



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 14, 2019 – 02:19 AM EST

PDB ID : 6D6R
EMDB ID: : EMD-7809
Title : Human nuclear exosome-MTR4 RNA complex - composite map after focused reconstruction
Authors : Weick, E.-M.; Lima, C.D.
Deposited on : 2018-04-22
Resolution : 3.45 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

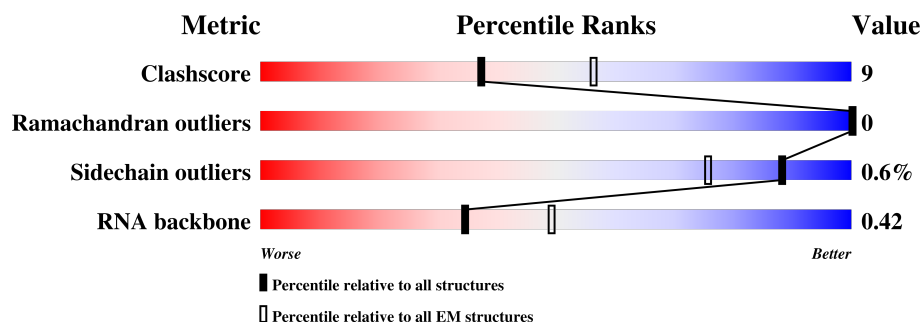
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 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.



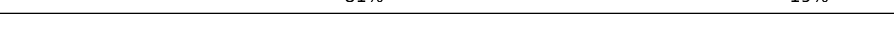
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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	473	45% 16% 39%
2	B	249	78% 18% ..
3	C	278	74% 21% 5%
4	D	237	68% 20% 12%
5	E	293	81% 16% ..
6	F	272	81% 11% . 7%
7	G	277	68% 17% 14%
8	H	296	79% 18% ..

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Mol	Chain	Length	Quality of chain
9	I	197	
10	J	761	
11	K	960	
12	L	162	
13	M	1045	
14	N	16	
15	O	62	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 31639 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 Exosome complex component RRP45.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	287	Total	C	N	O	S	0	0
			2264	1423	404	419	18		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	expression tag	UNP Q06265
A	-15	GLY	-	expression tag	UNP Q06265
A	-14	SER	-	expression tag	UNP Q06265
A	-13	SER	-	expression tag	UNP Q06265
A	-12	HIS	-	expression tag	UNP Q06265
A	-11	HIS	-	expression tag	UNP Q06265
A	-10	HIS	-	expression tag	UNP Q06265
A	-9	HIS	-	expression tag	UNP Q06265
A	-8	HIS	-	expression tag	UNP Q06265
A	-7	HIS	-	expression tag	UNP Q06265
A	-6	SER	-	expression tag	UNP Q06265
A	-5	GLN	-	expression tag	UNP Q06265
A	-4	ASP	-	expression tag	UNP Q06265
A	-3	PRO	-	expression tag	UNP Q06265
A	-2	ASN	-	expression tag	UNP Q06265
A	-1	SER	-	expression tag	UNP Q06265
A	0	HIS	-	expression tag	UNP Q06265

- Molecule 2 is a protein called Exosome complex component RRP41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	241	Total	C	N	O	S	0	0
			1824	1126	345	344	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	expression tag	UNP Q9NPD3
B	-3	ALA	-	expression tag	UNP Q9NPD3
B	-2	ASP	-	expression tag	UNP Q9NPD3
B	-1	PRO	-	expression tag	UNP Q9NPD3

- Molecule 3 is a protein called Exosome complex component RRP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	265	Total	C	N	O	S	0	0
			2020	1272	337	397	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ASP	-	expression tag	UNP Q96B26
C	0	PRO	-	expression tag	UNP Q96B26

- Molecule 4 is a protein called Exosome complex component RRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1566	979	278	297	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	SER	-	expression tag	UNP Q9NQT4
D	0	LEU	-	expression tag	UNP Q9NQT4

- Molecule 5 is a protein called Exosome complex component RRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	286	Total	C	N	O	S	0	0
			2194	1373	374	432	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASP	-	expression tag	UNP Q15024
E	0	PRO	-	expression tag	UNP Q15024

- Molecule 6 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	252	Total	C	N	O	S	0	0
			1859	1154	353	345	7		

- Molecule 7 is a protein called Exosome complex component RRP40.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	237	Total	C	N	O	S	0	0
			1806	1136	329	329	12		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	ASP	-	expression tag	UNP Q9NQT5
G	0	PRO	-	expression tag	UNP Q9NQT5
G	225	HIS	TYR	variant	UNP Q9NQT5

- Molecule 8 is a protein called Exosome complex component RRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	289	Total	C	N	O	S	0	0
			2263	1424	405	419	15		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	ASP	-	expression tag	UNP Q13868
H	-1	PRO	-	expression tag	UNP Q13868
H	0	HIS	-	expression tag	UNP Q13868

- Molecule 9 is a protein called Exosome complex component CSL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	183	Total	C	N	O	S	0	0
			1407	884	247	266	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	ASP	-	expression tag	UNP Q9Y3B2
I	0	PRO	-	expression tag	UNP Q9Y3B2

- Molecule 10 is a protein called Exosome component 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	11	Total	C	N	O	0	0
			86	56	14	16		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	SER	-	expression tag	UNP Q01780
J	313	ASN	ASP	engineered mutation	UNP Q01780
J	649	SER	-	linker	UNP Q01780
J	650	ARG	-	linker	UNP Q01780
J	651	GLY	-	linker	UNP Q01780
J	652	SER	-	linker	UNP Q01780
J	653	GLY	-	linker	UNP Q01780
J	654	SER	-	linker	UNP Q01780
J	655	GLY	-	linker	UNP Q01780
J	656	SER	-	linker	UNP Q01780
J	657	GLY	-	linker	UNP Q01780
J	658	SER	-	linker	UNP Q01780
J	659	GLY	-	linker	UNP Q01780
J	660	SER	-	linker	UNP Q01780

- Molecule 11 is a protein called Exosome complex exonuclease RRP44.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	853	Total	C	N	O	S	0	0
			6856	4329	1233	1260	34		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	GLY	-	expression tag	UNP Q9Y2L1
K	0	SER	-	expression tag	UNP Q9Y2L1
K	146	ASN	ASP	engineered mutation	UNP Q9Y2L1
K	269	SER	ASN	variant	UNP Q9Y2L1
K	487	ASN	ASP	engineered mutation	UNP Q9Y2L1
K	843	ASN	LYS	variant	UNP Q9Y2L1

- Molecule 12 is a protein called M-phase phosphoprotein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	68	Total	C	N	O	S	0	0
			573	371	95	101	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-1	ASP	-	expression tag	UNP Q99547
L	0	PRO	-	expression tag	UNP Q99547

- Molecule 13 is a protein called Exosome RNA helicase MTR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	709	Total	C	N	O	S	0	0
			5648	3589	963	1052	44		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP P42285
M	-1	GLY	-	expression tag	UNP P42285
M	0	ASP	-	expression tag	UNP P42285

- Molecule 14 is a RNA chain called RNA (5'-R(*AP*GP*CP*AP*CP*CP*GP*UP*AP*AP*AP*GP*AP*CP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	13	Total	C	N	O	P	0	0
			278	126	56	84	12		

- Molecule 15 is DNA/RNA hybrid called DNA/RNA (62-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	48	Total	C	N	O	P	0	0
			966	443	172	304	47		

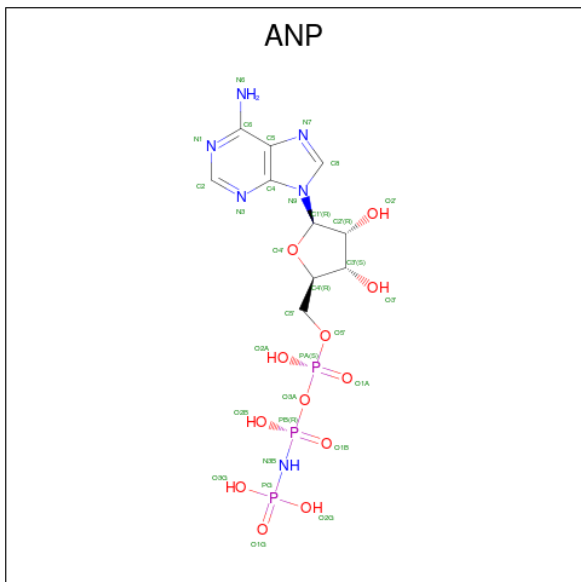
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	K	1	Total	Zn	0
			1	1	

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	K	1	Total	Mg	0
			1	1	

- Molecule 18 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

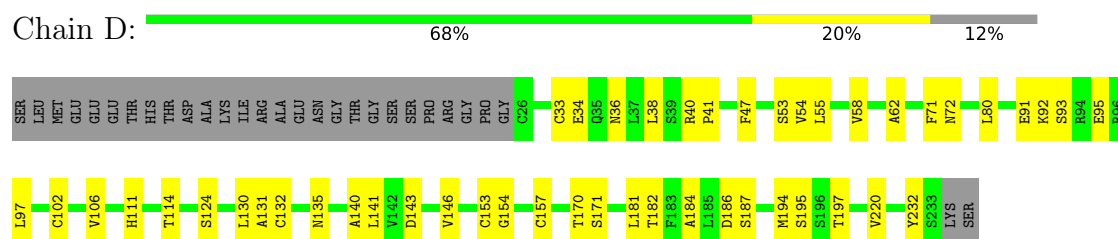


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	M	1	27	10	6	9	2	0

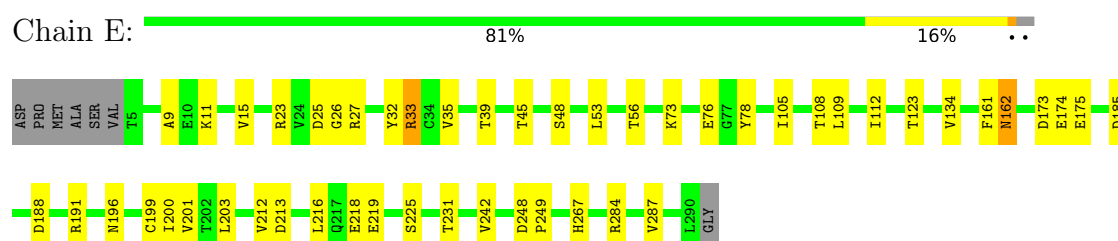
- Molecule 1: Exosome complex component RRP45



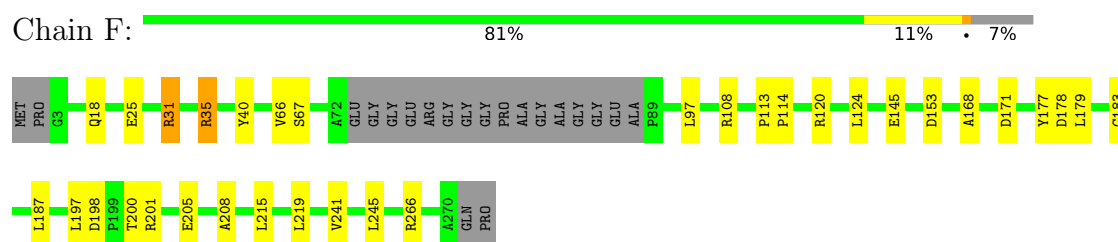
- Molecule 4: Exosome complex component RRP46



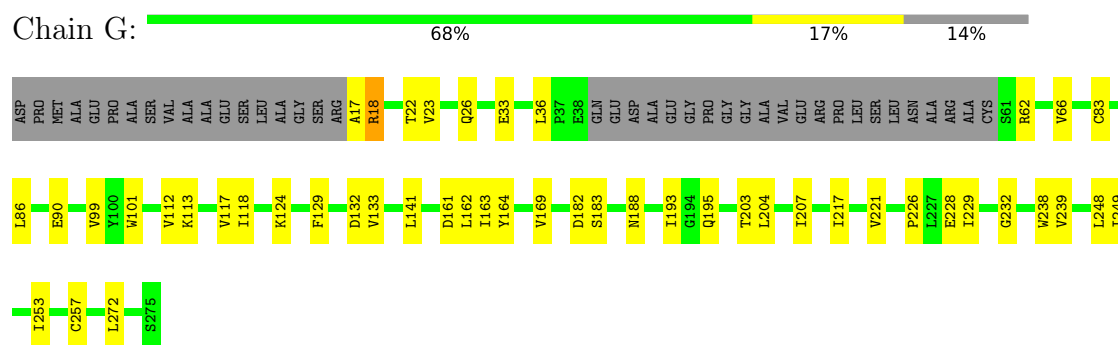
- Molecule 5: Exosome complex component RRP42



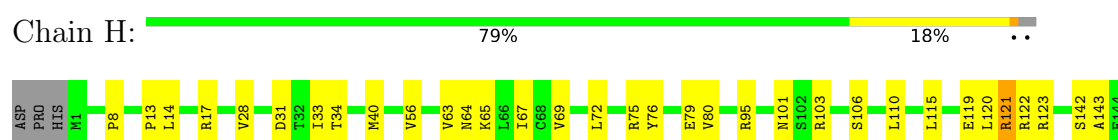
- Molecule 6: Exosome complex component MTR3



- Molecule 7: Exosome complex component RRP40



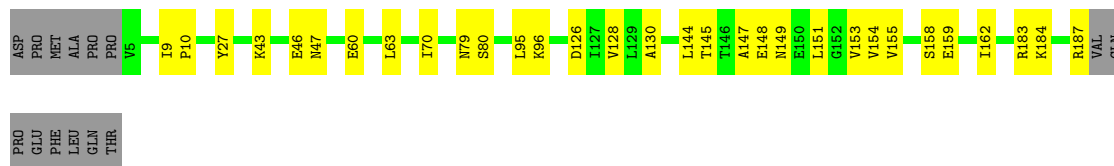
- Molecule 8: Exosome complex component RRP4



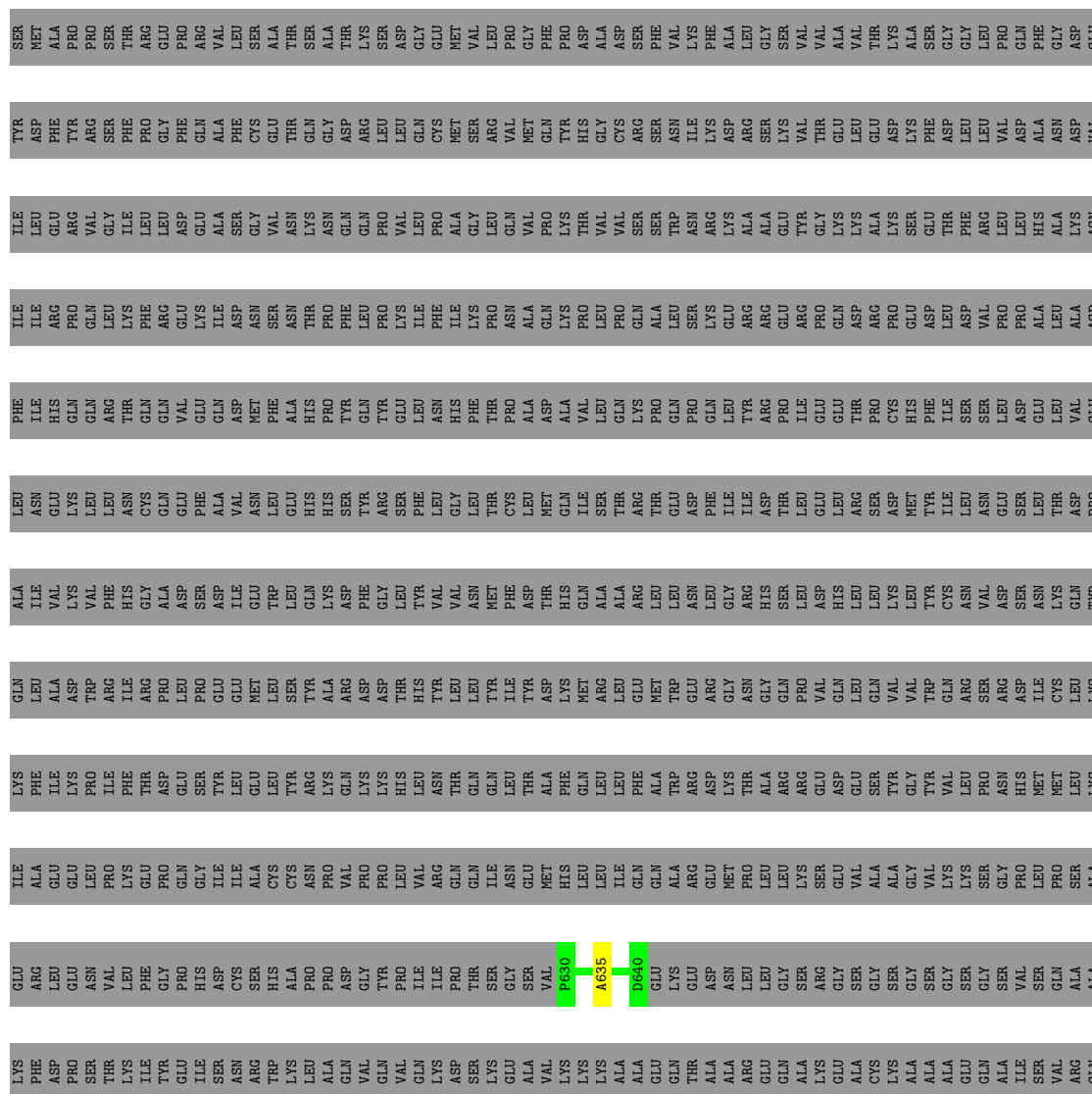
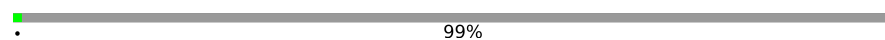


- Molecule 9: Exosome complex component CSL4

Chain I:



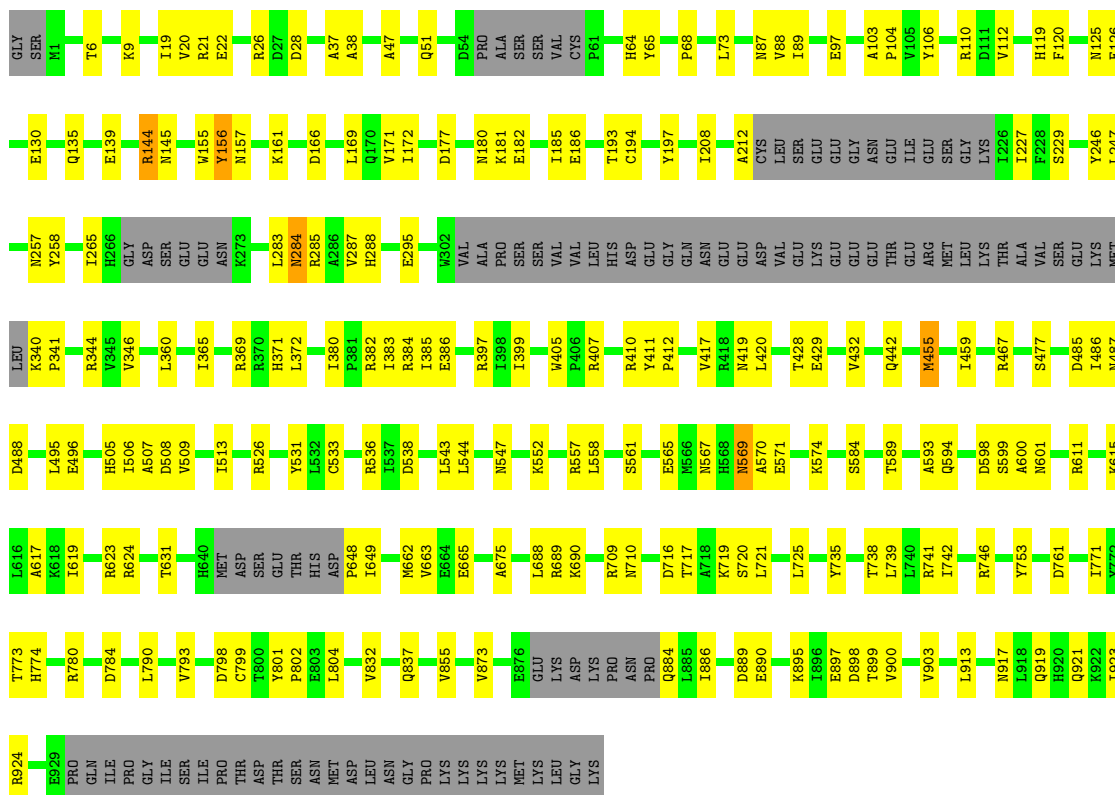
- Molecule 10: Exosome component 10

Chain J: 

GLN	VAL	VAL	LEU	GLU	ASN	ALA	ALA	LYS	LYS	ARG	GLU	ARG	ALA	THR	SER	ASP	PRO	ARG	THR	THR	GLU	GLN	LYS	GLN	GLU	LYS	LYS	ARG	ARG	LEU	LYS	ILE	SER	LYS	LYS
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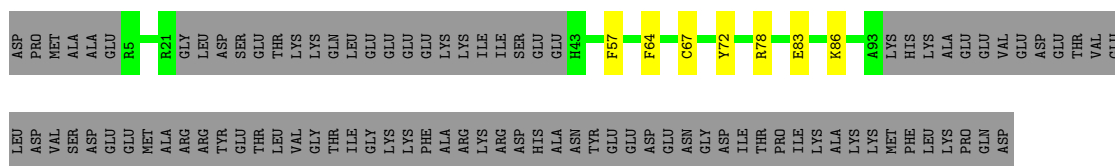
- Molecule 11: Exosome complex exonuclease RRP44

Chain K:  68% 20% • 11%



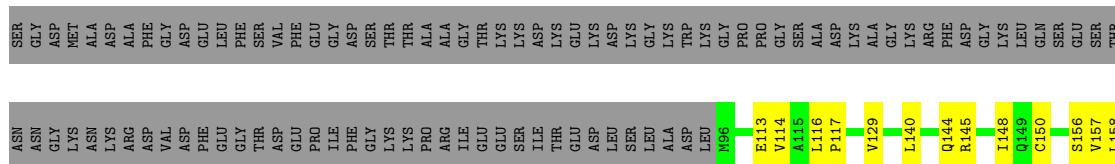
- Molecule 12: M-phase phosphoprotein 6

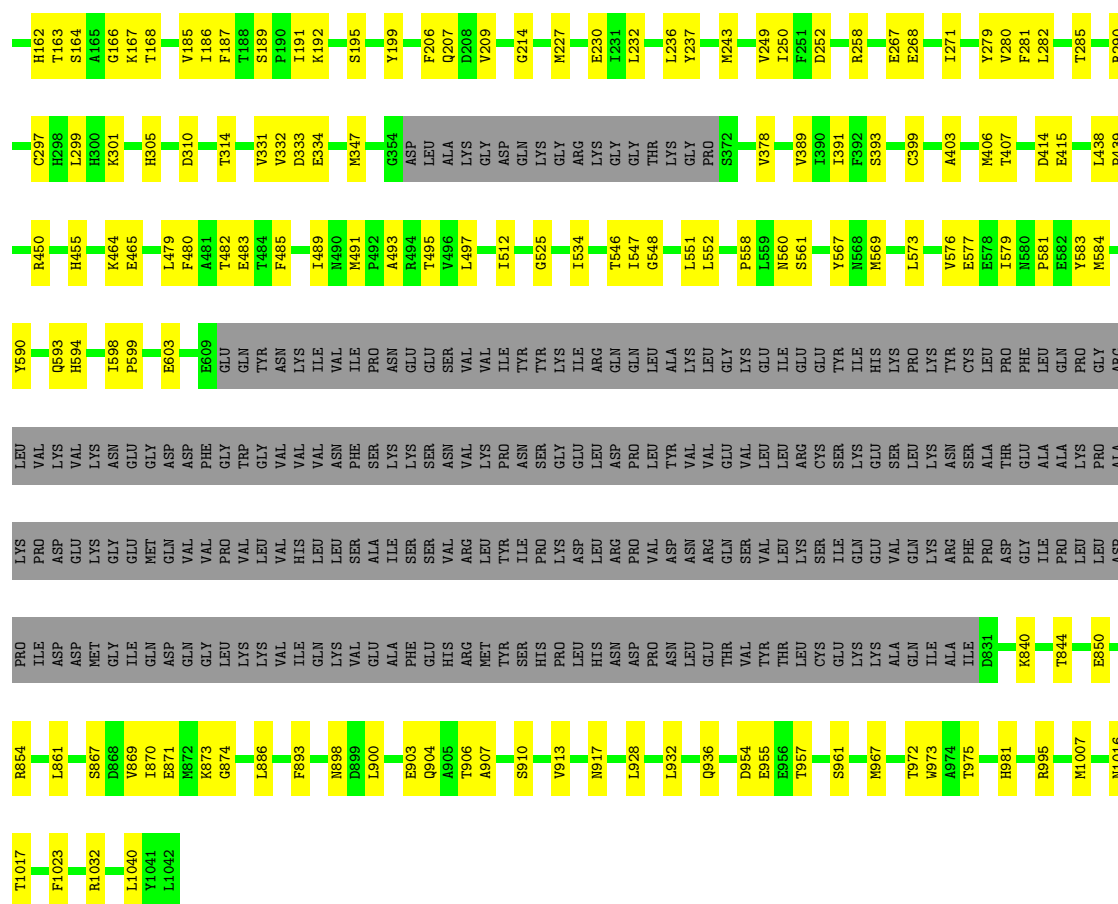
Chain L: 38% . 58%



- Molecule 13: Exosome RNA helicase MTR4

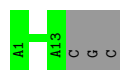
Chain M: 53% 15% 32%





- Molecule 14: RNA (5'-R(*AP*GP*CP*AP*CP*CP*GP*UP*AP*AP*AP*GP*AP*CP*GP*C)-3')

Chain N: 81% 19%



- Molecule 15: DNA/RNA (62-MER)

Chain O: 37% 29% 11% 23%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	122703	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	85.23	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ANP, 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	0.44	0/2297	0.51	0/3094
10	J	0.29	0/88	0.41	0/118
11	K	0.35	0/6991	0.48	1/9444 (0.0%)
12	L	0.31	0/583	0.44	0/776
13	M	0.35	0/5751	0.45	0/7752
14	N	0.22	0/312	0.76	0/485
15	O	0.50	1/1077 (0.1%)	0.87	1/1668 (0.1%)
2	B	0.43	0/1849	0.50	0/2500
3	C	0.43	0/2053	0.49	0/2786
4	D	0.45	0/1586	0.51	0/2145
5	E	0.46	0/2225	0.50	0/3007
6	F	0.41	0/1889	0.52	0/2562
7	G	0.41	0/1832	0.48	0/2467
8	H	0.42	0/2296	0.50	0/3092
9	I	0.33	0/1431	0.49	0/1932
All	All	0.40	1/32260 (0.0%)	0.51	2/43828 (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
11	K	0	1
2	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	17	C	P-O5'	8.76	1.68	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	648	PRO	CA-N-CD	-8.53	99.55	111.50
15	O	16	DT	O3'-P-O5'	5.79	115.00	104.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	201	ASP	Peptide
11	K	455	MET	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	2264	0	2315	62	0
2	B	1824	0	1823	36	0
3	C	2020	0	2035	42	0
4	D	1566	0	1605	31	0
5	E	2194	0	2205	41	0
6	F	1859	0	1889	22	0
7	G	1806	0	1865	35	0
8	H	2263	0	2337	42	0
9	I	1407	0	1432	20	0
10	J	86	0	86	1	0
11	K	6856	0	6907	138	0
12	L	573	0	575	5	0
13	M	5648	0	5681	104	0
14	N	278	0	144	0	0
15	O	966	0	518	23	0
16	K	1	0	0	0	0
17	K	1	0	0	0	0
18	M	27	0	12	2	0
All	All	31639	0	31429	563	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 9.

The worst 5 of 563 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)
11:K:157:ASN:OD1	11:K:171:VAL:CG1	2.06	1.04
11:K:157:ASN:OD1	11:K:171:VAL:HG12	1.61	0.98
3:C:111:ASP:OD1	3:C:115:ASN:ND2	1.96	0.98
15:O:42:C:O2'	15:O:43:A:O5'	1.82	0.96
13:M:393:SER:OG	13:M:399:CYS:SG	2.25	0.94

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/473 (60%)	263 (92%)	22 (8%)	0	100	100
2	B	239/249 (96%)	213 (89%)	26 (11%)	0	100	100
3	C	263/278 (95%)	238 (90%)	25 (10%)	0	100	100
4	D	206/237 (87%)	197 (96%)	9 (4%)	0	100	100
5	E	284/293 (97%)	248 (87%)	36 (13%)	0	100	100
6	F	248/272 (91%)	229 (92%)	19 (8%)	0	100	100
7	G	233/277 (84%)	211 (91%)	22 (9%)	0	100	100
8	H	285/296 (96%)	241 (85%)	44 (15%)	0	100	100
9	I	181/197 (92%)	158 (87%)	23 (13%)	0	100	100
10	J	9/761 (1%)	6 (67%)	3 (33%)	0	100	100
11	K	839/960 (87%)	750 (89%)	89 (11%)	0	100	100
12	L	64/162 (40%)	54 (84%)	10 (16%)	0	100	100
13	M	703/1045 (67%)	647 (92%)	56 (8%)	0	100	100
All	All	3839/5500 (70%)	3455 (90%)	384 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	252/411 (61%)	251 (100%)	1 (0%)	92	96
2	B	184/189 (97%)	182 (99%)	2 (1%)	76	89
3	C	227/237 (96%)	225 (99%)	2 (1%)	81	92
4	D	172/195 (88%)	172 (100%)	0	100	100
5	E	249/254 (98%)	247 (99%)	2 (1%)	83	93
6	F	179/188 (95%)	177 (99%)	2 (1%)	76	89
7	G	196/223 (88%)	195 (100%)	1 (0%)	90	96
8	H	251/257 (98%)	247 (98%)	4 (2%)	65	85
9	I	159/172 (92%)	159 (100%)	0	100	100
10	J	10/672 (2%)	10 (100%)	0	100	100
11	K	758/854 (89%)	753 (99%)	5 (1%)	85	94
12	L	63/148 (43%)	63 (100%)	0	100	100
13	M	618/911 (68%)	616 (100%)	2 (0%)	93	97
All	All	3318/4711 (70%)	3297 (99%)	21 (1%)	88	95

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	18	ARG
8	H	95	ARG
11	K	569	ASN
6	F	35	ARG
11	K	689	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	601	ASN
13	M	936	GLN
13	M	300	HIS
9	I	16	ASN
11	K	788	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	N	12/16 (75%)	0	0
15	O	33/62 (53%)	14 (42%)	2 (6%)
All	All	45/78 (57%)	14 (31%)	2 (4%)

5 of 14 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	O	24	C
15	O	26	A
15	O	29	C
15	O	42	C
15	O	43	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	O	42	C
15	O	53	A

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	ANP	M	2001	-	23,29,33	0.99	2 (8%)	23,45,52	1.07	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	ANP	M	2001	-	-	5/9/32/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	M	2001	ANP	PB-O1B	3.21	1.49	1.46
18	M	2001	ANP	PB-O3A	-2.21	1.56	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	M	2001	ANP	PA-O3A-PB	-3.78	120.22	132.49
18	M	2001	ANP	C5-C6-N6	2.21	123.86	120.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

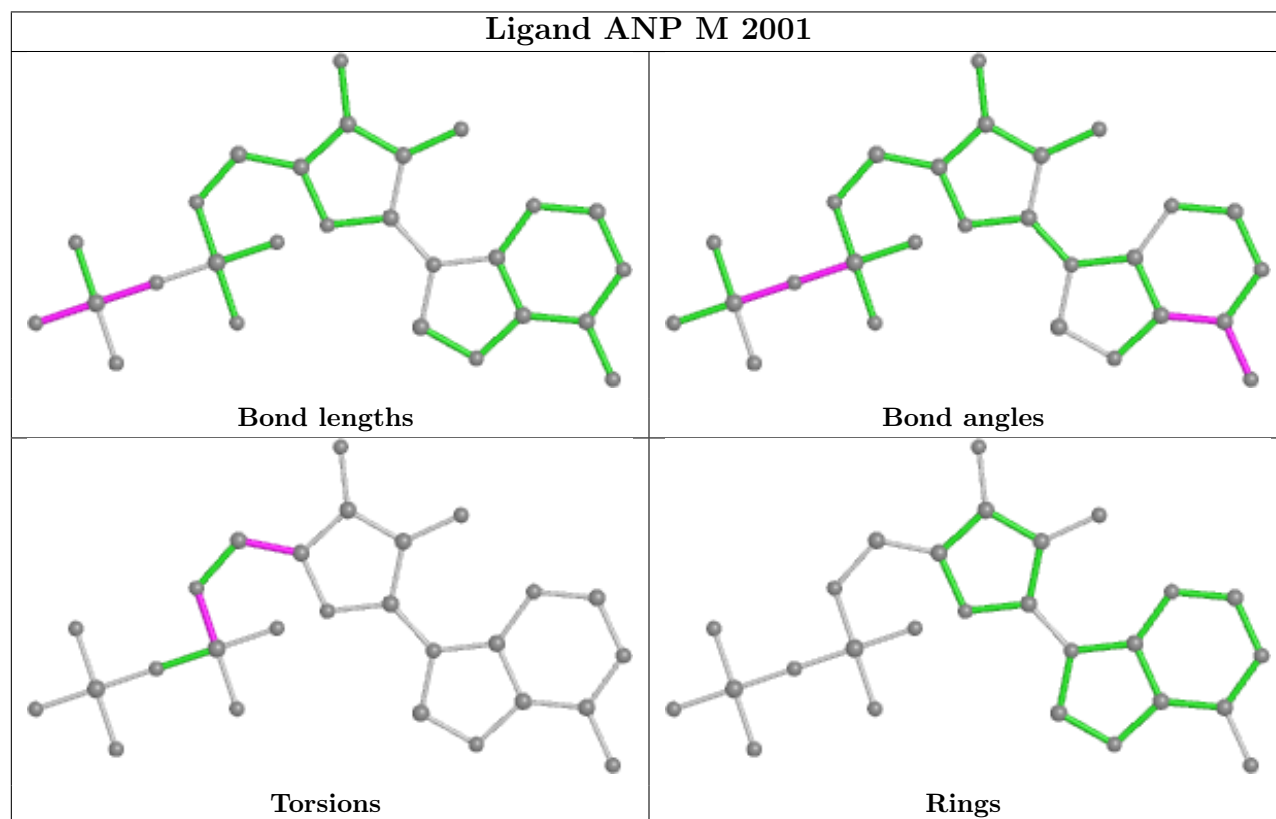
Mol	Chain	Res	Type	Atoms
18	M	2001	ANP	C5'-O5'-PA-O1A
18	M	2001	ANP	C5'-O5'-PA-O2A
18	M	2001	ANP	O4'-C4'-C5'-O5'
18	M	2001	ANP	C3'-C4'-C5'-O5'
18	M	2001	ANP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	M	2001	ANP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.