



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:10 AM UTC

PDB ID : 5C0W / pdb_00005c0w
Title : Structure of a 12-subunit nuclear exosome complex bound to single-stranded RNA substrates
Authors : Makino, D.L.; Conti, E.
Deposited on : 2015-06-12
Resolution : 4.60 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

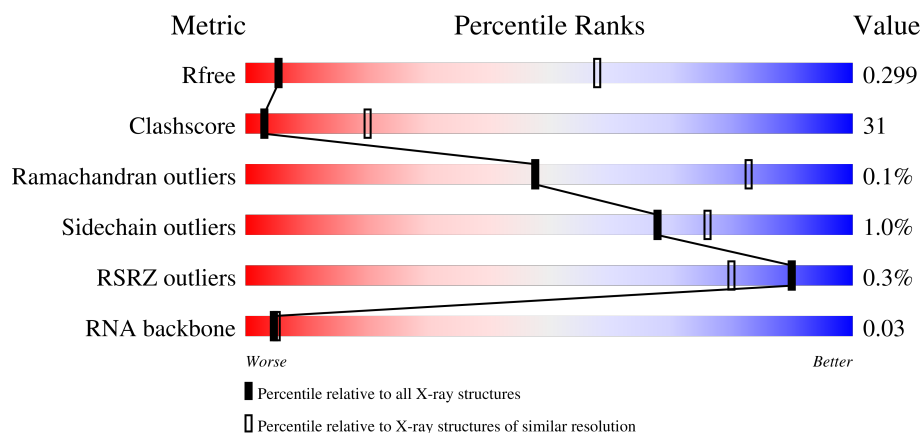
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 Å.

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



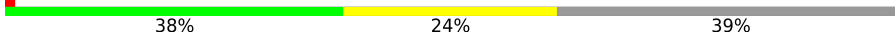
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1007 (5.28-3.92)
Clashscore	190562	1022 (5.26-3.94)
Ramachandran outliers	187476	1069 (5.30-3.90)
Sidechain outliers	187428	1051 (5.30-3.90)
RSRZ outliers	180081	1002 (5.28-3.92)
RNA backbone	3983	1041 (6.00-3.10)

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	 58% 39% ..
2	B	248	 61% 36% ..
3	C	394	 47% 33% 19%
4	D	245	 66% 22% 9%

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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	1004	
11	K	695	
12	L	184	
13	N	18	
13	R	18	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31160 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	298	Total	C	N	O	S	0	0	0
			2286	1434	389	446	17			

- 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
			1884	1176	339	360	9			

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	321	Total	C	N	O	S	0	0	0
			2431	1535	411	475	10			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	222	Total	C	N	O	S	0	0	0
			1689	1062	284	333	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	266	Total	C	N	O	S	0	0	0
			2046	1307	338	396	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	213	Total	C	N	O	S	0	0	0
			1627	1015	277	325	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	236	Total	C	N	O	S	0	0	0
			1813	1158	298	347	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	291	Total	C	N	O	S	0	0	0
			2196	1375	384	425	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	225	Total	C	N	O	S	0	0	0
			1690	1057	300	326	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	970	Total	C	N	O	S	0	1	0
			7645	4830	1334	1447	34			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-2	GLY	-	expression tag	UNP Q08162
J	-1	PRO	-	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	576	Total	C	N	O	S	0	0	0
			4605	2924	784	884	13			

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 protein called Exosome complex protein LRP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	113	Total	C	N	O	S	0	0	0
			894	565	151	174	4			

- Molecule 13 is a RNA chain called RNA synthetic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	12	Total	C	N	O	P	0	0	0
			224	100	40	72	12			
13	N	6	Total	C	N	O	P	0	0	0
			128	58	24	40	6			

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total	Mg	0	0
			1	1		

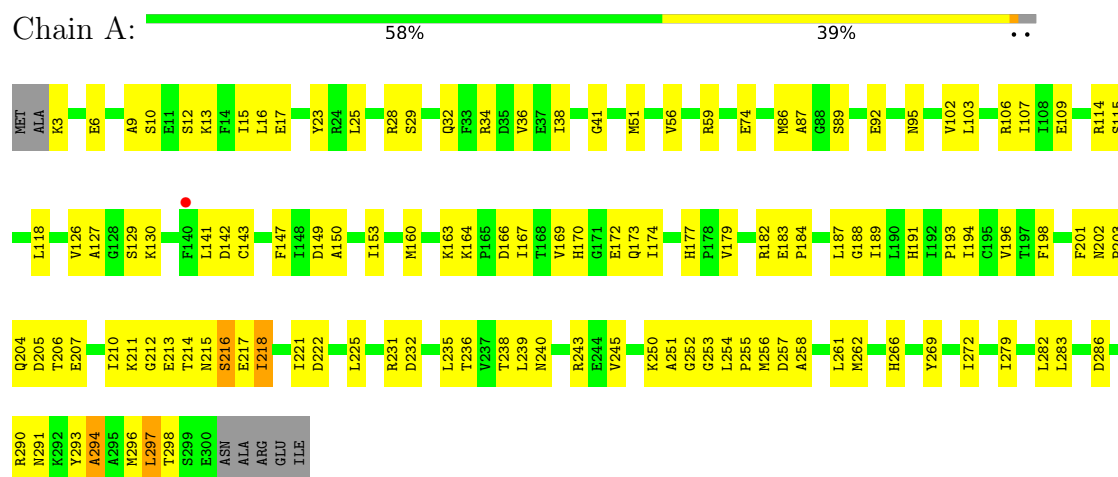
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

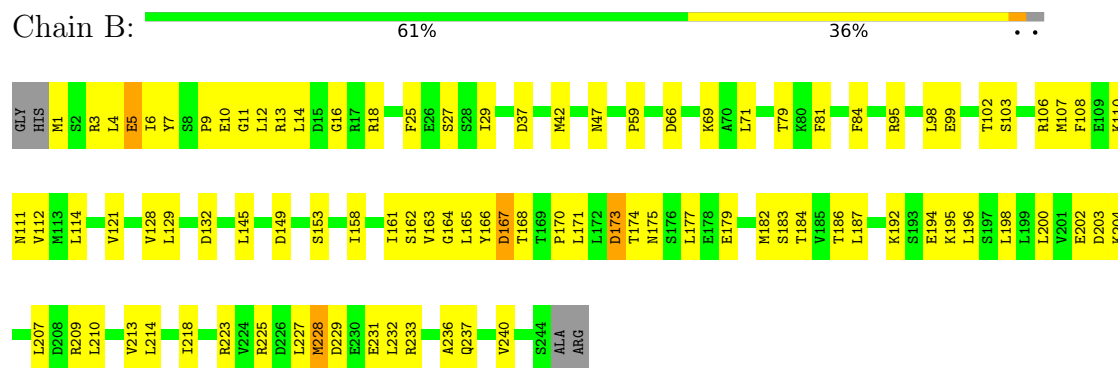
3 Residue-property plots

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.

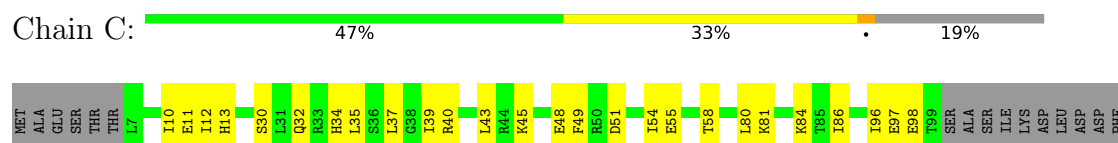
• Molecule 1: Exosome complex component RRP45

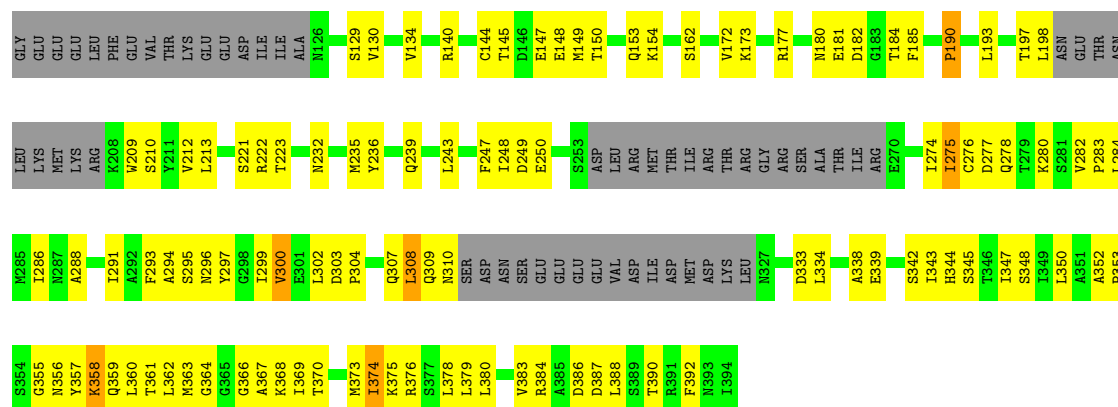


• Molecule 2: Exosome complex component SKI6



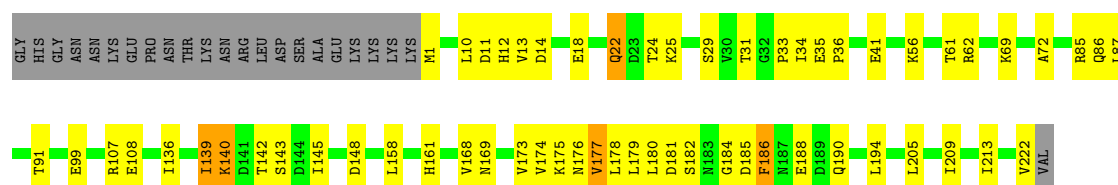
• Molecule 3: Exosome complex component RRP43





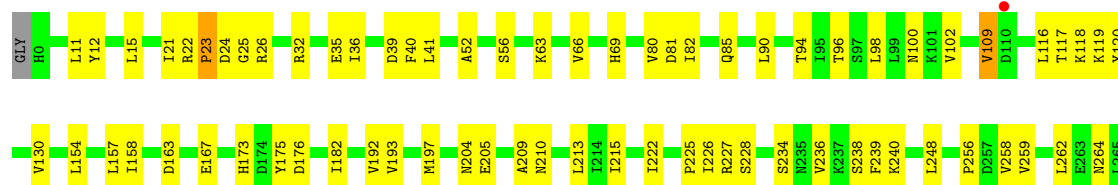
• Molecule 4: Exosome complex component RRP46

Chain D: 66% 22% 9%



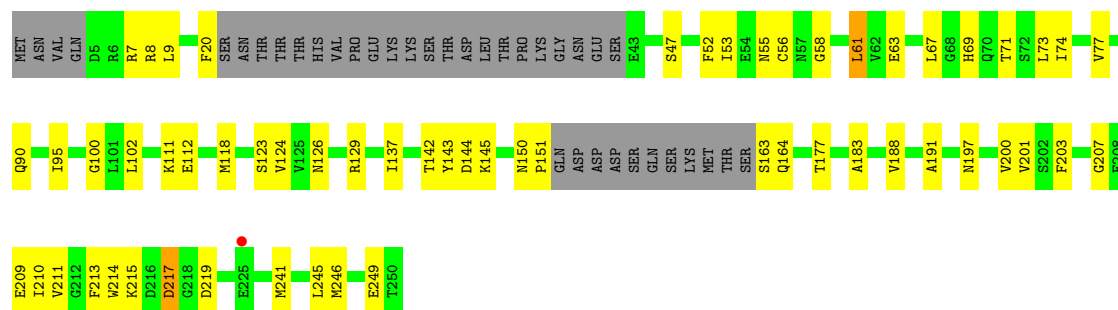
• Molecule 5: Exosome complex component RRP42

Chain E: 73% 26%



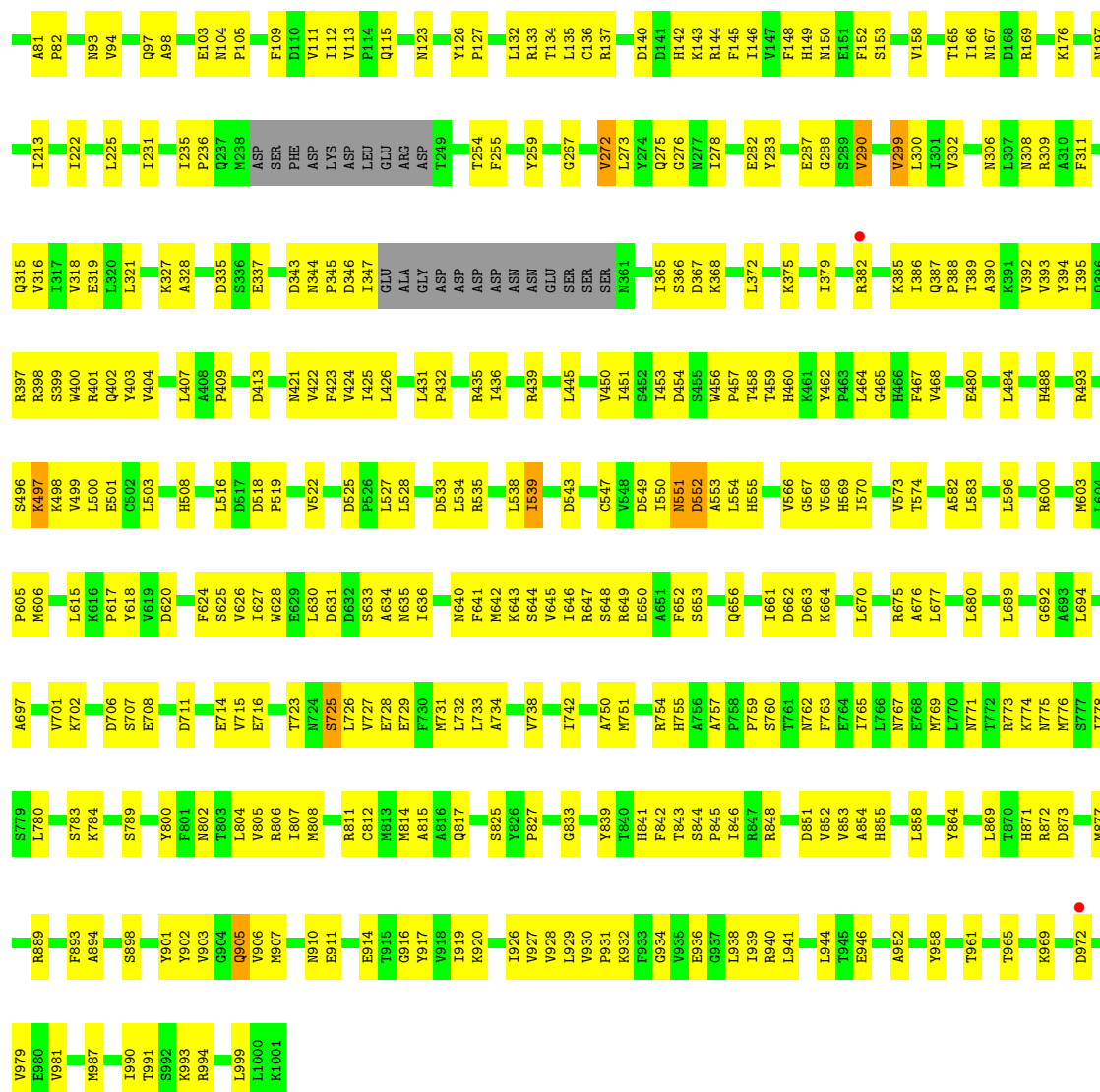
• Molecule 6: Exosome complex component MTR3

Chain F: 62% 23% 15%

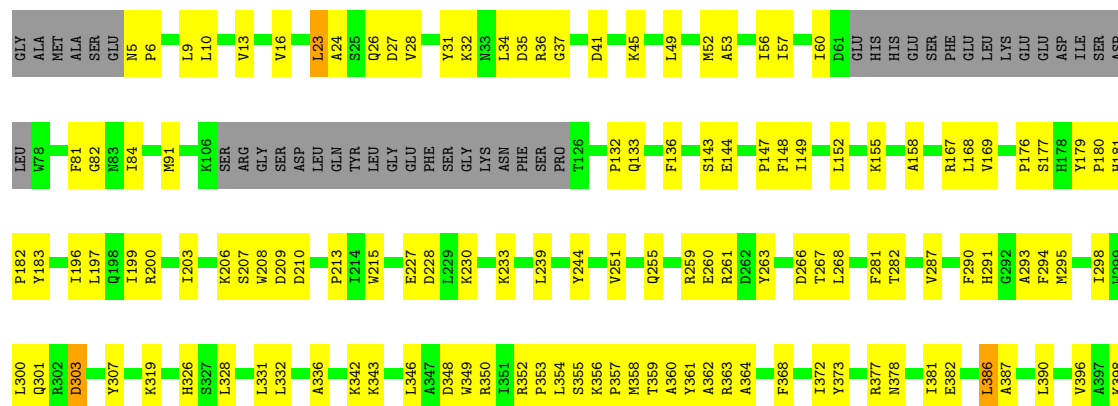


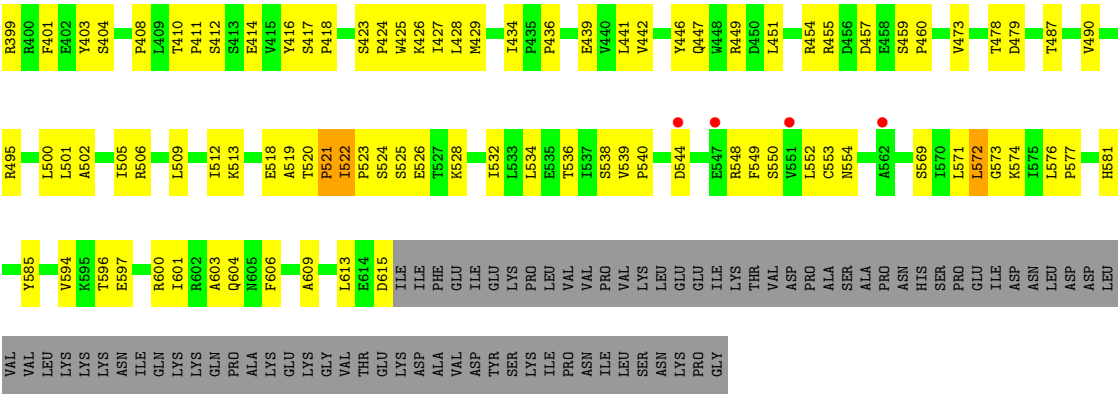
• Molecule 7: Exosome complex component RRP40

Chain G: 56% 40%

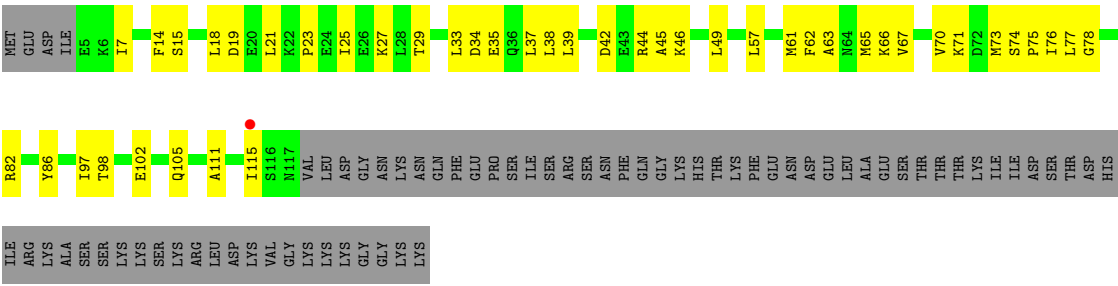


● Molecule 11: Exosome complex exonuclease RRP6

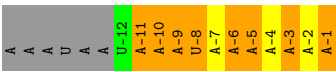
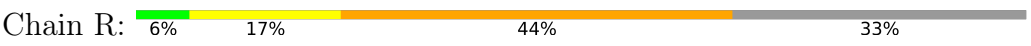




• Molecule 12: Exosome complex protein LRP1



• Molecule 13: RNA synthetic



• Molecule 13: RNA synthetic



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.38Å 195.38Å 463.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.09 – 4.60 59.09 – 4.60	Depositor EDS
% Data completeness (in resolution range)	69.5 (59.09-4.60) 69.5 (59.09-4.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 4.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.271 , 0.284 0.297 , 0.299	Depositor DCC
R_{free} test set	2007 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	262.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 563.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.379 for -h,-k,l	Xtriage
Reported twinning fraction	0.510 for -h,-k,l	Depositor
Outliers	0 of 40199 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	31160	wwPDB-VP
Average B, all atoms (Å ²)	341.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.43	0/2321	0.81	8/3136 (0.3%)
2	B	0.37	0/1907	0.76	1/2571 (0.0%)
3	C	0.34	0/2465	0.76	2/3351 (0.1%)
4	D	0.32	0/1707	0.77	4/2318 (0.2%)
5	E	0.33	0/2086	0.71	2/2838 (0.1%)
6	F	0.31	0/1650	0.70	2/2229 (0.1%)
7	G	0.28	0/1850	0.79	2/2513 (0.1%)
8	H	0.26	0/2229	0.72	1/3018 (0.0%)
9	I	0.36	0/1714	0.73	2/2325 (0.1%)
10	J	0.60	0/7797	0.91	11/10590 (0.1%)
11	K	0.52	0/4702	0.92	14/6392 (0.2%)
12	L	0.46	0/903	0.88	1/1210 (0.1%)
13	N	0.37	0/143	0.70	0/220
13	R	0.48	0/251	0.96	1/388 (0.3%)
All	All	0.45	0/31725	0.83	51/43099 (0.1%)

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	303	ASP	N-CA-C	9.54	121.76	111.36
10	J	272	VAL	N-CA-C	9.34	120.15	110.62
11	K	342	LYS	N-CA-C	9.25	121.44	111.36
13	R	-8	U	P-O3'-C3'	9.06	133.78	120.20
11	K	28	VAL	N-CA-C	8.73	120.46	112.43

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	2286	0	2254	174	0
2	B	1884	0	1923	215	0
3	C	2431	0	2414	224	0
4	D	1689	0	1733	124	0
5	E	2046	0	2069	119	0
6	F	1627	0	1577	61	0
7	G	1813	0	1784	180	0
8	H	2196	0	2158	145	0
9	I	1690	0	1661	93	0
10	J	7645	0	7573	581	1
11	K	4605	0	4538	301	1
12	L	894	0	917	58	0
13	N	128	0	65	6	0
13	R	224	0	113	25	0
14	J	1	0	0	0	0
15	J	1	0	0	0	0
All	All	31160	0	30779	1944	1

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 31.

The worst 5 of 1944 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)
2:B:16:GLY:HA2	10:J:152:PHE:CE1	1.44	1.50
2:B:16:GLY:HA2	10:J:152:PHE:CD1	1.47	1.49
10:J:630:LEU:HD11	10:J:680:LEU:CD2	1.47	1.45
11:K:196:ILE:CG2	11:K:287:VAL:HG21	1.46	1.44
10:J:630:LEU:CD1	10:J:680:LEU:HD21	1.44	1.43

All (1) 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)
10:J:872:ARG:NH2	11:K:82:GLY:O[2_544]	2.14	0.06

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	296/305 (97%)	290 (98%)	6 (2%)	0	100	100
2	B	242/248 (98%)	236 (98%)	5 (2%)	1 (0%)	30	67
3	C	311/394 (79%)	299 (96%)	11 (4%)	1 (0%)	36	71
4	D	220/245 (90%)	214 (97%)	6 (3%)	0	100	100
5	E	264/267 (99%)	248 (94%)	16 (6%)	0	100	100
6	F	207/250 (83%)	201 (97%)	6 (3%)	0	100	100
7	G	234/243 (96%)	230 (98%)	4 (2%)	0	100	100
8	H	285/361 (79%)	278 (98%)	7 (2%)	0	100	100
9	I	217/295 (74%)	206 (95%)	11 (5%)	0	100	100
10	J	965/1004 (96%)	939 (97%)	25 (3%)	1 (0%)	48	83
11	K	570/695 (82%)	549 (96%)	21 (4%)	0	100	100
12	L	111/184 (60%)	111 (100%)	0	0	100	100
All	All	3922/4491 (87%)	3801 (97%)	118 (3%)	3 (0%)	48	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	190	PRO
2	B	173	ASP
10	J	68	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	253/266 (95%)	251 (99%)	2 (1%)	73	77
2	B	210/219 (96%)	208 (99%)	2 (1%)	68	76
3	C	266/350 (76%)	260 (98%)	6 (2%)	44	63
4	D	194/216 (90%)	193 (100%)	1 (0%)	81	81
5	E	238/241 (99%)	235 (99%)	3 (1%)	61	72
6	F	178/219 (81%)	175 (98%)	3 (2%)	53	67
7	G	200/211 (95%)	197 (98%)	3 (2%)	57	70
8	H	237/313 (76%)	237 (100%)	0	100	100
9	I	177/242 (73%)	175 (99%)	2 (1%)	65	74
10	J	845/902 (94%)	837 (99%)	8 (1%)	70	76
11	K	514/636 (81%)	510 (99%)	4 (1%)	73	77
12	L	99/168 (59%)	98 (99%)	1 (1%)	68	76
All	All	3411/3983 (86%)	3376 (99%)	35 (1%)	68	76

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	905	GLN
10	J	969	LYS
11	K	572	LEU
5	E	154	LEU
5	E	109	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	197	ASN
10	J	905	GLN
10	J	306	ASN
10	J	755	HIS

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Mol	Chain	Res	Type
11	K	94	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	N	5/18 (27%)	5 (100%)	0
13	R	11/18 (61%)	9 (81%)	0
All	All	16/36 (44%)	14 (87%)	0

5 of 14 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	-11	A
13	R	-10	A
13	R	-9	A
13	R	-8	U
13	R	-7	A

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 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	298/305 (97%)	-0.62	1 (0%) 90 80	281, 296, 335, 355	0
2	B	244/248 (98%)	-0.72	0 100 100	294, 316, 360, 410	0
3	C	321/394 (81%)	-0.70	0 100 100	291, 331, 352, 375	0
4	D	222/245 (90%)	-0.69	0 100 100	288, 303, 338, 355	0
5	E	266/267 (99%)	-0.68	1 (0%) 88 77	285, 307, 399, 449	0
6	F	213/250 (85%)	-0.46	1 (0%) 87 75	324, 370, 391, 403	0
7	G	236/243 (97%)	-0.41	2 (0%) 82 68	292, 359, 394, 405	0
8	H	291/361 (80%)	-0.59	0 100 100	292, 338, 371, 394	0
9	I	225/295 (76%)	-0.25	1 (0%) 88 77	340, 374, 433, 442	0
10	J	970/1004 (96%)	-0.60	2 (0%) 91 82	203, 334, 407, 450	1 (0%)
11	K	576/695 (82%)	-0.54	4 (0%) 84 70	288, 349, 416, 459	0
12	L	113/184 (61%)	-0.27	1 (0%) 81 66	297, 366, 456, 482	0
13	N	6/18 (33%)	-0.81	0 100 100	338, 376, 392, 414	0
13	R	12/18 (66%)	-0.64	0 100 100	313, 328, 418, 422	0
All	All	3993/4527 (88%)	-0.57	13 (0%) 90 80	203, 338, 408, 482	1 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	551	VAL	4.6
11	K	547	GLU	4.0
11	K	544	ASP	3.4
5	E	110	ASP	3.0
7	G	199	GLU	2.8

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
14	MG	J	1101	1/1	0.99	0.04	320,320,320,320	0
15	ZN	J	1102	1/1	0.99	0.04	353,353,353,353	0

6.5 Other polymers [i](#)

There are no such residues in this entry.