



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 30, 2017 – 10:54 PM EDT

PDB ID : 5VZJ  
Title : STRUCTURE OF A TWELVE COMPONENT MPP6-NUCLEAR RNA EXOSOME COMPLEX BOUND TO RNA  
Authors : Lima, C.D.; Wasmuth, E.V.  
Deposited on : unknown  
Resolution : 3.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029824

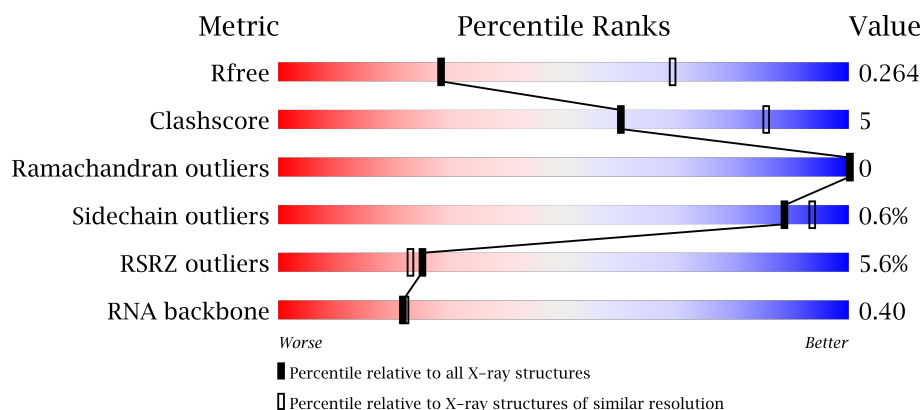
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)
RNA backbone	2435	1111 (3.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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>3%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
2	B	250	<div> <div>0%</div> <div>81%</div> <div>15%</div> <div>.</div> </div>
3	C	394	<div> <div>8%</div> <div>66%</div> <div>10%</div> <div>24%</div> </div>
4	D	225	<div> <div>3%</div> <div>77%</div> <div>21%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	269	
6	F	250	
7	G	244	
8	H	363	
9	I	296	
10	J	559	
11	K	1003	
12	L	42	
13	M	11	
14	N	19	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	SO4	G	302	-	-	-	X
16	GOL	A	402	-	-	-	X
16	GOL	K	2003	-	-	-	X

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 29498 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	302	Total	C	N	O	S	0	0	0
			2350	1473	401	459	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1896	1186	338	363	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P46948
B	-2	PRO	-	expression tag	UNP P46948
B	-1	ASP	-	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	299	Total	C	N	O	S	0	0	0
			2325	1482	397	436	10			

- 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
			1698	1068	288	333	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP P53256
D	0	SER	-	expression tag	UNP P53256

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	257	Total	C	N	O	S	0	0	0
			1979	1262	328	385	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP Q12277
E	-2	ASP	-	expression tag	UNP Q12277
E	-1	PRO	-	expression tag	UNP Q12277
E	0	HIS	-	expression tag	UNP Q12277

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	207	Total	C	N	O	S	0	0	0
			1589	998	265	316	10			

- 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
			1831	1169	302	349	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	expression tag	UNP Q08285
G	-2	ASP	-	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
			2249	1411	401	425	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-3	GLY	-	expression tag	UNP P38792
H	-2	ASP	-	expression tag	UNP P38792
H	-1	PRO	-	expression tag	UNP P38792
H	0	HIS	-	expression tag	UNP P38792

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	207	Total	C	N	O	S	0	0	0
			1579	986	285	301	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-3	GLY	-	expression tag	UNP P53859
I	-2	ASP	-	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 RRP6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	460	Total	C	N	O	S	0	0	0
			3784	2412	653	709	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	126	SER	-	expression tag	UNP Q12149
J	127	LEU	-	expression tag	UNP Q12149
J	128	MET	-	expression tag	UNP Q12149
J	238	ASN	ASP	engineered mutation	UNP Q12149

- Molecule 11 is a protein called Exosome complex exonuclease DIS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	956	Total	C	N	O	S	0	0	0
			7645	4834	1345	1430	36			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	SER	-	expression tag	UNP Q08162
K	0	LEU	-	expression tag	UNP Q08162
K	171	ASN	ASP	engineered mutation	UNP Q08162
K	551	ASN	ASP	engineered mutation	UNP Q08162

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	29	Total	C	N	O	0	0	0
			222	139	40	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	79	GLY	-	expression tag	UNP P53725
L	80	SER	-	expression tag	UNP P53725

- Molecule 13 is a RNA chain called RNA (11-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	5	Total	C	N	O	P	0	0	0
			101	45	21	30	5			

- Molecule 14 is a RNA chain called RNA (19-MER).

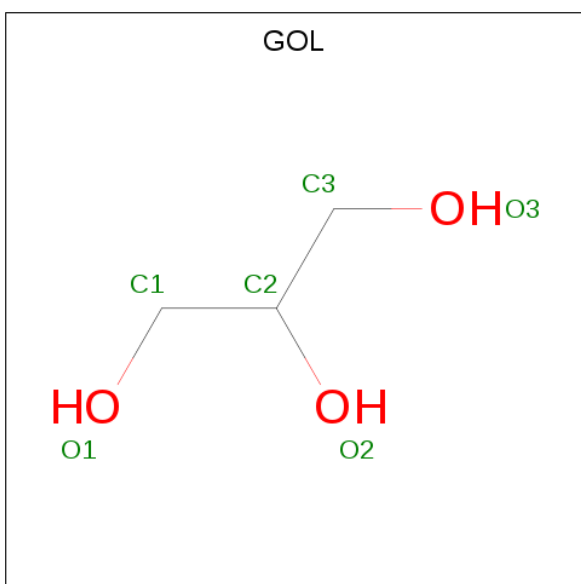
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	7	Total	C	N	O	P	0	0	0
			148	67	26	48	7			

- Molecule 15 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	O	S	0	0
			5	4	1		
15	B	1	Total	O	S	0	0
			5	4	1		
15	G	1	Total	O	S	0	0
			5	4	1		
15	G	1	Total	O	S	0	0
			5	4	1		
15	K	1	Total	O	S	0	0
			5	4	1		

- Molecule 16 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	C	O	0	0
			6	3	3		
16	K	1	Total	C	O	0	0
			6	3	3		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	K	1	Total	Zn	0	0
			1	1		

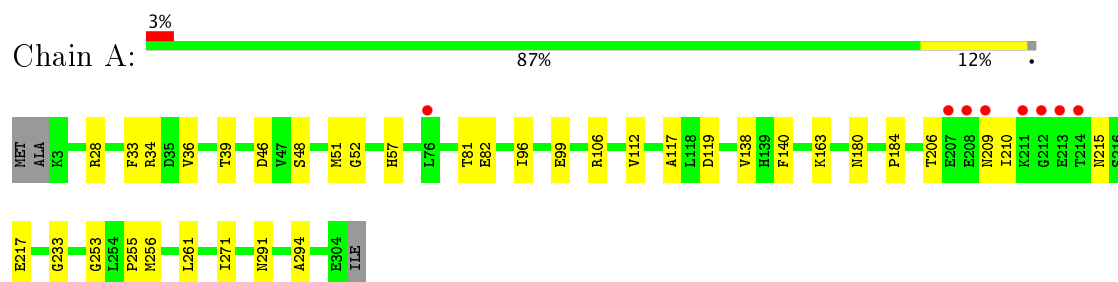
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	16	Total	O	0	0
			16	16		
18	B	17	Total	O	0	0
			17	17		
18	D	5	Total	O	0	0
			5	5		
18	E	1	Total	O	0	0
			1	1		
18	G	2	Total	O	0	0
			2	2		
18	H	3	Total	O	0	0
			3	3		
18	J	2	Total	O	0	0
			2	2		
18	K	18	Total	O	0	0
			18	18		

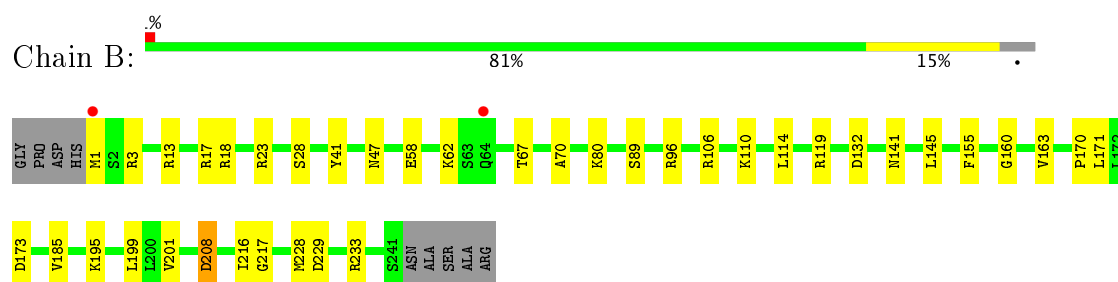
### 3 Residue-property plots [i](#)

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

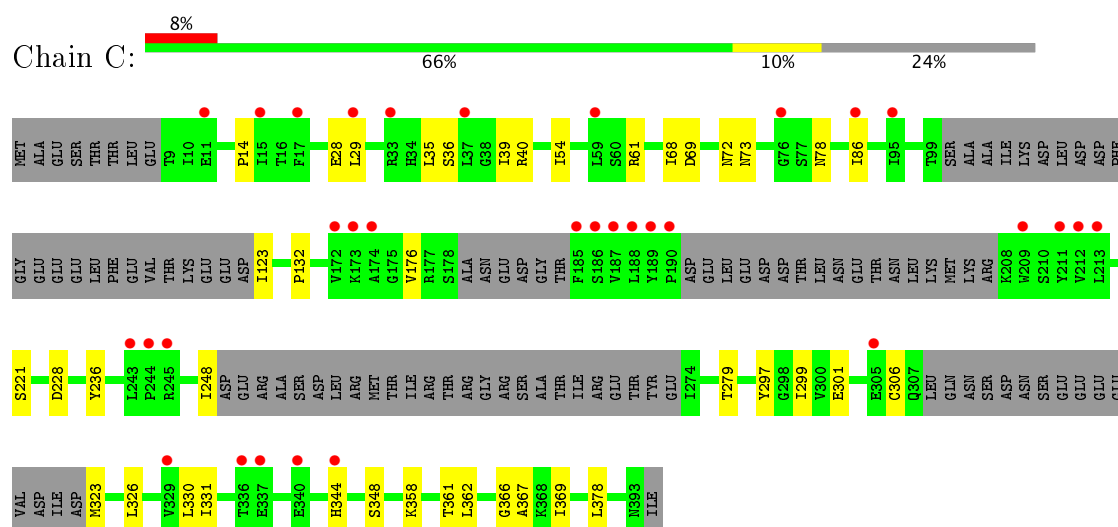
- Molecule 1: Exosome complex component RRP45



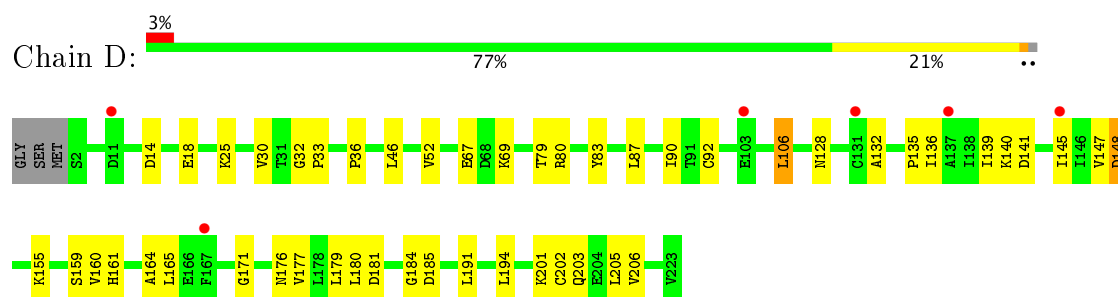
- Molecule 2: Exosome complex component SKI6



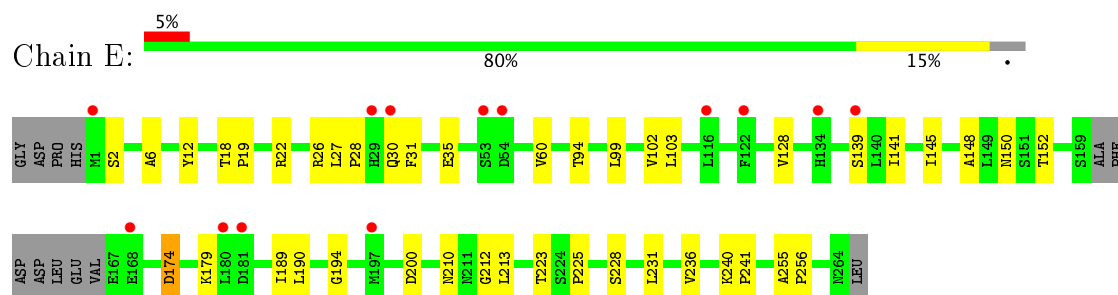
- Molecule 3: Exosome complex component RRP43



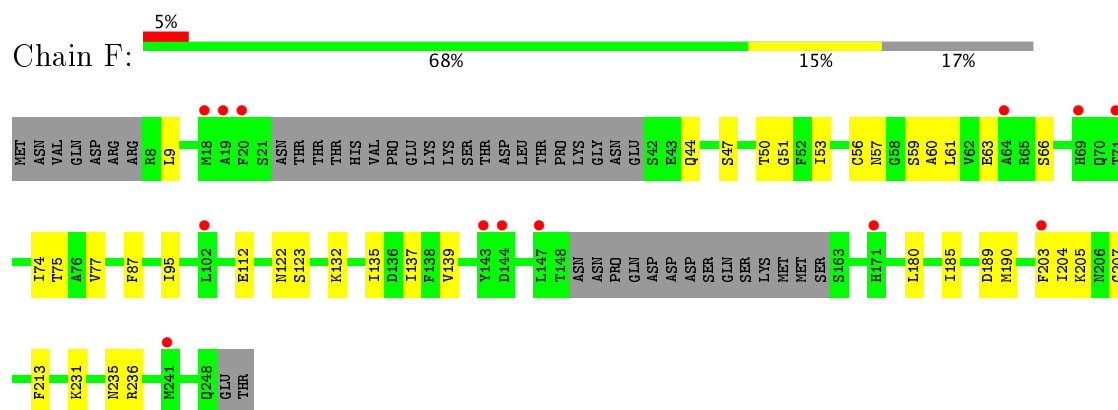
- Molecule 4: Exosome complex component RRP46



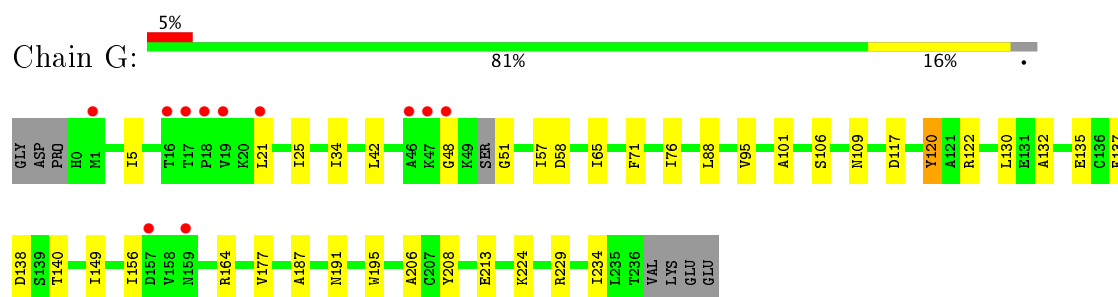
• Molecule 5: Exosome complex component RRP42



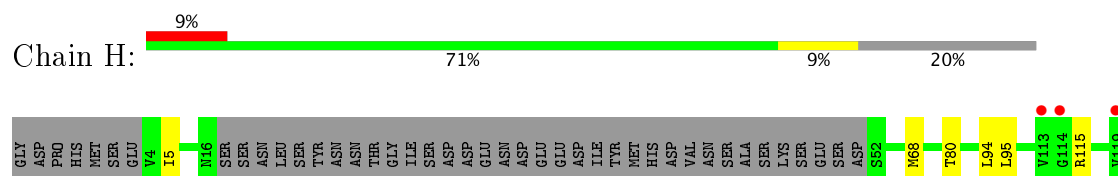
• Molecule 6: Exosome complex component MTR3

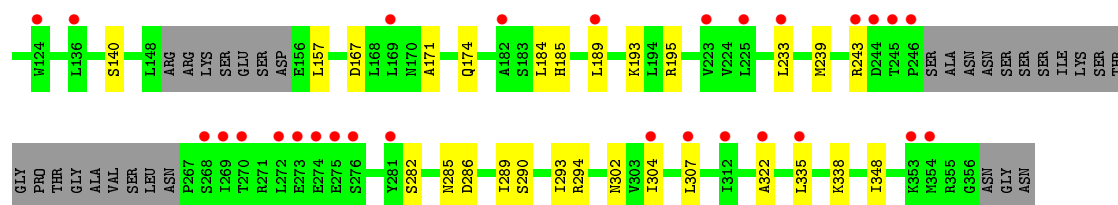


• Molecule 7: Exosome complex component RRP40

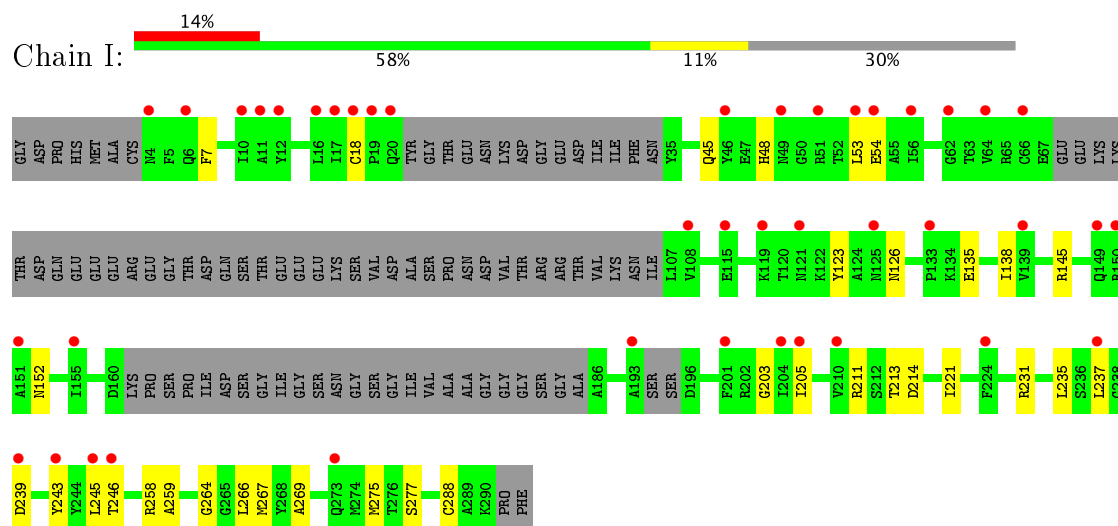


• Molecule 8: Exosome complex component RRP4

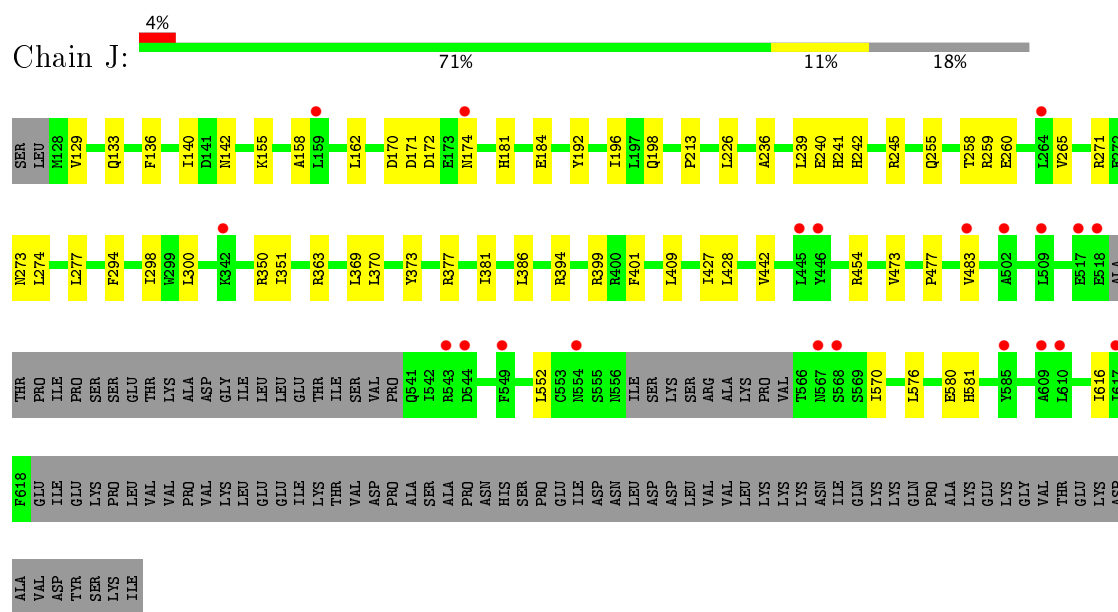




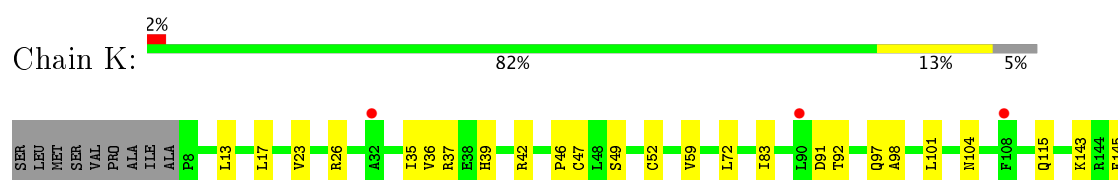
• Molecule 9: Exosome complex component CSL4

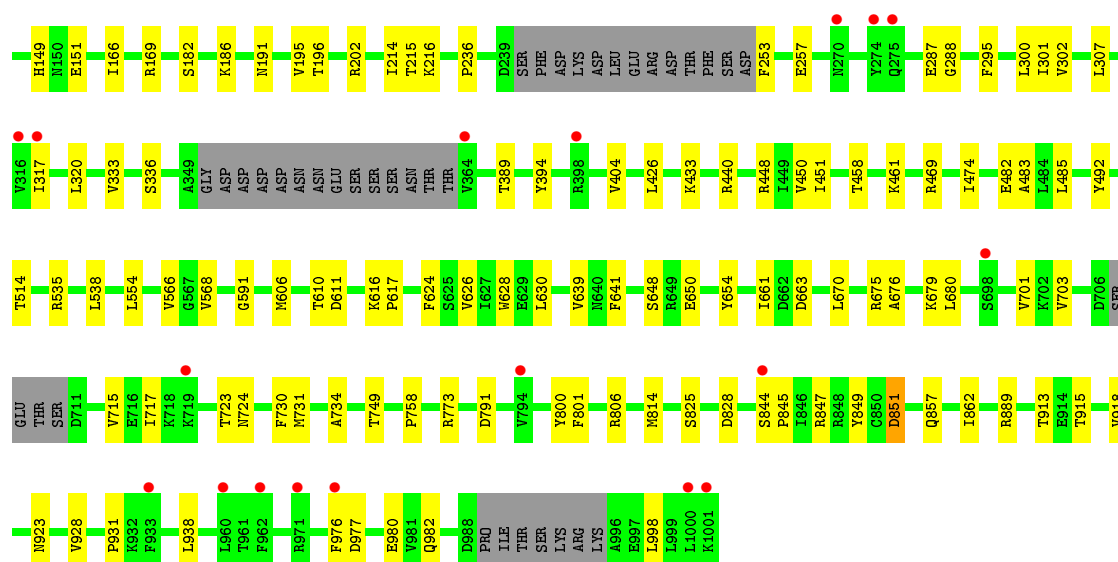


• Molecule 10: Exosome complex exonuclease RRP6

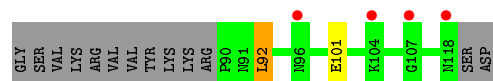


• Molecule 11: Exosome complex exonuclease DIS3

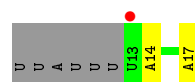
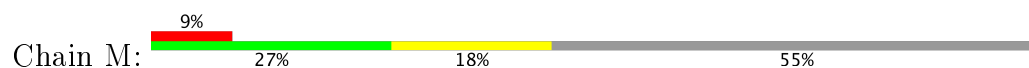




- Molecule 12: M-phase phosphoprotein 6 homolog



- Molecule 13: RNA (11-MER)



- Molecule 14: RNA (19-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.09Å 213.59Å 225.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.25 – 3.30 44.25 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (44.25-3.30) 97.4 (44.25-3.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.10 _2155	Depositor
R, $R_{free}$	0.217 , 0.266 0.215 , 0.264	Depositor DCC
$R_{free}$ test set	4990 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	100.2	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	29498	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, ZN, SO4

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	0.23	0/2386	0.39	0/3219
2	B	0.23	0/1920	0.40	0/2584
3	C	0.23	0/2359	0.41	0/3193
4	D	0.23	0/1716	0.42	0/2329
5	E	0.24	0/2016	0.41	0/2740
6	F	0.24	0/1611	0.43	0/2173
7	G	0.24	0/1868	0.41	0/2531
8	H	0.23	0/2284	0.42	0/3086
9	I	0.24	0/1599	0.43	0/2160
10	J	0.23	0/3869	0.38	0/5248
11	K	0.23	0/7794	0.39	0/10559
12	L	0.25	0/225	0.48	0/301
13	M	0.14	0/113	0.64	0/174
14	N	0.11	0/165	0.63	0/254
All	All	0.23	0/29925	0.41	0/40551

There are no bond length outliers.

There are no bond angle outliers.

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	2350	0	2335	22	0
2	B	1896	0	1954	29	0
3	C	2325	0	2408	27	0
4	D	1698	0	1754	31	0
5	E	1979	0	2010	27	0
6	F	1589	0	1571	27	0
7	G	1831	0	1819	24	0
8	H	2249	0	2263	21	0
9	I	1579	0	1584	22	0
10	J	3784	0	3776	36	0
11	K	7645	0	7684	79	0
12	L	222	0	225	3	0
13	M	101	0	52	1	0
14	N	148	0	75	2	0
15	A	5	0	0	0	0
15	B	5	0	0	0	0
15	G	10	0	0	0	0
15	K	5	0	0	0	0
16	A	6	0	8	0	0
16	K	6	0	8	1	0
17	K	1	0	0	0	0
18	A	16	0	0	0	0
18	B	17	0	0	1	0
18	D	5	0	0	0	0
18	E	1	0	0	0	0
18	G	2	0	0	0	0
18	H	3	0	0	0	0
18	J	2	0	0	0	0
18	K	18	0	0	1	0
All	All	29498	0	29526	313	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 5.

The worst 5 of 313 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:145:ILE:HG12	4:D:194:LEU:HB3	1.67	0.76
9:I:203:GLY:HA2	9:I:243:TYR:H	1.49	0.76
10:J:140:ILE:HD11	10:J:271:ARG:HH12	1.54	0.73
3:C:362:LEU:HB3	4:D:180:LEU:HB3	1.71	0.72
11:K:91:ASP:HB2	11:K:196:THR:HG22	1.70	0.71



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	300/305 (98%)	284 (95%)	16 (5%)	0	100	100
2	B	239/250 (96%)	226 (95%)	13 (5%)	0	100	100
3	C	287/394 (73%)	266 (93%)	21 (7%)	0	100	100
4	D	220/225 (98%)	207 (94%)	13 (6%)	0	100	100
5	E	253/269 (94%)	238 (94%)	15 (6%)	0	100	100
6	F	201/250 (80%)	185 (92%)	16 (8%)	0	100	100
7	G	232/244 (95%)	222 (96%)	10 (4%)	0	100	100
8	H	283/363 (78%)	264 (93%)	19 (7%)	0	100	100
9	I	197/296 (67%)	172 (87%)	25 (13%)	0	100	100
10	J	454/559 (81%)	424 (93%)	30 (7%)	0	100	100
11	K	946/1003 (94%)	891 (94%)	55 (6%)	0	100	100
12	L	27/42 (64%)	24 (89%)	3 (11%)	0	100	100
All	All	3639/4200 (87%)	3403 (94%)	236 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	263/266 (99%)	261 (99%)	2 (1%)	85	91
2	B	215/221 (97%)	214 (100%)	1 (0%)	91	94
3	C	263/349 (75%)	262 (100%)	1 (0%)	93	96
4	D	196/198 (99%)	193 (98%)	3 (2%)	70	85
5	E	232/243 (96%)	230 (99%)	2 (1%)	82	90
6	F	177/219 (81%)	177 (100%)	0	100	100
7	G	204/212 (96%)	203 (100%)	1 (0%)	91	94
8	H	248/314 (79%)	248 (100%)	0	100	100
9	I	168/243 (69%)	167 (99%)	1 (1%)	89	93
10	J	425/516 (82%)	422 (99%)	3 (1%)	87	92
11	K	857/903 (95%)	853 (100%)	4 (0%)	91	94
12	L	25/37 (68%)	24 (96%)	1 (4%)	36	70
All	All	3273/3721 (88%)	3254 (99%)	19 (1%)	89	93

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	174	ASP
9	I	53	LEU
11	K	624	PHE
5	E	12	TYR
11	K	851	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	M	4/11 (36%)	1 (25%)	0
14	N	6/19 (31%)	1 (16%)	0
All	All	10/30 (33%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	M	14	A

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Mol	Chain	Res	Type
14	N	12	U

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
15	SO4	A	401	-	4,4,4	0.14	0	6,6,6	0.07	0
16	GOL	A	402	-	5,5,5	0.34	0	5,5,5	0.26	0
15	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.06	0
15	SO4	G	301	-	4,4,4	0.15	0	6,6,6	0.06	0
15	SO4	G	302	-	4,4,4	0.14	0	6,6,6	0.06	0
15	SO4	K	2002	-	4,4,4	0.14	0	6,6,6	0.06	0
16	GOL	K	2003	-	5,5,5	0.35	0	5,5,5	0.24	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SO4	A	401	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	GOL	A	402	-	-	0/4/4/4	0/0/0/0
15	SO4	B	301	-	-	0/0/0/0	0/0/0/0
15	SO4	G	301	-	-	0/0/0/0	0/0/0/0
15	SO4	G	302	-	-	0/0/0/0	0/0/0/0
15	SO4	K	2002	-	-	0/0/0/0	0/0/0/0
16	GOL	K	2003	-	-	0/4/4/4	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	2003	GOL	1	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	302/305 (99%)	-0.04	8 (2%) 56 53	61, 98, 184, 237	0
2	B	241/250 (96%)	-0.08	2 (0%) 86 85	48, 83, 150, 194	0
3	C	299/394 (75%)	0.50	32 (10%) 7 6	125, 177, 245, 299	0
4	D	222/225 (98%)	0.09	6 (2%) 55 52	87, 132, 197, 240	0
5	E	257/269 (95%)	0.22	13 (5%) 29 26	81, 144, 202, 248	0
6	F	207/250 (82%)	0.29	13 (6%) 21 20	120, 170, 223, 254	0
7	G	236/244 (96%)	0.20	11 (4%) 32 30	72, 115, 206, 266	0
8	H	291/363 (80%)	0.44	31 (10%) 7 6	77, 160, 218, 260	0
9	I	207/296 (69%)	1.01	42 (20%) 1 1	94, 185, 257, 286	0
10	J	460/559 (82%)	0.14	21 (4%) 33 31	86, 128, 218, 288	0
11	K	956/1003 (95%)	-0.00	21 (2%) 62 60	74, 114, 189, 245	0
12	L	29/42 (69%)	0.74	4 (13%) 3 3	113, 180, 246, 276	0
13	M	5/11 (45%)	0.55	1 (20%) 1 1	129, 134, 180, 235	0
14	N	7/19 (36%)	1.62	2 (28%) 1 1	105, 108, 134, 203	0
All	All	3719/4230 (87%)	0.20	207 (5%) 25 23	48, 132, 217, 299	0

The worst 5 of 207 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	11	ALA	8.7
9	I	16	LEU	7.6
3	C	172	VAL	6.4
8	H	233	LEU	6.0
6	F	18	MET	5.9

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
16	GOL	A	402	6/6	0.86	0.66	6.83	73,108,120,124	0
16	GOL	K	2003	6/6	0.93	0.67	5.67	72,97,98,104	0
15	SO4	G	302	5/5	0.78	0.47	4.75	174,187,192,199	0
15	SO4	G	301	5/5	0.90	0.32	0.98	130,142,158,175	0
15	SO4	A	401	5/5	0.93	0.29	0.77	75,87,114,122	0
17	ZN	K	2001	1/1	0.99	0.19	0.33	125,125,125,125	0
15	SO4	K	2002	5/5	0.86	0.14	-	166,179,188,209	0
15	SO4	B	301	5/5	0.87	0.17	-	171,175,177,186	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.