wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 11:00 PM GMT

PDB ID	:	5C0W
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
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:

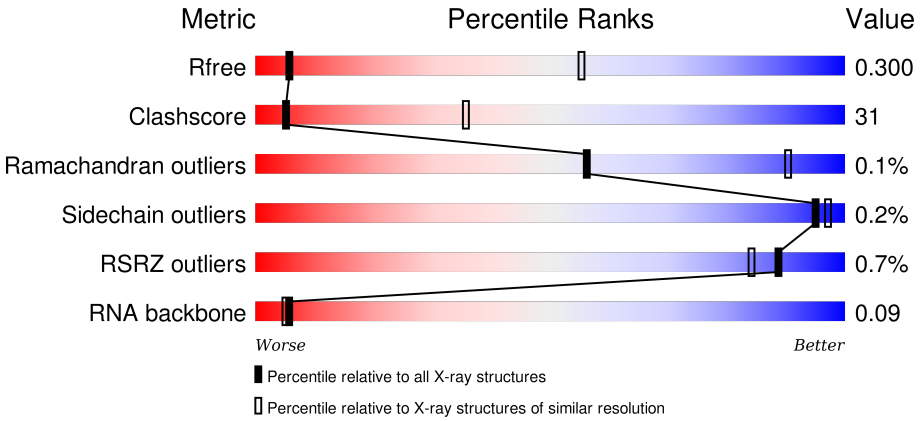
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 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}	91344	1089 (5.52-3.60)
Clashscore	102246	1004 (5.52-3.64)
Ramachandran outliers	100387	1131 (5.52-3.60)
Sidechain outliers	100360	1112 (5.50-3.60)
RSRZ outliers	91569	1092 (5.52-3.60)
RNA backbone	2183	1091 (6.22-2.80)

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	305	60% 38% ·
2	B	248	61% 37% ·
3	C	394	% 48% 32% · 19%
4	D	245	67% 24% 9%

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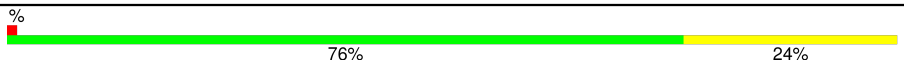
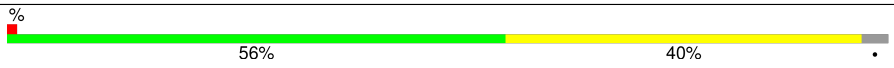
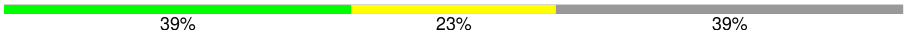
Mol	Chain	Length	Quality of chain
5	E	267	
6	F	250	
7	G	243	
8	H	361	
9	I	295	
10	J	1004	
11	K	695	
12	L	184	
13	N	18	
13	R	18	

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

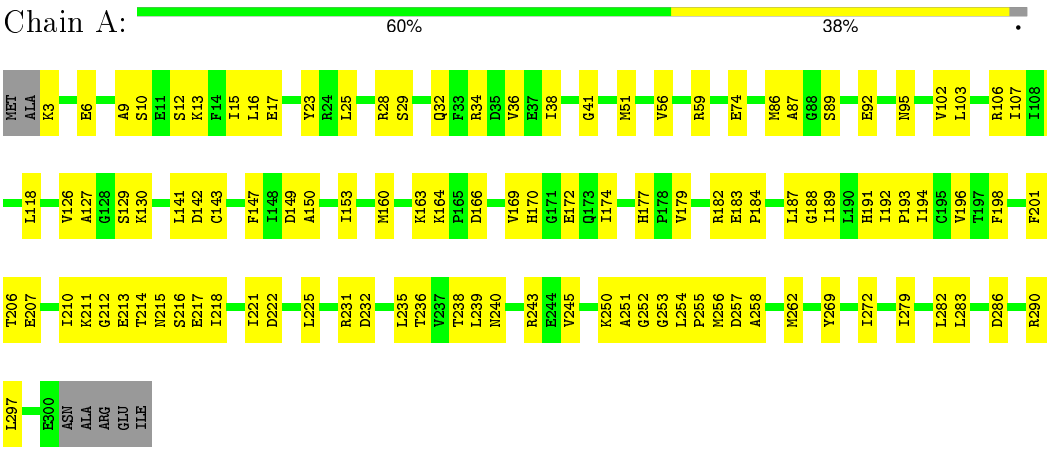
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	J	1	Total Zn 1 1	0	0

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.

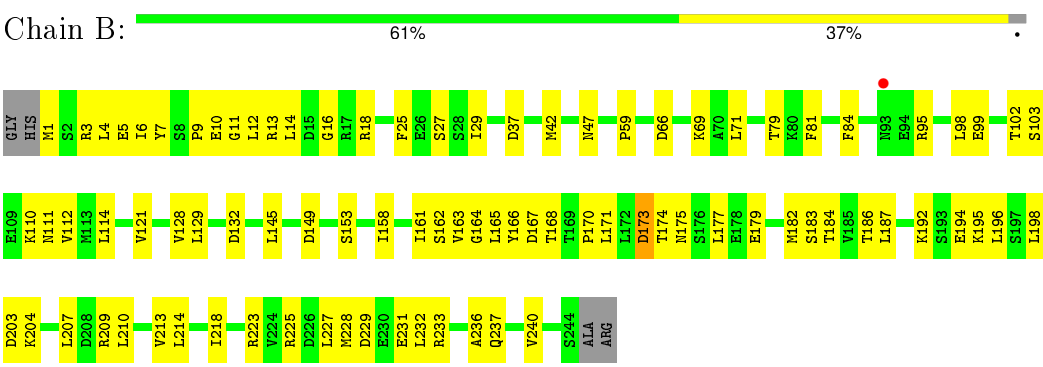
- Molecule 1: Exosome complex component RRP45

Chain A:



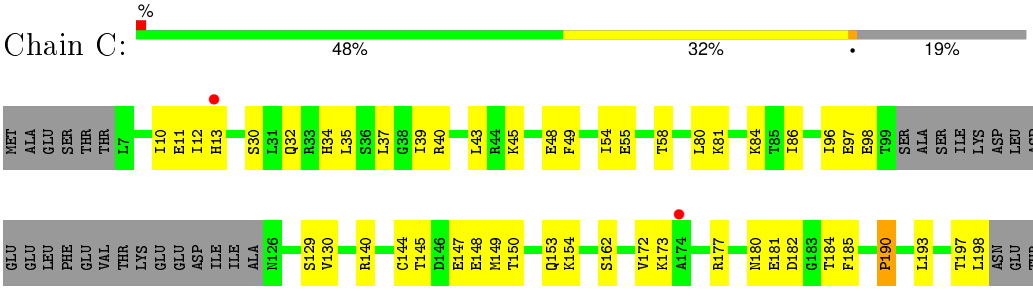
- Molecule 2: Exosome complex component SKI6

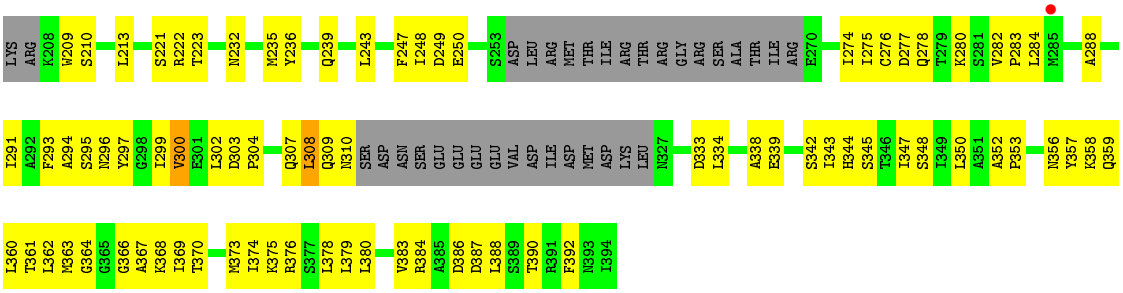
Chain B:



- Molecule 3: Exosome complex component RRP43

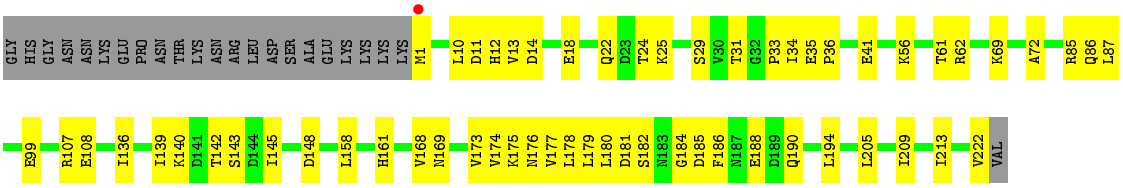
Chain C:





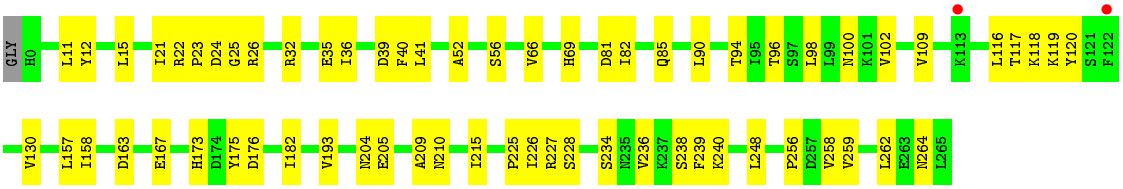
• Molecule 4: Exosome complex component RRP46

Chain D:



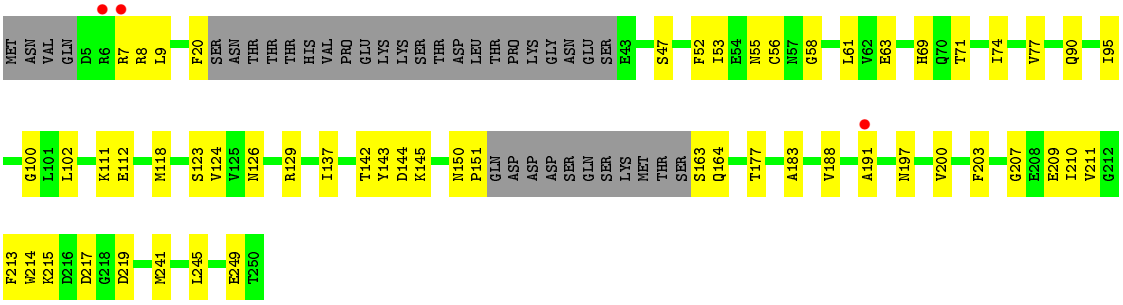
• Molecule 5: Exosome complex component RRP42

Chain E:



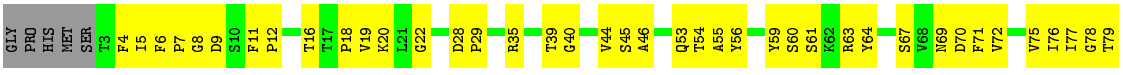
• Molecule 6: Exosome complex component MTR3

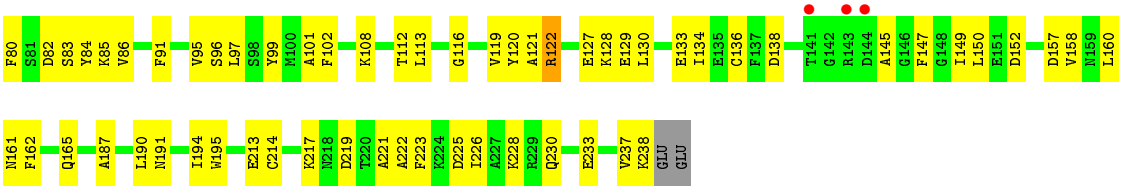
Chain F:



• Molecule 7: Exosome complex component RRP40

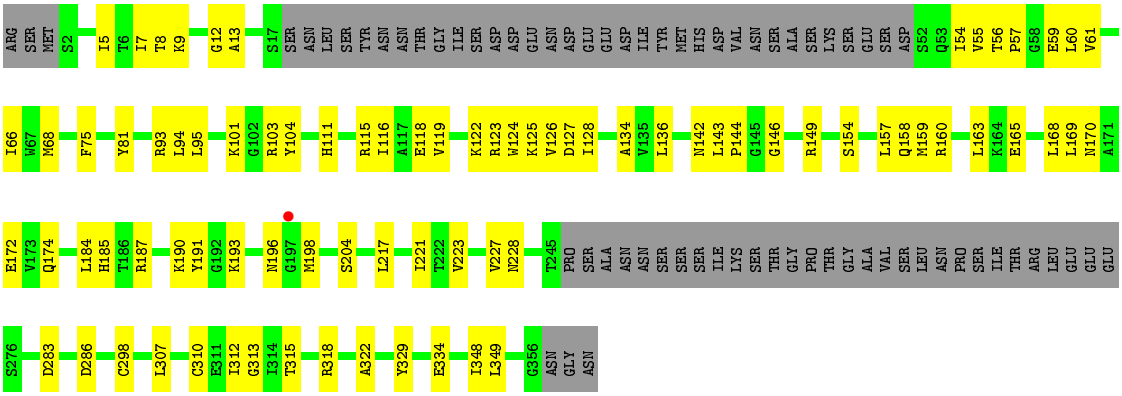
Chain G:





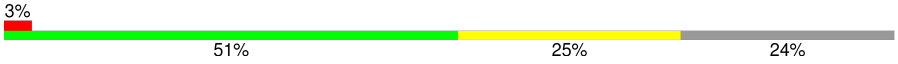
• Molecule 8: Exosome complex component RRP4

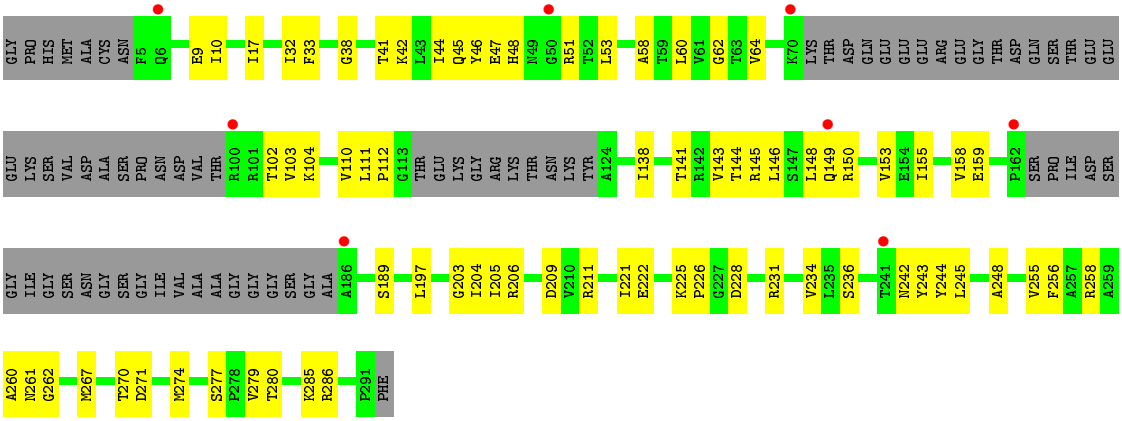
Chain H:



• Molecule 9: Exosome complex component CSL4

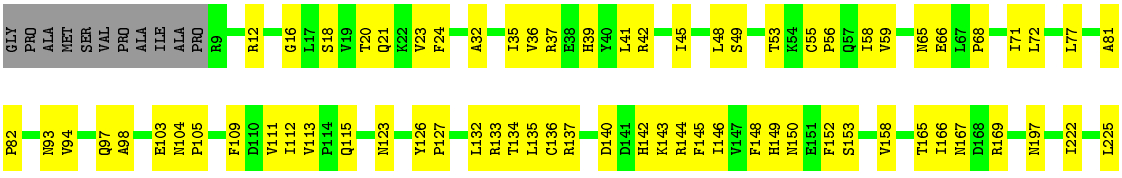
Chain I:

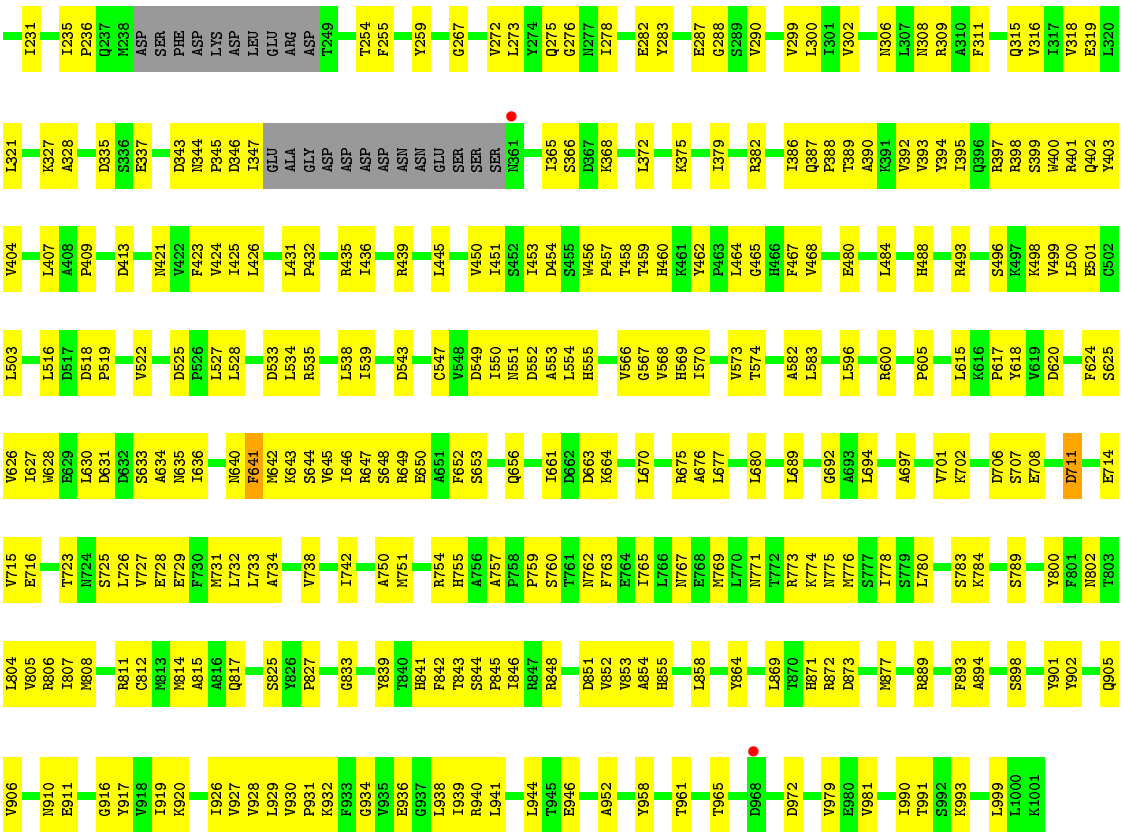




• Molecule 10: Exosome complex exonuclease DIS3

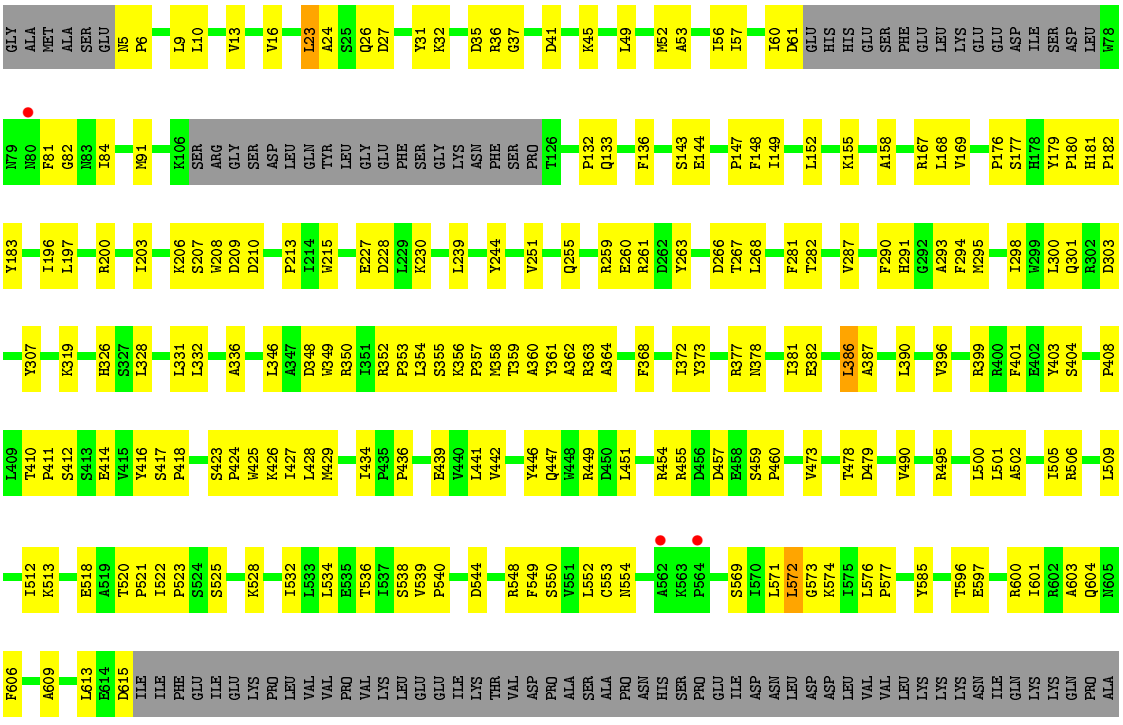
Chain J:





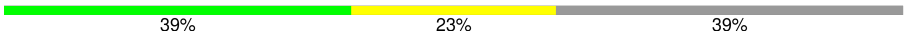
• Molecule 11: Exosome complex exonuclease RRP6

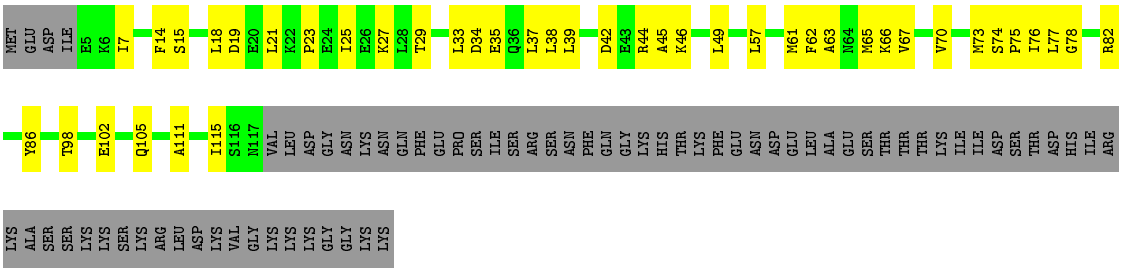
Chain K:



- Molecule 12: Exosome complex protein LRP1

Chain L:





- Molecule 13: RNA synthetic

Chain R:

- Molecule 13: RNA synthetic

Chain N:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.05 (at 4.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.271 , 0.284 0.295 , 0.300	Depositor DCC
R_{free} test set	2007 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	262.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 201.9	EDS
Estimated twinning fraction	0.510 for -h,-k,l 0.379 for -h,-k,l	Xtriage
Reported twinning fraction	0.510 for -h,-k,l	Depositor
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.17$	Xtriage
Outliers	0 of 40199 reflections	Xtriage
F_o,F_c correlation	0.89	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.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.31	0/2321	0.42	0/3136
2	B	0.25	0/1907	0.40	0/2571
3	C	0.26	0/2465	0.41	0/3351
4	D	0.22	0/1707	0.41	0/2318
5	E	0.23	0/2086	0.39	0/2838
6	F	0.23	0/1650	0.38	0/2229
7	G	0.22	0/1850	0.41	0/2513
8	H	0.21	0/2229	0.39	0/3018
9	I	0.24	0/1714	0.40	0/2325
10	J	0.46	0/7797	0.59	1/10590 (0.0%)
11	K	0.39	0/4702	0.53	1/6392 (0.0%)
12	L	0.35	0/903	0.53	0/1210
13	N	0.16	0/143	0.61	0/220
13	R	0.41	0/251	0.99	1/388 (0.3%)
All	All	0.34	0/31725	0.49	3/43099 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	R	-8	U	P-O3'-C3'	11.74	133.78	119.70
11	K	61	ASP	CB-CG-OD2	5.17	122.95	118.30
10	J	711	ASP	CB-CG-OD2	5.15	122.93	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	2286	0	2254	166	0
2	B	1884	0	1923	213	0
3	C	2431	0	2414	222	0
4	D	1689	0	1733	122	0
5	E	2046	0	2069	112	0
6	F	1627	0	1577	56	0
7	G	1813	0	1784	177	0
8	H	2196	0	2158	141	0
9	I	1690	0	1661	89	0
10	J	7645	0	7573	566	1
11	K	4605	0	4538	292	1
12	L	894	0	917	54	0
13	N	128	0	65	6	0
13	R	224	0	113	24	0
14	J	1	0	0	0	0
15	J	1	0	0	0	0
All	All	31160	0	30779	1893	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 1893 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%)	39	80
3	C	311/394 (79%)	299 (96%)	11 (4%)	1 (0%)	46	83
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%)	56	90
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%)	56	90

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 (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	253/266 (95%)	253 (100%)	0	100 100
2	B	210/219 (96%)	210 (100%)	0	100 100
3	C	266/350 (76%)	264 (99%)	2 (1%)	86 93
4	D	194/216 (90%)	194 (100%)	0	100 100
5	E	238/241 (99%)	238 (100%)	0	100 100
6	F	178/219 (81%)	178 (100%)	0	100 100
7	G	200/211 (95%)	198 (99%)	2 (1%)	82 92
8	H	237/313 (76%)	237 (100%)	0	100 100
9	I	177/242 (73%)	177 (100%)	0	100 100
10	J	845/902 (94%)	844 (100%)	1 (0%)	95 97
11	K	514/636 (81%)	511 (99%)	3 (1%)	90 95
12	L	99/168 (59%)	99 (100%)	0	100 100
All	All	3411/3983 (86%)	3403 (100%)	8 (0%)	95 97

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	122	ARG
11	K	572	LEU
11	K	23	LEU
7	G	19	VAL
10	J	641	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	158	GLN
10	J	97	GLN
11	K	516	ASN
8	H	185	HIS

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Mol	Chain	Res	Type
9	I	125	ASN

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 carbohydrates 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, 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	298/305 (97%)	-0.56	0 100 100	281, 296, 335, 355	0
2	B	244/248 (98%)	-0.56	1 (0%) 93 90	294, 316, 360, 410	0
3	C	321/394 (81%)	-0.37	3 (0%) 85 80	291, 331, 352, 375	0
4	D	222/245 (90%)	-0.57	1 (0%) 91 88	288, 303, 338, 355	0
5	E	266/267 (99%)	-0.52	2 (0%) 87 82	285, 307, 399, 449	0
6	F	213/250 (85%)	-0.33	3 (1%) 78 70	324, 370, 391, 403	0
7	G	236/243 (97%)	-0.46	3 (1%) 79 71	292, 359, 394, 405	0
8	H	291/361 (80%)	-0.37	1 (0%) 94 92	292, 338, 371, 394	0
9	I	225/295 (76%)	-0.14	8 (3%) 46 38	340, 374, 433, 442	0
10	J	970/1004 (96%)	-0.50	2 (0%) 95 94	279, 334, 407, 450	0
11	K	576/695 (82%)	-0.44	3 (0%) 91 88	288, 349, 416, 459	0
12	L	113/184 (61%)	-0.45	0 100 100	297, 366, 456, 482	0
13	N	6/18 (33%)	0.45	0 100 100	338, 376, 392, 414	0
13	R	12/18 (66%)	0.09	0 100 100	313, 328, 418, 422	0
All	All	3993/4527 (88%)	-0.45	27 (0%) 89 84	279, 338, 408, 482	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	285	MET	4.6
9	I	186	ALA	4.4
9	I	162	PRO	4.2
4	D	1	MET	4.2
9	I	50	GLY	4.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
14	MG	J	1101	1/1	0.90	0.13	-1.24	320,320,320,320	0
15	ZN	J	1102	1/1	0.96	0.09	-	353,353,353,353	0

6.5 Other polymers (i)

There are no such residues in this entry.