



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2020 – 10:01 AM BST

PDB ID : 5VYC
Title : Crystal structure of the human 40S ribosomal subunit in complex with DENR-MCT-1.
Authors : Lomakin, I.B.; Stolboushkina, E.A.; Vaidya, A.T.; Garber, M.B.; Dmitriev, S.E.; Steitz, T.A.
Deposited on : 2017-05-24
Resolution : 6.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

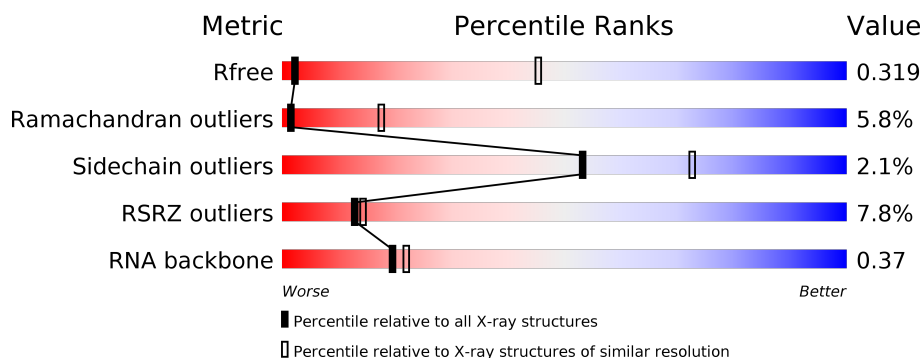
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 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.





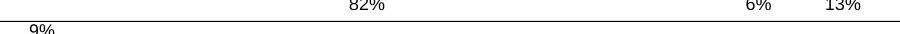


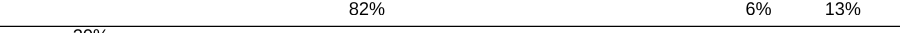

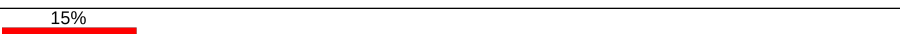


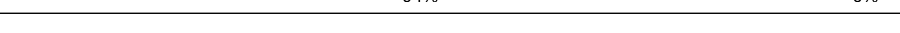
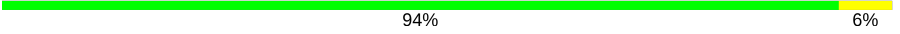

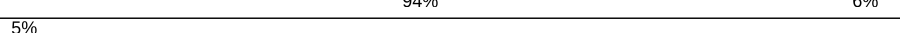


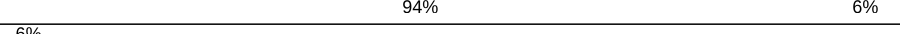




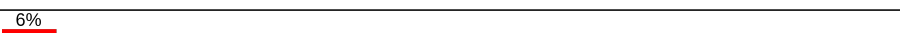



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1000 (8.00-3.88)
Ramachandran outliers	138981	1016 (8.00-3.86)
Sidechain outliers	138945	1017 (8.00-3.82)
RSRZ outliers	127900	1015 (8.20-3.78)
RNA backbone	3102	1076 (8.70-3.00)

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

Mol	Chain	Length	Quality of chain
1	T1	145	<div> <div>3%</div> <div>94%</div> <div>5%</div> </div>
1	T2	145	<div> <div>%</div> <div>94%</div> <div>5%</div> </div>
1	T3	145	<div> <div>%</div> <div>93%</div> <div>6%</div> </div>
1	T4	145	<div> <div>6%</div> <div>94%</div> <div>5%</div> </div>
1	T5	145	<div> <div>3%</div> <div>94%</div> <div>5%</div> </div>
1	T6	145	<div> <div>2%</div> <div>94%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
2	U1	119	
2	U2	119	
2	U3	119	
2	U4	119	
2	U5	119	
2	U6	119	
3	V1	83	
3	V2	83	
3	V3	83	
3	V4	83	
3	V5	83	
3	V6	83	
4	X1	143	
4	X2	143	
4	X3	143	
4	X4	143	
4	X5	143	
4	X6	143	
5	a1	115	
5	a2	115	
5	a3	115	
5	a4	115	
5	a5	115	
5	a6	115	
6	c1	69	

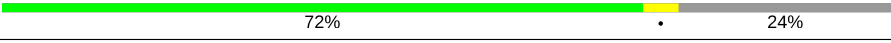















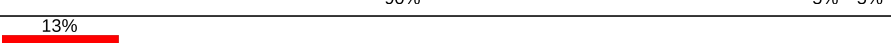
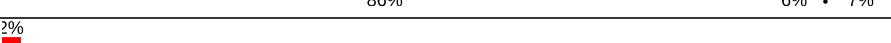
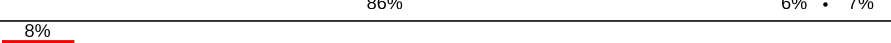

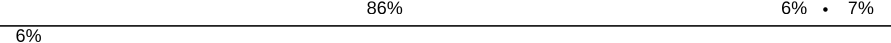
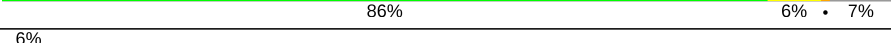



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Mol	Chain	Length	Quality of chain
6	c2	69	
6	c3	69	
6	c4	69	
6	c5	69	
6	c6	69	
7	d1	56	
7	d2	56	
7	d3	56	
7	d4	56	
7	d5	56	
7	d6	56	
8	f1	156	
8	f2	156	
8	f3	156	
8	f4	156	
8	f5	156	
8	f6	156	
9	g1	317	
9	g2	317	
9	g3	317	
9	g4	317	
9	g5	317	
9	g6	317	
10	C1	293	
10	C2	293	

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Mol	Chain	Length	Quality of chain
10	C3	293	
10	C4	293	
10	C5	293	
10	C6	293	
11	G1	249	
11	G2	249	
11	G3	249	
11	G4	249	
11	G5	249	
11	G6	249	
12	J1	194	
12	J2	194	
12	J3	194	
12	J4	194	
12	J5	194	
12	J6	194	
13	M1	132	
13	M2	132	
13	M3	132	
13	M4	132	
13	M5	132	
13	M6	132	
14	N1	151	
14	N2	151	
14	N3	151	

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Mol	Chain	Length	Quality of chain
14	N4	151	
14	N5	151	
14	N6	151	
15	O1	151	
15	O2	151	
15	O3	151	
15	O4	151	
15	O5	151	
15	O6	151	
16	W1	130	
16	W2	130	
16	W3	130	
16	W4	130	
16	W5	130	
16	W6	130	
17	Y1	133	
17	Y2	133	
17	Y3	133	
17	Y4	133	
17	Y5	133	
17	Y6	133	
18	Z1	125	
18	Z2	125	
18	Z3	125	
18	Z4	125	

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Mol	Chain	Length	Quality of chain
18	Z5	125	
18	Z6	125	
19	b1	84	
19	b2	84	
19	b3	84	
19	b4	84	
19	b5	84	
19	b6	84	
20	e1	133	
20	e2	133	
20	e3	133	
20	e4	133	
20	e5	133	
20	e6	133	
21	i1	1869	
21	i2	1869	
21	i3	1869	
21	i4	1869	
21	i5	1869	
21	i6	1869	
22	A1	295	
22	A2	295	
22	A3	295	
22	A4	295	
22	A5	295	

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Mol	Chain	Length	Quality of chain
22	A6	295	
23	B1	264	
23	B2	264	
23	B3	264	
23	B4	264	
23	B5	264	
23	B6	264	
24	D1	243	
24	D2	243	
24	D3	243	
24	D4	243	
24	D5	243	
24	D6	243	
25	E1	263	
25	E2	263	
25	E3	263	
25	E4	263	
25	E5	263	
25	E6	263	
26	F1	204	
26	F2	204	
26	F3	204	
26	F4	204	
26	F5	204	
26	F6	204	

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Mol	Chain	Length	Quality of chain
27	H1	194	
27	H2	194	
27	H3	194	
27	H4	194	
27	H5	194	
27	H6	194	
28	I1	208	
28	I2	208	
28	I3	208	
28	I4	208	
28	I5	208	
28	I6	208	
29	K1	165	
29	K2	165	
29	K3	165	
29	K4	165	
29	K5	165	
29	K6	165	
30	L1	158	
30	L2	158	
30	L3	158	
30	L4	158	
30	L5	158	
30	L6	158	
31	P1	145	





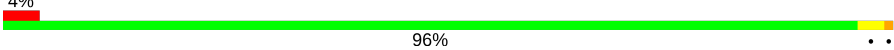


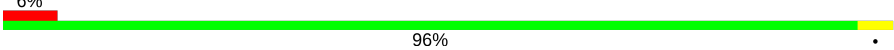
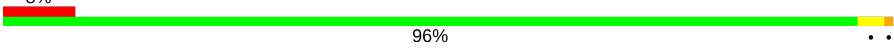
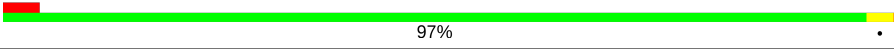





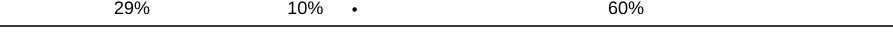
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Mol	Chain	Length	Quality of chain
31	P2	145	
31	P3	145	
31	P4	145	
31	P5	145	
31	P6	145	
32	Q1	146	
32	Q2	146	
32	Q3	146	
32	Q4	146	
32	Q5	146	
32	Q6	146	
33	R1	135	
33	R2	135	
33	R3	135	
33	R4	135	
33	R5	135	
33	R6	135	
34	S1	152	
34	S2	152	
34	S3	152	
34	S4	152	
34	S5	152	
34	S6	152	
35	j1	25	
35	j2	25	

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Mol	Chain	Length	Quality of chain
35	j3	25	
35	j4	25	
35	j5	25	
35	j6	25	
36	k1	181	
36	k2	181	
36	k3	181	
36	k4	181	
36	k5	181	
36	k6	181	
37	l1	198	
37	l2	198	
37	l3	198	
37	l4	198	
37	l5	198	
37	l6	198	

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 470574 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T1	143	Total	C	N	O	S	0	0	0
			1112	697	214	198	3			
1	T2	143	Total	C	N	O	S	0	0	0
			1112	697	214	198	3			
1	T3	143	Total	C	N	O	S	0	0	0
			1112	697	214	198	3			
1	T4	143	Total	C	N	O	S	0	0	0
			1112	697	214	198	3			
1	T5	143	Total	C	N	O	S	0	0	0
			1112	697	214	198	3			
1	T6	143	Total	C	N	O	S	0	0	0
			1112	697	214	198	3			

- Molecule 2 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U1	104	Total	C	N	O	S	0	0	0
			821	514	155	148	4			
2	U2	104	Total	C	N	O	S	0	0	0
			821	514	155	148	4			
2	U3	104	Total	C	N	O	S	0	0	0
			821	514	155	148	4			
2	U4	104	Total	C	N	O	S	0	0	0
			821	514	155	148	4			
2	U5	104	Total	C	N	O	S	0	0	0
			821	514	155	148	4			
2	U6	104	Total	C	N	O	S	0	0	0
			821	514	155	148	4			

- Molecule 3 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V1	83	Total	C	N	O	S	0	0	0
			636	393	117	121	5			
3	V2	83	Total	C	N	O	S	0	0	0
			636	393	117	121	5			
3	V3	83	Total	C	N	O	S	0	0	0
			636	393	117	121	5			
3	V4	83	Total	C	N	O	S	0	0	0
			636	393	117	121	5			
3	V5	83	Total	C	N	O	S	0	0	0
			636	393	117	121	5			
3	V6	83	Total	C	N	O	S	0	0	0
			636	393	117	121	5			

- Molecule 4 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X1	141	Total	C	N	O	S	0	0	0
			1098	693	219	183	3			
4	X2	141	Total	C	N	O	S	0	0	0
			1098	693	219	183	3			
4	X3	141	Total	C	N	O	S	0	0	0
			1098	693	219	183	3			
4	X4	141	Total	C	N	O	S	0	0	0
			1098	693	219	183	3			
4	X5	141	Total	C	N	O	S	0	0	0
			1098	693	219	183	3			
4	X6	141	Total	C	N	O	S	0	0	0
			1098	693	219	183	3			

- Molecule 5 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	a1	107	Total	C	N	O	S	0	0	0
			847	528	176	138	5			
5	a2	107	Total	C	N	O	S	0	0	0
			847	528	176	138	5			
5	a3	107	Total	C	N	O	S	0	0	0
			847	528	176	138	5			
5	a4	107	Total	C	N	O	S	0	0	0
			847	528	176	138	5			
5	a5	107	Total	C	N	O	S	0	0	0
			847	528	176	138	5			
5	a6	107	Total	C	N	O	S	0	0	0
			847	528	176	138	5			

- Molecule 6 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	c1	64	Total	C	N	O	S	0	0	0
			506	308	102	94	2			
6	c2	64	Total	C	N	O	S	0	0	0
			506	308	102	94	2			
6	c3	64	Total	C	N	O	S	0	0	0
			506	308	102	94	2			
6	c4	64	Total	C	N	O	S	0	0	0
			506	308	102	94	2			
6	c5	64	Total	C	N	O	S	0	0	0
			506	308	102	94	2			
6	c6	64	Total	C	N	O	S	0	0	0
			506	308	102	94	2			

- Molecule 7 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	d1	53	Total	C	N	O	S	0	0	0
			445	278	90	72	5			
7	d2	53	Total	C	N	O	S	0	0	0
			445	278	90	72	5			
7	d3	53	Total	C	N	O	S	0	0	0
			445	278	90	72	5			
7	d4	53	Total	C	N	O	S	0	0	0
			445	278	90	72	5			
7	d5	53	Total	C	N	O	S	0	0	0
			445	278	90	72	5			
7	d6	53	Total	C	N	O	S	0	0	0
			445	278	90	72	5			

- Molecule 8 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	f1	72	Total	C	N	O	S	0	0	0
			585	366	114	97	8			
8	f2	72	Total	C	N	O	S	0	0	0
			585	366	114	97	8			
8	f3	72	Total	C	N	O	S	0	0	0
			585	366	114	97	8			
8	f4	72	Total	C	N	O	S	0	0	0
			585	366	114	97	8			
8	f5	72	Total	C	N	O	S	0	0	0
			585	366	114	97	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	f6	72	Total	C	N	O	S	0	0	0
			585	366	114	97	8			

- Molecule 9 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	g1	313	Total	C	N	O	S	0	0	0
			2436	1535	424	465	12			
9	g2	313	Total	C	N	O	S	0	0	0
			2436	1535	424	465	12			
9	g3	313	Total	C	N	O	S	0	0	0
			2436	1535	424	465	12			
9	g4	313	Total	C	N	O	S	0	0	0
			2436	1535	424	465	12			
9	g5	313	Total	C	N	O	S	0	0	0
			2436	1535	424	465	12			
9	g6	313	Total	C	N	O	S	0	0	0
			2436	1535	424	465	12			

- Molecule 10 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	C1	222	Total	C	N	O	S	0	0	0
			1725	1115	298	302	10			
10	C2	222	Total	C	N	O	S	0	0	0
			1725	1115	298	302	10			
10	C3	222	Total	C	N	O	S	0	0	0
			1725	1115	298	302	10			
10	C4	222	Total	C	N	O	S	0	0	0
			1725	1115	298	302	10			
10	C5	222	Total	C	N	O	S	0	0	0
			1725	1115	298	302	10			
10	C6	222	Total	C	N	O	S	0	0	0
			1725	1115	298	302	10			

- Molecule 11 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G1	237	Total	C	N	O	S	0	0	0
			1923	1200	387	329	7			
11	G2	237	Total	C	N	O	S	0	0	0
			1923	1200	387	329	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G3	237	Total	C	N	O	S	0	0	0
			1923	1200	387	329	7			
11	G4	237	Total	C	N	O	S	0	0	0
			1923	1200	387	329	7			
11	G5	237	Total	C	N	O	S	0	0	0
			1923	1200	387	329	7			
11	G6	237	Total	C	N	O	S	0	0	0
			1923	1200	387	329	7			

- Molecule 12 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J1	185	Total	C	N	O	S	0	0	0
			1525	969	306	248	2			
12	J2	185	Total	C	N	O	S	0	0	0
			1525	969	306	248	2			
12	J3	185	Total	C	N	O	S	0	0	0
			1525	969	306	248	2			
12	J4	185	Total	C	N	O	S	0	0	0
			1525	969	306	248	2			
12	J5	185	Total	C	N	O	S	0	0	0
			1525	969	306	248	2			
12	J6	185	Total	C	N	O	S	0	0	0
			1525	969	306	248	2			

- Molecule 13 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M1	123	Total	C	N	O	S	0	0	0
			953	598	169	177	9			
13	M2	123	Total	C	N	O	S	0	0	0
			953	598	169	177	9			
13	M3	123	Total	C	N	O	S	0	0	0
			953	598	169	177	9			
13	M4	123	Total	C	N	O	S	0	0	0
			953	598	169	177	9			
13	M5	123	Total	C	N	O	S	0	0	0
			953	598	169	177	9			
13	M6	123	Total	C	N	O	S	0	0	0
			953	598	169	177	9			

- Molecule 14 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N1	150	Total	C	N	O	S	0	0	0
			1208	773	229	205	1			
14	N2	150	Total	C	N	O	S	0	0	0
			1208	773	229	205	1			
14	N3	150	Total	C	N	O	S	0	0	0
			1208	773	229	205	1			
14	N4	150	Total	C	N	O	S	0	0	0
			1208	773	229	205	1			
14	N5	150	Total	C	N	O	S	0	0	0
			1208	773	229	205	1			
14	N6	150	Total	C	N	O	S	0	0	0
			1208	773	229	205	1			

- Molecule 15 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O1	140	Total	C	N	O	S	0	0	0
			1049	642	204	197	6			
15	O2	140	Total	C	N	O	S	0	0	0
			1049	642	204	197	6			
15	O3	140	Total	C	N	O	S	0	0	0
			1049	642	204	197	6			
15	O4	140	Total	C	N	O	S	0	0	0
			1049	642	204	197	6			
15	O5	140	Total	C	N	O	S	0	0	0
			1049	642	204	197	6			
15	O6	140	Total	C	N	O	S	0	0	0
			1049	642	204	197	6			

- Molecule 16 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	W1	129	Total	C	N	O	S	0	0	0
			1034	659	193	176	6			
16	W2	129	Total	C	N	O	S	0	0	0
			1034	659	193	176	6			
16	W3	129	Total	C	N	O	S	0	0	0
			1034	659	193	176	6			
16	W4	129	Total	C	N	O	S	0	0	0
			1034	659	193	176	6			
16	W5	129	Total	C	N	O	S	0	0	0
			1034	659	193	176	6			
16	W6	129	Total	C	N	O	S	0	0	0
			1034	659	193	176	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y1	131	Total	C	N	O	S	0	0	0
			1065	673	209	178	5			
17	Y2	131	Total	C	N	O	S	0	0	0
			1065	673	209	178	5			
17	Y3	131	Total	C	N	O	S	0	0	0
			1065	673	209	178	5			
17	Y4	131	Total	C	N	O	S	0	0	0
			1065	673	209	178	5			
17	Y5	131	Total	C	N	O	S	0	0	0
			1065	673	209	178	5			
17	Y6	131	Total	C	N	O	S	0	0	0
			1065	673	209	178	5			

- Molecule 18 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z1	75	Total	C	N	O	S	0	0	0
			598	382	111	104	1			
18	Z2	75	Total	C	N	O	S	0	0	0
			598	382	111	104	1			
18	Z3	75	Total	C	N	O	S	0	0	0
			598	382	111	104	1			
18	Z4	75	Total	C	N	O	S	0	0	0
			598	382	111	104	1			
18	Z5	75	Total	C	N	O	S	0	0	0
			598	382	111	104	1			
18	Z6	75	Total	C	N	O	S	0	0	0
			598	382	111	104	1			

- Molecule 19 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	b1	83	Total	C	N	O	S	0	0	0
			651	408	121	115	7			
19	b2	83	Total	C	N	O	S	0	0	0
			651	408	121	115	7			
19	b3	83	Total	C	N	O	S	0	0	0
			651	408	121	115	7			
19	b4	83	Total	C	N	O	S	0	0	0
			651	408	121	115	7			
19	b5	83	Total	C	N	O	S	0	0	0
			651	408	121	115	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	b6	83	Total	C	N	O	S	0	0	0
			651	408	121	115	7			

- Molecule 20 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	e1	58	Total	C	N	O	S	0	0	0
			459	284	100	74	1			
20	e2	58	Total	C	N	O	S	0	0	0
			459	284	100	74	1			
20	e3	58	Total	C	N	O	S	0	0	0
			459	284	100	74	1			
20	e4	58	Total	C	N	O	S	0	0	0
			459	284	100	74	1			
20	e5	58	Total	C	N	O	S	0	0	0
			459	284	100	74	1			
20	e6	58	Total	C	N	O	S	0	0	0
			459	284	100	74	1			

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e1	-48	ALA	-	insertion	UNP E9PR30
e1	-47	HIS	-	insertion	UNP E9PR30
e1	-46	VAL	-	insertion	UNP E9PR30
e1	-45	ALA	-	insertion	UNP E9PR30
e1	-44	SER	-	insertion	UNP E9PR30
e1	-43	LEU	-	insertion	UNP E9PR30
e1	-42	GLU	-	insertion	UNP E9PR30
e1	-41	GLY	-	insertion	UNP E9PR30
e1	-40	ILE	-	insertion	UNP E9PR30
e1	-39	ALA	-	insertion	UNP E9PR30
e1	-38	PRO	-	insertion	UNP E9PR30
e1	-37	GLU	-	insertion	UNP E9PR30
e1	-36	ASP	-	insertion	UNP E9PR30
e1	-35	GLN	-	insertion	UNP E9PR30
e1	-34	VAL	-	insertion	UNP E9PR30
e1	-33	VAL	-	insertion	UNP E9PR30
e1	-32	LEU	-	insertion	UNP E9PR30
e1	-31	LEU	-	insertion	UNP E9PR30
e1	-30	ALA	-	insertion	UNP E9PR30
e1	-29	GLY	-	insertion	UNP E9PR30

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Chain	Residue	Modelled	Actual	Comment	Reference
e1	-28	ALA	-	insertion	UNP E9PR30
e1	-27	PRO	-	insertion	UNP E9PR30
e1	-26	LEU	-	insertion	UNP E9PR30
e1	-25	GLU	-	insertion	UNP E9PR30
e1	-24	ASP	-	insertion	UNP E9PR30
e1	-23	GLU	-	insertion	UNP E9PR30
e1	-22	ALA	-	insertion	UNP E9PR30
e1	-21	THR	-	insertion	UNP E9PR30
e1	-20	LEU	-	insertion	UNP E9PR30
e1	-19	GLY	-	insertion	UNP E9PR30
e1	-18	GLN	-	insertion	UNP E9PR30
e1	-17	CYS	-	insertion	UNP E9PR30
e1	-16	GLY	-	insertion	UNP E9PR30
e1	-15	VAL	-	insertion	UNP E9PR30
e1	-14	GLU	-	insertion	UNP E9PR30
e2	-48	ALA	-	insertion	UNP E9PR30
e2	-47	HIS	-	insertion	UNP E9PR30
e2	-46	VAL	-	insertion	UNP E9PR30
e2	-45	ALA	-	insertion	UNP E9PR30
e2	-44	SER	-	insertion	UNP E9PR30
e2	-43	LEU	-	insertion	UNP E9PR30
e2	-42	GLU	-	insertion	UNP E9PR30
e2	-41	GLY	-	insertion	UNP E9PR30
e2	-40	ILE	-	insertion	UNP E9PR30
e2	-39	ALA	-	insertion	UNP E9PR30
e2	-38	PRO	-	insertion	UNP E9PR30
e2	-37	GLU	-	insertion	UNP E9PR30
e2	-36	ASP	-	insertion	UNP E9PR30
e2	-35	GLN	-	insertion	UNP E9PR30
e2	-34	VAL	-	insertion	UNP E9PR30
e2	-33	VAL	-	insertion	UNP E9PR30
e2	-32	LEU	-	insertion	UNP E9PR30
e2	-31	LEU	-	insertion	UNP E9PR30
e2	-30	ALA	-	insertion	UNP E9PR30
e2	-29	GLY	-	insertion	UNP E9PR30
e2	-28	ALA	-	insertion	UNP E9PR30
e2	-27	PRO	-	insertion	UNP E9PR30
e2	-26	LEU	-	insertion	UNP E9PR30
e2	-25	GLU	-	insertion	UNP E9PR30
e2	-24	ASP	-	insertion	UNP E9PR30
e2	-23	GLU	-	insertion	UNP E9PR30
e2	-22	ALA	-	insertion	UNP E9PR30

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Chain	Residue	Modelled	Actual	Comment	Reference
e2	-21	THR	-	insertion	UNP E9PR30
e2	-20	LEU	-	insertion	UNP E9PR30
e2	-19	GLY	-	insertion	UNP E9PR30
e2	-18	GLN	-	insertion	UNP E9PR30
e2	-17	CYS	-	insertion	UNP E9PR30
e2	-16	GLY	-	insertion	UNP E9PR30
e2	-15	VAL	-	insertion	UNP E9PR30
e2	-14	GLU	-	insertion	UNP E9PR30
e3	-48	ALA	-	insertion	UNP E9PR30
e3	-47	HIS	-	insertion	UNP E9PR30
e3	-46	VAL	-	insertion	UNP E9PR30
e3	-45	ALA	-	insertion	UNP E9PR30
e3	-44	SER	-	insertion	UNP E9PR30
e3	-43	LEU	-	insertion	UNP E9PR30
e3	-42	GLU	-	insertion	UNP E9PR30
e3	-41	GLY	-	insertion	UNP E9PR30
e3	-40	ILE	-	insertion	UNP E9PR30
e3	-39	ALA	-	insertion	UNP E9PR30
e3	-38	PRO	-	insertion	UNP E9PR30
e3	-37	GLU	-	insertion	UNP E9PR30
e3	-36	ASP	-	insertion	UNP E9PR30
e3	-35	GLN	-	insertion	UNP E9PR30
e3	-34	VAL	-	insertion	UNP E9PR30
e3	-33	VAL	-	insertion	UNP E9PR30
e3	-32	LEU	-	insertion	UNP E9PR30
e3	-31	LEU	-	insertion	UNP E9PR30
e3	-30	ALA	-	insertion	UNP E9PR30
e3	-29	GLY	-	insertion	UNP E9PR30
e3	-28	ALA	-	insertion	UNP E9PR30
e3	-27	PRO	-	insertion	UNP E9PR30
e3	-26	LEU	-	insertion	UNP E9PR30
e3	-25	GLU	-	insertion	UNP E9PR30
e3	-24	ASP	-	insertion	UNP E9PR30
e3	-23	GLU	-	insertion	UNP E9PR30
e3	-22	ALA	-	insertion	UNP E9PR30
e3	-21	THR	-	insertion	UNP E9PR30
e3	-20	LEU	-	insertion	UNP E9PR30
e3	-19	GLY	-	insertion	UNP E9PR30
e3	-18	GLN	-	insertion	UNP E9PR30
e3	-17	CYS	-	insertion	UNP E9PR30
e3	-16	GLY	-	insertion	UNP E9PR30
e3	-15	VAL	-	insertion	UNP E9PR30

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Chain	Residue	Modelled	Actual	Comment	Reference
e3	-14	GLU	-	insertion	UNP E9PR30
e4	-48	ALA	-	insertion	UNP E9PR30
e4	-47	HIS	-	insertion	UNP E9PR30
e4	-46	VAL	-	insertion	UNP E9PR30
e4	-45	ALA	-	insertion	UNP E9PR30
e4	-44	SER	-	insertion	UNP E9PR30
e4	-43	LEU	-	insertion	UNP E9PR30
e4	-42	GLU	-	insertion	UNP E9PR30
e4	-41	GLY	-	insertion	UNP E9PR30
e4	-40	ILE	-	insertion	UNP E9PR30
e4	-39	ALA	-	insertion	UNP E9PR30
e4	-38	PRO	-	insertion	UNP E9PR30
e4	-37	GLU	-	insertion	UNP E9PR30
e4	-36	ASP	-	insertion	UNP E9PR30
e4	-35	GLN	-	insertion	UNP E9PR30
e4	-34	VAL	-	insertion	UNP E9PR30
e4	-33	VAL	-	insertion	UNP E9PR30
e4	-32	LEU	-	insertion	UNP E9PR30
e4	-31	LEU	-	insertion	UNP E9PR30
e4	-30	ALA	-	insertion	UNP E9PR30
e4	-29	GLY	-	insertion	UNP E9PR30
e4	-28	ALA	-	insertion	UNP E9PR30
e4	-27	PRO	-	insertion	UNP E9PR30
e4	-26	LEU	-	insertion	UNP E9PR30
e4	-25	GLU	-	insertion	UNP E9PR30
e4	-24	ASP	-	insertion	UNP E9PR30
e4	-23	GLU	-	insertion	UNP E9PR30
e4	-22	ALA	-	insertion	UNP E9PR30
e4	-21	THR	-	insertion	UNP E9PR30
e4	-20	LEU	-	insertion	UNP E9PR30
e4	-19	GLY	-	insertion	UNP E9PR30
e4	-18	GLN	-	insertion	UNP E9PR30
e4	-17	CYS	-	insertion	UNP E9PR30
e4	-16	GLY	-	insertion	UNP E9PR30
e4	-15	VAL	-	insertion	UNP E9PR30
e4	-14	GLU	-	insertion	UNP E9PR30
e5	-48	ALA	-	insertion	UNP E9PR30
e5	-47	HIS	-	insertion	UNP E9PR30
e5	-46	VAL	-	insertion	UNP E9PR30
e5	-45	ALA	-	insertion	UNP E9PR30
e5	-44	SER	-	insertion	UNP E9PR30
e5	-43	LEU	-	insertion	UNP E9PR30

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Chain	Residue	Modelled	Actual	Comment	Reference
e5	-42	GLU	-	insertion	UNP E9PR30
e5	-41	GLY	-	insertion	UNP E9PR30
e5	-40	ILE	-	insertion	UNP E9PR30
e5	-39	ALA	-	insertion	UNP E9PR30
e5	-38	PRO	-	insertion	UNP E9PR30
e5	-37	GLU	-	insertion	UNP E9PR30
e5	-36	ASP	-	insertion	UNP E9PR30
e5	-35	GLN	-	insertion	UNP E9PR30
e5	-34	VAL	-	insertion	UNP E9PR30
e5	-33	VAL	-	insertion	UNP E9PR30
e5	-32	LEU	-	insertion	UNP E9PR30
e5	-31	LEU	-	insertion	UNP E9PR30
e5	-30	ALA	-	insertion	UNP E9PR30
e5	-29	GLY	-	insertion	UNP E9PR30
e5	-28	ALA	-	insertion	UNP E9PR30
e5	-27	PRO	-	insertion	UNP E9PR30
e5	-26	LEU	-	insertion	UNP E9PR30
e5	-25	GLU	-	insertion	UNP E9PR30
e5	-24	ASP	-	insertion	UNP E9PR30
e5	-23	GLU	-	insertion	UNP E9PR30
e5	-22	ALA	-	insertion	UNP E9PR30
e5	-21	THR	-	insertion	UNP E9PR30
e5	-20	LEU	-	insertion	UNP E9PR30
e5	-19	GLY	-	insertion	UNP E9PR30
e5	-18	GLN	-	insertion	UNP E9PR30
e5	-17	CYS	-	insertion	UNP E9PR30
e5	-16	GLY	-	insertion	UNP E9PR30
e5	-15	VAL	-	insertion	UNP E9PR30
e5	-14	GLU	-	insertion	UNP E9PR30
e6	-48	ALA	-	insertion	UNP E9PR30
e6	-47	HIS	-	insertion	UNP E9PR30
e6	-46	VAL	-	insertion	UNP E9PR30
e6	-45	ALA	-	insertion	UNP E9PR30
e6	-44	SER	-	insertion	UNP E9PR30
e6	-43	LEU	-	insertion	UNP E9PR30
e6	-42	GLU	-	insertion	UNP E9PR30
e6	-41	GLY	-	insertion	UNP E9PR30
e6	-40	ILE	-	insertion	UNP E9PR30
e6	-39	ALA	-	insertion	UNP E9PR30
e6	-38	PRO	-	insertion	UNP E9PR30
e6	-37	GLU	-	insertion	UNP E9PR30
e6	-36	ASP	-	insertion	UNP E9PR30

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Chain	Residue	Modelled	Actual	Comment	Reference
e6	-35	GLN	-	insertion	UNP E9PR30
e6	-34	VAL	-	insertion	UNP E9PR30
e6	-33	VAL	-	insertion	UNP E9PR30
e6	-32	LEU	-	insertion	UNP E9PR30
e6	-31	LEU	-	insertion	UNP E9PR30
e6	-30	ALA	-	insertion	UNP E9PR30
e6	-29	GLY	-	insertion	UNP E9PR30
e6	-28	ALA	-	insertion	UNP E9PR30
e6	-27	PRO	-	insertion	UNP E9PR30
e6	-26	LEU	-	insertion	UNP E9PR30
e6	-25	GLU	-	insertion	UNP E9PR30
e6	-24	ASP	-	insertion	UNP E9PR30
e6	-23	GLU	-	insertion	UNP E9PR30
e6	-22	ALA	-	insertion	UNP E9PR30
e6	-21	THR	-	insertion	UNP E9PR30
e6	-20	LEU	-	insertion	UNP E9PR30
e6	-19	GLY	-	insertion	UNP E9PR30
e6	-18	GLN	-	insertion	UNP E9PR30
e6	-17	CYS	-	insertion	UNP E9PR30
e6	-16	GLY	-	insertion	UNP E9PR30
e6	-15	VAL	-	insertion	UNP E9PR30
e6	-14	GLU	-	insertion	UNP E9PR30

- Molecule 21 is a RNA chain called Human 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	i1	1742	Total	C	N	O	P	0	0	0
			36900	16458	6595	12106	1741			
21	i2	1742	Total	C	N	O	P	0	0	0
			36900	16458	6595	12106	1741			
21	i3	1742	Total	C	N	O	P	0	0	0
			36900	16458	6595	12106	1741			
21	i4	1742	Total	C	N	O	P	0	0	0
			36900	16458	6595	12106	1741			
21	i5	1742	Total	C	N	O	P	0	0	0
			36900	16458	6595	12106	1741			
21	i6	1742	Total	C	N	O	P	0	0	0
			36900	16458	6595	12106	1741			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i1	582	C	U	conflict	GB 36162

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Chain	Residue	Modelled	Actual	Comment	Reference
i1	583	C	A	conflict	GB 36162
i1	584	G	A	conflict	GB 36162
i1	798	A	G	conflict	GB 36162
i1	1095	U	C	conflict	GB 36162
i2	582	C	U	conflict	GB 36162
i2	583	C	A	conflict	GB 36162
i2	584	G	A	conflict	GB 36162
i2	798	A	G	conflict	GB 36162
i2	1095	U	C	conflict	GB 36162
i3	582	C	U	conflict	GB 36162
i3	583	C	A	conflict	GB 36162
i3	584	G	A	conflict	GB 36162
i3	798	A	G	conflict	GB 36162
i3	1095	U	C	conflict	GB 36162
i4	582	C	U	conflict	GB 36162
i4	583	C	A	conflict	GB 36162
i4	584	G	A	conflict	GB 36162
i4	798	A	G	conflict	GB 36162
i4	1095	U	C	conflict	GB 36162
i5	582	C	U	conflict	GB 36162
i5	583	C	A	conflict	GB 36162
i5	584	G	A	conflict	GB 36162
i5	798	A	G	conflict	GB 36162
i5	1095	U	C	conflict	GB 36162
i6	582	C	U	conflict	GB 36162
i6	583	C	A	conflict	GB 36162
i6	584	G	A	conflict	GB 36162
i6	798	A	G	conflict	GB 36162
i6	1095	U	C	conflict	GB 36162

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A1	222	Total	C	N	O	S	0	0	0
			1747	1109	306	324	8			
22	A2	222	Total	C	N	O	S	0	0	0
			1747	1109	306	324	8			
22	A3	222	Total	C	N	O	S	0	0	0
			1747	1109	306	324	8			
22	A4	222	Total	C	N	O	S	0	0	0
			1747	1109	306	324	8			
22	A5	222	Total	C	N	O	S	0	0	0
			1747	1109	306	324	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A6	222	Total	C	N	O	S	0	0	0
			1747	1109	306	324	8			

- Molecule 23 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	B1	214	Total	C	N	O	S	0	0	0
			1738	1103	310	311	14			
23	B2	214	Total	C	N	O	S	0	0	0
			1738	1103	310	311	14			
23	B3	214	Total	C	N	O	S	0	0	0
			1738	1103	310	311	14			
23	B4	214	Total	C	N	O	S	0	0	0
			1738	1103	310	311	14			
23	B5	214	Total	C	N	O	S	0	0	0
			1738	1103	310	311	14			
23	B6	214	Total	C	N	O	S	0	0	0
			1738	1103	310	311	14			

- Molecule 24 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	D1	227	Total	C	N	O	S	0	0	0
			1765	1125	317	315	8			
24	D2	227	Total	C	N	O	S	0	0	0
			1765	1125	317	315	8			
24	D3	227	Total	C	N	O	S	0	0	0
			1765	1125	317	315	8			
24	D4	227	Total	C	N	O	S	0	0	0
			1765	1125	317	315	8			
24	D5	227	Total	C	N	O	S	0	0	0
			1765	1125	317	315	8			
24	D6	227	Total	C	N	O	S	0	0	0
			1765	1125	317	315	8			

- Molecule 25 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	E1	262	Total	C	N	O	S	0	0	0
			2076	1324	386	358	8			
25	E2	262	Total	C	N	O	S	0	0	0
			2076	1324	386	358	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	E3	262	Total	C	N	O	S	0	0	0
			2076	1324	386	358	8			
25	E4	262	Total	C	N	O	S	0	0	0
			2076	1324	386	358	8			
25	E5	262	Total	C	N	O	S	0	0	0
			2076	1324	386	358	8			
25	E6	262	Total	C	N	O	S	0	0	0
			2076	1324	386	358	8			

- Molecule 26 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	F1	191	Total	C	N	O	S	0	0	0
			1509	943	286	273	7			
26	F2	191	Total	C	N	O	S	0	0	0
			1509	943	286	273	7			
26	F3	191	Total	C	N	O	S	0	0	0
			1509	943	286	273	7			
26	F4	191	Total	C	N	O	S	0	0	0
			1509	943	286	273	7			
26	F5	191	Total	C	N	O	S	0	0	0
			1509	943	286	273	7			
26	F6	191	Total	C	N	O	S	0	0	0
			1509	943	286	273	7			

- Molecule 27 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	H1	189	Total	C	N	O	S	0	0	0
			1521	969	280	271	1			
27	H2	189	Total	C	N	O	S	0	0	0
			1521	969	280	271	1			
27	H3	189	Total	C	N	O	S	0	0	0
			1521	969	280	271	1			
27	H4	189	Total	C	N	O	S	0	0	0
			1521	969	280	271	1			
27	H5	189	Total	C	N	O	S	0	0	0
			1521	969	280	271	1			
27	H6	189	Total	C	N	O	S	0	0	0
			1521	969	280	271	1			

- Molecule 28 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	I1	206	Total	C	N	O	S	0	0	0
			1686	1058	332	291	5			
28	I2	206	Total	C	N	O	S	0	0	0
			1686	1058	332	291	5			
28	I3	206	Total	C	N	O	S	0	0	0
			1686	1058	332	291	5			
28	I4	206	Total	C	N	O	S	0	0	0
			1686	1058	332	291	5			
28	I5	206	Total	C	N	O	S	0	0	0
			1686	1058	332	291	5			
28	I6	206	Total	C	N	O	S	0	0	0
			1686	1058	332	291	5			

- Molecule 29 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	K1	98	Total	C	N	O	S	0	0	0
			827	539	148	134	6			
29	K2	98	Total	C	N	O	S	0	0	0
			827	539	148	134	6			
29	K3	98	Total	C	N	O	S	0	0	0
			827	539	148	134	6			
29	K4	98	Total	C	N	O	S	0	0	0
			827	539	148	134	6			
29	K5	98	Total	C	N	O	S	0	0	0
			827	539	148	134	6			
29	K6	98	Total	C	N	O	S	0	0	0
			827	539	148	134	6			

- Molecule 30 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	L1	153	Total	C	N	O	S	0	0	0
			1247	793	234	214	6			
30	L2	153	Total	C	N	O	S	0	0	0
			1247	793	234	214	6			
30	L3	153	Total	C	N	O	S	0	0	0
			1247	793	234	214	6			
30	L4	153	Total	C	N	O	S	0	0	0
			1247	793	234	214	6			
30	L5	153	Total	C	N	O	S	0	0	0
			1247	793	234	214	6			
30	L6	153	Total	C	N	O	S	0	0	0
			1247	793	234	214	6			

- Molecule 31 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	P1	125	Total	C	N	O	S	0	0	0
			1033	656	196	174	7			
31	P2	125	Total	C	N	O	S	0	0	0
			1033	656	196	174	7			
31	P3	125	Total	C	N	O	S	0	0	0
			1033	656	196	174	7			
31	P4	125	Total	C	N	O	S	0	0	0
			1033	656	196	174	7			
31	P5	125	Total	C	N	O	S	0	0	0
			1033	656	196	174	7			
31	P6	125	Total	C	N	O	S	0	0	0
			1033	656	196	174	7			

- Molecule 32 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	Q1	146	Total	C	N	O	S	0	0	0
			1158	736	218	200	4			
32	Q2	146	Total	C	N	O	S	0	0	0
			1158	736	218	200	4			
32	Q3	146	Total	C	N	O	S	0	0	0
			1158	736	218	200	4			
32	Q4	146	Total	C	N	O	S	0	0	0
			1158	736	218	200	4			
32	Q5	146	Total	C	N	O	S	0	0	0
			1158	736	218	200	4			
32	Q6	146	Total	C	N	O	S	0	0	0
			1158	736	218	200	4			

- Molecule 33 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	R1	132	Total	C	N	O	S	0	0	0
			1072	673	199	195	5			
33	R2	132	Total	C	N	O	S	0	0	0
			1072	673	199	195	5			
33	R3	132	Total	C	N	O	S	0	0	0
			1072	673	199	195	5			
33	R4	132	Total	C	N	O	S	0	0	0
			1072	673	199	195	5			
33	R5	132	Total	C	N	O	S	0	0	0
			1072	673	199	195	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	R6	132	Total	C	N	O	S	0	0	0
			1072	673	199	195	5			

- Molecule 34 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	S1	143	Total	C	N	O	S	0	0	0
			1184	743	240	200	1			
34	S2	143	Total	C	N	O	S	0	0	0
			1184	743	240	200	1			
34	S3	143	Total	C	N	O	S	0	0	0
			1184	743	240	200	1			
34	S4	143	Total	C	N	O	S	0	0	0
			1184	743	240	200	1			
34	S5	143	Total	C	N	O	S	0	0	0
			1184	743	240	200	1			
34	S6	143	Total	C	N	O	S	0	0	0
			1184	743	240	200	1			

- Molecule 35 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	j1	25	Total	C	N	O	S	0	0	0
			239	145	64	27	3			
35	j2	25	Total	C	N	O	S	0	0	0
			239	145	64	27	3			
35	j3	25	Total	C	N	O	S	0	0	0
			239	145	64	27	3			
35	j4	25	Total	C	N	O	S	0	0	0
			239	145	64	27	3			
35	j5	25	Total	C	N	O	S	0	0	0
			239	145	64	27	3			
35	j6	25	Total	C	N	O	S	0	0	0
			239	145	64	27	3			

- Molecule 36 is a protein called Malignant T-cell-amplified sequence 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	k1	181	Total	C	N	O	S	0	0	0
			1421	926	234	250	11			
36	k2	181	Total	C	N	O	S	0	0	0
			1421	926	234	250	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	k3	181	Total	C	N	O	S	0	0	0
			1421	926	234	250	11			
36	k4	181	Total	C	N	O	S	0	0	0
			1421	926	234	250	11			
36	k5	181	Total	C	N	O	S	0	0	0
			1421	926	234	250	11			
36	k6	181	Total	C	N	O	S	0	0	0
			1421	926	234	250	11			

- Molecule 37 is a protein called Density-regulated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	l1	79	Total	C	N	O	S	0	0	0
			629	400	102	125	2			
37	l2	79	Total	C	N	O	S	0	0	0
			629	400	102	125	2			
37	l3	79	Total	C	N	O	S	0	0	0
			629	400	102	125	2			
37	l4	79	Total	C	N	O	S	0	0	0
			629	400	102	125	2			
37	l5	79	Total	C	N	O	S	0	0	0
			629	400	102	125	2			
37	l6	79	Total	C	N	O	S	0	0	0
			629	400	102	125	2			

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	f6	1	Total	Zn	0	0
			1	1		
38	f5	1	Total	Zn	0	0
			1	1		
38	f4	1	Total	Zn	0	0
			1	1		
38	f3	1	Total	Zn	0	0
			1	1		
38	f2	1	Total	Zn	0	0
			1	1		
38	f1	1	Total	Zn	0	0
			1	1		

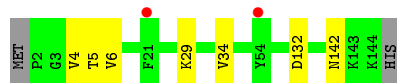
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

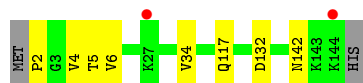
- Molecule 1: 40S ribosomal protein S19



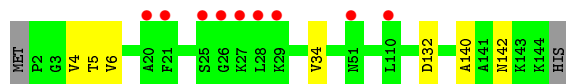
- Molecule 1: 40S ribosomal protein S19



- Molecule 1: 40S ribosomal protein S19



- Molecule 1: 40S ribosomal protein S19



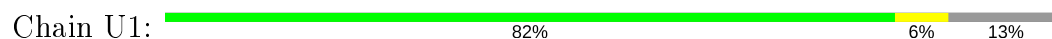
- Molecule 1: 40S ribosomal protein S19



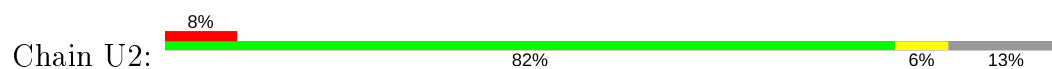
- Molecule 1: 40S ribosomal protein S19



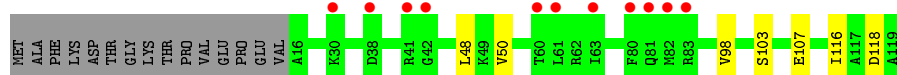
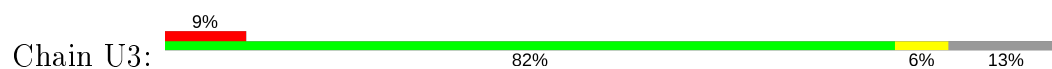
- Molecule 2: 40S ribosomal protein S20



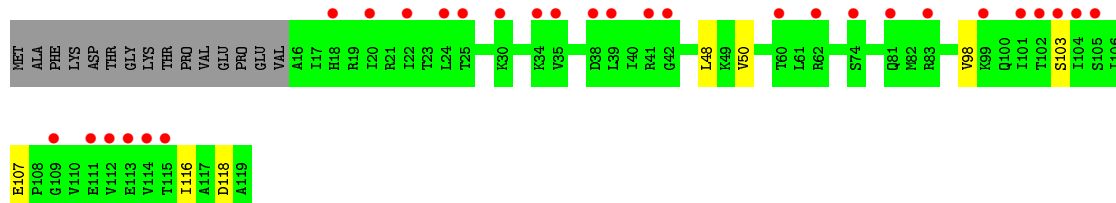
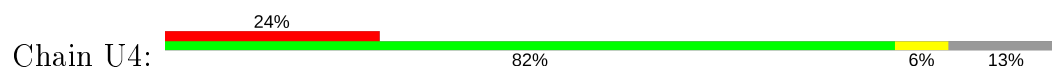
- Molecule 2: 40S ribosomal protein S20



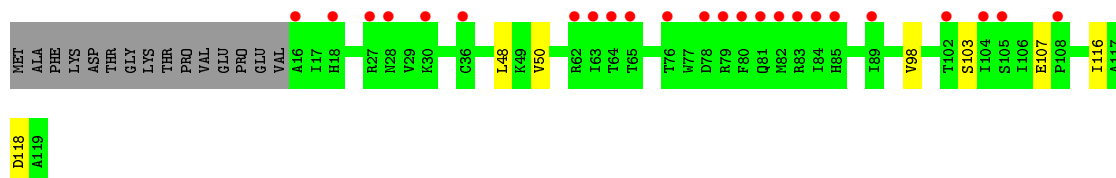
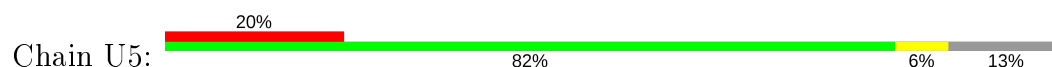
- Molecule 2: 40S ribosomal protein S20



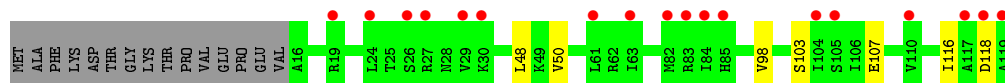
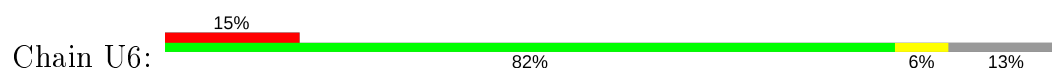
- Molecule 2: 40S ribosomal protein S20



- Molecule 2: 40S ribosomal protein S20



- Molecule 2: 40S ribosomal protein S20



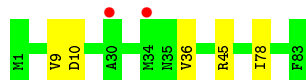
- Molecule 3: 40S ribosomal protein S21



- Molecule 3: 40S ribosomal protein S21



- Molecule 3: 40S ribosomal protein S21



- Molecule 3: 40S ribosomal protein S21



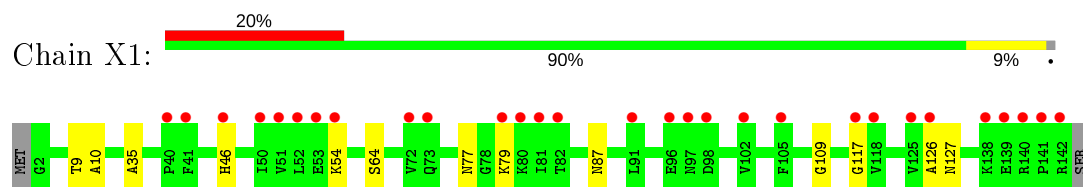
- Molecule 3: 40S ribosomal protein S21



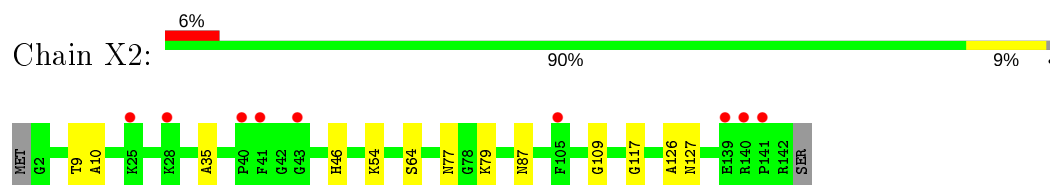
- Molecule 3: 40S ribosomal protein S21



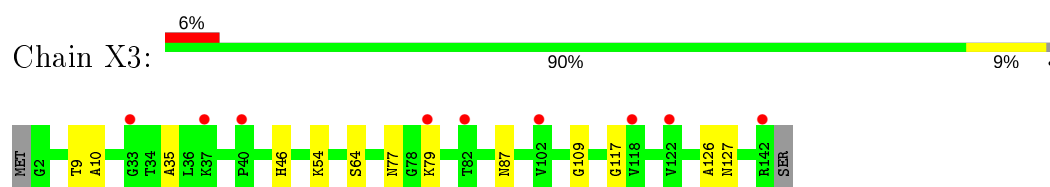
- Molecule 4: 40S ribosomal protein S23



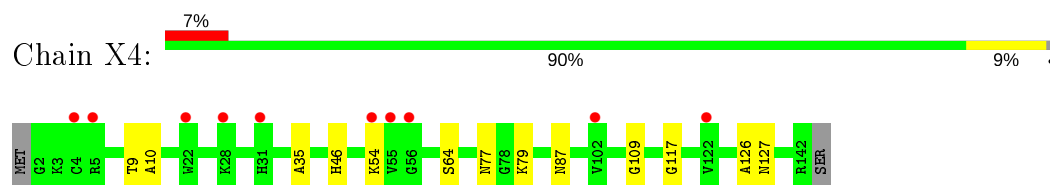
- Molecule 4: 40S ribosomal protein S23



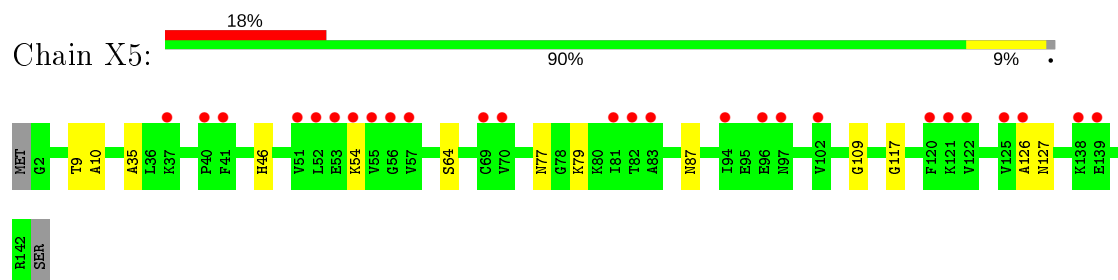
- Molecule 4: 40S ribosomal protein S23



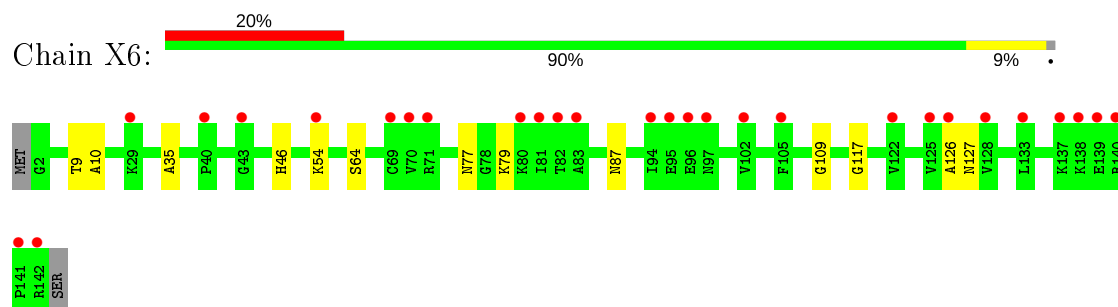
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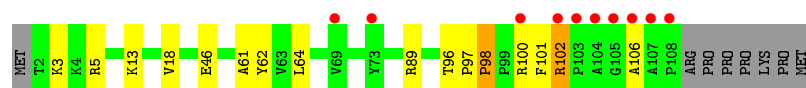
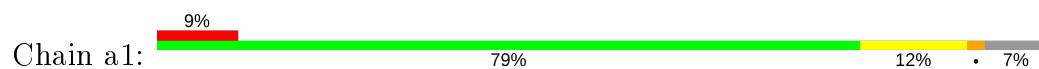
- Molecule 4: 40S ribosomal protein S23



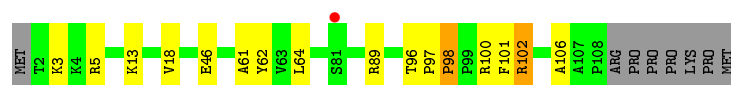
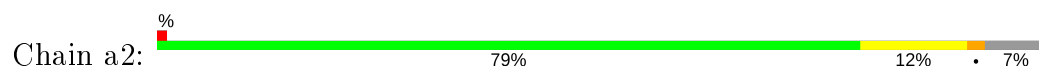
- Molecule 4: 40S ribosomal protein S23



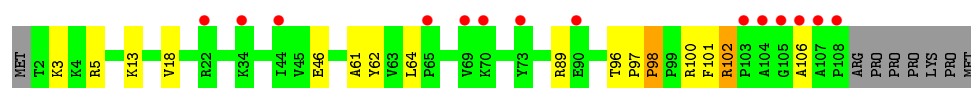
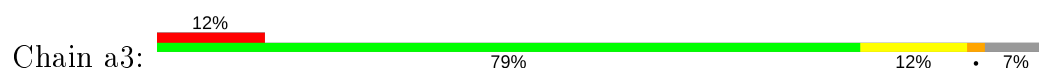
• Molecule 5: 40S ribosomal protein S26



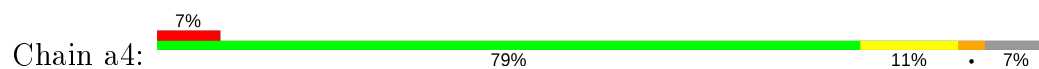
• Molecule 5: 40S ribosomal protein S26



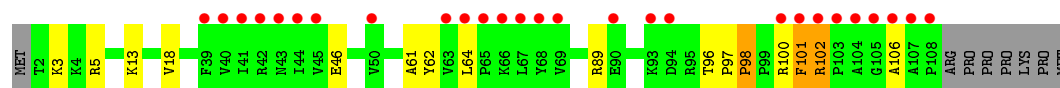
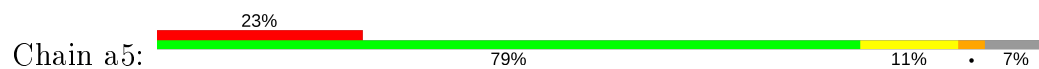
• Molecule 5: 40S ribosomal protein S26



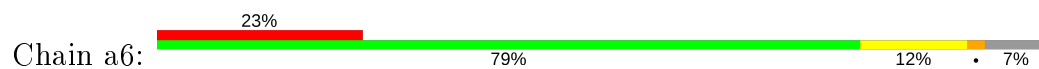
• Molecule 5: 40S ribosomal protein S26



• Molecule 5: 40S ribosomal protein S26

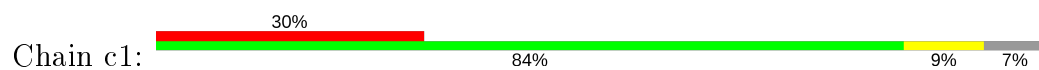


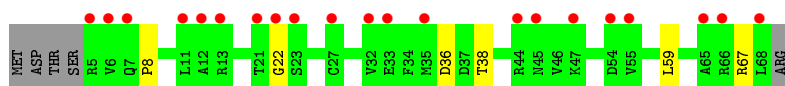
• Molecule 5: 40S ribosomal protein S26



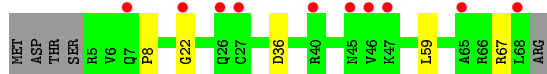
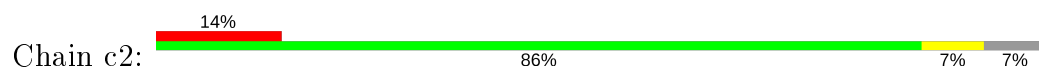
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• Molecule 6: 40S ribosomal protein S28

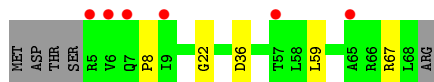
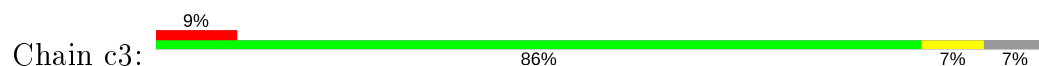




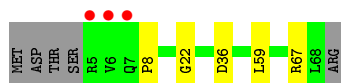
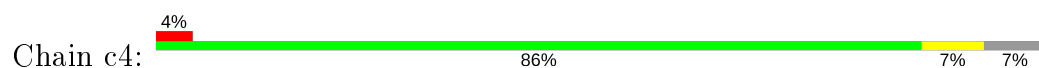
- Molecule 6: 40S ribosomal protein S28



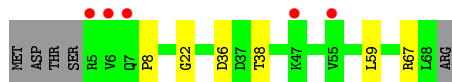
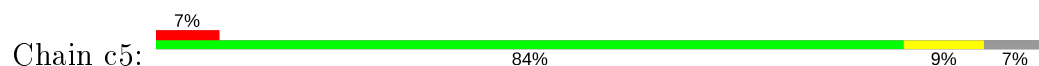
- Molecule 6: 40S ribosomal protein S28



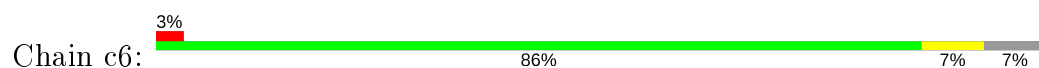
- Molecule 6: 40S ribosomal protein S28



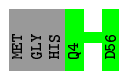
- Molecule 6: 40S ribosomal protein S28



- Molecule 6: 40S ribosomal protein S28



- Molecule 7: 40S ribosomal protein S29



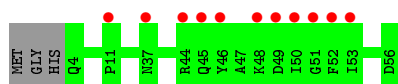
- Molecule 7: 40S ribosomal protein S29

Chain d2:  95% 5%



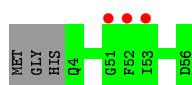
- Molecule 7: 40S ribosomal protein S29

Chain d3:  20% 95% 5%



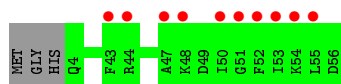
- Molecule 7: 40S ribosomal protein S29

Chain d4:  5% 95% 5%



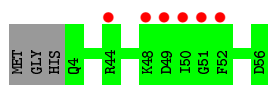
- Molecule 7: 40S ribosomal protein S29

Chain d5:  18% 95% 5%




- Molecule 7: 40S ribosomal protein S29

Chain d6:  11% 95% 5%




- Molecule 8: Ribosomal protein S27a

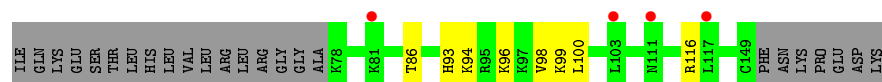
Chain f1:  3% 41% 5% 54%



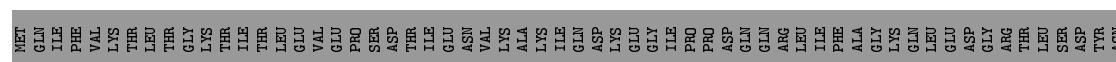
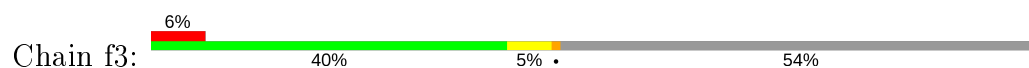
- Molecule 8: Ribosomal protein S27a

Chain f2:  3% 41% 5% 54%

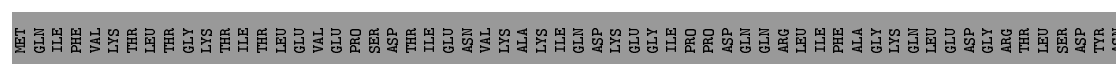
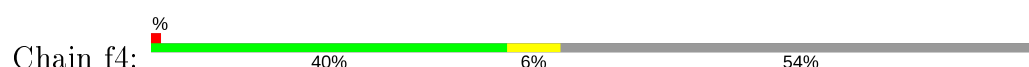




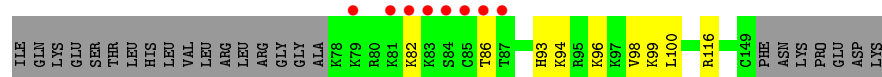
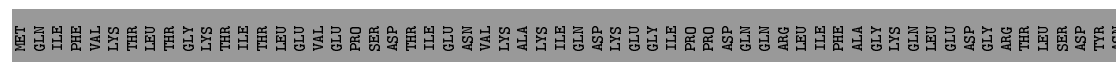
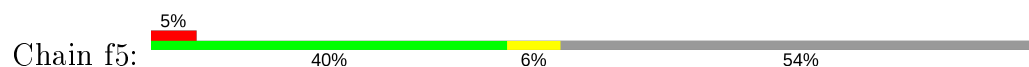
• Molecule 8: Ribosomal protein S27a



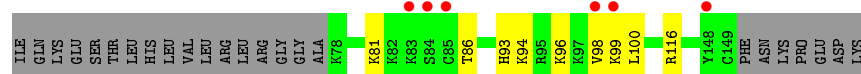
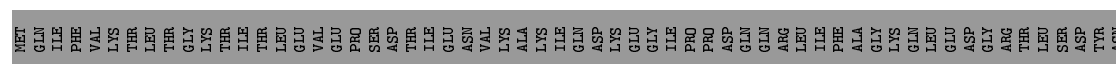
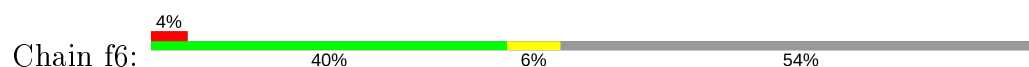
• Molecule 8: Ribosomal protein S27a



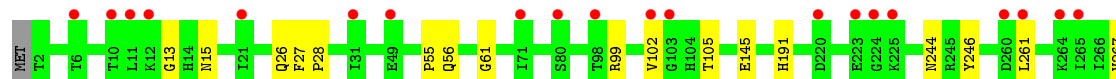
• Molecule 8: Ribosomal protein S27a

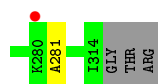


• Molecule 8: Ribosomal protein S27a

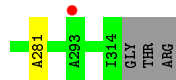


• Molecule 9: Receptor of activated protein C kinase 1

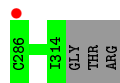
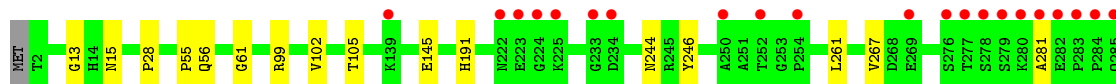
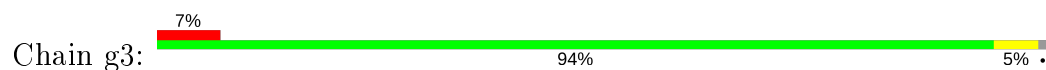




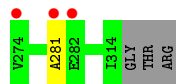
- Molecule 9: Receptor of activated protein C kinase 1



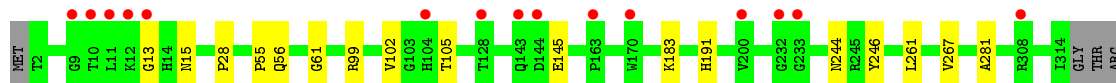
- Molecule 9: Receptor of activated protein C kinase 1



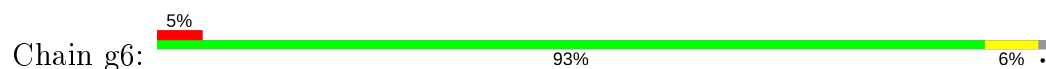
- Molecule 9: Receptor of activated protein C kinase 1

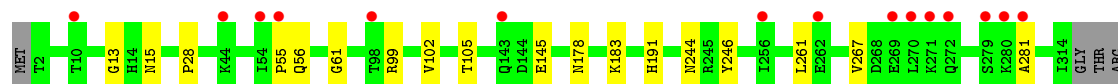


- Molecule 9: Receptor of activated protein C kinase 1

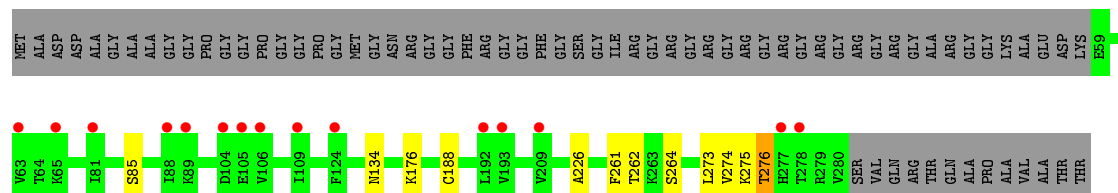
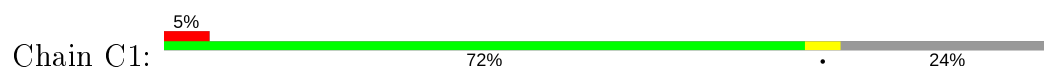


- Molecule 9: Receptor of activated protein C kinase 1

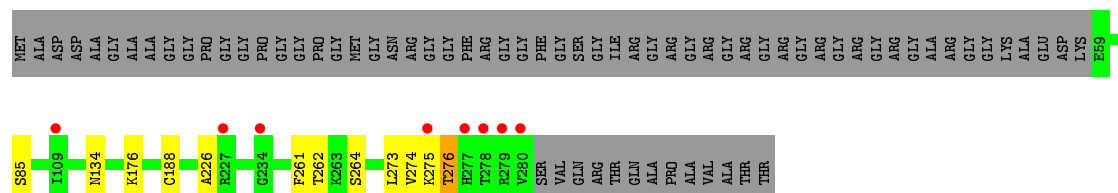




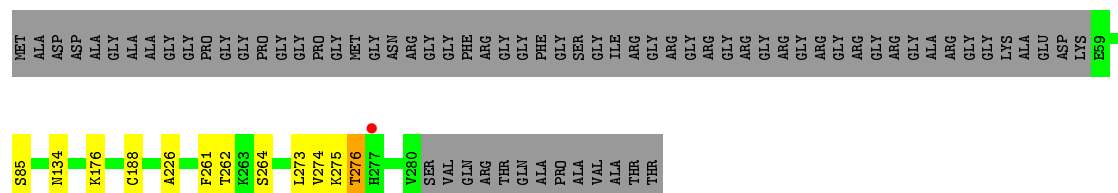
- Molecule 10: 40S ribosomal protein S2



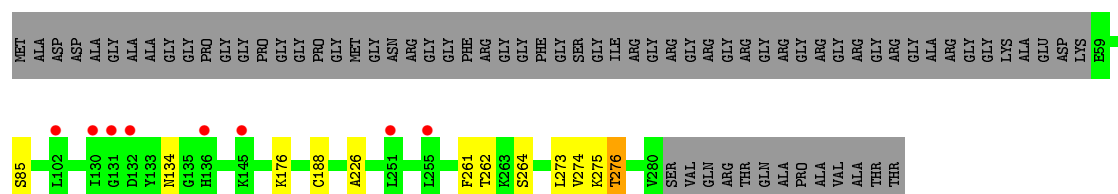
- Molecule 10: 40S ribosomal protein S2



- Molecule 10: 40S ribosomal protein S2

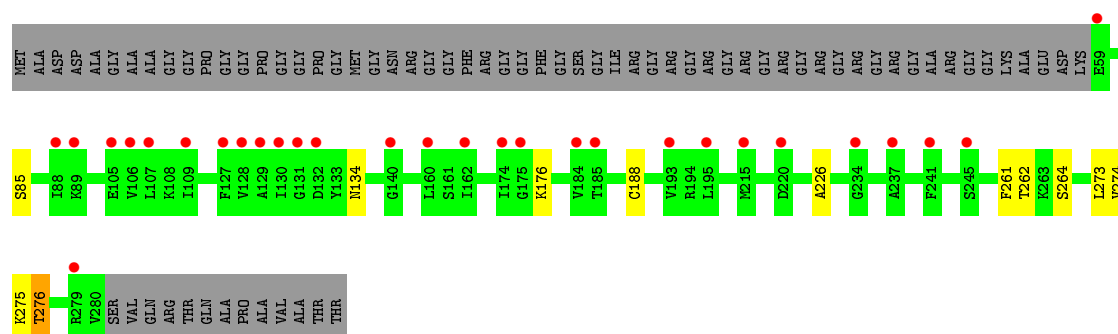


- Molecule 10: 40S ribosomal protein S2

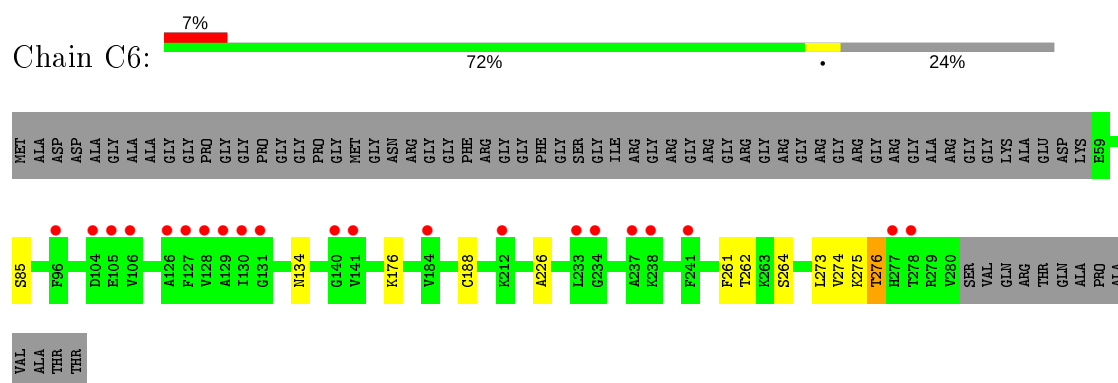


- Molecule 10: 40S ribosomal protein S2

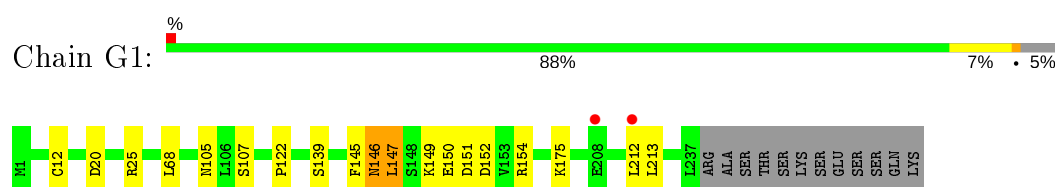




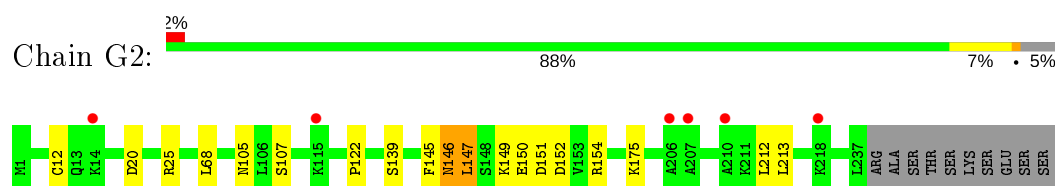
- Molecule 10: 40S ribosomal protein S2



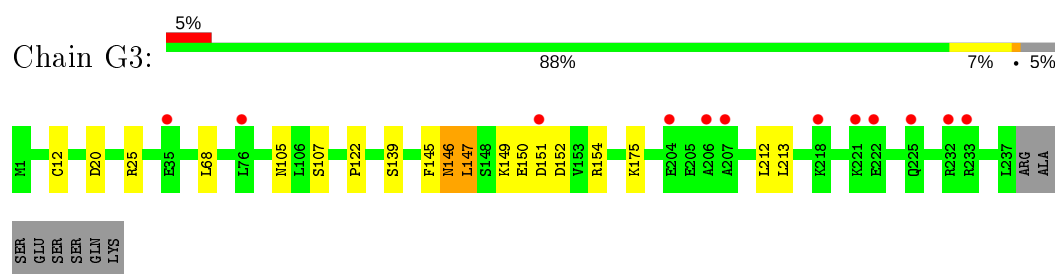
- Molecule 11: 40S ribosomal protein S6



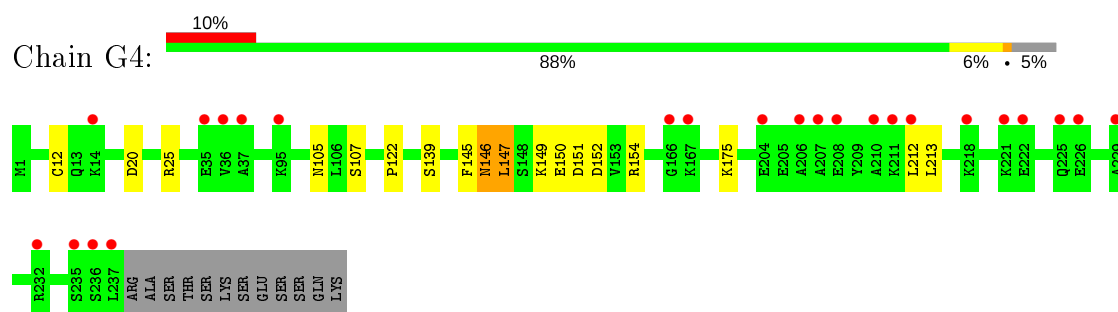
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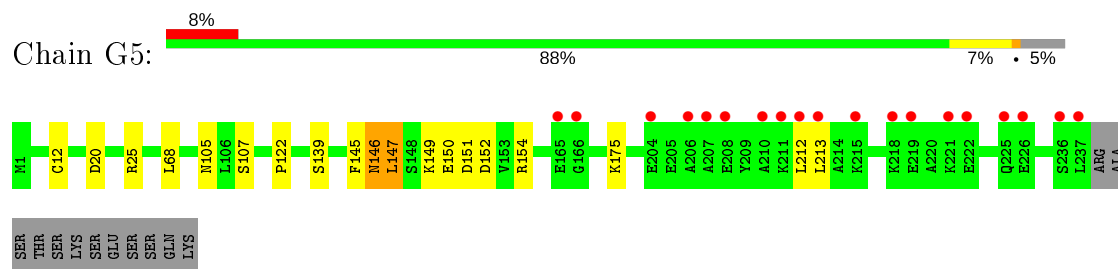
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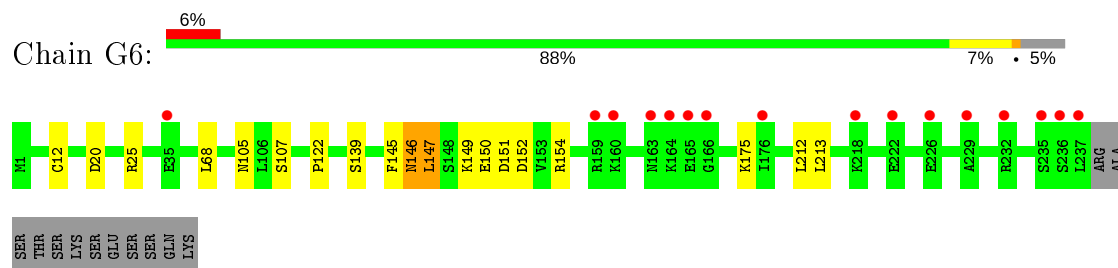
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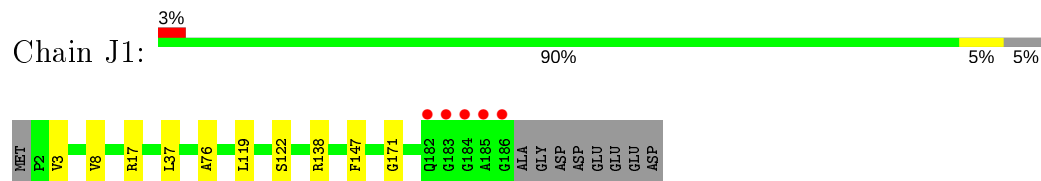
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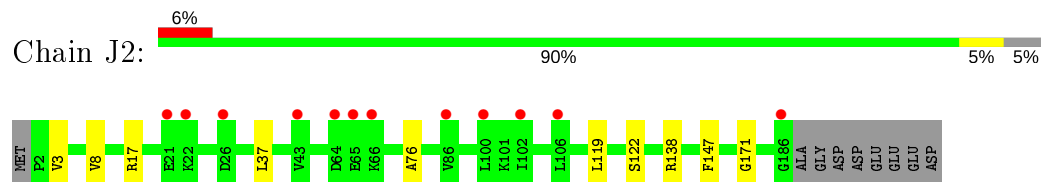
- Molecule 11: 40S ribosomal protein S6



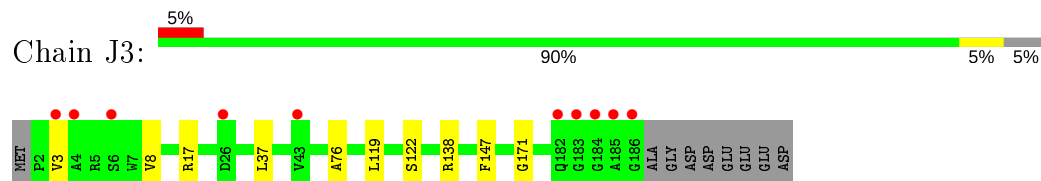
- Molecule 12: 40S ribosomal protein S9



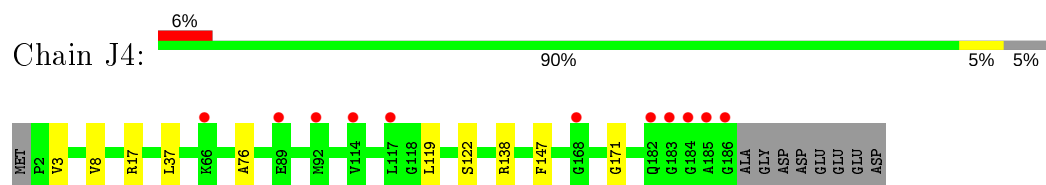
- Molecule 12: 40S ribosomal protein S9



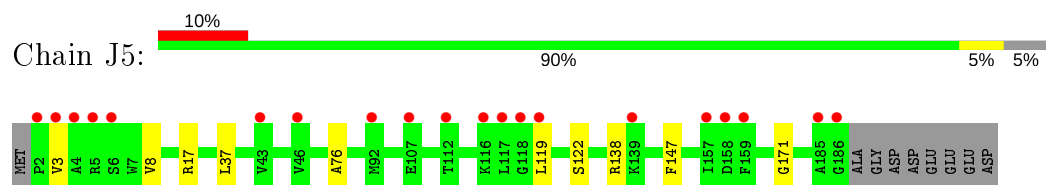
- Molecule 12: 40S ribosomal protein S9



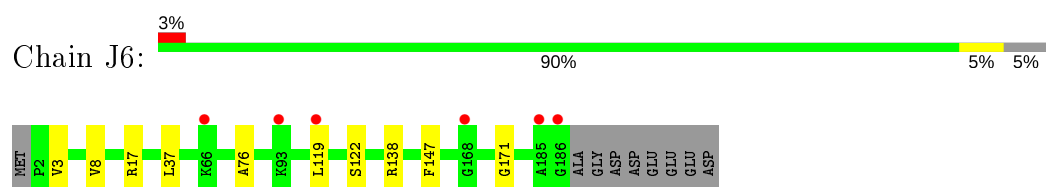
• Molecule 12: 40S ribosomal protein S9



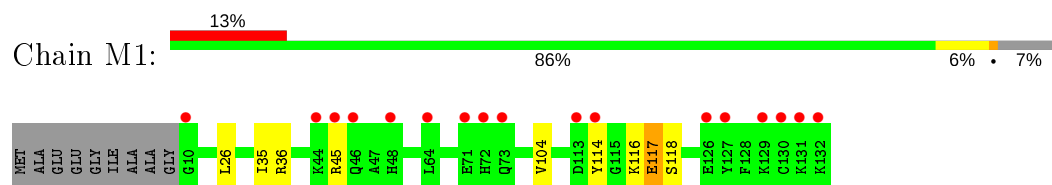
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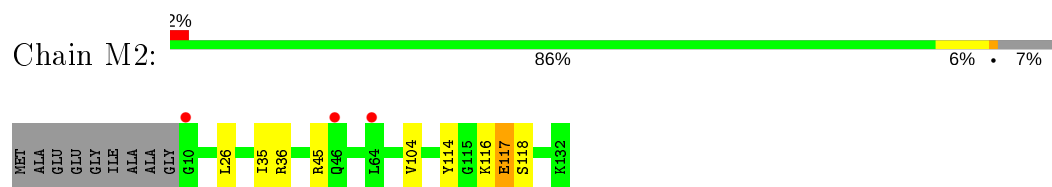
• Molecule 12: 40S ribosomal protein S9



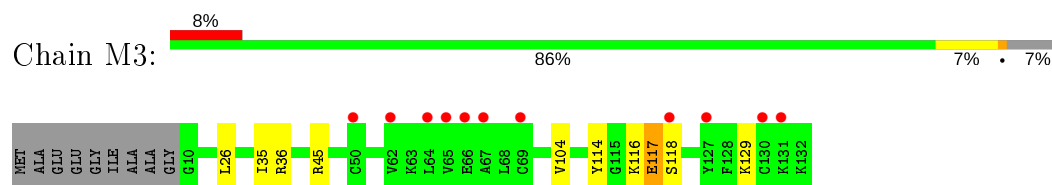
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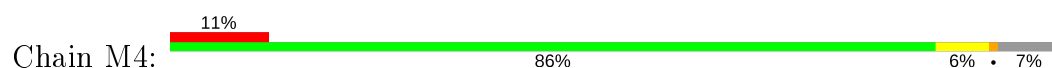
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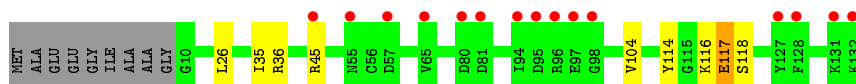


• Molecule 13: 40S ribosomal protein S12

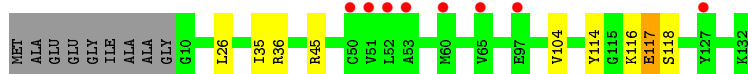
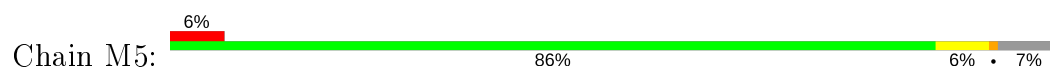


• Molecule 13: 40S ribosomal protein S12





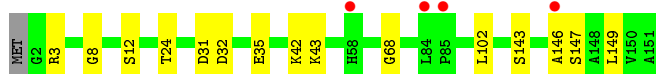
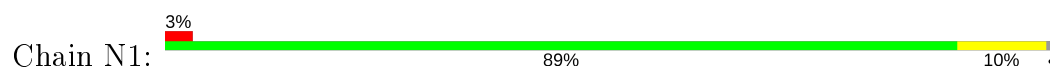
- Molecule 13: 40S ribosomal protein S12



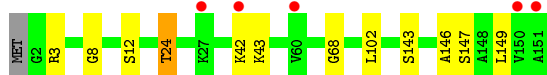
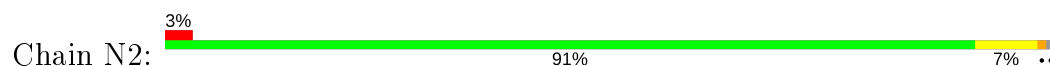
- Molecule 13: 40S ribosomal protein S12



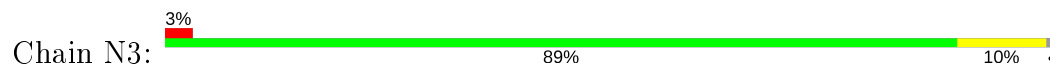
- Molecule 14: 40S ribosomal protein S13



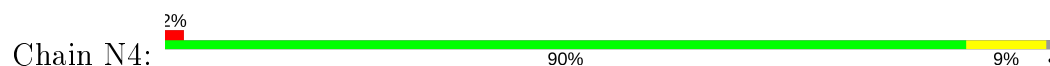
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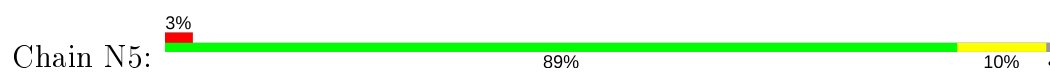
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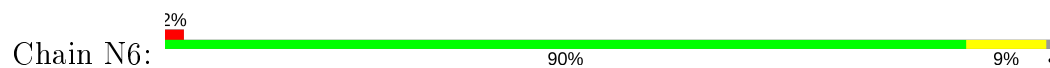
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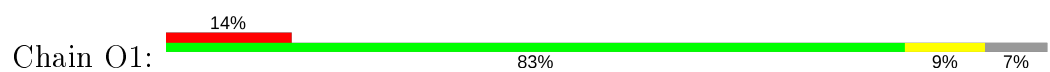
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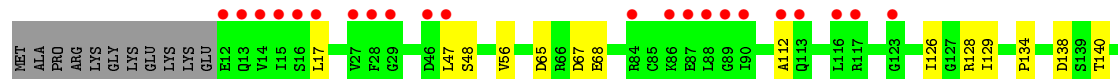
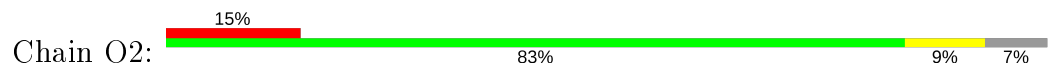
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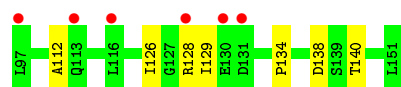
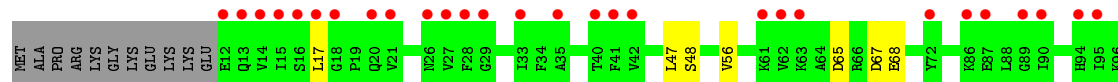
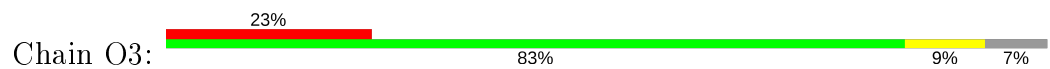
- Molecule 15: 40S ribosomal protein S14



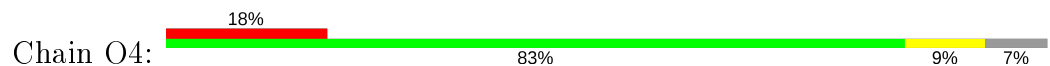
- Molecule 15: 40S ribosomal protein S14

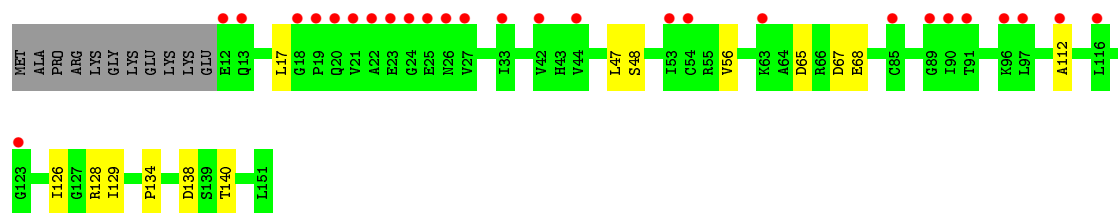


- Molecule 15: 40S ribosomal protein S14

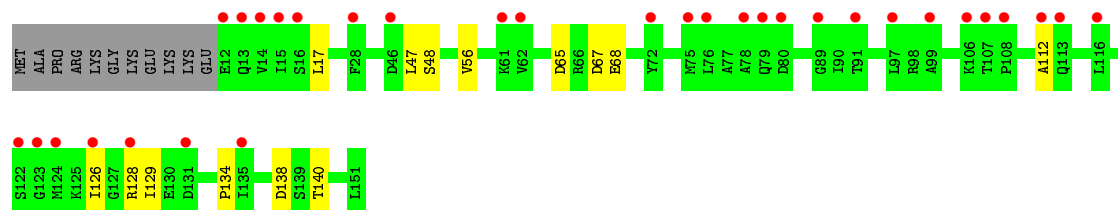
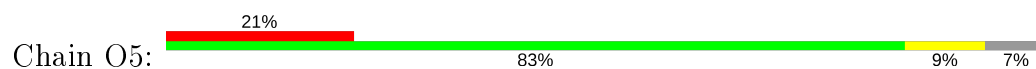


- Molecule 15: 40S ribosomal protein S14

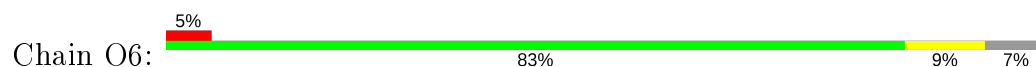




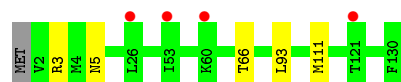
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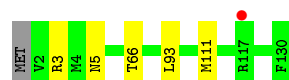
- Molecule 15: 40S ribosomal protein S14



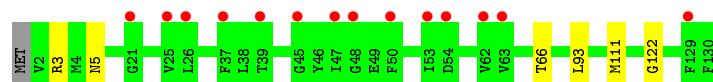
- Molecule 16: 40S ribosomal protein S15a



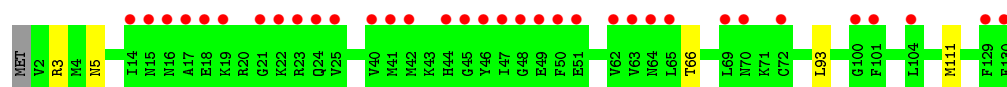
- Molecule 16: 40S ribosomal protein S15a



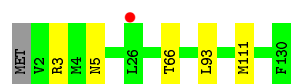
- Molecule 16: 40S ribosomal protein S15a



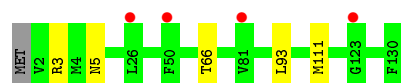
- Molecule 16: 40S ribosomal protein S15a



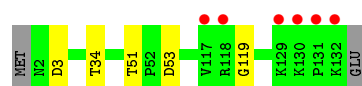
- Molecule 16: 40S ribosomal protein S15a



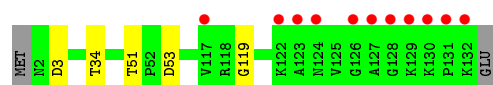
- Molecule 16: 40S ribosomal protein S15a



- Molecule 17: 40S ribosomal protein S24



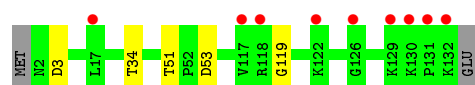
- Molecule 17: 40S ribosomal protein S24



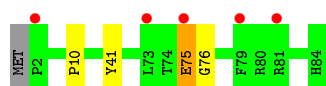
- Molecule 17: 40S ribosomal protein S24



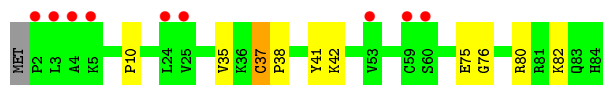
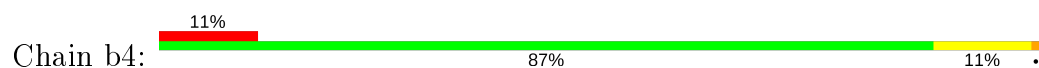
- Molecule 17: 40S ribosomal protein S24



- Molecule 18: 40S ribosomal protein S25



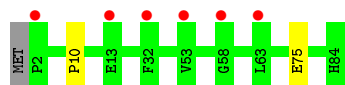
- Molecule 19: 40S ribosomal protein S27



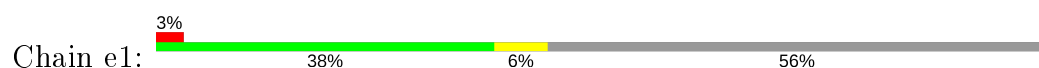
- Molecule 19: 40S ribosomal protein S27



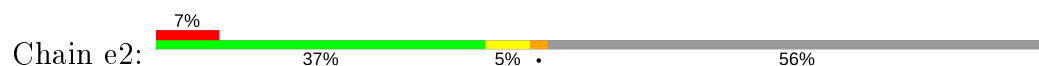
- Molecule 19: 40S ribosomal protein S27



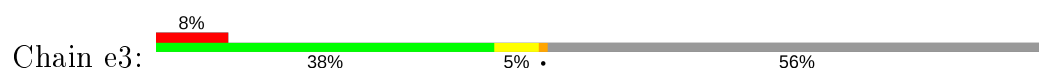
- Molecule 20: 40S ribosomal protein S30



- Molecule 20: 40S ribosomal protein S30

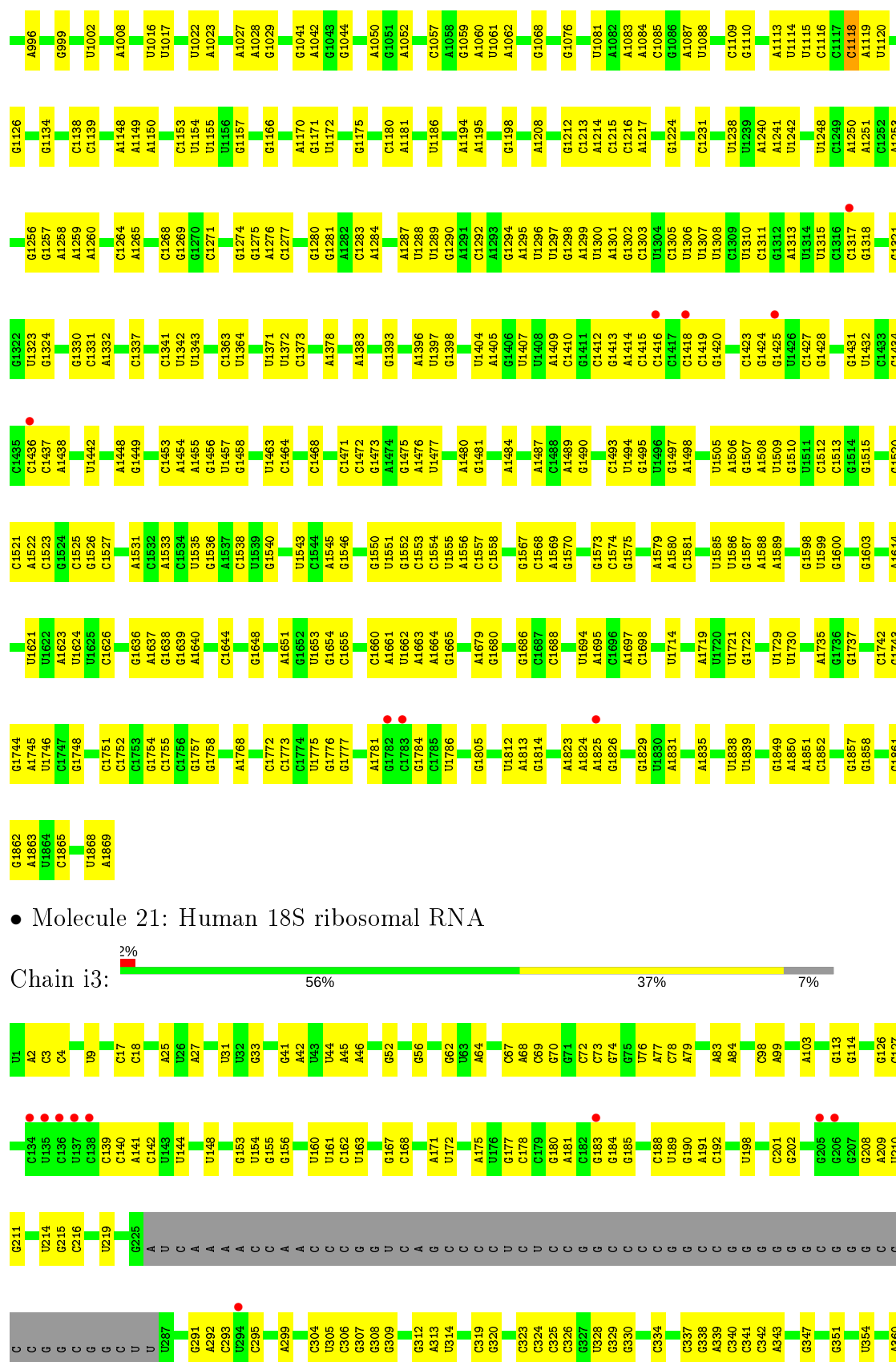


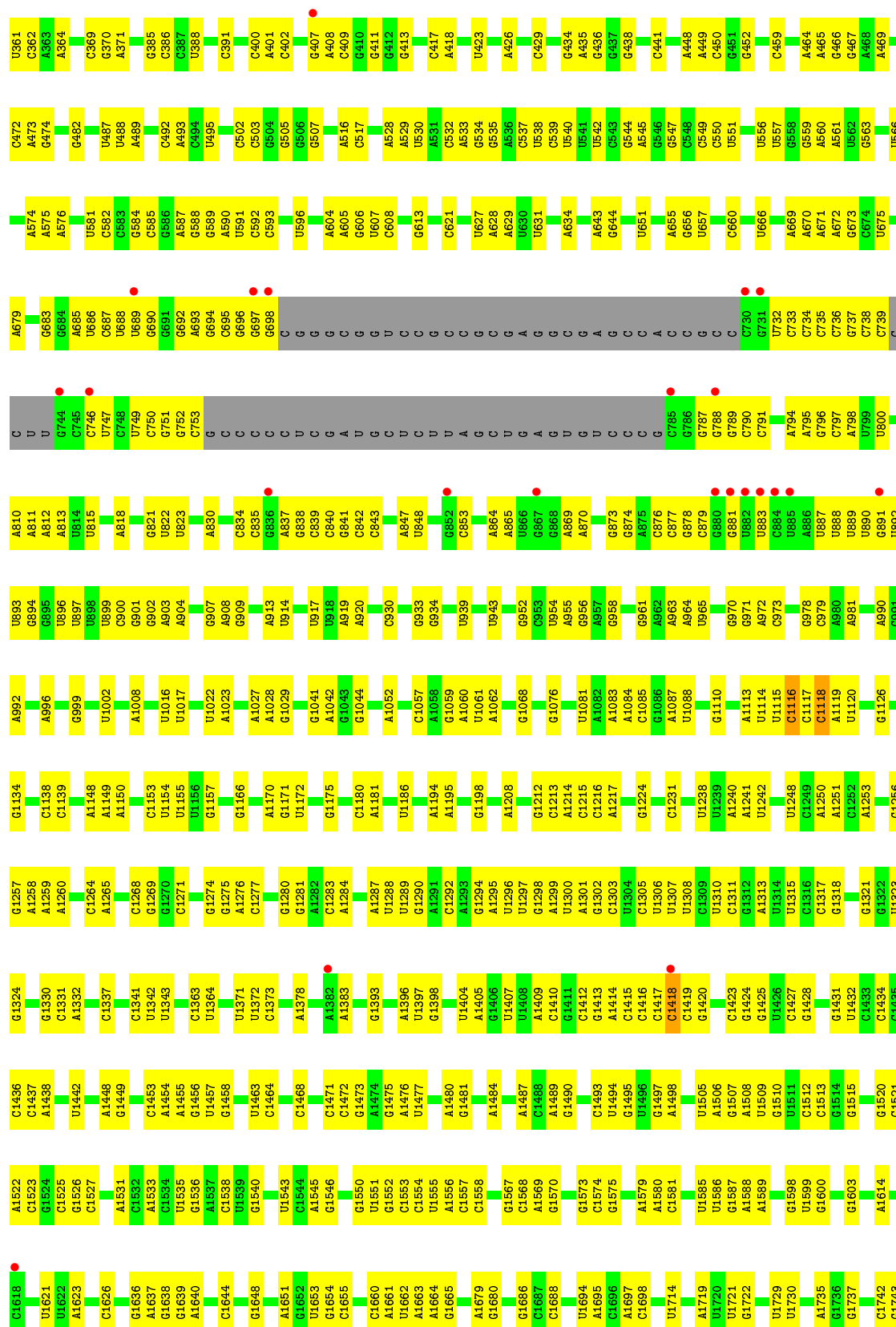
- Molecule 20: 40S ribosomal protein S30

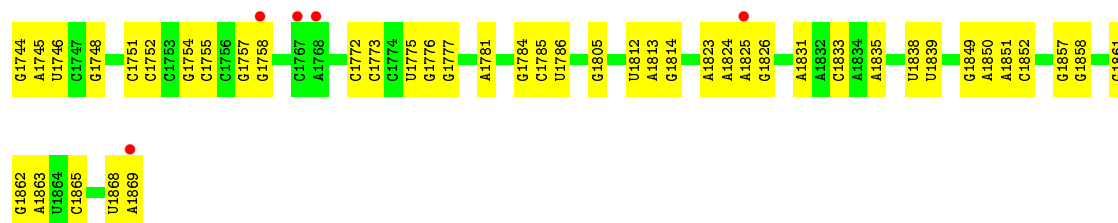




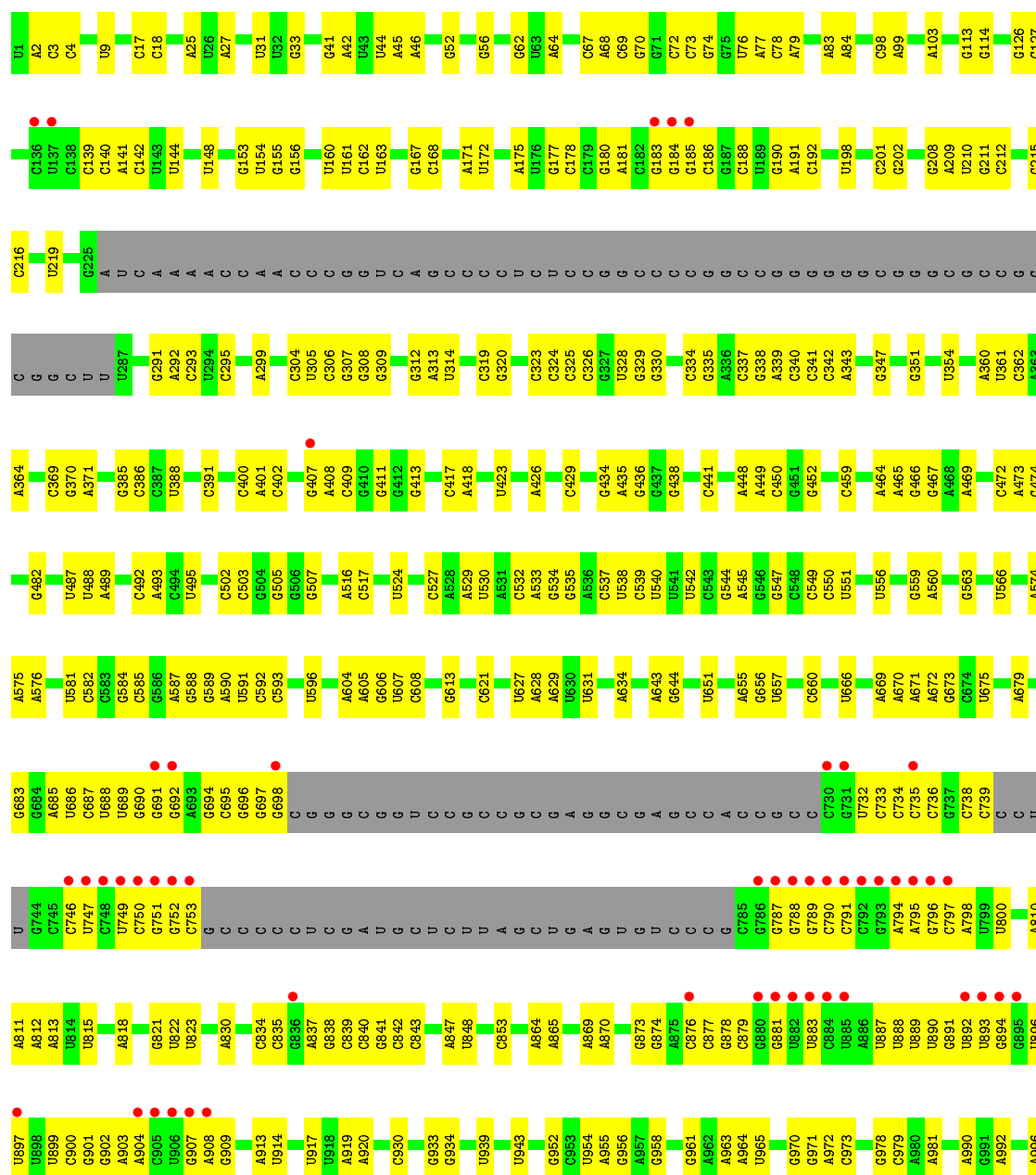






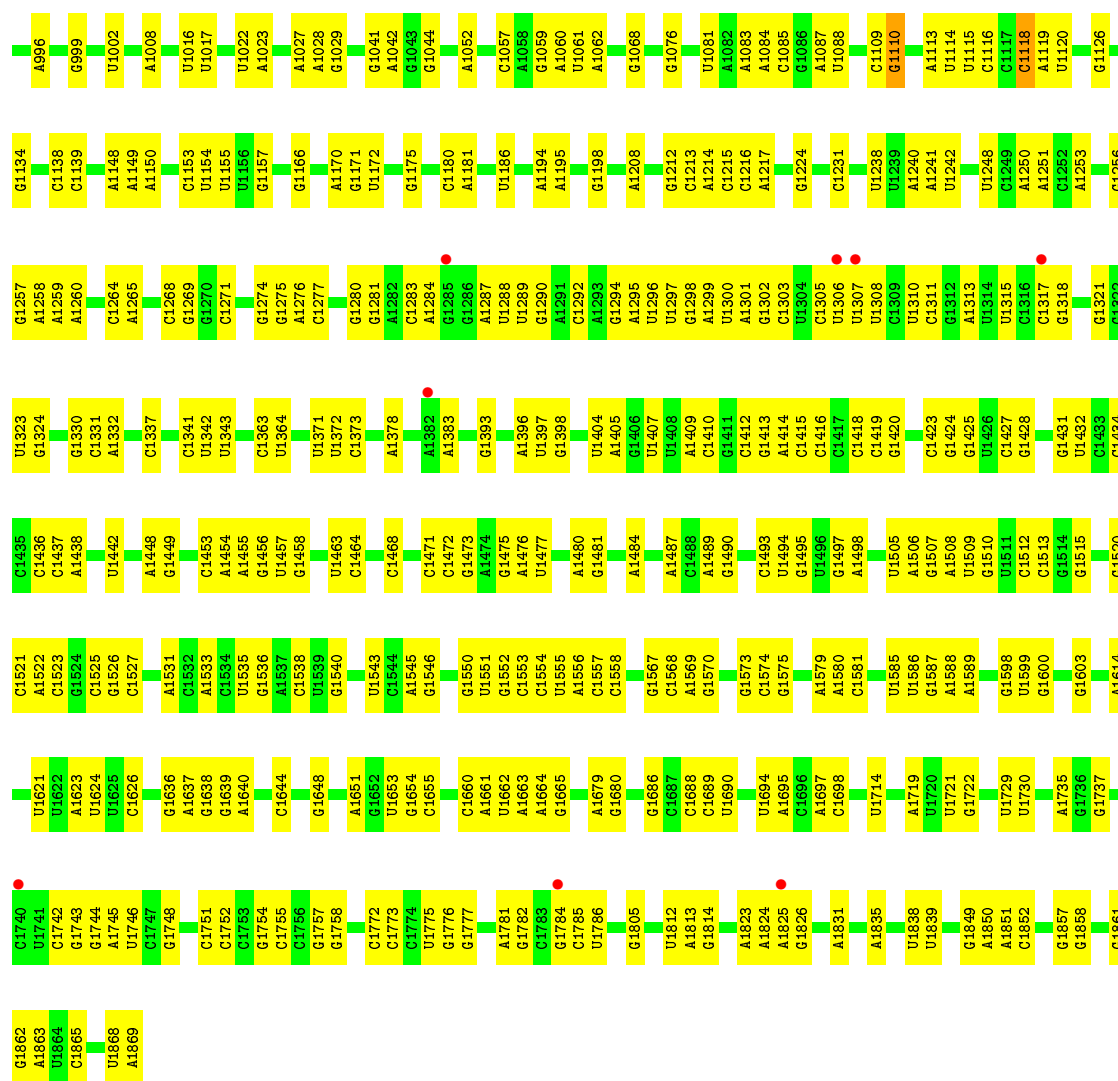


• Molecule 21: Human 18S ribosomal RNA

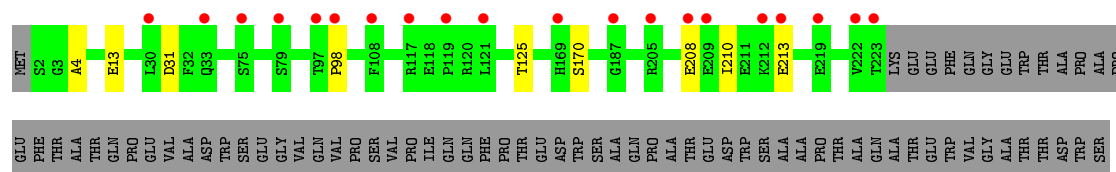




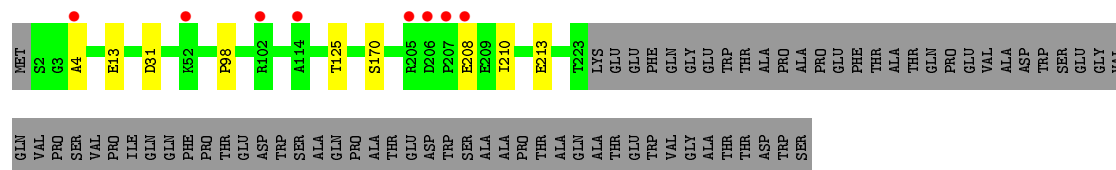
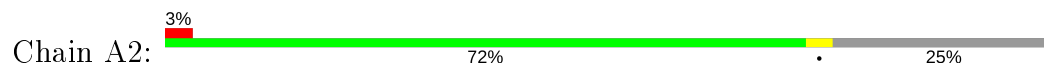
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U1622	C1436	U1323	G1138	A996	G895	U799	C738	G674	C472	U361
G1623	C1437	G1324	C1139	A998	U897	U800	C	U675	A473	C362
C1525	A1438	G1330	A1148	G999	U898	A810	C	U679	A363	A364
U1624	U1442	C1331	A1149	U1002	U899	A811	U	A574	G474	
C1626		A1332	A1150	U1008	C900	A812	G745	A575	G482	C369
	A1448	C1337	C1153	A1008	G901	A813	G746	A576		G370
A1531	G1449		C1154	U1016	A903	U814	U747		U487	A371
A1533	C1453	C1341	U1154	U1017	A904	U815	U748		U488	
G1638	A1454	U1342	U1155	U1022	G907	A818	C748		U489	
G1639	A1455	U1343	U1156	A1023	A908	G821	U749		C492	G355
A1640	G1456	G1270	G1157	U1022	G909	U822	C750		A493	C367
G1536	C1457	C1271	G1158	A1023	A909	U823	G751		U494	U388
A1537	G1458	G1274	G1166	A1023	G907	U823	G752		U495	
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U1539	G1464	C1276	G1168	A1023	G909	U823	C753			C502
G1540	U1463	U1371	A1170	A1023	A909	U823	G			C503
U1543	C1464	U1372	G1171	A1023	A909	U823	C			G504
G1544	C1468	C1373	U1172	A1023	A909	U823	C			G505
U1545	C1471	A1378	G1175	G1041	C934	C835	C			G506
G1546	C1472	A1383	G1176	A1042	U836	U836	C			G507
	C1473	A1383	C1180	G1043	A919	A837	C			C400
A1661	G1473	A1383	C1181	G1044	A920	U838	C			C401
U1551	A1474	G1393	A1181	A1052	G921	C839	C			C402
G1552	G1475		U1186	A1052	C930	C840	C			G407
A1553	A1476	U1396	U1287	C1057	U917	C840	C			A408
U1554	U1477	U1397	U1288	C1058	U918	C841	C			C409
G1555	U1477	U1397	U1289	A1058	U919	C842	C			G410
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C1557	G1481		A1291	G1060	A920	C843	C			G412
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	A1484	U1406	A1293	A1062	C930	U848	C			C417
G1567	A1487	U1407	A1294	G1068	U943	U848	C			A418
C1568	U1488	U1408	A1295	G1076	G952	C953	C			U423
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G1575	G1495	C1415	C1215	A1084	G958	G873	C			U436
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G1587	G1507	U1310	U1239	A1113	G880	C878	C			U448
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	G1510	A1313	U1242	C1116	U883	G789	C			G451
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U1599	C1512	G1428	C1118	C1118	U888	C791	C			C459
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	G1514	G1431	U1249	U1120	U890	A794	C			A464
A1735	G1515	U1432	C1252	G1126	G991	A795	C			A465
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			A1253							



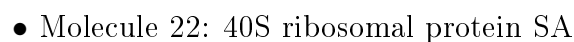
• Molecule 22: 40S ribosomal protein SA



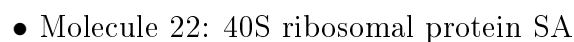
• Molecule 22: 40S ribosomal protein SA



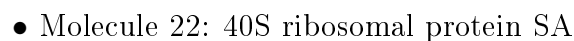
- Chain A3:



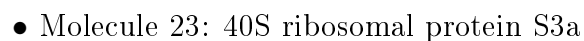
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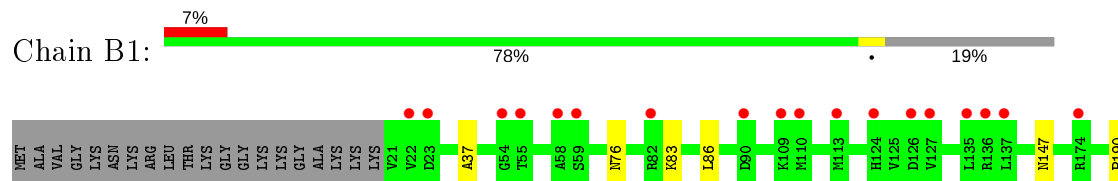
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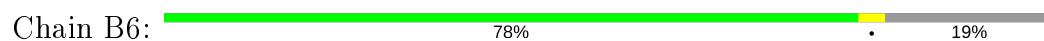


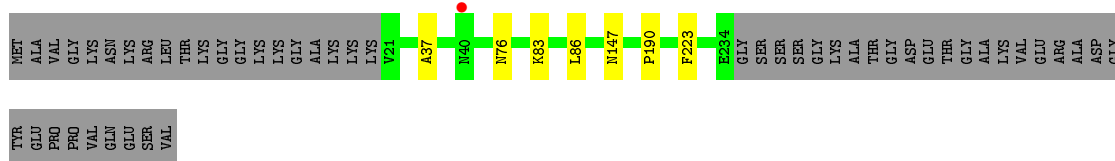
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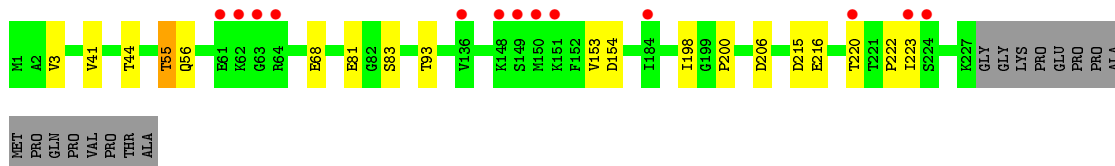
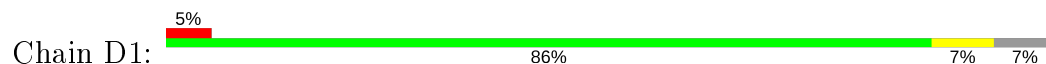
Chain B1:



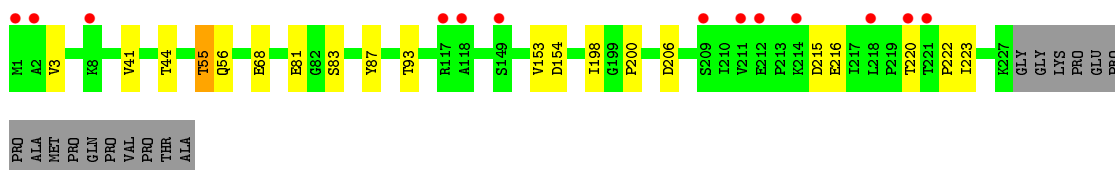
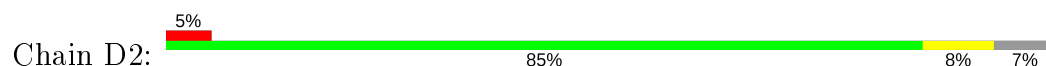




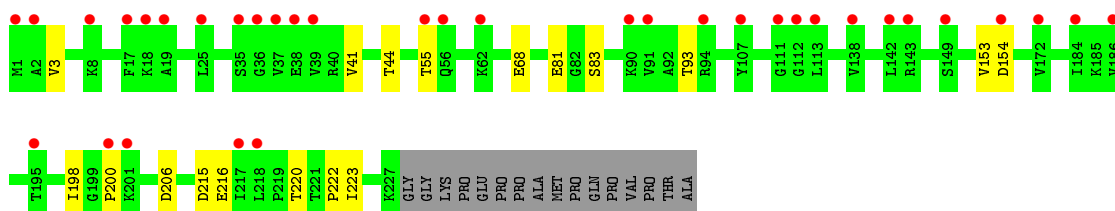
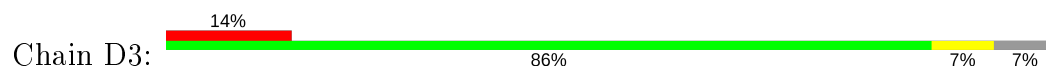
- Molecule 24: 40S ribosomal protein S3



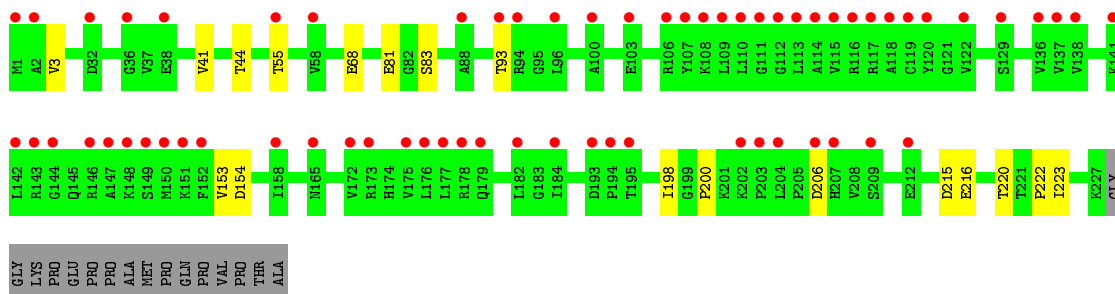
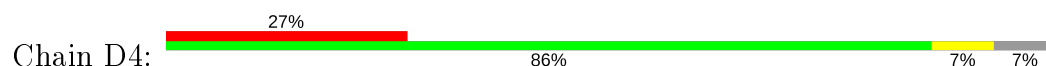
- Molecule 24: 40S ribosomal protein S3



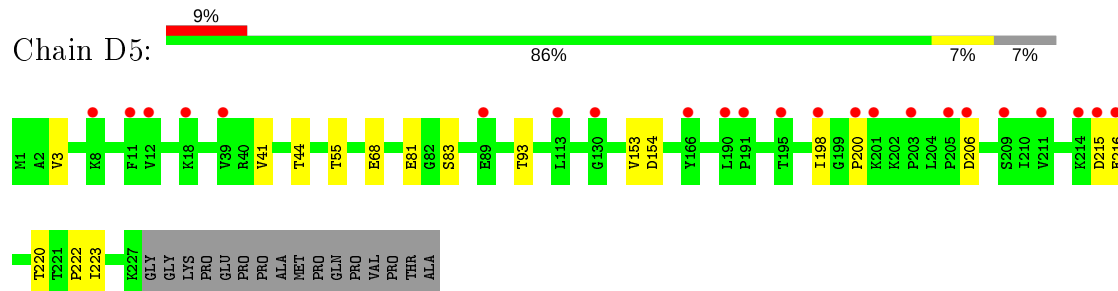
- Molecule 24: 40S ribosomal protein S3



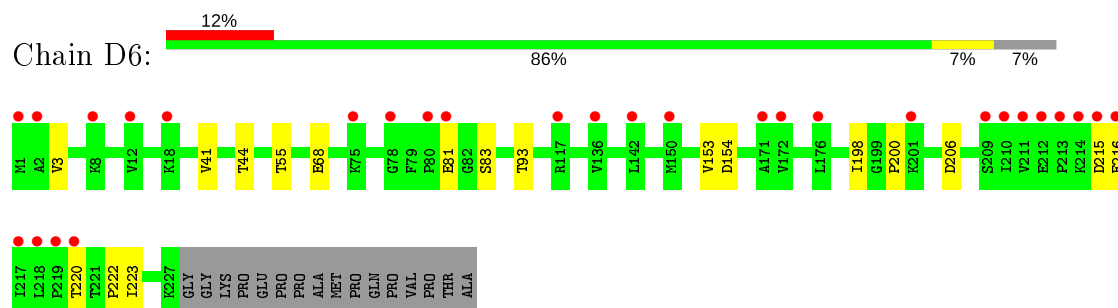
- Molecule 24: 40S ribosomal protein S3



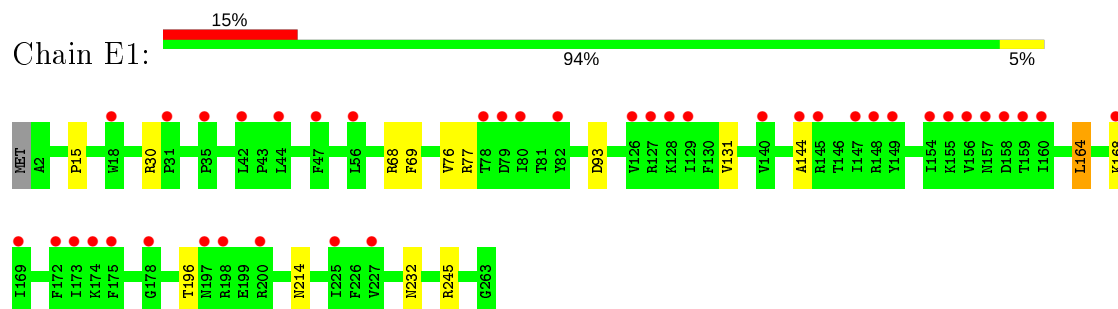
- Molecule 24: 40S ribosomal protein S3



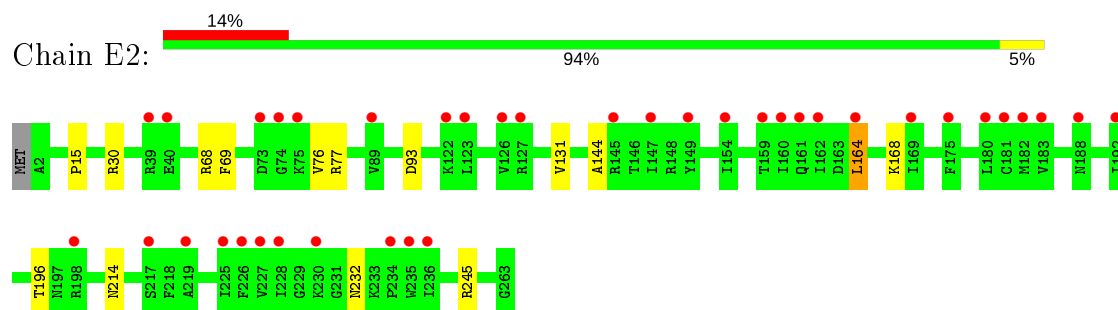
- Molecule 24: 40S ribosomal protein S3



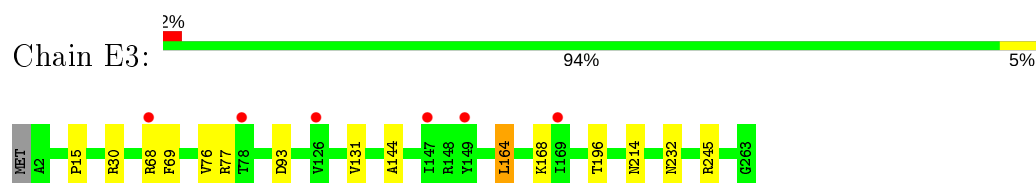
- Molecule 25: 40S ribosomal protein S4, X isoform



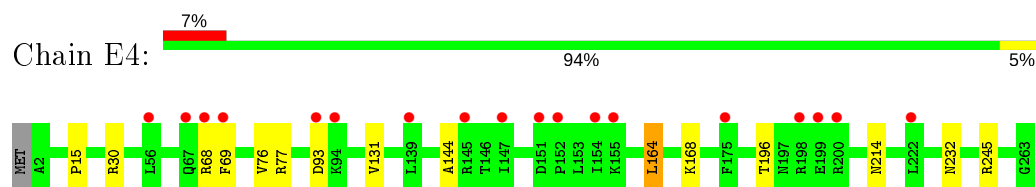
- Molecule 25: 40S ribosomal protein S4, X isoform



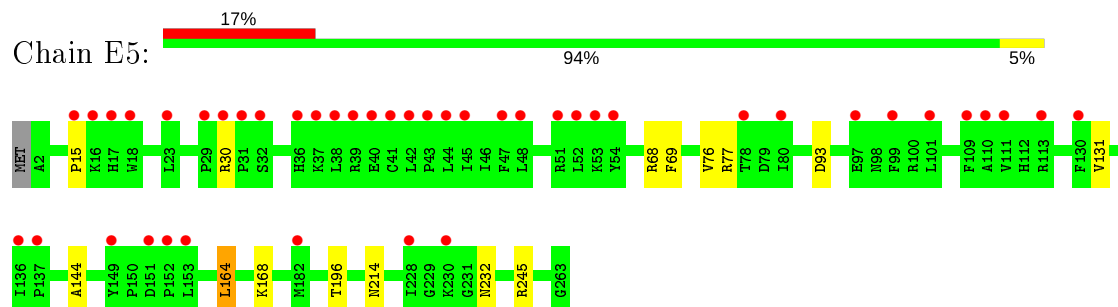
- Molecule 25: 40S ribosomal protein S4, X isoform



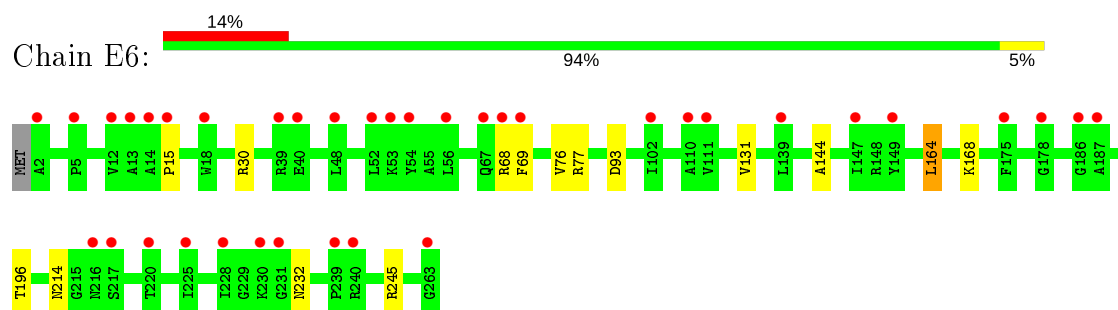
- Molecule 25: 40S ribosomal protein S4, X isoform



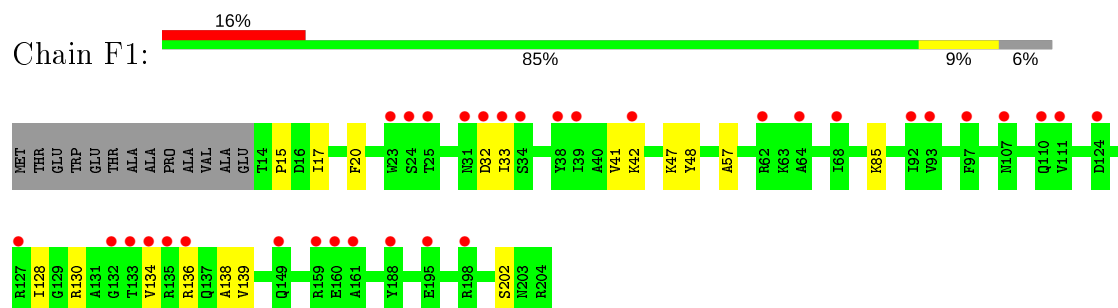
- Molecule 25: 40S ribosomal protein S4, X isoform



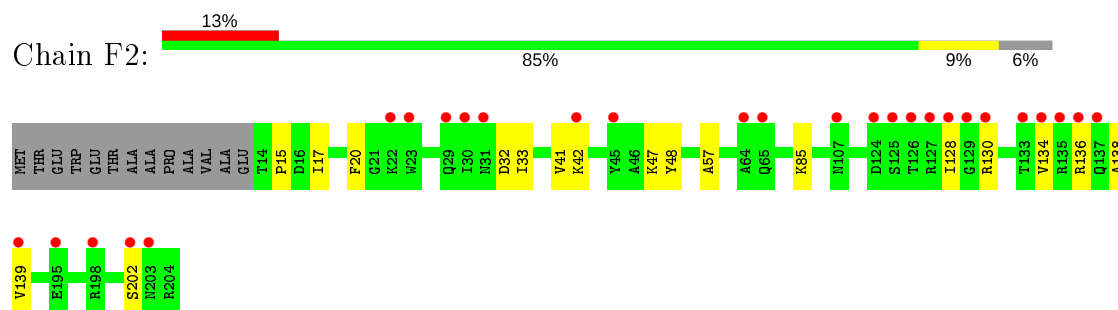
- Molecule 25: 40S ribosomal protein S4, X isoform




- Molecule 26: 40S ribosomal protein S5

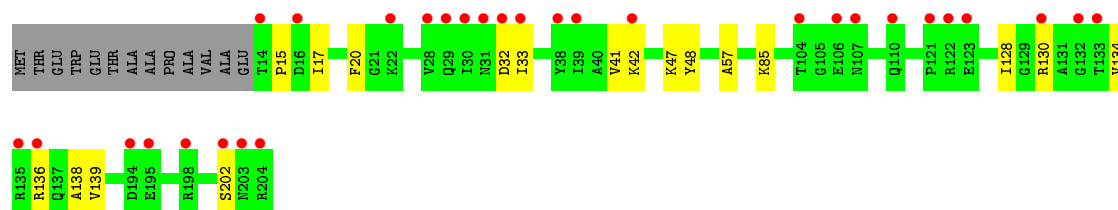


- Molecule 26: 40S ribosomal protein S5




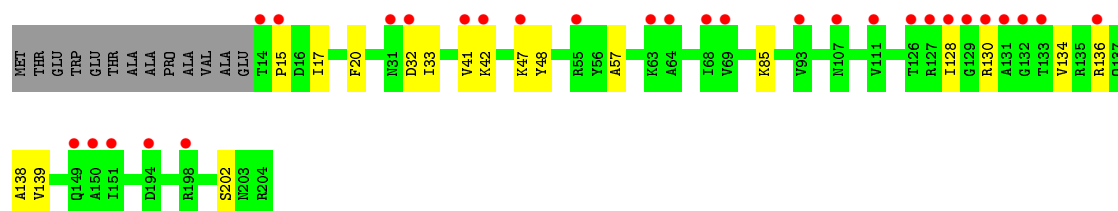
- Molecule 26: 40S ribosomal protein S5

Chain F3: 




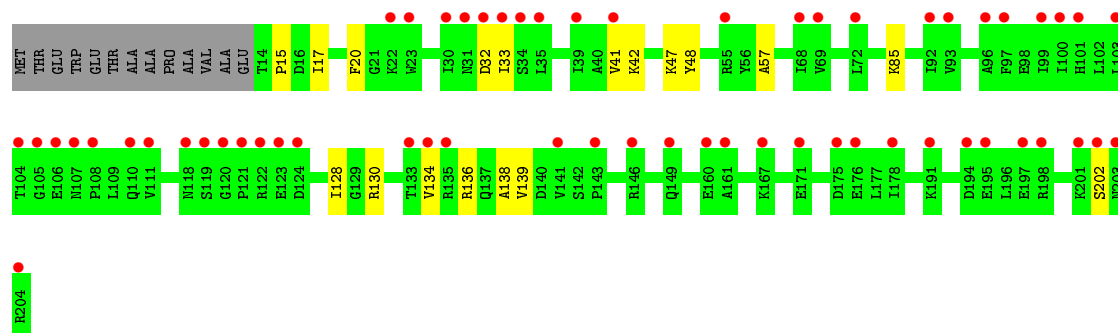
- Molecule 26: 40S ribosomal protein S5

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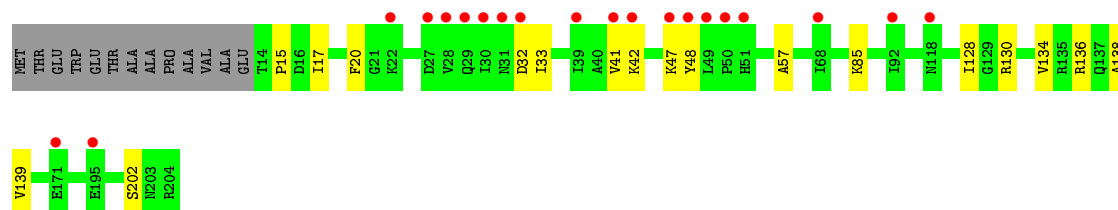
- Molecule 26: 40S ribosomal protein S5

Chain F5: 




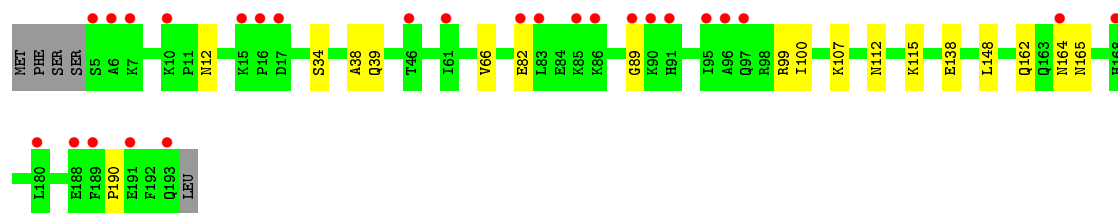
- Molecule 26: 40S ribosomal protein S5

Chain F6: 



- Molecule 27: 40S ribosomal protein S7

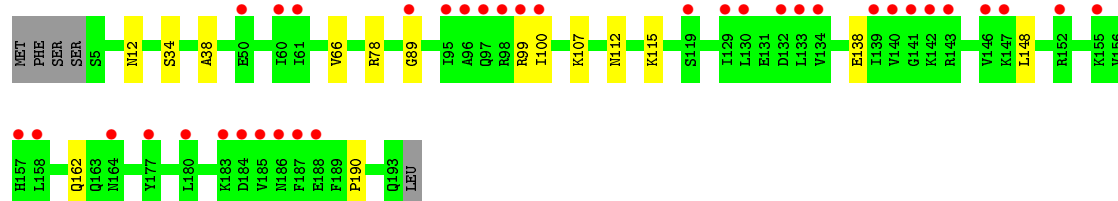
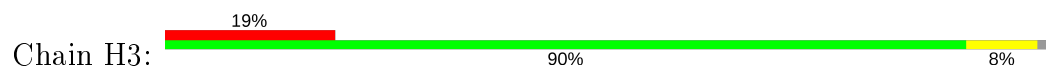
Chain H1: 



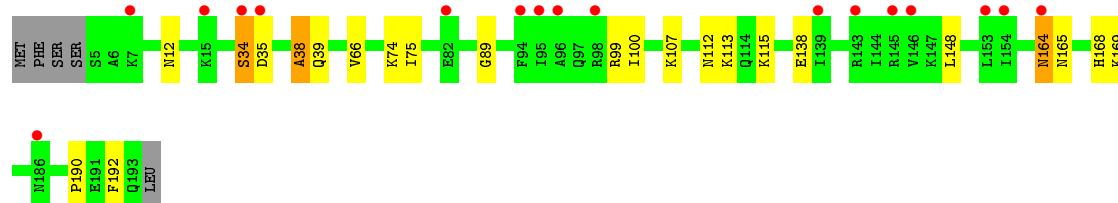
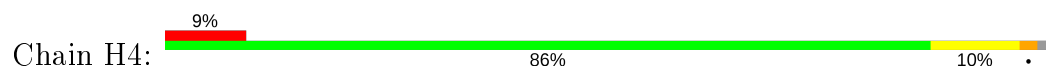
- Molecule 27: 40S ribosomal protein S7



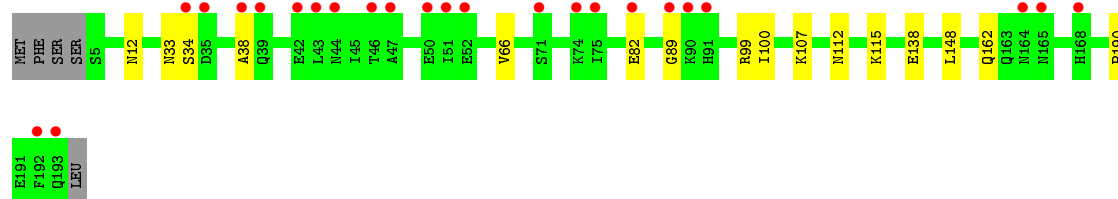
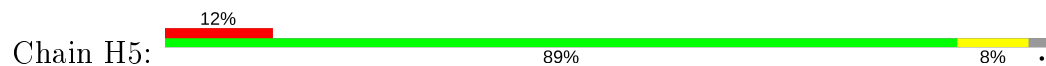
- Molecule 27: 40S ribosomal protein S7



- Molecule 27: 40S ribosomal protein S7

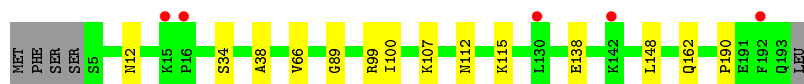


- Molecule 27: 40S ribosomal protein S7

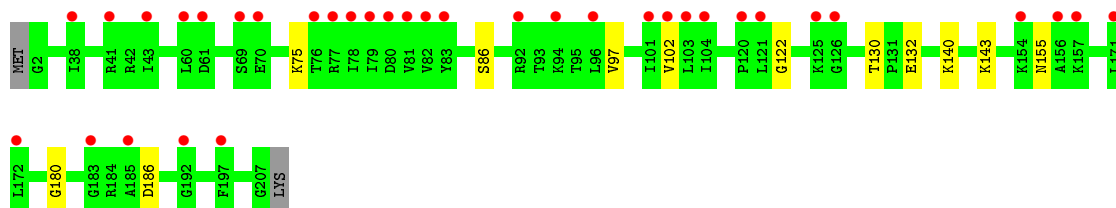


- Molecule 27: 40S ribosomal protein S7

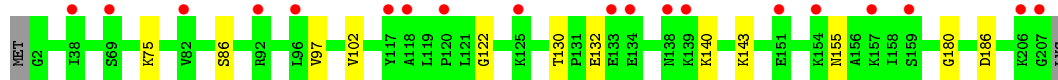
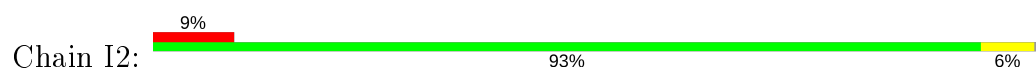




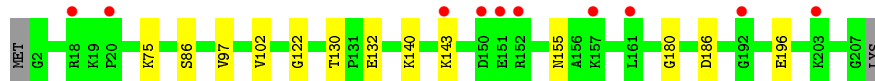
- Molecule 28: 40S ribosomal protein S8



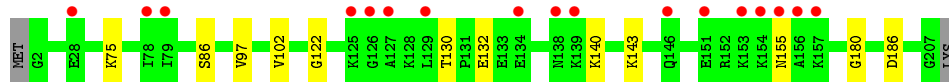
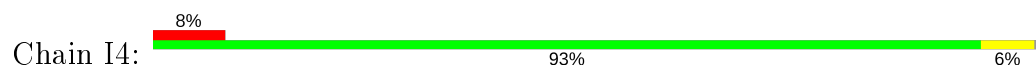
- Molecule 28: 40S ribosomal protein S8



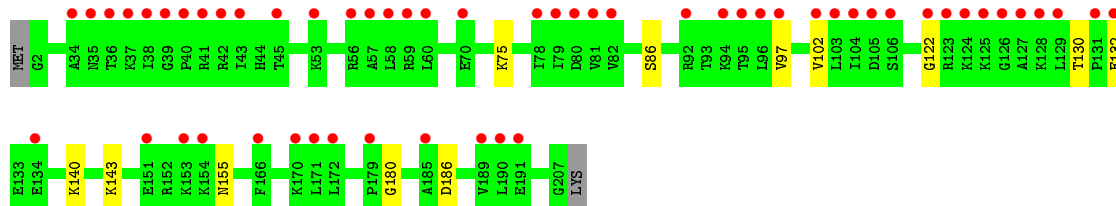
- Molecule 28: 40S ribosomal protein S8



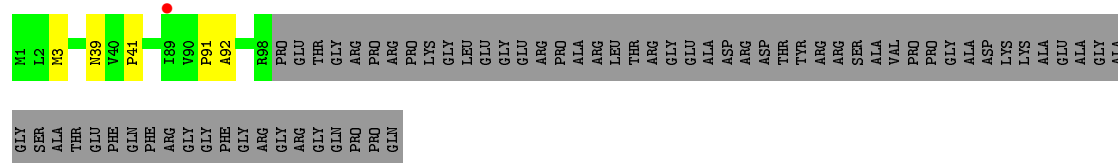
- Molecule 28: 40S ribosomal protein S8



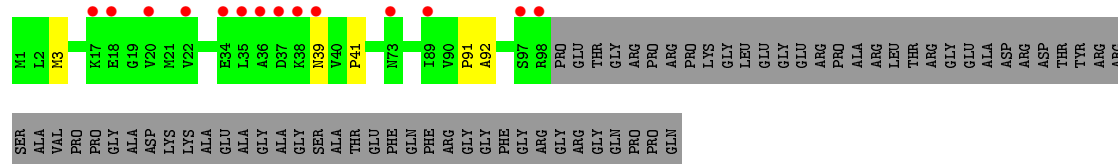
- Molecule 28: 40S ribosomal protein S8



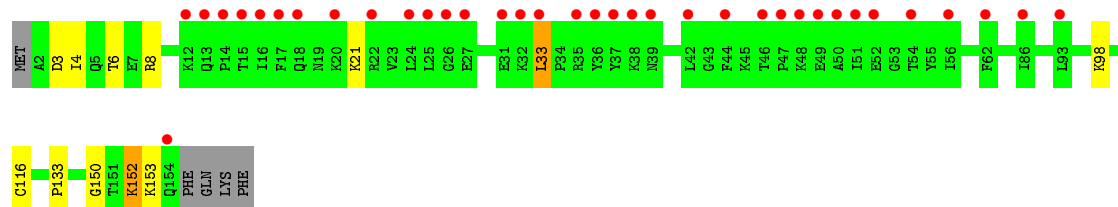
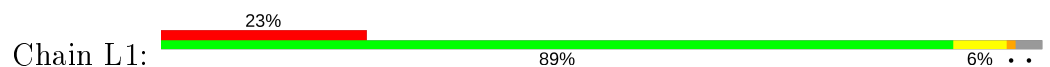
- Molecule 28: 40S ribosomal protein S8



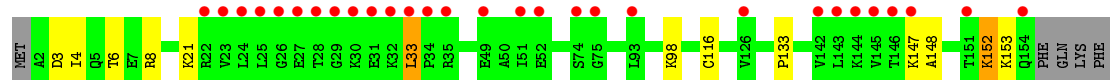
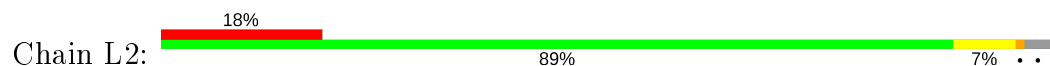
- Molecule 29: 40S ribosomal protein S10



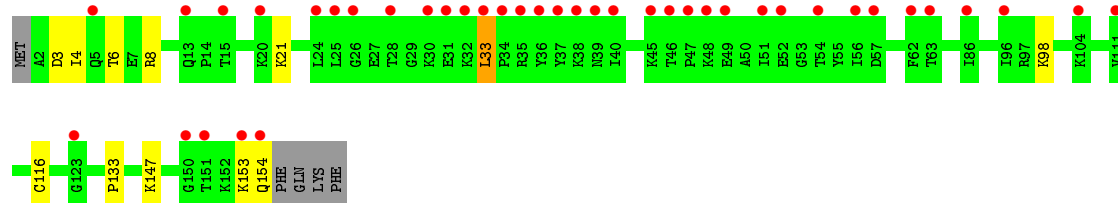
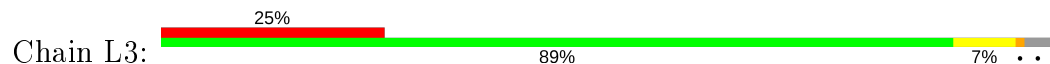
- Molecule 30: 40S ribosomal protein S11



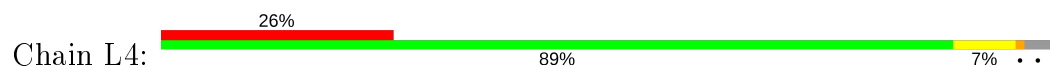
- Molecule 30: 40S ribosomal protein S11

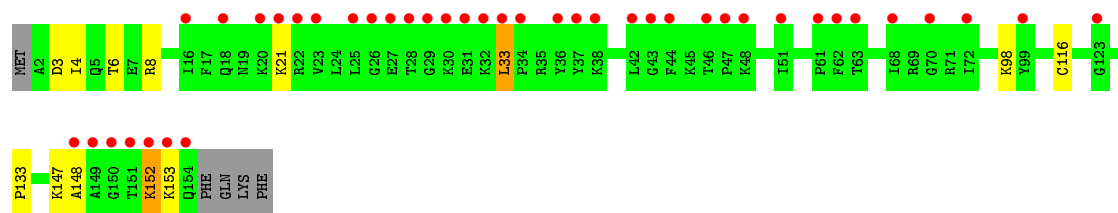


- Molecule 30: 40S ribosomal protein S11

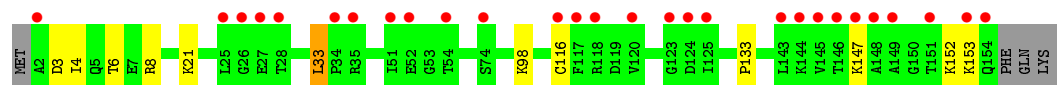
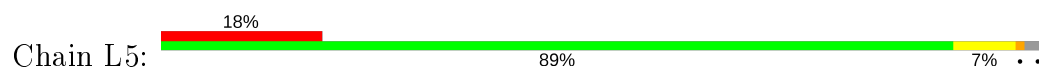


- Molecule 30: 40S ribosomal protein S11

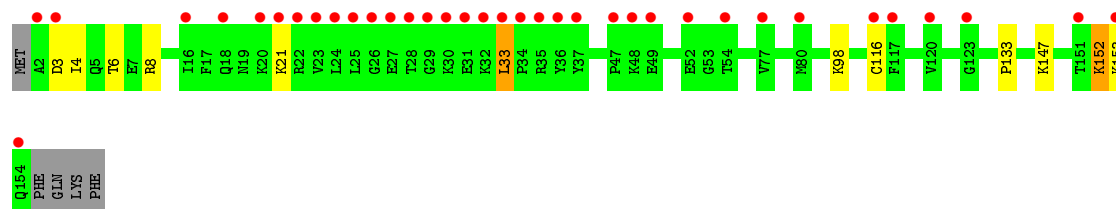
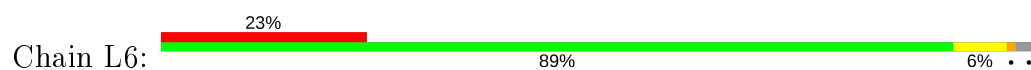




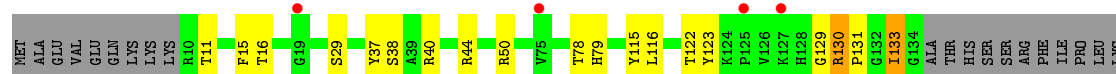
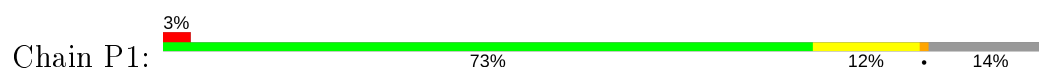
- Molecule 30: 40S ribosomal protein S11



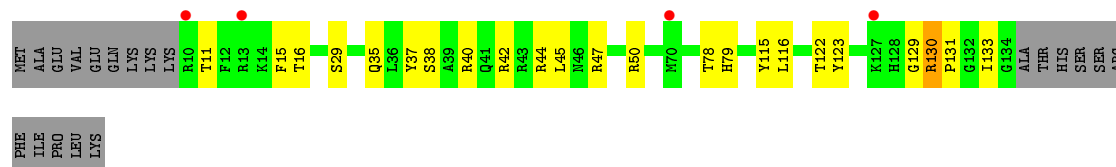
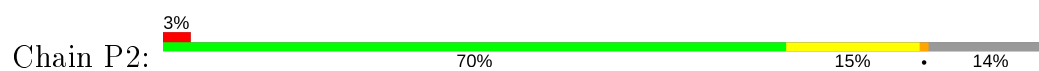
- Molecule 30: 40S ribosomal protein S11



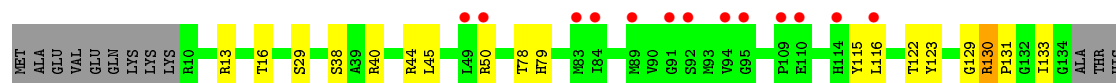
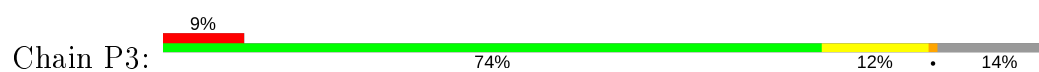
- Molecule 31: 40S ribosomal protein S15



- Molecule 31: 40S ribosomal protein S15

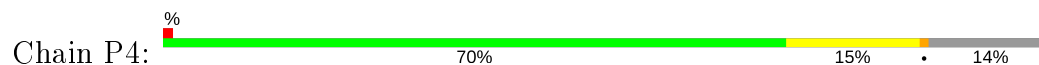


- Molecule 31: 40S ribosomal protein S15



SER
SER
GLU
ARG
PHE
ILE
PRO
LEU
LYS

- Molecule 31: 40S ribosomal protein S15



MET ALA GLU VAL GLN LYS LYS R10 T11 F15 T16 S29 Q35 Q36 Y37 S38 A39 R40 Q41 R42 R43 R44 L45 L49 R50 T78 H79 Y115 L116 T122 Y123 G129 R130 P131 G132 I133 G134 ALA THR HIS SER ARG PHE ILE PRO LEU LYS

- Molecule 31: 40S ribosomal protein S15



MET ALA GLU VAL GLN LYS LYS R10 K14 S29 Q35 L36 Y37 S38 A39 R40 Q41 R42 R43 R44 L45 R50 T78 H79 K108 P109 I112 Y115 L116 T122 Y123 G129 R130 P131 G132 I133 G134 ALA THR HIS SER ARG PHE ILE PRO LEU LYS

- Molecule 31: 40S ribosomal protein S15



MET ALA GLU VAL GLN LYS LYS R10 T11 F15 T16 S29 Y37 R40 R44 R45 R50 P69 M70 T77 T78 H79 P93 Q104 V105 E106 Y115 L116 T122 Y123 K124 P125 G129 R130 P131 G132 I133 G134 ALA THR HIS SER ARG PHE ILE PRO LEU LYS

ILE
PRO
LEU
LYS

- Molecule 32: 40S ribosomal protein S16



M1 G5 P6 K16 K17 L32 L39 I42 R45 T46 L47 Q48 L56 L57 V100 D101 R117 A122 D123 P135 S144 Y145 R146

- Molecule 32: 40S ribosomal protein S16



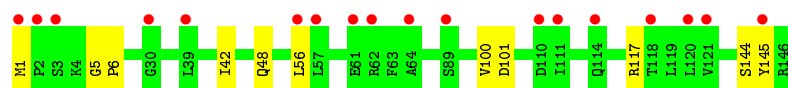
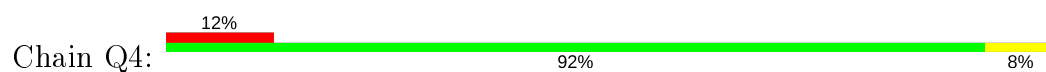
M1 P2 S3 K4 G5 P6 G14 L32 L39 I42 Q48 L52 L56 L57 V78 S89 L92 V100 D101 D110 R117 L120 V121 A122 S144 Y145 R146

- Molecule 32: 40S ribosomal protein S16

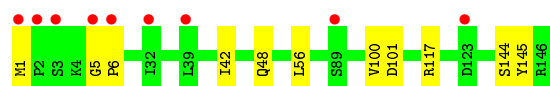


M1 P2 S3 K4 G5 P6 G30 I42 Q48 L56 L57 V100 D101 R117 L120 V121 S144 Y145 R146

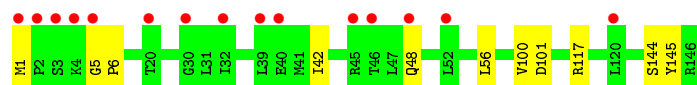
- Molecule 32: 40S ribosomal protein S16



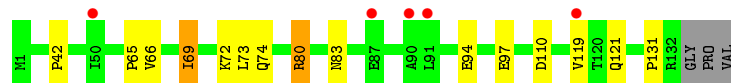
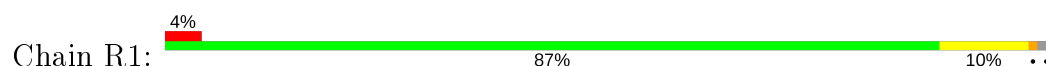
- Molecule 32: 40S ribosomal protein S16



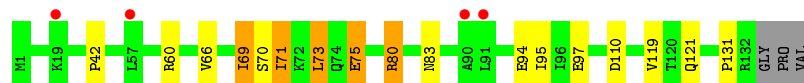
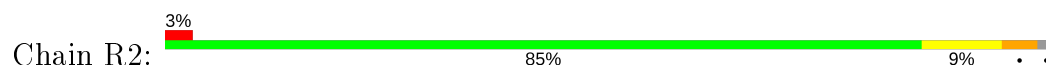
- Molecule 32: 40S ribosomal protein S16



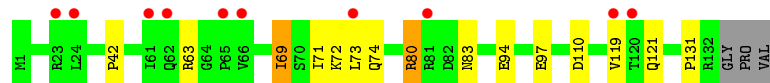
- Molecule 33: 40S ribosomal protein S17



- Molecule 33: 40S ribosomal protein S17



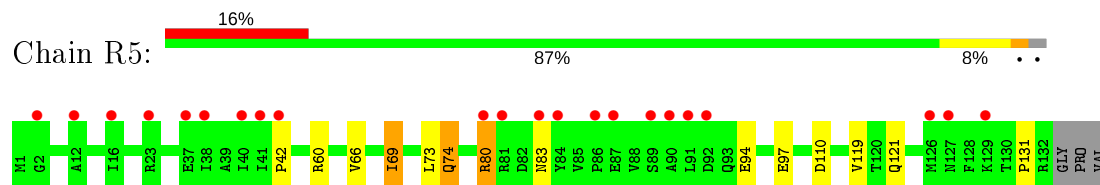
- Molecule 33: 40S ribosomal protein S17



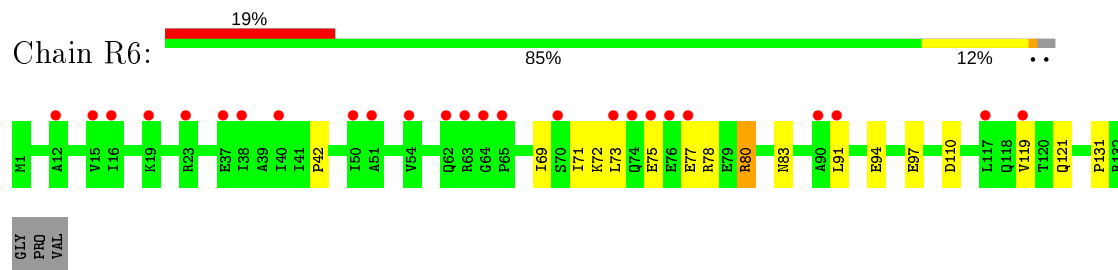
- Molecule 33: 40S ribosomal protein S17



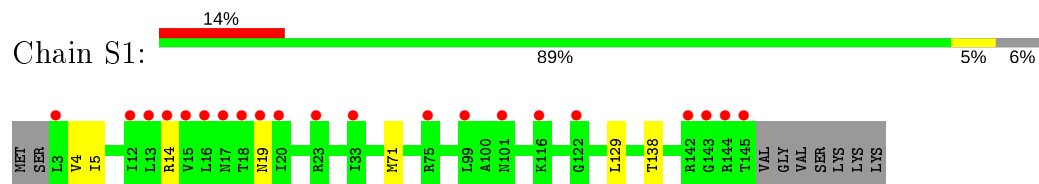
- Molecule 33: 40S ribosomal protein S17



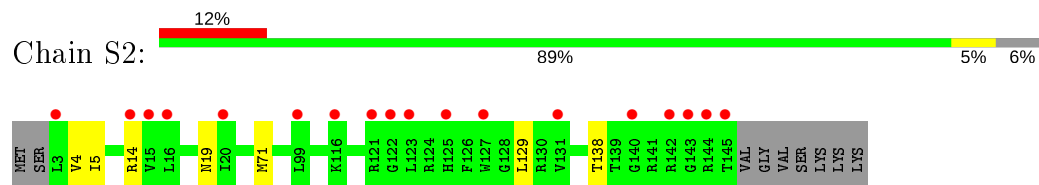
- Molecule 33: 40S ribosomal protein S17



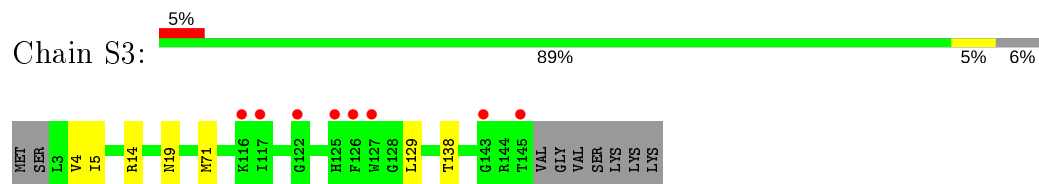
- Molecule 34: 40S ribosomal protein S18



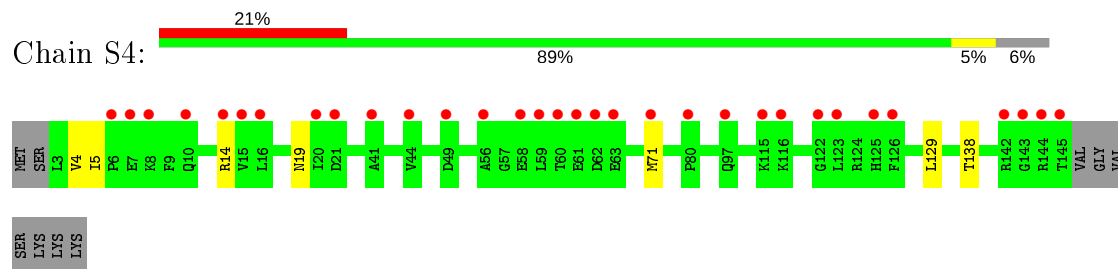
- Molecule 34: 40S ribosomal protein S18



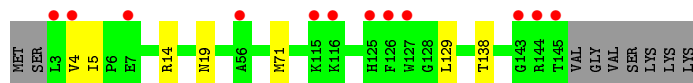
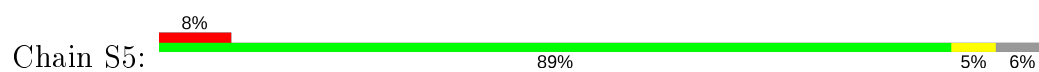
- Molecule 34: 40S ribosomal protein S18



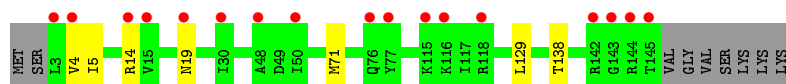
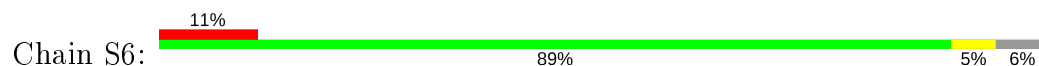
- Molecule 34: 40S ribosomal protein S18



- Molecule 34: 40S ribosomal protein S18



- Molecule 34: 40S ribosomal protein S18



- Molecule 35: 60S ribosomal protein L41



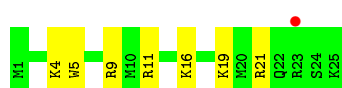
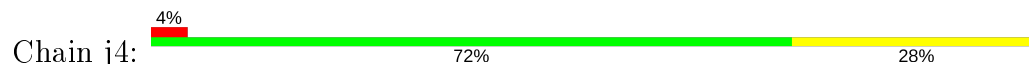
- Molecule 35: 60S ribosomal protein L41



- Molecule 35: 60S ribosomal protein L41



- Molecule 35: 60S ribosomal protein L41



- Molecule 35: 60S ribosomal protein L41



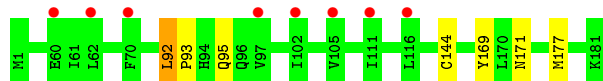
- Molecule 35: 60S ribosomal protein L41

Chain j6:  68% 32%



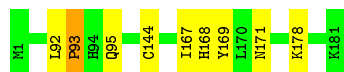
- Molecule 36: Malignant T-cell-amplified sequence 1

Chain k1:  4% 96% ..



- Molecule 36: Malignant T-cell-amplified sequence 1

Chain k2:  95% ..



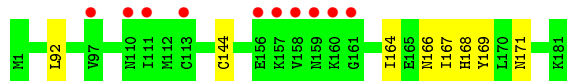
- Molecule 36: Malignant T-cell-amplified sequence 1

Chain k3:  97% ..



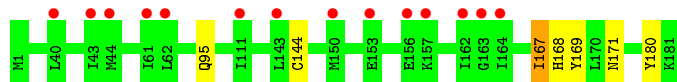
- Molecule 36: Malignant T-cell-amplified sequence 1

Chain k4:  6% 96% .



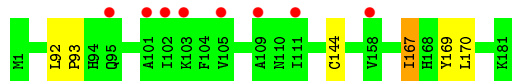
- Molecule 36: Malignant T-cell-amplified sequence 1

Chain k5:  8% 96% ..

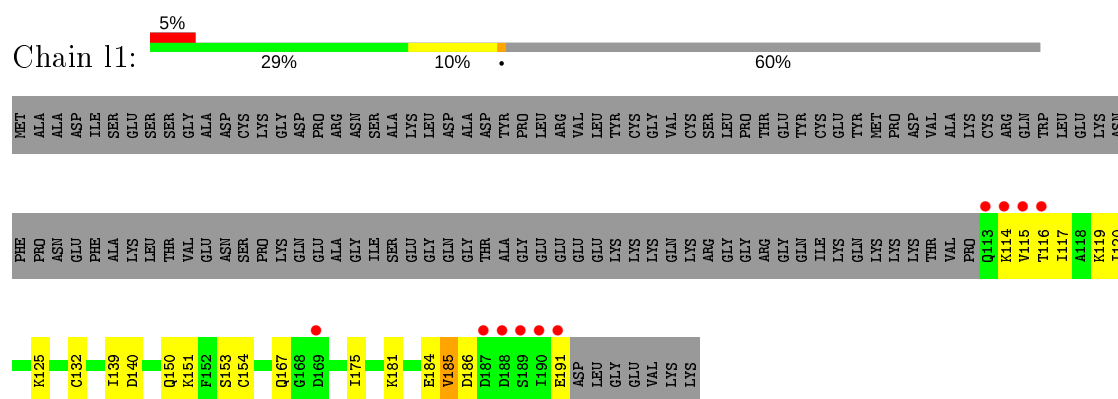


- Molecule 36: Malignant T-cell-amplified sequence 1

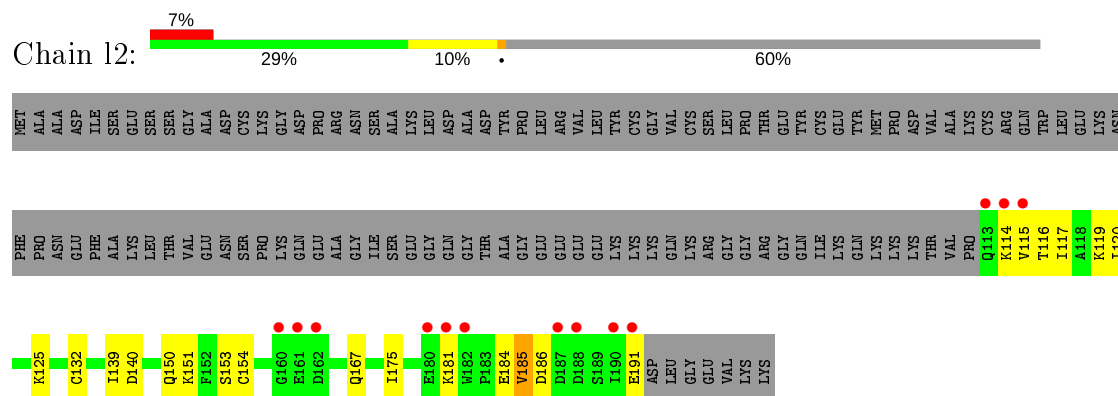
Chain k6:  4% 97% ..



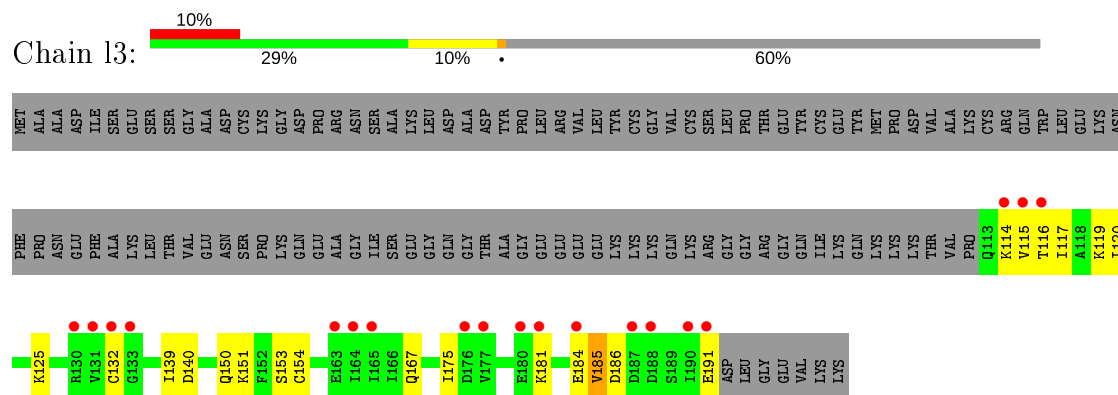
- Molecule 37: Density-regulated protein



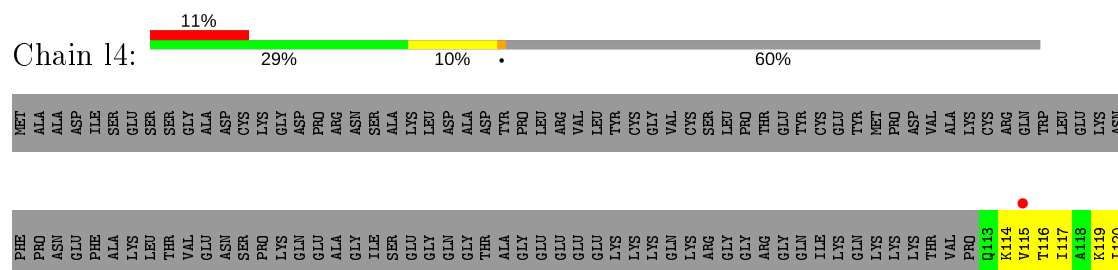
• Molecule 37: Density-regulated protein

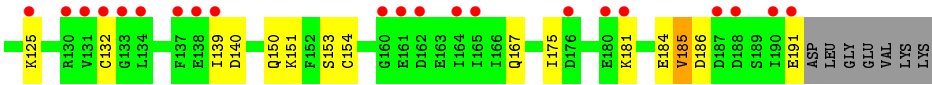


• Molecule 37: Density-regulated protein

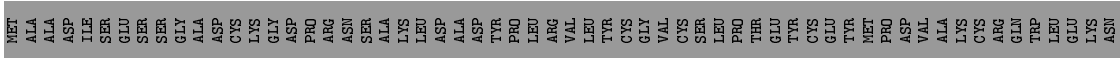


• Molecule 37: Density-regulated protein

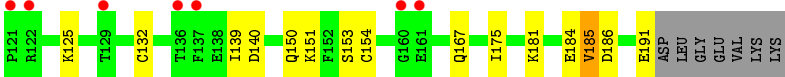
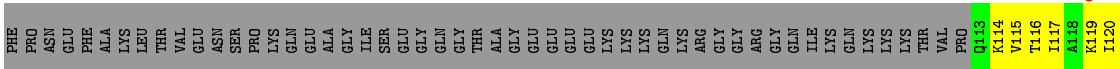
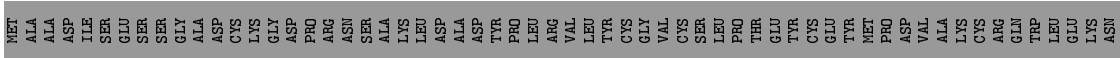




● Molecule 37: Density-regulated protein



● Molecule 37: Density-regulated protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	334.67Å 597.13Å 336.50Å 90.00° 120.29° 90.00°	Depositor
Resolution (Å)	116.93 – 6.00 116.93 – 5.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (116.93-6.00) 80.5 (116.93-5.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 5.12Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.323 , 0.321 0.322 , 0.319	Depositor DCC
R_{free} test set	19868 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	278.9	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , -31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.094 for -h-l,k,h 0.094 for l,k,-h-l 0.099 for l,-k,h 0.097 for h,-k,-h-l 0.118 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	470574	wwPDB-VP
Average B, all atoms (Å ²)	204.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	T1	0.26	0/1131	0.48	0/1515
1	T2	0.26	0/1131	0.48	0/1515
1	T3	0.26	0/1131	0.48	0/1515
1	T4	0.26	0/1131	0.48	0/1515
1	T5	0.26	0/1131	0.48	0/1515
1	T6	0.26	0/1131	0.48	0/1515
2	U1	0.29	0/831	0.55	0/1115
2	U2	0.29	0/831	0.55	0/1115
2	U3	0.29	0/831	0.56	0/1115
2	U4	0.28	0/831	0.56	0/1115
2	U5	0.29	0/831	0.56	0/1115
2	U6	0.29	0/831	0.56	0/1115
3	V1	0.27	0/643	0.44	0/860
3	V2	0.27	0/643	0.45	0/860
3	V3	0.27	0/643	0.45	0/860
3	V4	0.27	0/643	0.45	0/860
3	V5	0.26	0/643	0.45	0/860
3	V6	0.27	0/643	0.45	0/860
4	X1	0.30	0/1116	0.48	0/1490
4	X2	0.30	0/1116	0.48	0/1490
4	X3	0.30	0/1116	0.47	0/1490
4	X4	0.30	0/1116	0.48	0/1490
4	X5	0.30	0/1116	0.48	0/1490
4	X6	0.30	0/1116	0.48	0/1490
5	a1	0.49	0/863	0.65	3/1159 (0.3%)
5	a2	0.50	0/863	0.65	3/1159 (0.3%)
5	a3	0.49	0/863	0.65	3/1159 (0.3%)
5	a4	0.50	0/863	0.65	3/1159 (0.3%)
5	a5	0.50	0/863	0.65	3/1159 (0.3%)
5	a6	0.49	0/863	0.65	3/1159 (0.3%)
6	c1	0.26	0/508	0.51	0/680
6	c2	0.26	0/508	0.51	0/680

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	c3	0.27	0/508	0.51	0/680
6	c4	0.27	0/508	0.51	0/680
6	c5	0.26	0/508	0.51	0/680
6	c6	0.26	0/508	0.51	0/680
7	d1	0.27	0/455	0.42	0/603
7	d2	0.27	0/455	0.42	0/603
7	d3	0.27	0/455	0.42	0/603
7	d4	0.27	0/455	0.42	0/603
7	d5	0.27	0/455	0.42	0/603
7	d6	0.28	0/455	0.42	0/603
8	f1	0.27	0/595	0.43	0/785
8	f2	0.27	0/595	0.43	0/785
8	f3	0.27	0/595	0.43	0/785
8	f4	0.27	0/595	0.43	0/785
8	f5	0.26	0/595	0.43	0/785
8	f6	0.27	0/595	0.43	0/785
9	g1	0.25	0/2493	0.50	0/3394
9	g2	0.25	0/2493	0.50	0/3394
9	g3	0.25	0/2493	0.50	0/3394
9	g4	0.25	0/2493	0.50	0/3394
9	g5	0.25	0/2493	0.50	0/3394
9	g6	0.25	0/2493	0.50	0/3394
10	C1	0.29	0/1762	0.48	0/2381
10	C2	0.29	0/1762	0.48	0/2381
10	C3	0.29	0/1762	0.48	0/2381
10	C4	0.29	0/1762	0.48	0/2381
10	C5	0.29	0/1762	0.48	0/2381
10	C6	0.29	0/1762	0.48	0/2381
11	G1	0.26	0/1946	0.49	0/2590
11	G2	0.26	0/1946	0.49	0/2590
11	G3	0.26	0/1946	0.49	0/2590
11	G4	0.26	0/1946	0.49	0/2590
11	G5	0.26	0/1946	0.49	0/2590
11	G6	0.26	0/1946	0.49	0/2590
12	J1	0.27	0/1550	0.47	0/2069
12	J2	0.27	0/1550	0.47	0/2069
12	J3	0.27	0/1550	0.47	0/2069
12	J4	0.27	0/1550	0.48	0/2069
12	J5	0.27	0/1550	0.48	0/2069
12	J6	0.27	0/1550	0.48	0/2069
13	M1	0.33	0/963	0.49	0/1291
13	M2	0.33	0/963	0.49	0/1291
13	M3	0.33	0/963	0.48	0/1291

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
13	M4	0.33	0/963	0.49	0/1291
13	M5	0.33	0/963	0.49	0/1291
13	M6	0.33	0/963	0.49	0/1291
14	N1	0.30	0/1232	0.47	0/1656
14	N2	0.30	0/1232	0.47	0/1656
14	N3	0.29	0/1232	0.46	0/1656
14	N4	0.30	0/1232	0.47	0/1656
14	N5	0.29	0/1232	0.46	0/1656
14	N6	0.29	0/1232	0.47	0/1656
15	O1	0.30	0/1062	0.58	1/1425 (0.1%)
15	O2	0.30	0/1062	0.58	1/1425 (0.1%)
15	O3	0.30	0/1062	0.58	1/1425 (0.1%)
15	O4	0.30	0/1062	0.58	1/1425 (0.1%)
15	O5	0.30	0/1062	0.58	1/1425 (0.1%)
15	O6	0.30	0/1062	0.58	1/1425 (0.1%)
16	W1	0.30	0/1051	0.52	0/1406
16	W2	0.30	0/1051	0.52	0/1406
16	W3	0.30	0/1051	0.52	0/1406
16	W4	0.30	0/1051	0.52	0/1406
16	W5	0.30	0/1051	0.52	0/1406
16	W6	0.30	0/1051	0.52	0/1406
17	Y1	0.27	0/1083	0.47	0/1438
17	Y2	0.27	0/1083	0.47	0/1438
17	Y3	0.27	0/1083	0.47	0/1438
17	Y4	0.27	0/1083	0.47	0/1438
17	Y5	0.27	0/1083	0.47	0/1438
17	Y6	0.26	0/1083	0.47	0/1438
18	Z1	0.26	0/604	0.55	0/810
18	Z2	0.27	0/604	0.55	0/810
18	Z3	0.26	0/604	0.55	0/810
18	Z4	0.26	0/604	0.55	0/810
18	Z5	0.26	0/604	0.55	0/810
18	Z6	0.27	0/604	0.55	0/810
19	b1	0.27	0/665	0.66	1/891 (0.1%)
19	b2	0.28	0/665	0.51	0/891
19	b3	0.28	0/665	0.51	0/891
19	b4	0.27	0/665	0.71	1/891 (0.1%)
19	b5	0.28	0/665	0.51	0/891
19	b6	0.28	0/665	0.51	0/891
20	e1	0.25	0/465	0.86	1/612 (0.2%)
20	e2	0.33	0/465	0.48	1/612 (0.2%)
20	e3	0.33	0/465	0.50	1/612 (0.2%)
20	e4	0.32	0/465	0.47	1/612 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	e5	0.24	0/465	0.40	0/612
20	e6	0.33	0/465	0.50	1/612 (0.2%)
21	i1	0.37	1/41243 (0.0%)	0.78	14/64257 (0.0%)
21	i2	0.37	0/41242	0.77	11/64253 (0.0%)
21	i3	0.38	0/41242	0.77	9/64253 (0.0%)
21	i4	0.39	1/41243 (0.0%)	0.78	14/64257 (0.0%)
21	i5	0.44	1/41243 (0.0%)	0.78	14/64257 (0.0%)
21	i6	0.42	1/41243 (0.0%)	0.78	15/64257 (0.0%)
22	A1	0.26	0/1784	0.49	0/2424
22	A2	0.26	0/1784	0.48	0/2424
22	A3	0.27	0/1784	0.49	0/2424
22	A4	0.26	0/1784	0.49	0/2424
22	A5	0.27	0/1784	0.49	0/2424
22	A6	0.27	0/1784	0.49	0/2424
23	B1	0.29	0/1765	0.52	0/2362
23	B2	0.29	0/1765	0.53	0/2362
23	B3	0.29	0/1765	0.53	0/2362
23	B4	0.29	0/1765	0.53	0/2362
23	B5	0.29	0/1765	0.53	0/2362
23	B6	0.29	0/1765	0.52	0/2362
24	D1	0.27	0/1793	0.49	0/2414
24	D2	0.27	0/1793	0.49	0/2414
24	D3	0.27	0/1793	0.50	0/2414
24	D4	0.27	0/1793	0.50	0/2414
24	D5	0.27	0/1793	0.50	0/2414
24	D6	0.28	0/1793	0.50	0/2414
25	E1	0.27	0/2118	0.53	1/2849 (0.0%)
25	E2	0.27	0/2118	0.53	1/2849 (0.0%)
25	E3	0.27	0/2118	0.53	1/2849 (0.0%)
25	E4	0.27	0/2118	0.53	1/2849 (0.0%)
25	E5	0.27	0/2118	0.53	1/2849 (0.0%)
25	E6	0.27	0/2118	0.53	1/2849 (0.0%)
26	F1	0.28	0/1531	0.50	0/2059
26	F2	0.28	0/1531	0.50	0/2059
26	F3	0.28	0/1531	0.50	0/2059
26	F4	0.28	0/1531	0.50	0/2059
26	F5	0.28	0/1531	0.50	0/2059
26	F6	0.27	0/1531	0.50	0/2059
27	H1	0.27	0/1544	0.50	0/2068
27	H2	0.27	0/1544	0.50	0/2068
27	H3	0.27	0/1544	0.50	0/2068
27	H4	0.27	0/1544	0.50	0/2068
27	H5	0.27	0/1544	0.51	0/2068

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	H6	0.26	0/1544	0.50	0/2068
28	I1	0.28	0/1715	0.48	0/2287
28	I2	0.28	0/1715	0.49	0/2287
28	I3	0.28	0/1715	0.48	0/2287
28	I4	0.28	0/1715	0.48	0/2287
28	I5	0.28	0/1715	0.49	0/2287
28	I6	0.28	0/1715	0.48	0/2287
29	K1	0.27	0/851	0.49	0/1147
29	K2	0.28	0/851	0.49	0/1147
29	K3	0.28	0/851	0.49	0/1147
29	K4	0.28	0/851	0.49	0/1147
29	K5	0.28	0/851	0.49	0/1147
29	K6	0.28	0/851	0.49	0/1147
30	L1	0.30	0/1268	0.51	1/1696 (0.1%)
30	L2	0.30	0/1268	0.51	1/1696 (0.1%)
30	L3	0.30	0/1268	0.51	1/1696 (0.1%)
30	L4	0.30	0/1268	0.51	1/1696 (0.1%)
30	L5	0.30	0/1268	0.51	1/1696 (0.1%)
30	L6	0.30	0/1268	0.51	1/1696 (0.1%)
31	P1	0.28	0/1053	0.44	1/1406 (0.1%)
31	P2	0.28	0/1053	0.44	1/1406 (0.1%)
31	P3	0.28	0/1053	0.44	1/1406 (0.1%)
31	P4	0.28	0/1053	0.44	1/1406 (0.1%)
31	P5	0.27	0/1053	0.44	1/1406 (0.1%)
31	P6	0.28	0/1053	0.44	1/1406 (0.1%)
32	Q1	0.33	0/1177	0.50	0/1575
32	Q2	0.33	0/1177	0.50	0/1575
32	Q3	0.33	0/1177	0.51	0/1575
32	Q4	0.33	0/1177	0.51	0/1575
32	Q5	0.33	0/1177	0.50	0/1575
32	Q6	0.33	0/1177	0.51	0/1575
33	R1	0.27	0/1086	0.56	0/1457
33	R2	0.27	0/1086	0.56	0/1457
33	R3	0.27	0/1086	0.56	0/1457
33	R4	0.27	0/1086	0.55	0/1457
33	R5	0.27	0/1086	0.56	0/1457
33	R6	0.27	0/1086	0.56	0/1457
34	S1	0.36	0/1202	0.52	1/1610 (0.1%)
34	S2	0.36	0/1202	0.52	1/1610 (0.1%)
34	S3	0.36	0/1202	0.52	1/1610 (0.1%)
34	S4	0.36	0/1202	0.52	1/1610 (0.1%)
34	S5	0.36	0/1202	0.53	1/1610 (0.1%)
34	S6	0.36	0/1202	0.52	1/1610 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	j1	0.19	0/240	0.27	0/305
35	j2	0.19	0/240	0.26	0/305
35	j3	0.20	0/240	0.26	0/305
35	j4	0.19	0/240	0.26	0/305
35	j5	0.20	0/240	0.26	0/305
35	j6	0.20	0/240	0.27	0/305
36	k1	0.57	0/1455	0.60	1/1968 (0.1%)
36	k2	0.67	2/1455 (0.1%)	0.78	6/1968 (0.3%)
36	k3	0.59	0/1455	1.24	3/1968 (0.2%)
36	k4	0.58	0/1455	0.54	0/1968
36	k5	0.60	1/1455 (0.1%)	0.86	3/1968 (0.2%)
36	k6	0.58	0/1455	0.55	0/1968
37	l1	0.40	0/638	0.72	4/859 (0.5%)
37	l2	0.40	0/638	0.72	4/859 (0.5%)
37	l3	0.40	0/638	0.71	4/859 (0.5%)
37	l4	0.40	0/638	0.71	4/859 (0.5%)
37	l5	0.40	0/638	0.72	4/859 (0.5%)
37	l6	0.40	0/638	0.72	4/859 (0.5%)
All	All	0.35	7/500884 (0.0%)	0.67	169/725470 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
33	R1	0	1
33	R2	0	1
33	R3	0	1
33	R4	0	1
33	R5	0	1
36	k2	0	1
36	k3	0	2
36	k5	0	1
All	All	0	9

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	i5	1689	C	O3'-P	44.78	2.14	1.61
21	i6	1689	C	O3'-P	38.40	2.07	1.61
21	i4	1689	C	O3'-P	25.06	1.91	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	k2	92	LEU	C-N	11.28	1.55	1.34
36	k2	93	PRO	C-N	6.37	1.48	1.34

The worst 5 of 169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	k3	180	TYR	O-C-N	-37.78	62.25	122.70
21	i1	1689	C	P-O3'-C3'	-30.42	83.20	119.70
36	k5	167	ILE	O-C-N	-26.56	80.21	122.70
36	k3	180	TYR	CA-C-N	25.08	172.38	117.20
21	i4	1689	C	P-O3'-C3'	-25.00	89.69	119.70

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	R1	69	ILE	Peptide
33	R2	69	ILE	Peptide
33	R3	69	ILE	Peptide
33	R4	69	ILE	Peptide
33	R5	69	ILE	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 X-ray entries followed by that with respect to entries of similar resolution.

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	T1	141/145 (97%)	119 (84%)	15 (11%)	7 (5%)	2	20
1	T2	141/145 (97%)	119 (84%)	15 (11%)	7 (5%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T3	141/145 (97%)	119 (84%)	16 (11%)	6 (4%)	2	22
1	T4	141/145 (97%)	119 (84%)	16 (11%)	6 (4%)	2	22
1	T5	141/145 (97%)	119 (84%)	15 (11%)	7 (5%)	2	20
1	T6	141/145 (97%)	119 (84%)	16 (11%)	6 (4%)	2	22
2	U1	102/119 (86%)	84 (82%)	12 (12%)	6 (6%)	1	17
2	U2	102/119 (86%)	84 (82%)	12 (12%)	6 (6%)	1	17
2	U3	102/119 (86%)	84 (82%)	12 (12%)	6 (6%)	1	17
2	U4	102/119 (86%)	84 (82%)	12 (12%)	6 (6%)	1	17
2	U5	102/119 (86%)	84 (82%)	12 (12%)	6 (6%)	1	17
2	U6	102/119 (86%)	84 (82%)	12 (12%)	6 (6%)	1	17
3	V1	81/83 (98%)	65 (80%)	11 (14%)	5 (6%)	1	16
3	V2	81/83 (98%)	66 (82%)	10 (12%)	5 (6%)	1	16
3	V3	81/83 (98%)	65 (80%)	11 (14%)	5 (6%)	1	16
3	V4	81/83 (98%)	65 (80%)	11 (14%)	5 (6%)	1	16
3	V5	81/83 (98%)	65 (80%)	11 (14%)	5 (6%)	1	16
3	V6	81/83 (98%)	65 (80%)	11 (14%)	5 (6%)	1	16
4	X1	139/143 (97%)	114 (82%)	12 (9%)	13 (9%)	0	10
4	X2	139/143 (97%)	114 (82%)	12 (9%)	13 (9%)	0	10
4	X3	139/143 (97%)	114 (82%)	12 (9%)	13 (9%)	0	10
4	X4	139/143 (97%)	114 (82%)	12 (9%)	13 (9%)	0	10
4	X5	139/143 (97%)	114 (82%)	12 (9%)	13 (9%)	0	10
4	X6	139/143 (97%)	114 (82%)	12 (9%)	13 (9%)	0	10
5	a1	105/115 (91%)	73 (70%)	19 (18%)	13 (12%)	0	5
5	a2	105/115 (91%)	73 (70%)	19 (18%)	13 (12%)	0	5
5	a3	105/115 (91%)	73 (70%)	19 (18%)	13 (12%)	0	5
5	a4	105/115 (91%)	73 (70%)	19 (18%)	13 (12%)	0	5
5	a5	105/115 (91%)	73 (70%)	19 (18%)	13 (12%)	0	5
5	a6	105/115 (91%)	73 (70%)	19 (18%)	13 (12%)	0	5
6	c1	62/69 (90%)	47 (76%)	9 (14%)	6 (10%)	0	9
6	c2	62/69 (90%)	47 (76%)	10 (16%)	5 (8%)	1	12
6	c3	62/69 (90%)	47 (76%)	10 (16%)	5 (8%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	c4	62/69 (90%)	47 (76%)	10 (16%)	5 (8%)	1	12
6	c5	62/69 (90%)	47 (76%)	9 (14%)	6 (10%)	0	9
6	c6	62/69 (90%)	47 (76%)	10 (16%)	5 (8%)	1	12
7	d1	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
7	d2	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
7	d3	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
7	d4	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
7	d5	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
7	d6	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
8	f1	70/156 (45%)	56 (80%)	10 (14%)	4 (6%)	1	18
8	f2	70/156 (45%)	56 (80%)	10 (14%)	4 (6%)	1	18
8	f3	70/156 (45%)	56 (80%)	10 (14%)	4 (6%)	1	18
8	f4	70/156 (45%)	57 (81%)	9 (13%)	4 (6%)	1	18
8	f5	70/156 (45%)	56 (80%)	10 (14%)	4 (6%)	1	18
8	f6	70/156 (45%)	55 (79%)	11 (16%)	4 (6%)	1	18
9	g1	311/317 (98%)	237 (76%)	58 (19%)	16 (5%)	2	19
9	g2	311/317 (98%)	236 (76%)	59 (19%)	16 (5%)	2	19
9	g3	311/317 (98%)	236 (76%)	59 (19%)	16 (5%)	2	19
9	g4	311/317 (98%)	237 (76%)	58 (19%)	16 (5%)	2	19
9	g5	311/317 (98%)	237 (76%)	58 (19%)	16 (5%)	2	19
9	g6	311/317 (98%)	236 (76%)	59 (19%)	16 (5%)	2	19
10	C1	220/293 (75%)	182 (83%)	27 (12%)	11 (5%)	2	20
10	C2	220/293 (75%)	181 (82%)	28 (13%)	11 (5%)	2	20
10	C3	220/293 (75%)	182 (83%)	27 (12%)	11 (5%)	2	20
10	C4	220/293 (75%)	182 (83%)	27 (12%)	11 (5%)	2	20
10	C5	220/293 (75%)	182 (83%)	27 (12%)	11 (5%)	2	20
10	C6	220/293 (75%)	182 (83%)	27 (12%)	11 (5%)	2	20
11	G1	235/249 (94%)	194 (83%)	25 (11%)	16 (7%)	1	15
11	G2	235/249 (94%)	195 (83%)	24 (10%)	16 (7%)	1	15
11	G3	235/249 (94%)	194 (83%)	25 (11%)	16 (7%)	1	15
11	G4	235/249 (94%)	194 (83%)	26 (11%)	15 (6%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	G5	235/249 (94%)	194 (83%)	25 (11%)	16 (7%)	1	15
11	G6	235/249 (94%)	194 (83%)	25 (11%)	16 (7%)	1	15
12	J1	183/194 (94%)	157 (86%)	16 (9%)	10 (6%)	2	19
12	J2	183/194 (94%)	157 (86%)	16 (9%)	10 (6%)	2	19
12	J3	183/194 (94%)	157 (86%)	16 (9%)	10 (6%)	2	19
12	J4	183/194 (94%)	157 (86%)	16 (9%)	10 (6%)	2	19
12	J5	183/194 (94%)	157 (86%)	16 (9%)	10 (6%)	2	19
12	J6	183/194 (94%)	157 (86%)	16 (9%)	10 (6%)	2	19
13	M1	121/132 (92%)	111 (92%)	8 (7%)	2 (2%)	9	42
13	M2	121/132 (92%)	111 (92%)	8 (7%)	2 (2%)	9	42
13	M3	121/132 (92%)	111 (92%)	8 (7%)	2 (2%)	9	42
13	M4	121/132 (92%)	111 (92%)	8 (7%)	2 (2%)	9	42
13	M5	121/132 (92%)	111 (92%)	8 (7%)	2 (2%)	9	42
13	M6	121/132 (92%)	111 (92%)	8 (7%)	2 (2%)	9	42
14	N1	148/151 (98%)	125 (84%)	14 (10%)	9 (6%)	1	16
14	N2	148/151 (98%)	125 (84%)	14 (10%)	9 (6%)	1	16
14	N3	148/151 (98%)	124 (84%)	15 (10%)	9 (6%)	1	16
14	N4	148/151 (98%)	125 (84%)	14 (10%)	9 (6%)	1	16
14	N5	148/151 (98%)	124 (84%)	15 (10%)	9 (6%)	1	16
14	N6	148/151 (98%)	125 (84%)	13 (9%)	10 (7%)	1	15
15	O1	138/151 (91%)	101 (73%)	24 (17%)	13 (9%)	0	10
15	O2	138/151 (91%)	101 (73%)	24 (17%)	13 (9%)	0	10
15	O3	138/151 (91%)	101 (73%)	24 (17%)	13 (9%)	0	10
15	O4	138/151 (91%)	101 (73%)	24 (17%)	13 (9%)	0	10
15	O5	138/151 (91%)	101 (73%)	24 (17%)	13 (9%)	0	10
15	O6	138/151 (91%)	101 (73%)	24 (17%)	13 (9%)	0	10
16	W1	127/130 (98%)	109 (86%)	13 (10%)	5 (4%)	3	23
16	W2	127/130 (98%)	109 (86%)	13 (10%)	5 (4%)	3	23
16	W3	127/130 (98%)	108 (85%)	13 (10%)	6 (5%)	2	21
16	W4	127/130 (98%)	109 (86%)	13 (10%)	5 (4%)	3	23
16	W5	127/130 (98%)	109 (86%)	13 (10%)	5 (4%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	W6	127/130 (98%)	109 (86%)	13 (10%)	5 (4%)	3	23
17	Y1	129/133 (97%)	108 (84%)	16 (12%)	5 (4%)	3	23
17	Y2	129/133 (97%)	109 (84%)	15 (12%)	5 (4%)	3	23
17	Y3	129/133 (97%)	109 (84%)	15 (12%)	5 (4%)	3	23
17	Y4	129/133 (97%)	109 (84%)	15 (12%)	5 (4%)	3	23
17	Y5	129/133 (97%)	109 (84%)	15 (12%)	5 (4%)	3	23
17	Y6	129/133 (97%)	108 (84%)	16 (12%)	5 (4%)	3	23
18	Z1	73/125 (58%)	54 (74%)	15 (20%)	4 (6%)	2	19
18	Z2	73/125 (58%)	54 (74%)	15 (20%)	4 (6%)	2	19
18	Z3	73/125 (58%)	54 (74%)	15 (20%)	4 (6%)	2	19
18	Z4	73/125 (58%)	54 (74%)	15 (20%)	4 (6%)	2	19
18	Z5	73/125 (58%)	54 (74%)	15 (20%)	4 (6%)	2	19
18	Z6	73/125 (58%)	54 (74%)	15 (20%)	4 (6%)	2	19
19	b1	81/84 (96%)	64 (79%)	12 (15%)	5 (6%)	1	16
19	b2	81/84 (96%)	67 (83%)	12 (15%)	2 (2%)	5	32
19	b3	81/84 (96%)	67 (83%)	11 (14%)	3 (4%)	3	25
19	b4	81/84 (96%)	65 (80%)	11 (14%)	5 (6%)	1	16
19	b5	81/84 (96%)	67 (83%)	10 (12%)	4 (5%)	2	20
19	b6	81/84 (96%)	67 (83%)	12 (15%)	2 (2%)	5	32
20	e1	56/133 (42%)	41 (73%)	11 (20%)	4 (7%)	1	14
20	e2	56/133 (42%)	37 (66%)	12 (21%)	7 (12%)	0	5
20	e3	56/133 (42%)	38 (68%)	12 (21%)	6 (11%)	0	8
20	e4	56/133 (42%)	35 (62%)	15 (27%)	6 (11%)	0	8
20	e5	56/133 (42%)	38 (68%)	11 (20%)	7 (12%)	0	5
20	e6	56/133 (42%)	38 (68%)	12 (21%)	6 (11%)	0	8
22	A1	220/295 (75%)	181 (82%)	31 (14%)	8 (4%)	3	25
22	A2	220/295 (75%)	180 (82%)	32 (14%)	8 (4%)	3	25
22	A3	220/295 (75%)	181 (82%)	31 (14%)	8 (4%)	3	25
22	A4	220/295 (75%)	181 (82%)	31 (14%)	8 (4%)	3	25
22	A5	220/295 (75%)	181 (82%)	31 (14%)	8 (4%)	3	25
22	A6	220/295 (75%)	181 (82%)	31 (14%)	8 (4%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	B1	212/264 (80%)	174 (82%)	31 (15%)	7 (3%)	4	26
23	B2	212/264 (80%)	174 (82%)	29 (14%)	9 (4%)	3	22
23	B3	212/264 (80%)	174 (82%)	30 (14%)	8 (4%)	3	24
23	B4	212/264 (80%)	174 (82%)	30 (14%)	8 (4%)	3	24
23	B5	212/264 (80%)	174 (82%)	30 (14%)	8 (4%)	3	24
23	B6	212/264 (80%)	174 (82%)	31 (15%)	7 (3%)	4	26
24	D1	225/243 (93%)	183 (81%)	24 (11%)	18 (8%)	1	12
24	D2	225/243 (93%)	183 (81%)	24 (11%)	18 (8%)	1	12
24	D3	225/243 (93%)	183 (81%)	24 (11%)	18 (8%)	1	12
24	D4	225/243 (93%)	183 (81%)	24 (11%)	18 (8%)	1	12
24	D5	225/243 (93%)	183 (81%)	24 (11%)	18 (8%)	1	12
24	D6	225/243 (93%)	183 (81%)	24 (11%)	18 (8%)	1	12
25	E1	260/263 (99%)	215 (83%)	30 (12%)	15 (6%)	1	17
25	E2	260/263 (99%)	215 (83%)	30 (12%)	15 (6%)	1	17
25	E3	260/263 (99%)	215 (83%)	30 (12%)	15 (6%)	1	17
25	E4	260/263 (99%)	215 (83%)	30 (12%)	15 (6%)	1	17
25	E5	260/263 (99%)	215 (83%)	30 (12%)	15 (6%)	1	17
25	E6	260/263 (99%)	215 (83%)	30 (12%)	15 (6%)	1	17
26	F1	189/204 (93%)	144 (76%)	30 (16%)	15 (8%)	1	12
26	F2	189/204 (93%)	144 (76%)	30 (16%)	15 (8%)	1	12
26	F3	189/204 (93%)	144 (76%)	30 (16%)	15 (8%)	1	12
26	F4	189/204 (93%)	144 (76%)	30 (16%)	15 (8%)	1	12
26	F5	189/204 (93%)	144 (76%)	30 (16%)	15 (8%)	1	12
26	F6	189/204 (93%)	144 (76%)	30 (16%)	15 (8%)	1	12
27	H1	187/194 (96%)	145 (78%)	28 (15%)	14 (8%)	1	13
27	H2	187/194 (96%)	145 (78%)	28 (15%)	14 (8%)	1	13
27	H3	187/194 (96%)	145 (78%)	28 (15%)	14 (8%)	1	13
27	H4	187/194 (96%)	146 (78%)	27 (14%)	14 (8%)	1	13
27	H5	187/194 (96%)	146 (78%)	27 (14%)	14 (8%)	1	13
27	H6	187/194 (96%)	146 (78%)	27 (14%)	14 (8%)	1	13
28	I1	204/208 (98%)	168 (82%)	24 (12%)	12 (6%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	I2	204/208 (98%)	168 (82%)	24 (12%)	12 (6%)	1	17
28	I3	204/208 (98%)	168 (82%)	24 (12%)	12 (6%)	1	17
28	I4	204/208 (98%)	168 (82%)	24 (12%)	12 (6%)	1	17
28	I5	204/208 (98%)	168 (82%)	24 (12%)	12 (6%)	1	17
28	I6	204/208 (98%)	168 (82%)	24 (12%)	12 (6%)	1	17
29	K1	96/165 (58%)	76 (79%)	15 (16%)	5 (5%)	2	19
29	K2	96/165 (58%)	76 (79%)	15 (16%)	5 (5%)	2	19
29	K3	96/165 (58%)	76 (79%)	15 (16%)	5 (5%)	2	19
29	K4	96/165 (58%)	76 (79%)	15 (16%)	5 (5%)	2	19
29	K5	96/165 (58%)	76 (79%)	15 (16%)	5 (5%)	2	19
29	K6	96/165 (58%)	76 (79%)	15 (16%)	5 (5%)	2	19
30	L1	151/158 (96%)	129 (85%)	11 (7%)	11 (7%)	1	13
30	L2	151/158 (96%)	125 (83%)	15 (10%)	11 (7%)	1	13
30	L3	151/158 (96%)	128 (85%)	14 (9%)	9 (6%)	1	16
30	L4	151/158 (96%)	127 (84%)	13 (9%)	11 (7%)	1	13
30	L5	151/158 (96%)	128 (85%)	14 (9%)	9 (6%)	1	16
30	L6	151/158 (96%)	126 (83%)	15 (10%)	10 (7%)	1	15
31	P1	123/145 (85%)	111 (90%)	6 (5%)	6 (5%)	2	20
31	P2	123/145 (85%)	111 (90%)	6 (5%)	6 (5%)	2	20
31	P3	123/145 (85%)	108 (88%)	11 (9%)	4 (3%)	4	26
31	P4	123/145 (85%)	111 (90%)	6 (5%)	6 (5%)	2	20
31	P5	123/145 (85%)	112 (91%)	6 (5%)	5 (4%)	3	22
31	P6	123/145 (85%)	111 (90%)	6 (5%)	6 (5%)	2	20
32	Q1	144/146 (99%)	112 (78%)	22 (15%)	10 (7%)	1	14
32	Q2	144/146 (99%)	112 (78%)	22 (15%)	10 (7%)	1	14
32	Q3	144/146 (99%)	112 (78%)	22 (15%)	10 (7%)	1	14
32	Q4	144/146 (99%)	112 (78%)	22 (15%)	10 (7%)	1	14
32	Q5	144/146 (99%)	112 (78%)	22 (15%)	10 (7%)	1	14
32	Q6	144/146 (99%)	112 (78%)	22 (15%)	10 (7%)	1	14
33	R1	130/135 (96%)	94 (72%)	25 (19%)	11 (8%)	1	11
33	R2	130/135 (96%)	95 (73%)	22 (17%)	13 (10%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	R3	130/135 (96%)	95 (73%)	24 (18%)	11 (8%)	1	11
33	R4	130/135 (96%)	97 (75%)	23 (18%)	10 (8%)	1	13
33	R5	130/135 (96%)	93 (72%)	26 (20%)	11 (8%)	1	11
33	R6	130/135 (96%)	93 (72%)	27 (21%)	10 (8%)	1	13
34	S1	141/152 (93%)	135 (96%)	6 (4%)	0	100	100
34	S2	141/152 (93%)	135 (96%)	6 (4%)	0	100	100
34	S3	141/152 (93%)	135 (96%)	6 (4%)	0	100	100
34	S4	141/152 (93%)	135 (96%)	6 (4%)	0	100	100
34	S5	141/152 (93%)	135 (96%)	6 (4%)	0	100	100
34	S6	141/152 (93%)	135 (96%)	6 (4%)	0	100	100
35	j1	23/25 (92%)	23 (100%)	0	0	100	100
35	j2	23/25 (92%)	23 (100%)	0	0	100	100
35	j3	23/25 (92%)	23 (100%)	0	0	100	100
35	j4	23/25 (92%)	23 (100%)	0	0	100	100
35	j5	23/25 (92%)	23 (100%)	0	0	100	100
35	j6	23/25 (92%)	23 (100%)	0	0	100	100
36	k1	179/181 (99%)	162 (90%)	13 (7%)	4 (2%)	6	35
36	k2	179/181 (99%)	161 (90%)	16 (9%)	2 (1%)	14	52
36	k3	179/181 (99%)	164 (92%)	14 (8%)	1 (1%)	25	66
36	k4	179/181 (99%)	160 (89%)	17 (10%)	2 (1%)	14	52
36	k5	179/181 (99%)	164 (92%)	13 (7%)	2 (1%)	14	52
36	k6	179/181 (99%)	164 (92%)	13 (7%)	2 (1%)	14	52
37	l1	77/198 (39%)	44 (57%)	24 (31%)	9 (12%)	0	6
37	l2	77/198 (39%)	44 (57%)	24 (31%)	9 (12%)	0	6
37	l3	77/198 (39%)	44 (57%)	24 (31%)	9 (12%)	0	6
37	l4	77/198 (39%)	44 (57%)	24 (31%)	9 (12%)	0	6
37	l5	77/198 (39%)	44 (57%)	24 (31%)	9 (12%)	0	6
37	l6	77/198 (39%)	44 (57%)	24 (31%)	9 (12%)	0	6
All	All	30804/35724 (86%)	25074 (81%)	3953 (13%)	1777 (6%)	1	17

5 of 1777 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T1	4	VAL
2	U1	50	VAL
2	U1	103	SER
2	U1	107	GLU
2	U1	116	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	T1	113/115 (98%)	113 (100%)	0	100	100
1	T2	113/115 (98%)	113 (100%)	0	100	100
1	T3	113/115 (98%)	113 (100%)	0	100	100
1	T4	113/115 (98%)	113 (100%)	0	100	100
1	T5	113/115 (98%)	113 (100%)	0	100	100
1	T6	113/115 (98%)	113 (100%)	0	100	100
2	U1	94/107 (88%)	93 (99%)	1 (1%)	73	84
2	U2	94/107 (88%)	93 (99%)	1 (1%)	73	84
2	U3	94/107 (88%)	93 (99%)	1 (1%)	73	84
2	U4	94/107 (88%)	93 (99%)	1 (1%)	73	84
2	U5	94/107 (88%)	93 (99%)	1 (1%)	73	84
2	U6	94/107 (88%)	93 (99%)	1 (1%)	73	84
3	V1	67/67 (100%)	67 (100%)	0	100	100
3	V2	67/67 (100%)	67 (100%)	0	100	100
3	V3	67/67 (100%)	67 (100%)	0	100	100
3	V4	67/67 (100%)	67 (100%)	0	100	100
3	V5	67/67 (100%)	67 (100%)	0	100	100
3	V6	67/67 (100%)	67 (100%)	0	100	100
4	X1	113/115 (98%)	113 (100%)	0	100	100
4	X2	113/115 (98%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	X3	113/115 (98%)	113 (100%)	0	100	100
4	X4	113/115 (98%)	113 (100%)	0	100	100
4	X5	113/115 (98%)	113 (100%)	0	100	100
4	X6	113/115 (98%)	113 (100%)	0	100	100
5	a1	90/98 (92%)	88 (98%)	2 (2%)	52	71
5	a2	90/98 (92%)	88 (98%)	2 (2%)	52	71
5	a3	90/98 (92%)	88 (98%)	2 (2%)	52	71
5	a4	90/98 (92%)	87 (97%)	3 (3%)	38	61
5	a5	90/98 (92%)	87 (97%)	3 (3%)	38	61
5	a6	90/98 (92%)	88 (98%)	2 (2%)	52	71
6	c1	57/62 (92%)	57 (100%)	0	100	100
6	c2	57/62 (92%)	57 (100%)	0	100	100
6	c3	57/62 (92%)	57 (100%)	0	100	100
6	c4	57/62 (92%)	57 (100%)	0	100	100
6	c5	57/62 (92%)	57 (100%)	0	100	100
6	c6	57/62 (92%)	57 (100%)	0	100	100
7	d1	47/49 (96%)	47 (100%)	0	100	100
7	d2	47/49 (96%)	47 (100%)	0	100	100
7	d3	47/49 (96%)	47 (100%)	0	100	100
7	d4	47/49 (96%)	47 (100%)	0	100	100
7	d5	47/49 (96%)	47 (100%)	0	100	100
7	d6	47/49 (96%)	47 (100%)	0	100	100
8	f1	65/140 (46%)	61 (94%)	4 (6%)	18	43
8	f2	65/140 (46%)	61 (94%)	4 (6%)	18	43
8	f3	65/140 (46%)	60 (92%)	5 (8%)	13	37
8	f4	65/140 (46%)	59 (91%)	6 (9%)	9	29
8	f5	65/140 (46%)	60 (92%)	5 (8%)	13	37
8	f6	65/140 (46%)	60 (92%)	5 (8%)	13	37
9	g1	272/275 (99%)	272 (100%)	0	100	100
9	g2	272/275 (99%)	272 (100%)	0	100	100
9	g3	272/275 (99%)	272 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	g4	272/275 (99%)	272 (100%)	0	100	100
9	g5	272/275 (99%)	272 (100%)	0	100	100
9	g6	272/275 (99%)	272 (100%)	0	100	100
10	C1	188/225 (84%)	186 (99%)	2 (1%)	73	84
10	C2	188/225 (84%)	186 (99%)	2 (1%)	73	84
10	C3	188/225 (84%)	186 (99%)	2 (1%)	73	84
10	C4	188/225 (84%)	186 (99%)	2 (1%)	73	84
10	C5	188/225 (84%)	186 (99%)	2 (1%)	73	84
10	C6	188/225 (84%)	186 (99%)	2 (1%)	73	84
11	G1	207/218 (95%)	202 (98%)	5 (2%)	49	69
11	G2	207/218 (95%)	202 (98%)	5 (2%)	49	69
11	G3	207/218 (95%)	202 (98%)	5 (2%)	49	69
11	G4	207/218 (95%)	202 (98%)	5 (2%)	49	69
11	G5	207/218 (95%)	202 (98%)	5 (2%)	49	69
11	G6	207/218 (95%)	202 (98%)	5 (2%)	49	69
12	J1	161/168 (96%)	161 (100%)	0	100	100
12	J2	161/168 (96%)	161 (100%)	0	100	100
12	J3	161/168 (96%)	161 (100%)	0	100	100
12	J4	161/168 (96%)	161 (100%)	0	100	100
12	J5	161/168 (96%)	161 (100%)	0	100	100
12	J6	161/168 (96%)	161 (100%)	0	100	100
13	M1	104/108 (96%)	96 (92%)	8 (8%)	13	37
13	M2	104/108 (96%)	96 (92%)	8 (8%)	13	37
13	M3	104/108 (96%)	96 (92%)	8 (8%)	13	37
13	M4	104/108 (96%)	96 (92%)	8 (8%)	13	37
13	M5	104/108 (96%)	96 (92%)	8 (8%)	13	37
13	M6	104/108 (96%)	96 (92%)	8 (8%)	13	37
14	N1	130/131 (99%)	127 (98%)	3 (2%)	50	71
14	N2	130/131 (99%)	127 (98%)	3 (2%)	50	71
14	N3	130/131 (99%)	124 (95%)	6 (5%)	27	52
14	N4	130/131 (99%)	127 (98%)	3 (2%)	50	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N5	130/131 (99%)	124 (95%)	6 (5%)	27	52
14	N6	130/131 (99%)	127 (98%)	3 (2%)	50	71
15	O1	110/119 (92%)	110 (100%)	0	100	100
15	O2	110/119 (92%)	110 (100%)	0	100	100
15	O3	110/119 (92%)	110 (100%)	0	100	100
15	O4	110/119 (92%)	110 (100%)	0	100	100
15	O5	110/119 (92%)	110 (100%)	0	100	100
15	O6	110/119 (92%)	110 (100%)	0	100	100
16	W1	112/113 (99%)	112 (100%)	0	100	100
16	W2	112/113 (99%)	112 (100%)	0	100	100
16	W3	112/113 (99%)	112 (100%)	0	100	100
16	W4	112/113 (99%)	112 (100%)	0	100	100
16	W5	112/113 (99%)	112 (100%)	0	100	100
16	W6	112/113 (99%)	112 (100%)	0	100	100
17	Y1	113/115 (98%)	113 (100%)	0	100	100
17	Y2	113/115 (98%)	113 (100%)	0	100	100
17	Y3	113/115 (98%)	113 (100%)	0	100	100
17	Y4	113/115 (98%)	113 (100%)	0	100	100
17	Y5	113/115 (98%)	113 (100%)	0	100	100
17	Y6	113/115 (98%)	113 (100%)	0	100	100
18	Z1	66/103 (64%)	63 (96%)	3 (4%)	27	52
18	Z2	66/103 (64%)	63 (96%)	3 (4%)	27	52
18	Z3	66/103 (64%)	63 (96%)	3 (4%)	27	52
18	Z4	66/103 (64%)	63 (96%)	3 (4%)	27	52
18	Z5	66/103 (64%)	63 (96%)	3 (4%)	27	52
18	Z6	66/103 (64%)	63 (96%)	3 (4%)	27	52
19	b1	75/76 (99%)	75 (100%)	0	100	100
19	b2	75/76 (99%)	75 (100%)	0	100	100
19	b3	75/76 (99%)	75 (100%)	0	100	100
19	b4	75/76 (99%)	74 (99%)	1 (1%)	69	82
19	b5	75/76 (99%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	b6	75/76 (99%)	75 (100%)	0	100	100
20	e1	47/104 (45%)	44 (94%)	3 (6%)	17	42
20	e2	47/104 (45%)	44 (94%)	3 (6%)	17	42
20	e3	47/104 (45%)	45 (96%)	2 (4%)	29	54
20	e4	47/104 (45%)	42 (89%)	5 (11%)	6	24
20	e5	47/104 (45%)	43 (92%)	4 (8%)	10	33
20	e6	47/104 (45%)	45 (96%)	2 (4%)	29	54
22	A1	184/243 (76%)	183 (100%)	1 (0%)	88	93
22	A2	184/243 (76%)	183 (100%)	1 (0%)	88	93
22	A3	184/243 (76%)	183 (100%)	1 (0%)	88	93
22	A4	184/243 (76%)	183 (100%)	1 (0%)	88	93
22	A5	184/243 (76%)	183 (100%)	1 (0%)	88	93
22	A6	184/243 (76%)	183 (100%)	1 (0%)	88	93
23	B1	195/231 (84%)	195 (100%)	0	100	100
23	B2	195/231 (84%)	195 (100%)	0	100	100
23	B3	195/231 (84%)	195 (100%)	0	100	100
23	B4	195/231 (84%)	195 (100%)	0	100	100
23	B5	195/231 (84%)	195 (100%)	0	100	100
23	B6	195/231 (84%)	195 (100%)	0	100	100
24	D1	190/202 (94%)	190 (100%)	0	100	100
24	D2	190/202 (94%)	190 (100%)	0	100	100
24	D3	190/202 (94%)	190 (100%)	0	100	100
24	D4	190/202 (94%)	190 (100%)	0	100	100
24	D5	190/202 (94%)	190 (100%)	0	100	100
24	D6	190/202 (94%)	190 (100%)	0	100	100
25	E1	224/225 (100%)	224 (100%)	0	100	100
25	E2	224/225 (100%)	224 (100%)	0	100	100
25	E3	224/225 (100%)	224 (100%)	0	100	100
25	E4	224/225 (100%)	224 (100%)	0	100	100
25	E5	224/225 (100%)	224 (100%)	0	100	100
25	E6	224/225 (100%)	224 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	F1	161/170 (95%)	158 (98%)	3 (2%)	57	75
26	F2	161/170 (95%)	158 (98%)	3 (2%)	57	75
26	F3	161/170 (95%)	158 (98%)	3 (2%)	57	75
26	F4	161/170 (95%)	158 (98%)	3 (2%)	57	75
26	F5	161/170 (95%)	158 (98%)	3 (2%)	57	75
26	F6	161/170 (95%)	158 (98%)	3 (2%)	57	75
27	H1	169/174 (97%)	169 (100%)	0	100	100
27	H2	169/174 (97%)	169 (100%)	0	100	100
27	H3	169/174 (97%)	169 (100%)	0	100	100
27	H4	169/174 (97%)	167 (99%)	2 (1%)	71	84
27	H5	169/174 (97%)	169 (100%)	0	100	100
27	H6	169/174 (97%)	169 (100%)	0	100	100
28	I1	178/180 (99%)	178 (100%)	0	100	100
28	I2	178/180 (99%)	178 (100%)	0	100	100
28	I3	178/180 (99%)	177 (99%)	1 (1%)	86	92
28	I4	178/180 (99%)	178 (100%)	0	100	100
28	I5	178/180 (99%)	178 (100%)	0	100	100
28	I6	178/180 (99%)	178 (100%)	0	100	100
29	K1	89/136 (65%)	89 (100%)	0	100	100
29	K2	89/136 (65%)	89 (100%)	0	100	100
29	K3	89/136 (65%)	89 (100%)	0	100	100
29	K4	89/136 (65%)	89 (100%)	0	100	100
29	K5	89/136 (65%)	89 (100%)	0	100	100
29	K6	89/136 (65%)	89 (100%)	0	100	100
30	L1	137/142 (96%)	135 (98%)	2 (2%)	65	80
30	L2	137/142 (96%)	134 (98%)	3 (2%)	52	71
30	L3	137/142 (96%)	134 (98%)	3 (2%)	52	71
30	L4	137/142 (96%)	134 (98%)	3 (2%)	52	71
30	L5	137/142 (96%)	134 (98%)	3 (2%)	52	71
30	L6	137/142 (96%)	134 (98%)	3 (2%)	52	71
31	P1	112/130 (86%)	98 (88%)	14 (12%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	P2	112/130 (86%)	95 (85%)	17 (15%)	3	15
31	P3	112/130 (86%)	98 (88%)	14 (12%)	4	19
31	P4	112/130 (86%)	95 (85%)	17 (15%)	3	15
31	P5	112/130 (86%)	94 (84%)	18 (16%)	2	13
31	P6	112/130 (86%)	99 (88%)	13 (12%)	5	21
32	Q1	121/121 (100%)	120 (99%)	1 (1%)	81	89
32	Q2	121/121 (100%)	120 (99%)	1 (1%)	81	89
32	Q3	121/121 (100%)	120 (99%)	1 (1%)	81	89
32	Q4	121/121 (100%)	120 (99%)	1 (1%)	81	89
32	Q5	121/121 (100%)	120 (99%)	1 (1%)	81	89
32	Q6	121/121 (100%)	120 (99%)	1 (1%)	81	89
33	R1	120/122 (98%)	115 (96%)	5 (4%)	30	54
33	R2	120/122 (98%)	113 (94%)	7 (6%)	20	45
33	R3	120/122 (98%)	115 (96%)	5 (4%)	30	54
33	R4	120/122 (98%)	113 (94%)	7 (6%)	20	45
33	R5	120/122 (98%)	115 (96%)	5 (4%)	30	54
33	R6	120/122 (98%)	113 (94%)	7 (6%)	20	45
34	S1	124/132 (94%)	118 (95%)	6 (5%)	25	51
34	S2	124/132 (94%)	118 (95%)	6 (5%)	25	51
34	S3	124/132 (94%)	118 (95%)	6 (5%)	25	51
34	S4	124/132 (94%)	118 (95%)	6 (5%)	25	51
34	S5	124/132 (94%)	118 (95%)	6 (5%)	25	51
34	S6	124/132 (94%)	118 (95%)	6 (5%)	25	51
35	j1	24/24 (100%)	16 (67%)	8 (33%)	0	2
35	j2	24/24 (100%)	16 (67%)	8 (33%)	0	2
35	j3	24/24 (100%)	16 (67%)	8 (33%)	0	2
35	j4	24/24 (100%)	17 (71%)	7 (29%)	0	2
35	j5	24/24 (100%)	16 (67%)	8 (33%)	0	2
35	j6	24/24 (100%)	16 (67%)	8 (33%)	0	2
36	k1	152/159 (96%)	149 (98%)	3 (2%)	55	74
36	k2	152/159 (96%)	147 (97%)	5 (3%)	38	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k3	152/159 (96%)	148 (97%)	4 (3%)	46	67
36	k4	152/159 (96%)	146 (96%)	6 (4%)	32	56
36	k5	152/159 (96%)	149 (98%)	3 (2%)	55	74
36	k6	152/159 (96%)	147 (97%)	5 (3%)	38	61
37	l1	69/168 (41%)	58 (84%)	11 (16%)	2	14
37	l2	69/168 (41%)	58 (84%)	11 (16%)	2	14
37	l3	69/168 (41%)	58 (84%)	11 (16%)	2	14
37	l4	69/168 (41%)	58 (84%)	11 (16%)	2	14
37	l5	69/168 (41%)	58 (84%)	11 (16%)	2	14
37	l6	69/168 (41%)	58 (84%)	11 (16%)	2	14
All	All	26880/30402 (88%)	26325 (98%)	555 (2%)	53	72

5 of 555 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	N4	149	LEU
5	a5	101	PHE
37	l3	119	LYS
20	e4	12	VAL
31	P4	79	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 297 such sidechains are listed below:

Mol	Chain	Res	Type
34	S3	101	ASN
27	H4	33	ASN
36	k1	10	ASN
4	X4	63	ASN
11	G4	146	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	i1	1716/1869 (91%)	685 (39%)	0
21	i2	1715/1869 (91%)	687 (40%)	0
21	i3	1715/1869 (91%)	683 (39%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	i4	1716/1869 (91%)	684 (39%)	0
21	i5	1716/1869 (91%)	683 (39%)	0
21	i6	1716/1869 (91%)	683 (39%)	0
All	All	10294/11214 (91%)	4105 (39%)	0

5 of 4105 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	i1	2	A
21	i1	3	C
21	i1	4	C
21	i1	9	U
21	i1	17	C

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	i2	1
21	i4	1
21	i3	1
21	i6	1
21	i5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i2	1689:C	O3'	1690:U	P	2.39
1	i3	1689:C	O3'	1690:U	P	2.27
1	i5	1689:C	O3'	1690:U	P	2.14
1	i6	1689:C	O3'	1690:U	P	2.07
1	i4	1689:C	O3'	1690:U	P	1.91

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	T1	143/145 (98%)	-0.54	4 (2%)	53	46	166, 196, 227, 240	0
1	T2	143/145 (98%)	-0.44	2 (1%)	75	66	164, 191, 211, 219	0
1	T3	143/145 (98%)	-0.22	2 (1%)	75	66	235, 251, 270, 279	0
1	T4	143/145 (98%)	-0.20	9 (6%)	20	19	302, 349, 376, 382	0
1	T5	143/145 (98%)	-0.20	4 (2%)	53	46	182, 217, 239, 247	0
1	T6	143/145 (98%)	-0.43	3 (2%)	63	56	177, 203, 220, 229	0
2	U1	104/119 (87%)	-0.38	0	100	100	155, 178, 205, 213	0
2	U2	104/119 (87%)	0.28	10 (9%)	8	10	153, 168, 189, 197	0
2	U3	104/119 (87%)	0.18	11 (10%)	6	8	222, 235, 250, 257	0
2	U4	104/119 (87%)	0.98	29 (27%)	0	2	241, 266, 296, 311	0
2	U5	104/119 (87%)	1.25	24 (23%)	0	2	173, 200, 224, 233	0
2	U6	104/119 (87%)	0.51	18 (17%)	1	4	168, 180, 196, 203	0
3	V1	83/83 (100%)	0.37	7 (8%)	11	13	134, 163, 202, 215	0
3	V2	83/83 (100%)	-0.28	0	100	100	128, 151, 181, 191	0
3	V3	83/83 (100%)	-0.04	2 (2%)	59	52	169, 194, 239, 250	0
3	V4	83/83 (100%)	-0.14	4 (4%)	30	29	161, 194, 236, 248	0
3	V5	83/83 (100%)	-0.11	2 (2%)	59	52	162, 193, 232, 245	0
3	V6	83/83 (100%)	0.12	5 (6%)	21	21	153, 179, 211, 222	0
4	X1	141/143 (98%)	0.74	29 (20%)	1	3	112, 126, 143, 151	0
4	X2	141/143 (98%)	0.11	9 (6%)	19	18	116, 130, 146, 153	0
4	X3	141/143 (98%)	0.15	9 (6%)	19	18	131, 151, 176, 187	0
4	X4	141/143 (98%)	0.27	10 (7%)	16	16	129, 166, 204, 218	0
4	X5	141/143 (98%)	0.76	26 (18%)	1	3	137, 151, 168, 180	0
4	X6	141/143 (98%)	0.64	28 (19%)	1	3	138, 152, 169, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	a1	107/115 (93%)	0.18	10 (9%) 8 11	111, 122, 148, 157	0
5	a2	107/115 (93%)	-0.34	1 (0%) 84 77	113, 123, 149, 155	0
5	a3	107/115 (93%)	0.57	14 (13%) 3 7	144, 161, 211, 220	0
5	a4	107/115 (93%)	0.24	8 (7%) 14 15	136, 154, 197, 204	0
5	a5	107/115 (93%)	1.31	27 (25%) 0 2	135, 144, 180, 188	0
5	a6	107/115 (93%)	1.02	27 (25%) 0 2	133, 141, 171, 176	0
6	c1	64/69 (92%)	1.21	21 (32%) 0 2	182, 206, 232, 243	0
6	c2	64/69 (92%)	0.66	10 (15%) 2 4	191, 213, 235, 252	0
6	c3	64/69 (92%)	0.58	6 (9%) 8 11	209, 217, 229, 241	0
6	c4	64/69 (92%)	-0.03	3 (4%) 31 30	237, 252, 280, 296	0
6	c5	64/69 (92%)	0.53	5 (7%) 13 14	187, 203, 217, 222	0
6	c6	64/69 (92%)	-0.31	2 (3%) 49 42	196, 216, 234, 238	0
7	d1	53/56 (94%)	-0.35	0 100 100	156, 160, 181, 189	0
7	d2	53/56 (94%)	-0.31	0 100 100	154, 156, 172, 179	0
7	d3	53/56 (94%)	0.93	11 (20%) 1 3	217, 249, 308, 321	0
7	d4	53/56 (94%)	-0.19	3 (5%) 23 23	244, 285, 361, 375	0
7	d5	53/56 (94%)	0.37	10 (18%) 1 3	175, 179, 191, 197	0
7	d6	53/56 (94%)	-0.02	6 (11%) 5 8	169, 171, 191, 199	0
8	f1	72/156 (46%)	0.04	4 (5%) 24 24	179, 218, 268, 285	0
8	f2	72/156 (46%)	-0.06	4 (5%) 24 24	174, 207, 248, 257	0
8	f3	72/156 (46%)	0.20	10 (13%) 2 6	282, 365, 385, 393	0
8	f4	72/156 (46%)	-0.48	1 (1%) 75 66	317, 397, 425, 435	0
8	f5	72/156 (46%)	0.09	8 (11%) 5 8	182, 223, 255, 263	0
8	f6	72/156 (46%)	0.21	6 (8%) 11 13	185, 229, 268, 282	0
9	g1	313/317 (98%)	0.06	21 (6%) 17 17	191, 230, 269, 290	0
9	g2	313/317 (98%)	-0.04	20 (6%) 19 18	175, 207, 237, 248	0
9	g3	313/317 (98%)	0.02	22 (7%) 16 16	208, 228, 248, 255	0
9	g4	313/317 (98%)	-0.11	18 (5%) 23 23	223, 250, 276, 286	0
9	g5	313/317 (98%)	0.07	15 (4%) 30 29	204, 232, 260, 267	0
9	g6	313/317 (98%)	-0.16	15 (4%) 30 29	191, 224, 256, 271	0
10	C1	222/293 (75%)	0.16	15 (6%) 17 17	117, 147, 182, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
10	C2	222/293 (75%)	-0.08	8 (3%) 42 38	118, 140, 168, 176	0
10	C3	222/293 (75%)	-0.44	1 (0%) 91 86	145, 179, 221, 235	0
10	C4	222/293 (75%)	-0.19	8 (3%) 42 38	145, 186, 226, 241	0
10	C5	222/293 (75%)	0.31	29 (13%) 3 7	144, 176, 211, 221	0
10	C6	222/293 (75%)	0.25	21 (9%) 8 10	141, 166, 194, 203	0
11	G1	237/249 (95%)	-0.43	2 (0%) 86 79	160, 218, 269, 295	0
11	G2	237/249 (95%)	-0.30	6 (2%) 57 50	168, 228, 256, 271	0
11	G3	237/249 (95%)	-0.20	12 (5%) 28 27	166, 225, 250, 256	0
11	G4	237/249 (95%)	0.07	24 (10%) 7 9	174, 239, 267, 288	0
11	G5	237/249 (95%)	-0.19	19 (8%) 12 14	209, 290, 320, 341	0
11	G6	237/249 (95%)	-0.05	16 (6%) 17 17	212, 290, 318, 339	0
12	J1	185/194 (95%)	-0.30	5 (2%) 54 47	129, 171, 222, 262	0
12	J2	185/194 (95%)	-0.05	12 (6%) 18 18	128, 162, 204, 236	0
12	J3	185/194 (95%)	-0.20	10 (5%) 25 26	157, 197, 258, 306	0
12	J4	185/194 (95%)	-0.06	11 (5%) 22 22	164, 213, 300, 317	0
12	J5	185/194 (95%)	0.17	20 (10%) 5 8	158, 209, 259, 296	0
12	J6	185/194 (95%)	-0.35	6 (3%) 47 41	154, 195, 238, 271	0
13	M1	123/132 (93%)	0.42	17 (13%) 2 6	215, 248, 278, 291	0
13	M2	123/132 (93%)	-0.23	3 (2%) 59 52	201, 226, 255, 268	0
13	M3	123/132 (93%)	0.13	11 (8%) 9 12	339, 364, 377, 381	0
13	M4	123/132 (93%)	0.34	15 (12%) 4 8	369, 398, 417, 422	0
13	M5	123/132 (93%)	-0.06	8 (6%) 18 18	217, 237, 257, 269	0
13	M6	123/132 (93%)	-0.04	8 (6%) 18 18	212, 236, 257, 268	0
14	N1	150/151 (99%)	-0.08	4 (2%) 54 47	130, 172, 211, 221	0
14	N2	150/151 (99%)	-0.13	5 (3%) 46 40	124, 158, 185, 191	0
14	N3	150/151 (99%)	-0.17	5 (3%) 46 40	144, 166, 206, 219	0
14	N4	150/151 (99%)	-0.24	3 (2%) 65 58	138, 166, 208, 222	0
14	N5	150/151 (99%)	-0.32	5 (3%) 46 40	148, 182, 217, 230	0
14	N6	150/151 (99%)	-0.39	3 (2%) 65 58	144, 178, 207, 216	0
15	O1	140/151 (92%)	0.73	21 (15%) 2 5	121, 151, 185, 197	0
15	O2	140/151 (92%)	0.60	22 (15%) 2 4	124, 154, 181, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
15	O3	140/151 (92%)	1.16	34 (24%) 0 2	150, 202, 247, 260	0
15	O4	140/151 (92%)	0.73	27 (19%) 1 3	147, 199, 237, 259	0
15	O5	140/151 (92%)	0.76	32 (22%) 0 2	139, 177, 213, 227	0
15	O6	140/151 (92%)	-0.11	8 (5%) 23 23	138, 169, 197, 211	0
16	W1	129/130 (99%)	0.02	4 (3%) 49 42	132, 149, 167, 175	0
16	W2	129/130 (99%)	0.07	1 (0%) 86 79	127, 141, 155, 162	0
16	W3	129/130 (99%)	0.69	14 (10%) 5 8	146, 165, 180, 186	0
16	W4	129/130 (99%)	1.11	34 (26%) 0 2	140, 162, 178, 187	0
16	W5	129/130 (99%)	-0.25	1 (0%) 86 79	156, 178, 195, 207	0
16	W6	129/130 (99%)	0.05	4 (3%) 49 42	152, 169, 184, 194	0
17	Y1	131/133 (98%)	-0.35	6 (4%) 32 30	159, 196, 223, 237	0
17	Y2	131/133 (98%)	-0.22	11 (8%) 11 13	164, 191, 214, 225	0
17	Y3	131/133 (98%)	0.05	13 (9%) 7 10	180, 221, 252, 267	0
17	Y4	131/133 (98%)	-0.11	9 (6%) 16 16	191, 239, 278, 300	0
17	Y5	131/133 (98%)	0.16	10 (7%) 13 15	210, 252, 285, 302	0
17	Y6	131/133 (98%)	0.16	12 (9%) 9 11	208, 239, 266, 280	0
18	Z1	75/125 (60%)	0.60	11 (14%) 2 5	196, 226, 255, 258	0
18	Z2	75/125 (60%)	0.71	14 (18%) 1 3	191, 228, 254, 264	0
18	Z3	75/125 (60%)	-0.07	6 (8%) 12 14	241, 264, 288, 300	0
18	Z4	75/125 (60%)	-0.11	6 (8%) 12 14	325, 359, 372, 379	0
18	Z5	75/125 (60%)	1.62	24 (32%) 0 2	205, 223, 244, 248	0
18	Z6	75/125 (60%)	1.13	18 (24%) 0 2	195, 217, 236, 244	0
19	b1	83/84 (98%)	0.62	11 (13%) 3 6	146, 177, 216, 229	0
19	b2	83/84 (98%)	-0.34	0 100 100	136, 156, 185, 194	0
19	b3	83/84 (98%)	0.03	5 (6%) 21 21	166, 192, 221, 235	0
19	b4	83/84 (98%)	0.01	9 (10%) 5 8	157, 182, 219, 236	0
19	b5	83/84 (98%)	0.20	4 (4%) 30 29	169, 191, 221, 235	0
19	b6	83/84 (98%)	0.41	6 (7%) 15 16	160, 179, 207, 219	0
20	e1	58/133 (43%)	0.10	4 (6%) 16 16	134, 160, 176, 179	0
20	e2	58/133 (43%)	0.33	9 (15%) 2 4	143, 155, 166, 168	0
20	e3	58/133 (43%)	0.48	10 (17%) 1 4	163, 198, 215, 218	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
20	e4	58/133 (43%)	0.41	10 (17%) 1 4	199, 226, 246, 253	0
20	e5	58/133 (43%)	0.14	7 (12%) 4 8	154, 186, 202, 204	0
20	e6	58/133 (43%)	0.01	7 (12%) 4 8	158, 181, 191, 194	0
21	i1	1742/1869 (93%)	0.10	49 (2%) 53 46	110, 170, 323, 428	0
21	i2	1742/1869 (93%)	0.01	34 (1%) 65 58	113, 169, 301, 421	0
21	i3	1742/1869 (93%)	-0.05	37 (2%) 63 56	130, 200, 353, 478	0
21	i4	1742/1869 (93%)	0.07	59 (3%) 45 40	128, 212, 362, 457	0
21	i5	1742/1869 (93%)	-0.00	36 (2%) 63 56	133, 191, 362, 430	0
21	i6	1742/1869 (93%)	0.09	62 (3%) 42 38	132, 188, 335, 417	0
22	A1	222/295 (75%)	0.28	20 (9%) 9 11	134, 159, 193, 212	0
22	A2	222/295 (75%)	-0.11	8 (3%) 42 38	128, 149, 178, 190	0
22	A3	222/295 (75%)	-0.04	13 (5%) 22 22	172, 206, 247, 272	0
22	A4	222/295 (75%)	-0.52	0 100 100	161, 197, 237, 252	0
22	A5	222/295 (75%)	0.26	29 (13%) 3 7	162, 191, 229, 245	0
22	A6	222/295 (75%)	0.02	11 (4%) 28 28	154, 177, 211, 222	0
23	B1	214/264 (81%)	0.24	19 (8%) 9 12	127, 168, 205, 214	0
23	B2	214/264 (81%)	0.18	23 (10%) 6 9	124, 157, 193, 204	0
23	B3	214/264 (81%)	-0.02	13 (6%) 21 20	166, 208, 248, 254	0
23	B4	214/264 (81%)	0.33	19 (8%) 9 12	151, 197, 248, 262	0
23	B5	214/264 (81%)	-0.35	5 (2%) 60 53	150, 186, 220, 228	0
23	B6	214/264 (81%)	-0.42	1 (0%) 91 86	144, 172, 204, 210	0
24	D1	227/243 (93%)	0.20	13 (5%) 23 23	159, 173, 203, 250	0
24	D2	227/243 (93%)	-0.07	13 (5%) 23 23	156, 173, 205, 233	0
24	D3	227/243 (93%)	0.72	35 (15%) 2 5	211, 244, 269, 286	0
24	D4	227/243 (93%)	1.26	65 (28%) 0 2	217, 260, 298, 310	0
24	D5	227/243 (93%)	0.27	23 (10%) 7 9	180, 191, 221, 254	0
24	D6	227/243 (93%)	0.42	29 (12%) 3 7	171, 184, 221, 250	0
25	E1	262/263 (99%)	0.72	40 (15%) 2 5	149, 195, 227, 237	0
25	E2	262/263 (99%)	0.59	38 (14%) 2 5	151, 188, 219, 227	0
25	E3	262/263 (99%)	-0.23	6 (2%) 60 53	154, 197, 221, 238	0
25	E4	262/263 (99%)	0.10	18 (6%) 16 16	158, 209, 239, 261	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)		Q<0.9	
25	E5	262/263 (99%)	0.72	44 (16%)	1	4	190, 242, 280, 296	0
25	E6	262/263 (99%)	0.59	37 (14%)	2	6	189, 232, 270, 280	0
26	F1	191/204 (93%)	0.81	33 (17%)	1	4	175, 204, 228, 236	0
26	F2	191/204 (93%)	0.70	27 (14%)	2	6	172, 203, 224, 232	0
26	F3	191/204 (93%)	0.51	30 (15%)	2	4	209, 229, 245, 255	0
26	F4	191/204 (93%)	0.28	29 (15%)	2	5	242, 289, 324, 338	0
26	F5	191/204 (93%)	1.38	59 (30%)	0	2	185, 201, 218, 223	0
26	F6	191/204 (93%)	0.30	20 (10%)	6	9	180, 203, 216, 221	0
27	H1	189/194 (97%)	0.40	26 (13%)	2	6	173, 225, 287, 300	0
27	H2	189/194 (97%)	-0.16	5 (2%)	56	49	156, 196, 245, 258	0
27	H3	189/194 (97%)	0.58	36 (19%)	1	3	172, 222, 267, 278	0
27	H4	189/194 (97%)	0.22	17 (8%)	9	11	176, 228, 290, 303	0
27	H5	189/194 (97%)	0.35	24 (12%)	3	7	196, 242, 297, 312	0
27	H6	189/194 (97%)	-0.31	5 (2%)	56	49	183, 227, 279, 291	0
28	I1	206/208 (99%)	0.71	35 (16%)	1	4	135, 223, 315, 326	0
28	I2	206/208 (99%)	0.18	19 (9%)	9	11	139, 220, 301, 318	0
28	I3	206/208 (99%)	-0.09	10 (4%)	29	28	136, 188, 250, 272	0
28	I4	206/208 (99%)	0.07	17 (8%)	11	13	139, 204, 286, 313	0
28	I5	206/208 (99%)	1.03	56 (27%)	0	2	163, 250, 344, 364	0
28	I6	206/208 (99%)	1.06	53 (25%)	0	2	166, 255, 345, 361	0
29	K1	98/165 (59%)	1.14	24 (24%)	0	2	164, 190, 213, 221	0
29	K2	98/165 (59%)	0.19	8 (8%)	11	13	159, 181, 202, 210	0
29	K3	98/165 (59%)	-0.00	4 (4%)	37	34	255, 297, 324, 332	0
29	K4	98/165 (59%)	-0.11	7 (7%)	16	16	283, 331, 365, 374	0
29	K5	98/165 (59%)	-0.23	1 (1%)	82	75	182, 201, 219, 224	0
29	K6	98/165 (59%)	0.27	14 (14%)	2	5	174, 192, 204, 210	0
30	L1	153/158 (96%)	0.92	36 (23%)	0	2	124, 177, 257, 284	0
30	L2	153/158 (96%)	1.04	29 (18%)	1	3	124, 169, 239, 265	0
30	L3	153/158 (96%)	1.27	40 (26%)	0	2	138, 161, 209, 227	0
30	L4	153/158 (96%)	1.20	41 (26%)	0	2	136, 167, 234, 258	0
30	L5	153/158 (96%)	0.70	28 (18%)	1	3	152, 202, 272, 302	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
30	L6	153/158 (96%)	1.24	36 (23%) 0 2	150, 200, 273, 303	0
31	P1	125/145 (86%)	-0.27	4 (3%) 47 41	174, 193, 217, 230	0
31	P2	125/145 (86%)	-0.33	4 (3%) 47 41	174, 193, 222, 231	0
31	P3	125/145 (86%)	0.03	13 (10%) 6 9	265, 327, 365, 374	0
31	P4	125/145 (86%)	-0.33	2 (1%) 72 64	306, 383, 399, 409	0
31	P5	125/145 (86%)	-0.31	0 100 100	182, 204, 223, 228	0
31	P6	125/145 (86%)	-0.07	9 (7%) 15 16	187, 212, 240, 251	0
32	Q1	146/146 (100%)	0.01	10 (6%) 17 17	156, 200, 232, 265	0
32	Q2	146/146 (100%)	0.56	17 (11%) 4 8	156, 182, 200, 218	0
32	Q3	146/146 (100%)	-0.04	11 (7%) 14 15	212, 223, 233, 243	0
32	Q4	146/146 (100%)	0.31	18 (12%) 4 8	249, 279, 311, 317	0
32	Q5	146/146 (100%)	0.01	9 (6%) 20 20	174, 209, 233, 258	0
32	Q6	146/146 (100%)	0.45	15 (10%) 6 9	170, 194, 210, 229	0
33	R1	132/135 (97%)	-0.13	5 (3%) 40 36	127, 177, 194, 201	0
33	R2	132/135 (97%)	-0.26	4 (3%) 50 43	124, 171, 196, 202	0
33	R3	132/135 (97%)	0.06	10 (7%) 13 15	171, 211, 240, 249	0
33	R4	132/135 (97%)	-0.03	6 (4%) 33 31	154, 216, 227, 235	0
33	R5	132/135 (97%)	0.56	22 (16%) 1 4	153, 202, 220, 228	0
33	R6	132/135 (97%)	0.62	25 (18%) 1 3	146, 196, 217, 224	0
34	S1	143/152 (94%)	0.54	21 (14%) 2 5	171, 201, 229, 247	0
34	S2	143/152 (94%)	0.25	18 (12%) 3 7	172, 210, 240, 258	0
34	S3	143/152 (94%)	-0.31	8 (5%) 24 24	268, 296, 323, 339	0
34	S4	143/152 (94%)	0.92	32 (22%) 0 2	321, 375, 385, 388	0
34	S5	143/152 (94%)	-0.12	12 (8%) 11 13	181, 213, 234, 246	0
34	S6	143/152 (94%)	0.28	17 (11%) 4 8	183, 215, 233, 243	0
35	j1	25/25 (100%)	0.21	0 100 100	113, 121, 137, 140	0
35	j2	25/25 (100%)	-0.13	0 100 100	119, 127, 143, 146	0
35	j3	25/25 (100%)	-0.56	0 100 100	137, 141, 145, 149	0
35	j4	25/25 (100%)	-0.26	1 (4%) 38 34	139, 147, 157, 163	0
35	j5	25/25 (100%)	-0.89	0 100 100	133, 138, 152, 153	0
35	j6	25/25 (100%)	-0.11	0 100 100	134, 141, 155, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
36	k1	181/181 (100%)	-0.04	8 (4%) 34 32	146, 198, 267, 284	0
36	k2	181/181 (100%)	-0.41	0 100 100	147, 195, 253, 268	0
36	k3	181/181 (100%)	-0.54	0 100 100	158, 205, 256, 270	0
36	k4	181/181 (100%)	-0.12	10 (5%) 25 25	168, 233, 302, 315	0
36	k5	181/181 (100%)	0.26	14 (7%) 13 14	157, 199, 256, 270	0
36	k6	181/181 (100%)	-0.06	8 (4%) 34 32	155, 193, 242, 252	0
37	l1	79/198 (39%)	0.63	10 (12%) 3 7	174, 212, 268, 279	0
37	l2	79/198 (39%)	0.74	13 (16%) 1 4	185, 206, 233, 240	0
37	l3	79/198 (39%)	0.70	19 (24%) 0 2	237, 298, 351, 357	0
37	l4	79/198 (39%)	1.21	22 (27%) 0 2	237, 274, 309, 327	0
37	l5	79/198 (39%)	0.13	6 (7%) 13 15	199, 234, 288, 302	0
37	l6	79/198 (39%)	0.36	8 (10%) 7 9	185, 220, 273, 287	0
All	All	41688/46938 (88%)	0.15	3270 (7%) 13 14	110, 198, 315, 478	0

The worst 5 of 3270 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	L6	28	THR	20.9
32	Q5	2	PRO	19.7
21	i6	788	G	18.8
5	a4	105	GLY	18.4
15	O1	12	GLU	18.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
38	ZN	f5	500	1/1	0.34	0.07	80,80,80,80	0
38	ZN	f4	500	1/1	0.59	0.10	80,80,80,80	0
38	ZN	f6	500	1/1	0.72	0.07	80,80,80,80	0
38	ZN	f2	500	1/1	0.84	0.12	80,80,80,80	0
38	ZN	f3	500	1/1	0.91	0.12	80,80,80,80	0
38	ZN	f1	500	1/1	0.98	0.13	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.