



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Dec 20, 2016 – 07:59 AM EST

PDB ID : 5MLC
EMDB ID: : EMD-3525
Title : Cryo-EM structure of the spinach chloroplast ribosome reveals the location of plastid-specific ribosomal proteins and extensions
Authors : Graf, M.; Arenz, S.; Huter, P.; Doenhoefer, A.; Novacek, J.; Wilson, D.N.
Deposited on : 2016-12-06
Resolution : 3.90 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

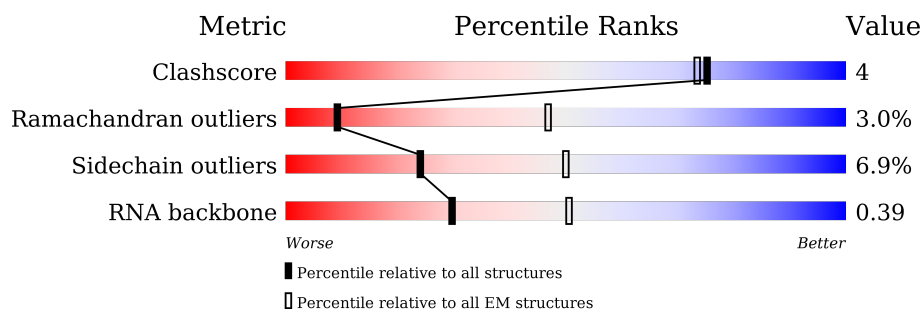
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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
















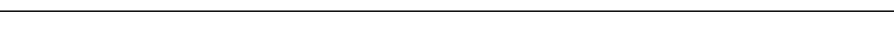
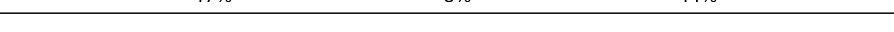
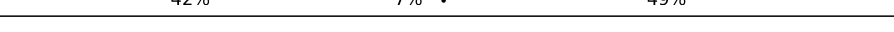
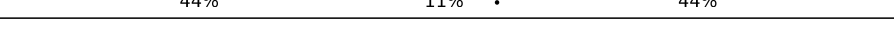
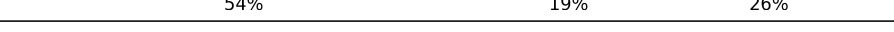



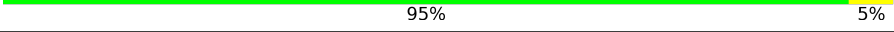


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	2811	59% 33% 6% .
2	B	121	73% 23% . .
3	C	103	53% 31% 6% 10%
4	D	272	74% 14% . 10%
5	E	305	62% 9% 28%
6	F	293	59% 10% . 30%
7	G	220	73% 9% 19%
8	H	220	70% 10% 19%

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Mol	Chain	Length	Quality of chain
9	I	196	
10	L	250	
11	M	121	
12	N	271	
13	O	135	
14	P	126	
15	Q	166	
16	R	233	
17	S	128	
18	T	256	
19	U	199	
20	V	198	
21	W	191	
22	X	194	
23	Y	148	
24	Z	168	
25	2	57	
26	3	66	
27	4	152	
28	5	159	
29	6	37	
30	9	271	
31	7	142	
32	8	116	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 90647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2750	Total	C	N	O	P	0	0
			59074	26351	10944	19029	2750		

- Molecule 2 is a RNA chain called 5S ribosomal RNA, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2564	1145	464	835	120		

- Molecule 3 is a RNA chain called 4.8S ribosomal RNA, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	93	Total	C	N	O	P	0	0
			2001	893	374	641	93		

- Molecule 4 is a protein called 50S ribosomal protein L2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	246	Total	C	N	O	S	0	0
			1895	1175	388	326	6		

- Molecule 5 is a protein called 50S ribosomal protein L3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	219	Total	C	N	O	S	0	0
			1669	1056	304	298	11		

- Molecule 6 is a protein called 50S ribosomal protein L4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	205	Total	C	N	O	S	0	0
			1617	1024	303	287	3		

- Molecule 7 is a protein called 50S ribosomal protein L5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	179	Total	C	N	O	S	0	0
			1387	883	241	255	8		

- Molecule 8 is a protein called 50S ribosomal protein L6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	178	Total	C	N	O	S	0	0
			1386	874	255	253	4		

- Molecule 9 is a protein called 50S ribosomal protein L9, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	45	Total	C	N	O	0	0
			359	237	65	57		

- Molecule 10 is a protein called 50S ribosomal protein L13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	196	Total	C	N	O	S	0	0
			1489	942	280	264	3		

- Molecule 11 is a protein called 50S ribosomal protein L14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	120	Total	C	N	O	S	0	0
			934	582	178	169	5		

- Molecule 12 is a protein called 50S ribosomal protein L15, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	182	Total	C	N	O	S	0	0
			1385	864	273	242	6		

- Molecule 13 is a protein called 50S ribosomal protein L16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	135	Total	C	N	O	S	0	0
			1075	677	218	174	6		

- Molecule 14 is a protein called 50S ribosomal protein L17, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	116	Total	C	N	O	S	0	0
			945	592	193	156	4		

- Molecule 15 is a protein called 50S ribosomal protein L18, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	118	Total	C	N	O	S	0	0
			931	579	179	168	5		

- Molecule 16 is a protein called 50S ribosomal protein L19, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	114	Total	C	N	O	S	0	0
			915	586	178	150	1		

- Molecule 17 is a protein called 50S ribosomal protein L20, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	116	Total	C	N	O	S	0	0
			1003	637	209	155	2		

- Molecule 18 is a protein called 50S ribosomal protein L21, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	T	134	Total	C	N	O	0	0
			1017	653	183	181		

- Molecule 19 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	152	Total	C	N	O	S	0	0
			1165	738	212	208	7		

- Molecule 20 is a protein called 50S ribosomal protein L23, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	91	Total	C	N	O	S	0	0
			734	474	127	131	2		

- Molecule 21 is a protein called 50S ribosomal protein L24, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	129	Total	C	N	O	S	0	0
			1018	641	193	182	2		

- Molecule 22 is a protein called 50S ribosomal protein L27, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	108	Total	C	N	O	S	0	0
			866	545	172	149			

- Molecule 23 is a protein called 50S ribosomal protein L28, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	75	Total	C	N	O	S	0	0
			616	391	125	99	1		

- Molecule 24 is a protein called 50S ribosomal protein L29, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	94	Total	C	N	O	S	0	0
			788	492	156	137	3		

- Molecule 25 is a protein called 50S ribosomal protein L32, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	42	Total	C	N	O	S	0	0
			341	223	65	53			

- Molecule 26 is a protein called 50S ribosomal protein L33, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	60	Total	C	N	O	S	0	0
			489	304	98	83	4		

- Molecule 27 is a protein called 50S ribosomal protein L34, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	61	Total	C	N	O	S	0	0
			471	284	108	76	3		

- Molecule 28 is a protein called 50S ribosomal protein L35, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	70	Total	C	N	O	S	0	0
			575	362	121	91	1		

- Molecule 29 is a protein called 50S ribosomal protein L36, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	37	Total	C	N	O	S	0	0
			305	186	70	45	4		

- Molecule 30 is a protein called Ribosome-recycling factor, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	9	107	Total	C	N	O	S	0	0
			881	545	158	175	3		

- Molecule 31 is a protein called PSRP5alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	7	46	Total	C	N	O	S	0	0
			378	241	77	56	4		

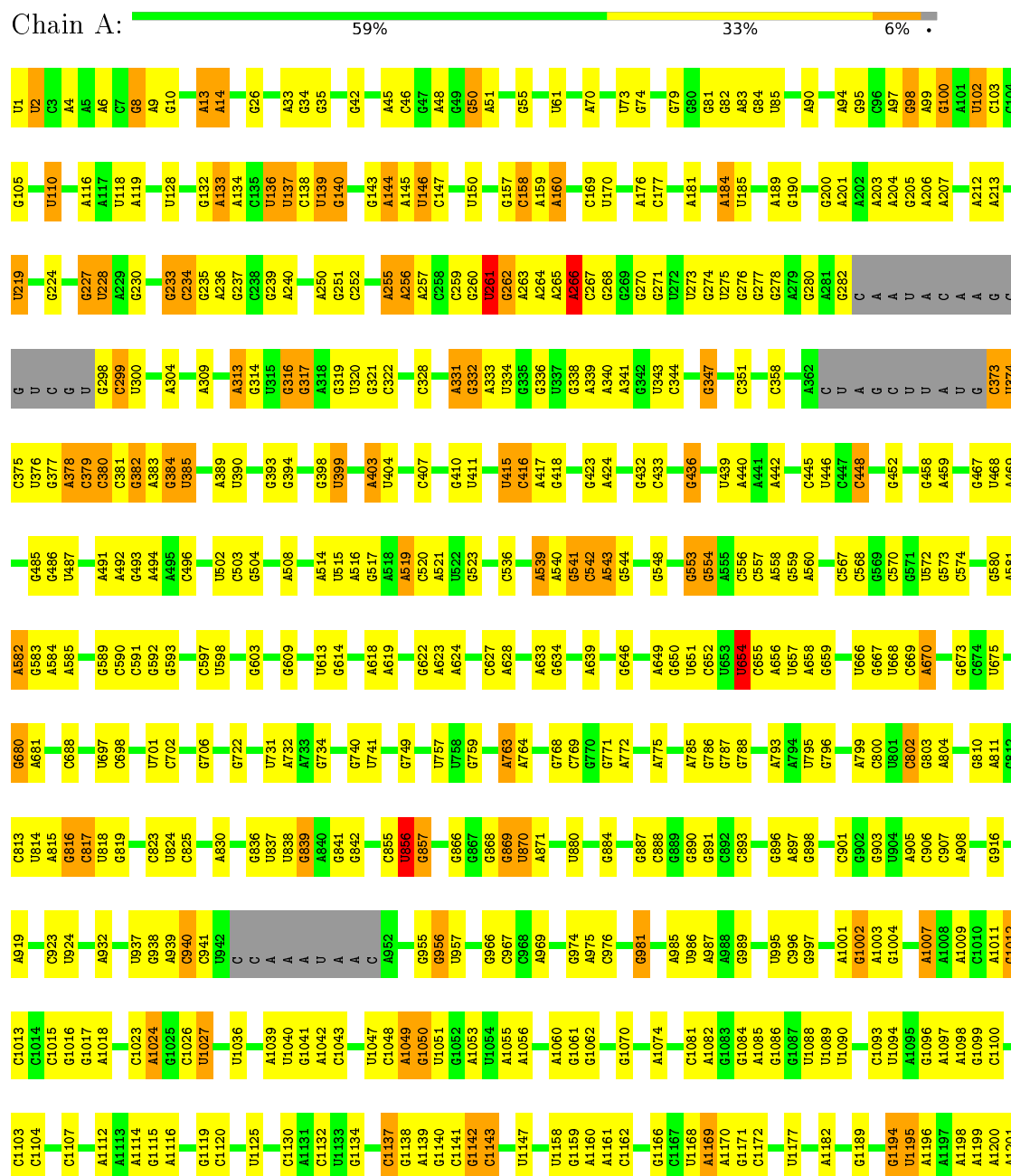
- Molecule 32 is a protein called PSRP6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	8	47	Total	C	N	O	S	0	0
			374	240	72	61	1		

3 Residue-property plots

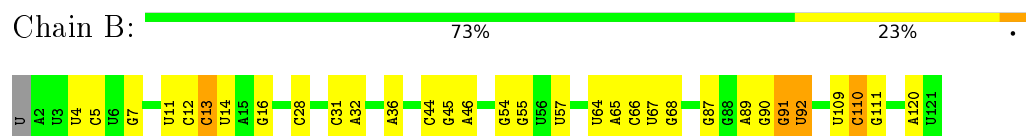
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S ribosomal RNA, chloroplastic

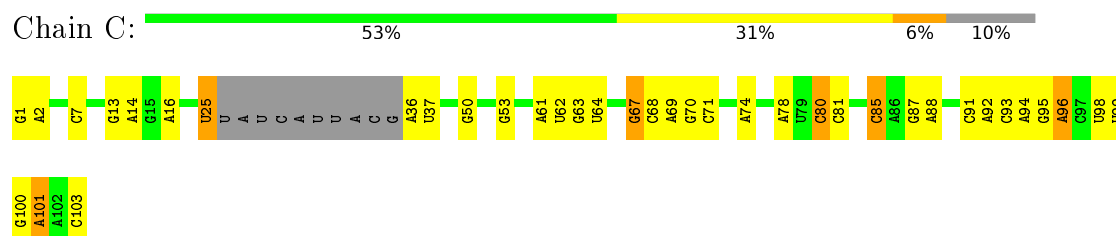




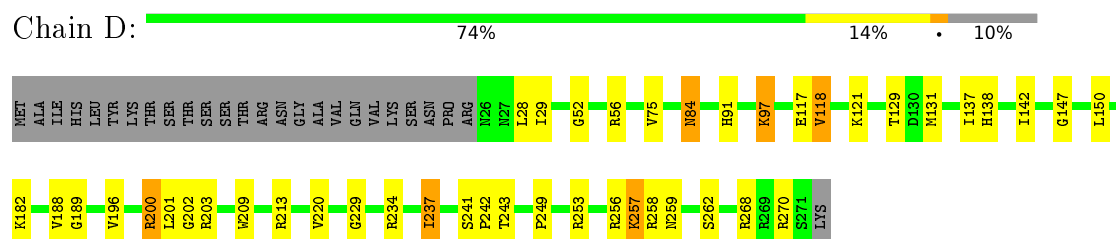

- Molecule 2: 5S ribosomal RNA, chloroplastic



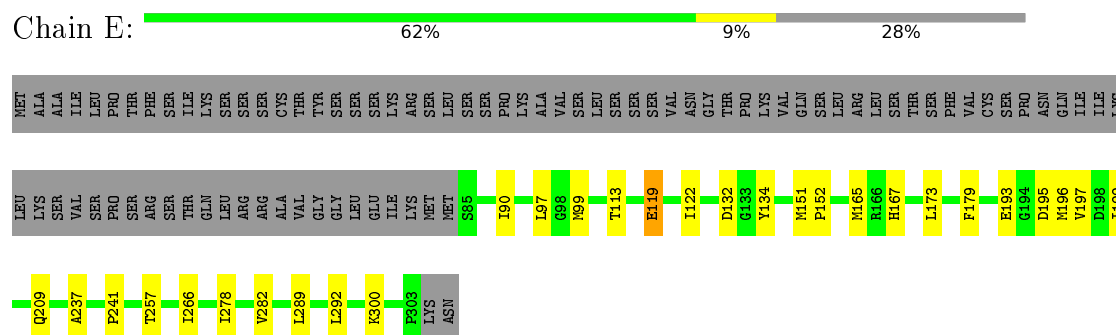
- Molecule 3: 4.8S ribosomal RNA, chloroplastic



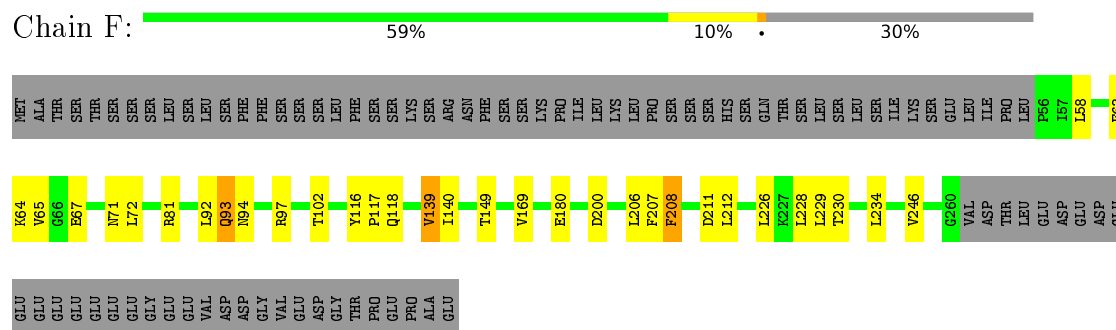
- Molecule 4: 50S ribosomal protein L2, chloroplastic



- Molecule 5: 50S ribosomal protein L3, chloroplastic

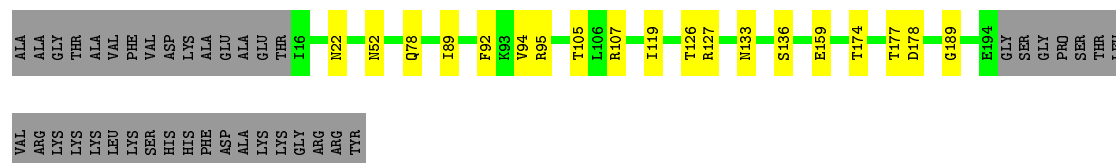


- Molecule 6: 50S ribosomal protein L4, chloroplastic



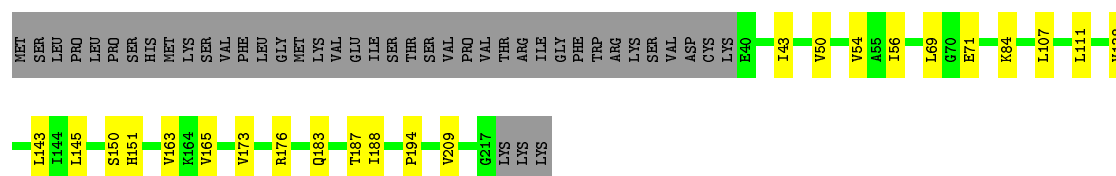
- Molecule 7: 50S ribosomal protein L5, chloroplastic

Chain G:  73% 9% 19%



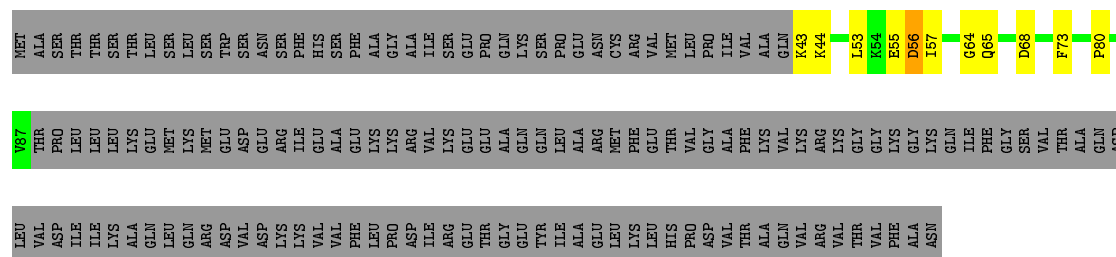
- Molecule 8: 50S ribosomal protein L6, chloroplastic

Chain H: 70% 10% 19%



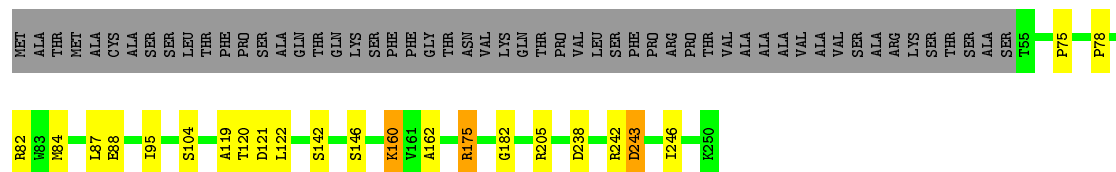
- Molecule 9: 50S ribosomal protein L9, chloroplastic

Chain I:  17% 5% 77%



- Molecule 10: 50S ribosomal protein L13, chloroplastic

Chain L: 69% 8% 22%



- Molecule 11: 50S ribosomal protein L14, chloroplastic

Chain M: 79% 21%



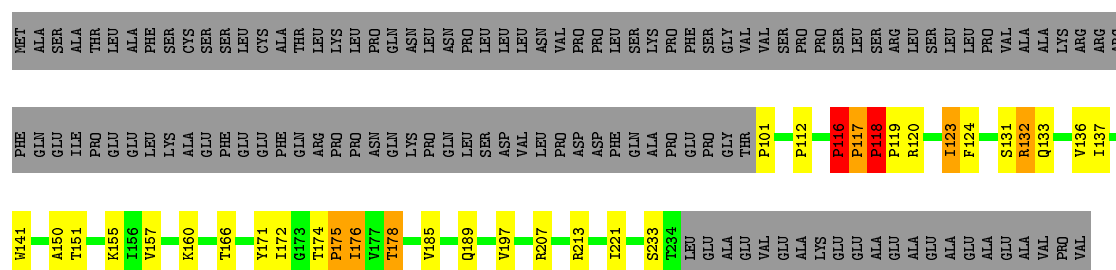
- Molecule 12: 50S ribosomal protein L15, chloroplastic

Chain S:  73% 18% 9%



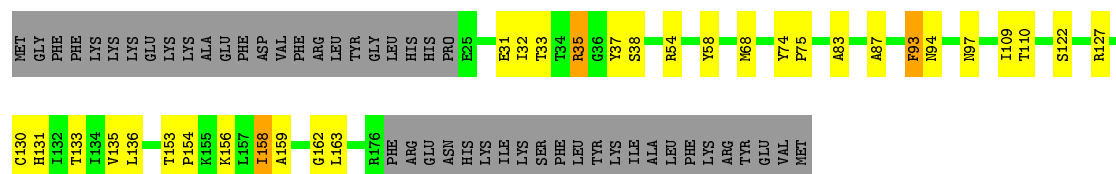
- Molecule 18: 50S ribosomal protein L21, chloroplastic

Chain T: 39% 10% 2% 48%

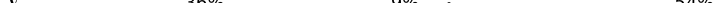


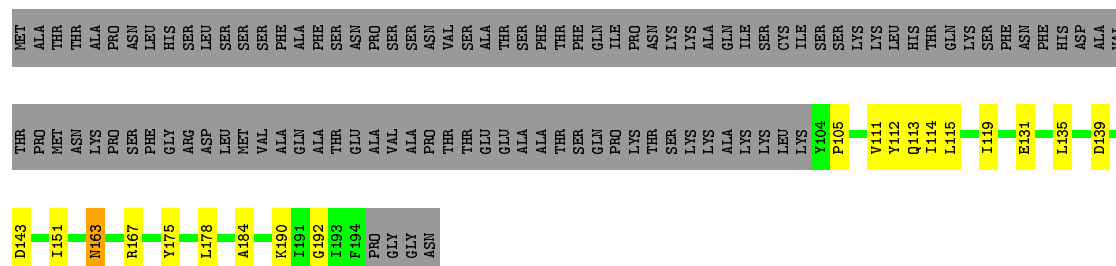
- Molecule 19: 50S ribosomal protein L22, chloroplastic

Chain U:  60% 15% 24%



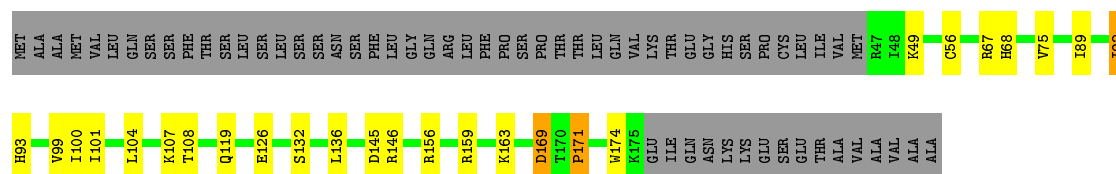
- Molecule 20: 50S ribosomal protein L23, chloroplastic

Chain V:  36% 9% . 54%



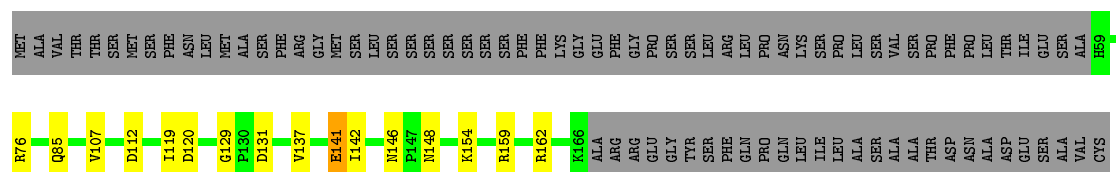
- Molecule 21: 50S ribosomal protein L24, chloroplastic

Chain W:  54% 12% 2% 32%



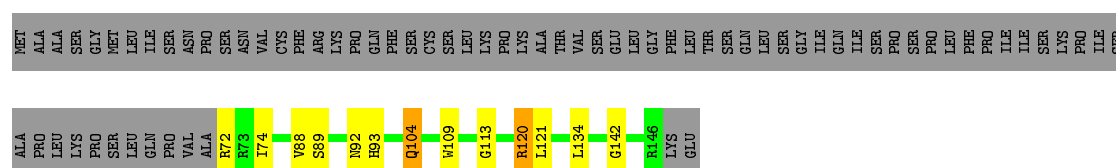
- Molecule 22: 50S ribosomal protein L27, chloroplastic

Chain X:  47% 8% 44%



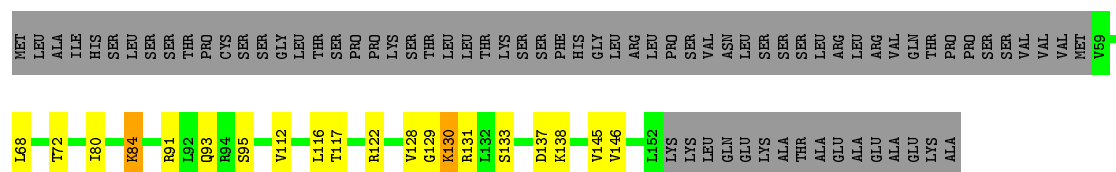
- Molecule 23: 50S ribosomal protein L28, chloroplastic

Chain Y: 42% 7% • 49%



- Molecule 24: 50S ribosomal protein L29, chloroplastic

Chain Z:  44% 11% • 44%



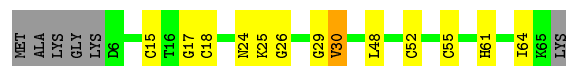
- Molecule 25: 50S ribosomal protein L32, chloroplastic

Chain 2:  54% 19% 26%



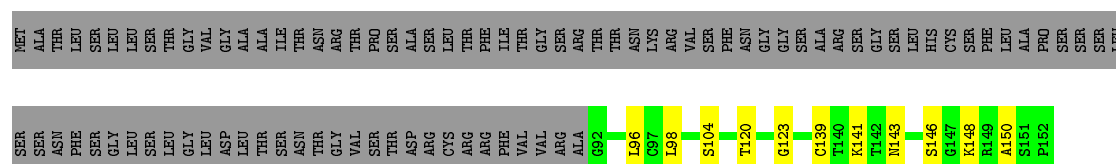
- Molecule 26: 50S ribosomal protein L33, chloroplastic

Chain 3:  71% 18% • 9%



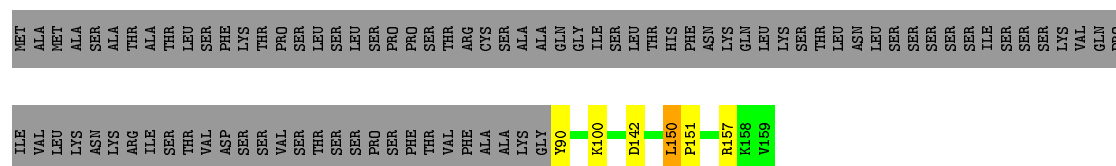
- Molecule 27: 50S ribosomal protein L34, chloroplastic

Chain 4: 33% 7% 60%



- Molecule 28: 50S ribosomal protein L35, chloroplatic

Chain 5:  40% 56%



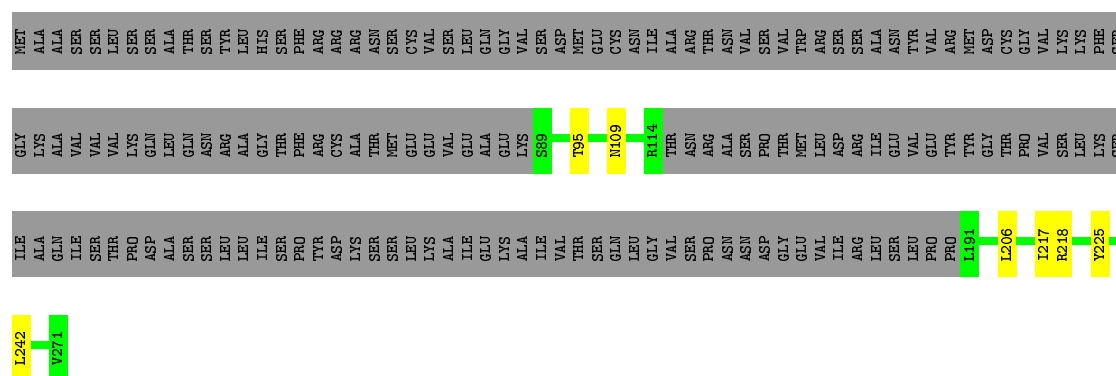
- Molecule 29: 50S ribosomal protein L36, chloroplatic

Chain 6:  95% 5%



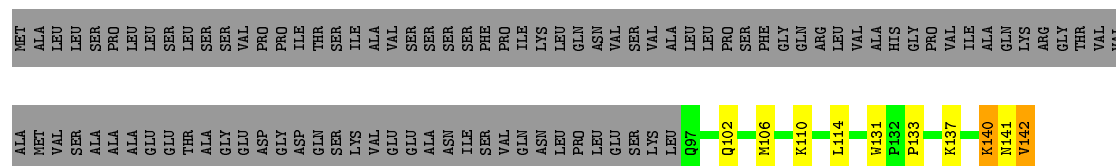
- Molecule 30: Ribosome-recycling factor, chloroplatic

Chain 9:  37% 61%



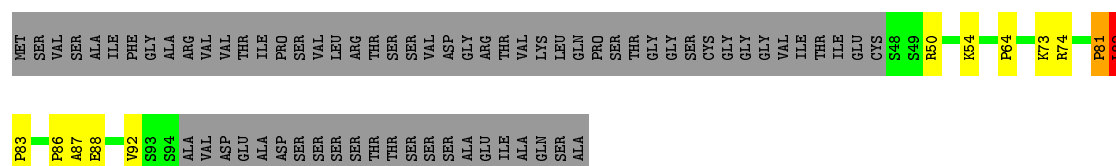
- Molecule 31: PSRP5alpha, chloroplatic

Chain 7:  25% 6% 68%



- Molecule 32: PSRP6, chloroplatic

Chain 8:  30% 9% 59%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	37636	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z > 2	RMSZ	# Z > 2
1	A	0.40	19/66169 (0.0%)	0.73	32/103225 (0.0%)
10	L	0.47	1/1521 (0.1%)	0.72	2/2062 (0.1%)
11	M	0.41	0/943	0.69	0/1271
12	N	0.44	0/1405	0.78	0/1864
13	O	0.43	0/1097	0.76	0/1471
14	P	0.47	0/960	0.82	0/1280
15	Q	0.43	0/946	0.69	0/1268
16	R	0.48	1/928 (0.1%)	0.71	0/1248
17	S	0.46	0/1020	0.82	0/1361
18	T	0.81	1/1034 (0.1%)	0.82	5/1405 (0.4%)
19	U	0.86	1/1184 (0.1%)	0.73	0/1593
2	B	0.29	0/2868	0.71	0/4469
20	V	0.50	1/744 (0.1%)	0.67	0/1000
21	W	0.55	1/1030 (0.1%)	0.71	1/1374 (0.1%)
22	X	0.41	0/882	0.64	1/1172 (0.1%)
23	Y	0.45	0/626	0.76	0/833
24	Z	0.42	0/796	0.77	0/1056
25	2	0.59	0/348	0.74	0/462
26	3	0.42	0/497	0.75	0/664
27	4	0.45	0/474	0.92	0/624
28	5	0.39	0/581	0.81	0/768
29	6	0.39	0/307	0.80	0/403
3	C	0.28	0/2241	0.69	0/3492
30	9	0.41	0/883	0.57	0/1169
31	7	0.45	0/381	0.75	0/498
32	8	0.45	0/388	0.73	0/528
4	D	0.43	0/1928	0.74	0/2588
5	E	0.41	0/1696	0.71	0/2269
6	F	0.56	2/1648 (0.1%)	0.72	0/2215
7	G	0.46	0/1408	0.58	0/1896
8	H	0.57	2/1407 (0.1%)	0.61	0/1892
9	I	0.47	0/362	0.69	0/480
All	All	0.43	29/98702 (0.0%)	0.73	41/147900 (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
18	T	0	1

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1554	C	O3'-P	-23.08	1.33	1.61
19	U	158	ILE	C-N	22.12	1.84	1.34
18	T	118	PRO	C-N	19.55	1.71	1.34
1	A	1435	U	O3'-P	-13.97	1.44	1.61
8	H	71	GLU	CD-OE2	12.96	1.40	1.25

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	U	N1-C1'-C2'	-11.30	99.31	114.00
1	A	1618	C	P-O3'-C3'	-10.44	107.17	119.70
1	A	763	A	C2'-C3'-O3'	8.73	128.71	109.50
1	A	50	G	C2'-C3'-O3'	7.76	126.57	109.50
1	A	261	U	C2'-C3'-O3'	7.38	125.74	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	T	116	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59074	0	29746	385	0
2	B	2564	0	1295	7	0
3	C	2001	0	1008	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1895	0	1977	18	0
5	E	1669	0	1753	11	0
6	F	1617	0	1677	10	0
7	G	1387	0	1443	7	0
8	H	1386	0	1448	12	0
9	I	359	0	415	3	0
10	L	1489	0	1434	8	0
11	M	934	0	985	10	0
12	N	1385	0	1464	13	0
13	O	1075	0	1134	13	0
14	P	945	0	1004	11	0
15	Q	931	0	952	3	0
16	R	915	0	1008	8	0
17	S	1003	0	1069	6	0
18	T	1017	0	1017	15	0
19	U	1165	0	1175	11	0
20	V	734	0	780	9	0
21	W	1018	0	1072	7	0
22	X	866	0	909	7	0
23	Y	616	0	665	7	0
24	Z	788	0	849	23	0
25	2	341	0	379	5	0
26	3	489	0	511	5	0
27	4	471	0	529	2	0
28	5	575	0	642	3	0
29	6	305	0	344	0	0
30	9	881	0	932	4	0
31	7	378	0	445	6	0
32	8	374	0	391	5	0
All	All	90647	0	60452	576	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 576 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:A:C6	24:Z:131:ARG:NH1	1.78	1.50
1:A:133:A:C2	24:Z:131:ARG:NH2	1.80	1.45
18:T:118:PRO:C	18:T:119:PRO:N	1.71	1.42
1:A:133:A:C5	24:Z:131:ARG:NH1	1.78	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:158:ILE:C	19:U:159:ALA:N	1.84	1.27

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	244/272 (90%)	200 (82%)	34 (14%)	10 (4%)	3	36
5	E	217/305 (71%)	191 (88%)	24 (11%)	2 (1%)	21	65
6	F	203/293 (69%)	170 (84%)	28 (14%)	5 (2%)	7	48
7	G	177/220 (80%)	160 (90%)	15 (8%)	2 (1%)	17	63
8	H	176/220 (80%)	152 (86%)	23 (13%)	1 (1%)	30	73
9	I	43/196 (22%)	33 (77%)	7 (16%)	3 (7%)	1	23
10	L	194/250 (78%)	171 (88%)	19 (10%)	4 (2%)	9	51
11	M	118/121 (98%)	101 (86%)	15 (13%)	2 (2%)	11	55
12	N	180/271 (66%)	142 (79%)	26 (14%)	12 (7%)	1	25
13	O	133/135 (98%)	120 (90%)	10 (8%)	3 (2%)	8	50
14	P	114/126 (90%)	102 (90%)	10 (9%)	2 (2%)	11	54
15	Q	116/166 (70%)	103 (89%)	11 (10%)	2 (2%)	11	55
16	R	112/233 (48%)	95 (85%)	16 (14%)	1 (1%)	21	65
17	S	114/128 (89%)	105 (92%)	7 (6%)	2 (2%)	11	54
18	T	132/256 (52%)	99 (75%)	23 (17%)	10 (8%)	1	20
19	U	150/199 (75%)	119 (79%)	29 (19%)	2 (1%)	15	59
20	V	89/198 (45%)	77 (86%)	9 (10%)	3 (3%)	5	42
21	W	127/191 (66%)	102 (80%)	20 (16%)	5 (4%)	4	37
22	X	106/194 (55%)	99 (93%)	5 (5%)	2 (2%)	10	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	Y	73/148 (49%)	64 (88%)	6 (8%)	3 (4%)	3	36
24	Z	92/168 (55%)	73 (79%)	14 (15%)	5 (5%)	2	30
25	2	40/57 (70%)	36 (90%)	3 (8%)	1 (2%)	7	48
26	3	58/66 (88%)	43 (74%)	9 (16%)	6 (10%)	1	12
27	4	59/152 (39%)	55 (93%)	2 (3%)	2 (3%)	5	42
28	5	68/159 (43%)	60 (88%)	8 (12%)	0	100	100
29	6	35/37 (95%)	31 (89%)	3 (9%)	1 (3%)	6	45
30	9	103/271 (38%)	100 (97%)	3 (3%)	0	100	100
31	7	44/142 (31%)	39 (89%)	2 (4%)	3 (7%)	1	24
32	8	45/116 (39%)	32 (71%)	6 (13%)	7 (16%)	0	5
All	All	3362/5290 (64%)	2874 (86%)	387 (12%)	101 (3%)	9	44

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	118	VAL
4	D	201	LEU
4	D	253	ARG
4	D	257	LYS
12	N	201	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	194/217 (89%)	181 (93%)	13 (7%)	20	60
5	E	180/259 (70%)	170 (94%)	10 (6%)	26	65
6	F	171/254 (67%)	160 (94%)	11 (6%)	22	61
7	G	152/183 (83%)	145 (95%)	7 (5%)	33	70
8	H	150/190 (79%)	147 (98%)	3 (2%)	63	86
9	I	39/170 (23%)	35 (90%)	4 (10%)	9	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	L	142/213 (67%)	134 (94%)	8 (6%)	26	65
11	M	100/101 (99%)	94 (94%)	6 (6%)	24	63
12	N	139/215 (65%)	125 (90%)	14 (10%)	9	41
13	O	108/108 (100%)	100 (93%)	8 (7%)	17	56
14	P	96/103 (93%)	83 (86%)	13 (14%)	5	30
15	Q	97/139 (70%)	93 (96%)	4 (4%)	37	73
16	R	100/207 (48%)	89 (89%)	11 (11%)	8	38
17	S	103/115 (90%)	90 (87%)	13 (13%)	5	31
18	T	101/223 (45%)	91 (90%)	10 (10%)	10	42
19	U	119/176 (68%)	107 (90%)	12 (10%)	9	41
20	V	80/171 (47%)	74 (92%)	6 (8%)	17	56
21	W	111/171 (65%)	101 (91%)	10 (9%)	12	47
22	X	90/163 (55%)	86 (96%)	4 (4%)	35	71
23	Y	65/130 (50%)	62 (95%)	3 (5%)	33	70
24	Z	87/153 (57%)	82 (94%)	5 (6%)	25	65
25	2	35/50 (70%)	31 (89%)	4 (11%)	7	36
26	3	56/60 (93%)	55 (98%)	1 (2%)	66	87
27	4	50/125 (40%)	45 (90%)	5 (10%)	9	42
28	5	61/140 (44%)	58 (95%)	3 (5%)	31	69
29	6	34/34 (100%)	33 (97%)	1 (3%)	50	79
30	9	101/244 (41%)	101 (100%)	0	100	100
31	7	41/121 (34%)	37 (90%)	4 (10%)	10	43
32	8	41/96 (43%)	38 (93%)	3 (7%)	17	57
All	All	2843/4531 (63%)	2647 (93%)	196 (7%)	24	59

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	P	25	ASP
16	R	225	LYS
27	4	98	LEU
14	P	52	SER
15	Q	102	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
14	P	26	GLN
20	V	153	ASN
30	9	216	ASN
14	P	101	ASN
16	R	202	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2745/2811 (97%)	824 (30%)	128 (4%)
2	B	119/121 (98%)	29 (24%)	3 (2%)
3	C	92/103 (89%)	28 (30%)	2 (2%)
All	All	2956/3035 (97%)	881 (29%)	133 (4%)

5 of 881 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	4	A
1	A	8	G
1	A	9	A
1	A	10	G

5 of 133 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1158	U
1	A	1439	U
1	A	2628	C
1	A	1169	A
1	A	1257	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
18	T	1
19	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	158:ILE	C	159:ALA	N	1.84
1	T	118:PRO	C	119:PRO	N	1.71
1	A	1554:C	O3'	1555:G	P	1.33