



Full wwPDB EM Validation Report ⓘ

Apr 2, 2025 – 02:34 am BST

PDB ID : 6EM1 / pdb_00006em1
EMDB ID : EMD-3893
Title : State C (Nsa1-TAP Flag-Ytm1) - Visualizing the assembly pathway of nuclear pre-60S ribosomes
Authors : Kater, L.; Cheng, J.; Barrio-Garcia, C.; Hurt, E.; Beckmann, R.
Deposited on : 2017-10-01
Resolution : 3.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

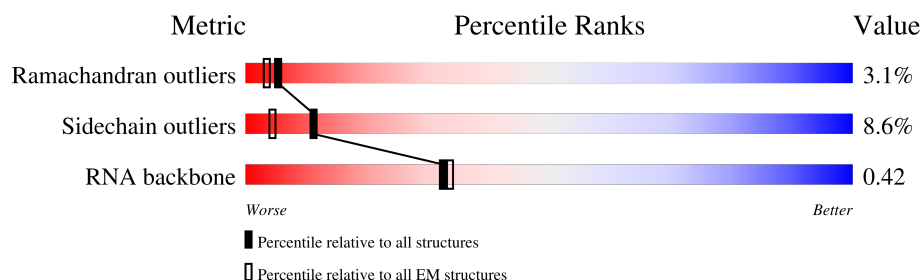
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



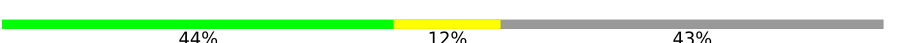






The reported resolution of this entry is 3.60 Å.

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



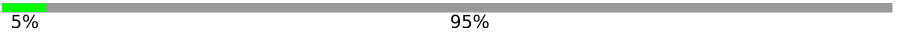
















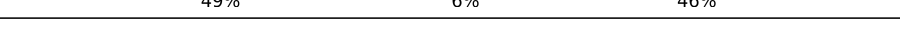







Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	x	295	
2	F	244	
3	3	306	
4	4	278	
5	5	463	
6	A	291	
7	b	647	
8	J	427	
9	r	261	









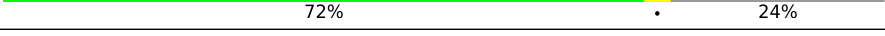
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Mol	Chain	Length	Quality of chain
10	s	520	 5% 95%
11	u	199	 55% 42%
12	v	231	 52% 44%
13	W	236	 93% 5%
14	y	245	 88% 8%
15	z	106	 52% 48%
16	B	387	 78% 8% 14%
17	C	362	 80% 15% 5%
18	e	130	 83% 13%
19	E	176	 81% 5% 14%
20	f	107	 86% 12% ..
21	G	256	 54% 9% 38%
22	h	120	 88% 10% ..
23	H	191	 91% 8%
24	i	100	 64% 10% 26%
25	j	88	 69% 10% 19%
26	L	199	 49% 6% 46%
27	M	138	 92% 5%
28	N	204	 74% 13% 13%
29	O	199	 42% 47% 10%
30	P	184	 65% 9% 26%
31	Q	186	 65% 6% 30%
32	S	172	 87% 11% ..
33	V	137	 90% 8%
34	Y	127	 87% 10% ..

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Mol	Chain	Length	Quality of chain
35	1	3396	
36	2	158	
37	6	232	
38	K	376	
39	m	807	
40	D	505	
41	o	220	
42	n	605	
43	t	322	

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 99980 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosome production factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	x	267	Total	C	N	O	S	0	0
			2268	1444	413	407	4		

- Molecule 2 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	241	Total	C	N	O	S	0	0
			1936	1246	351	338	1		

- Molecule 3 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	173	Total	C	N	O	S	0	0
			1434	901	274	250	9		

- Molecule 4 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	217	Total	C	N	O	S	0	0
			1853	1208	319	323	3		

- Molecule 5 is a protein called Ribosome biogenesis protein NSA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	385	Total	C	N	O	S	0	0
			3055	1957	514	573	11		

- Molecule 6 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	145	Total	C	N	O	S	0	0
			1211	780	218	210	3		

- Molecule 7 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	421	Total	C	N	O	S	0	0
			3410	2180	585	627	18		

- Molecule 8 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	66	Total	C	N	O	S	0	0
			549	341	97	110	1		

- Molecule 9 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	r	73	Total	C	N	O	S	0	0
			628	388	133	106	1		

- Molecule 10 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	s	27	Total	C	N	O	S	0	0
			224	136	51	37			

- Molecule 11 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	u	116	Total	C	N	O	S	0	0
			976	612	200	155	9		

- Molecule 12 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	v	130	Total	C	N	O	S	0	0
			1087	678	211	195	3		

- Molecule 13 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	232	Total	C	N	O	S	0	0
			1870	1184	321	360	5		

- Molecule 14 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	y	225	Total	C	N	O	S	0	0
			1701	1056	295	343	7		

- Molecule 15 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	z	55	Total	C	N	O	0	0
			444	273	88	83		

- Molecule 16 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B	333	Total	C	N	O	S	0	0
			2646	1680	490	470	6		

- Molecule 17 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	C	343	Total	C	N	O	S	0	0
			2611	1643	499	466	3		

- Molecule 18 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	e	125	Total	C	N	O	S	0	0
			1009	641	203	164	1		

- Molecule 19 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	151	Total	C	N	O	S	0	0
			1205	780	215	209	1		

- Molecule 20 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 21 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	159	Total	C	N	O	S	0	0
			1231	794	209	226	2		

- Molecule 22 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 23 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	H	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 24 is a protein called 60S ribosomal protein L36-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	74	Total	C	N	O	S	0	0
			594	367	125	101	1		

- Molecule 25 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	71	Total	C	N	O	S	0	0
			566	344	123	94	5		

- Molecule 26 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L	108	Total	C	N	O		0	0
			864	541	180	143			

- Molecule 27 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	M	134	Total	C	N	O	S	0	0
			1041	668	197	174	2		

- Molecule 28 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	N	177	Total	C	N	O	S	0	0
			1513	948	320	244	1		

- Molecule 29 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 30 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	P	137	Total	C	N	O	S	0	0
			1062	666	198	198			

- Molecule 31 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Q	131	Total	C	N	O	S	0	0
			1009	645	190	173	1		

- Molecule 32 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	170	Total	C	N	O	S	0	0
			1432	922	265	242	3		

- Molecule 33 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	V	126	Total	C	N	O	S	0	0
			936	588	176	165	7		

- Molecule 34 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Y	125	Total	C	N	O	S	0	0
			984	620	191	173			

- Molecule 35 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1	1785	Total	C	N	O	P	0	0
			38221	17064	6918	12454	1785		

- Molecule 36 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 37 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	6	65	Total	C	N	O	P	0	0
			1370	614	228	463	65		

- Molecule 38 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	K	257	Total	C	N	O	S	0	0
			2073	1337	341	392	3		

- Molecule 39 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	161	Total	C	N	O	S	0	0
			1362	867	238	253	4		

- Molecule 40 is a protein called ATP-dependent RNA helicase HAS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	D	194	Total	C	N	O	S	0	0
			1590	1030	268	287	5		

- Molecule 41 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	133	Total	C	N	O	S	0	0
			1107	716	198	189	4		

- Molecule 42 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	334	Total	C	N	O	S	0	0
			2734	1787	457	482	8		

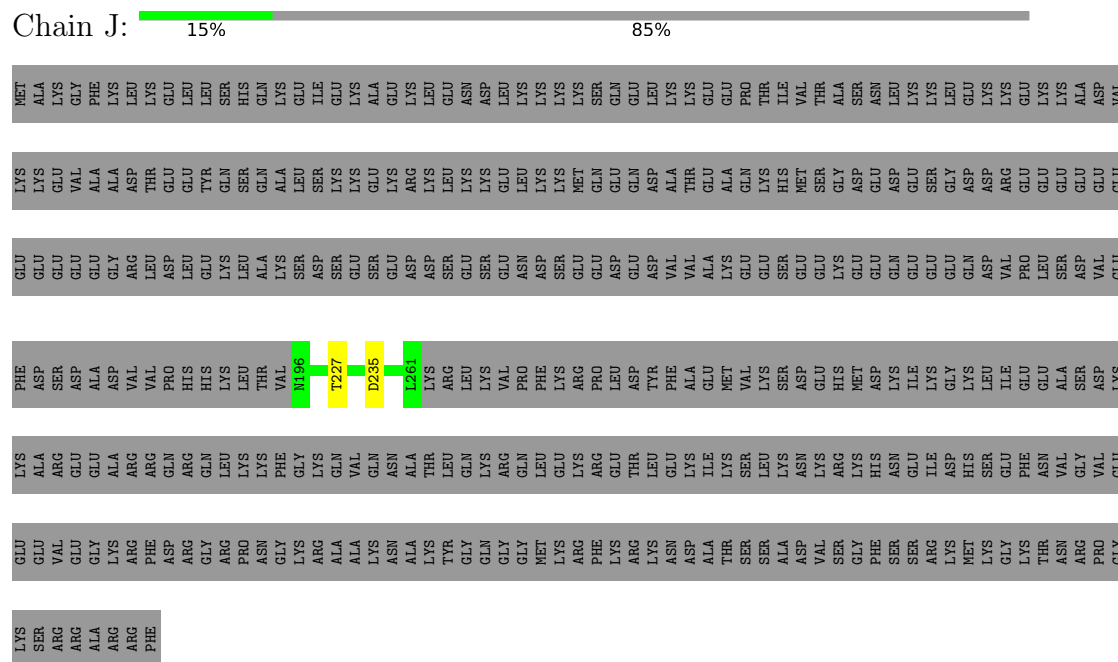
- Molecule 43 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	t	244	Total	C	N	O	S	0	0
			1935	1233	345	354	3		

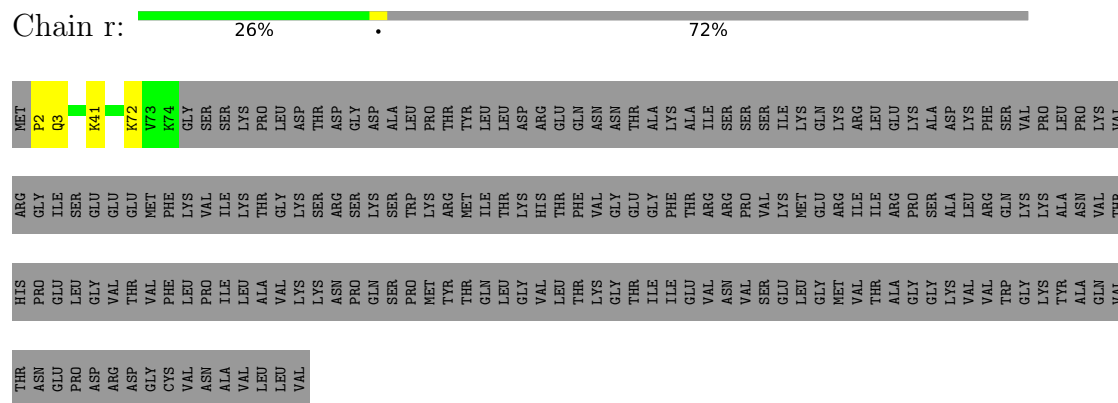
- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
44	u	1	Total	Zn	0
			1	1	
44	j	1	Total	Zn	0
			1	1	

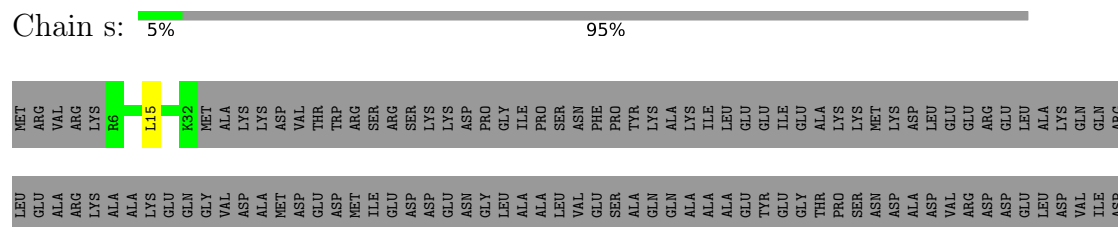
- Molecule 8: rRNA-processing protein EBP2

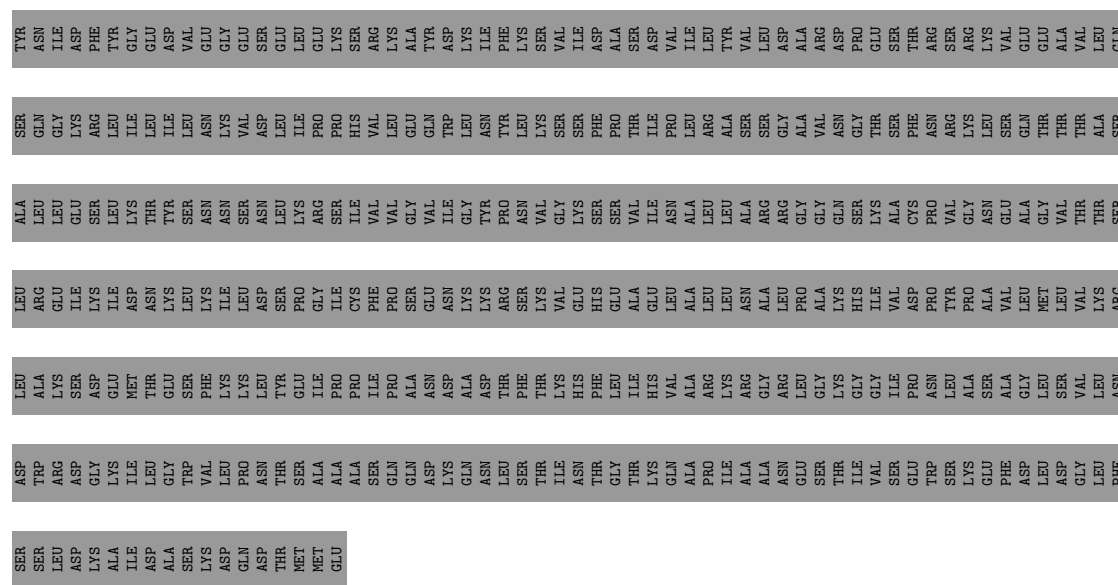


- Molecule 9: Ribosome biogenesis protein NSA2

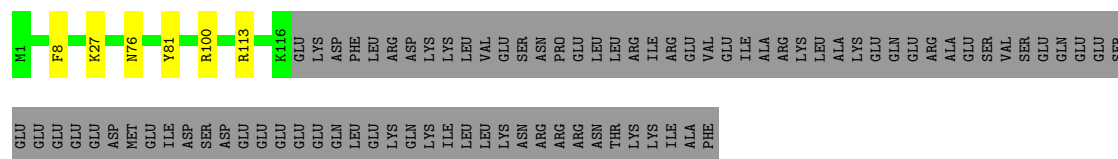


- Molecule 10: Nuclear GTP-binding protein NUG1

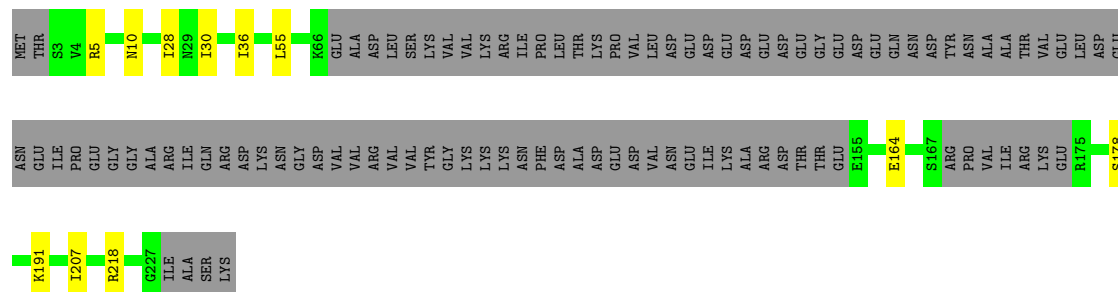




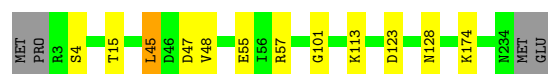
- Molecule 11: Ribosome biogenesis protein RLP24



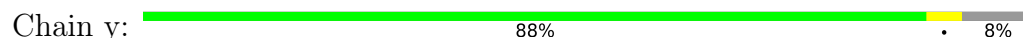
- Molecule 12: Nucleolar protein 16

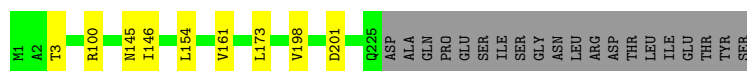


- Molecule 13: Ribosome assembly factor MRT4

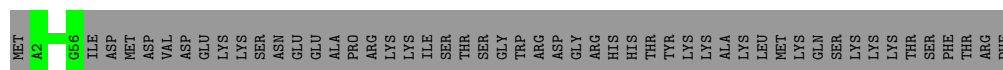


- Molecule 14: Eukaryotic translation initiation factor 6

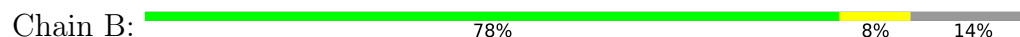




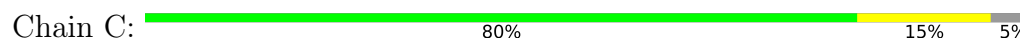
- Molecule 15: UPF0642 protein YBL028C



- Molecule 16: 60S ribosomal protein L3

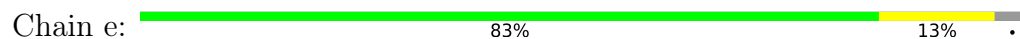


- Molecule 17: 60S ribosomal protein L4-A

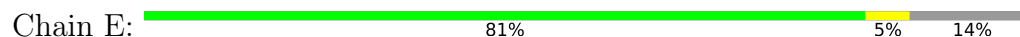


ASP

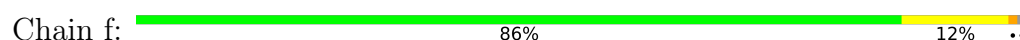
- Molecule 18: 60S ribosomal protein L32



- Molecule 19: 60S ribosomal protein L6-A



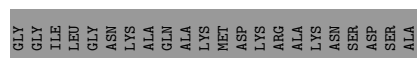
- Molecule 20: 60S ribosomal protein L33-A





- Molecule 21: 60S ribosomal protein L8-A

Chain G: 54% 9% 38%



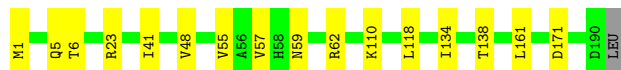
- Molecule 22: 60S ribosomal protein L35-A

Chain h: 88% 10% ..



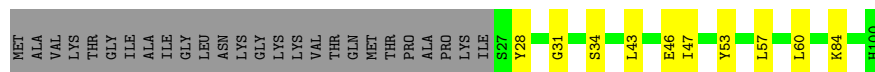
- Molecule 23: 60S ribosomal protein L9-A

Chain H: 91% 8% .



- Molecule 24: 60S ribosomal protein L36-B

Chain i: 64% 10% 26%



- Molecule 25: 60S ribosomal protein L37-A

Chain j: 69% 10% . 19%



- Molecule 26: 60S ribosomal protein L13-A

Chain L: 49% 6% 46%



PRO ILE ALA GLN PRO PRO THR ASP VAL GLU ALA ARG ALA VAL GLN ASP ASN GLY SER ALA PHE ARG THR LEU ARG ALA ALA SER GLY LEU ARG ALA LYS LYS PHE ARG GLY ILE ARG GLU LYS ALA GLU ALA GLU LYS LYS

• Molecule 27: 60S ribosomal protein L14-A

Chain M:  92% 5%

MET SER THR D4 V15 A29 I39 V63 T69 T80 K125 K137 ALA

• Molecule 28: 60S ribosomal protein L15-A

Chain N:  74% 13% 13%

MET G2 L7 L10 L19 L22 L29 R38 D46 R49 V66 G69 ASN ARG LYS ARG VAL PRO PRO LYS GLY ALA THR TYR GLY LYS PRO THR ASN GLN GLY VAL ASN GLU LEU LYS TYR R96 R105 R108 L116 V121 M122 T126

V132 I133 I142 R143 R144 D145 D153 P154 V155 T167 S171 A20 K179 G186 R187 K204

• Molecule 29: 60S ribosomal protein L16-A

Chain O:  42% 47% 10%

MET SER V3 V7 A83 I9 D10 G11 K12 L15 L16 G17 R18 L19 R20 A21 S21 V22 K25 Q26 L27 L28 N29 G30 Q31 V34 R37 R38 E39 M42 I43 E46 F47 F48 R49 N50 K53 P56 R59 K60 A61 T62 A63 F64 P70 R74 A75 P76 S77

R78 I79 F80 Y81 K82 A83 L84 R85 G86 M87 V88 S89 H90 K91 T92 A93 R94 G95 L99 E100 R101 L102 L105 K116 R117 V118 P121 Q122 A123 L124 R125 V126 L127 R128 G132 R133 K134 L138 G139 K140 L141 S142 T143 S144 V145 Y149 E150 D151 V152 V153 A154 K155 L156

E157 A158 K159 R160 V162 S163 S164 A166 E167 Y168 A169 K170 F174 T175 K176 K177 V178 A179 T184 A185 A186 E187 S188 D189 V190 A191 K192 Q193 L194 Y199

• Molecule 30: 60S ribosomal protein L17-A

Chain P:  65% 9% 26%

MET ALA ARG TYR GLY ALA THR SER N10 S16 V24 T29 R30 L41 T42 L52 K74 V78 P84 S87 Q86 V119 N120 K124 GLN ARG ARG ARG THR TYR ARG ALA HIS GLY ILE ARG MET ARG ASN LYS TYR E140 A156 V157 A158 K159 A160 A161

GLU LYS VAL VAL ARG LEU THR SER ARG GLN ARG GLY ARG ILE ALA ALA GLN LYS ARG ILE ALA


• Molecule 31: 60S ribosomal protein L18-A

Chain Q:  65% 6% 30%

MET GLY ILE ASP HIS THR SER LYS GLN HIS LYS ARG ARG GLY H15 K20 S21 D22 V23 V24 L28 L49 S55 K56 V64 R69 R92 N136 H145 SER ARG GLU PHE ALA VAL ARG HIS PHE GLY MET GLY PRO LYS LYS GLY LYS ALA PRO ARG ARG ILE LEU SER


THR
GLY
ARG
LYS
PHE
GLU
ARG
ALA
ARG
GLY
PHE
LYS
VAL

• Molecule 32: 60S ribosomal protein L20-A

Chain S:  87% 11% ..


MET
ALA
R3
R12
R13
L14
E21
P22
R23
L24
S32
S80
K71
I94
R95
D96
L106
R115
H122
D134
H154
K158
R167
P168
S169
Y172

• Molecule 33: 60S ribosomal protein L23-A

Chain V:  90% 8% ..

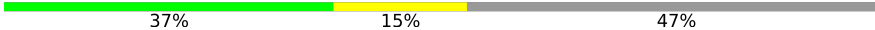
MET
SER
GLY
ASN
GLY
ALA
GLN
THR
PHE
R12
L54
K64
L93
Y137

• Molecule 34: 60S ribosomal protein L26-A

Chain Y:  87% 10% ..

MET
A2
S5
K17
K37
R51
R52
D53
D54
E55
V56
L57
V58
Y59
K64
Y74
T107
L111
L126
GLU

• Molecule 35: 25S ribosomal RNA

Chain 1:  37% 15% 47%

G1
U2
U3
A6
C7
A11
G18
A26
G30
A39
A40
C41
C42
A43
A48
A49
U50
A57
G58
G59
A60
A65
A66
C72
C73
G74
G75
G92
C93
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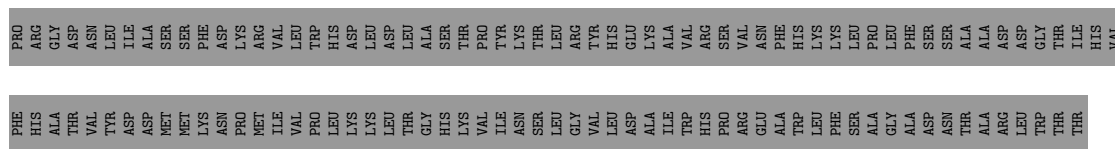
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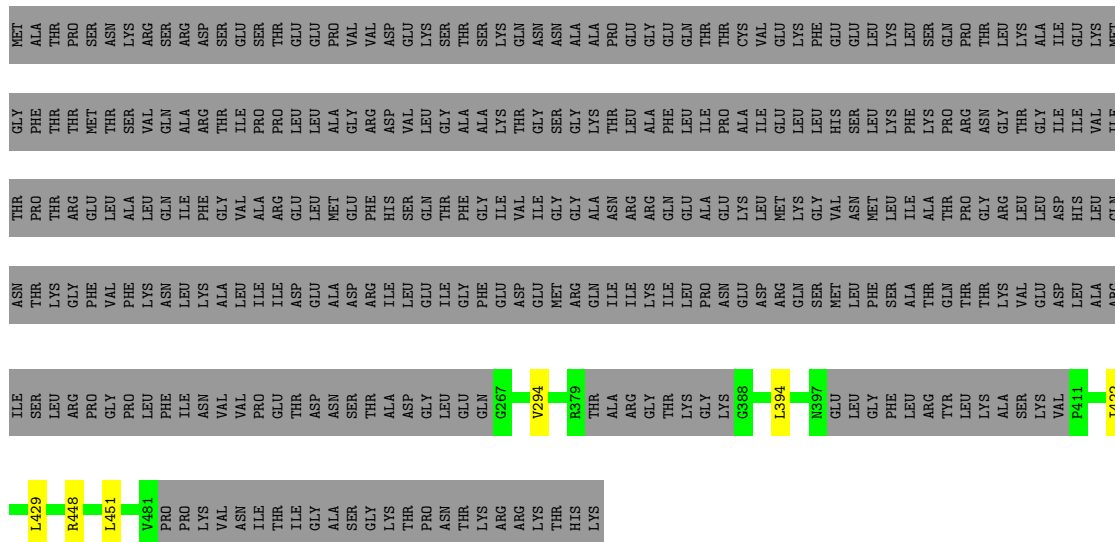
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C695
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A705
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G721
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A761
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U776
A780
G781
U782
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G785
A786

U794
G799
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U814
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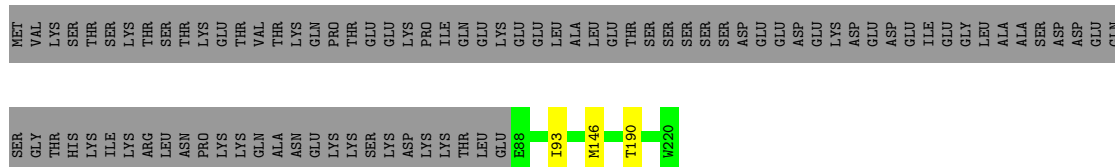




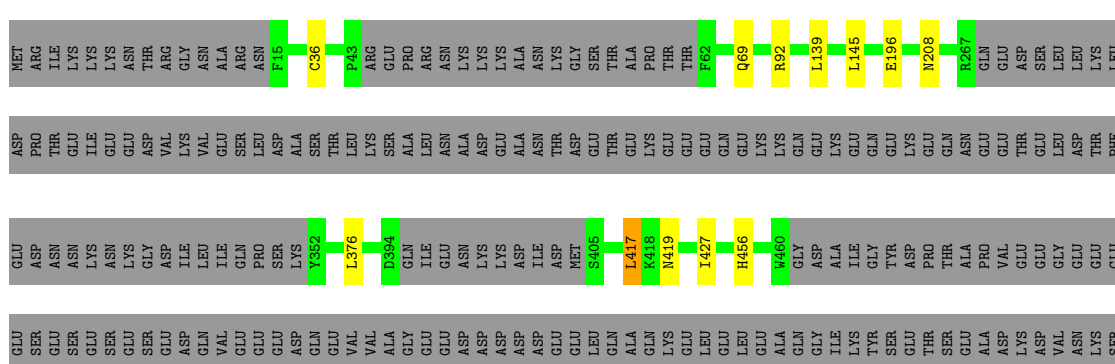
- Molecule 40: ATP-dependent RNA helicase HAS1



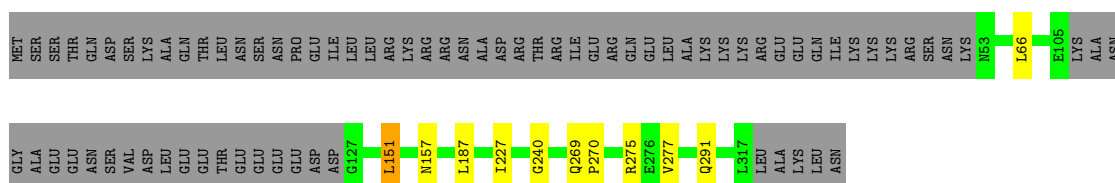
- Molecule 41: Ribosome biogenesis protein 15



- Molecule 42: Pescadillo homolog



- Molecule 43: Ribosome biogenesis protein RLP7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	156937	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor

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	x	0.55	1/2312 (0.0%)	0.80	1/3097 (0.0%)
2	F	0.49	0/1974	0.73	2/2654 (0.1%)
3	3	0.64	0/1461	0.93	2/1958 (0.1%)
4	4	0.47	0/1895	0.81	2/2549 (0.1%)
5	5	0.44	0/3109	0.68	0/4187
6	A	0.47	0/1243	0.64	0/1679
7	b	0.43	0/3474	0.64	1/4683 (0.0%)
8	J	0.44	0/559	0.58	0/754
9	r	0.41	0/638	0.61	0/837
10	s	0.44	0/224	0.64	0/288
11	u	0.42	0/996	0.61	0/1324
12	v	0.46	0/1100	0.63	0/1456
13	W	0.42	0/1902	0.62	1/2564 (0.0%)
14	y	0.41	0/1722	0.63	0/2343
15	z	0.39	0/445	0.60	0/585
16	B	0.44	0/2699	0.70	1/3626 (0.0%)
17	C	0.56	0/2660	0.86	4/3601 (0.1%)
18	e	0.56	0/1030	0.82	2/1379 (0.1%)
19	E	0.47	0/1226	0.72	0/1648
20	f	0.56	0/868	0.79	0/1168
21	G	0.44	0/1252	0.71	0/1695
22	h	0.42	0/978	0.70	1/1301 (0.1%)
23	H	0.43	0/1531	0.65	0/2062
24	i	0.41	0/599	0.70	0/793
25	j	0.55	0/578	0.85	0/767
26	L	0.51	0/877	0.84	0/1179
27	M	0.42	0/1056	0.69	0/1421
28	N	0.56	2/1544 (0.1%)	0.78	3/2065 (0.1%)
29	O	0.70	1/1585 (0.1%)	0.88	2/2128 (0.1%)
30	P	0.49	0/1080	0.70	0/1455
31	Q	0.47	0/1024	0.74	0/1385
32	S	0.47	0/1468	0.69	0/1973

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	V	0.41	0/950	0.61	0/1279
34	Y	0.59	1/995 (0.1%)	0.77	0/1329
35	1	0.35	0/42777	0.69	10/66679 (0.0%)
36	2	0.35	0/3740	0.69	1/5808 (0.0%)
37	6	0.27	0/1527	0.75	0/2371
38	K	0.42	0/2107	0.65	0/2845
39	m	0.40	0/1401	0.64	0/1895
40	D	0.44	0/1626	0.65	0/2193
41	o	0.42	0/1129	0.65	0/1502
42	n	0.42	0/2802	0.62	1/3791 (0.0%)
43	t	0.40	0/1961	0.65	0/2639
All	All	0.42	5/106124 (0.0%)	0.70	34/152935 (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
3	3	0	1
4	4	0	3
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	Y	126	LEU	C-O	11.24	1.44	1.23
29	O	100	GLU	CD-OE2	8.32	1.34	1.25
28	N	105	ARG	CZ-NH1	7.06	1.42	1.33
1	x	180	GLU	C-O	5.37	1.33	1.23
28	N	105	ARG	NE-CZ	5.00	1.39	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	1	649	A	C2'-C3'-O3'	8.99	129.27	109.50
29	O	19	LEU	CA-CB-CG	-8.57	95.58	115.30
17	C	313	LEU	CA-CB-CG	8.43	134.69	115.30
35	1	1347	U	C4'-C3'-O3'	7.64	128.28	113.00
28	N	105	ARG	NE-CZ-NH1	7.48	124.04	120.30
28	N	105	ARG	NE-CZ-NH2	-7.11	116.75	120.30
35	1	1102	A	C2'-C3'-O3'	7.06	125.03	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	157	LEU	CA-CB-CG	6.91	131.19	115.30
35	1	480	C	C2'-C3'-O3'	6.75	124.50	113.70
3	3	15	CYS	CA-CB-SG	6.70	126.07	114.00
35	1	1356	U	C2'-C3'-O3'	6.66	124.35	113.70
36	2	114	G	C2'-C3'-O3'	6.50	124.09	113.70
4	4	154	LEU	CA-CB-CG	6.33	129.87	115.30
7	b	277	LEU	CA-CB-CG	6.28	129.75	115.30
2	F	218	ARG	NE-CZ-NH2	-6.19	117.20	120.30
35	1	1389	G	N9-C1'-C2'	-6.14	105.24	112.00
17	C	156	LEU	CA-CB-CG	6.14	129.42	115.30
42	n	417	LEU	CA-CB-CG	6.11	129.35	115.30
18	e	85	LEU	CB-CG-CD1	-6.09	100.64	111.00
18	e	82	LEU	CA-CB-CG	6.09	129.30	115.30
29	O	102	LEU	CA-CB-CG	-5.85	101.84	115.30
17	C	138	ARG	NE-CZ-NH1	5.83	123.22	120.30
28	N	116	LEU	CA-CB-CG	5.67	128.33	115.30
22	h	28	LEU	CA-CB-CG	5.62	128.24	115.30
13	W	45	LEU	CA-CB-CG	5.60	128.17	115.30
1	x	81	LEU	CA-CB-CG	5.54	128.05	115.30
17	C	327	LEU	CA-CB-CG	5.47	127.89	115.30
35	1	694	C	C2'-C3'-O3'	5.47	122.45	113.70
16	B	351	LEU	CA-CB-CG	5.46	127.87	115.30
3	3	62	LEU	CA-CB-CG	5.43	127.79	115.30
2	F	239	LEU	CA-CB-CG	5.34	127.59	115.30
35	1	1178	G	O5'-P-OP2	5.16	116.89	110.70
35	1	441	U	C2'-C3'-O3'	5.14	121.92	113.70
35	1	456	U	C2'-C3'-O3'	5.05	121.79	113.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	118	VAL	Peptide
4	4	135	TYR	Peptide
4	4	136	LEU	Mainchain
4	4	225	VAL	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	x	259/295 (88%)	203 (78%)	44 (17%)	12 (5%)	2	18
2	F	239/244 (98%)	212 (89%)	23 (10%)	4 (2%)	7	37
3	3	171/306 (56%)	122 (71%)	38 (22%)	11 (6%)	1	13
4	4	209/278 (75%)	173 (83%)	26 (12%)	10 (5%)	2	17
5	5	377/463 (81%)	338 (90%)	33 (9%)	6 (2%)	8	38
6	A	139/291 (48%)	122 (88%)	12 (9%)	5 (4%)	3	23
7	b	413/647 (64%)	381 (92%)	27 (6%)	5 (1%)	11	43
8	J	64/427 (15%)	58 (91%)	4 (6%)	2 (3%)	3	26
9	r	71/261 (27%)	65 (92%)	4 (6%)	2 (3%)	4	27
10	s	25/520 (5%)	25 (100%)	0	0	100	100
11	u	114/199 (57%)	109 (96%)	4 (4%)	1 (1%)	14	48
12	v	124/231 (54%)	115 (93%)	9 (7%)	0	100	100
13	W	230/236 (98%)	213 (93%)	15 (6%)	2 (1%)	14	48
14	y	223/245 (91%)	210 (94%)	13 (6%)	0	100	100
15	z	53/106 (50%)	49 (92%)	4 (8%)	0	100	100
16	B	329/387 (85%)	289 (88%)	30 (9%)	10 (3%)	3	26
17	C	341/362 (94%)	295 (86%)	30 (9%)	16 (5%)	2	18
18	e	123/130 (95%)	113 (92%)	9 (7%)	1 (1%)	16	51
19	E	147/176 (84%)	131 (89%)	16 (11%)	0	100	100
20	f	104/107 (97%)	98 (94%)	4 (4%)	2 (2%)	6	35
21	G	155/256 (60%)	134 (86%)	17 (11%)	4 (3%)	4	28
22	h	117/120 (98%)	104 (89%)	8 (7%)	5 (4%)	2	19
23	H	188/191 (98%)	167 (89%)	20 (11%)	1 (0%)	25	59
24	i	72/100 (72%)	66 (92%)	4 (6%)	2 (3%)	4	27
25	j	69/88 (78%)	62 (90%)	5 (7%)	2 (3%)	3	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	L	106/199 (53%)	97 (92%)	7 (7%)	2 (2%)	6	35
27	M	132/138 (96%)	121 (92%)	9 (7%)	2 (2%)	8	39
28	N	173/204 (85%)	150 (87%)	22 (13%)	1 (1%)	22	55
29	O	195/199 (98%)	66 (34%)	44 (23%)	85 (44%)	0	0
30	P	133/184 (72%)	118 (89%)	13 (10%)	2 (2%)	8	39
31	Q	129/186 (69%)	117 (91%)	12 (9%)	0	100	100
32	S	168/172 (98%)	143 (85%)	18 (11%)	7 (4%)	2	20
33	V	124/137 (90%)	113 (91%)	11 (9%)	0	100	100
34	Y	123/127 (97%)	110 (89%)	11 (9%)	2 (2%)	8	38
38	K	253/376 (67%)	231 (91%)	20 (8%)	2 (1%)	16	51
39	m	159/807 (20%)	144 (91%)	14 (9%)	1 (1%)	22	55
40	D	188/505 (37%)	167 (89%)	21 (11%)	0	100	100
41	o	131/220 (60%)	121 (92%)	9 (7%)	1 (1%)	16	51
42	n	326/605 (54%)	302 (93%)	22 (7%)	2 (1%)	22	55
43	t	240/322 (74%)	214 (89%)	20 (8%)	6 (2%)	4	29
All	All	6936/11047 (63%)	6068 (88%)	652 (9%)	216 (3%)	5	26

All (216) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	x	119	PRO
1	x	128	PHE
1	x	222	PRO
2	F	160	ARG
2	F	164	SER
3	3	13	SER
3	3	31	GLU
3	3	133	HIS
4	4	137	GLN
4	4	212	THR
5	5	340	LYS
6	A	43	TYR
7	b	198	ALA
16	B	34	LYS
17	C	339	LEU
25	j	68	LYS
27	M	29	ALA

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Mol	Chain	Res	Type
29	O	9	ILE
29	O	16	VAL
29	O	17	GLY
29	O	18	ARG
29	O	20	ALA
29	O	21	SER
29	O	43	ILE
29	O	46	GLU
29	O	48	PHE
29	O	53	LYS
29	O	60	LYS
29	O	64	PHE
29	O	76	PRO
29	O	77	SER
29	O	81	TYR
29	O	82	LYS
29	O	83	ALA
29	O	85	ARG
29	O	93	ALA
29	O	99	LEU
29	O	118	VAL
29	O	121	PRO
29	O	122	GLN
29	O	126	VAL
29	O	127	LEU
29	O	138	LEU
29	O	139	GLY
29	O	142	SER
29	O	143	THR
29	O	144	SER
29	O	149	TYR
29	O	150	GLU
29	O	153	VAL
29	O	154	ALA
29	O	156	LEU
29	O	158	ALA
29	O	162	VAL
29	O	163	SER
29	O	168	TYR
29	O	169	ALA
29	O	170	LYS
29	O	175	THR

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Mol	Chain	Res	Type
29	O	176	LYS
29	O	179	ALA
29	O	189	ASP
29	O	190	VAL
29	O	191	ALA
29	O	192	LYS
41	o	190	THR
43	t	227	ILE
43	t	269	GLN
2	F	157	ASN
2	F	159	GLN
3	3	86	TYR
6	A	63	PRO
9	r	3	GLN
16	B	142	ALA
16	B	155	ALA
16	B	174	LYS
16	B	187	SER
17	C	90	PHE
17	C	140	HIS
17	C	141	ARG
17	C	268	ALA
18	e	86	THR
22	h	86	ARG
24	i	31	GLY
26	L	50	PRO
29	O	8	VAL
29	O	10	ASP
29	O	12	LYS
29	O	63	ALA
29	O	88	VAL
29	O	89	SER
29	O	91	LYS
29	O	125	ARG
29	O	152	VAL
29	O	155	LYS
29	O	167	TYR
29	O	178	VAL
29	O	185	ALA
29	O	187	GLU
29	O	193	GLN
30	P	156	ALA

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Mol	Chain	Res	Type
34	Y	52	ARG
39	m	328	LYS
43	t	277	VAL
1	x	132	LEU
1	x	155	LYS
1	x	281	GLU
1	x	290	LYS
4	4	82	ASN
4	4	157	LEU
5	5	305	GLN
6	A	94	HIS
6	A	105	PRO
7	b	14	ALA
7	b	432	MET
13	W	4	SER
16	B	279	ASN
17	C	3	ARG
17	C	174	ALA
17	C	311	HIS
17	C	320	ASN
21	G	79	GLN
21	G	232	HIS
22	h	42	PRO
22	h	91	ALA
24	i	34	SER
25	j	55	ARG
29	O	19	LEU
29	O	25	LYS
29	O	34	VAL
29	O	61	ALA
29	O	90	HIS
29	O	116	LYS
29	O	123	ALA
29	O	165	ALA
29	O	174	PHE
29	O	194	LEU
32	S	13	ARG
32	S	14	LEU
32	S	22	PRO
1	x	167	GLU
3	3	3	ASP
3	3	16	SER

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Mol	Chain	Res	Type
3	3	17	HIS
3	3	42	SER
3	3	157	LYS
4	4	61	PRO
4	4	87	GLU
4	4	213	PRO
5	5	129	LYS
5	5	211	GLU
8	J	235	ASP
9	r	41	LYS
11	u	81	TYR
16	B	139	GLN
16	B	300	ARG
16	B	333	LYS
17	C	4	PRO
17	C	232	SER
20	f	86	ARG
23	H	110	LYS
29	O	59	ARG
29	O	70	PRO
29	O	128	ARG
32	S	24	LEU
32	S	115	ARG
38	K	284	ASN
43	t	240	GLY
43	t	270	PRO
1	x	201	ASN
1	x	292	LYS
3	3	128	ARG
4	4	77	PHE
7	b	74	VAL
17	C	233	LEU
17	C	269	SER
17	C	317	PRO
17	C	328	ASN
21	G	137	ASN
22	h	85	THR
29	O	37	ARG
29	O	159	LYS
29	O	160	ARG
30	P	84	PRO
38	K	256	PRO

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Mol	Chain	Res	Type
42	n	196	GLU
42	n	456	HIS
43	t	151	LEU
1	x	270	LEU
3	3	73	PRO
5	5	116	ASP
7	b	434	GLU
8	J	227	THR
16	B	108	GLU
22	h	84	LYS
26	L	56	PRO
29	O	50	ASN
29	O	56	ASP
29	O	95	GLY
32	S	167	ARG
17	C	181	VAL
20	f	80	VAL
29	O	145	VAL
4	4	60	ARG
6	A	104	PRO
27	M	39	ILE
29	O	132	GLY
34	Y	59	VAL
1	x	101	VAL
5	5	131	VAL
32	S	21	GLU
13	W	101	GLY
29	O	30	GLY
4	4	153	VAL
21	G	159	PRO
28	N	186	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	252/276 (91%)	206 (82%)	46 (18%)	1	8
2	F	204/205 (100%)	191 (94%)	13 (6%)	14	43
3	3	155/274 (57%)	129 (83%)	26 (17%)	1	11
4	4	203/257 (79%)	177 (87%)	26 (13%)	3	19
5	5	343/410 (84%)	323 (94%)	20 (6%)	17	46
6	A	137/263 (52%)	129 (94%)	8 (6%)	17	46
7	b	377/573 (66%)	345 (92%)	32 (8%)	8	33
8	J	61/383 (16%)	61 (100%)	0	100	100
9	r	65/229 (28%)	63 (97%)	2 (3%)	35	62
10	s	24/445 (5%)	23 (96%)	1 (4%)	25	54
11	u	101/180 (56%)	96 (95%)	5 (5%)	20	49
12	v	116/205 (57%)	105 (90%)	11 (10%)	7	30
13	W	209/213 (98%)	199 (95%)	10 (5%)	21	51
14	y	193/211 (92%)	184 (95%)	9 (5%)	22	51
15	z	48/95 (50%)	48 (100%)	0	100	100
16	B	280/323 (87%)	259 (92%)	21 (8%)	11	37
17	C	273/289 (94%)	238 (87%)	35 (13%)	3	19
18	e	108/111 (97%)	94 (87%)	14 (13%)	3	19
19	E	131/153 (86%)	123 (94%)	8 (6%)	15	44
20	f	90/91 (99%)	77 (86%)	13 (14%)	2	16
21	G	128/208 (62%)	110 (86%)	18 (14%)	3	17
22	h	104/105 (99%)	96 (92%)	8 (8%)	10	36
23	H	170/171 (99%)	155 (91%)	15 (9%)	8	32
24	i	61/81 (75%)	53 (87%)	8 (13%)	3	19
25	j	59/71 (83%)	50 (85%)	9 (15%)	2	14
26	L	87/159 (55%)	78 (90%)	9 (10%)	6	27
27	M	106/109 (97%)	101 (95%)	5 (5%)	22	51
28	N	153/176 (87%)	128 (84%)	25 (16%)	2	12
29	O	160/162 (99%)	114 (71%)	46 (29%)	0	2
30	P	109/146 (75%)	94 (86%)	15 (14%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Q	107/151 (71%)	96 (90%)	11 (10%)	6	27
32	S	155/156 (99%)	141 (91%)	14 (9%)	8	32
33	V	98/105 (93%)	95 (97%)	3 (3%)	35	62
34	Y	108/110 (98%)	96 (89%)	12 (11%)	5	25
38	K	238/346 (69%)	233 (98%)	5 (2%)	48	71
39	m	150/723 (21%)	146 (97%)	4 (3%)	40	65
40	D	175/440 (40%)	169 (97%)	6 (3%)	32	60
41	o	118/199 (59%)	116 (98%)	2 (2%)	56	75
42	n	302/548 (55%)	292 (97%)	10 (3%)	33	61
43	t	216/287 (75%)	210 (97%)	6 (3%)	38	64
All	All	6174/9639 (64%)	5643 (91%)	531 (9%)	11	33

All (531) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	x	15	ARG
1	x	60	ILE
1	x	79	ASP
1	x	81	LEU
1	x	87	SER
1	x	88	ASN
1	x	99	THR
1	x	100	ASN
1	x	101	VAL
1	x	104	LYS
1	x	113	ILE
1	x	115	ILE
1	x	121	VAL
1	x	124	VAL
1	x	125	LYS
1	x	126	ARG
1	x	132	LEU
1	x	133	LYS
1	x	138	ILE
1	x	149	ILE
1	x	150	ILE
1	x	154	LYS
1	x	161	THR

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Mol	Chain	Res	Type
1	x	163	ILE
1	x	165	LEU
1	x	170	THR
1	x	176	SER
1	x	179	VAL
1	x	191	THR
1	x	197	LEU
1	x	204	THR
1	x	209	THR
1	x	217	ILE
1	x	223	ASP
1	x	232	LEU
1	x	235	GLN
1	x	239	ILE
1	x	241	PHE
1	x	242	ARG
1	x	247	VAL
1	x	263	PHE
1	x	266	LYS
1	x	270	LEU
1	x	274	ILE
1	x	279	GLU
1	x	290	LYS
2	F	8	THR
2	F	13	LEU
2	F	30	ARG
2	F	34	LYS
2	F	89	ILE
2	F	93	ASN
2	F	119	VAL
2	F	124	LEU
2	F	129	LEU
2	F	179	LEU
2	F	183	ASP
2	F	196	LYS
2	F	244	ASN
3	3	8	GLN
3	3	16	SER
3	3	28	CYS
3	3	29	ARG
3	3	33	ASN
3	3	39	THR

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Mol	Chain	Res	Type
3	3	40	ARG
3	3	49	LYS
3	3	52	THR
3	3	66	THR
3	3	71	HIS
3	3	75	LYS
3	3	76	LEU
3	3	78	GLU
3	3	79	ARG
3	3	84	LYS
3	3	87	THR
3	3	92	GLN
3	3	102	LYS
3	3	106	HIS
3	3	109	LYS
3	3	111	ARG
3	3	142	LYS
3	3	144	ARG
3	3	153	LEU
3	3	158	ILE
4	4	5	ASN
4	4	15	ARG
4	4	20	ASN
4	4	30	THR
4	4	45	LEU
4	4	50	TYR
4	4	57	ASP
4	4	64	ARG
4	4	75	LEU
4	4	92	ASP
4	4	97	LYS
4	4	99	SER
4	4	109	GLU
4	4	111	PHE
4	4	118	LEU
4	4	123	LEU
4	4	125	ILE
4	4	150	ILE
4	4	151	LYS
4	4	157	LEU
4	4	171	ILE
4	4	177	LEU

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Mol	Chain	Res	Type
4	4	179	ASP
4	4	229	ASN
4	4	234	LEU
4	4	242	LEU
5	5	6	SER
5	5	57	GLU
5	5	63	ASN
5	5	126	LEU
5	5	134	THR
5	5	136	LEU
5	5	190	LEU
5	5	204	ILE
5	5	213	LEU
5	5	219	ILE
5	5	263	LYS
5	5	280	THR
5	5	293	GLN
5	5	299	ASN
5	5	337	ASP
5	5	340	LYS
5	5	351	MET
5	5	352	LEU
5	5	376	LEU
5	5	408	VAL
6	A	51	ASP
6	A	65	LEU
6	A	72	GLN
6	A	84	ASN
6	A	87	LEU
6	A	101	LEU
6	A	106	ASN
6	A	189	ARG
7	b	8	ILE
7	b	17	LEU
7	b	22	LEU
7	b	31	THR
7	b	48	ARG
7	b	51	LYS
7	b	53	THR
7	b	55	GLU
7	b	70	ASN
7	b	86	TYR

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Mol	Chain	Res	Type
7	b	87	GLU
7	b	88	LYS
7	b	94	SER
7	b	116	LEU
7	b	125	CYS
7	b	159	ARG
7	b	168	ARG
7	b	170	LEU
7	b	180	LYS
7	b	184	LEU
7	b	189	LYS
7	b	221	THR
7	b	270	LEU
7	b	277	LEU
7	b	281	LYS
7	b	305	LEU
7	b	338	LYS
7	b	417	LYS
7	b	428	LYS
7	b	445	LEU
7	b	448	GLU
7	b	456	LEU
9	r	2	PRO
9	r	72	LYS
10	s	15	LEU
11	u	8	PHE
11	u	27	LYS
11	u	76	ASN
11	u	100	ARG
11	u	113	ARG
12	v	5	ARG
12	v	10	ASN
12	v	28	ILE
12	v	30	ILE
12	v	36	ILE
12	v	55	LEU
12	v	164	GLU
12	v	178	SER
12	v	191	LYS
12	v	207	ILE
12	v	218	ARG
13	W	15	THR

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Mol	Chain	Res	Type
13	W	45	LEU
13	W	47	ASP
13	W	48	VAL
13	W	55	GLU
13	W	57	ARG
13	W	113	LYS
13	W	123	ASP
13	W	128	ASN
13	W	174	LYS
14	y	3	THR
14	y	100	ARG
14	y	145	ASN
14	y	146	ILE
14	y	154	LEU
14	y	161	VAL
14	y	173	LEU
14	y	198	VAL
14	y	201	ASP
16	B	17	LEU
16	B	19	ARG
16	B	24	SER
16	B	25	ILE
16	B	28	ARG
16	B	29	VAL
16	B	37	ARG
16	B	45	SER
16	B	79	VAL
16	B	85	VAL
16	B	102	LEU
16	B	114	VAL
16	B	152	LYS
16	B	164	THR
16	B	184	ASN
16	B	305	ILE
16	B	306	THR
16	B	332	ARG
16	B	337	THR
16	B	364	LYS
16	B	385	LYS
17	C	22	LEU
17	C	32	PRO
17	C	35	VAL

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Mol	Chain	Res	Type
17	C	40	THR
17	C	47	ARG
17	C	52	VAL
17	C	60	THR
17	C	61	SER
17	C	74	ILE
17	C	92	ASN
17	C	105	THR
17	C	118	LYS
17	C	120	TYR
17	C	122	THR
17	C	124	SER
17	C	136	LEU
17	C	141	ARG
17	C	147	GLU
17	C	148	ILE
17	C	163	LYS
17	C	179	LEU
17	C	187	LEU
17	C	193	LYS
17	C	196	ASN
17	C	201	GLN
17	C	220	ARG
17	C	222	VAL
17	C	230	VAL
17	C	259	ASP
17	C	278	SER
17	C	295	ILE
17	C	299	ILE
17	C	306	THR
17	C	322	GLN
17	C	326	ARG
18	e	11	LYS
18	e	21	HIS
18	e	27	ARG
18	e	33	ARG
18	e	34	LYS
18	e	50	ILE
18	e	52	GLN
18	e	73	THR
18	e	80	LYS
18	e	90	LYS

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Mol	Chain	Res	Type
18	e	91	THR
18	e	120	THR
18	e	125	ARG
18	e	128	LEU
19	E	9	TRP
19	E	15	VAL
19	E	26	ARG
19	E	29	LYS
19	E	31	ARG
19	E	79	VAL
19	E	101	PHE
19	E	155	LEU
20	f	3	GLU
20	f	9	VAL
20	f	10	LYS
20	f	14	LEU
20	f	20	LYS
20	f	31	LYS
20	f	53	TYR
20	f	81	VAL
20	f	86	ARG
20	f	97	SER
20	f	98	VAL
20	f	100	ILE
20	f	102	LEU
21	G	71	VAL
21	G	83	ASP
21	G	84	ARG
21	G	107	GLU
21	G	111	LYS
21	G	142	LEU
21	G	143	ILE
21	G	145	ASN
21	G	150	LEU
21	G	162	LEU
21	G	163	VAL
21	G	166	LEU
21	G	180	VAL
21	G	197	VAL
21	G	200	LEU
21	G	204	ARG
21	G	214	LEU

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Mol	Chain	Res	Type
21	G	229	VAL
22	h	21	LEU
22	h	28	LEU
22	h	36	LEU
22	h	49	LYS
22	h	69	LEU
22	h	83	LYS
22	h	102	GLU
22	h	119	LYS
23	H	1	MET
23	H	5	GLN
23	H	6	THR
23	H	23	ARG
23	H	41	ILE
23	H	48	VAL
23	H	55	VAL
23	H	57	VAL
23	H	59	ASN
23	H	62	ARG
23	H	118	LEU
23	H	134	ILE
23	H	138	THR
23	H	161	LEU
23	H	171	ASP
24	i	28	TYR
24	i	43	LEU
24	i	46	GLU
24	i	47	ILE
24	i	53	TYR
24	i	57	LEU
24	i	60	LEU
24	i	84	LYS
25	j	17	THR
25	j	21	ARG
25	j	29	VAL
25	j	36	SER
25	j	58	THR
25	j	61	THR
25	j	67	LEU
25	j	68	LYS
25	j	75	LYS
26	L	41	THR

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Mol	Chain	Res	Type
26	L	45	LYS
26	L	69	VAL
26	L	70	ARG
26	L	77	LEU
26	L	100	ARG
26	L	101	ARG
26	L	108	ILE
26	L	123	ILE
27	M	15	VAL
27	M	53	VAL
27	M	69	THR
27	M	80	THR
27	M	125	LYS
28	N	7	LEU
28	N	10	LEU
28	N	19	LEU
28	N	22	LEU
28	N	29	GLU
28	N	38	ARG
28	N	46	ASP
28	N	49	ARG
28	N	66	VAL
28	N	108	ARG
28	N	116	LEU
28	N	121	VAL
28	N	122	ASN
28	N	126	THR
28	N	132	VAL
28	N	133	ILE
28	N	142	ILE
28	N	144	ARG
28	N	145	ASP
28	N	153	ASP
28	N	155	VAL
28	N	167	THR
28	N	171	SER
28	N	179	LYS
28	N	187	ARG
29	O	7	VAL
29	O	10	ASP
29	O	12	LYS
29	O	15	LEU

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Mol	Chain	Res	Type
29	O	16	VAL
29	O	22	VAL
29	O	27	LEU
29	O	28	LEU
29	O	31	GLN
29	O	34	VAL
29	O	39	GLU
29	O	42	ASN
29	O	46	GLU
29	O	48	PHE
29	O	49	ARG
29	O	50	ASN
29	O	56	ASP
29	O	60	LYS
29	O	62	THR
29	O	64	PHE
29	O	74	ARG
29	O	78	ARG
29	O	79	ILE
29	O	80	PHE
29	O	82	LYS
29	O	84	LEU
29	O	87	MET
29	O	89	SER
29	O	94	ARG
29	O	99	LEU
29	O	105	PHE
29	O	117	ARG
29	O	118	VAL
29	O	124	LEU
29	O	134	LYS
29	O	138	LEU
29	O	140	LYS
29	O	142	SER
29	O	151	ASP
29	O	153	VAL
29	O	156	LEU
29	O	157	GLU
29	O	164	SER
29	O	166	GLU
29	O	184	THR
29	O	189	ASP

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Mol	Chain	Res	Type
30	P	16	SER
30	P	24	VAL
30	P	29	THR
30	P	30	ARG
30	P	41	LEU
30	P	42	THR
30	P	52	LEU
30	P	74	LYS
30	P	78	VAL
30	P	87	SER
30	P	96	GLN
30	P	119	VAL
30	P	120	ASN
30	P	157	VAL
30	P	159	LYS
31	Q	20	LYS
31	Q	22	ASP
31	Q	24	VAL
31	Q	28	LEU
31	Q	49	LEU
31	Q	55	SER
31	Q	56	LYS
31	Q	64	VAL
31	Q	69	ARG
31	Q	92	ARG
31	Q	136	ASN
32	S	12	ARG
32	S	32	SER
32	S	60	SER
32	S	71	LYS
32	S	94	ILE
32	S	96	ASP
32	S	106	LEU
32	S	115	ARG
32	S	122	HIS
32	S	134	ASP
32	S	154	HIS
32	S	158	LYS
32	S	169	SER
32	S	172	TYR
33	V	54	LEU
33	V	64	LYS

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Mol	Chain	Res	Type
33	V	93	LEU
34	Y	5	SER
34	Y	17	LYS
34	Y	37	LYS
34	Y	51	ARG
34	Y	54	ASP
34	Y	56	VAL
34	Y	57	LEU
34	Y	64	LYS
34	Y	74	TYR
34	Y	107	THR
34	Y	111	LEU
34	Y	126	LEU
38	K	75	LYS
38	K	240	ARG
38	K	248	LEU
38	K	256	PRO
38	K	262	ASN
39	m	263	LYS
39	m	323	HIS
39	m	324	LEU
39	m	390	ARG
40	D	294	VAL
40	D	394	LEU
40	D	422	ILE
40	D	429	LEU
40	D	448	ARG
40	D	451	LEU
41	o	93	ILE
41	o	146	MET
42	n	36	CYS
42	n	69	GLN
42	n	92	ARG
42	n	139	LEU
42	n	145	LEU
42	n	208	ASN
42	n	376	LEU
42	n	417	LEU
42	n	419	ASN
42	n	427	ILE
43	t	66	LEU
43	t	151	LEU

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Mol	Chain	Res	Type
43	t	157	ASN
43	t	187	LEU
43	t	275	ARG
43	t	291	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	x	31	HIS
1	x	88	ASN
1	x	187	HIS
1	x	228	GLN
1	x	235	GLN
3	3	11	ASN
3	3	25	GLN
3	3	41	GLN
3	3	106	HIS
4	4	14	ASN
4	4	63	GLN
4	4	73	HIS
4	4	172	HIS
5	5	191	GLN
5	5	237	ASN
5	5	269	GLN
5	5	285	GLN
5	5	305	GLN
7	b	23	ASN
7	b	26	GLN
7	b	217	GLN
7	b	245	HIS
8	J	215	HIS
8	J	228	ASN
12	v	33	ASN
13	W	14	GLN
13	W	205	GLN
13	W	223	ASN
13	W	232	ASN
14	y	33	ASN
14	y	86	ASN
16	B	293	ASN
17	C	58	HIS
17	C	114	ASN

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Mol	Chain	Res	Type
17	C	260	GLN
17	C	291	ASN
17	C	304	GLN
20	f	13	HIS
20	f	42	GLN
21	G	95	ASN
21	G	137	ASN
21	G	145	ASN
22	h	59	ASN
22	h	62	GLN
23	H	58	HIS
23	H	125	ASN
23	H	157	ASN
26	L	37	ASN
26	L	112	ASN
28	N	57	GLN
29	O	31	GLN
29	O	42	ASN
29	O	90	HIS
29	O	122	GLN
30	P	55	GLN
30	P	116	HIS
31	Q	136	ASN
32	S	62	ASN
32	S	74	ASN
32	S	142	GLN
33	V	98	ASN
33	V	132	ASN
38	K	42	ASN
38	K	262	ASN
40	D	310	ASN
41	o	113	GLN
42	n	69	GLN
42	n	164	ASN
42	n	419	ASN
42	n	437	ASN
43	t	238	GLN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	1	1772/3396 (52%)	498 (28%)	49 (2%)
36	2	152/158 (96%)	36 (23%)	6 (3%)
37	6	63/232 (27%)	30 (47%)	2 (3%)
All	All	1987/3786 (52%)	564 (28%)	57 (2%)

All (564) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	1	3	U
35	1	6	A
35	1	7	C
35	1	11	A
35	1	18	G
35	1	26	A
35	1	30	G
35	1	39	A
35	1	40	A
35	1	41	G
35	1	43	A
35	1	48	A
35	1	49	A
35	1	50	U
35	1	57	A
35	1	59	G
35	1	60	A
35	1	65	A
35	1	66	A
35	1	72	C
35	1	74	G
35	1	75	G
35	1	92	G
35	1	94	G
35	1	96	G
35	1	105	C
35	1	110	G
35	1	111	C
35	1	116	A
35	1	117	U
35	1	119	U
35	1	120	G
35	1	122	A

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Mol	Chain	Res	Type
35	1	125	C
35	1	134	U
35	1	135	C
35	1	136	G
35	1	143	G
35	1	146	U
35	1	148	G
35	1	155	G
35	1	156	G
35	1	157	A
35	1	161	G
35	1	164	A
35	1	165	A
35	1	166	C
35	1	170	G
35	1	171	G
35	1	173	G
35	1	190	U
35	1	191	U
35	1	200	C
35	1	206	G
35	1	210	U
35	1	211	A
35	1	213	A
35	1	218	G
35	1	219	A
35	1	220	G
35	1	221	A
35	1	240	U
35	1	241	G
35	1	243	G
35	1	249	U
35	1	250	U
35	1	251	G
35	1	265	A
35	1	267	G
35	1	268	A
35	1	269	G
35	1	270	U
35	1	277	G
35	1	281	G
35	1	282	G

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Mol	Chain	Res	Type
35	1	283	G
35	1	284	A
35	1	285	A
35	1	286	U
35	1	287	G
35	1	295	A
35	1	298	U
35	1	299	G
35	1	304	G
35	1	305	U
35	1	311	C
35	1	315	C
35	1	323	A
35	1	324	A
35	1	329	U
35	1	338	A
35	1	346	C
35	1	349	A
35	1	352	A
35	1	354	U
35	1	368	G
35	1	370	U
35	1	374	A
35	1	376	G
35	1	377	A
35	1	383	G
35	1	385	A
35	1	386	A
35	1	387	A
35	1	388	G
35	1	390	G
35	1	395	A
35	1	398	A
35	1	400	G
35	1	401	U
35	1	402	A
35	1	403	C
35	1	421	G
35	1	422	A
35	1	429	U
35	1	436	A
35	1	438	A

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Mol	Chain	Res	Type
35	1	439	C
35	1	440	A
35	1	442	G
35	1	449	U
35	1	452	G
35	1	454	C
35	1	455	C
35	1	457	C
35	1	459	G
35	1	462	C
35	1	463	C
35	1	465	U
35	1	466	G
35	1	467	U
35	1	468	G
35	1	474	G
35	1	478	A
35	1	479	U
35	1	480	C
35	1	481	U
35	1	482	C
35	1	494	G
35	1	495	G
35	1	498	A
35	1	503	C
35	1	510	G
35	1	515	C
35	1	517	G
35	1	518	G
35	1	519	A
35	1	521	A
35	1	523	A
35	1	527	A
35	1	533	A
35	1	535	G
35	1	543	C
35	1	544	C
35	1	546	C
35	1	547	G
35	1	549	U
35	1	551	A
35	1	552	G

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Mol	Chain	Res	Type
35	1	555	U
35	1	556	U
35	1	557	A
35	1	559	A
35	1	569	A
35	1	570	A
35	1	572	A
35	1	578	A
35	1	579	G
35	1	590	G
35	1	592	A
35	1	597	G
35	1	602	A
35	1	604	G
35	1	611	A
35	1	618	C
35	1	619	A
35	1	629	U
35	1	636	C
35	1	642	U
35	1	644	G
35	1	645	A
35	1	647	A
35	1	648	C
35	1	649	A
35	1	650	C
35	1	660	A
35	1	661	G
35	1	675	C
35	1	677	A
35	1	681	U
35	1	691	A
35	1	695	C
35	1	704	U
35	1	705	A
35	1	720	A
35	1	721	G
35	1	722	G
35	1	742	G
35	1	750	G
35	1	756	U
35	1	757	C

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Mol	Chain	Res	Type
35	1	776	U
35	1	780	A
35	1	781	G
35	1	783	A
35	1	784	A
35	1	785	G
35	1	786	A
35	1	794	U
35	1	799	G
35	1	806	A
35	1	808	A
35	1	813	G
35	1	814	U
35	1	815	G
35	1	933	A
35	1	936	A
35	1	937	G
35	1	938	C
35	1	941	G
35	1	943	U
35	1	944	C
35	1	953	G
35	1	957	C
35	1	959	C
35	1	961	C
35	1	962	A
35	1	978	G
35	1	979	U
35	1	980	A
35	1	984	G
35	1	985	U
35	1	1103	A
35	1	1104	G
35	1	1111	U
35	1	1112	A
35	1	1116	G
35	1	1117	G
35	1	1124	U
35	1	1125	U
35	1	1128	U
35	1	1129	A
35	1	1130	A

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Mol	Chain	Res	Type
35	1	1132	C
35	1	1143	A
35	1	1144	U
35	1	1151	U
35	1	1153	A
35	1	1155	C
35	1	1157	G
35	1	1159	A
35	1	1160	C
35	1	1161	G
35	1	1177	G
35	1	1178	G
35	1	1179	A
35	1	1180	A
35	1	1181	U
35	1	1182	A
35	1	1186	G
35	1	1192	C
35	1	1193	A
35	1	1196	C
35	1	1197	A
35	1	1198	C
35	1	1199	C
35	1	1200	A
35	1	1201	C
35	1	1204	A
35	1	1212	A
35	1	1220	U
35	1	1221	A
35	1	1222	G
35	1	1227	C
35	1	1233	G
35	1	1234	G
35	1	1235	U
35	1	1239	C
35	1	1241	U
35	1	1242	G
35	1	1244	A
35	1	1245	A
35	1	1246	G
35	1	1253	U
35	1	1258	U

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Mol	Chain	Res	Type
35	1	1262	G
35	1	1263	A
35	1	1264	G
35	1	1265	U
35	1	1277	C
35	1	1278	A
35	1	1279	C
35	1	1285	G
35	1	1286	A
35	1	1287	A
35	1	1301	A
35	1	1302	A
35	1	1303	A
35	1	1304	A
35	1	1305	U
35	1	1307	G
35	1	1308	A
35	1	1309	U
35	1	1318	A
35	1	1325	U
35	1	1330	A
35	1	1332	A
35	1	1345	G
35	1	1347	U
35	1	1348	U
35	1	1349	G
35	1	1350	A
35	1	1351	U
35	1	1352	A
35	1	1353	U
35	1	1354	G
35	1	1355	A
35	1	1357	G
35	1	1359	C
35	1	1379	G
35	1	1386	A
35	1	1390	A
35	1	1391	C
35	1	1392	G
35	1	1397	C
35	1	1399	A
35	1	1400	G

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Mol	Chain	Res	Type
35	1	1408	G
35	1	1417	G
35	1	1419	A
35	1	1434	G
35	1	1437	C
35	1	1443	G
35	1	1446	A
35	1	1450	G
35	1	1452	A
35	1	2364	G
35	1	2371	G
35	1	2372	A
35	1	2374	C
35	1	2375	G
35	1	2377	G
35	1	2381	G
35	1	2393	G
35	1	2394	G
35	1	2826	U
35	1	2828	G
35	1	2833	A
35	1	2836	C
35	1	2837	A
35	1	2843	U
35	1	2845	A
35	1	2847	A
35	1	2857	C
35	1	2858	U
35	1	2877	G
35	1	2878	G
35	1	2879	C
35	1	2887	A
35	1	2889	C
35	1	2894	C
35	1	2899	C
35	1	2903	A
35	1	2916	U
35	1	2919	A
35	1	2921	U
35	1	2923	U
35	1	2924	U
35	1	2925	C

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Mol	Chain	Res	Type
35	1	2926	A
35	1	2927	C
35	1	2929	C
35	1	2930	A
35	1	2935	U
35	1	2936	A
35	1	2938	G
35	1	2941	A
35	1	2942	C
35	1	2943	G
35	1	2944	U
35	1	2945	G
35	1	2946	A
35	1	2947	G
35	1	2984	C
35	1	2986	U
35	1	2987	A
35	1	2990	G
35	1	2992	U
35	1	2996	U
35	1	2997	G
35	1	3003	G
35	1	3006	A
35	1	3012	A
35	1	3019	U
35	1	3021	A
35	1	3022	G
35	1	3023	U
35	1	3027	A
35	1	3028	G
35	1	3029	A
35	1	3030	G
35	1	3032	A
35	1	3037	U
35	1	3046	A
35	1	3049	A
35	1	3054	U
35	1	3055	U
35	1	3057	U
35	1	3058	U
35	1	3059	G
35	1	3069	G

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Mol	Chain	Res	Type
35	1	3070	A
35	1	3074	G
35	1	3075	G
35	1	3078	U
35	1	3086	A
35	1	3088	G
35	1	3092	C
35	1	3094	A
35	1	3099	C
35	1	3100	U
35	1	3101	G
35	1	3109	G
35	1	3116	G
35	1	3121	U
35	1	3122	A
35	1	3124	G
35	1	3129	A
35	1	3130	A
35	1	3131	U
35	1	3142	A
35	1	3143	C
35	1	3173	G
35	1	3174	A
35	1	3176	G
35	1	3179	U
35	1	3180	A
35	1	3181	C
35	1	3187	A
35	1	3188	G
35	1	3194	C
35	1	3195	U
35	1	3196	U
35	1	3198	U
35	1	3199	G
35	1	3207	U
35	1	3213	A
35	1	3217	C
35	1	3218	A
35	1	3219	G
35	1	3228	C
35	1	3229	G
35	1	3234	A

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Mol	Chain	Res	Type
35	1	3242	G
35	1	3243	A
35	1	3244	A
35	1	3245	A
35	1	3246	G
35	1	3247	G
35	1	3249	C
35	1	3256	G
35	1	3259	U
35	1	3263	G
35	1	3268	A
35	1	3270	U
35	1	3273	A
35	1	3275	U
35	1	3276	G
35	1	3286	G
35	1	3288	G
35	1	3289	G
35	1	3290	G
35	1	3304	U
35	1	3313	U
35	1	3316	A
35	1	3317	U
35	1	3319	U
35	1	3320	A
35	1	3330	A
35	1	3340	G
35	1	3341	U
35	1	3345	G
35	1	3346	U
35	1	3347	A
35	1	3351	U
35	1	3352	U
35	1	3355	U
35	1	3356	G
35	1	3360	C
35	1	3363	U
35	1	3368	U
35	1	3369	G
35	1	3375	A
35	1	3376	A
35	1	3378	C

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Mol	Chain	Res	Type
35	1	3382	U
35	1	3390	G
35	1	3396	U
36	2	12	A
36	2	13	A
36	2	23	U
36	2	33	A
36	2	34	U
36	2	35	C
36	2	39	G
36	2	40	A
36	2	52	A
36	2	59	A
36	2	62	C
36	2	63	G
36	2	75	G
36	2	81	U
36	2	82	U
36	2	83	C
36	2	84	C
36	2	85	G
36	2	86	U
36	2	87	G
36	2	90	U
36	2	95	G
36	2	97	A
36	2	100	U
36	2	105	A
36	2	106	C
36	2	107	G
36	2	113	U
36	2	115	C
36	2	116	G
36	2	121	U
36	2	123	G
36	2	144	G
36	2	148	G
36	2	152	G
36	2	157	U
37	6	4	U
37	6	5	C
37	6	6	U

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Mol	Chain	Res	Type
37	6	7	C
37	6	8	A
37	6	9	A
37	6	13	U
37	6	14	U
37	6	15	C
37	6	16	U
37	6	17	G
37	6	23	U
37	6	24	A
37	6	34	A
37	6	36	U
37	6	39	U
37	6	40	U
37	6	42	G
37	6	43	A
37	6	47	A
37	6	52	G
37	6	53	A
37	6	54	A
37	6	56	U
37	6	57	U
37	6	58	G
37	6	59	C
37	6	228	U
37	6	231	A
37	6	232	A

All (57) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	1	93	C
35	1	133	U
35	1	156	G
35	1	190	U
35	1	239	G
35	1	285	A
35	1	297	G
35	1	398	A
35	1	406	G
35	1	438	A
35	1	456	U

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Mol	Chain	Res	Type
35	1	480	C
35	1	518	G
35	1	533	A
35	1	548	G
35	1	588	G
35	1	607	A
35	1	618	C
35	1	644	G
35	1	649	A
35	1	720	A
35	1	1102	A
35	1	1104	G
35	1	1128	U
35	1	1160	C
35	1	1177	G
35	1	1241	U
35	1	1302	A
35	1	1307	G
35	1	1329	U
35	1	1347	U
35	1	1354	G
35	1	1356	U
35	1	1418	A
35	1	1434	G
35	1	2392	C
35	1	2828	G
35	1	2857	C
35	1	2986	U
35	1	3022	G
35	1	3069	G
35	1	3121	U
35	1	3205	G
35	1	3217	C
35	1	3218	A
35	1	3228	C
35	1	3267	A
35	1	3269	U
35	1	3350	C
36	2	39	G
36	2	48	A
36	2	71	A
36	2	84	C

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Mol	Chain	Res	Type
36	2	85	G
36	2	114	G
37	6	16	U
37	6	56	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
36	2	6
1	x	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	124:G	O3'	125:U	P	7.11
1	2	110:C	O3'	111:A	P	6.92
1	2	125:U	O3'	126:A	P	6.42
1	2	113:U	O3'	114:G	P	4.42
1	2	126:A	O3'	127:U	P	3.70
1	2	128:U	O3'	129:C	P	3.37
1	x	285:GLU	C	286:MET	N	2.75

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3893. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.