



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Feb 14, 2017 – 02:23 PM EST

PDB ID : 5T6R
EMDB ID: : EMD-8368
Title : Nmd3 is a structural mimic of eIF5A, and activates the cpGTPase Lsg1 during
60S ribosome biogenesis: 60S-Nmd3 Complex
Authors : Malyutin, A.G.; Musalgaonkar, S.; Patchett, S.; Frank, J.; Johnson, A.W.
Deposited on : 2016-09-01
Resolution : 4.50 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

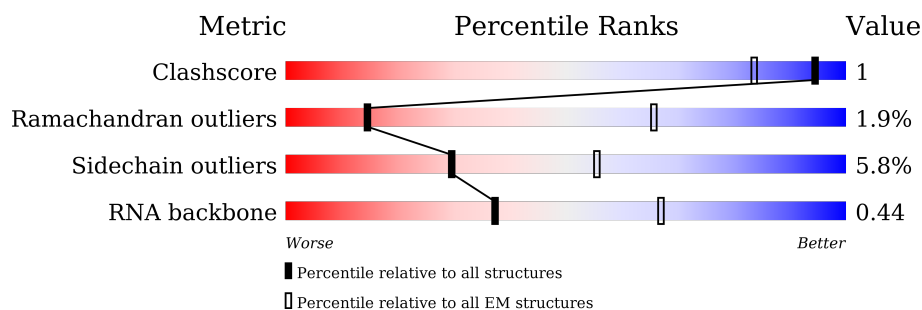
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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










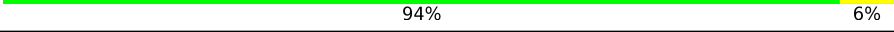
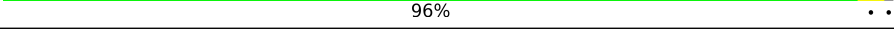
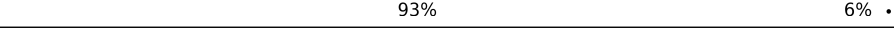
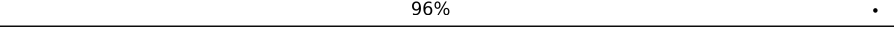
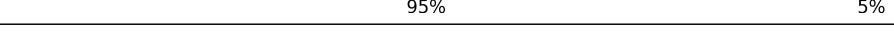
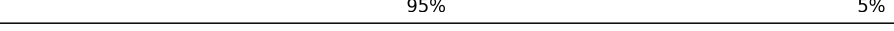


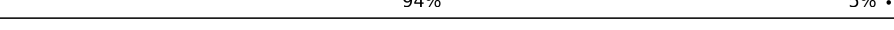


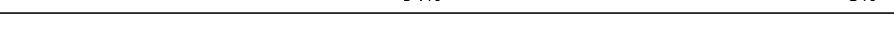
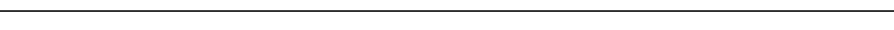

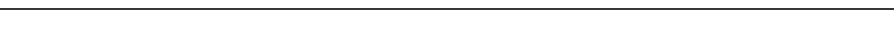
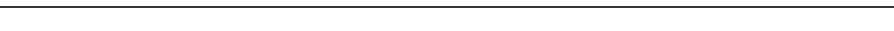


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	3396	69% 23% 6%
2	B	121	81% 18% .
3	C	158	75% 24% .
4	D	254	95% . .
5	E	387	94% 6%
6	F	362	91% 9%
7	G	297	89% 10% .
8	H	176	84% 5% 11%





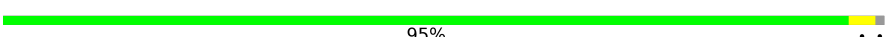

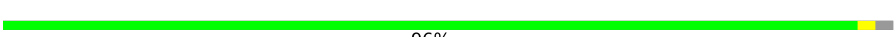



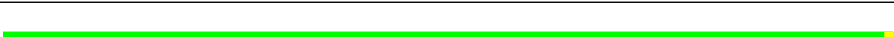

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Mol	Chain	Length	Quality of chain
9	I	244	
10	J	256	
11	K	191	
12	L	221	
13	M	174	
14	N	199	
15	O	138	
16	a	204	
17	b	199	
18	c	184	
19	d	186	
20	e	189	
21	f	172	
22	g	160	
23	h	121	
24	i	137	
25	j	155	
26	k	142	
27	l	127	
28	m	136	
29	n	149	
30	o	59	
31	p	105	
32	q	113	
33	r	130	

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Mol	Chain	Length	Quality of chain
34	s	107	 46% 53%
35	t	121	 89% 7%
36	u	120	 91% 8%
37	v	100	 91% 8%
38	w	88	 95%
39	x	78	 92% 6%
40	y	51	 96%
41	z	128	 37% 59%
42	Q	106	 88% 11%
43	R	92	 96%
44	S	210	 99%
45	V	917	 19% 6% 73%

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 126616 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 25S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3204	Total	C	N	O	P	0	0
			68535	30613	12358	22360	3204		

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 3 is a RNA chain called 5.8S Ribosomal RNA.

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

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	211	Total	C	N	O	S	0	0
			1705	1083	322	294	6		

- Molecule 13 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	c	183	Total	C	N	O	0	0
			1420	882	281	257		

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	e	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	f	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	h	100	Total	C	N	O	S	0	0
			796	516	131	149			

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	98	Total	C	N	O	S	0	0
			699	443	137	118	1		

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	k	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	l	126	Total	C	N	O	S	0	0
			993	625	192	176			

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	m	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 29 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	n	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	o	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	p	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	q	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	r	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	50	Total	C	N	O	0	0
			406	258	77	71		

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	t	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	v	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	w	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	x	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	y	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	z	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 42 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Q	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 43 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	R	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 44 is a protein called Ribosomal Protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	S	210	Total	C	N	O		0	0
			1050	630	210	210			

- Molecule 45 is a protein called Maltose binding protein, 60S ribosomal export protein Nmd3 fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	V	251	Total	C	N	O	S	0	0
			1975	1263	333	372	7		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-396	ILE	THR	conflict	UNP A0A0F8NYV9
V	-15	HIS	-	linker	UNP A0A0F8NYV9
V	-14	HIS	-	linker	UNP A0A0F8NYV9
V	-13	HIS	-	linker	UNP A0A0F8NYV9
V	-12	HIS	-	linker	UNP A0A0F8NYV9
V	-11	HIS	-	linker	UNP A0A0F8NYV9
V	-10	HIS	-	linker	UNP A0A0F8NYV9
V	-9	HIS	-	linker	UNP A0A0F8NYV9
V	-8	HIS	-	linker	UNP A0A0F8NYV9
V	-7	HIS	-	linker	UNP A0A0F8NYV9
V	-6	HIS	-	linker	UNP A0A0F8NYV9
V	-5	GLU	-	linker	UNP A0A0F8NYV9
V	-4	ASN	-	linker	UNP A0A0F8NYV9
V	-3	LEU	-	linker	UNP A0A0F8NYV9
V	-2	TYR	-	linker	UNP A0A0F8NYV9
V	-1	PHE	-	linker	UNP A0A0F8NYV9
V	0	GLN	-	linker	UNP A0A0F8NYV9
V	1	GLY	-	linker	UNP A0A0F8NYV9

- Molecule 46 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
46	A	84	Total 84	Mg 84	0
46	C	1	Total 1	Mg 1	0
46	i	1	Total 1	Mg 1	0

- Molecule 47 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
47	A	3	Total 3	K 3	0

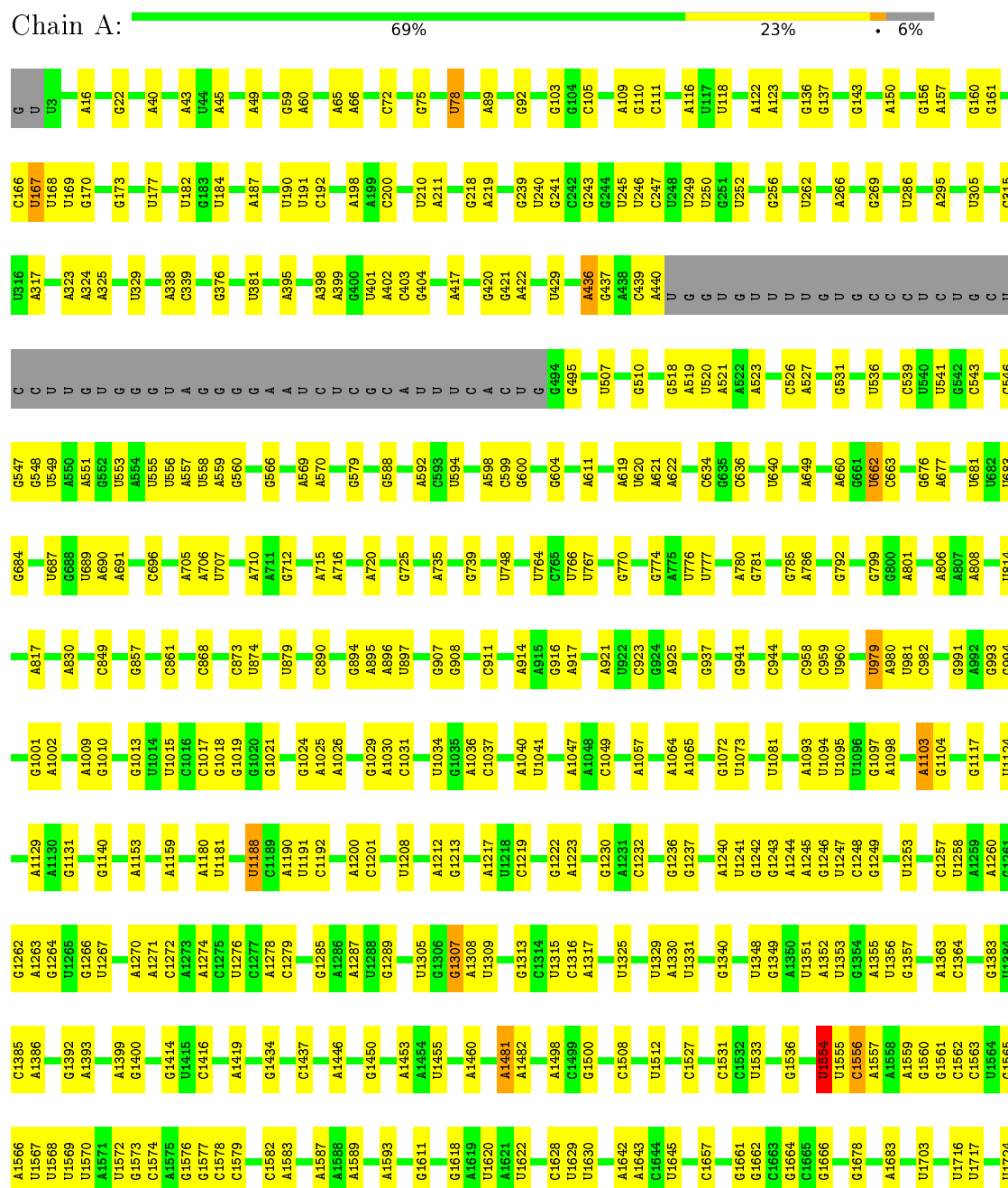
- Molecule 48 is water.

Mol	Chain	Residues	Atoms		AltConf
48	A	10	Total 10	O 10	0
48	c	1	Total 1	O 1	0
48	e	1	Total 1	O 1	0

3 Residue-property plots

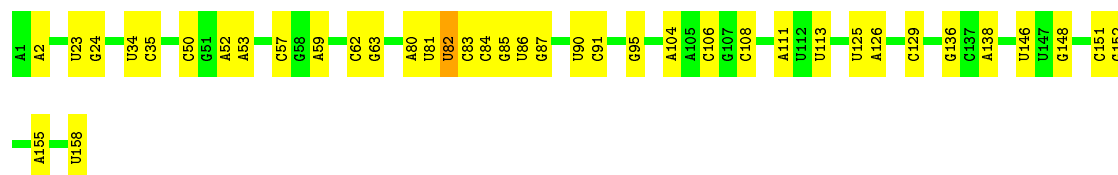
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: 25S Ribosomal RNA



- Molecule 3: 5.8S Ribosomal RNA

Chain C: 75% 24%



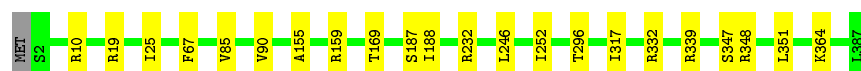
- Molecule 4: 60S ribosomal protein L2-A

Chain D: 95%

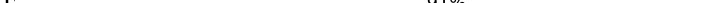


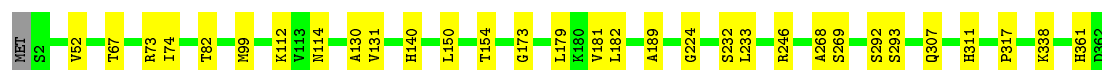
- Molecule 5: 60S ribosomal protein L3

Chain E: 94% 6%



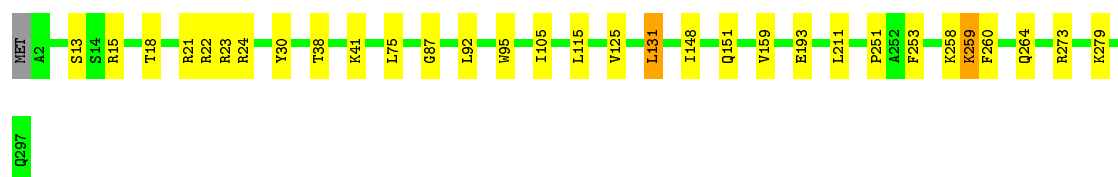
- Molecule 6: 60S ribosomal protein L4-A

Chain F:  91% 9%

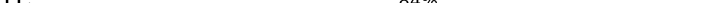


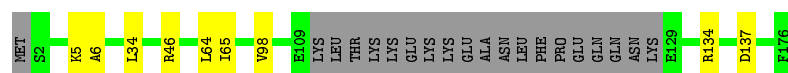
- Molecule 7: 60S ribosomal protein L5

Chain G: 89% 10%

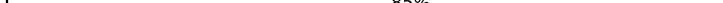


- Molecule 8: 60S ribosomal protein L6-A

Chain H:  84% 5% 11%



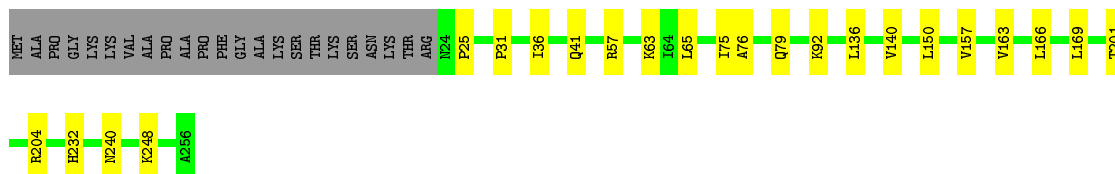
- Molecule 9: 60S ribosomal protein L7-A

Chain I:  85% 6% 9%



- Molecule 10: 60S ribosomal protein L8-A

Chain J: 82% 9% 9%



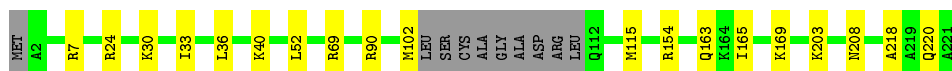
- Molecule 11: 60S ribosomal protein L9-A

Chain K: 91% 8%



- Molecule 12: 60S ribosomal protein L10

Chain L: 87% 9% 5%



- Molecule 13: 60S ribosomal protein L11-A

Chain M: 87% 9% 2%



- Molecule 14: 60S ribosomal protein L13-A

Chain N: 88% 9% 3%



- Molecule 15: 60S ribosomal protein L14-A

Chain O: 92% 7% 1%



- Molecule 16: 60S ribosomal protein L15-A

Chain a: 94% 6%



- Molecule 17: 60S ribosomal protein L16-A

Chain b: 96%



- Molecule 18: 60S ribosomal protein L17-A

Chain c: 93%



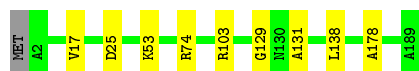
- Molecule 19: 60S ribosomal protein L18-A

Chain d: 96%



- Molecule 20: 60S ribosomal protein L19-A

Chain e: 95%



- Molecule 21: 60S ribosomal protein L20-A

Chain f: 95%



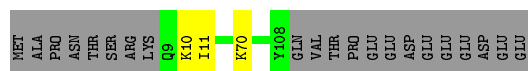
- Molecule 22: 60S ribosomal protein L21-A

Chain g: 91%



- Molecule 23: 60S ribosomal protein L22-A

Chain h: 80%



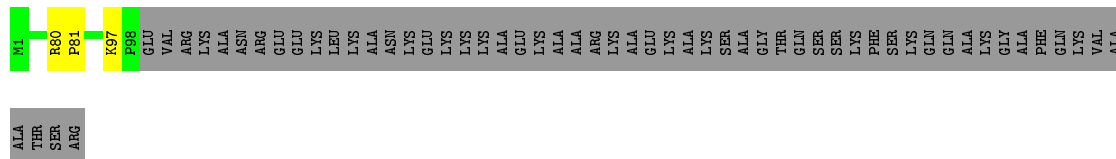
- Molecule 24: 60S ribosomal protein L23-A

Chain i:  94% 5% .




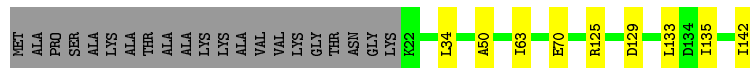
- Molecule 25: 60S ribosomal protein L24-A

Chain j:  61% . 37%



- Molecule 26: 60S ribosomal protein L25

Chain k:  79% 6% 15%



- Molecule 27: 60S ribosomal protein L26-A

Chain l:  94% 5% ..




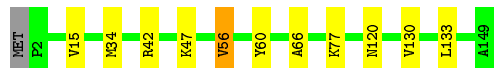
- Molecule 28: 60S ribosomal protein L27-A

Chain m:  93% 7% .




- Molecule 29: 60S ribosomal protein L28

Chain n:  92% 7% ..




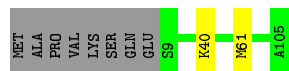
- Molecule 30: 60S ribosomal protein L29

Chain o:  88% 8% . .




- Molecule 31: 60S ribosomal protein L30

Chain p:  90% 8%




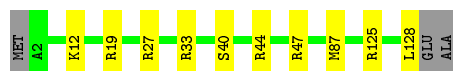
- Molecule 32: 60S ribosomal protein L31-A

Chain q:  90% 6%



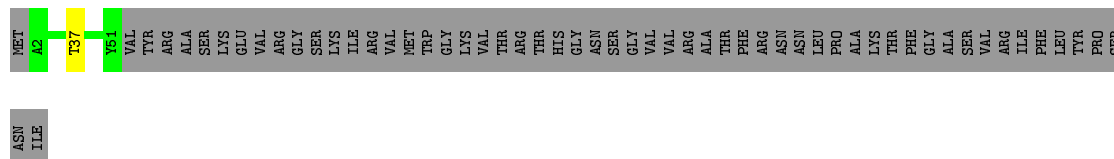
- Molecule 33: 60S ribosomal protein L32

Chain r:  90% 8%




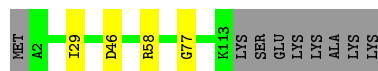
- Molecule 34: 60S ribosomal protein L33-A

Chain s:  46% 53%



- Molecule 35: 60S ribosomal protein L34-A

Chain t:  89% 7%



- Molecule 36: 60S ribosomal protein L35-A

Chain u:  91% 8%



- Molecule 37: 60S ribosomal protein L36-A

Chain v:  91% 8%



- Molecule 38: 60S ribosomal protein L37-A

Chain w:  95% ..



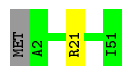
- Molecule 39: 60S ribosomal protein L38

Chain x:  92% 6% .



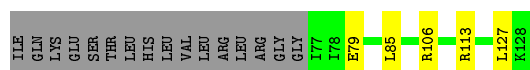
- Molecule 40: 60S ribosomal protein L39

Chain y:  96% ..




- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain z:  37% . 59%



- Molecule 42: 60S ribosomal protein L42-A

Chain Q:  88% 11% .



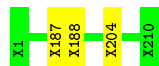
- Molecule 43: 60S ribosomal protein L43-A

Chain R:  96% ..

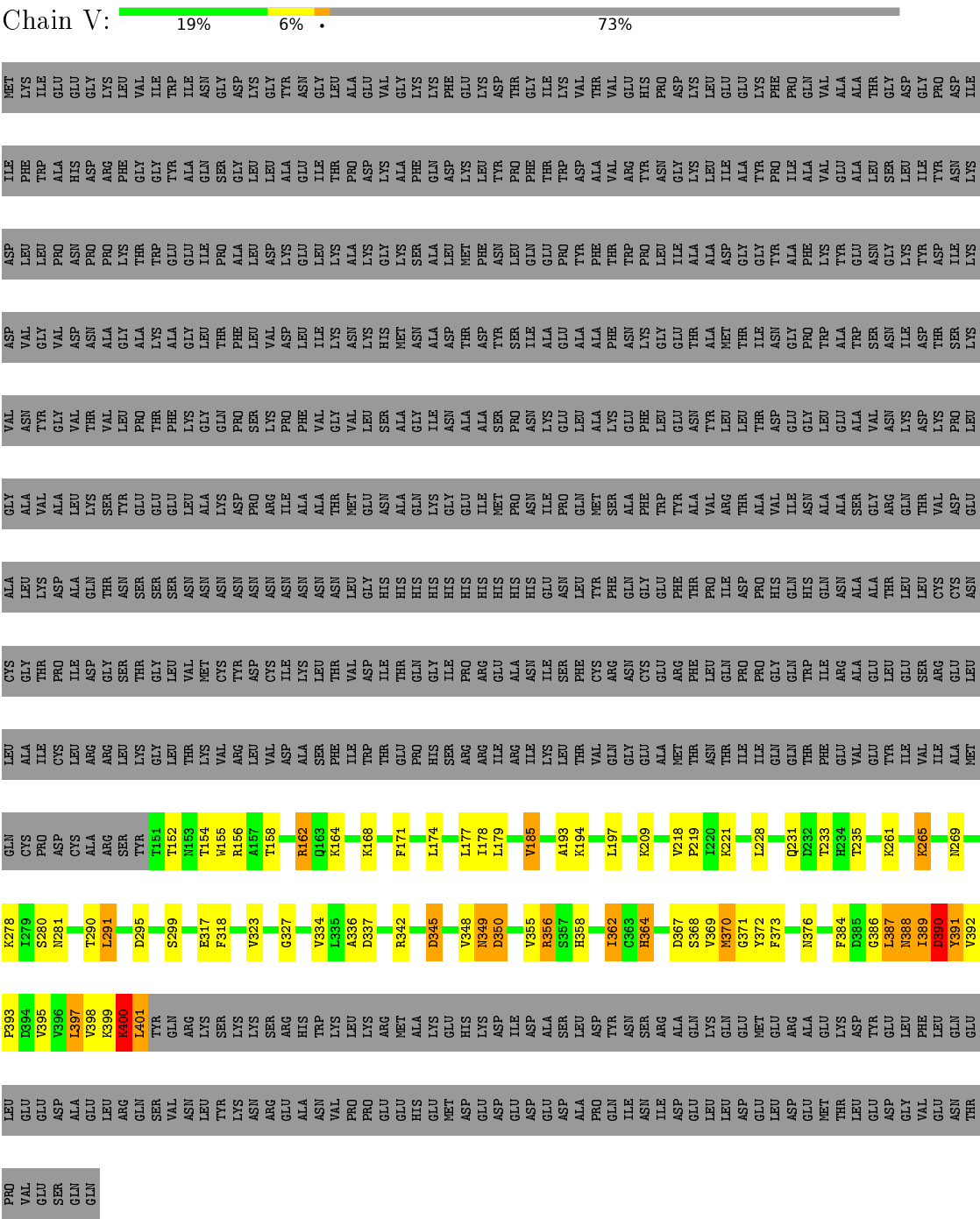


- Molecule 44: Ribosomal Protein uL1

Chain S:  99% .



- Molecule 45: Maltose binding protein, 60S ribosomal export protein Nmd3 fusion



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	65650	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	31000	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.24	1/76717 (0.0%)	0.69	8/119611 (0.0%)
10	J	0.37	0/1836	0.54	0/2481
11	K	0.36	0/1539	0.57	0/2073
12	L	0.38	0/1741	0.61	0/2335
13	M	0.38	0/1374	0.64	0/1842
14	N	0.39	0/1568	0.65	0/2106
15	O	0.36	0/1068	0.59	0/1438
16	a	0.38	0/1757	0.68	0/2354
17	b	0.37	0/1585	0.55	0/2128
18	c	0.36	0/1443	0.62	0/1944
19	d	0.37	0/1465	0.65	0/1965
2	B	0.24	0/2883	0.67	0/4491
20	e	0.36	0/1538	0.62	0/2050
21	f	0.36	0/1481	0.59	0/1990
22	g	0.36	0/1300	0.58	0/1743
23	h	0.39	0/812	0.51	0/1099
24	i	0.36	0/1018	0.59	0/1369
25	j	0.38	0/712	0.58	0/958
26	k	0.35	0/979	0.55	0/1321
27	l	0.36	0/1004	0.60	0/1341
28	m	0.37	0/1118	0.54	0/1497
29	n	0.35	0/1204	0.62	0/1612
3	C	0.23	0/3746	0.68	1/5832 (0.0%)
30	o	0.37	0/473	0.61	0/629
31	p	0.36	0/751	0.50	0/1008
32	q	0.35	0/890	0.60	0/1196
33	r	0.36	0/1041	0.60	0/1394
34	s	0.36	0/414	0.58	0/556
35	t	0.35	0/890	0.63	0/1189
36	u	0.37	0/978	0.60	0/1301
37	v	0.40	0/778	0.60	0/1034
38	w	0.39	0/696	0.66	0/923

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	x	0.35	0/618	0.56	0/826
4	D	0.35	0/1948	0.63	0/2617
40	y	0.39	0/443	0.64	0/588
41	z	0.38	0/423	0.61	0/562
42	Q	0.37	0/860	0.60	0/1136
43	R	0.37	0/701	0.65	0/934
45	V	0.39	0/2015	0.75	3/2738 (0.1%)
5	E	0.36	0/3146	0.62	0/4228
6	F	0.37	0/2800	0.58	0/3790
7	G	0.38	0/2425	0.60	1/3271 (0.0%)
8	H	0.37	0/1260	0.56	0/1694
9	I	0.38	0/1821	0.57	0/2451
All	All	0.30	1/135259 (0.0%)	0.66	13/199645 (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
30	o	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2595	A	C5-C6	5.44	1.46	1.41

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	V	386	GLY	C-N-CA	14.40	157.70	121.70
45	V	386	GLY	O-C-N	-13.14	101.67	122.70
45	V	386	GLY	CA-C-N	9.55	138.20	117.20
1	A	2249	G	C2'-C3'-O3'	7.62	126.26	109.50
1	A	1307	G	C2'-C3'-O3'	7.11	125.14	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	o	20	GLY	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	68535	0	34437	205	0
2	B	2579	0	1304	1	0
3	C	3353	0	1695	0	0
4	D	1914	0	1981	3	0
5	E	3075	0	3142	4	0
6	F	2748	0	2859	1	0
7	G	2375	0	2325	2	0
8	H	1239	0	1326	0	0
9	I	1784	0	1862	5	0
10	J	1804	0	1877	2	0
11	K	1518	0	1587	3	0
12	L	1705	0	1736	11	0
13	M	1353	0	1383	0	0
14	N	1543	0	1608	2	0
15	O	1053	0	1149	0	0
16	a	1720	0	1779	0	0
17	b	1555	0	1659	0	0
18	c	1420	0	1437	0	0
19	d	1441	0	1543	0	0
20	e	1521	0	1617	0	0
21	f	1445	0	1487	0	0
22	g	1276	0	1323	0	0
23	h	796	0	812	0	0
24	i	1003	0	1048	0	0
25	j	699	0	640	0	0
26	k	964	0	1025	0	0
27	l	993	0	1081	0	0
28	m	1092	0	1155	0	0
29	n	1173	0	1215	0	0
30	o	462	0	491	0	0
31	p	743	0	797	0	0
32	q	876	0	912	0	0
33	r	1020	0	1090	0	0
34	s	406	0	416	0	0
35	t	880	0	945	0	0
36	u	969	0	1078	0	0
37	v	771	0	849	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	w	681	0	687	0	0
39	x	612	0	682	0	0
40	y	436	0	475	0	0
41	z	417	0	459	0	0
42	Q	847	0	918	0	0
43	R	694	0	738	0	0
44	S	1050	0	247	2	0
45	V	1975	0	1984	70	0
46	A	84	0	0	0	0
46	C	1	0	0	0	0
46	i	1	0	0	0	0
47	A	3	0	0	0	0
48	A	10	0	0	2	0
48	c	1	0	0	0	0
48	e	1	0	0	0	0
All	All	126616	0	90860	286	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 1.

The worst 5 of 286 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:2434:U:O4	1:A:2595:A:N1	1.60	1.33
12:L:102:MET:CG	45:V:152:THR:HA	1.58	1.32
12:L:102:MET:HG3	45:V:152:THR:CA	1.63	1.28
45:V:388:ASN:O	45:V:390:ASP:N	1.73	1.21
1:A:2410:U:O4	1:A:2801:A:N1	1.87	1.06

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	250/254 (98%)	228 (91%)	20 (8%)	2 (1%)	24	70
5	E	384/387 (99%)	343 (89%)	34 (9%)	7 (2%)	11	55
6	F	359/362 (99%)	311 (87%)	32 (9%)	16 (4%)	3	33
7	G	294/297 (99%)	267 (91%)	19 (6%)	8 (3%)	6	47
8	H	152/176 (86%)	137 (90%)	12 (8%)	3 (2%)	9	53
9	I	220/244 (90%)	203 (92%)	14 (6%)	3 (1%)	14	59
10	J	231/256 (90%)	202 (87%)	24 (10%)	5 (2%)	8	51
11	K	189/191 (99%)	173 (92%)	16 (8%)	0	100	100
12	L	207/221 (94%)	187 (90%)	17 (8%)	3 (1%)	14	59
13	M	167/174 (96%)	145 (87%)	15 (9%)	7 (4%)	3	35
14	N	191/199 (96%)	170 (89%)	19 (10%)	2 (1%)	19	65
15	O	134/138 (97%)	125 (93%)	5 (4%)	4 (3%)	5	44
16	a	201/204 (98%)	189 (94%)	9 (4%)	3 (2%)	13	58
17	b	195/199 (98%)	187 (96%)	7 (4%)	1 (0%)	34	77
18	c	181/184 (98%)	161 (89%)	20 (11%)	0	100	100
19	d	183/186 (98%)	169 (92%)	11 (6%)	3 (2%)	12	57
20	e	186/189 (98%)	175 (94%)	7 (4%)	4 (2%)	8	51
21	f	170/172 (99%)	158 (93%)	10 (6%)	2 (1%)	16	62
22	g	157/160 (98%)	142 (90%)	12 (8%)	3 (2%)	10	54
23	h	98/121 (81%)	84 (86%)	13 (13%)	1 (1%)	19	65
24	i	134/137 (98%)	126 (94%)	7 (5%)	1 (1%)	26	71
25	j	96/155 (62%)	83 (86%)	10 (10%)	3 (3%)	5	44
26	k	119/142 (84%)	111 (93%)	7 (6%)	1 (1%)	24	70
27	l	124/127 (98%)	115 (93%)	7 (6%)	2 (2%)	12	57
28	m	133/136 (98%)	113 (85%)	18 (14%)	2 (2%)	13	58
29	n	146/149 (98%)	125 (86%)	16 (11%)	5 (3%)	5	42
30	o	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	2	30
31	p	95/105 (90%)	89 (94%)	6 (6%)	0	100	100
32	q	107/113 (95%)	98 (92%)	7 (6%)	2 (2%)	10	54
33	r	125/130 (96%)	115 (92%)	8 (6%)	2 (2%)	12	57
34	s	48/107 (45%)	46 (96%)	2 (4%)	0	100	100
35	t	110/121 (91%)	105 (96%)	3 (3%)	2 (2%)	11	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	u	117/120 (98%)	108 (92%)	6 (5%)	3 (3%)	7	47
37	v	97/100 (97%)	88 (91%)	7 (7%)	2 (2%)	9	52
38	w	85/88 (97%)	76 (89%)	9 (11%)	0	100	100
39	x	75/78 (96%)	68 (91%)	4 (5%)	3 (4%)	4	37
40	y	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
41	z	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	9	53
42	Q	103/106 (97%)	88 (85%)	11 (11%)	4 (4%)	4	37
43	R	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
45	V	249/917 (27%)	222 (89%)	20 (8%)	7 (3%)	6	46
All	All	6355/7475 (85%)	5756 (91%)	479 (8%)	120 (2%)	14	54

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	292	SER
9	I	178	ILE
10	J	31	PRO
10	J	157	VAL
14	N	47	ALA

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	193/196 (98%)	187 (97%)	6 (3%)	47	78
5	E	318/323 (98%)	304 (96%)	14 (4%)	35	71
6	F	288/289 (100%)	275 (96%)	13 (4%)	34	70
7	G	244/245 (100%)	224 (92%)	20 (8%)	14	51
8	H	134/153 (88%)	128 (96%)	6 (4%)	34	70
9	I	186/205 (91%)	176 (95%)	10 (5%)	27	66
10	J	187/208 (90%)	173 (92%)	14 (8%)	17	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	171/171 (100%)	158 (92%)	13 (8%)	16	55
12	L	177/187 (95%)	164 (93%)	13 (7%)	17	57
13	M	147/150 (98%)	136 (92%)	11 (8%)	17	56
14	N	154/159 (97%)	141 (92%)	13 (8%)	14	51
15	O	107/109 (98%)	102 (95%)	5 (5%)	32	69
16	a	175/176 (99%)	166 (95%)	9 (5%)	29	67
17	b	160/162 (99%)	155 (97%)	5 (3%)	47	78
18	c	140/146 (96%)	129 (92%)	11 (8%)	15	53
19	d	150/151 (99%)	146 (97%)	4 (3%)	52	80
20	e	153/154 (99%)	148 (97%)	5 (3%)	45	77
21	f	156/156 (100%)	149 (96%)	7 (4%)	34	70
22	g	136/137 (99%)	125 (92%)	11 (8%)	15	52
23	h	87/107 (81%)	85 (98%)	2 (2%)	58	83
24	i	104/105 (99%)	98 (94%)	6 (6%)	25	64
25	j	57/129 (44%)	57 (100%)	0	100	100
26	k	104/118 (88%)	96 (92%)	8 (8%)	16	55
27	l	109/110 (99%)	103 (94%)	6 (6%)	27	66
28	m	115/116 (99%)	108 (94%)	7 (6%)	23	62
29	n	118/119 (99%)	111 (94%)	7 (6%)	24	63
30	o	46/47 (98%)	43 (94%)	3 (6%)	21	60
31	p	81/88 (92%)	79 (98%)	2 (2%)	55	82
32	q	92/97 (95%)	87 (95%)	5 (5%)	27	66
33	r	109/111 (98%)	101 (93%)	8 (7%)	17	57
34	s	43/91 (47%)	42 (98%)	1 (2%)	58	83
35	t	95/103 (92%)	93 (98%)	2 (2%)	61	85
36	u	104/105 (99%)	97 (93%)	7 (7%)	20	59
37	v	81/82 (99%)	75 (93%)	6 (7%)	17	56
38	w	70/71 (99%)	67 (96%)	3 (4%)	35	71
39	x	68/69 (99%)	66 (97%)	2 (3%)	50	79
40	y	45/46 (98%)	44 (98%)	1 (2%)	60	84
41	z	47/116 (40%)	43 (92%)	4 (8%)	13	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	Q	90/91 (99%)	82 (91%)	8 (9%)	12	47
43	R	71/72 (99%)	68 (96%)	3 (4%)	36	72
45	V	224/791 (28%)	193 (86%)	31 (14%)	4	29
All	All	5336/6261 (85%)	5024 (94%)	312 (6%)	29	64

5 of 312 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	a	133	ILE
21	f	61	ILE
45	V	185	VAL
16	a	183	THR
18	c	125	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
16	a	87	GLN
19	d	73	GLN
45	V	160	GLN
12	L	14	ASN
45	V	163	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3201/3396 (94%)	770 (24%)	77 (2%)
2	B	120/121 (99%)	22 (18%)	2 (1%)
3	C	157/158 (99%)	38 (24%)	3 (1%)
All	All	3478/3675 (94%)	830 (23%)	82 (2%)

5 of 830 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	16	A
1	A	22	G
1	A	40	A
1	A	43	A
1	A	45	A

5 of 82 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1841	A
1	A	2269	U
1	A	3351	U
1	A	1846	C
1	A	2112	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 89 ligands modelled in this entry, 89 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](#)

There are no chain breaks in this entry.