wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 04:38 AM GMT

PDB ID	:	2NN6
Title	:	Structure of the human RNA exosome composed of Rrp41, Rrp45, Rrp46, Rrp43, Mtr3, Rrp42, Csl4, Rrp4, and Rrp40
Authors	:	Lima, C.D.
Deposited on	:	2006-10-23
Resolution	:	3.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

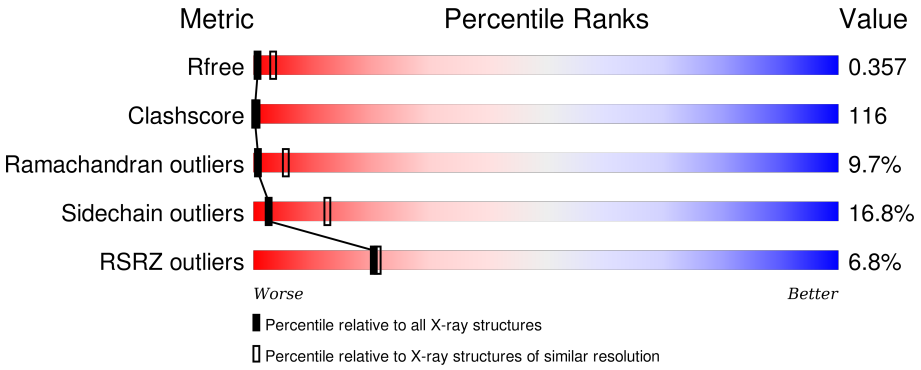
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	358	3% 15% 55% 23% • 5%
2	B	249	3% 12% 63% 18% • 6%
3	C	278	5% 10% 68% 17% • •
4	D	237	3% 11% 59% 16% 14%
5	E	305	12% 11% 63% 15% • 10%

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Mol	Chain	Length	Quality of chain
6	F	272	7% 12% 56% 14% 18%
7	G	289	2% 15% 46% 19% 18%
8	H	308	4% 15% 54% 12% 19%
9	I	209	16% 15% 56% 15% 14%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 16858 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Polymyositis/scleroderma autoantigen 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2611	1651	464	477	19			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	CLONING ARTIFACT	UNP Q86Y41
A	-15	GLY	-	CLONING ARTIFACT	UNP Q86Y41
A	-14	SER	-	CLONING ARTIFACT	UNP Q86Y41
A	-13	SER	-	CLONING ARTIFACT	UNP Q86Y41
A	-12	HIS	-	CLONING ARTIFACT	UNP Q86Y41
A	-11	HIS	-	CLONING ARTIFACT	UNP Q86Y41
A	-10	HIS	-	CLONING ARTIFACT	UNP Q86Y41
A	-9	HIS	-	CLONING ARTIFACT	UNP Q86Y41
A	-8	HIS	-	CLONING ARTIFACT	UNP Q86Y41
A	-7	HIS	-	CLONING ARTIFACT	UNP Q86Y41
A	-6	SER	-	CLONING ARTIFACT	UNP Q86Y41
A	-5	GLN	-	CLONING ARTIFACT	UNP Q86Y41
A	-4	ASP	-	CLONING ARTIFACT	UNP Q86Y41
A	-3	PRO	-	CLONING ARTIFACT	UNP Q86Y41
A	-2	ASN	-	CLONING ARTIFACT	UNP Q86Y41
A	-1	SER	-	CLONING ARTIFACT	UNP Q86Y41
A	0	HIS	-	CLONING ARTIFACT	UNP Q86Y41

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	0
			1779	1095	339	336	9			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	CLONING ARTIFACT	UNP Q9NPD3
B	-3	ALA	-	CLONING ARTIFACT	UNP Q9NPD3
B	-2	ASP	-	CLONING ARTIFACT	UNP Q9NPD3
B	-1	PRO	-	CLONING ARTIFACT	UNP Q9NPD3
B	0	MET	-	CLONING ARTIFACT	UNP Q9NPD3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	270	Total	C	N	O	S	0	0	0
			2058	1298	344	402	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ASP	-	CLONING ARTIFACT	UNP Q96B26
C	0	PRO	-	CLONING ARTIFACT	UNP Q96B26

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	205	Total	C	N	O	S	0	0	0
			1534	956	275	291	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	SER	-	CLONING ARTIFACT	UNP Q9NQT4
D	0	LEU	-	CLONING ARTIFACT	UNP Q9NQT4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	275	Total	C	N	O	S	0	0	0
			2109	1320	361	413	15			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-13	MET	-	CLONING ARTIFACT	UNP Q15024
E	-12	GLY	-	CLONING ARTIFACT	UNP Q15024
E	-11	SER	-	CLONING ARTIFACT	UNP Q15024

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	SER	-	CLONING ARTIFACT	UNP Q15024
E	-9	HIS	-	CLONING ARTIFACT	UNP Q15024
E	-8	HIS	-	CLONING ARTIFACT	UNP Q15024
E	-7	HIS	-	CLONING ARTIFACT	UNP Q15024
E	-6	HIS	-	CLONING ARTIFACT	UNP Q15024
E	-5	HIS	-	CLONING ARTIFACT	UNP Q15024
E	-4	HIS	-	CLONING ARTIFACT	UNP Q15024
E	-3	SER	-	CLONING ARTIFACT	UNP Q15024
E	-2	GLN	-	CLONING ARTIFACT	UNP Q15024
E	-1	ASP	-	CLONING ARTIFACT	UNP Q15024
E	0	PRO	-	CLONING ARTIFACT	UNP Q15024
E	274	VAL	LEU	VARIANT	UNP Q15024

- Molecule 6 is a protein called Exosome component 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	223	Total	C	N	O	S	0	0	0
			1635	1019	311	298	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	236	Total	C	N	O	S	0	0	0
			1793	1128	318	337	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	MET	-	CLONING ARTIFACT	UNP Q9NQT5
G	-13	GLY	-	CLONING ARTIFACT	UNP Q9NQT5
G	-12	SER	-	CLONING ARTIFACT	UNP Q9NQT5
G	-11	SER	-	CLONING ARTIFACT	UNP Q9NQT5
G	-10	HIS	-	CLONING ARTIFACT	UNP Q9NQT5
G	-9	HIS	-	CLONING ARTIFACT	UNP Q9NQT5
G	-8	HIS	-	CLONING ARTIFACT	UNP Q9NQT5
G	-7	HIS	-	CLONING ARTIFACT	UNP Q9NQT5
G	-6	HIS	-	CLONING ARTIFACT	UNP Q9NQT5
G	-5	HIS	-	CLONING ARTIFACT	UNP Q9NQT5
G	-4	SER	-	CLONING ARTIFACT	UNP Q9NQT5
G	-3	GLN	-	CLONING ARTIFACT	UNP Q9NQT5
G	-2	ASP	-	CLONING ARTIFACT	UNP Q9NQT5
G	-1	PRO	-	CLONING ARTIFACT	UNP Q9NQT5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	250	Total	C	N	O	S	0	0	0
			1956	1238	341	365	12			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-14	MET	-	CLONING ARTIFACT	UNP Q13868
H	-13	GLY	-	CLONING ARTIFACT	UNP Q13868
H	-12	SER	-	CLONING ARTIFACT	UNP Q13868
H	-11	SER	-	CLONING ARTIFACT	UNP Q13868
H	-10	HIS	-	CLONING ARTIFACT	UNP Q13868
H	-9	HIS	-	CLONING ARTIFACT	UNP Q13868
H	-8	HIS	-	CLONING ARTIFACT	UNP Q13868
H	-7	HIS	-	CLONING ARTIFACT	UNP Q13868
H	-6	HIS	-	CLONING ARTIFACT	UNP Q13868
H	-5	HIS	-	CLONING ARTIFACT	UNP Q13868
H	-4	SER	-	CLONING ARTIFACT	UNP Q13868
H	-3	GLN	-	CLONING ARTIFACT	UNP Q13868
H	-2	ASP	-	CLONING ARTIFACT	UNP Q13868
H	-1	PRO	-	CLONING ARTIFACT	UNP Q13868
H	0	HIS	-	CLONING ARTIFACT	UNP Q13868

- Molecule 9 is a protein called 3'-5' exoribonuclease CSL4 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	180	Total	C	N	O	S	0	0	0
			1383	870	241	262	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-13	MET	-	CLONING ARTIFACT	UNP Q9Y3B2
I	-12	GLY	-	CLONING ARTIFACT	UNP Q9Y3B2
I	-11	SER	-	CLONING ARTIFACT	UNP Q9Y3B2
I	-10	SER	-	CLONING ARTIFACT	UNP Q9Y3B2
I	-9	HIS	-	CLONING ARTIFACT	UNP Q9Y3B2
I	-8	HIS	-	CLONING ARTIFACT	UNP Q9Y3B2
I	-7	HIS	-	CLONING ARTIFACT	UNP Q9Y3B2
I	-6	HIS	-	CLONING ARTIFACT	UNP Q9Y3B2
I	-5	HIS	-	CLONING ARTIFACT	UNP Q9Y3B2
I	-4	HIS	-	CLONING ARTIFACT	UNP Q9Y3B2

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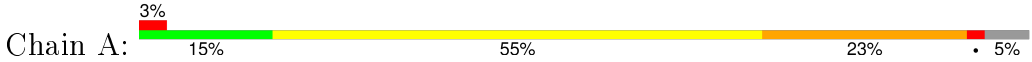
Chain	Residue	Modelled	Actual	Comment	Reference
I	-3	SER	-	CLONING ARTIFACT	UNP Q9Y3B2
I	-2	GLN	-	CLONING ARTIFACT	UNP Q9Y3B2
I	-1	ASP	-	CLONING ARTIFACT	UNP Q9Y3B2
I	0	PRO	-	CLONING ARTIFACT	UNP Q9Y3B2

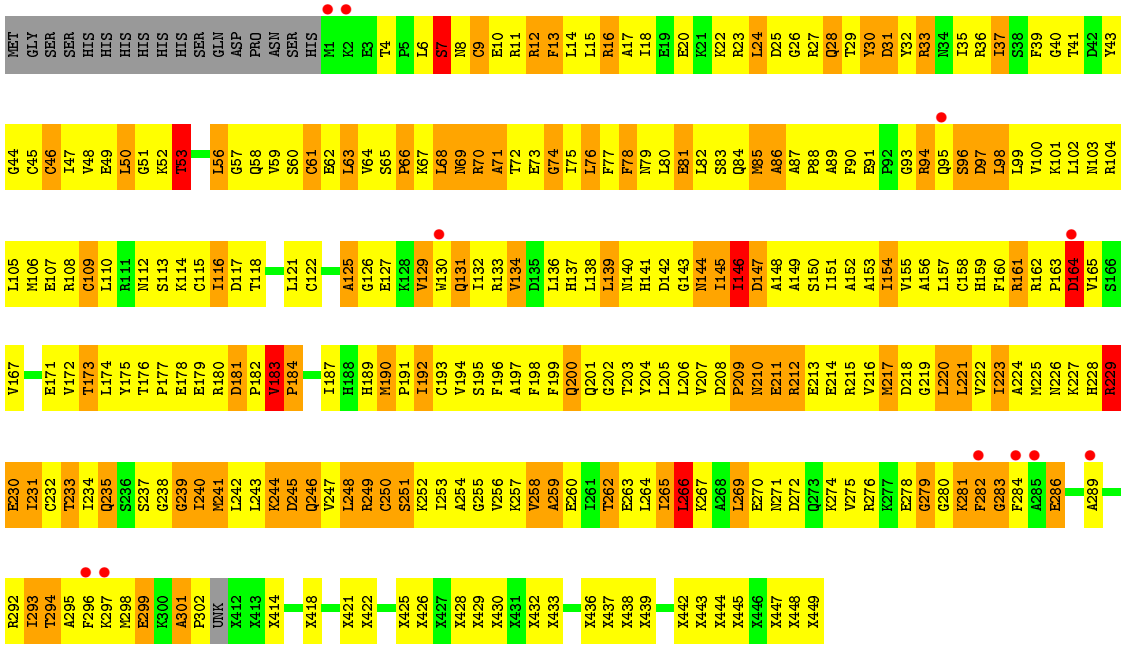
3 Residue-property plots (i)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Polymyositis/scleroderma autoantigen 1

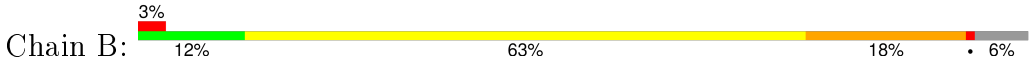
Chain A:

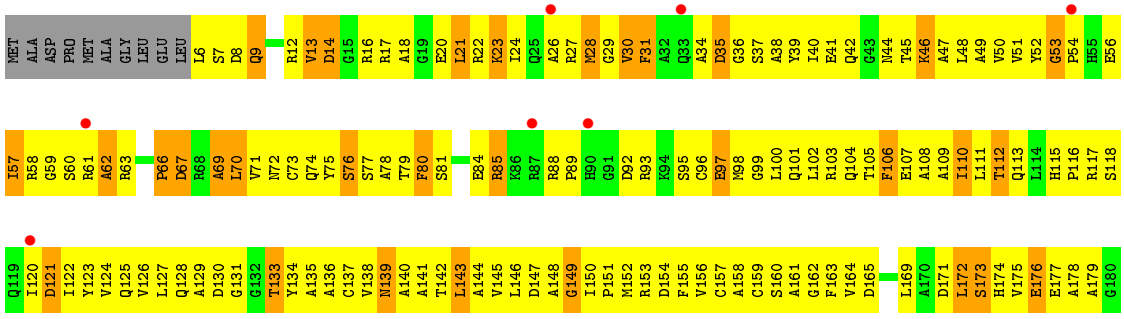




- Molecule 2: Exosome complex exonuclease RRP41

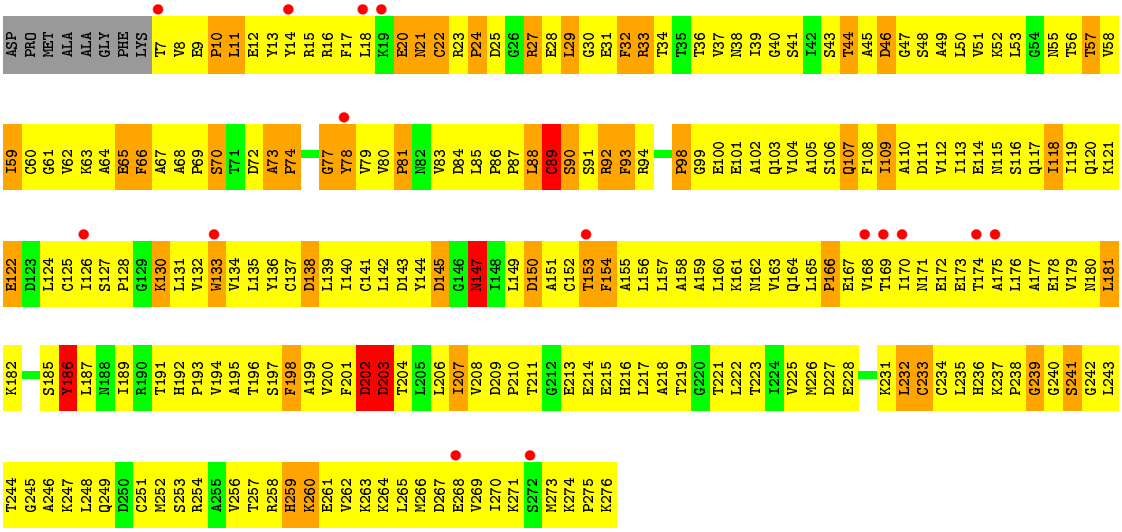
Chain B:





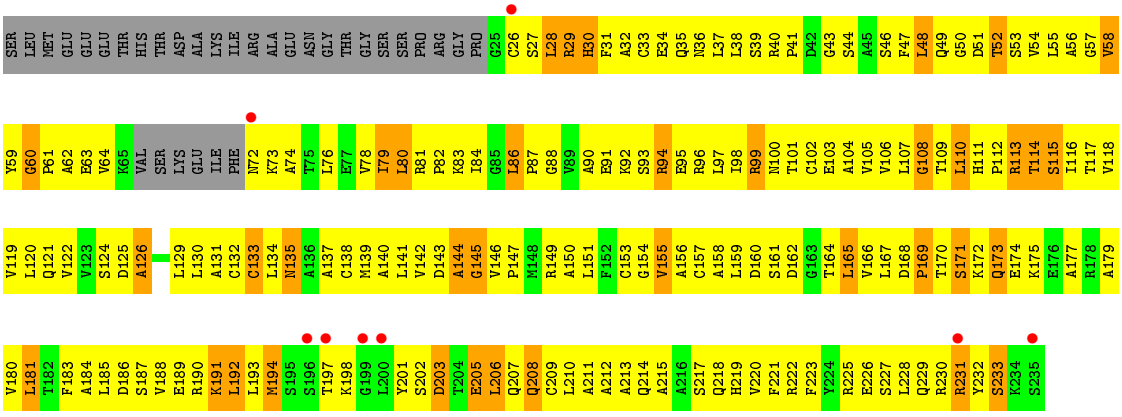
• Molecule 3: Exosome complex exonuclease RRP43

Chain C:



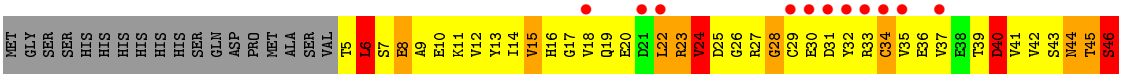
• Molecule 4: Exosome complex exonuclease RRP46

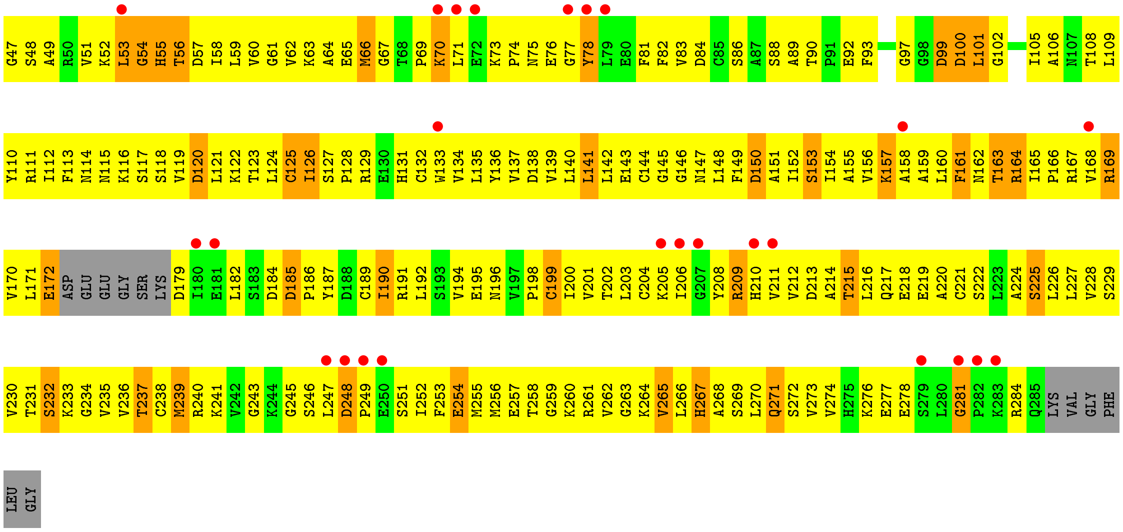
Chain D:



• Molecule 5: Exosome complex exonuclease RRP42

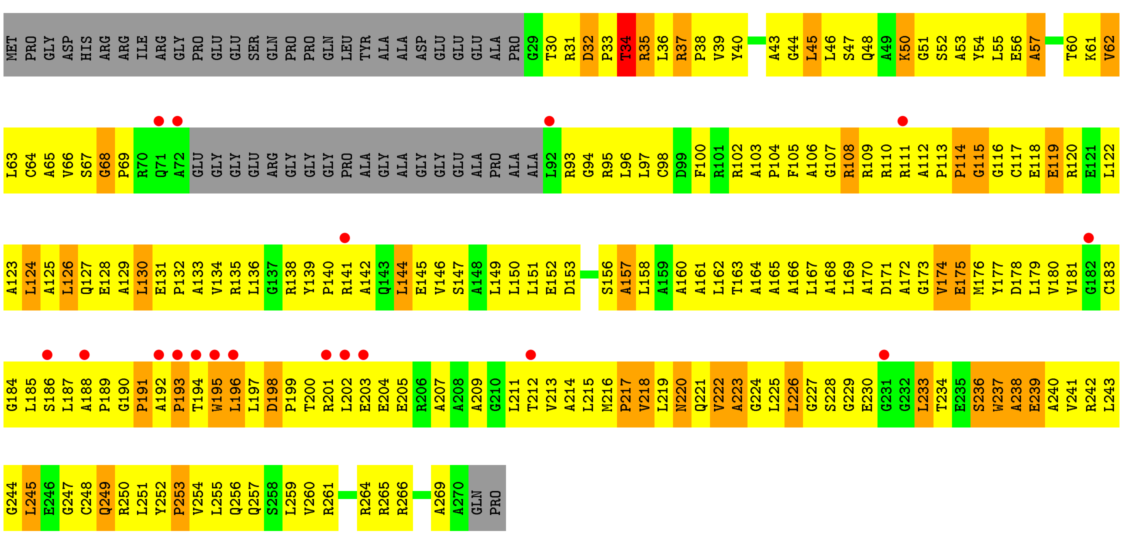
Chain E:





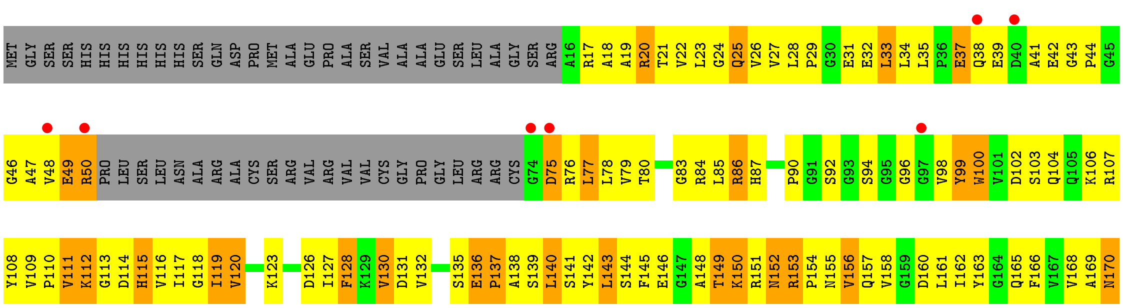
- Molecule 6: Exosome component 6

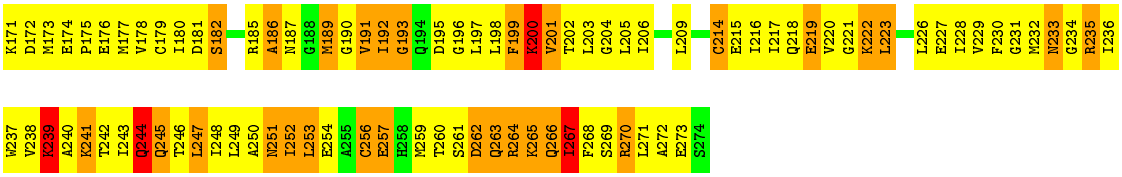
Chain F:



- Molecule 7: Exosome complex exonuclease RRP40

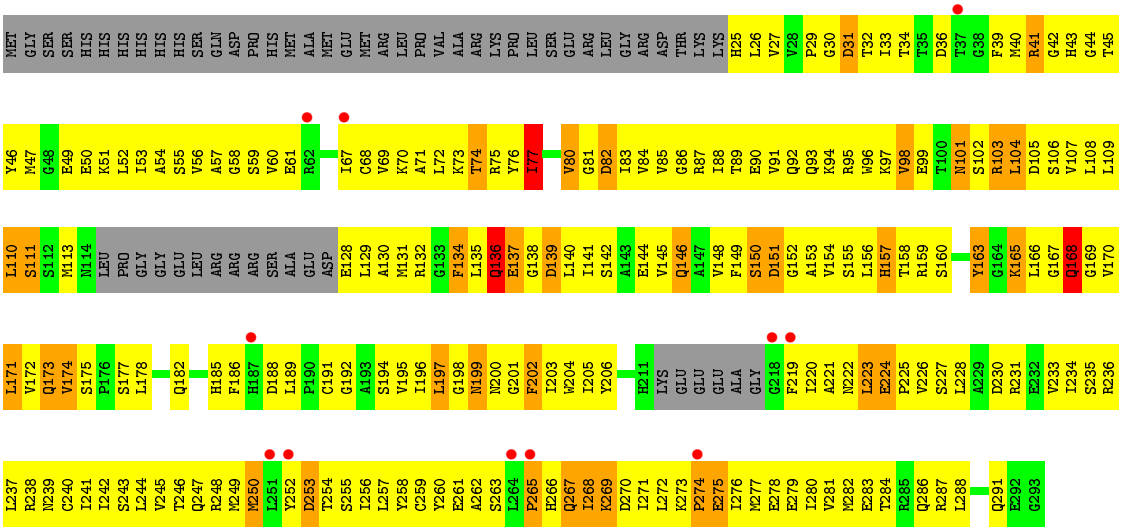
Chain G:





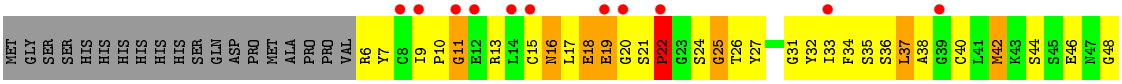
• Molecule 8: Exosome complex exonuclease RRP4

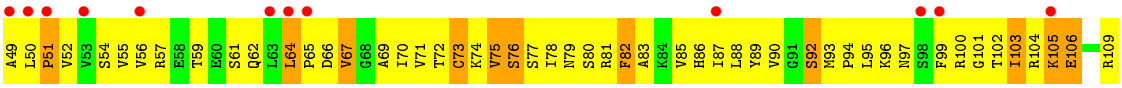
Chain H:

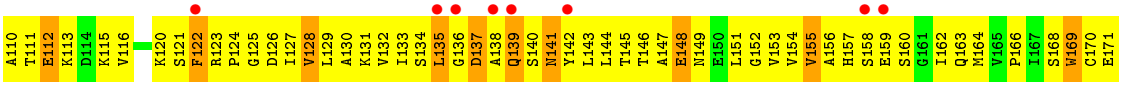


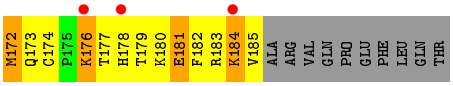
• Molecule 9: 3'-5' exoribonuclease CSL4 homolog

Chain I:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 3 2	Depositor
Cell constants a, b, c, α, β, γ	307.80Å 307.80Å 307.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 3.35 34.85 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.7 (14.98-3.35) 97.8 (34.85-3.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 3.32Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.291 , 0.344 0.308 , 0.357	Depositor DCC
R_{free} test set	3465 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	87.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 62.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.17$	Xtriage
Outliers	1 of 69964 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	16858	wwPDB-VP
Average B, all atoms (Å^2)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.62	0/2418	0.87	4/3256 (0.1%)
2	B	0.51	0/1804	0.81	2/2439 (0.1%)
3	C	0.46	0/2092	0.73	0/2839
4	D	0.54	0/1552	0.79	1/2097 (0.0%)
5	E	0.41	0/2138	0.72	0/2890
6	F	0.41	0/1658	0.69	0/2247
7	G	0.62	0/1819	0.91	2/2451 (0.1%)
8	H	0.39	0/1985	0.72	0/2679
9	I	0.41	0/1407	0.74	1/1899 (0.1%)
All	All	0.50	0/16873	0.78	10/22797 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	266	LEU	CA-CB-CG	-7.27	98.57	115.30
7	G	253	LEU	CA-CB-CG	-6.87	99.50	115.30
1	A	53	THR	N-CA-C	-6.70	92.92	111.00
1	A	33	ARG	N-CA-C	-5.80	95.33	111.00
7	G	193	GLY	N-CA-C	5.79	127.58	113.10

There are no chirality outliers.

There are no planarity outliers.

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	2611	0	2673	640	0
2	B	1779	0	1770	414	0
3	C	2058	0	2084	608	0
4	D	1534	0	1572	415	0
5	E	2109	0	2122	495	0
6	F	1635	0	1686	409	0
7	G	1793	0	1827	495	0
8	H	1956	0	2002	414	0
9	I	1383	0	1405	329	0
All	All	16858	0	17141	3953	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 116.

The worst 5 of 3953 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)
4:D:202:SER:N	4:D:205:GLU:HG3	1.49	1.25
8:H:220:ILE:HA	8:H:223:LEU:HD13	1.26	1.18
1:A:230:GLU:HB3	2:B:205:HIS:HA	1.22	1.18
9:I:24:SER:HB3	9:I:54:SER:HB2	1.24	1.18
3:C:126:ILE:HB	3:C:131:LEU:HB3	1.25	1.17

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	300/358 (84%)	209 (70%)	60 (20%)	31 (10%)	1 5
2	B	233/249 (94%)	156 (67%)	56 (24%)	21 (9%)	1 7
3	C	268/278 (96%)	193 (72%)	44 (16%)	31 (12%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	201/237 (85%)	157 (78%)	29 (14%)	15 (8%)	1 11
5	E	271/305 (89%)	200 (74%)	47 (17%)	24 (9%)	1 7
6	F	219/272 (80%)	166 (76%)	32 (15%)	21 (10%)	1 6
7	G	232/289 (80%)	152 (66%)	51 (22%)	29 (12%)	0 2
8	H	244/308 (79%)	182 (75%)	41 (17%)	21 (9%)	1 8
9	I	178/209 (85%)	122 (68%)	40 (22%)	16 (9%)	1 7
All	All	2146/2505 (86%)	1537 (72%)	400 (19%)	209 (10%)	1 5

5 of 209 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	68	LEU
1	A	69	ASN
1	A	94	ARG
1	A	227	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	264/280 (94%)	196 (74%)	68 (26%)	0 2
2	B	179/189 (95%)	146 (82%)	33 (18%)	2 9
3	C	232/237 (98%)	201 (87%)	31 (13%)	5 21
4	D	168/195 (86%)	144 (86%)	24 (14%)	4 19
5	E	240/265 (91%)	205 (85%)	35 (15%)	4 18
6	F	157/188 (84%)	135 (86%)	22 (14%)	4 20
7	G	192/234 (82%)	150 (78%)	42 (22%)	1 5
8	H	219/268 (82%)	194 (89%)	25 (11%)	7 29
9	I	157/183 (86%)	133 (85%)	24 (15%)	3 16
All	All	1808/2039 (89%)	1504 (83%)	304 (17%)	2 12

5 of 304 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	58	VAL
5	E	78	TYR
9	I	16	ASN
4	D	94	ARG
4	D	208	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	173	GLN
5	E	162	ASN
9	I	16	ASN
4	D	207	GLN
5	E	114	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no ligands in this entry.

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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	302/358 (84%)	0.02	11 (3%) 46 46	15, 86, 175, 194	0
2	B	235/249 (94%)	0.10	7 (2%) 54 54	21, 99, 145, 181	0
3	C	270/278 (97%)	0.15	15 (5%) 28 27	66, 117, 171, 203	0
4	D	205/237 (86%)	0.08	8 (3%) 43 42	38, 94, 128, 157	0
5	E	275/305 (90%)	0.55	36 (13%) 5 4	87, 133, 181, 195	0
6	F	223/272 (81%)	0.11	18 (8%) 15 14	77, 131, 174, 189	0
7	G	236/289 (81%)	-0.07	7 (2%) 54 54	19, 98, 153, 189	0
8	H	250/308 (81%)	0.28	11 (4%) 38 37	94, 146, 185, 204	0
9	I	180/209 (86%)	0.60	34 (18%) 2 2	88, 142, 178, 193	0
All	All	2176/2505 (86%)	0.19	147 (6%) 20 21	15, 118, 176, 204	0

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	133	TRP	7.3
5	E	282	PRO	6.9
8	H	265	PRO	6.6
8	H	264	LEU	5.9
9	I	53	VAL	5.8

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.