



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 08:16 AM EDT

PDB ID : 5C0X
Title : Structure of a 12-subunit nuclear exosome complex bound to structured RNA
Authors : Makino, D.L.; Conti, E.
Deposited on : 2015-06-12
Resolution : 3.81 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

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

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:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

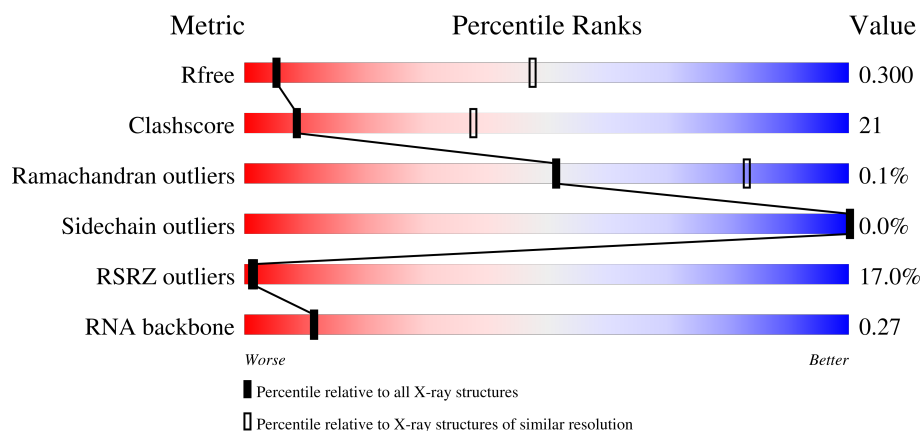
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 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.





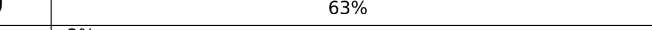

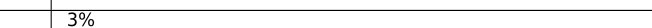
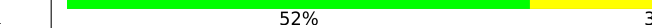

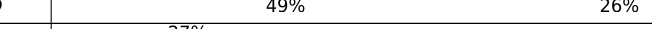
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1231 (4.04-3.60)
Clashscore	141614	1031 (4.02-3.62)
Ramachandran outliers	138981	1261 (4.04-3.60)
Sidechain outliers	138945	1255 (4.04-3.60)
RSRZ outliers	127900	1139 (4.04-3.60)
RNA backbone	3102	1037 (4.62-3.00)

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 of the lower 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 $\leq 5\%$. 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	305	<div> <div>7%</div> <div>77%</div> <div>21%</div> <div>•</div> </div>
2	B	248	<div> <div>8%</div> <div>76%</div> <div>22%</div> <div>•</div> </div>
3	C	394	<div> <div>7%</div> <div>61%</div> <div>25%</div> <div>14%</div> </div>
4	D	245	<div> <div>5%</div> <div>74%</div> <div>17%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	267	
6	F	250	
7	G	243	
8	H	361	
9	I	295	
10	J	1003	
11	K	695	
12	R	45	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 27816 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 Exosome complex component RRP45.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2304	1444	393	451	16			

- Molecule 2 is a protein called Exosome complex component SKI6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1886	1177	335	366	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P46948
B	0	HIS	-	expression tag	UNP P46948

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	339	Total	C	N	O	S	0	1	0
			2589	1640	441	497	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	102	SER	ALA	engineered mutation	UNP P25359
C	363	MET	VAL	engineered mutation	UNP P25359

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	223	Total	C	N	O	S	0	1	0
			1701	1072	285	334	10			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	GLY	-	expression tag	UNP P53256
D	-20	HIS	-	expression tag	UNP P53256
D	-19	GLY	-	expression tag	UNP P53256
D	-18	ASN	-	expression tag	UNP P53256
D	-17	ASN	-	expression tag	UNP P53256
D	-16	LYS	-	expression tag	UNP P53256
D	-15	GLU	-	expression tag	UNP P53256
D	-14	PRO	-	expression tag	UNP P53256
D	-13	ASN	-	expression tag	UNP P53256
D	-12	THR	-	expression tag	UNP P53256
D	-11	LYS	-	expression tag	UNP P53256
D	-10	ASN	-	expression tag	UNP P53256
D	-9	ARG	-	expression tag	UNP P53256
D	-8	LEU	-	expression tag	UNP P53256
D	-7	ASP	-	expression tag	UNP P53256
D	-6	SER	-	expression tag	UNP P53256
D	-5	ALA	-	expression tag	UNP P53256
D	-4	GLU	-	expression tag	UNP P53256
D	-3	LYS	-	expression tag	UNP P53256
D	-2	LYS	-	expression tag	UNP P53256
D	-1	LYS	-	expression tag	UNP P53256
D	0	LYS	-	expression tag	UNP P53256

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	267	Total	C	N	O	S	0	1	0
			2050	1308	338	399	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP Q12277
E	0	HIS	-	expression tag	UNP Q12277
E	138	ILE	VAL	engineered mutation	UNP Q12277

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	215	Total	C	N	O	S	0	0	0
			1638	1023	273	332	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	75	SER	THR	engineered mutation	UNP P48240
F	161	THR	MET	engineered mutation	UNP P48240

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	237	Total	C	N	O	S	0	0	0
			1792	1143	295	344	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	GLY	-	expression tag	UNP Q08285
G	-1	PRO	-	expression tag	UNP Q08285
G	0	HIS	-	expression tag	UNP Q08285

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	293	Total	C	N	O	S	0	0	0
			2236	1393	403	428	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	ARG	-	expression tag	UNP P38792
H	0	SER	-	expression tag	UNP P38792

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	222	Total	C	N	O	S	0	0	0
			1653	1034	287	325	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	GLY	-	expression tag	UNP P53859
I	-1	PRO	-	expression tag	UNP P53859
I	0	HIS	-	expression tag	UNP P53859

- Molecule 10 is a protein called Exosome complex exonuclease DIS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	944	Total	C	N	O	S	0	1	0
			7427	4693	1304	1395	35			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-1	GLY	-	expression tag	UNP Q08162
J	0	ALA	-	expression tag	UNP Q08162
J	171	ASN	ASP	engineered mutation	UNP Q08162
J	551	ASN	ASP	engineered mutation	UNP Q08162

- Molecule 11 is a protein called Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	350	Total	C	N	O	S	0	0	0
			1982	1212	379	389	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	GLY	-	expression tag	UNP Q12149
K	0	ALA	-	expression tag	UNP Q12149
K	2	ALA	THR	engineered mutation	UNP Q12149
K	296	ASN	ASP	engineered mutation	UNP Q12149

- Molecule 12 is a RNA chain called RNA synthetic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	R	31	Total	C	N	O	P	0	0	0
			557	244	71	211	31			

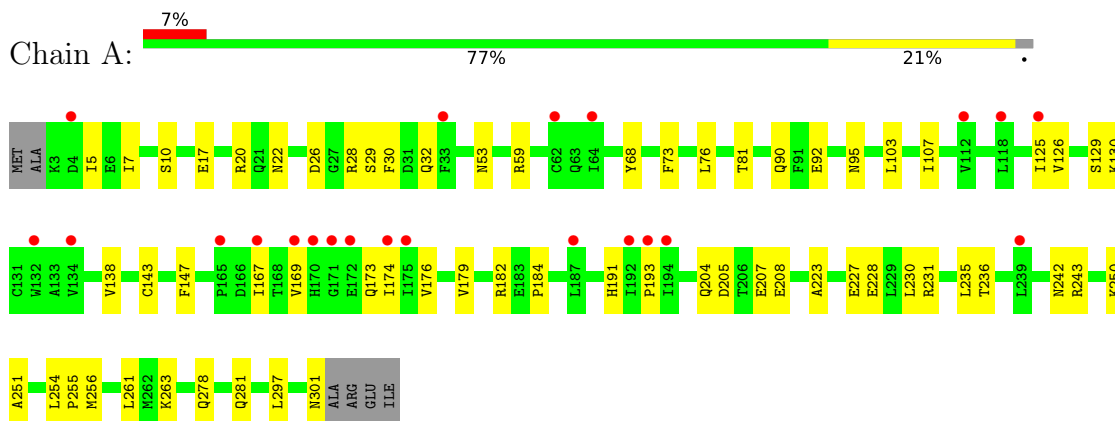
- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

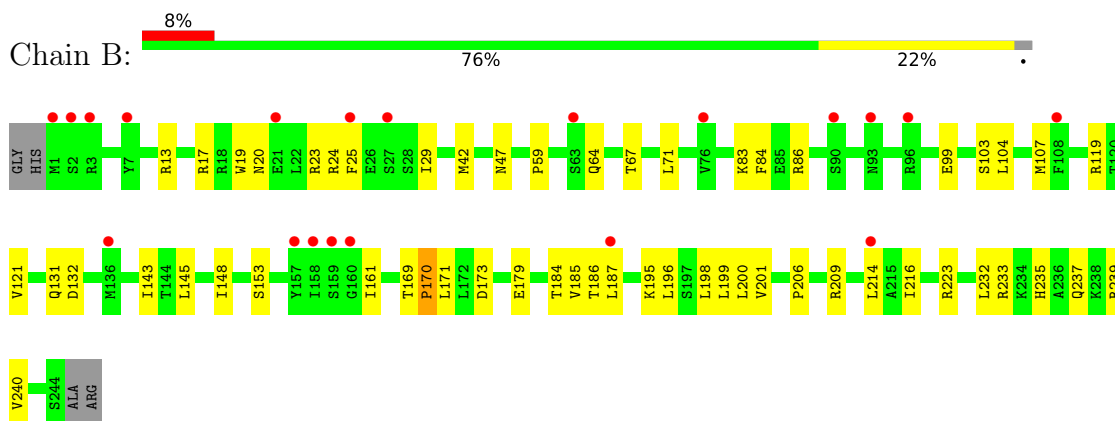
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

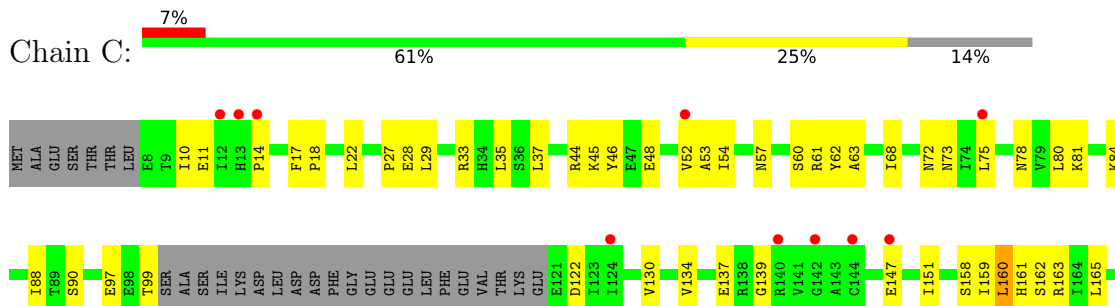
• Molecule 1: Exosome complex component RRP45

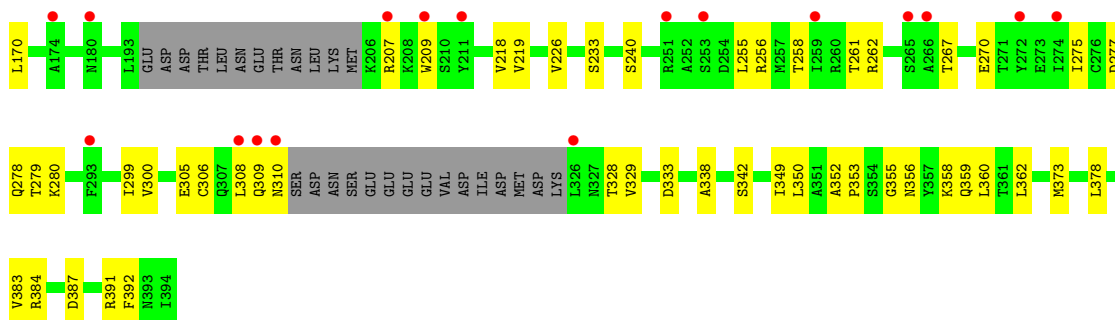


• Molecule 2: Exosome complex component SKI6

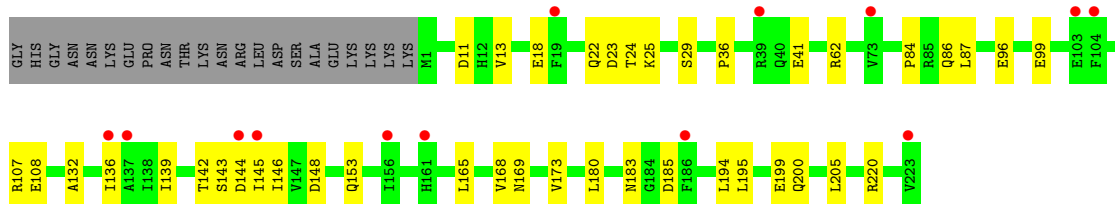
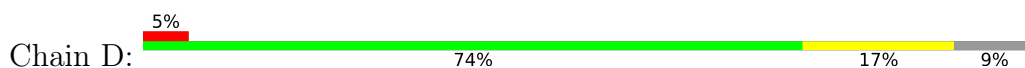


• Molecule 3: Exosome complex component RRP43

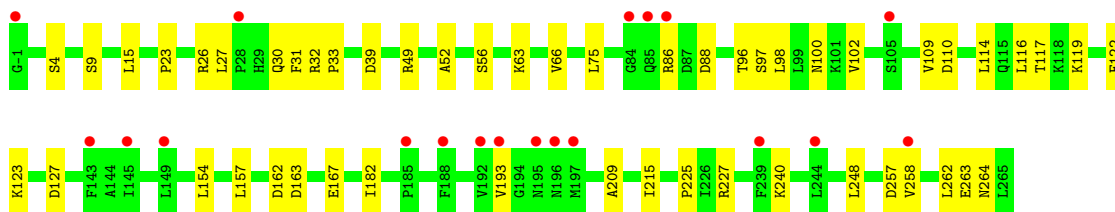
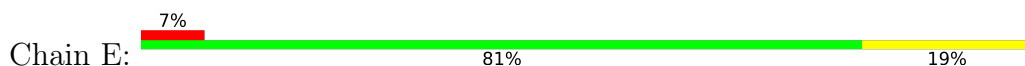




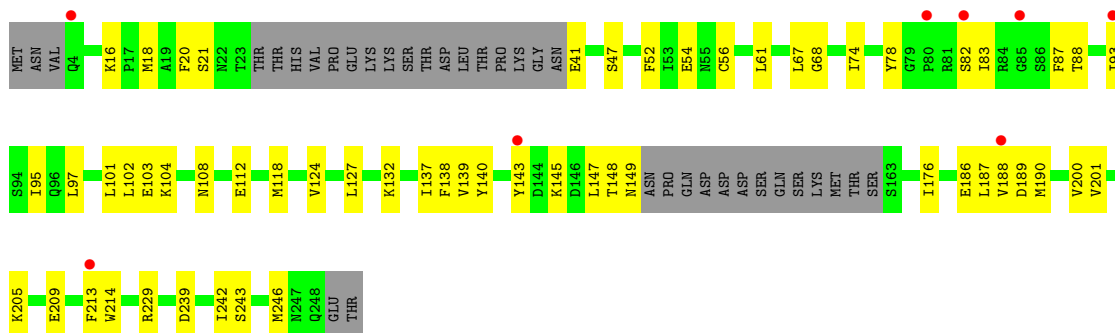
● Molecule 4: Exosome complex component RRP46



● Molecule 5: Exosome complex component RRP42

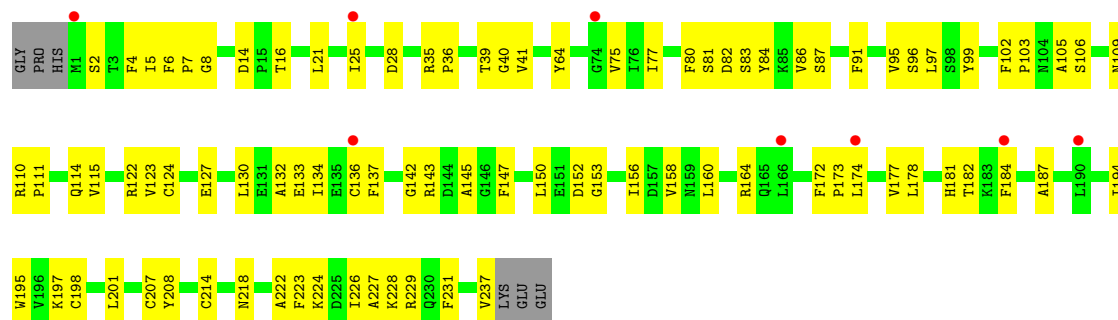


● Molecule 6: Exosome complex component MTR3

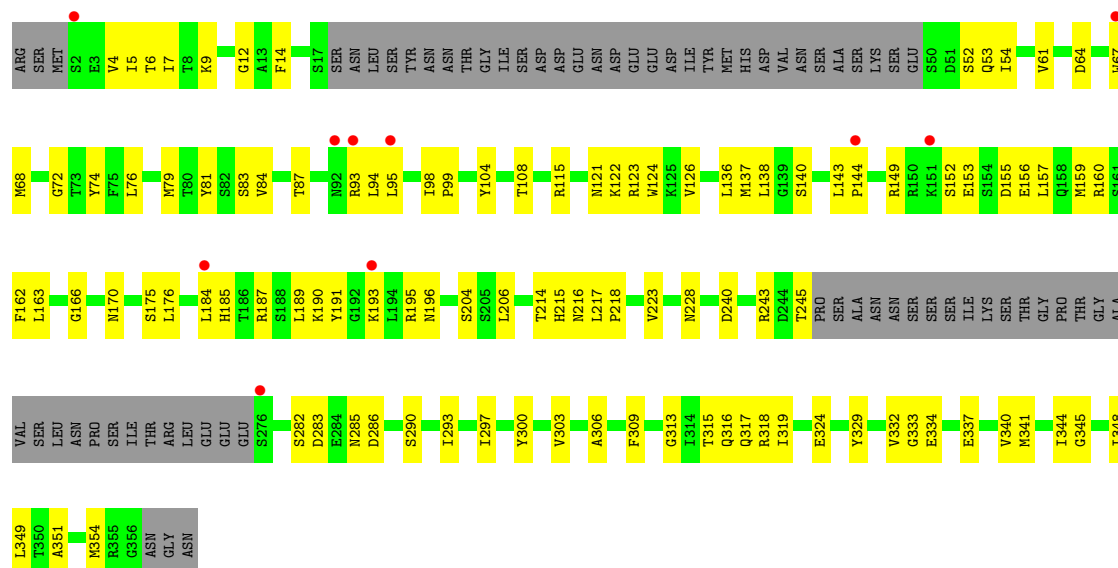


● Molecule 7: Exosome complex component RRP40

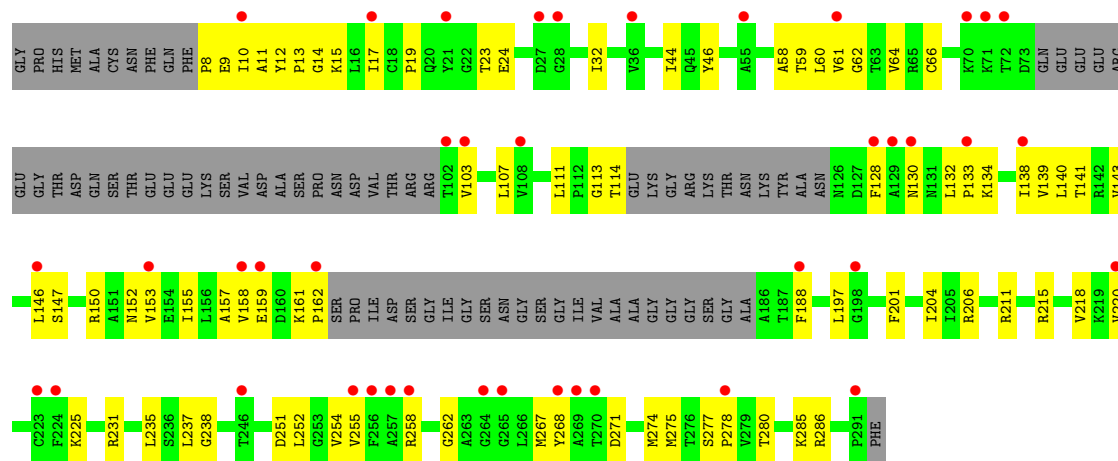




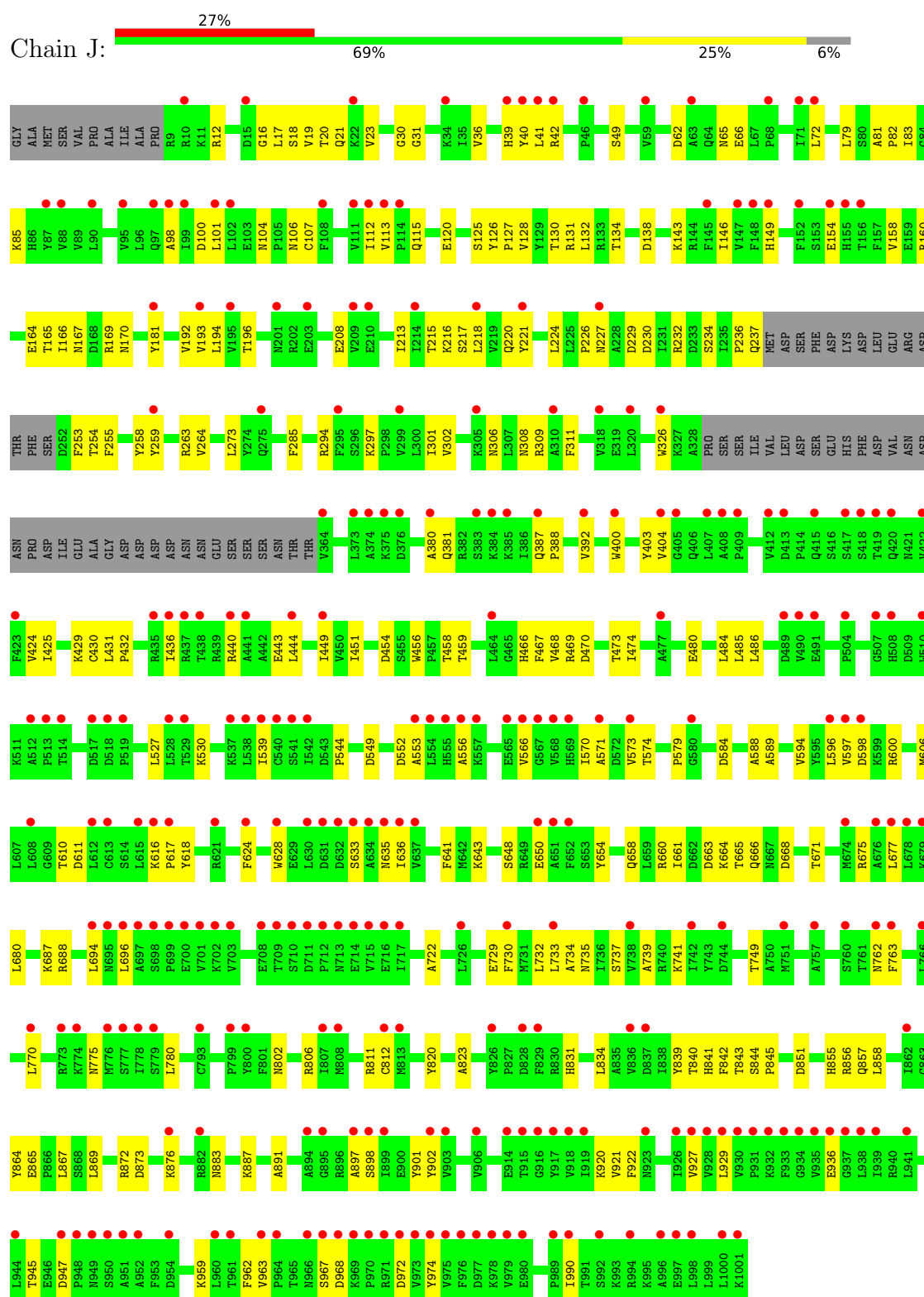
• Molecule 8: Exosome complex component RRP4



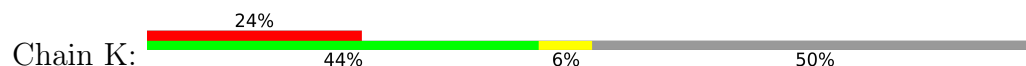
• Molecule 9: Exosome complex component CSL4

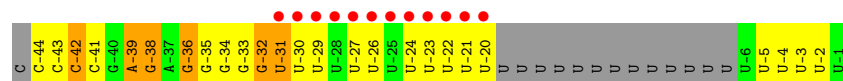


• Molecule 10: Exosome complex exonuclease DIS3



• Molecule 11: Exosome complex exonuclease RRP6





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.15Å 177.39Å 299.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.89 – 3.81 57.89 – 3.81	Depositor EDS
% Data completeness (in resolution range)	81.5 (57.89-3.81) 81.6 (57.89-3.81)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.295 , 0.300 0.295 , 0.300	Depositor DCC
R_{free} test set	2292 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	159.6	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 181.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	27816	wwPDB-VP
Average B, all atoms (Å ²)	270.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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

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	0.25	0/2340	0.37	0/3161
2	B	0.28	0/1910	0.43	0/2579
3	C	0.25	0/2629	0.41	0/3569
4	D	0.23	0/1722	0.40	0/2339
5	E	0.24	0/2093	0.39	1/2849 (0.0%)
6	F	0.24	0/1660	0.40	0/2241
7	G	0.25	0/1828	0.43	0/2486
8	H	0.26	0/2269	0.40	0/3066
9	I	0.22	0/1676	0.43	0/2277
10	J	0.28	0/7575	0.40	1/10290 (0.0%)
11	K	0.30	0/2001	0.56	0/2778
12	R	0.26	0/615	0.70	0/951
All	All	0.26	0/28318	0.43	2/38586 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	947	ASP	CB-CG-OD2	5.20	122.97	118.30
5	E	110	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2304	0	2265	85	0
2	B	1886	0	1904	59	0
3	C	2589	0	2607	135	0
4	D	1701	0	1755	39	3
5	E	2050	0	2063	74	1
6	F	1638	0	1590	108	0
7	G	1792	0	1747	133	1
8	H	2236	0	2215	159	4
9	I	1653	0	1616	142	0
10	J	7427	0	7352	284	0
11	K	1982	0	1255	45	2
12	R	557	0	281	45	1
13	J	1	0	0	0	0
All	All	27816	0	26650	1120	6

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 21.

The worst 5 of 1120 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)
5:E:257:ASP:CB	8:H:4:VAL:HG21	1.35	1.57
10:J:467:PHE:CZ	10:J:469:ARG:O	1.63	1.50
5:E:257:ASP:CB	8:H:4:VAL:CG2	2.08	1.30
10:J:467:PHE:CZ	10:J:469:ARG:C	2.04	1.29
1:A:242:ASN:HB3	10:J:872:ARG:NH2	1.45	1.28

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:200:GLN:NE2	8:H:329:TYR:CE1[1_655]	1.52	0.68
7:G:229:ARG:NH1	12:R:-39:A:N6[4_545]	1.88	0.32
8:H:245:THR:C	11:K:202:GLU:O[1_455]	1.88	0.32
5:E:162:ASP:OD1	11:K:543:ARG:NH2[3_554]	1.97	0.23
4:D:200:GLN:NE2	8:H:329:TYR:CD1[1_655]	1.98	0.22

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 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	297/305 (97%)	290 (98%)	7 (2%)	0	100	100
2	B	242/248 (98%)	237 (98%)	4 (2%)	1 (0%)	34	70
3	C	332/394 (84%)	312 (94%)	19 (6%)	1 (0%)	41	74
4	D	222/245 (91%)	218 (98%)	4 (2%)	0	100	100
5	E	266/267 (100%)	250 (94%)	16 (6%)	0	100	100
6	F	209/250 (84%)	197 (94%)	12 (6%)	0	100	100
7	G	235/243 (97%)	226 (96%)	9 (4%)	0	100	100
8	H	287/361 (80%)	278 (97%)	8 (3%)	1 (0%)	41	74
9	I	214/295 (72%)	208 (97%)	6 (3%)	0	100	100
10	J	939/1003 (94%)	899 (96%)	39 (4%)	1 (0%)	51	83
11	K	344/695 (50%)	330 (96%)	14 (4%)	0	100	100
All	All	3587/4306 (83%)	3445 (96%)	138 (4%)	4 (0%)	51	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	333	GLY
2	B	170	PRO
10	J	598	ASP
3	C	18	PRO

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 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	255/266 (96%)	255 (100%)	0	100	100
2	B	210/219 (96%)	210 (100%)	0	100	100
3	C	282/350 (81%)	281 (100%)	1 (0%)	91	95
4	D	196/216 (91%)	196 (100%)	0	100	100
5	E	238/241 (99%)	238 (100%)	0	100	100
6	F	181/219 (83%)	181 (100%)	0	100	100
7	G	194/211 (92%)	194 (100%)	0	100	100
8	H	243/313 (78%)	243 (100%)	0	100	100
9	I	174/242 (72%)	174 (100%)	0	100	100
10	J	816/901 (91%)	816 (100%)	0	100	100
11	K	81/636 (13%)	81 (100%)	0	100	100
All	All	2870/3814 (75%)	2869 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	160	LEU

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

Mol	Chain	Res	Type
10	J	855	HIS
7	G	218	ASN
6	F	49	HIS
3	C	73	ASN
6	F	206	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	R	29/45 (64%)	15 (51%)	0

5 of 15 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	R	-42	C
12	R	-39	A

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Mol	Chain	Res	Type
12	R	-38	G
12	R	-36	G
12	R	-32	G

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	299/305 (98%)	0.35	22 (7%) 14 11	168, 206, 270, 304	0
2	B	244/248 (98%)	0.58	20 (8%) 11 9	162, 209, 280, 314	0
3	C	339/394 (86%)	0.51	27 (7%) 12 10	205, 234, 301, 333	0
4	D	223/245 (91%)	0.44	13 (5%) 23 18	170, 206, 259, 300	0
5	E	267/267 (100%)	0.47	19 (7%) 16 12	179, 216, 267, 309	0
6	F	215/250 (86%)	0.34	8 (3%) 41 33	189, 221, 266, 308	0
7	G	237/243 (97%)	0.19	8 (3%) 45 37	167, 203, 253, 283	0
8	H	293/361 (81%)	0.21	10 (3%) 45 37	175, 209, 263, 286	0
9	I	222/295 (75%)	0.94	41 (18%) 1 1	205, 244, 291, 345	0
10	J	944/1003 (94%)	1.46	274 (29%) 0 0	238, 377, 429, 458	0
11	K	350/695 (50%)	2.51	170 (48%) 0 0	227, 378, 404, 428	0
12	R	31/45 (68%)	3.37	12 (38%) 0 0	265, 295, 398, 401	0
All	All	3664/4351 (84%)	0.93	624 (17%) 1 1	162, 242, 405, 458	0

The worst 5 of 624 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	270	LEU	16.1
10	J	553	ALA	15.2
12	R	-27	U	14.3
12	R	-26	U	13.5
12	R	-28	U	13.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	ZN	J	1101	1/1	0.73	0.04	298,298,298,298	0

6.5 Other polymers [i](#)

There are no such residues in this entry.