26	113.33	110.70
20	2	728	C	N3-C2-O2	-5.26	118.22	121.90
20	2	1532	C	C6-N1-C2	-5.26	118.19	120.30
20	2	421	G	C4-C5-N7	5.26	112.91	110.80
20	2	1684	C	N3-C2-O2	-5.26	118.22	121.90
20	2	1177	U	N1-C2-O2	5.26	126.48	122.80
20	2	479	C	N1-C2-O2	5.26	122.05	118.90
20	2	806	U	N3-C2-O2	-5.26	118.52	122.20
20	2	158	A	C5-C6-N1	5.25	120.32	117.70
20	2	539	C	N3-C4-N4	5.25	121.67	118.00
20	2	958	G	N7-C8-N9	5.25	115.72	113.10
20	2	56	G	N9-C4-C5	-5.25	103.30	105.40
20	2	851	C	C6-N1-C1'	-5.25	114.50	120.80
20	2	1079	C	N1-C2-O2	5.25	122.05	118.90
20	2	1113	A	N9-C4-C5	-5.24	103.70	105.80
20	2	394	G	N3-C4-N9	5.24	129.15	126.00
20	2	966	U	N1-C2-O2	5.24	126.47	122.80
20	2	401	A	C5-C6-N1	5.24	120.32	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	816	A	C2-N3-C4	5.24	113.22	110.60
16	j	113	GLY	N-CA-C	-5.24	100.00	113.10
20	2	795	A	N1-C6-N6	-5.24	115.46	118.60
20	2	1415	C	C6-N1-C2	-5.24	118.20	120.30
20	2	104	A	C5-C6-N1	5.24	120.32	117.70
20	2	1288	U	C2-N1-C1'	5.23	123.98	117.70
20	2	810	A	N1-C2-N3	-5.23	126.69	129.30
20	2	195	C	N3-C2-O2	-5.23	118.24	121.90
20	2	723	C	C5-C6-N1	5.23	123.61	121.00
20	2	1123	C	C2-N3-C4	5.23	122.51	119.90
43	K	76	ASN	C-N-CA	5.23	134.77	121.70
20	2	548	C	C6-N1-C2	-5.22	118.21	120.30
20	2	1016	U	C5-C6-N1	5.22	125.31	122.70
20	2	193	C	N3-C2-O2	-5.22	118.25	121.90
20	2	34	U	N3-C2-O2	-5.21	118.55	122.20
20	2	295	C	C2-N1-C1'	5.21	124.53	118.80
20	2	1182	A	C4-C5-N7	5.21	113.31	110.70
20	2	1559	C	C6-N1-C2	-5.21	118.22	120.30
20	2	501	C	C2-N3-C4	5.21	122.50	119.90
20	2	863	U	O4'-C1'-N1	5.21	112.37	108.20
20	2	1053	C	C2-N1-C1'	5.21	124.53	118.80
20	2	1596	U	N3-C2-O2	-5.21	118.56	122.20
20	2	1603	G	C2-N3-C4	5.21	114.50	111.90
20	2	822	U	N1-C2-O2	5.21	126.44	122.80
20	2	1854	U	C5-C6-N1	5.21	125.30	122.70
20	2	315	C	C6-N1-C2	-5.20	118.22	120.30
20	2	1125	C	C5-C6-N1	5.20	123.60	121.00
20	2	1164	G	C4-N9-C1'	5.20	133.26	126.50
1	a	60	LEU	CA-CB-CG	5.20	127.26	115.30
20	2	447	A	C4-C5-C6	-5.20	114.40	117.00
20	2	489	A	N1-C2-N3	-5.20	126.70	129.30
20	2	555	A	C4-C5-C6	-5.20	114.40	117.00
20	2	852	G	C4-C5-N7	5.20	112.88	110.80
20	2	973	C	C2-N1-C1'	5.20	124.52	118.80
20	2	988	C	C5-C6-N1	5.20	123.60	121.00
20	2	1231	C	N1-C2-O2	5.19	122.02	118.90
20	2	1389	C	C6-N1-C1'	-5.19	114.57	120.80
20	2	1504	U	N1-C2-O2	5.19	126.43	122.80
20	2	1103	C	C5-C6-N1	5.19	123.60	121.00
20	2	389	A	C5-C6-N6	-5.19	119.55	123.70
20	2	69	C	C5-C6-N1	5.19	123.59	121.00
20	2	120	U	C2-N1-C1'	5.19	123.93	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	152	U	N3-C2-O2	-5.19	118.57	122.20
20	2	208	G	N3-C4-N9	5.19	129.11	126.00
20	2	209	A	N9-C4-C5	-5.19	103.72	105.80
20	2	886	A	N7-C8-N9	5.19	116.39	113.80
20	2	401	A	N1-C6-N6	-5.18	115.49	118.60
20	2	1172	U	C6-N1-C2	-5.18	117.89	121.00
20	2	1348	G	C4-N9-C1'	5.18	133.24	126.50
20	2	394	G	C4-N9-C1'	5.18	133.24	126.50
20	2	1645	C	C6-N1-C2	-5.18	118.23	120.30
20	2	438	G	N3-C4-C5	-5.18	126.01	128.60
20	2	585	C	N1-C2-O2	5.18	122.00	118.90
20	2	1180	C	C5-C6-N1	5.18	123.59	121.00
20	2	585	C	C6-N1-C2	-5.17	118.23	120.30
20	2	660	C	C2-N1-C1'	5.17	124.49	118.80
20	2	1530	U	C5-C6-N1	5.17	125.29	122.70
20	2	424	C	N3-C2-O2	-5.17	118.28	121.90
20	2	1276	A	N1-C6-N6	-5.17	115.50	118.60
20	2	648	A	N1-C2-N3	-5.16	126.72	129.30
20	2	958	G	C8-N9-C1'	-5.16	120.29	127.00
20	2	1164	G	N3-C4-N9	5.16	129.10	126.00
20	2	1592	C	C6-N1-C2	-5.16	118.23	120.30
20	2	1747	C	N3-C2-O2	-5.16	118.29	121.90
20	2	583	A	N1-C2-N3	-5.16	126.72	129.30
20	2	5	U	N3-C2-O2	-5.16	118.59	122.20
20	2	1544	C	O4'-C1'-N1	5.16	112.33	108.20
20	2	1624	U	N1-C2-O2	5.16	126.41	122.80
20	2	207	G	N3-C4-C5	-5.16	126.02	128.60
20	2	649	U	N1-C2-O2	5.16	126.41	122.80
43	K	112	CYS	CA-CB-SG	5.15	123.28	114.00
20	2	930	C	N3-C2-O2	-5.15	118.30	121.90
20	2	1109	C	C6-N1-C2	-5.15	118.24	120.30
20	2	638	C	O4'-C1'-N1	5.15	112.32	108.20
20	2	565	G	N9-C4-C5	5.14	107.46	105.40
20	2	1837	G	C8-N9-C1'	5.14	133.69	127.00
20	2	424	C	C6-N1-C2	-5.14	118.24	120.30
20	2	655	A	C5-N7-C8	-5.14	101.33	103.90
20	2	664	A	N1-C6-N6	-5.14	115.52	118.60
38	A	511	LEU	CA-CB-CG	5.14	127.12	115.30
20	2	1080	A	N1-C6-N6	-5.14	115.52	118.60
20	2	1224	G	C4-N9-C1'	5.14	133.18	126.50
20	2	1561	A	C2-N3-C4	5.14	113.17	110.60
10	c	169	ARG	NE-CZ-NH1	5.13	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	362	C	N1-C2-O2	5.13	121.98	118.90
20	2	543	C	N1-C2-O2	5.13	121.98	118.90
20	2	1779	G	N7-C8-N9	5.13	115.67	113.10
20	2	1363	C	C2-N1-C1'	5.13	124.44	118.80
20	2	19	A	N1-C2-N3	-5.13	126.73	129.30
20	2	1310	U	C2-N1-C1'	5.13	123.85	117.70
20	2	28	U	C6-N1-C2	-5.13	117.92	121.00
20	2	464	A	O4'-C1'-N9	-5.12	104.10	108.20
20	2	372	U	N1-C2-O2	5.12	126.39	122.80
20	2	690	G	N7-C8-N9	5.12	115.66	113.10
20	2	830	A	C5-C6-N1	5.12	120.26	117.70
20	2	917	U	N1-C2-O2	5.12	126.38	122.80
31	P	96	LEU	CA-CB-CG	5.12	127.08	115.30
20	2	1368	U	C6-N1-C2	-5.12	117.93	121.00
20	2	93	U	N1-C2-O2	5.12	126.38	122.80
20	2	1165	G	C6-C5-N7	-5.12	127.33	130.40
20	2	1465	A	C5-N7-C8	-5.12	101.34	103.90
20	2	1849	A	C5-C6-N6	-5.12	119.61	123.70
24	e	196	LEU	CA-CB-CG	5.11	127.05	115.30
20	2	422	U	O4'-C1'-N1	5.11	112.28	108.20
20	2	1602	U	C2-N1-C1'	5.10	123.82	117.70
20	2	1391	C	C5-C6-N1	5.10	123.55	121.00
20	2	428	U	O4'-C1'-N1	-5.10	104.12	108.20
20	2	615	C	C5-C6-N1	5.10	123.55	121.00
20	2	1651	A	N1-C2-N3	-5.10	126.75	129.30
20	2	212	C	C6-N1-C2	-5.10	118.26	120.30
20	2	439	A	N1-C2-N3	-5.10	126.75	129.30
20	2	1536	G	C4-N9-C1'	5.10	133.13	126.50
20	2	1353	A	N1-C2-N3	-5.10	126.75	129.30
20	2	1751	C	N3-C2-O2	-5.10	118.33	121.90
20	2	862	A	O4'-C1'-N9	5.09	112.28	108.20
20	2	1626	C	C6-N1-C2	-5.09	118.26	120.30
20	2	1856	C	C6-N1-C1'	5.09	126.91	120.80
20	2	200	G	C8-N9-C4	-5.09	104.36	106.40
20	2	417	C	C6-N1-C2	-5.09	118.26	120.30
20	2	619	A	N1-C2-N3	-5.09	126.75	129.30
20	2	1163	C	C6-N1-C2	-5.09	118.26	120.30
20	2	650	A	N1-C2-N3	-5.09	126.76	129.30
20	2	870	A	N1-C2-N3	-5.08	126.76	129.30
20	2	565	G	N1-C6-O6	-5.08	116.85	119.90
20	2	814	U	C6-N1-C1'	-5.08	114.08	121.20
20	2	1782	G	C4-N9-C1'	5.08	133.10	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	1149	A	N1-C2-N3	-5.08	126.76	129.30
20	2	100	U	N1-C2-O2	5.08	126.35	122.80
20	2	803	C	N3-C2-O2	-5.08	118.35	121.90
20	2	526	A	N1-C6-N6	-5.07	115.56	118.60
20	2	1116	C	C5-C6-N1	5.07	123.53	121.00
20	2	1288	U	N3-C2-O2	-5.07	118.65	122.20
20	2	550	C	N3-C2-O2	-5.07	118.35	121.90
20	2	678	U	C6-N1-C2	-5.07	117.96	121.00
20	2	187	G	C8-N9-C4	-5.06	104.37	106.40
20	2	576	A	N9-C4-C5	-5.06	103.77	105.80
20	2	479	C	N3-C2-O2	-5.06	118.36	121.90
20	2	1229	G	N7-C8-N9	5.06	115.63	113.10
20	2	716	G	C4-C5-N7	5.06	112.82	110.80
20	2	169	U	N1-C2-O2	5.06	126.34	122.80
20	2	1804	U	C5-C6-N1	5.06	125.23	122.70
20	2	186	C	C2-N1-C1'	5.06	124.36	118.80
20	2	1202	U	C6-N1-C2	-5.06	117.97	121.00
20	2	1832	A	N1-C2-N3	-5.06	126.77	129.30
20	2	447	A	C8-N9-C4	5.06	107.82	105.80
20	2	1608	U	N1-C2-O2	5.06	126.34	122.80
20	2	710	C	N1-C2-O2	5.05	121.93	118.90
20	2	207	G	N3-C4-N9	5.05	129.03	126.00
20	2	1272	C	C5-C6-N1	5.05	123.53	121.00
20	2	86	C	N3-C2-O2	-5.05	118.36	121.90
20	2	1825	A	N1-C2-N3	-5.04	126.78	129.30
20	2	701	G	C8-N9-C4	-5.04	104.38	106.40
20	2	734	C	C5-C6-N1	5.04	123.52	121.00
20	2	1259	A	C4-C5-N7	5.04	113.22	110.70
20	2	1801	A	N1-C2-N3	-5.04	126.78	129.30
20	2	489	A	C4-C5-N7	5.04	113.22	110.70
20	2	1170	A	C5-C6-N1	5.04	120.22	117.70
20	2	1661	A	C4-N9-C1'	5.04	135.37	126.30
20	2	124	U	N1-C2-O2	5.03	126.32	122.80
20	2	680	G	C8-N9-C4	-5.03	104.39	106.40
20	2	1177	U	C5-C6-N1	5.03	125.22	122.70
20	2	901	G	N3-C2-N2	-5.03	116.38	119.90
20	2	699	C	C6-N1-C2	-5.03	118.29	120.30
20	2	352	U	N1-C2-O2	5.03	126.32	122.80
20	2	1265	A	C5-N7-C8	-5.03	101.39	103.90
20	2	1512	C	N1-C2-O2	5.03	121.92	118.90
20	2	1524	G	N3-C4-N9	5.03	129.02	126.00
20	2	289	G	N3-C4-N9	-5.03	122.98	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	394	G	C8-N9-C1'	-5.03	120.47	127.00
20	2	645	C	C5-C6-N1	5.03	123.51	121.00
20	2	1559	C	C2-N1-C1'	5.03	124.33	118.80
20	2	179	C	C2-N1-C1'	5.02	124.33	118.80
20	2	293	C	C6-N1-C1'	-5.02	114.77	120.80
20	2	340	C	N3-C2-O2	-5.02	118.39	121.90
20	2	561	A	N1-C2-N3	-5.02	126.79	129.30
20	2	165	G	C8-N9-C4	-5.02	104.39	106.40
20	2	295	C	N3-C2-O2	-5.02	118.39	121.90
20	2	603	C	C5-C6-N1	5.02	123.51	121.00
20	2	26	U	C6-N1-C2	-5.02	117.99	121.00
45	M	71	LEU	CA-CB-CG	5.01	126.83	115.30
20	2	1349	G	C8-N9-C1'	-5.01	120.48	127.00
20	2	454	U	C5-C6-N1	5.01	125.20	122.70
20	2	1098	C	C5-C6-N1	5.01	123.50	121.00
20	2	1280	G	C2-N3-C4	5.01	114.41	111.90
20	2	1464	C	C5-C6-N1	5.01	123.50	121.00
20	2	1465	A	OP2-P-O3'	5.01	116.22	105.20
20	2	411	G	C8-N9-C4	-5.00	104.40	106.40
20	2	341	C	N1-C2-O2	5.00	121.90	118.90
20	2	483	C	C5-C6-N1	5.00	123.50	121.00
20	2	1178	U	C5-C6-N1	5.00	125.20	122.70

There are no chirality outliers.

All (77) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
46	1	189	ASP	Peptide
46	1	263	ILE	Peptide
46	1	33	ARG	Peptide
46	1	357	MET	Peptide
46	1	528	LEU	Peptide
37	B	256	ASP	Peptide
37	B	292	ASN	Peptide
37	B	332	ARG	Peptide
37	B	442	THR	Peptide
37	B	443	LEU	Peptide
37	B	445	THR	Peptide
37	B	678	ASP	Peptide
39	C	416	PRO	Peptide
39	C	422	GLU	Peptide
39	C	424	ILE	Peptide

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Mol	Chain	Res	Type	Group
39	C	427	GLU	Peptide
39	C	437	PRO	Peptide
39	C	708	ARG	Peptide
39	C	759	GLU	Peptide
48	D	242	GLN	Peptide
48	D	25	PHE	Peptide
48	D	39	LEU	Peptide
40	E	176	GLU	Peptide
40	E	31	ILE	Peptide
41	F	126	LYS	Peptide
41	F	194	ALA	Peptide
41	F	203	ASP	Peptide
41	F	211	MET	Peptide
41	F	228	MET	Peptide
41	F	265	LEU	Peptide
42	H	313	ARG	Peptide
42	H	41	ILE	Peptide
42	H	55	GLU	Peptide
42	H	59	GLY	Peptide
36	I	146	ASP	Peptide
36	I	147	SER	Peptide
36	I	175	ALA	Peptide
43	K	150	TYR	Peptide
43	K	182	ASP	Peptide
43	K	195	SER	Peptide
43	K	199	LYS	Peptide
43	K	42	TYR	Peptide
44	L	261	GLY	Peptide
44	L	345	ARG	Peptide
44	L	403	LYS	Peptide
44	L	432	HIS	Peptide
44	L	500	LEU	Peptide
45	M	113	MET	Peptide
45	M	116	ASN	Peptide
45	M	236	LEU	Peptide
45	M	318	THR	Peptide
45	M	96	GLY	Peptide
32	S	35	MET	Peptide
35	V	143	GLN	Peptide
35	V	174	VAL	Peptide
35	V	175	LYS	Peptide
35	V	241	PHE	Peptide

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Mol	Chain	Res	Type	Group
35	V	293	ALA	Peptide
35	V	75	GLY	Peptide
3	d	133	TYR	Peptide
3	d	135	GLY	Peptide
24	e	42	LYS	Peptide
24	e	65	GLN	Peptide
24	e	77	MET	Peptide
15	f	54	ASP	Peptide
15	f	65	LEU	Peptide
28	k	99	LEU	Peptide
33	l	12	ARG	Peptide
5	q	132	GLY	Peptide
5	q	184	THR	Peptide
5	q	87	MET	Peptide
8	s	134	VAL	Peptide
21	w	42	PRO	Peptide
21	w	60	ARG	Peptide
21	w	71	ILE	Peptide
17	z	10	ARG	Peptide
17	z	102	THR	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	214/216 (99%)	214 (100%)	0	0	100	100
2	p	209/211 (99%)	209 (100%)	0	0	100	100
3	d	214/216 (99%)	214 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	99/101 (98%)	99 (100%)	0	0	100	100
5	q	253/255 (99%)	250 (99%)	3 (1%)	0	100	100
6	W	22/24 (92%)	22 (100%)	0	0	100	100
7	r	220/222 (99%)	220 (100%)	0	0	100	100
8	s	165/181 (91%)	165 (100%)	0	0	100	100
9	t	195/205 (95%)	195 (100%)	0	0	100	100
10	c	178/180 (99%)	178 (100%)	0	0	100	100
11	n	131/144 (91%)	131 (100%)	0	0	100	100
12	m	147/149 (99%)	147 (100%)	0	0	100	100
13	i	123/125 (98%)	123 (100%)	0	0	100	100
14	y	80/82 (98%)	80 (100%)	0	0	100	100
15	f	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
16	j	137/139 (99%)	135 (98%)	2 (2%)	0	100	100
17	z	120/122 (98%)	120 (100%)	0	0	100	100
18	R	80/82 (98%)	80 (100%)	0	0	100	100
19	T	40/44 (91%)	40 (100%)	0	0	100	100
21	w	124/130 (95%)	124 (100%)	0	0	100	100
22	g	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
23	b	222/224 (99%)	221 (100%)	1 (0%)	0	100	100
24	e	187/189 (99%)	185 (99%)	2 (1%)	0	100	100
25	u	93/95 (98%)	93 (100%)	0	0	100	100
26	v	107/116 (92%)	107 (100%)	0	0	100	100
27	o	117/119 (98%)	117 (100%)	0	0	100	100
28	k	138/140 (99%)	138 (100%)	0	0	100	100
29	x	139/141 (99%)	139 (100%)	0	0	100	100
30	h	96/98 (98%)	96 (100%)	0	0	100	100
31	P	68/70 (97%)	68 (100%)	0	0	100	100
32	S	59/61 (97%)	59 (100%)	0	0	100	100
33	l	52/54 (96%)	52 (100%)	0	0	100	100
34	U	53/62 (86%)	53 (100%)	0	0	100	100
35	V	290/309 (94%)	287 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	I	301/316 (95%)	301 (100%)	0	0	100	100
37	B	528/566 (93%)	528 (100%)	0	0	100	100
38	A	682/722 (94%)	682 (100%)	0	0	100	100
39	C	615/743 (83%)	613 (100%)	2 (0%)	0	100	100
40	E	406/429 (95%)	406 (100%)	0	0	100	100
41	F	267/269 (99%)	266 (100%)	1 (0%)	0	100	100
42	H	289/318 (91%)	289 (100%)	0	0	100	100
43	K	215/217 (99%)	215 (100%)	0	0	100	100
44	L	370/372 (100%)	366 (99%)	4 (1%)	0	100	100
45	M	330/362 (91%)	330 (100%)	0	0	100	100
46	1	572/595 (96%)	570 (100%)	2 (0%)	0	100	100
47	N	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
48	D	441/527 (84%)	441 (100%)	0	0	100	100
49	Y	76/78 (97%)	76 (100%)	0	0	100	100
50	G	68/258 (26%)	68 (100%)	0	0	100	100
50	J	71/258 (28%)	71 (100%)	0	0	100	100
All	All	9955/10894 (91%)	9931 (100%)	24 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	180/180 (100%)	175 (97%)	5 (3%)	43	68
2	p	192/192 (100%)	191 (100%)	1 (0%)	88	94
3	d	182/182 (100%)	179 (98%)	3 (2%)	62	79
4	Q	88/88 (100%)	88 (100%)	0	100	100
5	q	220/220 (100%)	219 (100%)	1 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	W	23/23 (100%)	23 (100%)	0	100	100
7	r	193/193 (100%)	190 (98%)	3 (2%)	62	79
8	s	155/163 (95%)	154 (99%)	1 (1%)	86	92
9	t	174/178 (98%)	173 (99%)	1 (1%)	86	92
10	c	160/160 (100%)	160 (100%)	0	100	100
11	n	125/132 (95%)	124 (99%)	1 (1%)	81	89
12	m	130/130 (100%)	129 (99%)	1 (1%)	81	89
13	i	98/98 (100%)	98 (100%)	0	100	100
14	y	66/66 (100%)	64 (97%)	2 (3%)	41	66
15	f	112/112 (100%)	112 (100%)	0	100	100
16	j	111/111 (100%)	109 (98%)	2 (2%)	59	77
17	z	106/106 (100%)	106 (100%)	0	100	100
18	R	74/74 (100%)	73 (99%)	1 (1%)	67	81
19	T	35/35 (100%)	34 (97%)	1 (3%)	42	67
21	w	111/118 (94%)	109 (98%)	2 (2%)	59	77
22	g	114/114 (100%)	111 (97%)	3 (3%)	46	69
23	b	188/188 (100%)	186 (99%)	2 (1%)	73	85
24	e	159/159 (100%)	156 (98%)	3 (2%)	57	76
25	u	86/86 (100%)	85 (99%)	1 (1%)	71	84
26	v	94/98 (96%)	93 (99%)	1 (1%)	73	85
27	o	107/107 (100%)	106 (99%)	1 (1%)	78	88
28	k	122/122 (100%)	120 (98%)	2 (2%)	62	79
29	x	111/111 (100%)	109 (98%)	2 (2%)	59	77
30	h	91/91 (100%)	90 (99%)	1 (1%)	73	85
31	P	62/62 (100%)	62 (100%)	0	100	100
32	S	54/54 (100%)	54 (100%)	0	100	100
33	l	47/47 (100%)	47 (100%)	0	100	100
34	U	51/55 (93%)	50 (98%)	1 (2%)	55	75
35	V	256/268 (96%)	253 (99%)	3 (1%)	71	84
37	B	90/508 (18%)	90 (100%)	0	100	100
38	A	546/667 (82%)	541 (99%)	5 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	C	554/662 (84%)	545 (98%)	9 (2%)	62 79
40	E	380/393 (97%)	376 (99%)	4 (1%)	73 85
41	F	237/237 (100%)	231 (98%)	6 (2%)	47 70
42	H	269/290 (93%)	265 (98%)	4 (2%)	65 81
43	K	192/192 (100%)	190 (99%)	2 (1%)	76 86
44	L	342/342 (100%)	337 (98%)	5 (2%)	65 81
45	M	305/324 (94%)	301 (99%)	4 (1%)	69 82
46	1	506/523 (97%)	498 (98%)	8 (2%)	62 79
47	N	77/78 (99%)	74 (96%)	3 (4%)	32 60
48	D	398/473 (84%)	389 (98%)	9 (2%)	50 72
All	All	7973/8812 (90%)	7869 (99%)	104 (1%)	70 82

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	97	THR
1	a	102	ARG
1	a	107	THR
1	a	140	VAL
1	a	212	LYS
2	p	153	THR
3	d	132	ASP
3	d	170	TRP
3	d	248	TYR
5	q	247	THR
7	r	126	ASP
7	r	162	LEU
7	r	180	VAL
8	s	66	VAL
9	t	47	ARG
11	n	69	ARG
12	m	39	LYS
14	y	9	VAL
14	y	10	ASP
16	j	85	VAL
16	j	112	VAL
18	R	53	VAL
19	T	18	LYS

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Mol	Chain	Res	Type
21	w	41	ILE
21	w	72	LYS
22	g	12	VAL
22	g	27	ARG
22	g	102	GLU
23	b	76	ARG
23	b	107	TYR
24	e	26	ASP
24	e	168	THR
24	e	187	SER
25	u	2	LEU
26	v	36	ARG
27	o	37	TYR
28	k	136	THR
28	k	142	ARG
29	x	35	ASP
29	x	75	MET
30	h	90	ASP
34	U	89	LYS
35	V	23	THR
35	V	111	VAL
35	V	113	PHE
38	A	309	ASN
38	A	311	THR
38	A	336	THR
38	A	407	VAL
38	A	462	VAL
39	C	324	ILE
39	C	378	ILE
39	C	413	PHE
39	C	440	VAL
39	C	633	LEU
39	C	709	MET
39	C	712	LYS
39	C	726	LEU
39	C	733	MET
40	E	136	LYS
40	E	331	ASP
40	E	339	PHE
40	E	342	GLU
41	F	210	ARG
41	F	219	THR

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Mol	Chain	Res	Type
41	F	230	VAL
41	F	254	LYS
41	F	261	ARG
41	F	322	ASP
42	H	36	VAL
42	H	110	VAL
42	H	133	LEU
42	H	233	LEU
43	K	32	TYR
43	K	90	ASP
44	L	244	LEU
44	L	346	THR
44	L	391	ARG
44	L	501	VAL
44	L	503	THR
45	M	82	LEU
45	M	117	THR
45	M	121	TYR
45	M	285	MET
46	1	11	VAL
46	1	55	CYS
46	1	158	LYS
46	1	241	ASP
46	1	433	ARG
46	1	436	TYR
46	1	493	ASP
46	1	543	THR
47	N	57	LYS
47	N	90	ARG
47	N	91	LYS
48	D	3	LYS
48	D	234	VAL
48	D	272	VAL
48	D	291	VAL
48	D	368	ASP
48	D	446	TYR
48	D	468	THR
48	D	491	LEU
48	D	520	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	9	GLN
1	a	111	GLN
2	p	157	GLN
2	p	160	GLN
4	Q	25	ASN
4	Q	72	HIS
5	q	98	ASN
5	q	216	ASN
5	q	224	ASN
7	r	13	GLN
7	r	59	GLN
8	s	73	GLN
8	s	91	HIS
9	t	7	ASN
9	t	35	ASN
9	t	64	ASN
9	t	146	GLN
9	t	165	GLN
10	c	132	GLN
11	n	13	GLN
13	i	38	ASN
13	i	79	GLN
15	f	113	HIS
17	z	22	GLN
18	R	83	GLN
19	T	44	ASN
21	w	26	ASN
22	g	142	GLN
23	b	179	GLN
24	e	74	ASN
24	e	82	ASN
24	e	148	ASN
24	e	149	GLN
25	u	7	ASN
25	u	32	HIS
25	u	77	GLN
27	o	32	GLN
28	k	42	HIS
28	k	105	ASN
28	k	120	HIS
29	x	11	GLN
29	x	128	GLN
30	h	47	ASN

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Mol	Chain	Res	Type
30	h	81	GLN
31	P	46	ASN
33	l	3	HIS
33	l	16	GLN
33	l	26	ASN
35	V	178	ASN
35	V	311	GLN
37	B	508	ASN
38	A	10	ASN
38	A	16	ASN
38	A	236	GLN
38	A	316	GLN
38	A	432	GLN
38	A	442	GLN
38	A	549	GLN
38	A	573	GLN
39	C	62	ASN
39	C	460	GLN
39	C	478	GLN
39	C	575	HIS
39	C	637	GLN
39	C	713	GLN
39	C	717	GLN
39	C	784	GLN
39	C	870	ASN
40	E	49	ASN
40	E	121	HIS
40	E	143	ASN
40	E	210	GLN
40	E	216	HIS
40	E	225	HIS
40	E	252	HIS
40	E	321	ASN
40	E	335	ASN
40	E	377	ASN
41	F	332	ASN
41	F	342	ASN
42	H	109	HIS
42	H	114	HIS
42	H	207	ASN
42	H	238	HIS
42	H	261	ASN

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Mol	Chain	Res	Type
42	H	270	GLN
42	H	336	GLN
42	H	337	ASN
43	K	6	GLN
43	K	36	GLN
43	K	55	GLN
43	K	76	ASN
43	K	91	GLN
43	K	151	GLN
44	L	195	GLN
44	L	243	GLN
44	L	364	ASN
44	L	402	GLN
45	M	14	GLN
45	M	79	GLN
45	M	138	GLN
45	M	259	ASN
45	M	302	GLN
46	1	175	GLN
46	1	556	ASN
46	1	593	ASN
47	N	95	GLN
48	D	392	ASN
48	D	469	GLN
48	D	479	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	2	1710/1720 (99%)	524 (30%)	10 (0%)

All (524) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	2	2	A
20	2	6	G
20	2	25	A
20	2	41	G
20	2	44	U
20	2	45	A
20	2	46	A

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Mol	Chain	Res	Type
20	2	47	G
20	2	49	C
20	2	56	G
20	2	60	A
20	2	62	G
20	2	64	A
20	2	65	C
20	2	67	C
20	2	68	A
20	2	69	C
20	2	71	G
20	2	72	C
20	2	74	G
20	2	76	U
20	2	79	A
20	2	92	A
20	2	99	A
20	2	103	A
20	2	112	U
20	2	113	G
20	2	114	G
20	2	115	U
20	2	126	G
20	2	128	U
20	2	129	C
20	2	130	G
20	2	143	U
20	2	147	A
20	2	149	A
20	2	155	G
20	2	163	U
20	2	170	A
20	2	175	A
20	2	178	C
20	2	182	C
20	2	187	G
20	2	190	G
20	2	195	C
20	2	196	C
20	2	197	U
20	2	198	U
20	2	199	C

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Mol	Chain	Res	Type
20	2	200	G
20	2	202	G
20	2	204	G
20	2	206	G
20	2	207	G
20	2	208	G
20	2	220	U
20	2	222	U
20	2	223	C
20	2	291	G
20	2	305	U
20	2	307	G
20	2	308	G
20	2	309	G
20	2	312	G
20	2	313	A
20	2	332	G
20	2	333	G
20	2	344	U
20	2	345	U
20	2	346	C
20	2	347	G
20	2	362	C
20	2	364	A
20	2	368	U
20	2	369	C
20	2	370	G
20	2	381	C
20	2	384	U
20	2	385	G
20	2	386	C
20	2	399	C
20	2	400	C
20	2	408	A
20	2	409	C
20	2	418	A
20	2	421	G
20	2	435	A
20	2	438	G
20	2	439	A
20	2	445	A
20	2	448	A

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Mol	Chain	Res	Type
20	2	449	A
20	2	450	C
20	2	451	G
20	2	455	A
20	2	461	U
20	2	464	A
20	2	465	A
20	2	472	C
20	2	474	G
20	2	482	G
20	2	483	C
20	2	487	U
20	2	488	U
20	2	492	C
20	2	493	A
20	2	494	C
20	2	500	A
20	2	501	C
20	2	508	A
20	2	509	G
20	2	523	A
20	2	525	A
20	2	529	A
20	2	537	C
20	2	538	U
20	2	539	C
20	2	541	U
20	2	542	U
20	2	543	C
20	2	544	G
20	2	546	G
20	2	547	G
20	2	548	C
20	2	549	C
20	2	551	U
20	2	556	U
20	2	559	G
20	2	560	A
20	2	564	A
20	2	568	C
20	2	570	C
20	2	574	A

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Mol	Chain	Res	Type
20	2	576	A
20	2	587	A
20	2	588	G
20	2	589	G
20	2	591	U
20	2	593	C
20	2	594	A
20	2	600	G
20	2	603	C
20	2	604	A
20	2	606	G
20	2	607	U
20	2	608	C
20	2	609	U
20	2	614	C
20	2	615	C
20	2	617	G
20	2	623	G
20	2	627	U
20	2	628	A
20	2	629	A
20	2	630	U
20	2	639	C
20	2	640	A
20	2	643	A
20	2	644	G
20	2	655	A
20	2	660	C
20	2	662	G
20	2	666	U
20	2	668	A
20	2	669	A
20	2	671	A
20	2	672	A
20	2	673	G
20	2	675	U
20	2	684	G
20	2	687	C
20	2	690	G
20	2	691	G
20	2	698	G
20	2	707	C

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Mol	Chain	Res	Type
20	2	709	G
20	2	710	C
20	2	713	C
20	2	714	G
20	2	716	G
20	2	717	G
20	2	719	G
20	2	723	C
20	2	727	G
20	2	733	C
20	2	734	C
20	2	735	C
20	2	739	C
20	2	749	U
20	2	750	C
20	2	751	G
20	2	752	G
20	2	792	C
20	2	793	G
20	2	794	A
20	2	796	G
20	2	798	G
20	2	799	U
20	2	801	U
20	2	810	A
20	2	811	A
20	2	816	A
20	2	821	G
20	2	822	U
20	2	823	U
20	2	824	C
20	2	827	A
20	2	830	A
20	2	847	A
20	2	869	A
20	2	870	A
20	2	871	U
20	2	872	A
20	2	873	G
20	2	874	G
20	2	878	G
20	2	881	G

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Mol	Chain	Res	Type
20	2	883	U
20	2	884	C
20	2	885	U
20	2	886	A
20	2	887	U
20	2	888	U
20	2	889	U
20	2	890	U
20	2	891	G
20	2	892	U
20	2	893	U
20	2	894	G
20	2	895	G
20	2	897	U
20	2	898	U
20	2	899	U
20	2	901	G
20	2	902	G
20	2	903	A
20	2	907	G
20	2	908	A
20	2	909	G
20	2	913	A
20	2	919	A
20	2	920	A
20	2	921	G
20	2	922	A
20	2	930	C
20	2	933	G
20	2	938	A
20	2	943	U
20	2	952	G
20	2	953	C
20	2	961	G
20	2	963	A
20	2	970	G
20	2	971	G
20	2	973	C
20	2	989	C
20	2	990	A
20	2	992	A
20	2	997	A

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Mol	Chain	Res	Type
20	2	1008	A
20	2	1017	U
20	2	1023	A
20	2	1026	C
20	2	1027	A
20	2	1029	G
20	2	1030	A
20	2	1045	U
20	2	1049	A
20	2	1053	C
20	2	1054	G
20	2	1056	U
20	2	1058	A
20	2	1060	A
20	2	1061	U
20	2	1064	C
20	2	1082	A
20	2	1083	A
20	2	1085	C
20	2	1087	A
20	2	1096	G
20	2	1097	G
20	2	1109	C
20	2	1113	A
20	2	1114	U
20	2	1115	U
20	2	1116	C
20	2	1117	C
20	2	1118	C
20	2	1120	U
20	2	1138	C
20	2	1143	A
20	2	1149	A
20	2	1153	C
20	2	1154	U
20	2	1155	U
20	2	1156	U
20	2	1157	G
20	2	1166	G
20	2	1168	G
20	2	1170	A
20	2	1171	G

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Mol	Chain	Res	Type
20	2	1181	A
20	2	1188	A
20	2	1194	A
20	2	1195	A
20	2	1207	G
20	2	1208	A
20	2	1210	G
20	2	1211	G
20	2	1215	C
20	2	1216	C
20	2	1221	G
20	2	1224	G
20	2	1229	G
20	2	1236	G
20	2	1237	C
20	2	1240	A
20	2	1242	U
20	2	1248	U
20	2	1249	C
20	2	1250	A
20	2	1251	A
20	2	1253	A
20	2	1256	G
20	2	1257	G
20	2	1258	A
20	2	1259	A
20	2	1260	A
20	2	1263	U
20	2	1264	C
20	2	1265	A
20	2	1271	C
20	2	1273	C
20	2	1274	G
20	2	1275	G
20	2	1277	C
20	2	1280	G
20	2	1285	G
20	2	1286	G
20	2	1287	A
20	2	1289	U
20	2	1293	A
20	2	1295	A

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Mol	Chain	Res	Type
20	2	1297	U
20	2	1299	A
20	2	1301	A
20	2	1302	G
20	2	1306	U
20	2	1313	A
20	2	1315	U
20	2	1317	C
20	2	1321	G
20	2	1322	G
20	2	1328	G
20	2	1330	G
20	2	1341	C
20	2	1342	U
20	2	1352	G
20	2	1354	G
20	2	1355	C
20	2	1358	U
20	2	1362	U
20	2	1363	C
20	2	1369	A
20	2	1371	U
20	2	1372	U
20	2	1378	A
20	2	1381	G
20	2	1382	A
20	2	1397	U
20	2	1398	G
20	2	1401	A
20	2	1402	A
20	2	1403	C
20	2	1405	A
20	2	1428	G
20	2	1429	G
20	2	1430	C
20	2	1447	G
20	2	1449	G
20	2	1452	A
20	2	1454	A
20	2	1462	U
20	2	1463	U
20	2	1464	C

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Mol	Chain	Res	Type
20	2	1466	G
20	2	1473	G
20	2	1475	G
20	2	1477	U
20	2	1478	U
20	2	1480	A
20	2	1484	A
20	2	1489	A
20	2	1490	G
20	2	1493	C
20	2	1497	G
20	2	1498	A
20	2	1499	U
20	2	1506	A
20	2	1507	G
20	2	1508	A
20	2	1519	U
20	2	1520	G
20	2	1521	C
20	2	1522	A
20	2	1531	A
20	2	1533	A
20	2	1536	G
20	2	1544	C
20	2	1547	C
20	2	1548	G
20	2	1551	U
20	2	1552	G
20	2	1553	C
20	2	1554	C
20	2	1556	A
20	2	1558	C
20	2	1559	C
20	2	1560	U
20	2	1568	C
20	2	1575	G
20	2	1578	U
20	2	1580	A
20	2	1582	C
20	2	1584	G
20	2	1585	U
20	2	1587	G

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Mol	Chain	Res	Type
20	2	1588	A
20	2	1599	U
20	2	1601	A
20	2	1603	G
20	2	1604	G
20	2	1606	G
20	2	1620	A
20	2	1621	U
20	2	1623	A
20	2	1624	U
20	2	1629	C
20	2	1632	G
20	2	1634	A
20	2	1636	G
20	2	1637	A
20	2	1648	G
20	2	1654	G
20	2	1660	C
20	2	1661	A
20	2	1664	A
20	2	1665	G
20	2	1669	G
20	2	1671	G
20	2	1677	U
20	2	1680	G
20	2	1683	C
20	2	1686	G
20	2	1694	U
20	2	1695	A
20	2	1697	A
20	2	1700	C
20	2	1702	G
20	2	1718	G
20	2	1720	U
20	2	1721	U
20	2	1722	G
20	2	1723	G
20	2	1725	U
20	2	1726	G
20	2	1730	U
20	2	1733	U
20	2	1742	C

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Mol	Chain	Res	Type
20	2	1744	G
20	2	1751	C
20	2	1752	C
20	2	1753	C
20	2	1755	C
20	2	1756	C
20	2	1757	G
20	2	1758	G
20	2	1759	G
20	2	1760	G
20	2	1772	C
20	2	1773	C
20	2	1774	C
20	2	1777	G
20	2	1778	C
20	2	1780	G
20	2	1781	A
20	2	1783	C
20	2	1784	G
20	2	1785	C
20	2	1787	G
20	2	1791	A
20	2	1799	G
20	2	1800	A
20	2	1805	G
20	2	1806	A
20	2	1808	U
20	2	1810	U
20	2	1811	C
20	2	1814	G
20	2	1816	G
20	2	1820	G
20	2	1821	U
20	2	1822	A
20	2	1823	A
20	2	1824	A
20	2	1825	A
20	2	1826	G
20	2	1829	G
20	2	1831	A
20	2	1834	A
20	2	1835	A

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Mol	Chain	Res	Type
20	2	1837	G
20	2	1838	U
20	2	1848	U
20	2	1849	A
20	2	1851	A
20	2	1857	G
20	2	1861	G
20	2	1862	G
20	2	1863	A
20	2	1865	C
20	2	1866	A
20	2	1867	U
20	2	1869	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	2	332	G
20	2	367	U
20	2	368	U
20	2	550	C
20	2	912	C
20	2	1060	A
20	2	1292	C
20	2	1474	A
20	2	1581	C
20	2	1807	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
53	ADP	1	603	54	24,29,29	0.95	1 (4%)	29,45,45	1.46	4 (13%)
52	SF4	1	601	-	0,12,12	-	-	-		
55	ATP	1	605	54	26,33,33	0.93	1 (3%)	31,52,52	1.61	5 (16%)
52	SF4	1	602	-	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
53	ADP	1	603	54	-	6/12/32/32	0/3/3/3
52	SF4	1	601	-	-	-	0/6/5/5
55	ATP	1	605	54	-	2/18/38/38	0/3/3/3
52	SF4	1	602	-	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1	605	ATP	C5-C4	2.50	1.47	1.40
53	1	603	ADP	C5-C4	2.48	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	1	603	ADP	PA-O3A-PB	-3.72	120.07	132.83
55	1	605	ATP	PB-O3B-PG	-3.65	120.31	132.83
55	1	605	ATP	PA-O3A-PB	-3.49	120.84	132.83
55	1	605	ATP	C3'-C2'-C1'	3.42	106.13	100.98
55	1	605	ATP	N3-C2-N1	-3.16	123.74	128.68
53	1	603	ADP	N3-C2-N1	-3.16	123.75	128.68
53	1	603	ADP	C3'-C2'-C1'	2.95	105.41	100.98
55	1	605	ATP	C4-C5-N7	-2.75	106.54	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	1	603	ADP	C4-C5-N7	-2.68	106.61	109.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

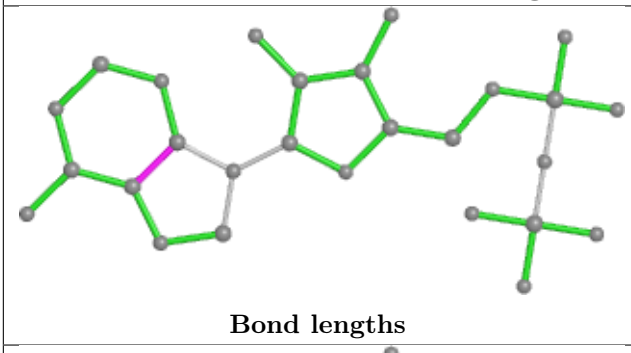
Mol	Chain	Res	Type	Atoms
53	1	603	ADP	C5'-O5'-PA-O1A
53	1	603	ADP	C5'-O5'-PA-O2A
55	1	605	ATP	O4'-C4'-C5'-O5'
53	1	603	ADP	PA-O3A-PB-O2B
53	1	603	ADP	PA-O3A-PB-O3B
53	1	603	ADP	C5'-O5'-PA-O3A
55	1	605	ATP	C3'-C4'-C5'-O5'
53	1	603	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

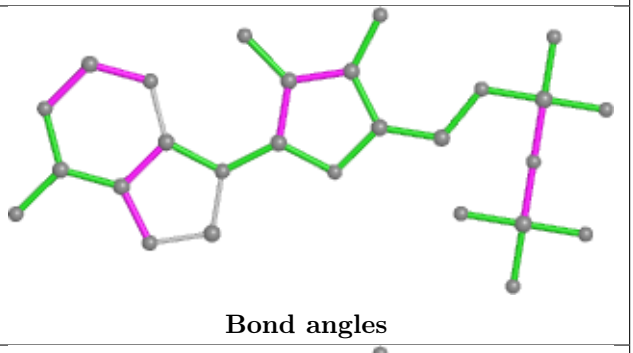
No monomer is involved in short contacts.

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

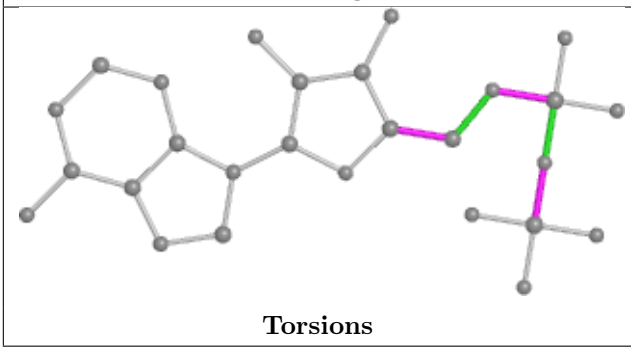
Ligand ADP 1 603



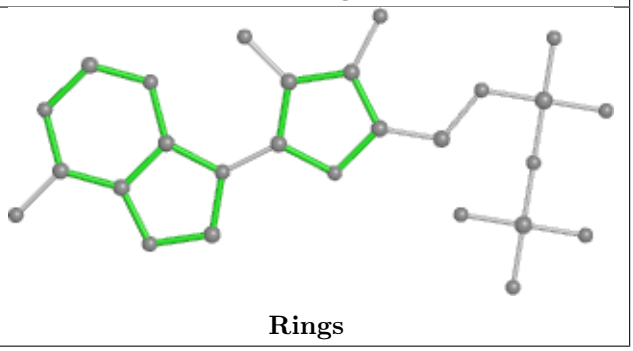
Bond lengths



Bond angles

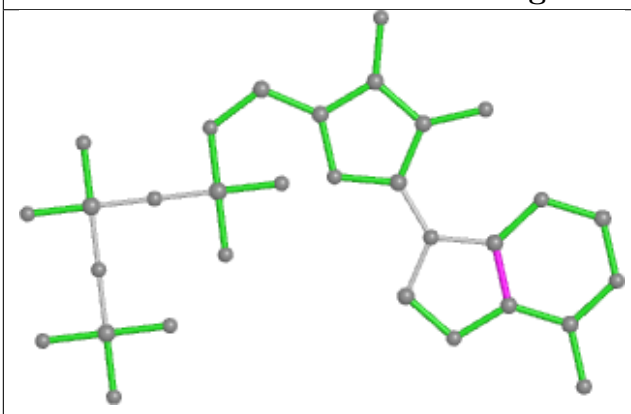


Torsions

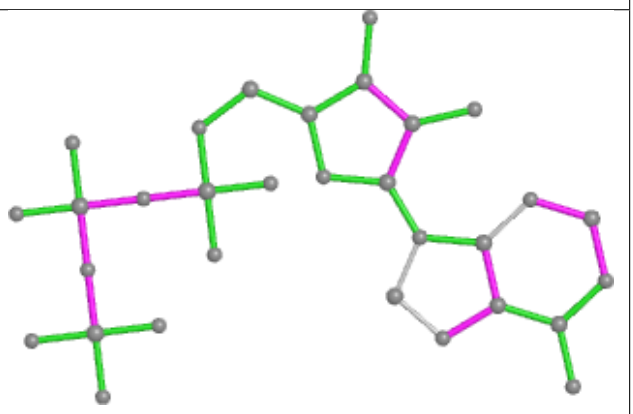


Rings

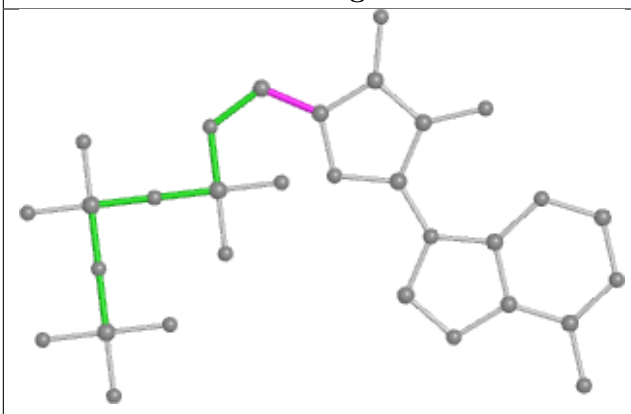
Ligand ATP 1 605



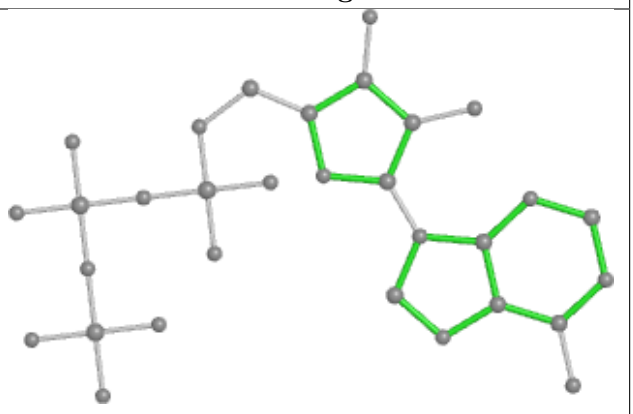
Bond lengths



Bond angles



Torsions



Rings

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
39	C	1
8	s	1
11	n	1
20	2	1
19	T	1
40	E	1
15	f	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	149:ASN	C	320:LYS	N	53.70
1	s	12:ASN	C	18:GLU	N	15.89
1	n	23:VAL	C	33:LEU	N	14.18
1	2	739:C	O3'	747:U	P	13.90
1	T	45:VAL	C	54:GLY	N	10.18
1	E	95:PHE	C	99:GLU	N	10.11
1	f	93:LEU	C	94:LEU	N	1.19

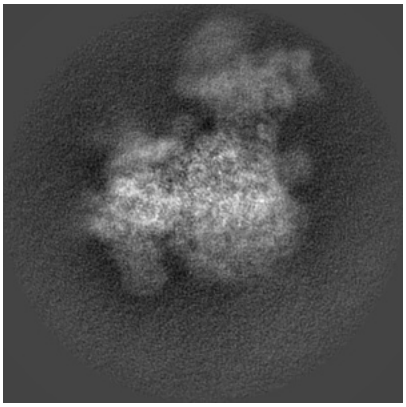
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11458. These allow visual inspection of the internal detail of the map and identification of artifacts.

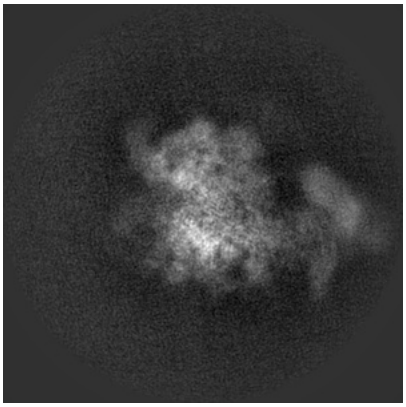
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

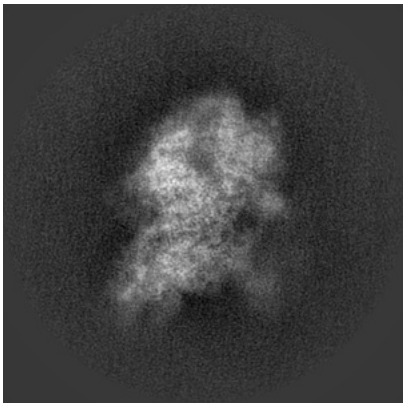
6.1.1 Primary map



X



Y

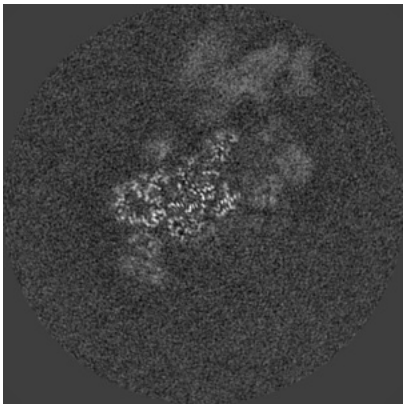


Z

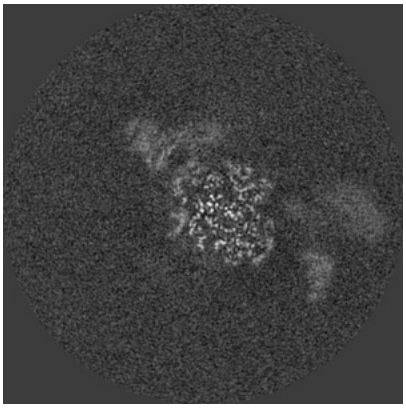
The images above show the map projected in three orthogonal directions.

6.2 Central slices

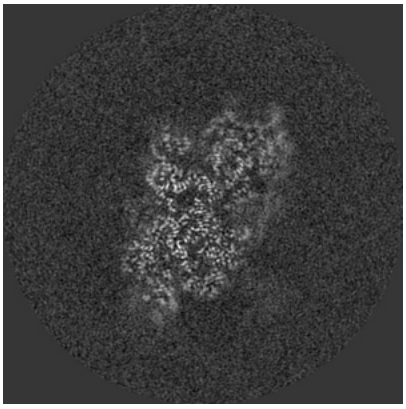
6.2.1 Primary map



X Index: 200



Y Index: 200

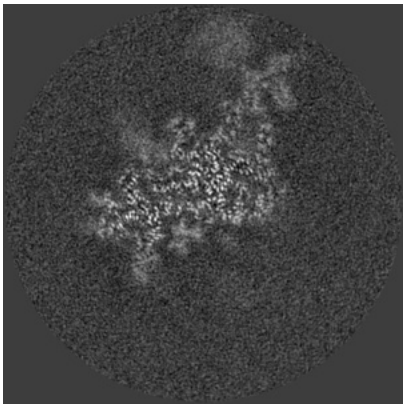


Z Index: 200

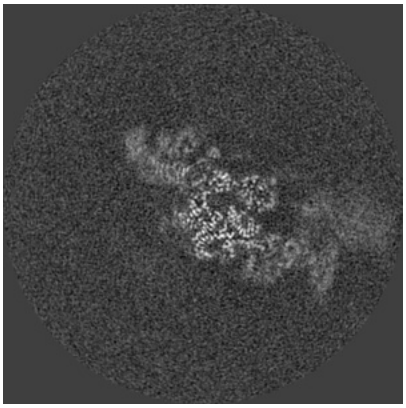
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

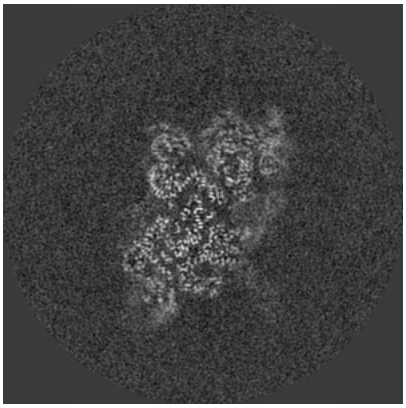
6.3.1 Primary map



X Index: 166



Y Index: 218

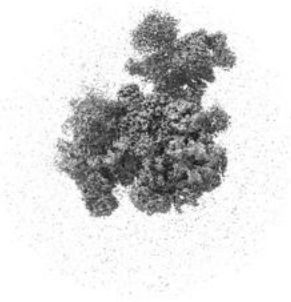


Z Index: 202

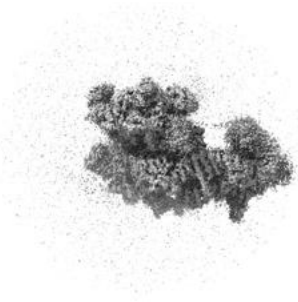
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

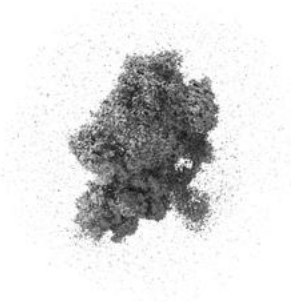
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

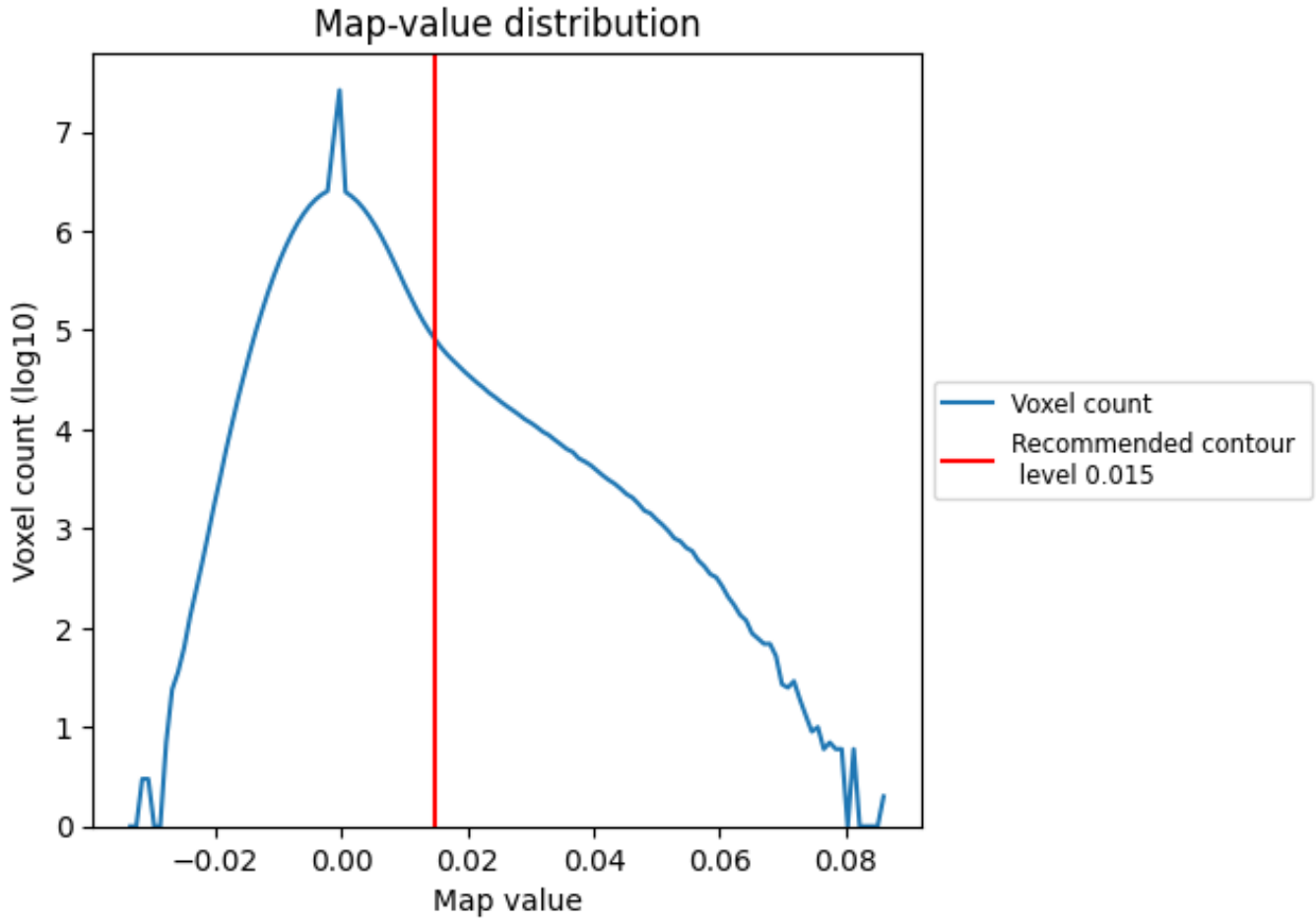
6.5 Mask visualisation (i)

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

7 Map analysis

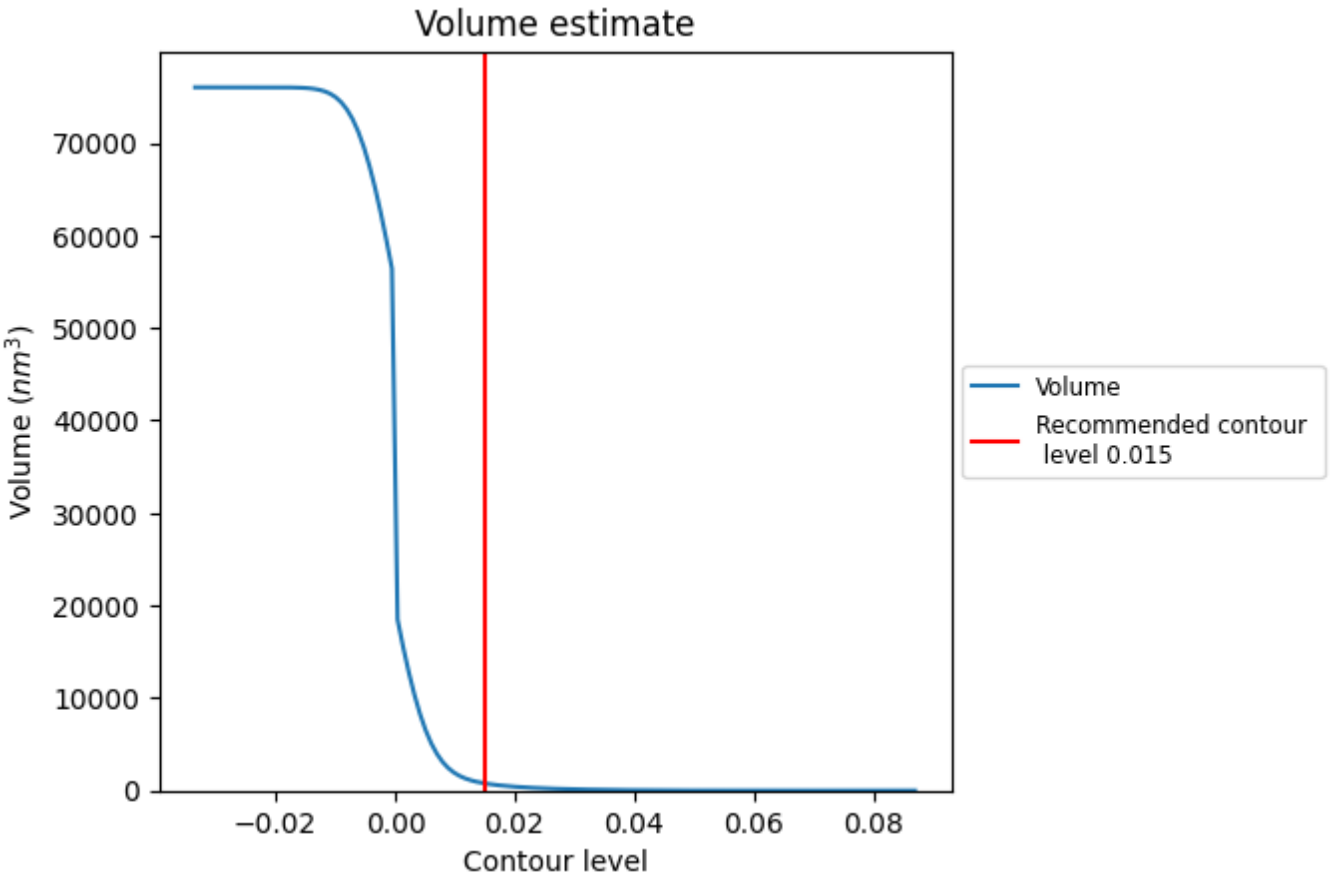
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

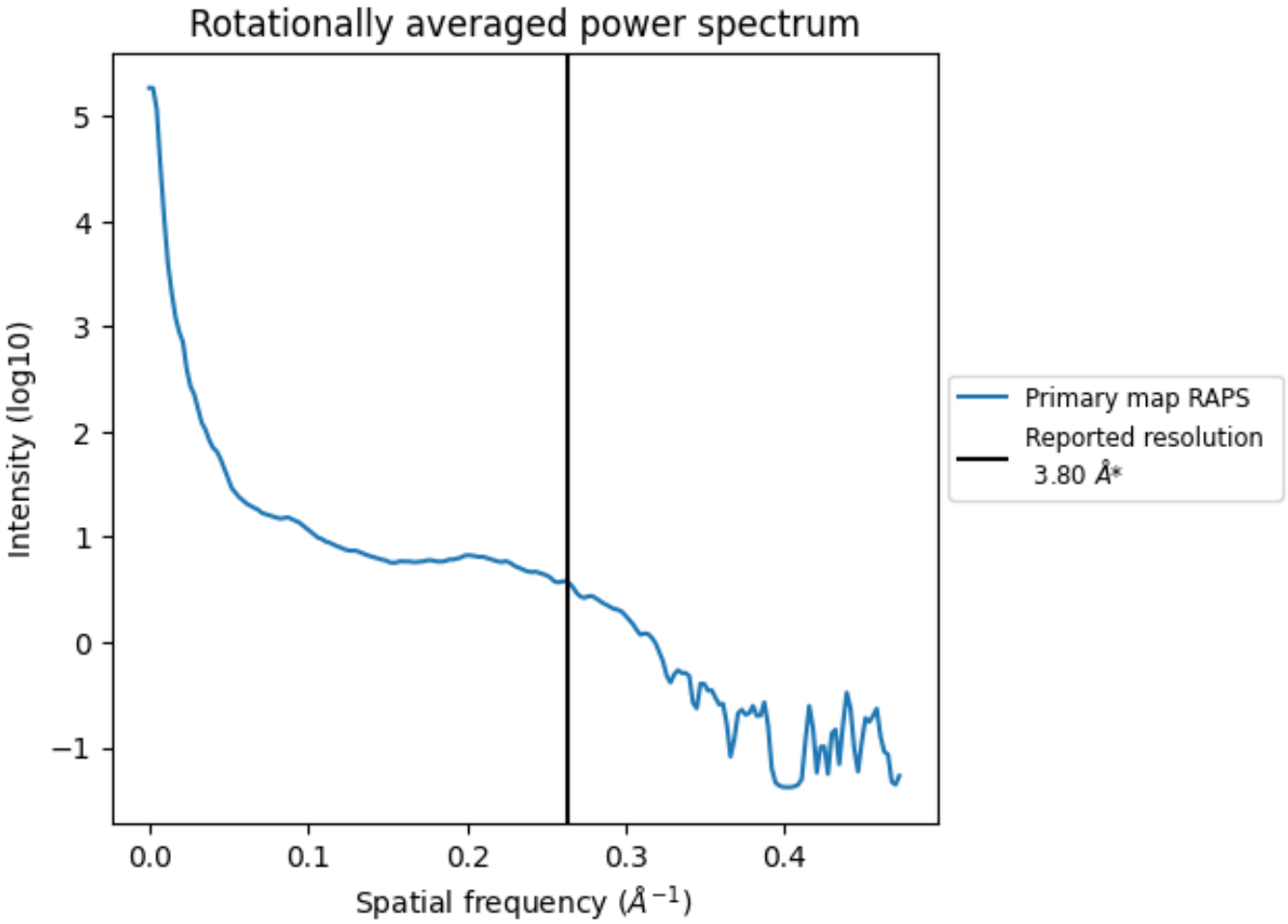
7.2 Volume estimate (i)



The volume at the recommended contour level is 779 nm^3; this corresponds to an approximate mass of 704 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 (i)

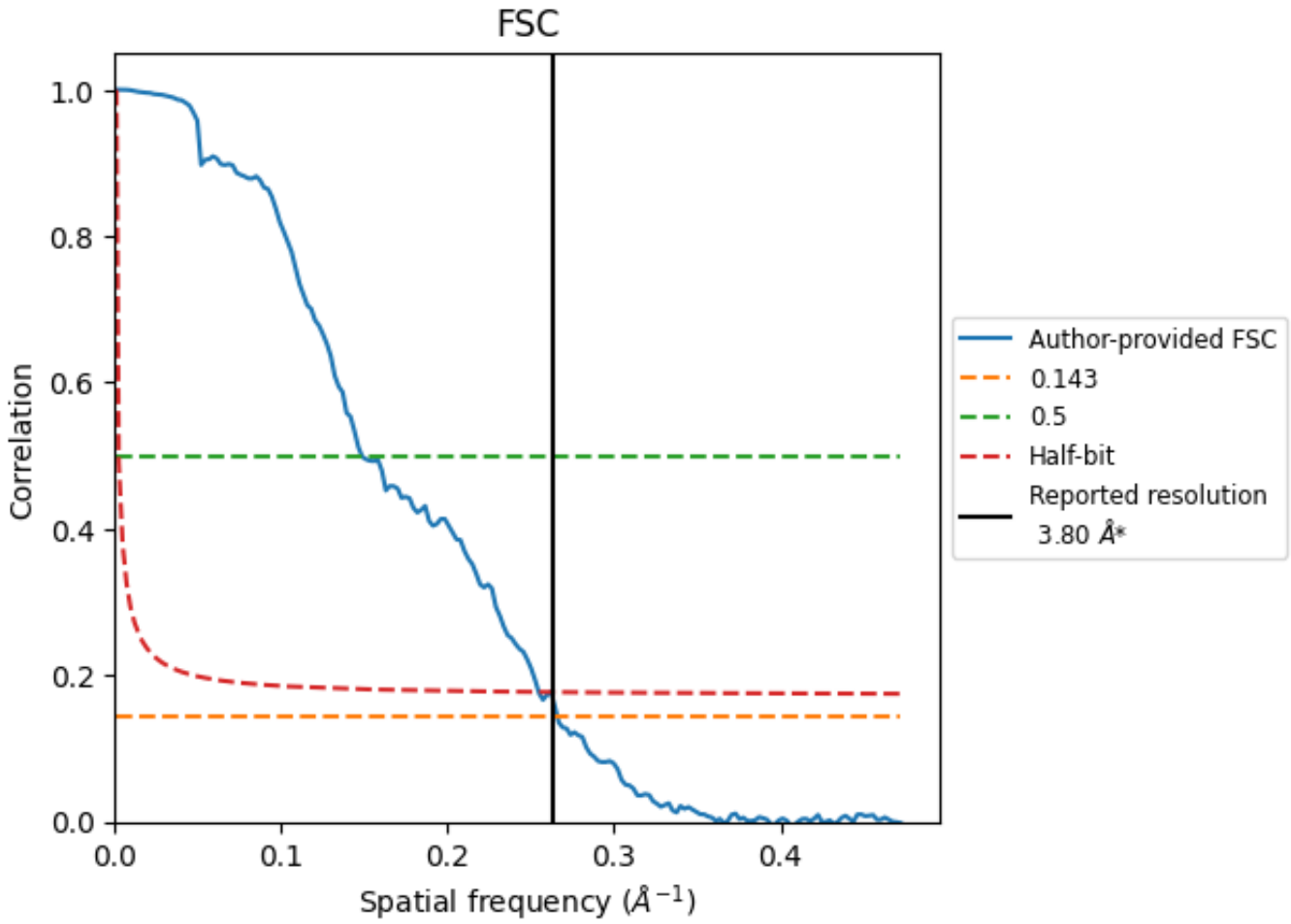


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

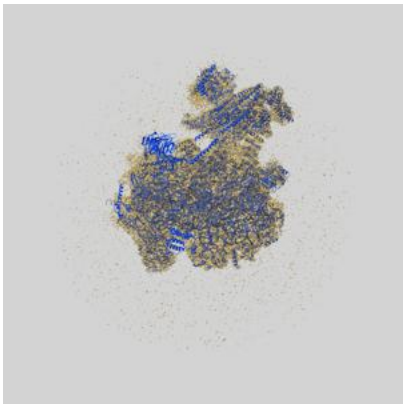
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.76	6.74	3.93
Unmasked-calculated*	-	-	-

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

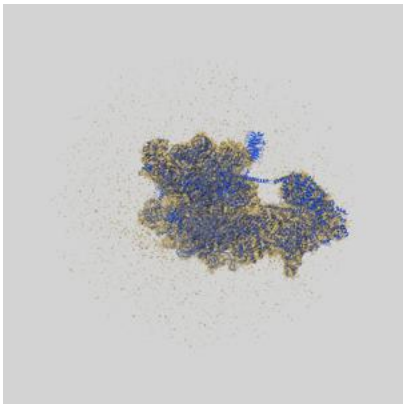
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11458 and PDB model 6ZVJ. Per-residue inclusion information can be found in section 3 on page 16.

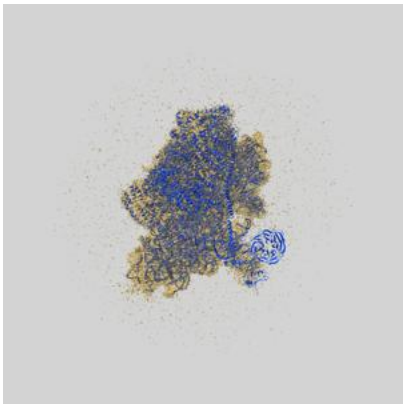
9.1 Map-model overlay



X



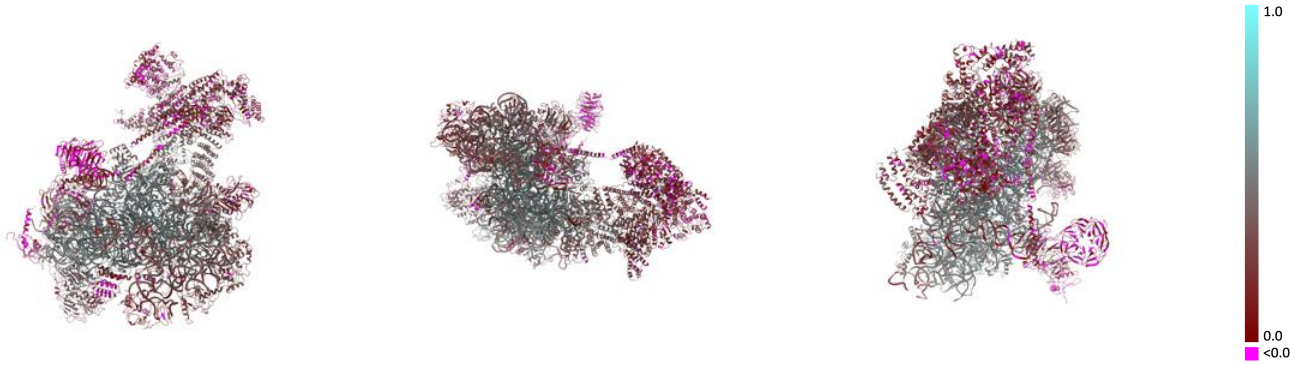
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

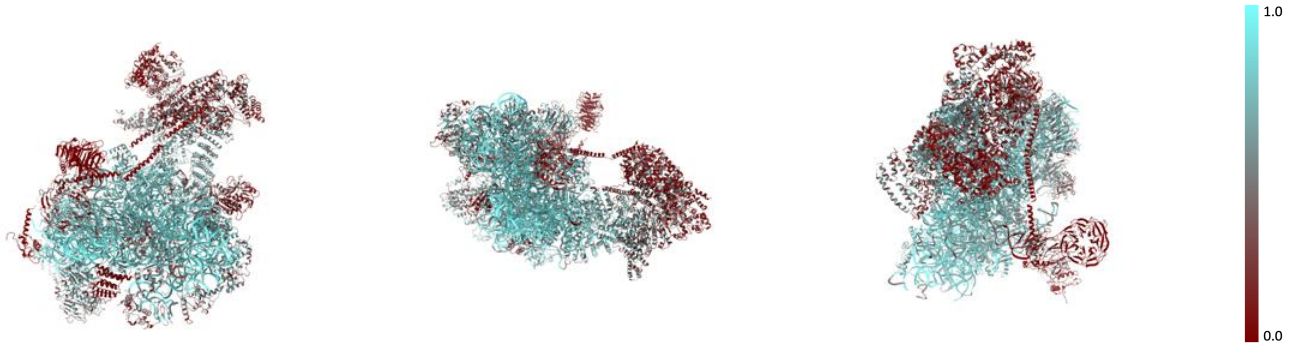
9.2 Q-score mapped to coordinate model



X Y Z

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

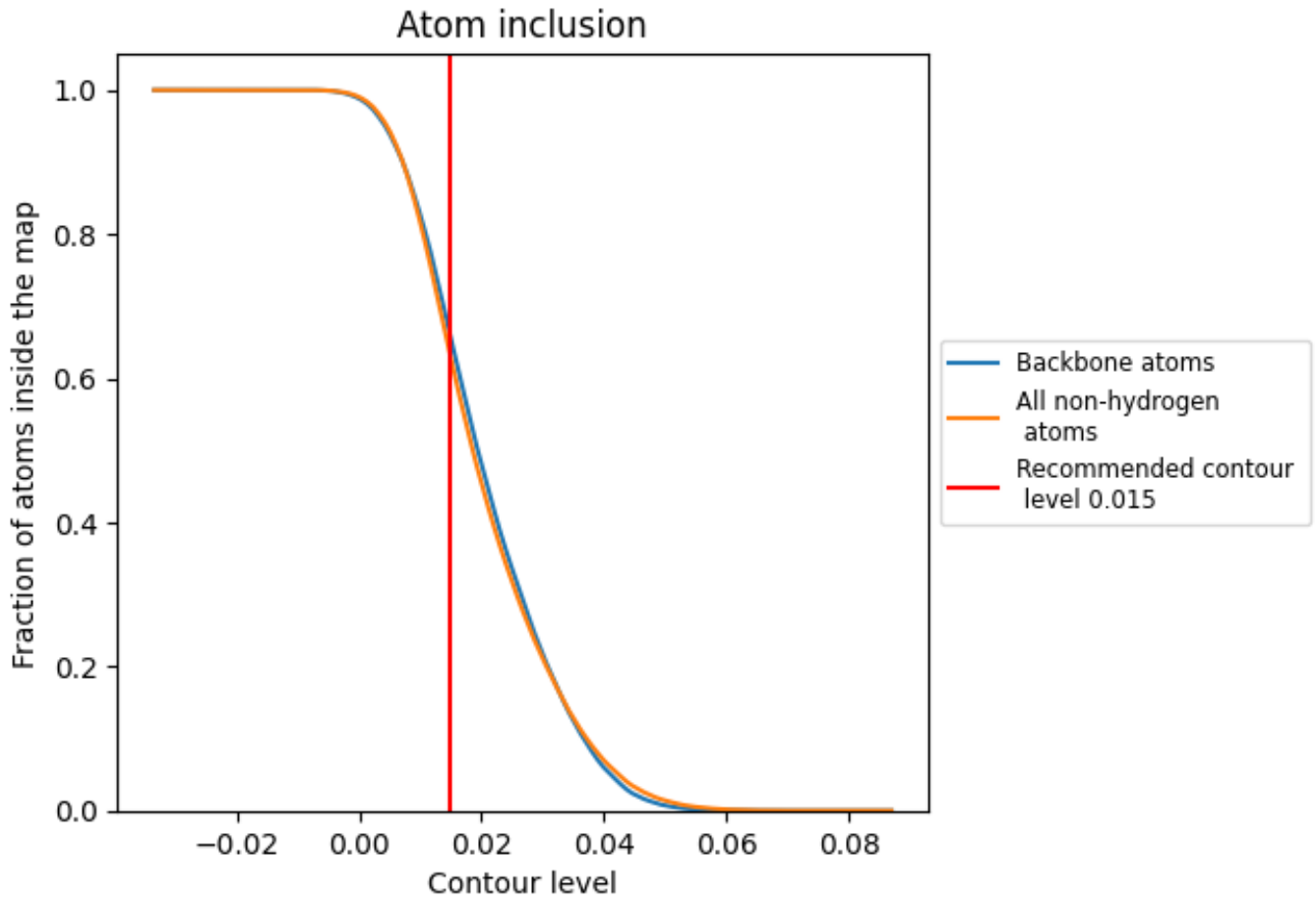
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 63% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6281	0.3650
1	0.5522	0.3700
2	0.8922	0.4510
A	0.4593	0.2820
B	0.1581	0.1870
C	0.5257	0.3210
D	0.2236	0.2230
E	0.3827	0.2210
F	0.2055	0.1790
G	0.0230	0.0940
H	0.1979	0.1700
I	0.0013	0.0250
J	0.0055	0.1020
K	0.1223	0.1540
L	0.1222	0.1220
M	0.2459	0.1820
N	0.1227	0.2020
P	0.5119	0.2920
Q	0.7676	0.4840
R	0.7806	0.4910
S	0.5022	0.3380
T	0.7735	0.4720
U	0.4216	0.2280
V	0.5930	0.3130
W	0.6381	0.4350
Y	0.3333	0.2290
a	0.7940	0.4990
b	0.6248	0.3870
c	0.7993	0.4990
d	0.7998	0.5040
e	0.6176	0.3680
f	0.8376	0.5370
g	0.6823	0.4140
h	0.6053	0.3840
i	0.7783	0.4680

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Chain	Atom inclusion	Q-score
j	0.7926	0.5160
k	0.5286	0.3190
l	0.7535	0.4120
m	0.8012	0.4880
n	0.8240	0.5230
o	0.4411	0.2630
p	0.7847	0.4830
q	0.8294	0.5100
r	0.7597	0.4440
s	0.7225	0.4310
t	0.8089	0.4720
u	0.5384	0.3070
v	0.3847	0.2290
w	0.6977	0.4320
x	0.6423	0.3460
y	0.7941	0.4940
z	0.8031	0.4900