wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:36 PM BST

PDB ID	:	5FL8
EMDB ID:	:	3199
Title	:	CRYO-EM STRUCTURE OF THE RIX1-REA1 PRE-60S PARTICLE
Authors	:	BARRIO-GARCIA, C.; THOMS, M.; FLEMMING, D.; KATER, L.; BERNINGHAUSEN, O.; BASSLER, J.; BECKMANN, R.; HURT, E.
Deposited on	:	2015-10-22
Resolution	:	9.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

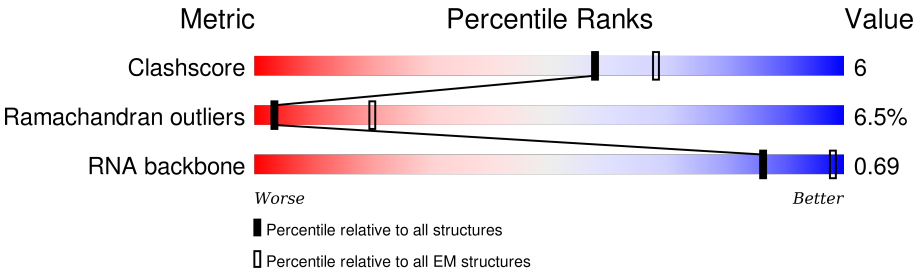
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	A	254	85% 13% • •
2	B	387	92% 7% •
3	C	362	90% 9% •
4	D	297	95% •
5	E	176	84% 5% 11%
6	F	244	85% 6% 9%
7	G	256	87% • 9%
8	H	191	95% 5% •
9	I	217	94% 6%

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Mol	Chain	Length	Quality of chain
10	J	174	75% 20%
11	K	165	67% 10% 23%
12	L	199	88% 8%
13	M	138	93% 6%
14	N	204	92% 8%
15	O	199	87% 11%
16	P	184	92% 7%
17	Q	186	93% 6%
18	R	189	88% 12%
19	S	172	95% 5%
20	T	160	79% 18%
21	U	121	76% 7% 17%
22	V	137	95%
23	X	142	80% 5% 15%
24	Y	127	92% 7%
25	Z	136	93% 6%
26	a	149	88% 9%
27	c	105	91% 8%
28	d	113	93%
29	e	130	96%
30	f	107	92% 6%
31	g	121	88% 7%
32	h	120	96%
33	i	100	93% 6%
34	j	88	91% 7%

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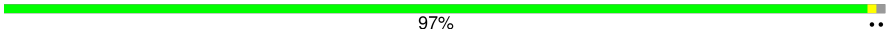
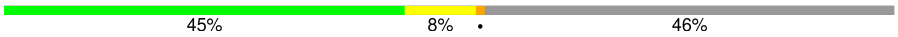
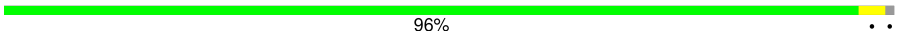
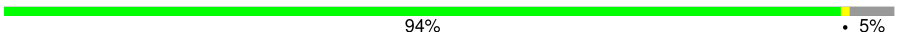
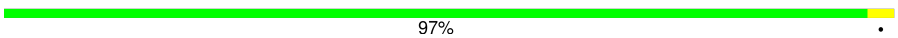
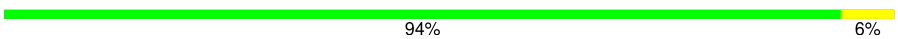
Mol	Chain	Length	Quality of chain
35	k	78	
36	l	51	
37	m	245	
38	n	236	
39	o	647	
40	p	92	
41	q	515	
42	r	767	
43	s	4914	
44	t	199	
45	u	380	
46	x	2779	
47	y	158	
48	z	121	

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 105808 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 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	252	Total	C	N	O	0	0
			1007	504	252	251		

- Molecule 2 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	386	Total	C	N	O	0	0
			1543	772	386	385		

- Molecule 3 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	361	Total	C	N	O	0	0
			1443	722	361	360		

- Molecule 4 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	296	Total	C	N	O	0	0
			1183	592	296	295		

- Molecule 5 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	156	Total	C	N	O	0	0
			622	312	156	154		

- Molecule 6 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	222	Total	C	N	O	0	0
			887	444	222	221		

- Molecule 7 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	233	Total 931	C 466	N 233	O 232	0	0

- Molecule 8 is a protein called Rpl9ap.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	191	Total 763	C 382	N 191	O 190	0	0

- Molecule 9 is a protein called 60S ribosomal protein L1-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	217	Total 867	C 434	N 217	O 216	0	0

- Molecule 10 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	169	Total 675	C 338	N 169	O 168	0	0

- Molecule 11 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	127	Total 507	C 254	N 127	O 126	0	0

- Molecule 12 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	193	Total 771	C 386	N 193	O 192	0	0

- Molecule 13 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	136	Total 543	C 272	N 136	O 135	0	0

- Molecule 14 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	203	Total 811	C 406	N 203	O 202	0	0

- Molecule 15 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	197	Total 787	C 394	N 197	O 196	0	0

- Molecule 16 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	183	Total 731	C 366	N 183	O 182	0	0

- Molecule 17 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	185	Total 739	C 370	N 185	O 184	0	0

- Molecule 18 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	188	Total 751	C 376	N 188	O 187	0	0

- Molecule 19 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	172	Total 687	C 344	N 172	O 171	0	0

- Molecule 20 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	159	Total 635	C 318	N 159	O 158	0	0

- Molecule 21 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	100	Total 399	C 200	N 100	O 99	0	0

- Molecule 22 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	136	Total 543	C 272	N 136	O 135	0	0

- Molecule 23 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	121	Total 483	C 242	N 121	O 120	0	0

- Molecule 24 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Y	126	Total 503	C 252	N 126	O 125	0	0

- Molecule 25 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Z	135	Total 539	C 270	N 135	O 134	0	0

- Molecule 26 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	a	148	Total 591	C 296	N 148	O 147	0	0

- Molecule 27 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	c	97	Total 387	C 194	N 97	O 96	0	0

- Molecule 28 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	d	109	Total 435	C 218	N 109	O 108	0	0

- Molecule 29 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	e	127	Total 507	C 254	N 127	O 126	0	0

- Molecule 30 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	f	106	Total 423	C 212	N 106	O 105	0	0

- Molecule 31 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	g	112	Total 447	C 224	N 112	O 111	0	0

- Molecule 32 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	h	119	Total 475	C 238	N 119	O 118	0	0

- Molecule 33 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	i	99	Total 395	C 198	N 99	O 98	0	0

- Molecule 34 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	j	87	Total 347	C 174	N 87	O 86	0	0

- Molecule 35 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	k	77	Total	C	N	O	0	0
			307	154	77	76		

- Molecule 36 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	l	50	Total	C	N	O	0	0
			199	100	50	49		

- Molecule 37 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	m	224	Total	C	N	O	0	0
			895	448	224	223		

- Molecule 38 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	n	212	Total	C	N	O	0	0
			847	424	212	211		

- Molecule 39 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	o	347	Total	C	N	O	0	0
			1387	694	347	346		

- Molecule 40 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	p	91	Total	C	N	O	0	0
			363	182	91	90		

- Molecule 41 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	q	488	Total	C	N	O	0	0
			1951	976	488	487		

- Molecule 42 is a protein called Protein SDA1.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	r	333	Total	C	N	O	0	0
			1304	666	333	305		

- Molecule 43 is a protein called Midasin.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	s	2008	Total	C	N	O	0	0
			8027	4016	2008	2003		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
s	804	ASN	-	insertion	UNP Q12019
s	805	SER	-	insertion	UNP Q12019
s	999	LYS	-	insertion	UNP Q12019
s	1643	ALA	-	insertion	UNP Q12019

- Molecule 44 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	t	63	Total	C	N	O	0	0
			251	126	63	62		

- Molecule 45 is a protein called ARX1.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	u	380	Total	C	N	O	0	0
			1519	760	380	379		

- Molecule 46 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	x	2779	Total	C	N	O	P	0	0
			59475	26560	10747	19390	2778		

- Molecule 47 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	y	158	Total	C	N	O	P	0	0
			3350	1500	586	1107	157		

- Molecule 48 is a RNA chain called 5S ribosomal RNA.

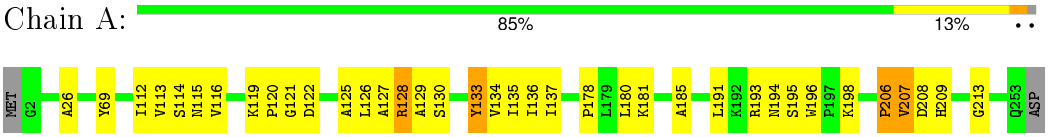
Mol	Chain	Residues	Atoms					AltConf	Trace
48	z	121	Total	C	N	O	P	0	0
			2576	1152	461	843	120		

3 Residue-property plots (i)

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

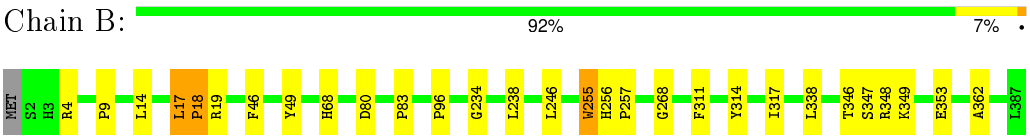
- Molecule 1: 60S ribosomal protein L2-A

Chain A:



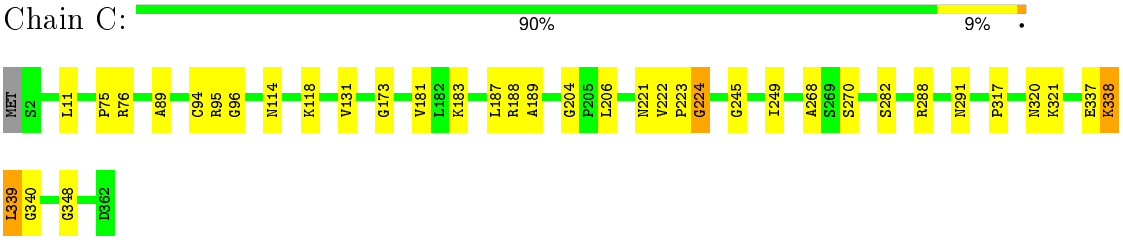
- Molecule 2: 60S ribosomal protein L3

Chain B:



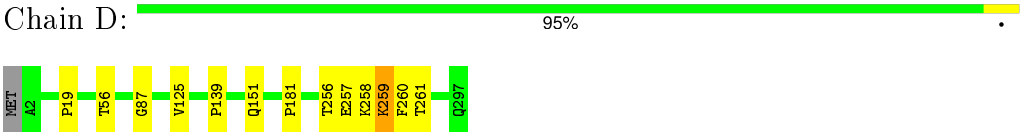
- Molecule 3: 60S ribosomal protein L4-A

Chain C:



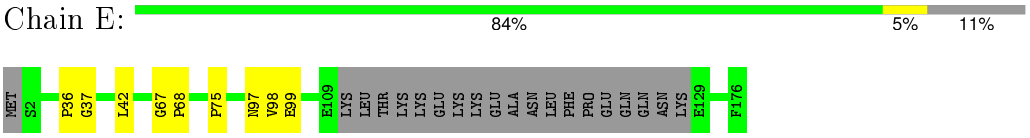
- Molecule 4: 60S ribosomal protein L5

Chain D:



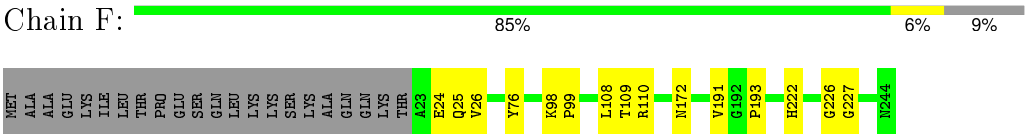
- Molecule 5: 60S ribosomal protein L6-A

Chain E:



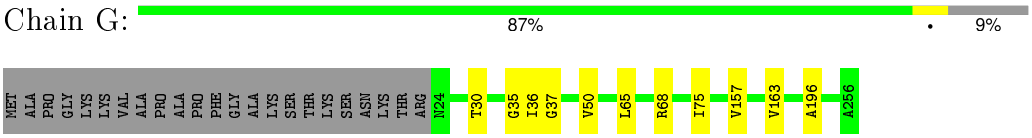
- Molecule 6: 60S ribosomal protein L7-A

Chain F:



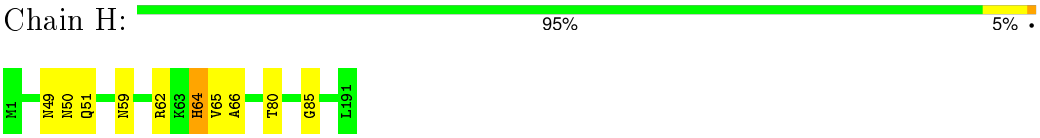
- Molecule 7: 60S ribosomal protein L8-A

Chain G:



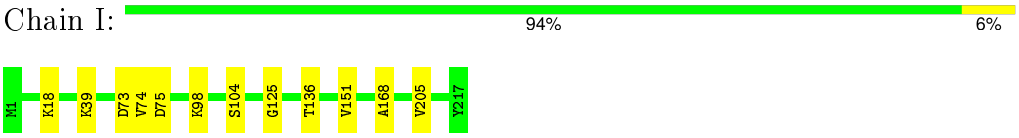
- Molecule 8: Rpl9ap

Chain H:



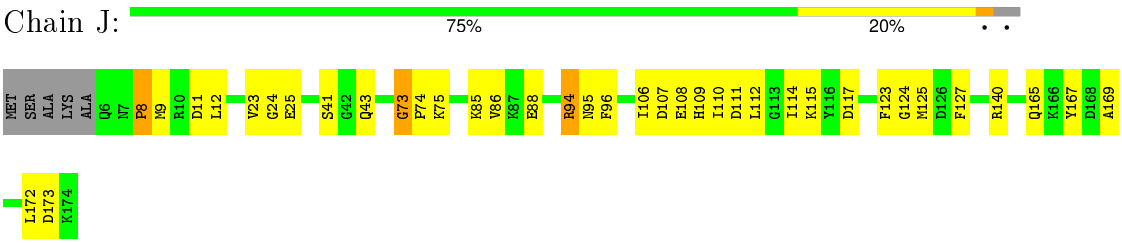
- Molecule 9: 60S ribosomal protein L1-B

Chain I:



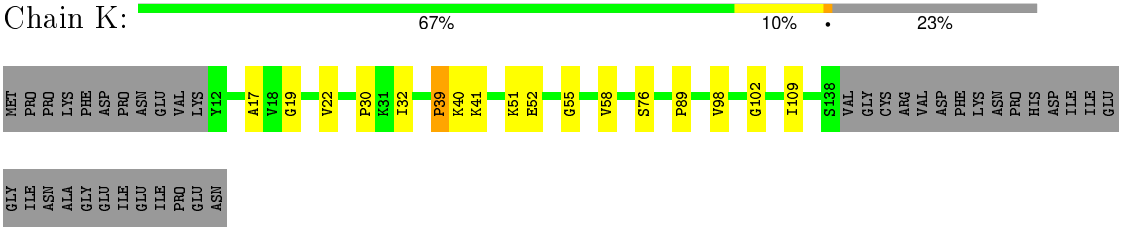
- Molecule 10: 60S ribosomal protein L11-A

Chain J:



- Molecule 11: 60S ribosomal protein L12-A

Chain K:



- Molecule 12: 60S ribosomal protein L13-A

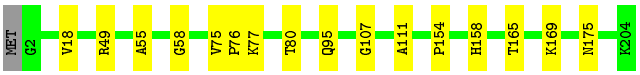
Chain L:

• Molecule 13: 60S ribosomal protein L14-A

Chain M:

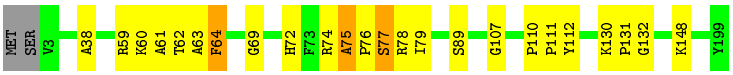
• Molecule 14: 60S ribosomal protein L15-A

Chain N:



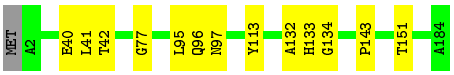
• Molecule 15: 60S ribosomal protein L16-A

Chain O:



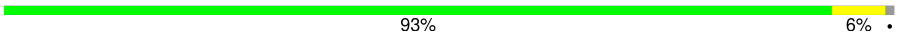
• Molecule 16: 60S ribosomal protein L17-A

Chain P:



• Molecule 17: 60S ribosomal protein L18-A

Chain Q:

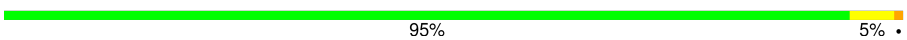


• Molecule 18: 60S ribosomal protein L19-A

Chain R:

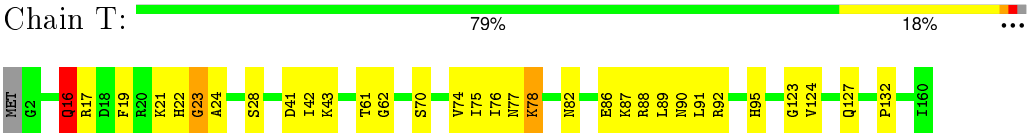
• Molecule 19: 60S ribosomal protein L20-A

Chain S:



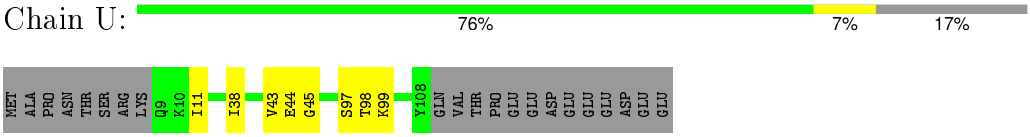
• Molecule 20: 60S ribosomal protein L21-A

Chain T:



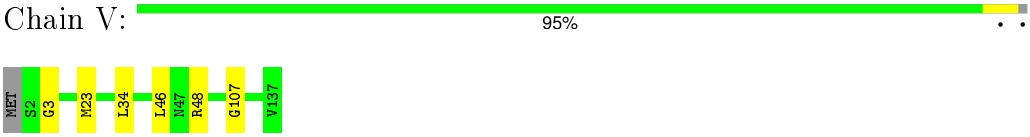
• Molecule 21: 60S ribosomal protein L22-A

Chain U:



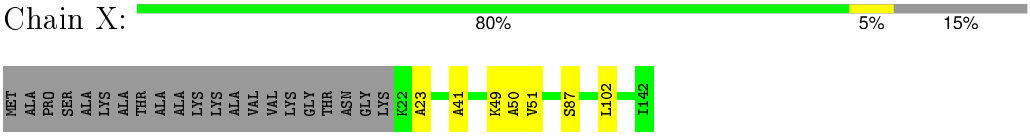
• Molecule 22: 60S ribosomal protein L23-A

Chain V:



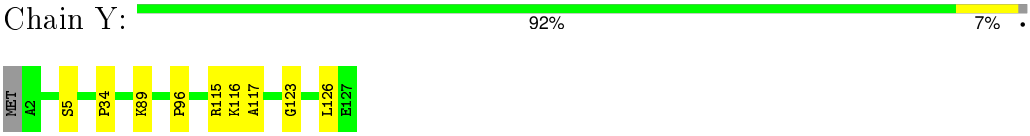
• Molecule 23: 60S ribosomal protein L25

Chain X:



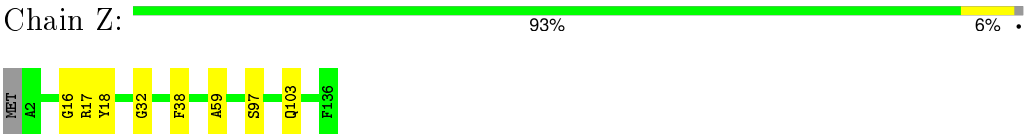
• Molecule 24: 60S ribosomal protein L26-A

Chain Y:



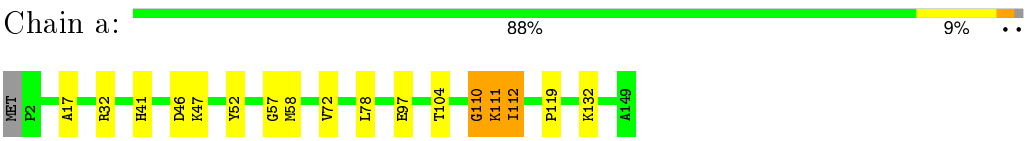
• Molecule 25: 60S ribosomal protein L27-A

Chain Z:



• Molecule 26: 60S ribosomal protein L28

Chain a:

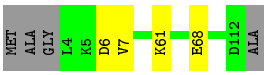


• Molecule 27: 60S ribosomal protein L30

Chain c:

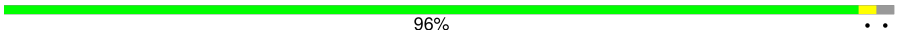
• Molecule 28: 60S ribosomal protein L31-A

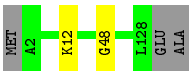
Chain d:



• Molecule 29: 60S ribosomal protein L32

Chain e:



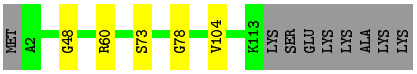


• Molecule 30: 60S ribosomal protein L33-A

Chain f:

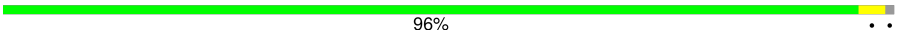
• Molecule 31: 60S ribosomal protein L34-A

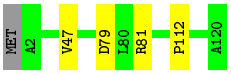
Chain g:



• Molecule 32: 60S ribosomal protein L35-A

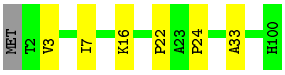
Chain h:





• Molecule 33: 60S ribosomal protein L36-A

Chain i:

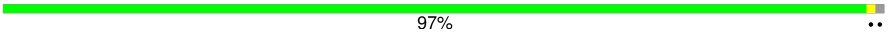


• Molecule 34: 60S ribosomal protein L37-A

Chain j:

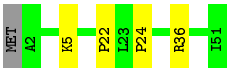
• Molecule 35: 60S ribosomal protein L38

Chain k:



• Molecule 36: 60S ribosomal protein L39

Chain l:



• Molecule 37: Eukaryotic translation initiation factor 6

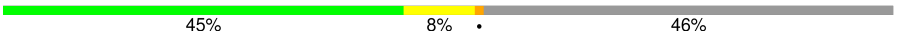
Chain m:

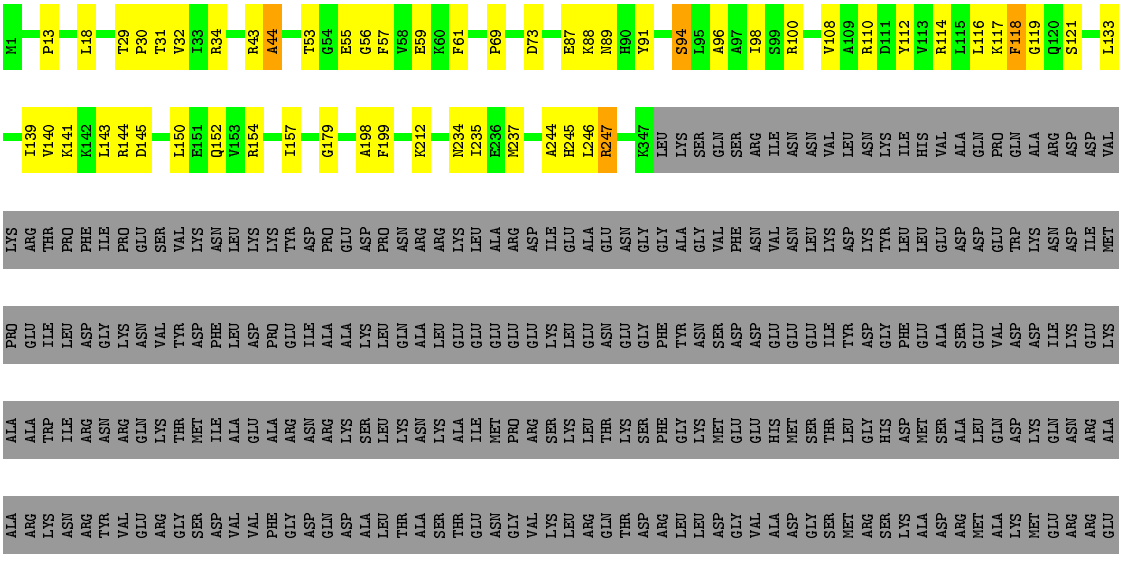
• Molecule 38: Ribosome assembly factor MRT4

Chain n:

• Molecule 39: Nucleolar GTP-binding protein 1

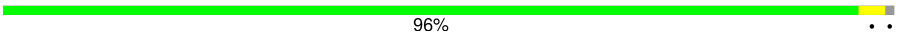
Chain o:





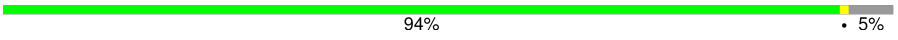
- Molecule 40: 60S ribosomal protein L43-A

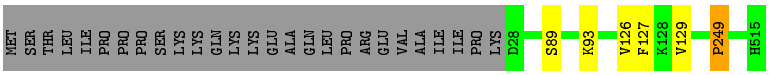
Chain p:



- Molecule 41: Ribosome assembly protein 4

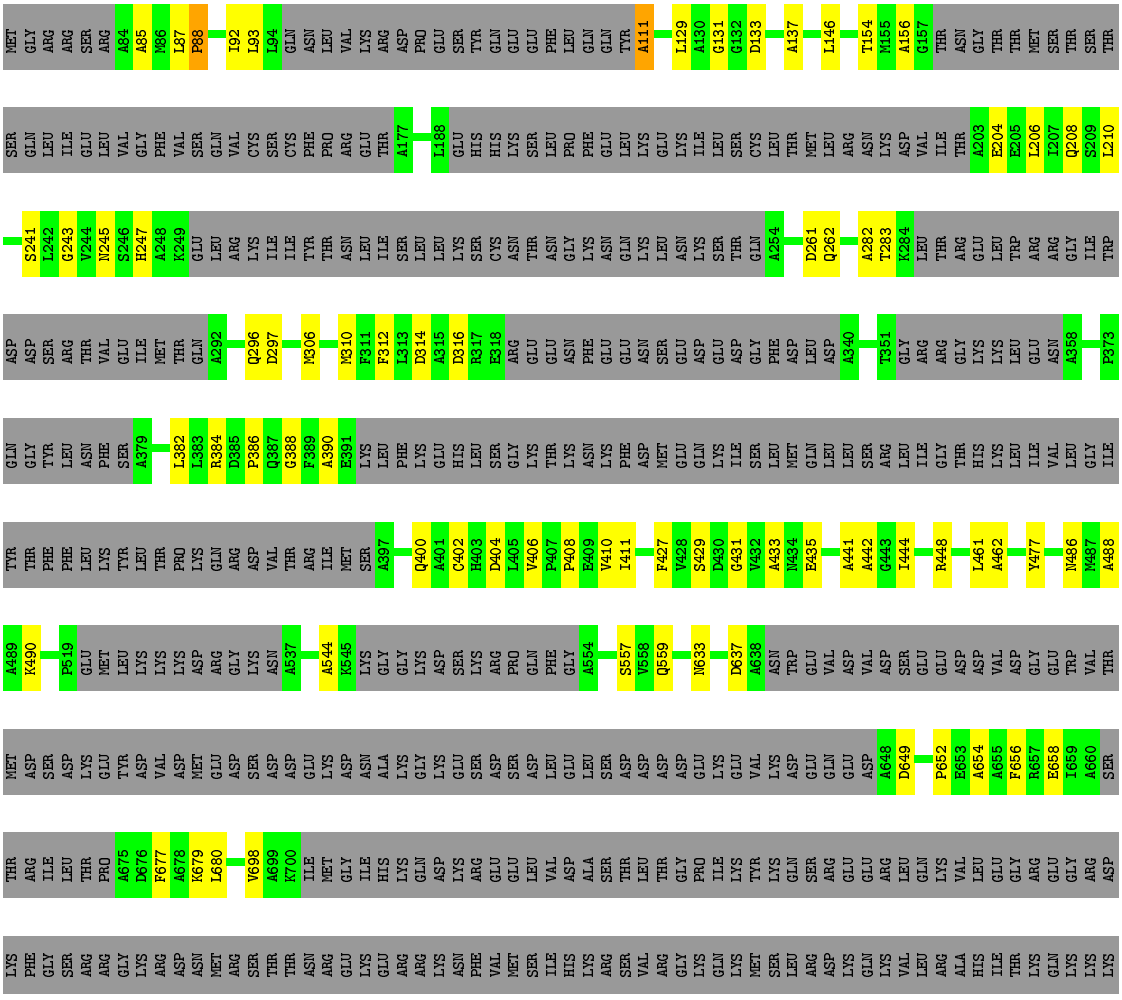
Chain q:

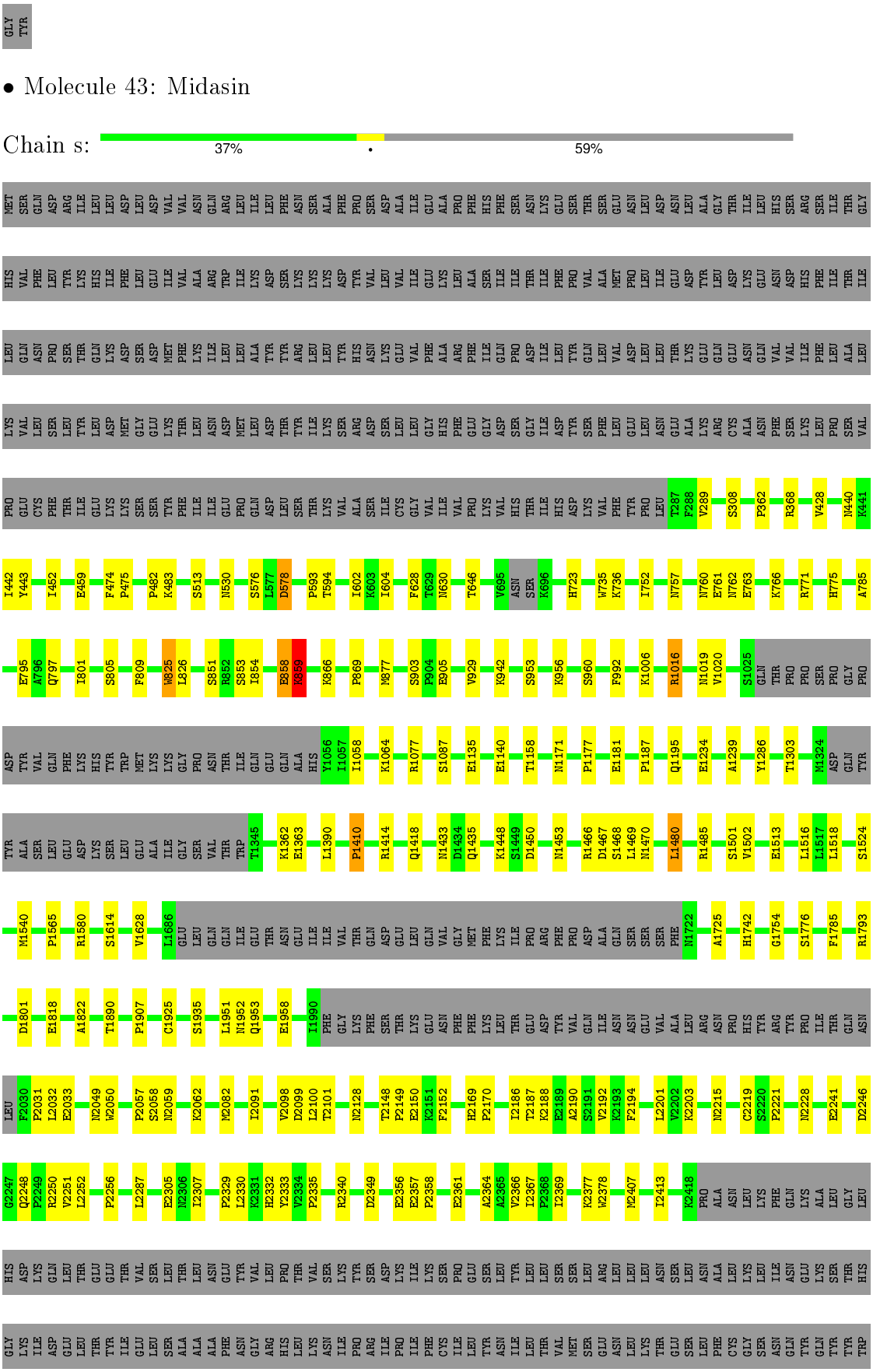


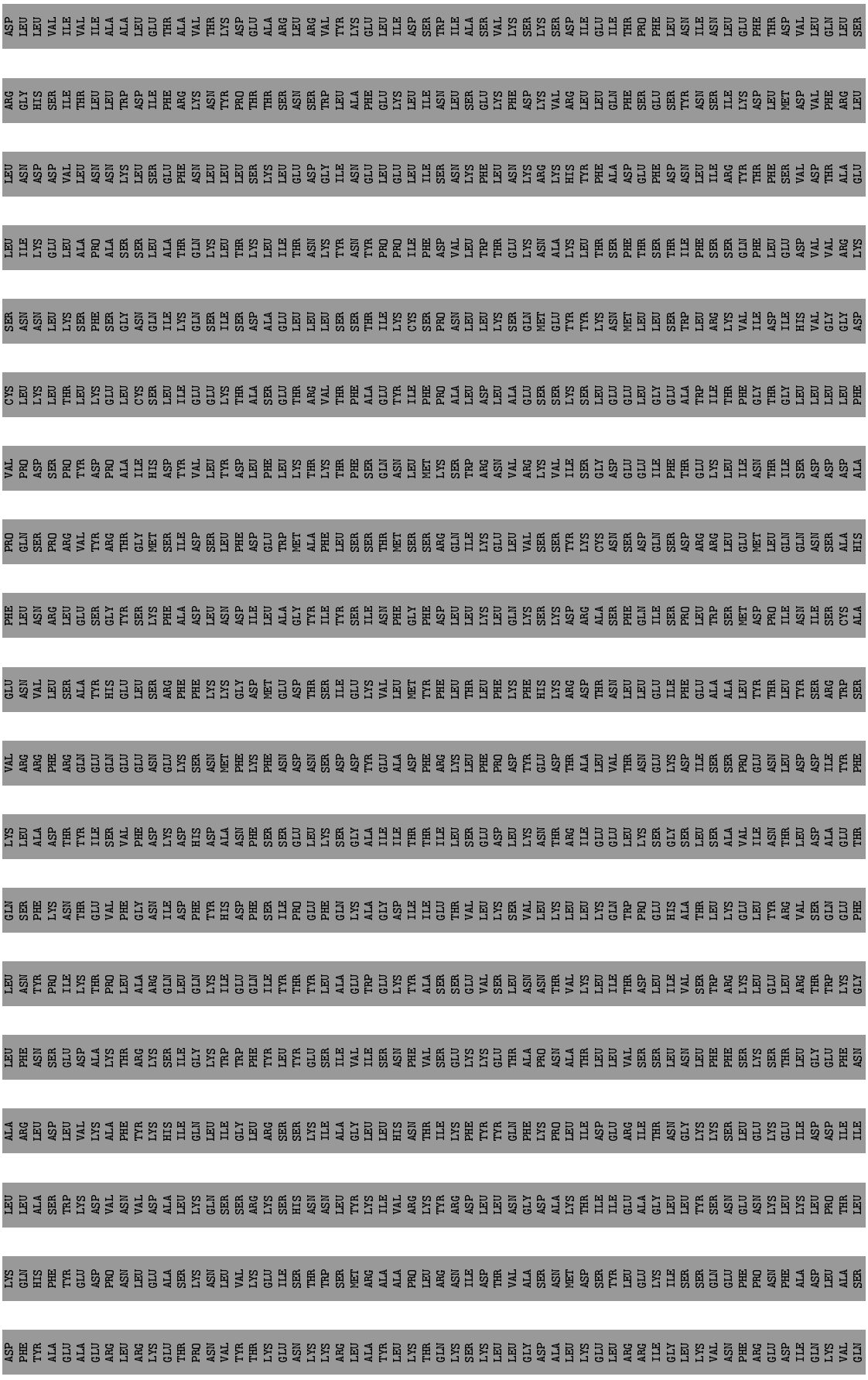


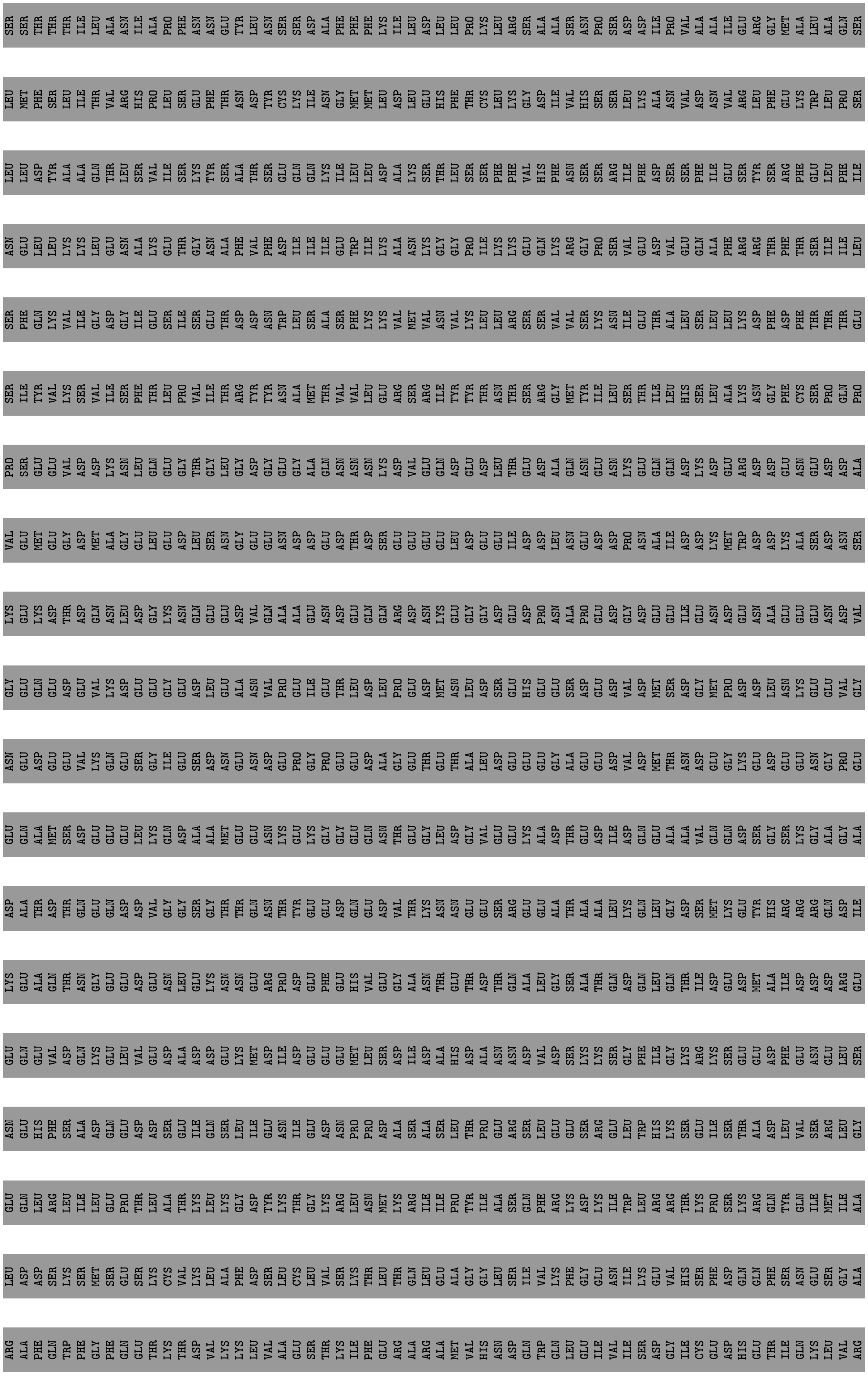
- Molecule 42: Protein SDA1

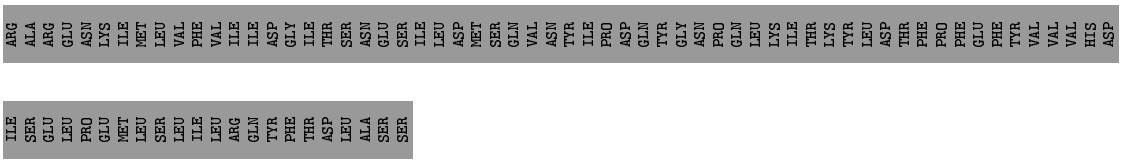
Chain r:




GLY TYR
• Molecule 43: Midasin
Chain s:
37%
59%

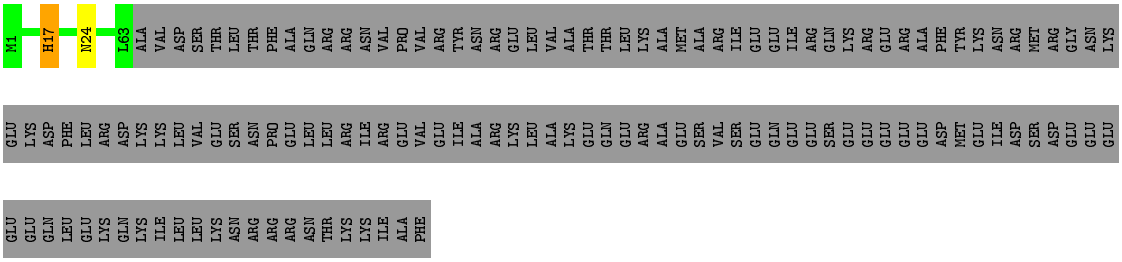



SER SER THR THR ILE LEU ALA ASN ILE ALA PRO PHE ASN ASN GLU TYR LEU ASN SER SER ASP ALA PHE PHE PHE LYS ILE LEU ASP LEU LEU PRO LYS LEU ARG SER ALA ALA SER ASN PRO SER ASP ASP ILE PRO VAL ALA ALA ILE GLU ARG GLY MET ALA LEU ALA GLN SER
LEU MET PHE SER LEU ILE THR VAL ARG HIS PRO LEU SER GLU PHE THR ASN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



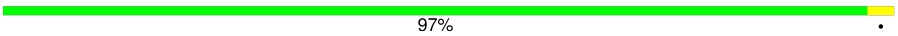
• Molecule 44: Ribosome biogenesis protein RLP24

Chain t:



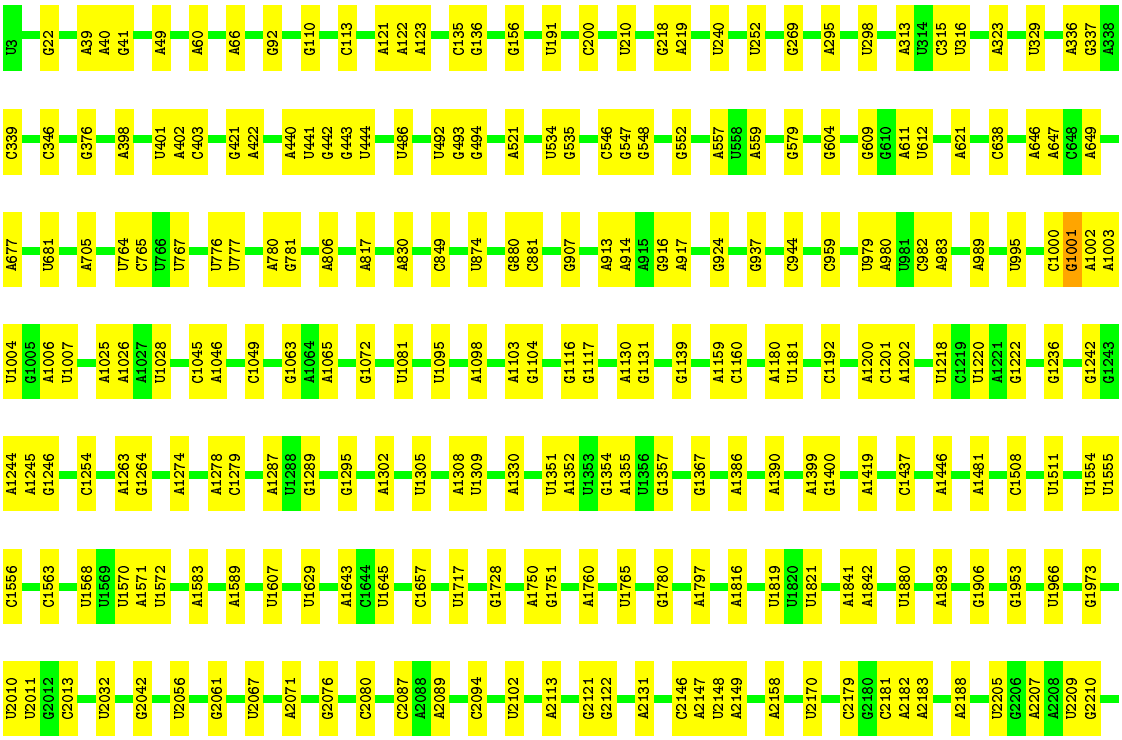
• Molecule 45: ARX1

Chain u:



• Molecule 46: 25S ribosomal RNA

Chain x:

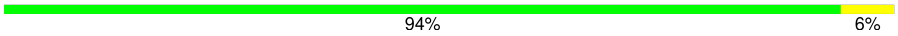


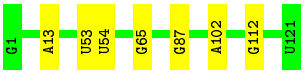
- Molecule 47: 5.8S ribosomal RNA

Chain y:

- Molecule 48: 5S ribosomal RNA

Chain z:





4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	SUBVOLUMES, Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	4200	Depositor
Magnification	75000	Depositor
Image detector	TVIPS	Depositor

5 Model quality

5.1 Standard geometry

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.35	1/1006 (0.1%)	0.47	0/1256
10	J	0.53	0/674	0.78	0/841
11	K	0.18	0/506	0.35	0/631
12	L	0.17	0/770	0.35	0/961
13	M	0.17	0/542	0.30	0/676
14	N	0.19	0/810	0.38	0/1011
15	O	0.20	0/786	0.47	1/981 (0.1%)
16	P	0.17	0/730	0.33	0/911
17	Q	0.17	0/738	0.30	0/921
18	R	0.20	0/750	0.41	0/936
19	S	0.16	0/686	0.32	0/856
2	B	0.32	1/1542 (0.1%)	0.44	2/1926 (0.1%)
20	T	0.44	1/634 (0.2%)	0.64	2/791 (0.3%)
21	U	0.17	0/398	0.31	0/496
22	V	0.22	0/542	0.34	0/676
23	X	0.17	0/482	0.29	0/601
24	Y	0.17	0/502	0.30	0/626
25	Z	0.17	0/538	0.31	0/671
26	a	0.80	3/590 (0.5%)	0.71	3/736 (0.4%)
27	c	0.17	0/386	0.27	0/481
28	d	0.17	0/434	0.31	0/541
29	e	0.17	0/506	0.32	0/631
3	C	0.19	0/1442	0.37	1/1801 (0.1%)
30	f	0.49	1/422 (0.2%)	0.71	1/526 (0.2%)
31	g	0.17	0/446	0.32	0/556
32	h	0.17	0/474	0.29	0/591
33	i	0.17	0/394	0.31	0/491
34	j	0.57	1/346 (0.3%)	0.57	1/431 (0.2%)
35	k	0.17	0/306	0.29	0/381
36	l	0.17	0/198	0.36	0/246
37	m	0.17	0/894	0.30	0/1116
38	n	0.17	0/846	0.31	0/1056
39	o	0.60	3/1386 (0.2%)	0.86	9/1731 (0.5%)
4	D	0.17	0/1182	0.32	0/1476

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
40	p	0.17	0/362	0.30	0/451
41	q	0.94	0/1950	0.91	1/2436 (0.0%)
42	r	0.56	1/1276 (0.1%)	0.92	4/1553 (0.3%)
43	s	0.43	4/8022 (0.0%)	0.50	9/10020 (0.1%)
44	t	0.34	0/250	0.52	0/311
45	u	0.92	0/1518	0.86	1/1896 (0.1%)
46	x	0.26	5/66581 (0.0%)	0.76	154/103823 (0.1%)
47	y	0.11	0/3743	0.64	0/5828
48	z	0.12	0/2880	0.64	0/4487
5	E	0.55	1/620 (0.2%)	0.70	4/772 (0.5%)
6	F	0.17	0/886	0.32	0/1106
7	G	0.17	0/930	0.32	0/1161
8	H	0.17	0/762	0.30	0/951
9	I	0.17	0/866	0.31	0/1081
All	All	0.32	22/113534 (0.0%)	0.69	193/164435 (0.1%)

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
1	A	0	1
10	J	0	1
2	B	0	3
20	T	0	3
26	a	0	1
30	f	0	2
39	o	0	1
42	r	0	3
43	s	0	12
44	t	0	1
5	E	0	1
All	All	0	29

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	x	2699	G	O3'-P	41.80	2.11	1.61
43	s	825	TRP	C-N	-18.64	0.91	1.34
43	s	826	LEU	N-CA	17.84	1.82	1.46
26	a	111	LYS	N-CA	14.18	1.74	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	110	GLY	C-N	9.94	1.56	1.34
5	E	67	GLY	CA-C	-9.76	1.36	1.51
43	s	805	SER	C-O	8.98	1.40	1.23
34	j	39	TYR	C-O	-8.62	1.06	1.23
2	B	18	PRO	C-N	7.71	1.51	1.34
46	x	2638	C	O3'-P	-7.37	1.52	1.61
30	f	100	ILE	C-N	7.04	1.50	1.34
43	s	2364	ALA	C-O	6.99	1.36	1.23
39	o	56	GLY	C-O	6.14	1.33	1.23
20	T	16	GLN	N-CA	6.10	1.58	1.46
46	x	443	G	O3'-P	5.83	1.68	1.61
39	o	44	ALA	CA-C	5.76	1.68	1.52
46	x	1025	A	C6-N6	5.62	1.38	1.33
46	x	1130	A	O3'-P	5.55	1.67	1.61
42	r	111	ALA	C-N	5.50	1.46	1.34
26	a	112	ILE	N-CA	-5.46	1.35	1.46
1	A	207	VAL	N-CA	5.30	1.56	1.46
39	o	44	ALA	C-O	5.03	1.32	1.23

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	x	2699	G	P-O3'-C3'	-26.90	87.42	119.70
46	x	2700	G	O5'-P-OP2	26.12	142.05	110.70
46	x	2700	G	O5'-P-OP1	-25.82	79.71	110.70
43	s	858	GLU	O-C-N	-21.29	88.64	122.70
46	x	440	A	O5'-P-OP1	-19.66	87.11	110.70
46	x	2699	G	O3'-P-O5'	-17.51	70.72	104.00
46	x	440	A	O5'-P-OP2	17.49	131.69	110.70
46	x	2638	C	P-O3'-C3'	-16.84	99.49	119.70
46	x	2700	G	OP1-P-OP2	-14.38	98.04	119.60
46	x	440	A	P-O5'-C5'	14.22	143.66	120.90
46	x	494	G	P-O5'-C5'	13.59	142.64	120.90
46	x	2699	G	OP1-P-O3'	13.00	133.81	105.20
46	x	1026	A	N1-C6-N6	12.33	126.00	118.60
46	x	913	A	N1-C6-N6	12.08	125.85	118.60
46	x	2183	A	N1-C6-N6	11.74	125.64	118.60
46	x	2705	A	N1-C6-N6	11.73	125.64	118.60
46	x	2182	A	N1-C6-N6	11.69	125.62	118.60
46	x	1025	A	N1-C6-N6	11.58	125.55	118.60
46	x	494	G	C4'-C3'-O3'	11.50	135.99	113.00
46	x	40	A	C4'-C3'-O3'	-11.49	85.27	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	x	2147	A	N1-C6-N6	11.37	125.42	118.60
46	x	2149	A	N1-C6-N6	11.33	125.40	118.60
46	x	2617	U	C4'-C3'-O3'	-11.24	85.81	109.40
5	E	67	GLY	N-CA-C	-11.04	85.50	113.10
46	x	1218	U	P-O5'-C5'	10.90	138.34	120.90
26	a	110	GLY	CA-C-O	-10.67	101.40	120.60
46	x	1002	A	P-O5'-C5'	10.66	137.96	120.90
30	f	100	ILE	O-C-N	-10.16	106.44	122.70
43	s	1016	ARG	O-C-N	-10.16	106.44	122.70
46	x	313	A	P-O3'-C3'	-10.06	107.63	119.70
46	x	442	G	C4'-C3'-O3'	9.87	132.74	113.00
46	x	2403	G	C4'-C3'-O3'	-9.58	89.28	109.40
46	x	2728	G	N1-C6-O6	9.34	125.50	119.90
46	x	1131	G	O4'-C4'-C3'	-9.29	94.71	104.00
46	x	2637	A	C4'-C3'-O3'	-9.07	90.36	109.40
46	x	2699	G	OP2-P-O3'	-9.00	85.40	105.20
46	x	2639	G	P-O5'-C5'	8.90	135.14	120.90
46	x	315	C	C5'-C4'-O4'	-8.87	98.45	109.10
46	x	2638	C	C4'-C3'-O3'	8.82	130.64	113.00
46	x	2700	G	N1-C6-O6	8.69	125.11	119.90
46	x	315	C	C2'-C3'-O3'	8.57	128.36	109.50
46	x	2728	G	O4'-C1'-N9	8.57	115.05	108.20
46	x	315	C	P-O5'-C5'	-8.54	107.23	120.90
46	x	1000	C	C4'-C3'-O3'	8.49	129.98	113.00
46	x	2259	A	C4'-C3'-O3'	8.43	129.87	113.00
46	x	1130	A	C4'-C3'-O3'	8.26	129.52	113.00
46	x	2319	U	C2'-C3'-O3'	-8.24	91.37	109.50
39	o	247	ARG	N-CA-C	8.24	133.24	111.00
46	x	1001	G	C2'-C3'-O3'	-8.22	91.41	109.50
46	x	2403	G	P-O3'-C3'	8.21	129.55	119.70
46	x	1001	G	C4'-C3'-O3'	8.17	129.34	113.00
46	x	2254	U	C4'-C3'-O3'	7.96	128.92	113.00
46	x	2181	C	O4'-C1'-N1	7.83	114.47	108.20
39	o	119	GLY	O-C-N	7.81	135.20	122.70
46	x	1003	A	N9-C1'-C2'	-7.75	103.48	112.00
46	x	2319	U	C4'-C3'-O3'	7.73	128.46	113.00
26	a	110	GLY	CA-C-N	7.63	133.99	117.20
46	x	2404	A	C5'-C4'-C3'	7.59	128.14	116.00
46	x	1554	U	P-O3'-C3'	7.56	128.77	119.70
46	x	39	A	C4'-C3'-O3'	-7.48	93.69	109.40
46	x	1025	A	O4'-C1'-N9	7.45	114.16	108.20
26	a	110	GLY	C-N-CA	7.34	140.06	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	o	119	GLY	CA-C-N	-7.33	101.08	117.20
46	x	2319	U	C5'-C4'-O4'	7.24	117.79	109.10
46	x	2256	A	C2'-C3'-O3'	7.22	125.38	109.50
46	x	2617	U	P-O5'-C5'	7.12	132.29	120.90
39	o	119	GLY	C-N-CA	7.12	139.49	121.70
45	u	285	PRO	N-CA-C	7.02	130.34	112.10
46	x	1130	A	O3'-P-O5'	7.01	117.32	104.00
43	s	630	ASN	C-N-CA	-6.99	104.23	121.70
46	x	2146	C	P-O3'-C3'	-6.92	111.39	119.70
46	x	2640	A	P-O5'-C5'	-6.87	109.91	120.90
46	x	2617	U	C2'-C3'-O3'	6.83	124.62	113.70
46	x	2585	G	C4'-C3'-O3'	-6.77	95.18	109.40
46	x	983	A	C4'-C3'-O3'	-6.72	95.28	109.40
46	x	2585	G	P-O5'-C5'	6.70	131.62	120.90
20	T	16	GLN	N-CA-C	6.69	129.06	111.00
46	x	313	A	O3'-P-O5'	6.58	116.51	104.00
46	x	41	G	C4'-C3'-O3'	-6.51	95.73	109.40
43	s	801	ILE	O-C-N	-6.49	112.31	122.70
46	x	2700	G	C5-C6-O6	-6.45	124.73	128.60
39	o	44	ALA	N-CA-C	6.44	128.40	111.00
15	O	59	ARG	N-CA-C	6.44	128.39	111.00
46	x	39	A	P-O5'-C5'	6.44	131.20	120.90
46	x	2639	G	O5'-C5'-C4'	-6.42	99.49	111.70
46	x	2705	A	C4-C5-C6	6.42	120.21	117.00
46	x	1025	A	C4-C5-C6	6.42	120.21	117.00
20	T	16	GLN	C-N-CA	6.40	137.70	121.70
46	x	1002	A	O5'-C5'-C4'	-6.40	99.55	111.70
46	x	444	U	P-O5'-C5'	6.38	131.12	120.90
46	x	2210	G	C4'-C3'-O3'	6.38	125.76	113.00
46	x	494	G	O5'-C5'-C4'	-6.36	99.61	111.70
46	x	2586	G	C4'-C3'-O3'	6.36	125.72	113.00
46	x	440	A	O5'-C5'-C4'	-6.34	99.65	111.70
46	x	2182	A	O4'-C1'-N9	6.30	113.24	108.20
46	x	2183	A	C4-C5-C6	6.29	120.15	117.00
46	x	40	A	N9-C1'-C2'	-6.23	105.14	112.00
46	x	2258	U	O5'-P-OP2	-6.22	100.10	105.70
46	x	1003	A	O3'-P-O5'	-6.21	92.19	104.00
46	x	2701	U	O4'-C1'-N1	6.21	113.17	108.20
34	j	38	GLY	O-C-N	-6.19	112.80	122.70
46	x	1218	U	O5'-C5'-C4'	-6.18	99.96	111.70
46	x	1554	U	C4'-C3'-O3'	6.12	125.24	113.00
39	o	117	LYS	C-N-CA	6.11	136.97	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	67	GLY	C-N-CA	-6.08	96.44	122.00
46	x	2182	A	C4-C5-C6	6.08	120.04	117.00
46	x	913	A	C4-C5-C6	6.04	120.02	117.00
5	E	68	PRO	CA-C-N	-5.96	104.08	117.20
46	x	1026	A	C4-C5-C6	5.95	119.97	117.00
46	x	1026	A	C5-C6-N6	-5.94	118.95	123.70
46	x	2586	G	O4'-C1'-N9	-5.93	103.45	108.20
46	x	1131	G	P-O5'-C5'	5.93	130.38	120.90
46	x	2316	G	C4'-C3'-O3'	5.92	124.84	113.00
42	r	88	PRO	N-CA-C	-5.91	96.72	112.10
46	x	2728	G	C5-C6-O6	-5.91	125.05	128.60
46	x	1004	U	C5'-C4'-C3'	5.90	125.44	116.00
46	x	441	U	P-O3'-C3'	5.87	126.75	119.70
46	x	2318	U	O4'-C1'-N1	5.87	112.89	108.20
46	x	1556	C	O4'-C1'-N1	5.87	112.89	108.20
46	x	2587	U	C4'-C3'-O3'	-5.82	97.18	109.40
46	x	2319	U	P-O3'-C3'	5.82	126.68	119.70
5	E	68	PRO	N-CA-C	-5.81	97.00	112.10
46	x	1556	C	N1-C1'-C2'	5.80	121.55	114.00
46	x	2616	C	C2'-C3'-O3'	5.79	122.97	113.70
46	x	2147	A	O4'-C1'-N9	5.79	112.83	108.20
46	x	2147	A	C4-C5-C6	5.78	119.89	117.00
46	x	443	G	C4'-C3'-O3'	5.77	124.54	113.00
46	x	493	G	O3'-P-O5'	5.77	114.96	104.00
46	x	40	A	O4'-C4'-C3'	-5.76	98.24	104.00
46	x	1000	C	P-O3'-C3'	5.74	126.58	119.70
46	x	1002	A	P-O3'-C3'	5.73	126.58	119.70
46	x	2183	A	O4'-C1'-N9	5.72	112.78	108.20
46	x	913	A	C5-C6-N6	-5.70	119.14	123.70
42	r	442	ALA	N-CA-C	-5.70	95.62	111.00
46	x	1025	A	C5-C6-N6	-5.68	119.16	123.70
43	s	1480	LEU	O-C-N	-5.65	113.67	122.70
46	x	2320	A	C5'-C4'-C3'	5.64	125.02	116.00
43	s	630	ASN	N-CA-C	-5.62	95.83	111.00
46	x	1131	G	O4'-C1'-N9	5.62	112.70	108.20
46	x	2617	U	N1-C1'-C2'	-5.62	105.82	112.00
39	o	237	MET	N-CA-C	-5.60	95.87	111.00
46	x	2207	A	C4'-C3'-O3'	5.59	124.18	113.00
46	x	2256	A	C4'-C3'-O3'	-5.58	97.68	109.40
46	x	2637	A	C2'-C3'-O3'	5.58	122.63	113.70
46	x	2586	G	C2'-C3'-O3'	5.57	122.62	113.70
46	x	2403	G	N9-C1'-C2'	5.56	121.23	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	x	2404	A	O5'-C5'-C4'	5.56	122.26	111.70
46	x	913	A	O4'-C1'-N9	5.55	112.64	108.20
46	x	2405	C	O5'-C5'-C4'	-5.54	101.17	111.70
46	x	2616	C	P-O3'-C3'	5.54	126.35	119.70
46	x	2700	G	O4'-C1'-N9	5.52	112.62	108.20
46	x	2705	A	C5-C6-N1	-5.51	114.94	117.70
46	x	1220	U	P-O3'-C3'	-5.50	113.11	119.70
46	x	2183	A	C5-C6-N6	-5.49	119.31	123.70
46	x	443	G	O3'-P-O5'	5.49	114.43	104.00
46	x	1220	U	O4'-C1'-N1	5.49	112.59	108.20
46	x	2149	A	C5-C6-N6	-5.49	119.31	123.70
3	C	187	LEU	N-CA-C	-5.48	96.19	111.00
46	x	2181	C	N3-C4-N4	5.47	121.83	118.00
46	x	2147	A	C5-C6-N1	-5.45	114.97	117.70
46	x	494	G	C2'-C3'-O3'	-5.42	97.58	109.50
46	x	2182	A	C5-C6-N6	-5.41	119.38	123.70
43	s	1410	PRO	CA-C-N	-5.39	105.35	117.20
46	x	2182	A	C5-C6-N1	-5.38	115.01	117.70
46	x	913	A	C5-C6-N1	-5.38	115.01	117.70
2	B	18	PRO	C-N-CA	5.38	135.14	121.70
46	x	2615	G	C4'-C3'-O3'	5.37	123.73	113.00
46	x	2705	A	C5-C6-N6	-5.35	119.42	123.70
46	x	2181	C	N3-C4-C5	-5.33	119.77	121.90
42	r	306	MET	N-CA-C	-5.32	96.64	111.00
43	s	578	ASP	N-CA-C	-5.32	96.65	111.00
46	x	2585	G	P-O3'-C3'	5.31	126.07	119.70
46	x	2183	A	C5-C6-N1	-5.29	115.05	117.70
39	o	118	PHE	CA-C-N	5.29	126.78	116.20
46	x	1026	A	C5-C6-N1	-5.29	115.06	117.70
46	x	2209	U	C5'-C4'-O4'	-5.23	102.82	109.10
46	x	2258	U	C4'-C3'-O3'	5.22	123.43	113.00
46	x	2319	U	O4'-C4'-C3'	-5.22	98.78	104.00
42	r	129	LEU	N-CA-C	-5.20	96.97	111.00
41	q	249	PRO	N-CA-C	5.18	125.58	112.10
2	B	17	LEU	O-C-N	-5.17	111.27	121.10
46	x	2149	A	C4-C5-C6	5.17	119.58	117.00
39	o	94	SER	N-CA-C	-5.16	97.06	111.00
46	x	2618	G	P-O5'-C5'	5.16	129.16	120.90
46	x	2269	U	P-O5'-C5'	5.12	129.09	120.90
46	x	2147	A	C5-C6-N6	-5.12	119.60	123.70
46	x	441	U	O5'-C5'-C4'	-5.11	102.00	111.70
46	x	1556	C	C5'-C4'-O4'	5.10	115.22	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	x	1555	U	C4'-C3'-O3'	5.09	123.17	113.00
43	s	859	LYS	C-N-CA	-5.07	111.65	122.30
46	x	2728	G	C1'-O4'-C4'	-5.07	105.85	109.90
46	x	2618	G	O5'-C5'-C4'	-5.04	102.13	111.70
46	x	2148	U	O4'-C1'-N1	5.01	112.21	108.20

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	LYS	Peptide
2	B	18	PRO	Peptide
2	B	255	TRP	Peptide
2	B	256	HIS	Peptide
5	E	42	LEU	Mainchain
10	J	8	PRO	Peptide
20	T	16	GLN	Mainchain
20	T	23	GLY	Peptide
20	T	86	GLU	Peptide
26	a	111	LYS	Peptide
30	f	100	ILE	Mainchain
30	f	103	TYR	Peptide
39	o	43	ARG	Mainchain
42	r	111	ALA	Mainchain
42	r	461	LEU	Peptide
42	r	462	ALA	Peptide
43	s	1016	ARG	Mainchain
43	s	1019	ASN	Peptide
43	s	1467	ASP	Peptide
43	s	1480	LEU	Mainchain
43	s	576	SER	Mainchain,Peptide
43	s	578	ASP	Peptide
43	s	628	PHE	Peptide
43	s	825	TRP	Mainchain
43	s	858	GLU	Mainchain
43	s	859	LYS	Peptide
43	s	903	SER	Peptide
44	t	17	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1007	0	310	18	0
2	B	1543	0	433	4	0
3	C	1443	0	399	7	0
4	D	1183	0	325	1	0
5	E	622	0	160	1	0
6	F	887	0	241	3	0
7	G	931	0	242	1	0
8	H	763	0	215	3	0
9	I	867	0	230	2	0
10	J	675	0	191	11	0
11	K	507	0	140	1	0
12	L	771	0	199	4	0
13	M	543	0	145	2	0
14	N	811	0	221	3	0
15	O	787	0	214	7	0
16	P	731	0	197	4	0
17	Q	739	0	205	1	0
18	R	751	0	203	14	0
19	S	687	0	175	3	0
20	T	635	0	174	14	0
21	U	399	0	109	2	0
22	V	543	0	162	2	0
23	X	483	0	121	1	0
24	Y	503	0	134	1	0
25	Z	539	0	144	1	0
26	a	591	0	176	0	0
27	c	387	0	113	0	0
28	d	435	0	114	0	0
29	e	507	0	135	0	0
30	f	423	0	117	0	0
31	g	447	0	121	0	0
32	h	475	0	118	0	0
33	i	395	0	109	0	0
34	j	347	0	104	0	0
35	k	307	0	79	0	0
36	l	199	0	47	0	0
37	m	895	0	257	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	n	847	0	224	0	0
39	o	1387	0	358	0	0
40	p	363	0	108	0	0
41	q	1951	0	539	0	0
42	r	1304	0	336	0	0
43	s	8027	0	2141	0	0
44	t	251	0	68	0	0
45	u	1519	0	416	0	0
46	x	59475	0	29874	0	0
47	y	3350	0	1696	0	0
48	z	2576	0	1304	0	0
All	All	105808	0	43843	111	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:75:ALA:O	15:O:77:SER:N	1.85	1.10
20:T:62:GLY:N	20:T:75:ILE:H	1.51	1.08
20:T:43:LYS:O	20:T:95:HIS:CA	2.03	1.06
18:R:158:GLU:O	18:R:162:ARG:N	1.90	1.03
20:T:62:GLY:CA	20:T:75:ILE:H	1.72	1.03
20:T:62:GLY:HA3	20:T:75:ILE:N	1.80	0.96
20:T:41:ASP:O	20:T:43:LYS:N	2.00	0.93
1:A:114:SER:CA	1:A:134:VAL:H	1.81	0.89
1:A:206:PRO:O	1:A:208:ASP:N	2.06	0.88
18:R:158:GLU:O	18:R:161:ALA:N	2.08	0.86
1:A:119:LYS:O	1:A:121:GLY:N	2.12	0.82
1:A:115:ASN:CA	1:A:133:TYR:CA	2.58	0.81
20:T:62:GLY:CA	20:T:75:ILE:N	2.42	0.81
1:A:115:ASN:N	1:A:133:TYR:CA	2.45	0.80
10:J:106:ILE:O	10:J:125:MET:N	2.15	0.79
18:R:157:GLU:O	18:R:161:ALA:N	2.16	0.78
1:A:113:VAL:N	1:A:134:VAL:C	2.39	0.73
10:J:94:ARG:O	10:J:96:PHE:N	2.22	0.71
20:T:74:VAL:O	20:T:89:LEU:N	2.26	0.69
20:T:62:GLY:H	20:T:75:ILE:H	1.41	0.68
18:R:173:ARG:O	18:R:177:VAL:N	2.24	0.68
1:A:114:SER:C	1:A:133:TYR:CA	2.63	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:N	1:A:134:VAL:O	2.26	0.66
10:J:85:LYS:O	10:J:88:GLU:N	2.28	0.66
1:A:206:PRO:C	1:A:208:ASP:H	1.98	0.65
18:R:158:GLU:O	18:R:159:ALA:C	2.37	0.63
12:L:99:HIS:O	12:L:101:ARG:N	2.28	0.63
20:T:62:GLY:N	20:T:75:ILE:N	2.36	0.62
20:T:76:ILE:O	20:T:78:LYS:N	2.34	0.60
2:B:238:LEU:N	2:B:246:LEU:O	2.36	0.59
1:A:134:VAL:O	1:A:136:ILE:N	2.35	0.59
18:R:81:ARG:O	18:R:83:GLY:N	2.36	0.59
15:O:62:THR:O	15:O:64:PHE:N	2.29	0.58
18:R:79:GLY:O	18:R:81:ARG:N	2.36	0.58
7:G:35:GLY:O	7:G:37:GLY:N	2.37	0.58
1:A:125:ALA:O	1:A:127:ALA:N	2.37	0.58
18:R:158:GLU:O	18:R:161:ALA:CA	2.52	0.57
1:A:114:SER:C	1:A:134:VAL:H	2.07	0.56
10:J:94:ARG:C	10:J:96:PHE:H	2.09	0.56
16:P:95:LEU:O	16:P:97:ASN:N	2.38	0.55
1:A:125:ALA:C	1:A:127:ALA:H	2.10	0.54
15:O:110:PRO:O	15:O:112:TYR:N	2.41	0.54
20:T:61:THR:CA	20:T:75:ILE:O	2.55	0.54
20:T:43:LYS:C	20:T:95:HIS:CA	2.75	0.54
15:O:75:ALA:C	15:O:77:SER:N	2.59	0.54
22:V:46:LEU:O	22:V:48:ARG:N	2.41	0.53
14:N:107:GLY:O	14:N:111:ALA:N	2.41	0.53
18:R:150:GLN:O	18:R:154:ALA:N	2.40	0.53
20:T:61:THR:C	20:T:75:ILE:O	2.46	0.53
1:A:114:SER:CA	1:A:134:VAL:N	2.64	0.52
1:A:114:SER:C	1:A:134:VAL:N	2.63	0.52
3:C:94:CYS:O	3:C:96:GLY:N	2.42	0.52
19:S:132:THR:O	19:S:134:ASP:N	2.43	0.52
14:N:75:VAL:O	14:N:77:LYS:N	2.43	0.52
16:P:40:GLU:O	16:P:42:THR:N	2.42	0.52
20:T:74:VAL:O	20:T:88:ARG:CA	2.58	0.51
1:A:112:ILE:CA	1:A:134:VAL:O	2.59	0.51
1:A:125:ALA:C	1:A:127:ALA:N	2.63	0.51
9:I:39:LYS:N	9:I:205:VAL:O	2.40	0.50
14:N:165:THR:O	14:N:169:LYS:N	2.28	0.50
2:B:346:THR:O	2:B:348:ARG:N	2.45	0.49
2:B:46:PHE:O	2:B:338:LEU:N	2.45	0.49
4:D:257:GLU:O	4:D:259:LYS:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:23:VAL:O	10:J:25:GLU:N	2.39	0.49
16:P:132:ALA:O	16:P:134:GLY:N	2.45	0.49
10:J:73:GLY:O	10:J:75:LYS:N	2.46	0.49
3:C:181:VAL:O	3:C:183:LYS:N	2.43	0.49
12:L:164:GLU:O	12:L:166:ALA:N	2.45	0.49
13:M:34:ALA:O	13:M:47:ASP:N	2.46	0.48
8:H:80:THR:O	8:H:85:GLY:N	2.47	0.48
2:B:49:TYR:O	2:B:80:ASP:N	2.46	0.48
19:S:79:VAL:N	19:S:90:MET:O	2.45	0.48
15:O:62:THR:N	15:O:69:GLY:HA2	2.30	0.47
3:C:337:GLU:O	3:C:339:LEU:N	2.48	0.47
24:Y:115:ARG:O	24:Y:117:ALA:N	2.48	0.47
1:A:128:ARG:C	1:A:130:SER:H	2.17	0.47
11:K:39:PRO:O	11:K:41:LYS:N	2.47	0.47
18:R:85:ARG:O	18:R:89:LEU:N	2.48	0.47
18:R:81:ARG:C	18:R:83:GLY:H	2.18	0.46
25:Z:16:GLY:O	25:Z:18:TYR:N	2.48	0.46
6:F:108:LEU:O	6:F:110:ARG:N	2.48	0.46
12:L:27:ASP:O	12:L:29:ALA:N	2.49	0.46
3:C:114:ASN:O	3:C:118:LYS:N	2.42	0.46
12:L:165:SER:O	12:L:167:PHE:N	2.47	0.46
18:R:66:HIS:O	18:R:70:LYS:N	2.41	0.45
3:C:206:LEU:O	3:C:249:ILE:N	2.39	0.45
6:F:24:GLU:O	6:F:26:VAL:N	2.50	0.45
10:J:109:HIS:N	10:J:123:PHE:O	2.49	0.44
3:C:338:LYS:O	3:C:340:GLY:N	2.50	0.44
19:S:79:VAL:O	19:S:90:MET:N	2.49	0.44
23:X:49:LYS:O	23:X:51:VAL:N	2.51	0.44
6:F:222:HIS:O	6:F:227:GLY:N	2.51	0.44
17:Q:170:ARG:O	17:Q:172:PHE:N	2.51	0.43
3:C:222:VAL:O	3:C:224:GLY:N	2.52	0.43
8:H:49:ASN:O	8:H:51:GLN:N	2.51	0.43
9:I:73:ASP:O	9:I:75:ASP:N	2.51	0.43
10:J:110:ILE:C	10:J:112:LEU:H	2.21	0.43
21:U:97:SER:O	21:U:99:LYS:N	2.51	0.43
21:U:43:VAL:O	21:U:45:GLY:N	2.52	0.42
22:V:23:MET:O	22:V:34:LEU:N	2.43	0.42
10:J:107:ASP:CA	10:J:124:GLY:HA2	2.49	0.42
8:H:64:HIS:O	8:H:66:ALA:N	2.53	0.42
16:P:113:TYR:O	16:P:151:THR:N	2.48	0.42
18:R:158:GLU:C	18:R:161:ALA:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:130:LYS:O	15:O:132:GLY:N	2.53	0.42
5:E:97:ASN:O	5:E:99:GLU:N	2.53	0.41
10:J:41:SER:C	10:J:43:GLN:H	2.24	0.41
15:O:38:ALA:H	15:O:107:GLY:HA2	1.85	0.41
13:M:34:ALA:N	13:M:47:ASP:O	2.52	0.41
18:R:158:GLU:O	18:R:161:ALA:C	2.54	0.40
10:J:110:ILE:O	10:J:112:LEU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	250/254 (98%)	156 (62%)	70 (28%)	24 (10%)	1 15
2	B	384/387 (99%)	294 (77%)	71 (18%)	19 (5%)	3 31
3	C	359/362 (99%)	254 (71%)	80 (22%)	25 (7%)	1 22
4	D	294/297 (99%)	229 (78%)	53 (18%)	12 (4%)	3 35
5	E	152/176 (86%)	113 (74%)	35 (23%)	4 (3%)	7 45
6	F	220/244 (90%)	181 (82%)	30 (14%)	9 (4%)	3 35
7	G	231/256 (90%)	179 (78%)	43 (19%)	9 (4%)	4 36
8	H	189/191 (99%)	147 (78%)	37 (20%)	5 (3%)	7 45
9	I	215/217 (99%)	159 (74%)	48 (22%)	8 (4%)	4 38
10	J	167/174 (96%)	116 (70%)	29 (17%)	22 (13%)	0 7
11	K	125/165 (76%)	80 (64%)	29 (23%)	16 (13%)	0 8
12	L	191/199 (96%)	141 (74%)	39 (20%)	11 (6%)	2 27
13	M	134/138 (97%)	106 (79%)	22 (16%)	6 (4%)	3 33
14	N	201/204 (98%)	147 (73%)	44 (22%)	10 (5%)	3 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	O	195/199 (98%)	142 (73%)	38 (20%)	15 (8%)	1 20
16	P	181/184 (98%)	141 (78%)	35 (19%)	5 (3%)	6 44
17	Q	183/186 (98%)	143 (78%)	30 (16%)	10 (6%)	2 29
18	R	186/189 (98%)	136 (73%)	44 (24%)	6 (3%)	5 41
19	S	170/172 (99%)	133 (78%)	31 (18%)	6 (4%)	4 39
20	T	157/160 (98%)	90 (57%)	46 (29%)	21 (13%)	0 7
21	U	98/121 (81%)	77 (79%)	17 (17%)	4 (4%)	3 35
22	V	134/137 (98%)	95 (71%)	37 (28%)	2 (2%)	13 57
23	X	119/142 (84%)	91 (76%)	23 (19%)	5 (4%)	3 34
24	Y	124/127 (98%)	91 (73%)	26 (21%)	7 (6%)	2 28
25	Z	133/136 (98%)	97 (73%)	30 (23%)	6 (4%)	3 33
26	a	146/149 (98%)	91 (62%)	39 (27%)	16 (11%)	0 11
27	c	95/105 (90%)	84 (88%)	10 (10%)	1 (1%)	17 63
28	d	107/113 (95%)	88 (82%)	15 (14%)	4 (4%)	4 38
29	e	125/130 (96%)	99 (79%)	24 (19%)	2 (2%)	12 56
30	f	104/107 (97%)	78 (75%)	19 (18%)	7 (7%)	1 24
31	g	110/121 (91%)	78 (71%)	27 (24%)	5 (4%)	3 33
32	h	117/120 (98%)	92 (79%)	21 (18%)	4 (3%)	5 40
33	i	97/100 (97%)	78 (80%)	13 (13%)	6 (6%)	2 26
34	j	85/88 (97%)	53 (62%)	26 (31%)	6 (7%)	1 22
35	k	75/78 (96%)	66 (88%)	8 (11%)	1 (1%)	15 60
36	l	48/51 (94%)	33 (69%)	11 (23%)	4 (8%)	1 18
37	m	222/245 (91%)	170 (77%)	44 (20%)	8 (4%)	4 38
38	n	210/236 (89%)	156 (74%)	48 (23%)	6 (3%)	6 43
39	o	345/647 (53%)	218 (63%)	76 (22%)	51 (15%)	0 5
40	p	89/92 (97%)	72 (81%)	14 (16%)	3 (3%)	5 40
41	q	486/515 (94%)	459 (94%)	21 (4%)	6 (1%)	16 61
42	r	277/767 (36%)	152 (55%)	58 (21%)	67 (24%)	0 2
43	s	1998/4914 (41%)	1595 (80%)	228 (11%)	175 (9%)	1 17
44	t	61/199 (31%)	53 (87%)	6 (10%)	2 (3%)	5 40
45	u	378/380 (100%)	359 (95%)	9 (2%)	10 (3%)	7 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9967/14174 (70%)	7612 (76%)	1704 (17%)	651 (6%)	3 25

All (651) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ASP
1	A	128	ARG
1	A	133	TYR
1	A	135	ILE
1	A	137	ILE
1	A	196	TRP
1	A	206	PRO
1	A	207	VAL
2	B	19	ARG
3	C	95	ARG
3	C	188	ARG
3	C	317	PRO
6	F	99	PRO
10	J	8	PRO
10	J	11	ASP
10	J	12	LEU
10	J	74	PRO
10	J	94	ARG
10	J	127	PHE
10	J	165	GLN
11	K	30	PRO
11	K	58	VAL
12	L	100	ARG
13	M	49	PRO
15	O	63	ALA
15	O	72	HIS
15	O	74	ARG
15	O	75	ALA
15	O	76	PRO
15	O	79	ILE
16	P	143	PRO
18	R	80	LYS
18	R	144	GLN
20	T	17	ARG
20	T	42	ILE
20	T	70	SER
20	T	77	ASN

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Mol	Chain	Res	Type
20	T	87	LYS
20	T	90	ASN
20	T	91	LEU
20	T	92	ARG
20	T	132	PRO
26	a	32	ARG
26	a	112	ILE
26	a	119	PRO
30	f	103	TYR
30	f	104	PRO
34	j	5	THR
36	l	22	PRO
39	o	13	PRO
39	o	18	LEU
39	o	30	PRO
39	o	31	THR
39	o	32	VAL
39	o	55	GLU
39	o	59	GLU
39	o	61	PHE
39	o	88	LYS
39	o	98	ILE
39	o	100	ARG
39	o	108	VAL
39	o	110	ARG
39	o	112	TYR
39	o	114	ARG
39	o	116	LEU
39	o	139	ILE
39	o	143	LEU
39	o	145	ASP
39	o	157	ILE
39	o	234	ASN
39	o	245	HIS
39	o	246	LEU
39	o	247	ARG
42	r	92	ILE
42	r	137	ALA
42	r	154	THR
42	r	156	ALA
42	r	283	THR
42	r	382	LEU

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Mol	Chain	Res	Type
42	r	390	ALA
42	r	400	GLN
42	r	402	CYS
42	r	404	ASP
42	r	406	VAL
42	r	410	VAL
42	r	441	ALA
42	r	477	TYR
42	r	490	LYS
42	r	559	GLN
42	r	649	ASP
42	r	654	ALA
42	r	679	LYS
43	s	368	ARG
43	s	428	VAL
43	s	442	ILE
43	s	443	TYR
43	s	452	ILE
43	s	474	PHE
43	s	475	PRO
43	s	513	SER
43	s	735	TRP
43	s	736	LYS
43	s	752	ILE
43	s	757	ASN
43	s	760	ASN
43	s	771	ARG
43	s	775	HIS
43	s	797	GLN
43	s	809	PHE
43	s	853	SER
43	s	854	ILE
43	s	859	LYS
43	s	866	LYS
43	s	869	PRO
43	s	877	MET
43	s	929	VAL
43	s	1020	VAL
43	s	1077	ARG
43	s	1158	THR
43	s	1286	TYR
43	s	1362	LYS

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Mol	Chain	Res	Type
43	s	1363	GLU
43	s	1410	PRO
43	s	1433	ASN
43	s	1435	GLN
43	s	1468	SER
43	s	1469	LEU
43	s	1501	SER
43	s	1502	VAL
43	s	1518	LEU
43	s	1540	MET
43	s	1614	SER
43	s	1776	SER
43	s	1793	ARG
43	s	1907	PRO
43	s	1935	SER
43	s	2032	LEU
43	s	2049	ASN
43	s	2050	TRP
43	s	2057	PRO
43	s	2062	LYS
43	s	2091	ILE
43	s	2101	THR
43	s	2128	ASN
43	s	2148	THR
43	s	2149	PRO
43	s	2169	HIS
43	s	2186	ILE
43	s	2188	LYS
43	s	2192	VAL
43	s	2194	PHE
43	s	2203	LYS
43	s	2241	GLU
43	s	2246	ASP
43	s	2250	ARG
43	s	2252	LEU
43	s	2305	GLU
43	s	2329	PRO
43	s	2330	LEU
43	s	2358	PRO
43	s	2366	VAL
43	s	2369	ILE
43	s	2377	LYS

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Mol	Chain	Res	Type
43	s	2407	MET
45	u	70	VAL
45	u	136	PRO
45	u	187	ASN
45	u	206	GLN
45	u	250	ILE
1	A	116	VAL
1	A	126	LEU
1	A	185	ALA
1	A	194	ASN
2	B	4	ARG
2	B	14	LEU
2	B	96	PRO
3	C	76	ARG
3	C	189	ALA
3	C	224	GLY
3	C	270	SER
3	C	282	SER
3	C	338	LYS
4	D	56	THR
4	D	259	LYS
4	D	261	THR
6	F	25	GLN
6	F	109	THR
7	G	65	LEU
7	G	163	VAL
8	H	65	VAL
9	I	98	LYS
10	J	9	MET
10	J	73	GLY
10	J	86	VAL
10	J	115	LYS
10	J	167	TYR
11	K	98	VAL
12	L	28	GLN
13	M	8	LYS
14	N	18	VAL
14	N	76	PRO
15	O	60	LYS
15	O	61	ALA
15	O	64	PHE
15	O	77	SER

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Mol	Chain	Res	Type
15	O	78	ARG
15	O	111	PRO
15	O	148	LYS
17	Q	19	PRO
17	Q	97	PRO
17	Q	171	LYS
17	Q	173	GLU
18	R	82	LYS
19	S	22	PRO
19	S	50	LYS
20	T	16	GLN
20	T	19	PHE
20	T	21	LYS
20	T	24	ALA
20	T	78	LYS
20	T	124	VAL
21	U	44	GLU
21	U	98	THR
23	X	50	ALA
23	X	87	SER
23	X	102	LEU
24	Y	116	LYS
24	Y	126	LEU
25	Z	17	ARG
26	a	17	ALA
26	a	41	HIS
27	c	49	PRO
28	d	68	GLU
32	h	112	PRO
33	i	22	PRO
33	i	24	PRO
36	l	24	PRO
37	m	30	GLY
37	m	89	PRO
38	n	27	PHE
39	o	44	ALA
39	o	57	PHE
39	o	69	PRO
39	o	73	ASP
39	o	89	ASN
39	o	94	SER
39	o	118	PHE

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Mol	Chain	Res	Type
39	o	133	LEU
39	o	141	LYS
39	o	144	ARG
39	o	152	GLN
39	o	154	ARG
41	q	126	VAL
41	q	127	PHE
42	r	85	ALA
42	r	93	LEU
42	r	131	GLY
42	r	204	GLU
42	r	206	LEU
42	r	208	GLN
42	r	210	LEU
42	r	245	ASN
42	r	261	ASP
42	r	282	ALA
42	r	296	GLN
42	r	297	ASP
42	r	312	PHE
42	r	384	ARG
42	r	386	PRO
42	r	427	PHE
42	r	429	SER
42	r	433	ALA
42	r	486	ASN
42	r	488	ALA
42	r	557	SER
42	r	633	ASN
42	r	656	PHE
42	r	658	GLU
43	s	440	ASN
43	s	482	PRO
43	s	483	LYS
43	s	594	THR
43	s	723	HIS
43	s	761	GLU
43	s	766	LYS
43	s	942	LYS
43	s	960	SER
43	s	992	PHE
43	s	1058	ILE

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Mol	Chain	Res	Type
43	s	1135	GLU
43	s	1140	GLU
43	s	1418	GLN
43	s	1453	ASN
43	s	1466	ARG
43	s	1580	ARG
43	s	1742	HIS
43	s	1952	ASN
43	s	1953	GLN
43	s	2033	GLU
43	s	2058	SER
43	s	2150	GLU
43	s	2187	THR
43	s	2228	ASN
43	s	2248	GLN
43	s	2251	VAL
43	s	2287	LEU
43	s	2307	ILE
43	s	2335	PRO
43	s	2356	GLU
43	s	2361	GLU
43	s	2378	TRP
44	t	17	HIS
44	t	24	ASN
45	u	137	ILE
45	u	286	PHE
1	A	120	PRO
1	A	181	LYS
1	A	191	LEU
1	A	193	ARG
1	A	195	SER
2	B	68	HIS
2	B	255	TRP
2	B	257	PRO
2	B	311	PHE
2	B	347	SER
3	C	11	LEU
3	C	223	PRO
3	C	268	ALA
3	C	320	ASN
3	C	321	LYS
3	C	339	LEU

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Mol	Chain	Res	Type
4	D	151	GLN
5	E	37	GLY
5	E	98	VAL
6	F	98	LYS
6	F	193	PRO
6	F	226	GLY
8	H	50	ASN
9	I	18	LYS
9	I	74	VAL
9	I	136	THR
10	J	140	ARG
10	J	169	ALA
10	J	173	ASP
11	K	17	ALA
11	K	39	PRO
11	K	40	LYS
11	K	76	SER
11	K	89	PRO
12	L	61	PRO
12	L	62	THR
12	L	165	SER
12	L	166	ALA
14	N	80	THR
14	N	158	HIS
14	N	175	ASN
15	O	89	SER
16	P	41	LEU
16	P	96	GLN
16	P	133	HIS
17	Q	73	GLN
18	R	16	GLY
18	R	136	ARG
18	R	139	VAL
19	S	133	ALA
19	S	154	HIS
20	T	22	HIS
23	X	41	ALA
24	Y	5	SER
24	Y	89	LYS
25	Z	59	ALA
26	a	46	ASP
26	a	47	LYS

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Mol	Chain	Res	Type
26	a	52	TYR
26	a	58	MET
26	a	97	GLU
26	a	104	THR
26	a	132	LYS
28	d	6	ASP
28	d	61	LYS
29	e	12	LYS
30	f	20	LYS
30	f	91	ALA
31	g	48	GLY
31	g	60	ARG
31	g	78	GLY
33	i	16	LYS
34	j	10	LYS
34	j	39	TYR
34	j	72	ARG
34	j	77	GLY
35	k	18	ALA
36	l	36	ARG
38	n	50	THR
39	o	34	ARG
39	o	53	THR
39	o	91	TYR
39	o	96	ALA
39	o	150	LEU
39	o	199	PHE
39	o	244	ALA
40	p	23	ARG
40	p	24	ARG
41	q	89	SER
41	q	93	LYS
41	q	129	VAL
42	r	133	ASP
42	r	243	GLY
42	r	247	HIS
42	r	310	MET
42	r	314	ASP
42	r	316	ASP
42	r	388	GLY
42	r	408	PRO
42	r	637	ASP

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Mol	Chain	Res	Type
42	r	652	PRO
42	r	698	VAL
43	s	308	SER
43	s	362	PRO
43	s	459	GLU
43	s	763	GLU
43	s	785	ALA
43	s	851	SER
43	s	905	GLU
43	s	1064	LYS
43	s	1195	GLN
43	s	1234	GLU
43	s	1470	ASN
43	s	1513	GLU
43	s	1516	LEU
43	s	1524	SER
43	s	1725	ALA
43	s	1754	GLY
43	s	1822	ALA
43	s	1890	THR
43	s	1925	CYS
43	s	2031	PRO
43	s	2100	LEU
43	s	2170	PRO
43	s	2190	ALA
45	u	71	ASN
1	A	69	TYR
1	A	180	LEU
2	B	9	PRO
2	B	17	LEU
2	B	234	GLY
2	B	314	TYR
2	B	353	GLU
2	B	362	ALA
3	C	89	ALA
3	C	288	ARG
3	C	291	ASN
4	D	87	GLY
4	D	256	THR
4	D	258	LYS
5	E	75	PRO
6	F	76	TYR

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Mol	Chain	Res	Type
6	F	172	ASN
7	G	36	ILE
7	G	196	ALA
8	H	62	ARG
8	H	64	HIS
10	J	95	ASN
10	J	108	GLU
10	J	114	ILE
10	J	117	ASP
11	K	19	GLY
11	K	51	LYS
11	K	52	GLU
11	K	55	GLY
12	L	152	THR
13	M	9	ALA
14	N	95	GLN
17	Q	154	GLY
17	Q	166	LEU
19	S	32	SER
20	T	82	ASN
26	a	78	LEU
30	f	105	SER
31	g	73	SER
32	h	81	ARG
34	j	15	SER
37	m	31	SER
37	m	111	ASN
38	n	133	LEU
38	n	162	GLU
39	o	87	GLU
39	o	179	GLY
39	o	198	ALA
39	o	212	LYS
39	o	235	ILE
42	r	88	PRO
42	r	146	LEU
42	r	435	GLU
42	r	448	ARG
42	r	544	ALA
42	r	677	PHE
43	s	795	GLU
43	s	1181	GLU

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Mol	Chain	Res	Type
43	s	1390	LEU
43	s	1414	ARG
43	s	1485	ARG
43	s	1565	PRO
43	s	1785	PHE
43	s	1818	GLU
43	s	1951	LEU
43	s	1958	GLU
43	s	2059	ASN
43	s	2099	ASP
45	u	253	PRO
1	A	26	ALA
1	A	129	ALA
1	A	209	HIS
1	A	213	GLY
2	B	317	ILE
2	B	349	LYS
3	C	75	PRO
3	C	131	VAL
3	C	221	ASN
4	D	125	VAL
4	D	260	PHE
6	F	191	VAL
7	G	50	VAL
7	G	68	ARG
8	H	59	ASN
9	I	151	VAL
9	I	168	ALA
10	J	24	GLY
10	J	111	ASP
10	J	172	LEU
11	K	32	ILE
11	K	102	GLY
11	K	109	ILE
12	L	32	LYS
12	L	84	GLY
12	L	94	GLY
12	L	136	GLU
13	M	6	ILE
13	M	82	SER
13	M	90	VAL
14	N	49	ARG

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Mol	Chain	Res	Type
14	N	55	ALA
14	N	58	GLY
15	O	131	PRO
17	Q	9	GLN
17	Q	38	ARG
20	T	28	SER
20	T	127	GLN
21	U	11	ILE
21	U	38	ILE
23	X	23	ALA
24	Y	34	PRO
25	Z	32	GLY
25	Z	38	PHE
25	Z	97	SER
29	e	48	GLY
30	f	62	SER
32	h	79	ASP
33	i	3	VAL
36	l	5	LYS
37	m	112	ASP
38	n	130	LYS
40	p	7	LYS
41	q	249	PRO
42	r	87	LEU
42	r	241	SER
42	r	680	LEU
43	s	530	ASN
43	s	1177	PRO
43	s	1239	ALA
43	s	1303	THR
43	s	1448	LYS
43	s	1801	ASP
43	s	2082	MET
43	s	2201	LEU
43	s	2215	ASN
43	s	2221	PRO
43	s	2333	TYR
43	s	2349	ASP
43	s	2413	ILE
2	B	83	PRO
4	D	19	PRO
5	E	36	PRO

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Mol	Chain	Res	Type
7	G	157	VAL
9	I	104	SER
17	Q	175	ALA
19	S	132	THR
22	V	3	GLY
28	d	7	VAL
30	f	90	PRO
33	i	33	ALA
37	m	44	ASP
38	n	70	ARG
39	o	121	SER
39	o	140	VAL
43	s	593	PRO
43	s	602	ILE
43	s	646	THR
43	s	762	ASN
43	s	953	SER
43	s	1087	SER
43	s	1171	ASN
43	s	1450	ASP
43	s	2152	PHE
43	s	2219	CYS
43	s	2332	HIS
45	u	84	ASP
3	C	173	GLY
7	G	30	THR
25	Z	103	GLN
31	g	104	VAL
32	h	47	VAL
42	r	262	GLN
42	r	431	GLY
42	r	444	ILE
43	s	289	VAL
43	s	604	ILE
43	s	956	LYS
11	K	22	VAL
16	P	77	GLY
20	T	23	GLY
20	T	123	GLY
39	o	29	THR
43	s	2098	VAL
3	C	204	GLY

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Mol	Chain	Res	Type
3	C	245	GLY
3	C	348	GLY
4	D	181	PRO
24	Y	96	PRO
26	a	57	GLY
43	s	1187	PRO
43	s	1628	VAL
43	s	2340	ARG
1	A	178	PRO
24	Y	123	GLY
26	a	72	VAL
33	i	7	ILE
37	m	105	GLY
37	m	148	VAL
42	r	411	ILE
43	s	2367	ILE
2	B	268	GLY
4	D	139	PRO
7	G	75	ILE
9	I	125	GLY
14	N	154	PRO
22	V	107	GLY
26	a	110	GLY
43	s	1006	LYS
43	s	2256	PRO
43	s	2357	GLU

5.3.2 Protein sidechains

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

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	x	2778/2779 (99%)	291 (10%)	0
47	y	157/158 (99%)	20 (12%)	0
48	z	120/121 (99%)	7 (5%)	0
All	All	3055/3058 (99%)	318 (10%)	0

All (318) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	x	22	G
46	x	49	A
46	x	60	A
46	x	66	A
46	x	92	G
46	x	110	G
46	x	113	C
46	x	121	A
46	x	122	A
46	x	123	A
46	x	135	C
46	x	136	G
46	x	156	G
46	x	191	U
46	x	200	C
46	x	210	U
46	x	218	G
46	x	219	A
46	x	240	U
46	x	252	U
46	x	269	G
46	x	295	A
46	x	298	U
46	x	316	U
46	x	323	A
46	x	329	U
46	x	336	A
46	x	337	G
46	x	339	C
46	x	346	C
46	x	376	G
46	x	398	A
46	x	401	U
46	x	402	A
46	x	403	C
46	x	421	G
46	x	422	A
46	x	486	U
46	x	492	U
46	x	521	A
46	x	534	U
46	x	535	G
46	x	546	C

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Mol	Chain	Res	Type
46	x	547	G
46	x	548	G
46	x	552	G
46	x	557	A
46	x	559	A
46	x	579	G
46	x	604	G
46	x	609	G
46	x	611	A
46	x	612	U
46	x	621	A
46	x	638	C
46	x	646	A
46	x	647	A
46	x	649	A
46	x	677	A
46	x	681	U
46	x	705	A
46	x	764	U
46	x	765	C
46	x	767	U
46	x	776	U
46	x	777	U
46	x	780	A
46	x	781	G
46	x	806	A
46	x	817	A
46	x	830	A
46	x	849	C
46	x	874	U
46	x	880	G
46	x	881	C
46	x	907	G
46	x	914	A
46	x	916	G
46	x	917	A
46	x	924	G
46	x	937	G
46	x	944	C
46	x	959	C
46	x	979	U
46	x	980	A

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Mol	Chain	Res	Type
46	x	982	C
46	x	989	A
46	x	995	U
46	x	1001	G
46	x	1006	A
46	x	1007	U
46	x	1028	U
46	x	1045	C
46	x	1046	A
46	x	1049	C
46	x	1063	G
46	x	1065	A
46	x	1072	G
46	x	1081	U
46	x	1095	U
46	x	1098	A
46	x	1103	A
46	x	1104	G
46	x	1116	G
46	x	1117	G
46	x	1139	G
46	x	1159	A
46	x	1160	C
46	x	1180	A
46	x	1181	U
46	x	1192	C
46	x	1200	A
46	x	1201	C
46	x	1202	A
46	x	1222	G
46	x	1236	G
46	x	1242	G
46	x	1244	A
46	x	1245	A
46	x	1246	G
46	x	1254	C
46	x	1263	A
46	x	1264	G
46	x	1274	A
46	x	1278	A
46	x	1279	C
46	x	1287	A

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Mol	Chain	Res	Type
46	x	1289	G
46	x	1295	G
46	x	1302	A
46	x	1305	U
46	x	1308	A
46	x	1309	U
46	x	1330	A
46	x	1351	U
46	x	1352	A
46	x	1354	G
46	x	1355	A
46	x	1357	G
46	x	1367	G
46	x	1386	A
46	x	1390	A
46	x	1399	A
46	x	1400	G
46	x	1419	A
46	x	1437	C
46	x	1446	A
46	x	1481	A
46	x	1508	C
46	x	1511	U
46	x	1563	C
46	x	1568	U
46	x	1570	U
46	x	1571	A
46	x	1572	U
46	x	1583	A
46	x	1589	A
46	x	1607	U
46	x	1629	U
46	x	1643	A
46	x	1645	U
46	x	1657	C
46	x	1717	U
46	x	1728	G
46	x	1750	A
46	x	1751	G
46	x	1760	A
46	x	1765	U
46	x	1780	G

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Mol	Chain	Res	Type
46	x	1797	A
46	x	1816	A
46	x	1819	U
46	x	1821	U
46	x	1841	A
46	x	1842	A
46	x	1880	U
46	x	1893	A
46	x	1906	G
46	x	1953	G
46	x	1966	U
46	x	1973	G
46	x	2010	U
46	x	2011	U
46	x	2013	C
46	x	2032	U
46	x	2042	G
46	x	2056	U
46	x	2061	G
46	x	2067	U
46	x	2071	A
46	x	2076	G
46	x	2080	C
46	x	2087	C
46	x	2089	A
46	x	2094	C
46	x	2102	U
46	x	2113	A
46	x	2121	G
46	x	2122	G
46	x	2131	A
46	x	2158	A
46	x	2170	U
46	x	2179	C
46	x	2188	A
46	x	2205	U
46	x	2228	A
46	x	2244	A
46	x	2249	G
46	x	2255	A
46	x	2260	U
46	x	2273	G

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Mol	Chain	Res	Type
46	x	2275	A
46	x	2279	A
46	x	2281	A
46	x	2298	U
46	x	2307	G
46	x	2363	A
46	x	2374	C
46	x	2388	U
46	x	2397	A
46	x	2411	U
46	x	2418	G
46	x	2440	G
46	x	2446	U
46	x	2451	G
46	x	2453	U
46	x	2463	G
46	x	2469	G
46	x	2472	U
46	x	2477	G
46	x	2478	C
46	x	2479	C
46	x	2484	A
46	x	2490	C
46	x	2493	U
46	x	2494	A
46	x	2495	C
46	x	2496	C
46	x	2501	U
46	x	2502	A
46	x	2505	U
46	x	2508	U
46	x	2510	U
46	x	2514	U
46	x	2519	A
46	x	2523	A
46	x	2524	A
46	x	2526	C
46	x	2531	C
46	x	2538	U
46	x	2540	A
46	x	2541	U
46	x	2542	U

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Mol	Chain	Res	Type
46	x	2547	A
46	x	2548	C
46	x	2549	G
46	x	2552	C
46	x	2569	A
46	x	2570	U
46	x	2571	U
46	x	2572	C
46	x	2573	G
46	x	2590	A
46	x	2593	A
46	x	2601	A
46	x	2606	G
46	x	2614	G
46	x	2619	G
46	x	2621	G
46	x	2622	C
46	x	2627	C
46	x	2630	C
46	x	2636	A
46	x	2652	U
46	x	2656	A
46	x	2674	A
46	x	2677	G
46	x	2689	A
46	x	2691	A
46	x	2694	A
46	x	2696	A
46	x	2700	G
46	x	2714	G
46	x	2728	G
46	x	2729	U
46	x	2753	G
46	x	2760	C
46	x	2762	A
46	x	2772	C
46	x	2777	G
46	x	2778	G
47	y	17	A
47	y	34	U
47	y	35	C
47	y	37	A

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Mol	Chain	Res	Type
47	y	39	G
47	y	52	A
47	y	59	A
47	y	62	C
47	y	63	G
47	y	72	A
47	y	80	A
47	y	86	U
47	y	90	U
47	y	95	G
47	y	104	A
47	y	106	C
47	y	111	A
47	y	113	U
47	y	125	U
47	y	126	A
48	z	13	A
48	z	53	U
48	z	54	U
48	z	65	G
48	z	87	G
48	z	102	A
48	z	112	G

There are no RNA pucker outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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
42	r	14
46	x	1
43	s	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	576:GLY	C	629:GLU	N	23.87
1	r	472:VAL	C	476:GLU	N	19.67
1	r	121:MET	C	126:LEU	N	18.70
1	r	228:GLY	C	240:ASN	N	15.12
1	r	436:VAL	C	440:ALA	N	14.62
1	r	454:ALA	C	460:PRO	N	13.67
1	r	681:GLN	C	691:GLU	N	13.49
1	r	298:VAL	C	303:LYS	N	11.43
1	r	212:PRO	C	220:LEU	N	11.31
1	r	412:ASN	C	418:VAL	N	10.41
1	r	560:GLY	C	562:ILE	N	10.16
1	r	492:LEU	C	511:ILE	N	9.62
1	r	139:ASN	C	145:GLY	N	9.34
1	r	263:PRO	C	276:ASP	N	5.99
1	x	2699:G	O3'	2700:G	P	2.11
1	s	825:TRP	C	826:LEU	N	0.91