



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:03 AM GMT

PDB ID : 3CW1  
Title : Crystal Structure of Human Spliceosomal U1 snRNP  
Authors : Pomeranz Krummel, D.A.; Oubridge, C.; Leung, A.K.; Li, J.; Nagai, K.  
Deposited on : 2008-04-21  
Resolution : 5.49 Å(reported)

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

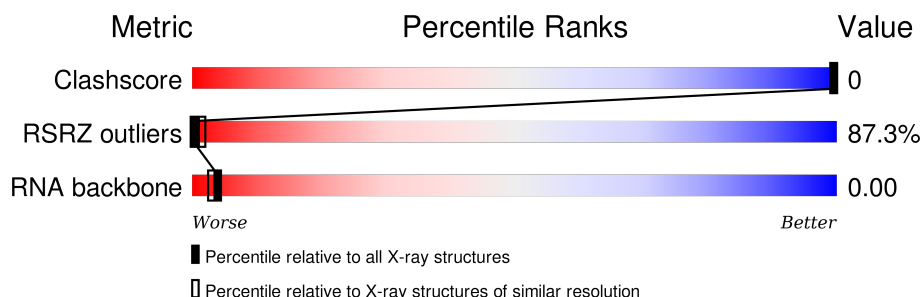
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 5.49 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.



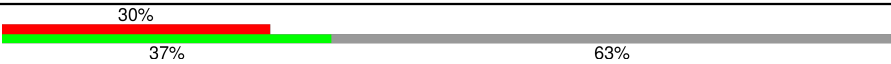


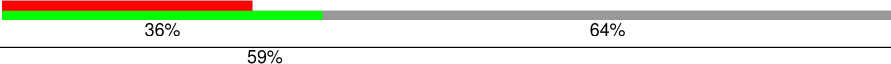






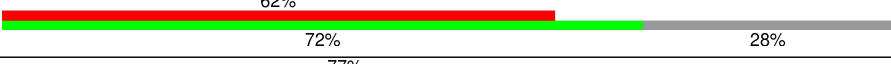







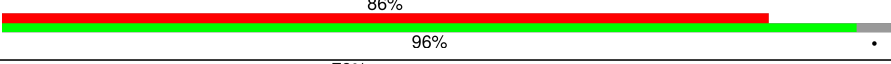
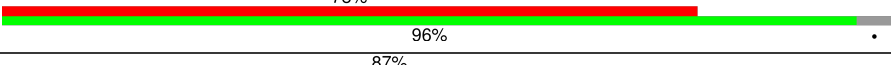
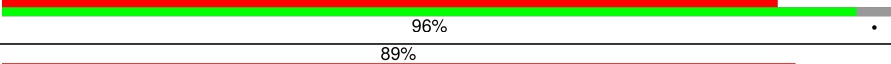
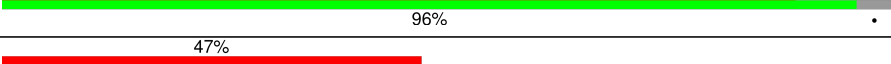
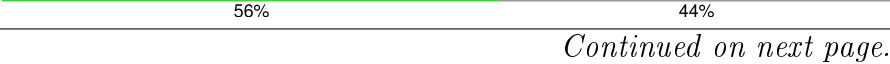


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1020 (7.10-3.70)
RSRZ outliers	91569	1014 (7.38-3.62)
RNA backbone	2183	1101 (7.80-2.80)

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	V	138	<div> <div>99%</div> <div>100%</div> </div>
1	v	138	<div> <div>100%</div> <div>99%</div> </div>
1	w	138	<div> <div>99%</div> <div>100%</div> </div>
1	x	138	<div> <div>99%</div> <div>100%</div> </div>
2	D	126	<div> <div>52%</div> <div>60%</div> <div>40%</div> </div>
2	S	126	<div> <div>49%</div> <div>60%</div> <div>40%</div> </div>
2	T	126	<div> <div>52%</div> <div>60%</div> <div>40%</div> </div>
2	U	126	<div> <div>53%</div> <div>60%</div> <div>40%</div> </div>




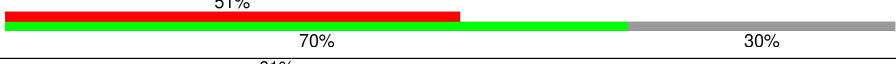
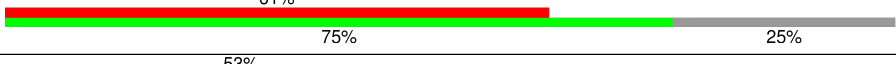
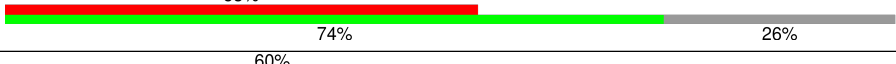
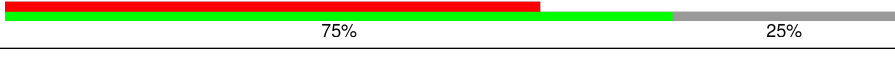
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Mol	Chain	Length	Quality of chain
3	A	174	
3	H	174	
3	I	174	
3	J	174	
4	B	119	
4	M	119	
4	N	119	
4	O	119	
5	C	118	
5	P	118	
5	Q	118	
5	R	118	
6	1	86	
6	2	86	
6	F	86	
6	Z	86	
7	E	92	
7	W	92	
7	X	92	
7	Y	92	
8	3	76	
8	4	76	
8	5	76	
8	G	76	
9	6	216	

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Mol	Chain	Length	Quality of chain
9	7	216	 <p>47% (Red), 56% (Green), 44% (Grey)</p>
9	8	216	 <p>47% (Red), 56% (Green), 44% (Grey)</p>
9	K	216	 <p>46% (Red), 55% (Green), 44% (Grey)</p>
10	0	77	 <p>51% (Red), 70% (Green), 30% (Grey)</p>
10	9	77	 <p>61% (Red), 75% (Green), 25% (Grey)</p>
10	L	77	 <p>53% (Red), 74% (Green), 26% (Grey)</p>
10	l	77	 <p>60% (Red), 75% (Green), 25% (Grey)</p>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 3365 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 RNA chain called U1 snRNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	V	138	Total P 138 138	0	0	138
1	v	138	Total P 138 138	0	0	138
1	w	138	Total P 138 138	0	0	138
1	x	138	Total P 138 138	0	0	138

- Molecule 2 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	76	Total C 76 76	0	0	76
2	S	76	Total C 76 76	0	0	76
2	T	76	Total C 76 76	0	0	76
2	U	76	Total C 76 76	0	0	76

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	66	CYS	SER	CONFLICT	UNP P62318
S	266	CYS	SER	CONFLICT	UNP P62318
T	466	CYS	SER	CONFLICT	UNP P62318
U	666	CYS	SER	CONFLICT	UNP P62318

- Molecule 3 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	A	64	Total C 64 64	0	0	64
3	H	64	Total C 64 64	0	0	64
3	I	63	Total C 63 63	0	0	63
3	J	63	Total C 63 63	0	0	63

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	B	77	Total C 77 77	0	0	77
4	M	77	Total C 77 77	0	0	77
4	N	76	Total C 76 76	0	0	76
4	O	77	Total C 77 77	0	0	77

- Molecule 5 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	C	88	Total C 88 88	0	0	88
5	P	86	Total C 86 86	0	0	86
5	Q	89	Total C 89 89	0	0	89
5	R	85	Total C 85 85	0	0	85

- Molecule 6 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	76	Total C 76 76	0	0	76
6	Z	70	Total C 70 70	0	0	70
6	1	75	Total C 75 75	0	0	75

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	2	76	Total C 76 76	0	0	76

- Molecule 7 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	E	75	Total C 75 75	0	0	75
7	W	75	Total C 75 75	0	0	75
7	X	75	Total C 75 75	0	0	75
7	Y	75	Total C 75 75	0	0	75

- Molecule 8 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	G	73	Total C 73 73	0	0	73
8	3	73	Total C 73 73	0	0	73
8	4	73	Total C 73 73	0	0	73
8	5	73	Total C 73 73	0	0	73

- Molecule 9 is a protein called U1 small nuclear ribonucleoprotein 70 kDa.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	K	120	Total C 120 120	0	0	120
9	6	120	Total C 120 120	0	0	120
9	7	120	Total C 120 120	0	0	120
9	8	120	Total C 120 120	0	0	120

- Molecule 10 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	L	57	Total C 57 57	0	0	57
10	9	58	Total C 58 58	0	0	58
10	0	54	Total C 54 54	0	0	54
10	1	58	Total C 58 58	0	0	58

There are 4 discrepancies between the modelled and reference sequences:

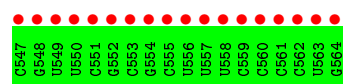
Chain	Residue	Modelled	Actual	Comment	Reference
L	39	CYS	GLN	CONFLICT	UNP P09234
9	239	CYS	GLN	CONFLICT	UNP P09234
0	439	CYS	GLN	CONFLICT	UNP P09234
1	639	CYS	GLN	CONFLICT	UNP P09234

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

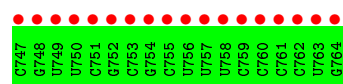
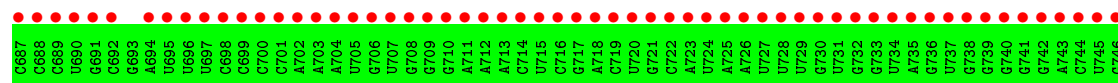
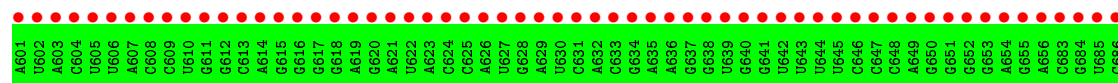
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	0	1	Total Zn 1 1	0	0
11	1	1	Total Zn 1 1	0	0
11	9	1	Total Zn 1 1	0	0
11	L	1	Total Zn 1 1	0	0



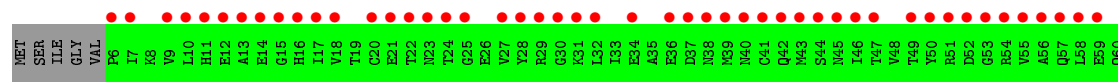




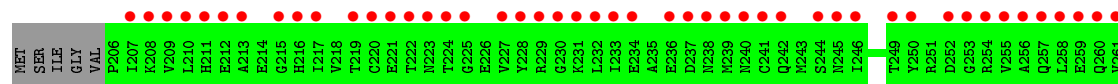
● Molecule 1: U1 snRNA



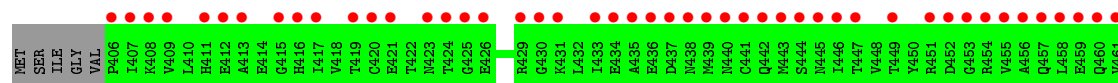
● Molecule 2: Small nuclear ribonucleoprotein Sm D3

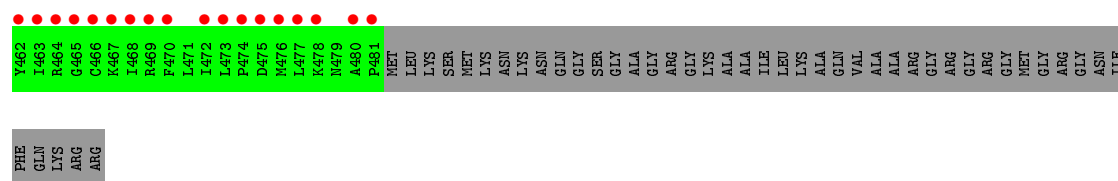


● Molecule 2: Small nuclear ribonucleoprotein Sm D3

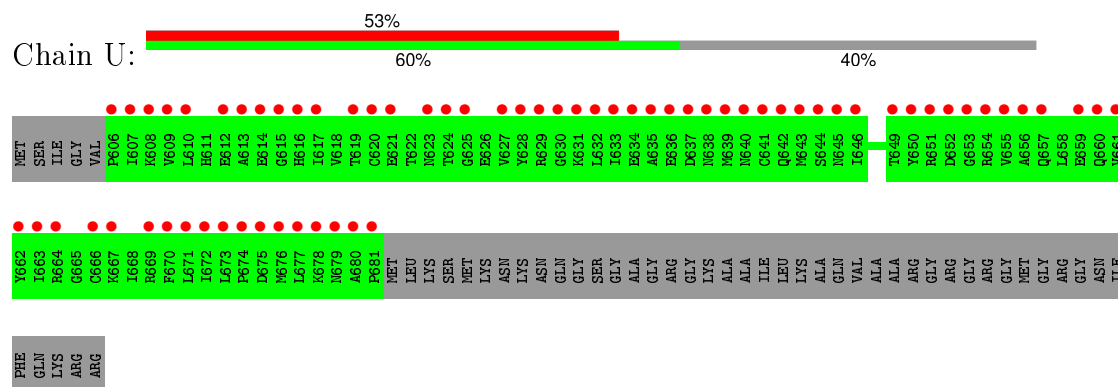


● Molecule 2: Small nuclear ribonucleoprotein Sm D3

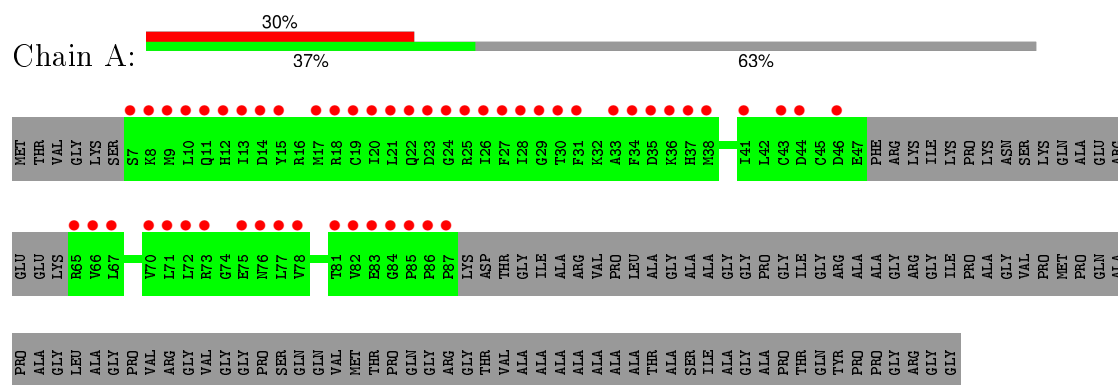




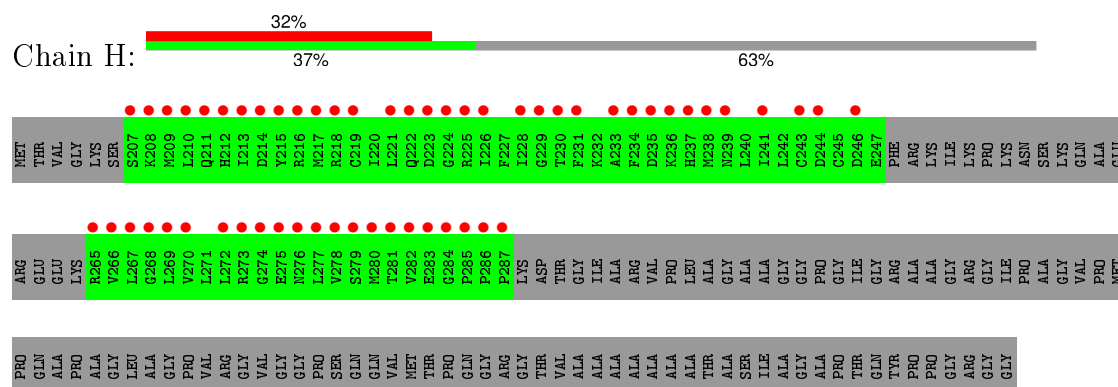
• Molecule 2: Small nuclear ribonucleoprotein Sm D3



• Molecule 3: Small nuclear ribonucleoprotein-associated proteins B and B

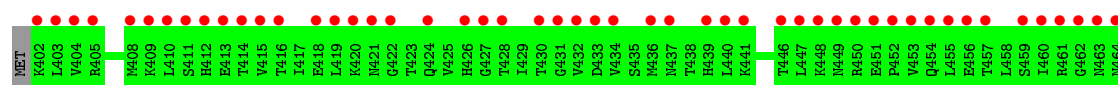


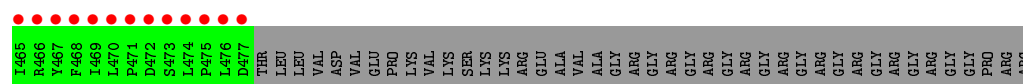
• Molecule 3: Small nuclear ribonucleoprotein-associated proteins B and B



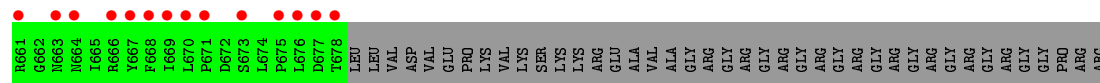
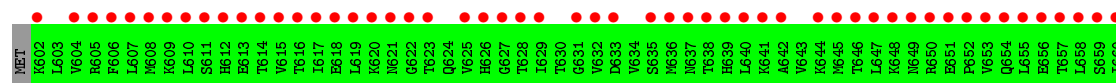
• Molecule 3: Small nuclear ribonucleoprotein-associated proteins B and B



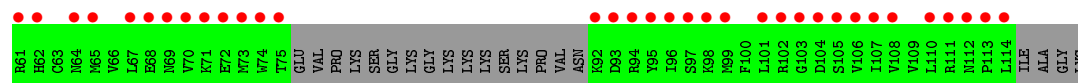
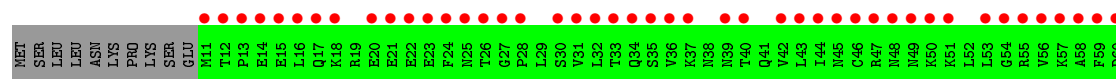
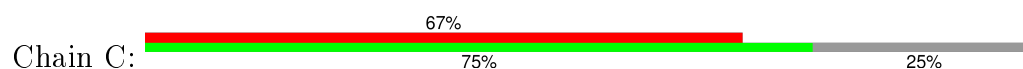




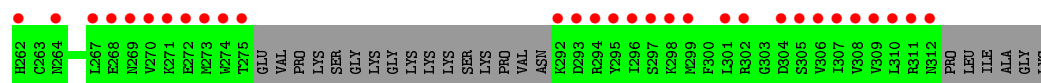
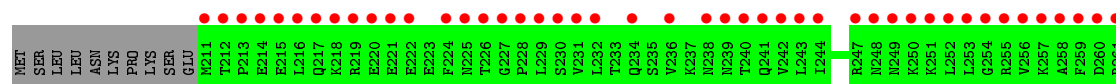
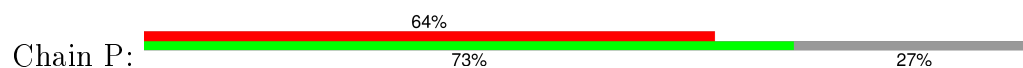
• Molecule 4: Small nuclear ribonucleoprotein Sm D1



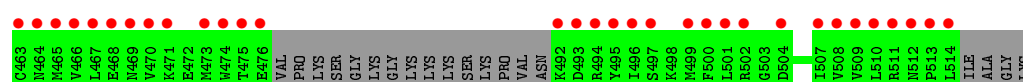
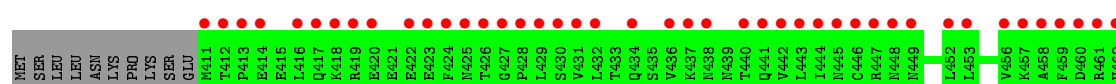
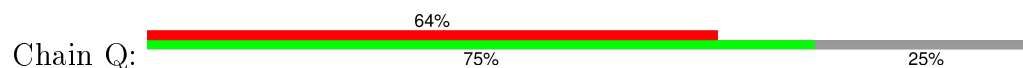
• Molecule 5: Small nuclear ribonucleoprotein Sm D2



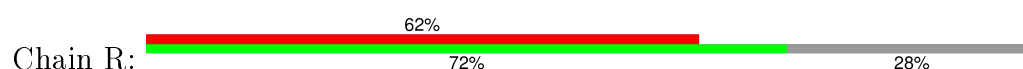
• Molecule 5: Small nuclear ribonucleoprotein Sm D2

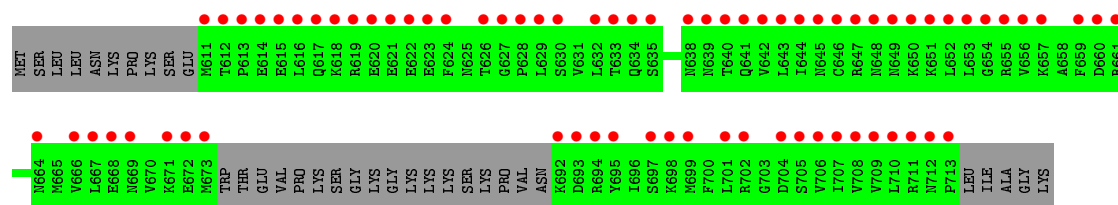


• Molecule 5: Small nuclear ribonucleoprotein Sm D2

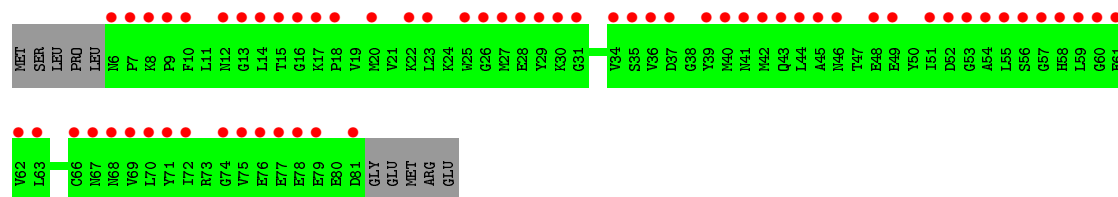
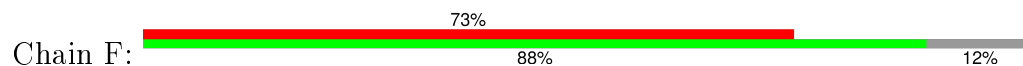


• Molecule 5: Small nuclear ribonucleoprotein Sm D2

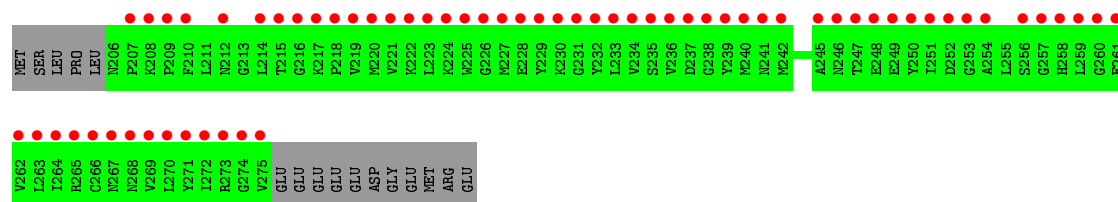
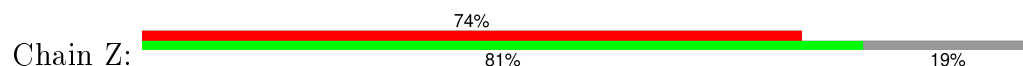




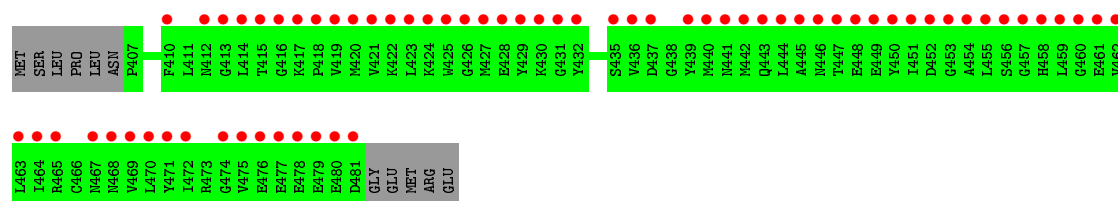
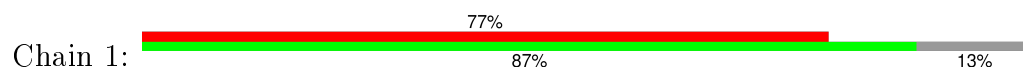
• Molecule 6: Small nuclear ribonucleoprotein F



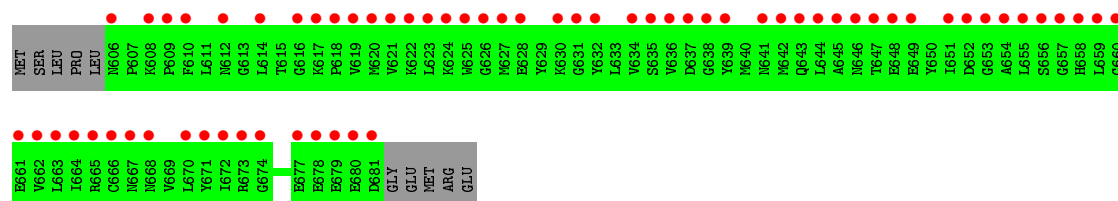
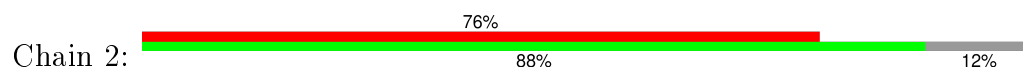
• Molecule 6: Small nuclear ribonucleoprotein F



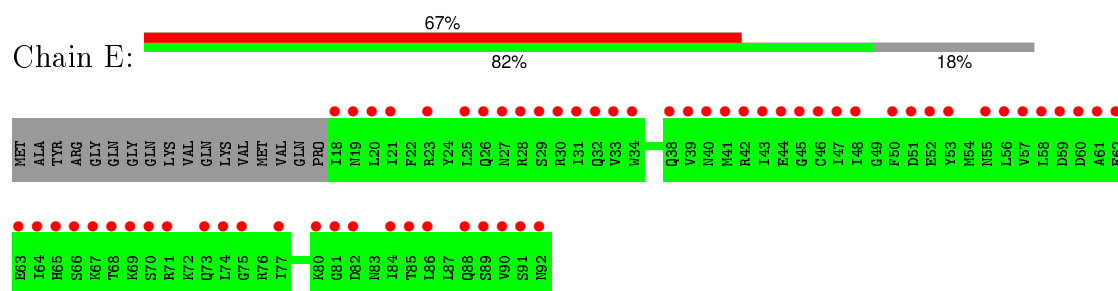
• Molecule 6: Small nuclear ribonucleoprotein F



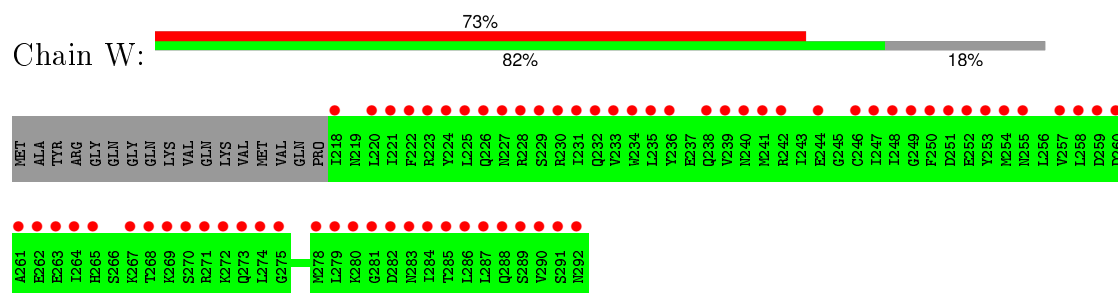
• Molecule 6: Small nuclear ribonucleoprotein F



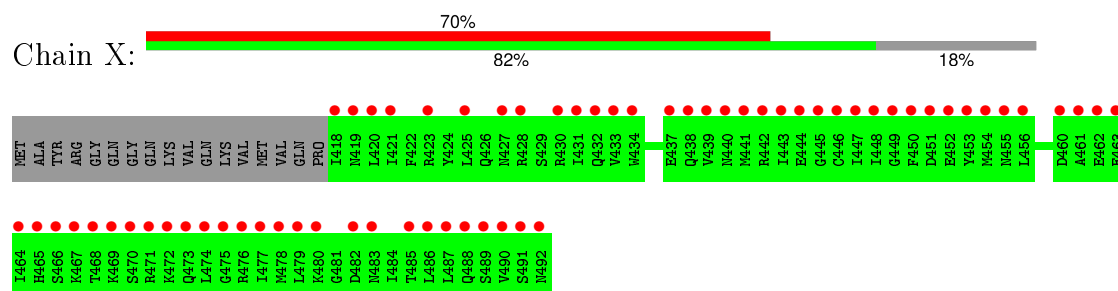
• Molecule 7: Small nuclear ribonucleoprotein E



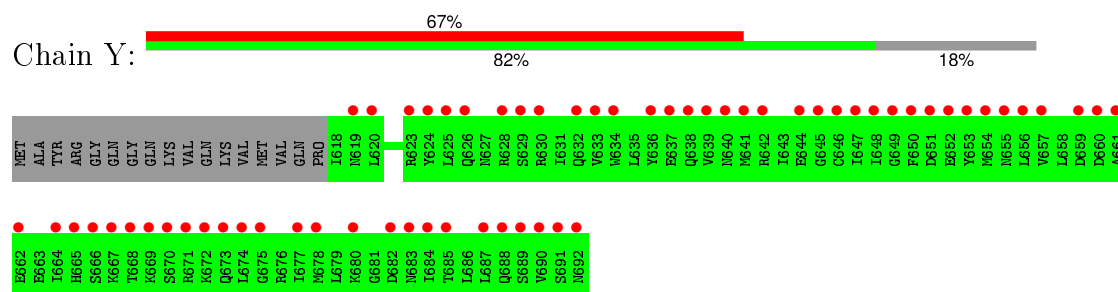
- Molecule 7: Small nuclear ribonucleoprotein E



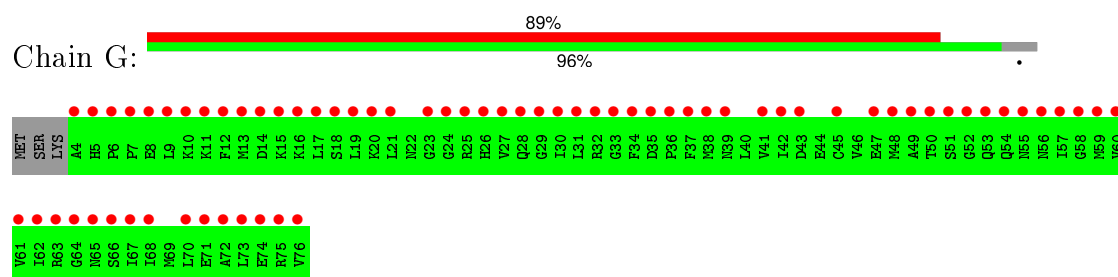
- Molecule 7: Small nuclear ribonucleoprotein E



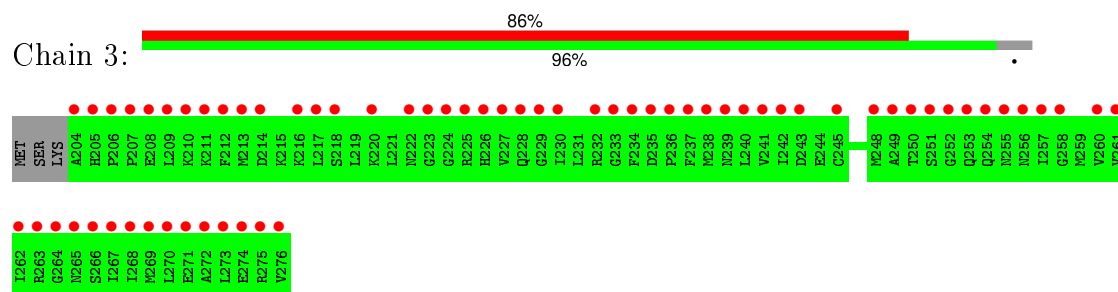
- Molecule 7: Small nuclear ribonucleoprotein E



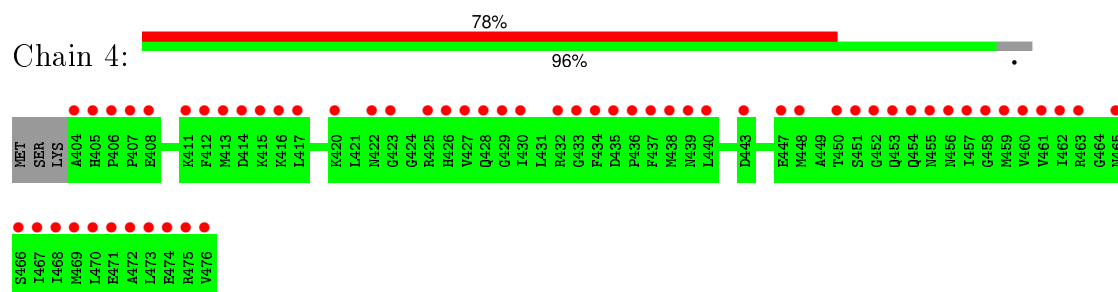
- Molecule 8: Small nuclear ribonucleoprotein G



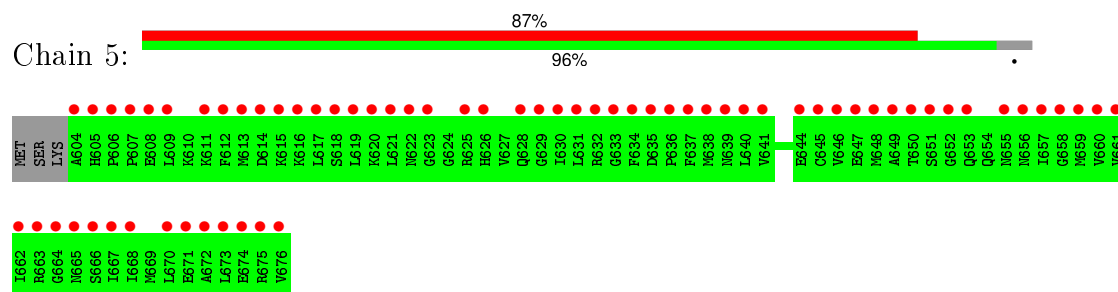
- Molecule 8: Small nuclear ribonucleoprotein G



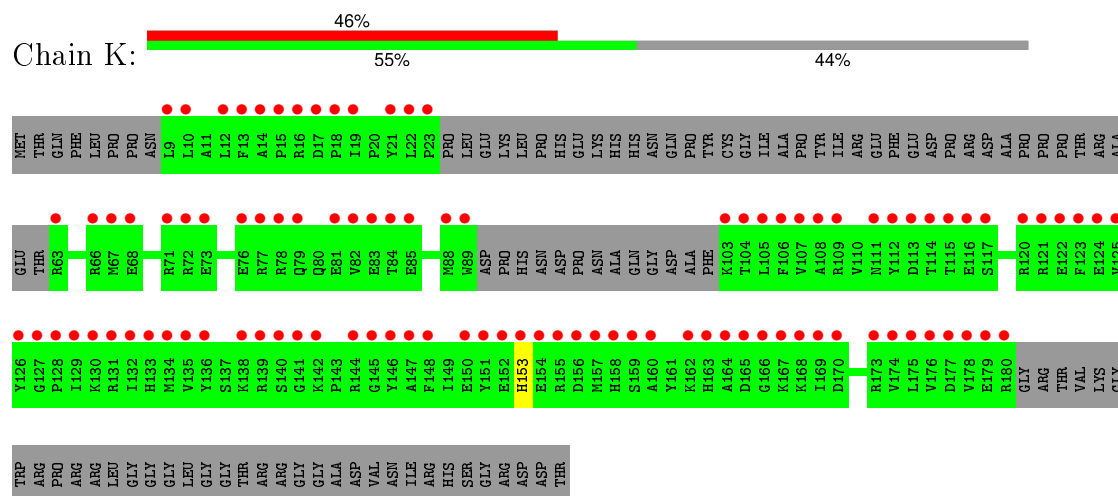
- Molecule 8: Small nuclear ribonucleoprotein G



- Molecule 8: Small nuclear ribonucleoprotein G

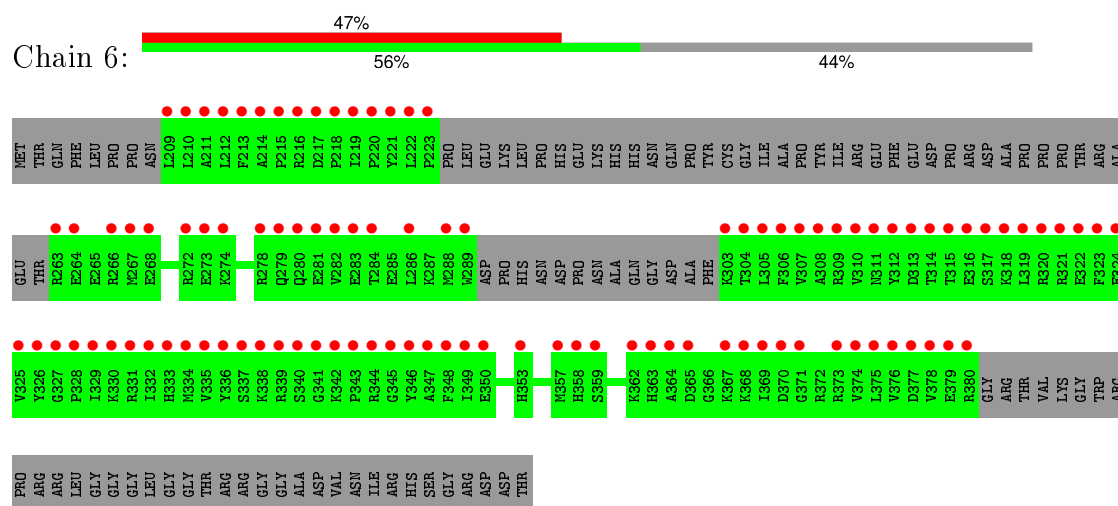


- Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa

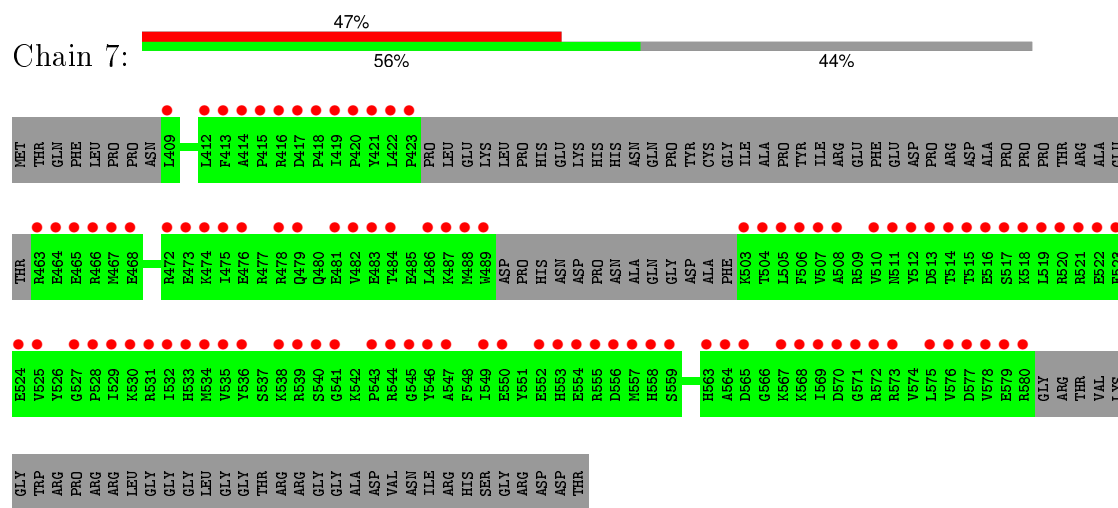


- Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa

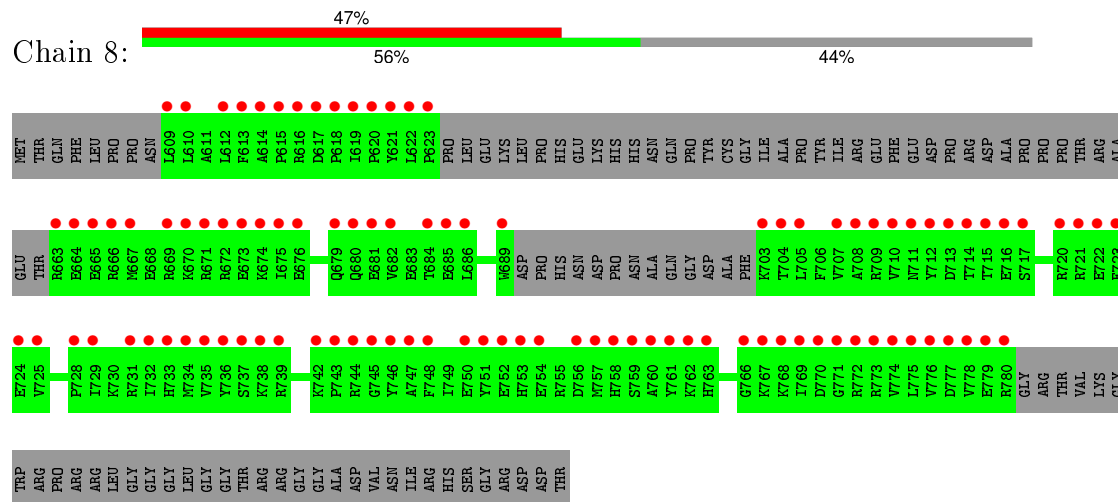




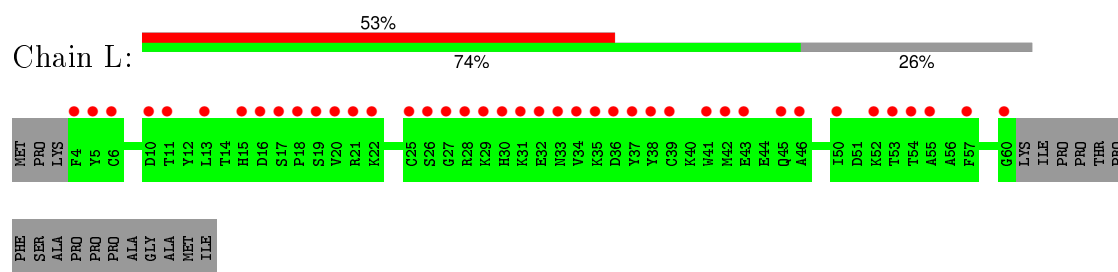
- Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa



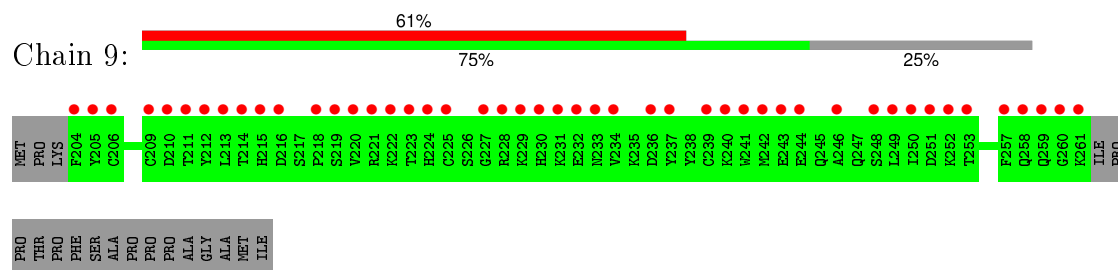
- Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa



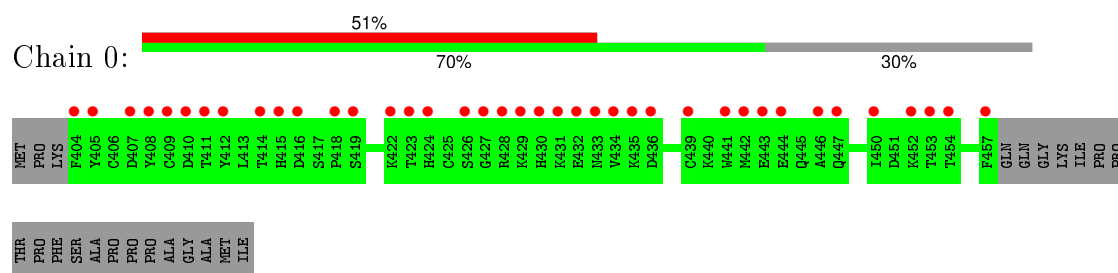
- Molecule 10: U1 small nuclear ribonucleoprotein C



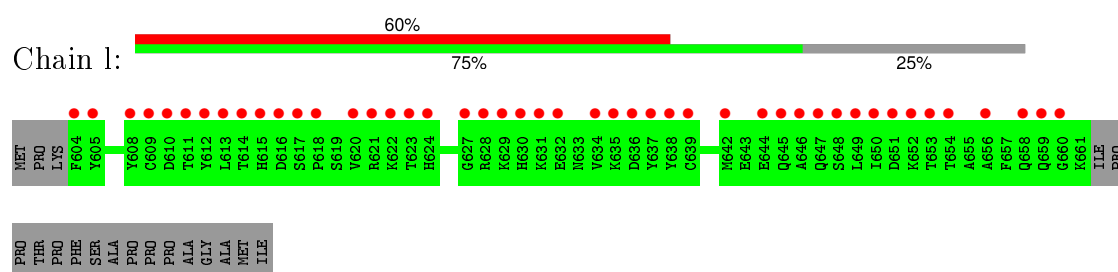
- Molecule 10: U1 small nuclear ribonucleoprotein C



- Molecule 10: U1 small nuclear ribonucleoprotein C



- Molecule 10: U1 small nuclear ribonucleoprotein C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.47Å 127.08Å 152.02Å 95.42° 105.92° 101.80°	Depositor
Resolution (Å)	123.09 – 5.49 122.79 – 5.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (123.09-5.49) 93.9 (122.79-5.49)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 5.42Å)	Xtriage
Refinement program	O, version 9.0.7	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.497 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	251.7	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.58 , -4.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 28397 reflections	Xtriage
$F_o, F_c$ correlation	0.72	EDS
Total number of atoms	3365	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	231.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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, 0.375 respectively for untwinned datasets, and 0.333, 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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 [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	V	138	0	0	0	0
1	v	138	0	0	0	1
1	w	138	0	0	0	0
1	x	138	0	0	0	0
2	D	76	0	0	0	0
2	S	76	0	0	0	0
2	T	76	0	0	0	0
2	U	76	0	0	0	0
3	A	64	0	0	0	0
3	H	64	0	0	0	0
3	I	63	0	0	0	0
3	J	63	0	0	0	0
4	B	77	0	0	0	0
4	M	77	0	0	0	0
4	N	76	0	0	0	0
4	O	77	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	88	0	0	0	0
5	P	86	0	0	0	0
5	Q	89	0	0	0	0
5	R	85	0	0	0	0
6	1	75	0	0	0	0
6	2	76	0	0	0	0
6	F	76	0	0	0	0
6	Z	70	0	0	0	0
7	E	75	0	0	0	0
7	W	75	0	0	0	0
7	X	75	0	0	0	0
7	Y	75	0	0	0	0
8	3	73	0	0	0	0
8	4	73	0	0	0	0
8	5	73	0	0	0	0
8	G	73	0	0	0	0
9	6	120	0	0	0	0
9	7	120	0	0	0	0
9	8	120	0	0	0	0
9	K	120	0	0	0	1
10	0	54	0	0	0	0
10	9	58	0	0	0	0
10	L	57	0	0	0	0
10	l	58	0	0	0	0
11	0	1	0	0	0	0
11	9	1	0	0	0	0
11	L	1	0	0	0	0
11	l	1	0	0	0	0
All	All	3365	0	0	0	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 0.

There are no clashes within the asymmetric unit.

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)
1:v:214:A:P	9:K:153:HIS:CA[1_545]	2.05	0.15

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	V	0/138	-	-
1	v	0/138	-	-
1	w	0/138	-	-
1	x	0/138	-	-
All	All	0/552	-	-

There are no RNA backbone outliers to report.

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 4 ligands modelled in this entry, 4 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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	V	138/138 (100%)	17.31	137 (99%) 0 0	232, 232, 232, 232	0
1	v	138/138 (100%)	18.02	138 (100%) 0 0	232, 232, 232, 232	0
1	w	138/138 (100%)	17.29	137 (99%) 0 0	232, 232, 232, 232	0
1	x	138/138 (100%)	16.71	137 (99%) 0 0	232, 232, 232, 232	0
2	D	76/126 (60%)	7.10	65 (85%) 0 1	232, 232, 232, 232	0
2	S	76/126 (60%)	7.23	62 (81%) 0 2	232, 232, 232, 232	0
2	T	76/126 (60%)	7.09	65 (85%) 0 1	232, 232, 232, 232	0
2	U	76/126 (60%)	6.64	67 (88%) 0 1	232, 232, 232, 232	0
3	A	64/174 (36%)	6.58	52 (81%) 0 2	232, 232, 232, 232	0
3	H	64/174 (36%)	6.58	56 (87%) 0 1	232, 232, 232, 232	0
3	I	63/174 (36%)	5.55	52 (82%) 0 2	232, 232, 232, 232	0
3	J	63/174 (36%)	6.23	49 (77%) 0 2	232, 232, 232, 232	0
4	B	77/119 (64%)	7.07	70 (90%) 0 1	232, 232, 232, 232	0
4	M	77/119 (64%)	5.89	67 (87%) 0 1	232, 232, 232, 232	0
4	N	76/119 (63%)	6.45	63 (82%) 0 2	232, 232, 232, 232	0
4	O	77/119 (64%)	6.24	68 (88%) 0 1	232, 232, 232, 232	0
5	C	88/118 (74%)	6.10	79 (89%) 0 1	232, 232, 232, 232	0
5	P	86/118 (72%)	6.33	75 (87%) 0 1	232, 232, 232, 232	0
5	Q	89/118 (75%)	6.05	75 (84%) 0 1	232, 232, 232, 232	0
5	R	85/118 (72%)	6.82	73 (85%) 0 1	232, 232, 232, 232	0
6	1	75/86 (87%)	7.00	66 (88%) 0 1	232, 232, 232, 232	0
6	2	76/86 (88%)	7.06	65 (85%) 0 1	232, 232, 232, 232	0
6	F	76/86 (88%)	6.73	63 (82%) 0 2	232, 232, 232, 232	0
6	Z	70/86 (81%)	6.30	64 (91%) 0 1	232, 232, 232, 232	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
7	E	75/92 (81%)	6.86	62 (82%) 0 2	232, 232, 232, 232	0
7	W	75/92 (81%)	6.16	67 (89%) 0 1	232, 232, 232, 232	0
7	X	75/92 (81%)	6.73	64 (85%) 0 1	232, 232, 232, 232	0
7	Y	75/92 (81%)	6.02	62 (82%) 0 2	232, 232, 232, 232	0
8	3	73/76 (96%)	6.22	65 (89%) 0 1	232, 232, 232, 232	0
8	4	73/76 (96%)	5.90	59 (80%) 0 2	232, 232, 232, 232	0
8	5	73/76 (96%)	6.80	66 (90%) 0 1	232, 232, 232, 232	0
8	G	73/76 (96%)	7.48	68 (93%) 0 1	232, 232, 232, 232	0
9	6	120/216 (55%)	6.54	102 (85%) 0 1	232, 232, 232, 232	0
9	7	120/216 (55%)	6.53	101 (84%) 0 2	232, 232, 232, 232	0
9	8	120/216 (55%)	6.08	101 (84%) 0 2	232, 232, 232, 232	0
9	K	120/216 (55%)	6.78	100 (83%) 0 2	232, 232, 232, 232	0
10	0	54/77 (70%)	6.15	39 (72%) 0 2	232, 232, 232, 232	0
10	9	58/77 (75%)	6.01	47 (81%) 0 2	232, 232, 232, 232	0
10	L	57/77 (74%)	5.62	41 (71%) 0 2	232, 232, 232, 232	0
10	l	58/77 (75%)	6.22	46 (79%) 0 2	232, 232, 232, 232	0
All	All	3361/4888 (68%)	8.27	2935 (87%) 0 1	232, 232, 232, 232	0

All (2935) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	w	489	C	56.4
1	V	56	A	56.3
1	V	110	G	55.0
1	v	342	G	54.3
1	w	564	G	54.3
1	V	7	A	52.6
1	V	12	G	51.4
1	V	109	G	47.9
1	w	532	G	47.6
1	x	721	G	47.1
1	v	364	G	45.1
1	x	751	C	44.9
1	V	161	C	44.5
1	v	346	G	42.9
1	V	23	A	42.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	v	220	G	42.1
1	x	761	C	42.0
1	V	163	U	41.4
1	w	454	A	41.3
1	w	557	U	41.0
1	v	283	C	40.6
1	V	139	G	40.3
1	V	150	U	39.8
1	w	539	G	39.6
1	v	290	U	39.6
1	v	285	U	39.2
1	w	509	G	38.9
1	v	321	G	38.9
1	w	525	A	38.2
1	v	212	G	38.1
1	w	547	C	38.0
1	v	203	A	38.0
1	w	440	G	37.8
1	w	560	C	37.7
1	x	615	G	37.5
1	V	53	G	37.4
1	x	636	A	36.8
1	x	649	A	36.3
1	v	305	U	36.3
1	w	436	A	36.2
1	v	252	G	35.6
1	x	687	C	35.5
1	v	210	U	35.5
1	v	217	G	35.4
1	v	284	G	35.3
1	x	698	C	35.0
1	v	245	U	34.9
1	v	214	A	34.8
1	V	2	U	34.4
1	w	548	G	34.2
1	v	250	G	33.1
1	v	339	G	33.0
1	V	84	G	32.9
1	x	684	G	32.9
1	x	759	C	32.8
1	x	730	G	32.2
1	v	318	A	31.9

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Mol	Chain	Res	Type	RSRZ
1	x	691	G	31.8
1	V	43	U	31.8
1	v	295	U	31.4
1	v	353	C	30.9
1	V	113	A	30.8
2	S	269	ARG	30.8
1	v	360	C	30.8
1	w	538	G	30.7
1	V	37	G	30.6
1	V	41	G	30.6
1	v	332	G	30.6
1	v	362	C	30.5
1	V	130	G	30.4
1	x	706	G	30.3
1	w	531	U	30.2
1	w	485	U	30.1
1	V	133	G	30.0
1	x	623	A	29.8
1	V	106	G	29.8
1	V	47	C	29.7
1	V	132	G	29.6
1	w	425	C	29.5
1	v	326	A	29.4
1	v	225	C	29.0
1	V	49	A	29.0
1	x	740	G	28.9
1	w	501	C	28.8
1	w	510	G	28.8
7	X	466	SER	28.7
9	K	84	THR	28.7
1	v	317	G	28.6
1	v	237	G	28.5
1	v	347	C	28.4
1	x	729	U	28.4
1	w	441	G	28.3
1	x	696	U	28.2
1	x	723	A	28.1
9	K	72	ARG	27.7
1	v	294	A	27.7
1	w	411	G	27.7
1	v	227	U	27.5
4	N	431	GLY	27.5

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Mol	Chain	Res	Type	RSRZ
1	V	155	C	27.3
5	R	649	ASN	27.2
1	v	209	C	27.1
1	x	727	U	27.1
1	V	94	A	27.0
1	x	717	G	26.9
1	V	91	G	26.8
1	w	541	G	26.7
1	v	351	C	26.4
1	x	635	A	26.3
1	v	358	U	26.3
1	x	643	U	26.3
1	w	408	C	26.1
1	V	126	A	26.0
1	V	95	U	26.0
1	x	654	A	26.0
1	v	236	A	25.8
1	V	5	U	25.8
9	6	353	HIS	25.6
10	l	627	GLY	25.5
1	w	496	U	25.4
1	v	240	G	25.4
1	x	648	C	25.4
1	x	614	A	25.2
1	w	428	G	25.2
1	V	55	G	25.1
1	v	253	G	25.0
1	w	444	U	24.9
1	V	162	C	24.7
1	v	229	A	24.7
3	A	77	LEU	24.5
2	S	272	ILE	24.5
1	V	30	U	24.4
1	v	302	A	24.3
1	x	626	A	24.2
1	w	520	U	24.2
1	x	731	U	24.1
5	R	629	LEU	24.1
1	x	747	C	24.1
1	w	507	U	24.0
1	x	656	A	24.0
1	x	604	C	23.9

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Mol	Chain	Res	Type	RSRZ
1	v	307	U	23.8
1	V	46	C	23.7
1	x	602	U	23.7
5	R	645	ASN	23.6
1	v	343	A	23.5
5	Q	437	LYS	23.5
1	V	36	A	23.4
1	v	301	C	23.4
1	v	311	A	23.4
1	V	15	G	23.3
8	3	235	ASP	23.3
1	w	518	A	23.1
1	w	513	A	23.0
8	4	435	ASP	22.8
1	w	423	A	22.8
1	V	86	C	22.7
1	x	726	A	22.7
7	Y	661	ALA	22.7
5	R	620	GLU	22.7
1	w	519	C	22.5
1	v	303	A	22.5
1	w	442	U	22.4
1	v	215	G	22.4
1	v	288	C	22.4
1	V	13	C	22.4
8	5	663	ARG	22.3
1	x	641	G	22.2
1	w	452	G	22.1
1	w	533	G	22.0
1	v	221	A	22.0
7	W	241	MET	21.9
7	E	41	MET	21.9
1	w	410	U	21.8
1	x	610	U	21.8
1	x	686	C	21.8
1	v	287	C	21.7
6	Z	228	GLU	21.6
1	w	503	A	21.6
1	w	488	C	21.5
1	V	108	G	21.4
6	2	668	ASN	21.4
1	V	115	U	21.4

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Mol	Chain	Res	Type	RSRZ
1	x	694	A	21.4
1	V	118	A	21.3
1	x	703	A	21.3
1	V	137	U	21.3
4	B	58	LEU	21.3
2	T	467	LYS	21.2
1	V	146	G	21.2
1	x	764	G	20.9
1	x	650	G	20.8
1	x	605	U	20.6
1	w	551	C	20.6
1	w	526	A	20.6
6	1	479	GLU	20.6
10	0	428	ARG	20.4
1	x	612	G	20.4
8	G	74	GLU	20.4
1	x	638	G	20.2
6	F	48	GLU	20.2
4	B	71	PRO	20.2
1	w	416	G	20.2
1	x	753	C	20.2
1	w	516	C	20.1
6	1	447	THR	20.1
6	2	672	ILE	20.1
10	9	233	ASN	20.1
7	X	440	ASN	20.1
2	D	13	ALA	20.1
1	v	352	G	20.1
1	v	322	C	19.9
1	V	100	C	19.9
1	v	232	A	19.9
9	K	116	GLU	19.8
5	C	26	THR	19.8
1	w	494	A	19.8
1	w	429	A	19.8
7	E	61	ALA	19.7
6	2	622	LYS	19.7
1	v	330	G	19.7
1	x	711	A	19.7
1	V	159	C	19.7
4	N	446	THR	19.7
8	3	267	ILE	19.6

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Mol	Chain	Res	Type	RSRZ
1	w	536	G	19.6
1	x	619	A	19.6
2	U	646	ILE	19.5
1	x	755	C	19.5
4	O	616	THR	19.5
1	v	291	G	19.3
1	x	607	A	19.3
1	V	103	A	19.2
1	x	688	C	19.2
1	v	202	U	19.2
1	V	27	U	19.1
1	w	521	G	19.1
10	9	224	HIS	19.0
1	V	104	A	19.0
1	V	127	U	18.9
9	6	350	GLU	18.9
1	x	690	U	18.8
9	6	311	ASN	18.8
1	w	491	G	18.7
1	w	493	G	18.6
1	v	286	C	18.6
3	H	284	GLY	18.6
7	X	445	GLY	18.6
1	x	644	U	18.5
10	0	407	ASP	18.5
1	v	310	G	18.5
1	v	238	G	18.5
6	F	28	GLU	18.5
1	x	653	G	18.5
9	7	479	GLN	18.4
1	V	54	A	18.3
1	w	545	U	18.3
1	x	640	G	18.3
1	w	549	U	18.3
9	8	620	PRO	18.2
9	7	467	MET	18.2
1	x	622	U	18.2
1	w	498	C	18.2
8	G	29	GLY	18.1
1	x	685	U	18.1
1	V	105	U	18.0
1	x	627	U	18.0

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Mol	Chain	Res	Type	RSRZ
1	V	98	C	17.9
5	P	307	ILE	17.8
1	V	10	U	17.8
3	I	428	GLY	17.8
1	v	336	G	17.8
1	w	517	G	17.8
9	6	283	GLU	17.8
5	C	27	GLY	17.8
1	V	1	A	17.8
1	x	709	G	17.7
2	D	14	GLU	17.7
5	C	64	ASN	17.7
6	l	451	ILE	17.7
1	v	324	U	17.6
2	T	420	CYS	17.6
1	w	438	G	17.6
1	V	88	C	17.6
1	w	562	C	17.6
1	v	231	C	17.6
4	M	259	SER	17.6
10	l	621	ARG	17.6
1	V	85	U	17.5
3	J	630	THR	17.4
1	v	223	A	17.3
6	F	17	LYS	17.3
1	w	422	U	17.1
9	K	163	HIS	17.1
1	x	732	G	17.1
9	7	573	ARG	17.1
1	w	431	C	17.0
1	w	490	U	17.0
1	v	333	G	17.0
1	V	83	C	17.0
1	x	624	C	17.0
6	Z	222	LYS	16.9
6	2	618	PRO	16.8
1	x	752	G	16.8
6	F	41	ASN	16.8
6	1	468	ASN	16.8
1	V	128	U	16.8
8	4	466	SER	16.8
1	V	24	C	16.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	w	530	G	16.8
1	x	701	C	16.7
9	K	152	GLU	16.6
10	0	427	GLY	16.6
1	v	211	G	16.6
2	D	28	TYR	16.6
1	V	151	C	16.6
1	w	522	C	16.5
8	G	71	GLU	16.5
7	X	490	VAL	16.5
1	x	642	U	16.4
4	B	28	THR	16.4
5	P	241	GLN	16.4
9	7	468	GLU	16.3
1	w	414	A	16.3
5	R	710	LEU	16.3
3	I	481	THR	16.3
1	V	111	A	16.3
1	w	435	A	16.3
1	V	160	C	16.2
4	M	254	GLN	16.2
2	U	653	GLY	16.2
3	A	81	THR	16.2
1	x	744	C	16.2
9	7	538	LYS	16.2
1	x	655	G	16.1
1	w	556	U	16.1
9	K	128	PRO	16.0
3	J	621	LEU	16.0
9	6	328	PRO	16.0
1	V	149	U	16.0
2	T	439	MET	15.9
3	H	282	VAL	15.9
8	G	70	LEU	15.9
5	P	239	ASN	15.9
10	L	25	CYS	15.9
8	5	646	VAL	15.8
9	7	553	HIS	15.8
1	v	335	A	15.8
2	S	231	LYS	15.8
8	G	49	ALA	15.8
1	w	512	A	15.8

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Mol	Chain	Res	Type	RSRZ
1	v	331	U	15.8
3	H	243	CYS	15.7
8	G	55	ASN	15.7
1	w	403	A	15.7
6	l	416	GLY	15.7
2	S	239	MET	15.6
1	V	131	U	15.6
6	l	475	VAL	15.6
1	w	559	C	15.6
1	V	97	U	15.6
1	x	754	G	15.5
4	B	66	ARG	15.5
1	V	9	C	15.5
9	7	564	ALA	15.4
1	V	121	G	15.4
1	v	355	C	15.4
6	F	72	ILE	15.4
10	l	616	ASP	15.4
1	v	230	U	15.3
7	E	29	SER	15.3
7	E	70	SER	15.3
1	w	508	G	15.3
10	L	32	GLU	15.3
1	w	453	G	15.3
1	w	439	U	15.3
9	8	716	GLU	15.3
4	B	31	GLY	15.3
1	w	506	G	15.2
1	x	741	G	15.2
1	x	645	U	15.2
1	w	514	C	15.1
9	6	346	TYR	15.1
1	x	630	U	15.1
1	w	546	G	15.1
7	W	263	GLU	15.1
7	W	251	ASP	15.0
5	R	615	GLU	15.0
1	V	102	A	15.0
4	B	10	LEU	15.0
1	x	621	A	15.0
9	8	732	ILE	15.0
10	L	52	LYS	15.0

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Mol	Chain	Res	Type	RSRZ
10	l	632	GLU	15.0
3	J	672	LEU	14.9
2	S	230	GLY	14.9
8	5	637	PHE	14.9
1	V	19	A	14.8
6	Z	217	LYS	14.8
2	U	638	ASN	14.8
4	B	40	LEU	14.8
1	x	702	A	14.8
8	5	634	PHE	14.8
1	w	561	C	14.8
1	V	119	C	14.8
4	M	233	ASP	14.7
2	S	275	ASP	14.7
6	1	477	GLU	14.7
2	S	217	ILE	14.7
9	7	484	THR	14.7
1	V	112	A	14.6
5	Q	420	GLU	14.6
1	w	504	A	14.6
1	v	206	U	14.6
4	O	633	ASP	14.6
5	R	698	LYS	14.6
4	N	459	SER	14.6
6	2	641	ASN	14.5
2	U	640	ASN	14.5
3	A	76	ASN	14.5
1	x	651	G	14.5
9	K	177	ASP	14.5
1	w	448	C	14.5
8	5	645	CYS	14.5
1	x	617	G	14.5
9	8	757	MET	14.5
4	O	654	GLN	14.5
7	Y	683	ASN	14.5
1	x	736	G	14.4
4	N	415	VAL	14.4
4	O	670	LEU	14.4
3	H	214	ASP	14.4
6	Z	226	GLY	14.4
9	7	478	ARG	14.4
1	V	144	C	14.4

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Mol	Chain	Res	Type	RSRZ
1	x	700	C	14.4
1	w	450	G	14.3
1	w	487	C	14.3
1	v	337	U	14.3
4	B	21	ASN	14.3
1	w	426	A	14.2
7	E	85	THR	14.2
1	x	763	U	14.2
9	7	483	GLU	14.2
5	C	48	ASN	14.1
9	6	358	HIS	14.1
9	K	146	TYR	14.1
2	D	71	LEU	14.1
6	F	59	LEU	14.1
1	x	608	C	14.1
1	x	609	C	14.1
1	V	125	A	14.0
6	F	67	ASN	14.0
8	4	416	LYS	14.0
6	F	54	ALA	14.0
5	Q	418	LYS	14.0
1	V	152	G	13.9
1	v	313	A	13.9
7	X	489	SER	13.9
4	N	427	GLY	13.9
4	B	77	ASP	13.9
5	P	232	LEU	13.9
2	T	445	ASN	13.9
7	X	438	GLN	13.9
1	w	443	U	13.9
6	F	53	GLY	13.8
1	v	344	C	13.8
5	P	242	VAL	13.8
8	3	240	LEU	13.8
1	x	625	C	13.8
6	1	418	PRO	13.8
1	v	350	U	13.8
9	7	505	LEU	13.8
7	E	46	CYS	13.7
9	7	557	MET	13.7
2	T	419	THR	13.7
2	T	425	GLY	13.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	0	432	GLU	13.7
10	9	223	THR	13.7
4	O	667	TYR	13.7
1	x	683	C	13.7
2	T	431	LYS	13.7
3	H	228	ILE	13.7
6	2	651	ILE	13.6
7	E	74	LEU	13.6
9	7	578	VAL	13.6
6	2	648	GLU	13.6
3	H	225	ARG	13.6
6	1	437	ASP	13.6
5	Q	412	THR	13.6
2	T	444	SER	13.6
1	w	505	U	13.6
2	S	260	GLN	13.6
8	5	636	PRO	13.6
8	5	658	GLY	13.5
3	H	233	ALA	13.5
6	Z	221	VAL	13.5
2	U	659	GLU	13.5
1	x	733	G	13.5
9	6	357	MET	13.5
7	Y	685	THR	13.5
8	G	25	ARG	13.5
4	O	656	GLU	13.4
10	0	423	THR	13.4
6	1	445	ALA	13.4
2	D	72	ILE	13.4
1	v	314	C	13.4
2	D	40	ASN	13.4
2	U	610	LEU	13.4
4	M	205	ARG	13.4
3	J	619	CYS	13.4
6	1	427	MET	13.4
4	N	433	ASP	13.3
5	C	18	LYS	13.3
1	w	420	G	13.3
4	N	451	GLU	13.3
8	4	465	ASN	13.3
10	l	623	THR	13.3
5	R	653	LEU	13.3

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Mol	Chain	Res	Type	RSRZ
1	v	361	C	13.3
2	D	6	PRO	13.3
1	w	424	C	13.3
1	v	207	A	13.2
4	O	614	THR	13.2
1	w	407	A	13.2
1	v	234	G	13.2
9	6	214	ALA	13.2
1	x	718	A	13.1
9	8	715	THR	13.1
1	v	356	U	13.1
2	D	12	GLU	13.1
2	D	39	MET	13.1
1	w	401	A	13.0
10	L	28	ARG	13.0
1	v	315	U	13.0
6	F	77	GLU	13.0
1	x	695	U	13.0
1	x	606	U	13.0
2	S	236	GLU	13.0
5	P	251	LYS	13.0
9	K	111	ASN	13.0
1	x	713	A	13.0
6	2	627	MET	13.0
8	3	216	LYS	13.0
9	7	413	PHE	13.0
1	w	412	G	13.0
1	w	434	G	13.0
1	V	140	G	12.9
1	V	96	U	12.9
9	8	775	LEU	12.9
1	V	52	G	12.9
6	F	74	GLY	12.9
1	w	451	G	12.9
4	B	27	GLY	12.9
2	S	257	GLN	12.9
4	N	405	ARG	12.9
1	x	697	U	12.9
6	2	667	ASN	12.8
10	9	228	ARG	12.8
1	V	42	U	12.8
7	Y	691	SER	12.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
8	5	671	GLU	12.8
8	G	65	ASN	12.7
3	A	83	GLU	12.7
7	X	474	LEU	12.7
1	w	449	A	12.7
1	x	748	G	12.7
1	V	25	C	12.6
7	X	485	THR	12.6
1	V	38	G	12.6
3	A	14	ASP	12.6
9	6	312	TYR	12.6
4	M	224	GLN	12.6
9	K	129	ILE	12.6
5	Q	509	VAL	12.6
1	v	228	G	12.6
2	T	474	PRO	12.6
8	4	458	GLY	12.6
4	B	59	SER	12.6
1	v	239	U	12.5
9	6	273	GLU	12.5
1	x	620	G	12.5
1	x	637	G	12.5
5	R	655	ARG	12.5
3	I	485	PRO	12.5
9	6	374	VAL	12.5
10	l	631	LYS	12.5
7	W	264	ILE	12.5
6	Z	247	THR	12.5
7	W	260	ASP	12.5
2	D	75	ASP	12.5
6	1	446	ASN	12.5
2	S	277	LEU	12.5
1	x	632	A	12.5
10	l	651	ASP	12.4
9	K	104	THR	12.4
5	R	628	PRO	12.4
8	G	10	LYS	12.4
5	C	59	PHE	12.4
8	3	212	PHE	12.4
2	T	434	GLU	12.4
1	x	725	A	12.4
5	P	231	VAL	12.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	S	212	GLU	12.3
7	E	88	GLN	12.3
6	F	20	MET	12.3
2	S	229	ARG	12.3
5	C	70	VAL	12.3
9	6	379	GLU	12.3
1	x	634	G	12.3
10	l	624	HIS	12.3
6	F	58	HIS	12.3
2	S	253	GLY	12.3
3	A	24	GLY	12.3
4	N	409	LYS	12.2
3	A	13	ILE	12.2
1	v	323	A	12.2
1	V	28	G	12.2
7	E	30	ARG	12.2
8	G	67	ILE	12.2
10	9	234	VAL	12.2
9	7	415	PRO	12.2
8	G	39	ASN	12.2
2	T	469	ARG	12.2
5	P	308	VAL	12.2
1	v	251	G	12.2
1	w	430	U	12.2
5	P	225	ASN	12.1
9	6	272	ARG	12.1
5	C	68	GLU	12.1
8	G	62	ILE	12.1
8	G	51	SER	12.1
9	K	133	HIS	12.1
1	V	135	A	12.1
1	v	296	U	12.1
5	P	221	GLU	12.1
8	G	58	GLY	12.1
2	U	674	PRO	12.1
9	7	539	ARG	12.0
9	K	131	ARG	12.0
3	J	643	CYS	12.0
9	8	756	ASP	12.0
1	v	242	U	12.0
1	w	497	U	12.0
1	x	616	G	12.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	v	243	U	12.0
1	x	628	G	12.0
1	w	527	U	12.0
6	2	646	ASN	12.0
7	Y	642	ARG	12.0
6	1	480	GLU	12.0
4	M	261	ARG	11.9
10	L	26	SER	11.9
4	B	20	LYS	11.9
1	x	749	U	11.9
2	U	624	THR	11.9
3	H	275	GLU	11.9
7	E	39	VAL	11.9
8	G	72	ALA	11.9
6	2	664	ILE	11.9
1	V	11	G	11.8
6	F	35	SER	11.8
1	v	354	G	11.8
6	2	678	GLU	11.8
5	R	664	ASN	11.8
9	K	159	SER	11.8
5	C	57	LYS	11.7
3	H	268	GLY	11.7
8	G	30	ILE	11.7
2	T	454	ARG	11.7
8	5	650	THR	11.7
8	3	260	VAL	11.7
3	A	34	PHE	11.7
9	K	164	ALA	11.7
8	G	47	GLU	11.7
9	6	220	PRO	11.6
7	E	58	LEU	11.6
9	K	23	PRO	11.6
9	6	370	ASP	11.6
7	W	240	ASN	11.6
10	l	654	THR	11.6
3	A	35	ASP	11.6
6	Z	235	SER	11.6
9	K	113	ASP	11.6
9	6	279	GLN	11.6
7	E	42	ARG	11.5
1	x	633	C	11.5

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Mol	Chain	Res	Type	RSRZ
1	w	502	A	11.5
5	Q	440	THR	11.5
7	Y	653	TYR	11.5
9	7	532	ILE	11.5
2	T	465	GLY	11.5
2	T	424	THR	11.5
9	K	122	GLU	11.5
7	Y	665	HIS	11.5
1	V	138	G	11.5
2	U	672	ILE	11.4
2	T	452	ASP	11.4
1	V	157	U	11.4
1	w	415	G	11.4
1	V	31	C	11.4
10	0	444	GLU	11.4
4	B	60	ILE	11.4
4	O	644	LYS	11.4
4	N	471	PRO	11.4
3	H	281	THR	11.4
1	V	17	G	11.4
6	F	51	ILE	11.4
7	E	92	ASN	11.4
7	X	476	ARG	11.4
9	8	779	GLU	11.4
3	J	677	LEU	11.4
9	8	712	TYR	11.4
2	D	69	ARG	11.4
5	R	612	THR	11.3
9	7	535	VAL	11.3
1	V	29	A	11.3
2	U	612	GLU	11.3
1	w	446	C	11.3
8	3	250	THR	11.3
2	T	466	CYS	11.3
5	R	622	GLU	11.3
1	V	35	A	11.3
2	U	627	VAL	11.3
3	J	637	HIS	11.3
9	6	376	VAL	11.3
1	x	722	C	11.3
9	8	761	TYR	11.3
2	U	635	ALA	11.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	Y	625	LEU	11.2
3	I	431	LYS	11.2
7	X	431	ILE	11.2
2	D	61	VAL	11.2
4	N	408	MET	11.2
10	0	452	LYS	11.1
9	8	728	PRO	11.1
5	C	17	GLN	11.1
1	v	249	A	11.1
4	O	659	SER	11.1
9	7	414	ALA	11.1
9	6	334	MET	11.1
5	P	264	ASN	11.1
3	I	446	GLU	11.1
8	3	265	ASN	11.1
2	D	27	VAL	11.1
1	w	555	C	11.1
5	C	32	LEU	11.1
1	x	710	G	11.1
2	D	62	TYR	11.0
4	B	48	LYS	11.0
1	w	524	U	11.0
6	2	654	ALA	11.0
7	W	288	GLN	11.0
7	W	282	ASP	11.0
3	I	410	GLN	11.0
7	E	68	THR	11.0
4	N	416	THR	11.0
6	2	635	SER	11.0
2	T	468	ILE	11.0
8	G	57	ILE	11.0
2	S	242	GLN	11.0
3	H	230	THR	11.0
3	H	276	ASN	10.9
1	V	90	U	10.9
8	3	217	LEU	10.9
10	0	411	THR	10.9
2	S	240	ASN	10.9
6	2	652	ASP	10.9
5	C	40	THR	10.9
7	X	492	ASN	10.9
9	K	108	ALA	10.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	v	340	G	10.9
7	X	488	GLN	10.9
8	5	651	SER	10.9
9	8	745	GLY	10.9
7	X	452	GLU	10.9
1	w	540	G	10.9
9	7	506	PHE	10.9
1	w	406	U	10.9
4	O	631	GLY	10.9
1	v	224	C	10.9
2	T	449	THR	10.9
5	Q	473	MET	10.9
8	5	614	ASP	10.9
10	0	443	GLU	10.8
7	Y	664	ILE	10.8
1	w	404	C	10.8
4	O	651	GLU	10.8
9	8	665	GLU	10.8
1	x	715	U	10.8
10	L	27	GLY	10.8
6	1	476	GLU	10.8
10	9	250	ILE	10.8
1	v	304	A	10.8
3	A	19	CYS	10.8
5	Q	468	GLU	10.8
10	L	6	CYS	10.8
10	l	605	TYR	10.8
1	V	124	U	10.8
3	A	75	GLU	10.8
8	5	622	ASN	10.8
1	w	419	A	10.7
8	5	666	SER	10.7
9	6	362	LYS	10.7
2	S	238	ASN	10.7
7	X	454	MET	10.7
3	I	413	ASP	10.7
6	F	55	LEU	10.7
1	w	537	U	10.7
7	W	233	VAL	10.7
4	N	447	LEU	10.7
5	C	104	ASP	10.7
2	D	45	ASN	10.7

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Mol	Chain	Res	Type	RSRZ
8	4	413	MET	10.7
1	v	218	G	10.7
1	v	235	A	10.7
2	S	223	ASN	10.7
6	Z	270	LEU	10.7
9	6	278	ARG	10.7
5	Q	464	ASN	10.6
9	8	666	ARG	10.6
2	S	262	TYR	10.6
1	x	692	C	10.6
2	U	652	ASP	10.6
1	v	292	C	10.6
1	x	631	C	10.6
8	3	213	MET	10.6
2	D	49	THR	10.6
3	A	12	HIS	10.6
5	P	214	GLU	10.6
1	x	699	C	10.6
10	9	260	GLY	10.6
9	8	748	PHE	10.6
2	D	25	GLY	10.5
8	4	463	ARG	10.5
5	R	646	CYS	10.5
10	L	38	TYR	10.5
8	3	251	SER	10.5
9	6	221	TYR	10.5
10	0	453	THR	10.5
2	T	426	GLU	10.5
5	P	301	LEU	10.5
1	x	712	A	10.5
1	w	544	C	10.5
8	5	623	GLY	10.5
4	B	52	PRO	10.5
4	M	209	LYS	10.5
10	0	424	HIS	10.5
7	X	453	TYR	10.5
1	x	601	A	10.5
2	D	42	GLN	10.5
7	E	40	ASN	10.4
4	B	9	LYS	10.4
6	F	71	TYR	10.4
2	U	628	TYR	10.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	M	220	LYS	10.4
6	2	662	VAL	10.4
9	K	145	GLY	10.4
6	1	464	ILE	10.4
1	v	205	U	10.4
2	U	654	ARG	10.4
4	B	78	THR	10.4
9	K	165	ASP	10.4
6	F	45	ALA	10.4
1	w	500	C	10.4
2	T	406	PRO	10.4
6	F	15	THR	10.4
7	X	447	ILE	10.4
10	0	418	PRO	10.4
7	Y	660	ASP	10.3
9	8	759	SER	10.3
5	C	12	THR	10.3
2	S	224	THR	10.3
5	R	647	ARG	10.3
6	F	9	PRO	10.3
4	B	15	VAL	10.3
7	E	47	ILE	10.3
10	9	210	ASP	10.3
8	4	454	GLN	10.3
2	S	245	ASN	10.3
8	4	451	SER	10.3
2	T	416	HIS	10.3
2	S	213	ALA	10.2
4	O	650	ARG	10.2
3	H	265	ARG	10.2
7	E	44	GLU	10.2
9	8	742	LYS	10.2
5	P	240	THR	10.2
8	3	270	LEU	10.2
8	G	54	GLN	10.2
3	A	7	SER	10.2
1	x	750	U	10.2
2	T	437	ASP	10.2
3	A	84	GLY	10.2
4	O	646	THR	10.2
9	8	750	GLU	10.2
10	0	442	MET	10.2

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Mol	Chain	Res	Type	RSRZ
7	E	50	PHE	10.2
9	8	753	HIS	10.2
8	3	254	GLN	10.2
4	N	473	SER	10.1
7	E	45	GLY	10.1
9	6	364	ALA	10.1
2	T	435	ALA	10.1
10	l	650	ILE	10.1
8	4	460	VAL	10.1
7	Y	654	MET	10.1
2	U	637	ASP	10.1
7	E	19	ASN	10.1
9	6	367	LYS	10.1
9	K	115	THR	10.1
5	Q	424	PHE	10.1
9	K	140	SER	10.1
4	N	441	LYS	10.1
6	1	429	TYR	10.1
7	E	28	ARG	10.0
9	6	333	HIS	10.0
7	W	272	LYS	10.0
6	2	642	MET	10.0
10	L	43	GLU	10.0
9	8	705	LEU	10.0
1	V	122	C	10.0
5	Q	496	ILE	10.0
2	D	24	THR	10.0
4	B	8	MET	10.0
1	x	705	U	10.0
1	V	87	C	9.9
1	V	44	U	9.9
3	I	445	ASP	9.9
9	K	173	ARG	9.9
9	7	523	PHE	9.9
4	O	606	PHE	9.9
4	B	72	ASP	9.9
7	W	239	VAL	9.9
3	J	671	LEU	9.9
8	5	605	HIS	9.9
9	K	151	TYR	9.9
10	l	637	TYR	9.9
5	R	711	ARG	9.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	Q	495	TYR	9.9
1	x	762	C	9.9
9	8	746	TYR	9.9
4	N	462	GLY	9.9
6	2	619	VAL	9.9
2	S	276	MET	9.8
10	9	216	ASP	9.8
8	5	674	GLU	9.8
7	W	259	ASP	9.8
5	C	33	THR	9.8
2	D	50	TYR	9.8
1	V	123	A	9.8
1	w	511	A	9.8
8	G	73	LEU	9.8
5	Q	453	LEU	9.8
1	v	328	U	9.8
1	v	201	A	9.8
9	7	417	ASP	9.8
3	I	477	LEU	9.8
4	B	17	ILE	9.8
5	P	295	TYR	9.8
5	R	613	PRO	9.8
9	8	724	GLU	9.8
10	l	611	THR	9.8
9	K	120	ARG	9.8
5	Q	500	PHE	9.7
6	1	449	GLU	9.7
7	W	267	LYS	9.7
2	S	207	ILE	9.7
6	Z	214	LEU	9.7
8	5	612	PHE	9.7
9	8	619	ILE	9.7
10	L	4	PHE	9.7
7	Y	640	ASN	9.7
6	2	606	ASN	9.7
3	J	628	ILE	9.7
6	Z	251	ILE	9.7
4	N	470	LEU	9.7
4	M	211	SER	9.7
9	8	615	PRO	9.7
2	S	208	LYS	9.7
4	B	4	VAL	9.7

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Mol	Chain	Res	Type	RSRZ
5	Q	513	PRO	9.7
4	B	75	PRO	9.6
5	Q	458	ALA	9.6
6	F	76	GLU	9.6
8	G	34	PHE	9.6
8	5	604	ALA	9.6
10	9	218	PRO	9.6
8	5	675	ARG	9.6
1	v	233	C	9.6
9	6	373	ARG	9.6
2	S	273	LEU	9.6
3	J	620	ILE	9.6
8	5	639	ASN	9.6
9	6	363	HIS	9.6
9	8	778	VAL	9.6
3	I	484	GLY	9.6
5	C	74	TRP	9.6
10	L	46	ALA	9.6
1	x	708	G	9.6
6	2	656	SER	9.6
8	5	667	ILE	9.6
3	A	36	LYS	9.6
6	2	647	THR	9.6
7	Y	666	SER	9.6
3	J	675	GLU	9.6
3	I	429	THR	9.6
7	W	228	ARG	9.5
1	w	445	U	9.5
1	v	204	C	9.5
1	x	611	G	9.5
1	V	114	C	9.5
1	w	484	G	9.5
6	1	441	ASN	9.5
2	T	436	GLU	9.5
2	D	67	LYS	9.5
6	Z	246	ASN	9.5
4	O	605	ARG	9.5
5	R	619	ARG	9.5
5	R	614	GLU	9.5
5	C	42	VAL	9.5
8	3	257	ILE	9.5
5	P	257	LYS	9.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	E	73	GLN	9.5
1	V	20	G	9.5
2	D	53	GLY	9.5
7	X	464	ILE	9.5
7	W	286	LEU	9.4
3	A	67	LEU	9.4
9	7	422	LEU	9.4
1	V	142	G	9.4
8	4	457	ILE	9.4
2	D	22	THR	9.4
3	J	676	ASN	9.4
4	O	637	ASN	9.4
6	1	452	ASP	9.4
8	G	23	GLY	9.4
9	K	85	GLU	9.4
9	K	153	HIS	9.4
8	3	204	ALA	9.4
3	J	611	GLN	9.4
8	3	225	ARG	9.4
8	4	450	THR	9.4
1	x	618	G	9.4
9	8	776	VAL	9.4
10	9	231	LYS	9.4
1	x	739	G	9.4
1	w	486	C	9.4
8	3	236	PRO	9.4
2	D	73	LEU	9.3
4	B	63	ASN	9.3
5	Q	494	ARG	9.3
4	B	74	LEU	9.3
2	D	80	ALA	9.3
1	v	327	U	9.3
2	T	417	ILE	9.3
4	M	260	ILE	9.3
9	6	222	LEU	9.3
1	v	208	C	9.3
9	6	216	ARG	9.3
3	H	266	VAL	9.3
6	2	621	VAL	9.3
2	T	407	ILE	9.3
6	Z	227	MET	9.3
9	6	331	ARG	9.3

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Mol	Chain	Res	Type	RSRZ
9	K	157	MET	9.3
9	7	552	GLU	9.3
10	0	431	LYS	9.3
3	J	622	GLN	9.3
5	R	639	ASN	9.3
9	6	365	ASP	9.3
9	6	218	PRO	9.2
3	I	432	ALA	9.2
6	2	628	GLU	9.2
2	T	438	ASN	9.2
7	W	270	SER	9.2
10	0	434	VAL	9.2
9	7	567	LYS	9.2
3	J	631	PHE	9.2
6	F	18	PRO	9.2
7	Y	623	ARG	9.2
9	K	123	PHE	9.2
4	N	453	VAL	9.2
2	U	634	GLU	9.2
10	L	19	SER	9.2
2	D	38	ASN	9.2
9	8	621	TYR	9.2
9	K	135	VAL	9.2
8	5	619	LEU	9.2
7	X	467	LYS	9.2
1	w	534	U	9.2
6	Z	265	ARG	9.2
8	5	632	ARG	9.2
2	D	77	LEU	9.1
5	P	260	ASP	9.1
8	4	436	PRO	9.1
1	v	338	G	9.1
9	8	773	ARG	9.1
9	6	217	ASP	9.1
9	7	547	ALA	9.1
8	4	432	ARG	9.1
1	v	319	C	9.1
8	5	665	ASN	9.1
3	H	239	ASN	9.1
7	Y	672	LYS	9.1
6	2	655	LEU	9.1
3	J	607	SER	9.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	W	247	ILE	9.1
9	K	67	MET	9.1
9	7	489	TRP	9.1
1	w	528	U	9.0
5	C	58	ALA	9.0
10	l	622	LYS	9.0
10	l	636	ASP	9.0
6	2	658	HIS	9.0
6	F	56	SER	9.0
10	9	258	GLN	9.0
7	W	273	GLN	9.0
3	J	667	LEU	9.0
3	H	272	LEU	9.0
1	V	148	G	9.0
2	D	9	VAL	9.0
3	H	229	GLY	9.0
10	9	257	PHE	9.0
7	X	473	GLN	9.0
4	O	649	ASN	8.9
1	V	3	A	8.9
4	N	466	ARG	8.9
2	T	477	LEU	8.9
3	H	223	ASP	8.9
7	X	423	ARG	8.9
6	F	8	LYS	8.9
5	C	102	ARG	8.9
10	0	410	ASP	8.9
3	H	207	SER	8.9
5	C	99	MET	8.9
1	v	289	C	8.9
1	x	716	C	8.9
10	L	33	ASN	8.9
9	7	569	ILE	8.9
10	9	242	MET	8.9
3	J	678	VAL	8.9
6	2	681	ASP	8.9
7	E	52	GLU	8.9
2	S	210	LEU	8.9
2	U	657	GLN	8.9
9	K	76	GLU	8.9
9	6	375	LEU	8.9
3	A	43	CYS	8.8

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Mol	Chain	Res	Type	RSRZ
5	P	311	ARG	8.8
9	8	713	ASP	8.8
5	P	227	GLY	8.8
7	Y	656	LEU	8.8
4	N	430	THR	8.8
1	x	728	U	8.8
9	7	536	TYR	8.8
3	I	438	ASN	8.8
4	B	50	ARG	8.8
2	S	255	VAL	8.8
7	W	236	TYR	8.8
5	P	248	ASN	8.8
1	v	244	U	8.8
4	M	215	VAL	8.8
6	2	644	LEU	8.8
9	6	329	ILE	8.8
8	5	629	GLY	8.8
7	X	465	HIS	8.8
1	w	495	U	8.8
3	J	686	PRO	8.8
4	M	258	LEU	8.7
9	6	344	ARG	8.7
10	l	638	TYR	8.7
9	8	754	GLU	8.7
9	7	420	PRO	8.7
3	J	684	GLY	8.7
1	V	4	C	8.7
8	G	7	PRO	8.7
8	3	208	GLU	8.7
10	L	10	ASP	8.7
10	L	36	ASP	8.7
8	4	428	GLN	8.7
1	x	757	U	8.7
10	9	211	THR	8.7
7	E	82	ASP	8.7
1	V	153	C	8.7
5	P	305	SER	8.7
7	X	482	ASP	8.7
5	C	23	GLU	8.7
7	W	248	ILE	8.7
6	Z	262	VAL	8.7
8	5	659	MET	8.7

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Mol	Chain	Res	Type	RSRZ
6	1	455	LEU	8.7
7	W	232	GLN	8.7
5	R	694	ARG	8.6
1	w	413	C	8.6
7	Y	688	GLN	8.6
9	8	767	LYS	8.6
6	Z	257	GLY	8.6
8	G	26	HIS	8.6
9	8	771	GLY	8.6
4	O	611	SER	8.6
5	C	44	ILE	8.6
4	O	638	THR	8.6
1	v	254	A	8.6
10	L	11	THR	8.6
8	4	470	LEU	8.6
10	9	239	CYS	8.6
6	1	457	GLY	8.6
9	K	144	ARG	8.6
4	M	208	MET	8.6
8	G	4	ALA	8.6
9	7	515	THR	8.6
9	7	558	HIS	8.6
3	A	8	LYS	8.6
5	P	216	LEU	8.6
9	7	550	GLU	8.6
6	Z	241	ASN	8.5
10	l	614	THR	8.5
4	M	271	PRO	8.5
2	D	81	PRO	8.5
4	O	609	LYS	8.5
3	J	626	ILE	8.5
1	V	16	G	8.5
8	3	274	GLU	8.5
1	x	707	U	8.5
5	Q	449	ASN	8.5
5	R	704	ASP	8.5
1	V	48	C	8.5
8	5	655	ASN	8.5
4	O	610	LEU	8.5
9	6	267	MET	8.5
4	M	237	ASN	8.5
6	Z	248	GLU	8.5

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Mol	Chain	Res	Type	RSRZ
9	6	325	VAL	8.5
9	8	729	ILE	8.5
8	G	13	MET	8.5
7	X	428	ARG	8.5
1	w	554	G	8.4
8	G	11	LYS	8.4
5	P	247	ARG	8.4
3	J	681	THR	8.4
6	F	68	ASN	8.4
8	5	660	VAL	8.4
1	x	743	A	8.4
2	U	615	GLY	8.4
5	Q	459	PHE	8.4
6	2	617	LYS	8.4
7	X	430	ARG	8.4
5	R	695	TYR	8.4
1	V	18	G	8.4
6	1	470	LEU	8.4
9	8	680	GLN	8.4
3	A	41	ILE	8.4
1	V	141	G	8.4
7	Y	680	LYS	8.4
10	L	42	MET	8.4
6	1	428	GLU	8.4
3	H	267	LEU	8.4
6	Z	224	LYS	8.4
8	4	405	HIS	8.4
3	J	617	MET	8.4
5	R	660	ASP	8.4
9	7	568	LYS	8.4
9	7	563	HIS	8.3
2	S	234	GLU	8.3
3	I	421	GLN	8.3
4	N	437	ASN	8.3
1	x	689	C	8.3
4	B	51	GLU	8.3
6	1	417	LYS	8.3
8	G	16	LYS	8.3
5	R	640	THR	8.3
6	F	43	GLN	8.3
2	U	677	LEU	8.3
2	U	642	GLN	8.3

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Mol	Chain	Res	Type	RSRZ
6	Z	245	ALA	8.3
7	Y	637	GLU	8.3
9	6	317	SER	8.3
3	A	87	PRO	8.3
3	H	224	GLY	8.3
7	E	91	SER	8.3
1	w	402	U	8.3
5	P	275	THR	8.3
2	D	59	GLU	8.3
8	4	430	ILE	8.3
7	Y	684	ILE	8.3
9	6	268	GLU	8.3
5	C	43	LEU	8.2
6	1	442	MET	8.2
3	H	274	GLY	8.2
9	8	616	ARG	8.2
9	K	16	ARG	8.2
2	D	52	ASP	8.2
6	2	680	GLU	8.2
5	R	648	ASN	8.2
6	1	474	GLY	8.2
1	w	405	U	8.2
3	H	213	ILE	8.2
3	I	407	LYS	8.2
2	S	221	GLU	8.2
4	N	440	LEU	8.2
10	0	435	LYS	8.2
1	V	154	G	8.2
1	x	629	A	8.2
1	V	117	G	8.2
2	S	267	LYS	8.2
9	K	147	ALA	8.2
4	B	47	LEU	8.1
6	1	465	ARG	8.1
7	E	84	ILE	8.1
7	Y	671	ARG	8.1
6	1	454	ALA	8.1
3	A	11	GLN	8.1
9	K	18	PRO	8.1
9	6	345	GLY	8.1
5	P	243	LEU	8.1
2	U	669	ARG	8.1

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Mol	Chain	Res	Type	RSRZ
3	A	17	MET	8.1
6	2	639	TYR	8.1
8	4	407	PRO	8.1
7	E	66	SER	8.1
2	U	643	MET	8.1
10	9	237	TYR	8.1
8	G	50	THR	8.1
4	B	54	GLN	8.1
6	Z	240	MET	8.1
8	G	48	MET	8.1
5	R	656	VAL	8.1
5	R	661	ARG	8.1
8	4	411	LYS	8.1
10	0	433	ASN	8.0
10	9	215	HIS	8.0
2	U	676	MET	8.0
9	7	549	ILE	8.0
2	T	442	GLN	8.0
5	C	75	THR	8.0
6	1	444	LEU	8.0
8	3	252	GLY	8.0
9	K	158	HIS	8.0
9	6	330	LYS	8.0
8	G	18	SER	8.0
5	Q	443	LEU	8.0
4	B	38	THR	8.0
9	8	769	ILE	8.0
8	G	56	ASN	8.0
1	w	550	U	8.0
3	A	30	THR	8.0
3	A	29	GLY	8.0
4	B	53	VAL	8.0
9	7	514	THR	8.0
10	L	54	THR	8.0
4	O	675	PRO	8.0
1	w	515	U	8.0
1	w	433	C	7.9
9	K	142	LYS	7.9
7	W	226	GLN	7.9
9	K	19	ILE	7.9
9	K	166	GLY	7.9
5	Q	457	LYS	7.9

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Mol	Chain	Res	Type	RSRZ
7	E	51	ASP	7.9
9	7	416	ARG	7.9
10	L	29	LYS	7.9
3	I	427	ILE	7.9
6	F	30	LYS	7.9
5	R	705	SER	7.9
6	1	458	HIS	7.9
8	G	59	MET	7.9
5	P	309	VAL	7.9
5	R	616	LEU	7.9
2	U	607	ILE	7.9
4	B	2	LYS	7.9
8	4	414	ASP	7.9
8	5	653	GLN	7.8
3	A	85	PRO	7.8
9	K	139	ARG	7.8
2	D	57	GLN	7.8
6	1	453	GLY	7.8
9	8	739	ARG	7.8
3	A	66	VAL	7.8
9	7	474	LYS	7.8
5	Q	467	LEU	7.8
5	Q	456	VAL	7.8
4	O	677	ASP	7.8
10	0	457	PHE	7.8
3	A	73	ARG	7.8
6	Z	253	GLY	7.8
2	U	681	PRO	7.8
6	2	661	GLU	7.8
2	U	675	ASP	7.8
2	U	651	ARG	7.8
4	M	253	VAL	7.8
5	P	256	VAL	7.8
9	K	78	ARG	7.8
8	3	258	GLY	7.8
3	I	482	VAL	7.7
5	C	107	ILE	7.8
3	J	636	LYS	7.7
2	S	216	HIS	7.7
2	T	458	LEU	7.7
10	0	450	ILE	7.7
1	w	432	A	7.7

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Mol	Chain	Res	Type	RSRZ
3	J	633	ALA	7.7
7	Y	633	VAL	7.7
9	K	117	SER	7.7
7	W	284	ILE	7.7
8	G	12	PHE	7.7
9	6	310	VAL	7.7
9	6	332	ILE	7.7
5	C	114	LEU	7.7
1	V	32	A	7.7
6	2	609	PRO	7.7
3	I	420	LEU	7.7
10	9	236	ASP	7.7
6	Z	231	GLY	7.7
6	F	6	ASN	7.7
4	N	452	PRO	7.7
9	8	689	TRP	7.7
2	U	623	ASN	7.7
9	K	14	ALA	7.7
2	D	17	ILE	7.7
3	I	467	LEU	7.7
9	8	722	GLU	7.7
10	9	212	TYR	7.7
3	A	46	ASP	7.7
1	v	256	A	7.7
9	8	738	LYS	7.7
1	x	742	G	7.7
9	6	281	GLU	7.7
4	N	439	HIS	7.6
8	4	455	ASN	7.6
1	V	21	A	7.6
9	6	213	PHE	7.6
2	D	29	ARG	7.6
7	E	80	LYS	7.6
8	4	404	ALA	7.6
6	F	39	TYR	7.6
4	B	61	ARG	7.6
9	8	686	LEU	7.6
7	X	472	LYS	7.6
7	Y	690	VAL	7.6
2	D	21	GLU	7.6
5	P	296	ILE	7.6
4	N	420	LYS	7.6

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Mol	Chain	Res	Type	RSRZ
6	Z	258	HIS	7.6
9	K	169	ILE	7.6
8	5	670	LEU	7.6
5	Q	422	GLU	7.6
9	K	167	LYS	7.6
7	X	471	ARG	7.6
3	J	685	PRO	7.6
9	7	504	THR	7.6
1	V	34	G	7.5
7	Y	668	THR	7.5
3	H	211	GLN	7.5
2	U	636	GLU	7.5
4	N	448	LYS	7.5
5	Q	474	TRP	7.5
4	M	263	ASN	7.5
2	D	15	GLY	7.5
5	P	211	MET	7.5
3	J	646	ASP	7.5
7	Y	636	TYR	7.5
7	W	253	TYR	7.5
4	N	460	ILE	7.5
6	2	659	LEU	7.5
2	U	625	GLY	7.5
8	3	232	ARG	7.5
8	3	275	ARG	7.5
10	9	240	LYS	7.5
9	7	473	GLU	7.5
7	W	234	TRP	7.5
1	x	760	C	7.5
4	O	632	VAL	7.5
2	S	250	TYR	7.5
9	8	703	LYS	7.5
10	0	412	TYR	7.5
9	6	378	VAL	7.5
7	W	283	ASN	7.4
8	4	420	LYS	7.4
6	Z	264	ILE	7.4
8	3	214	ASP	7.4
9	8	772	ARG	7.4
4	O	660	ILE	7.4
1	w	409	C	7.4
6	2	625	TRP	7.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	6	314	THR	7.4
4	M	250	ARG	7.4
8	3	230	ILE	7.4
8	3	266	SER	7.4
7	X	455	ASN	7.4
5	Q	427	GLY	7.4
9	K	21	TYR	7.4
5	Q	514	LEU	7.4
5	C	71	LYS	7.4
9	6	219	ILE	7.4
4	M	278	THR	7.4
4	O	608	MET	7.4
10	L	60	GLY	7.4
9	6	324	GLU	7.3
6	F	75	VAL	7.3
9	7	513	ASP	7.3
1	w	456	A	7.3
4	O	658	LEU	7.3
9	8	743	PRO	7.3
5	Q	504	ASP	7.3
5	Q	510	LEU	7.3
5	C	113	PRO	7.3
5	P	212	THR	7.3
10	L	30	HIS	7.3
9	8	613	PHE	7.3
7	E	90	VAL	7.3
1	V	143	A	7.3
4	M	231	GLY	7.3
9	6	308	ALA	7.3
9	8	725	VAL	7.3
1	v	222	U	7.3
5	Q	413	PRO	7.3
4	M	272	ASP	7.3
8	3	248	MET	7.3
6	Z	271	TYR	7.3
10	l	635	LYS	7.3
4	M	257	THR	7.3
8	G	45	CYS	7.3
5	R	638	ASN	7.3
1	V	134	U	7.3
10	l	618	PRO	7.3
1	V	164	G	7.3

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Mol	Chain	Res	Type	RSRZ
5	Q	432	LEU	7.3
10	9	244	GLU	7.3
8	G	35	ASP	7.3
5	Q	460	ASP	7.2
9	7	418	PRO	7.2
7	Y	650	PHE	7.2
9	7	511	ASN	7.2
4	O	669	ILE	7.2
6	1	481	ASP	7.2
5	P	270	VAL	7.2
9	7	423	PRO	7.2
1	v	248	C	7.2
6	1	435	SER	7.2
4	N	432	VAL	7.2
7	Y	692	ASN	7.2
9	7	531	ARG	7.2
4	B	49	ASN	7.2
5	Q	507	ILE	7.2
5	P	304	ASP	7.2
6	2	610	PHE	7.2
1	v	241	G	7.2
5	P	220	GLU	7.2
8	4	474	GLU	7.2
2	T	478	LYS	7.2
9	8	675	ILE	7.2
5	R	632	LEU	7.2
1	V	39	U	7.2
6	Z	208	LYS	7.1
1	w	417	G	7.1
5	C	106	VAL	7.1
6	F	60	GLY	7.1
9	K	174	VAL	7.1
1	x	737	U	7.1
5	C	96	ILE	7.1
5	P	215	GLU	7.1
1	x	646	C	7.1
5	Q	417	GLN	7.1
10	l	629	LYS	7.1
3	I	424	ARG	7.1
3	J	614	ASP	7.1
5	Q	492	LYS	7.1
7	X	451	ASP	7.1

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Mol	Chain	Res	Type	RSRZ
1	x	652	G	7.1
1	v	219	A	7.1
6	1	467	ASN	7.1
9	K	170	ASP	7.1
10	l	653	THR	7.1
1	V	129	U	7.1
4	O	625	VAL	7.1
5	P	306	VAL	7.1
1	v	298	C	7.0
9	K	83	GLU	7.0
2	T	411	HIS	7.0
2	U	630	GLY	7.0
6	1	412	ASN	7.0
10	9	209	CYS	7.0
3	J	644	ASP	7.0
9	6	307	VAL	7.0
3	H	285	PRO	7.0
6	F	14	LEU	7.0
7	Y	619	ASN	7.0
1	v	312	A	7.0
4	O	648	LYS	7.0
1	v	357	U	7.0
1	w	483	C	7.0
4	M	238	THR	7.0
2	T	429	ARG	7.0
6	2	624	LYS	7.0
2	U	663	ILE	7.0
5	P	219	ARG	7.0
4	M	206	PHE	7.0
3	A	15	TYR	7.0
10	l	615	HIS	7.0
9	8	780	ARG	7.0
1	v	348	G	7.0
8	4	440	LEU	7.0
2	D	78	LYS	6.9
1	V	99	C	6.9
5	R	657	LYS	6.9
9	7	487	LYS	6.9
10	l	608	TYR	6.9
4	B	73	SER	6.9
8	4	468	ILE	6.9
9	6	215	PRO	6.9

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Mol	Chain	Res	Type	RSRZ
9	8	614	ALA	6.9
7	X	470	SER	6.9
3	J	683	GLU	6.9
2	U	639	MET	6.9
9	8	760	ALA	6.9
4	B	5	ARG	6.9
9	7	525	VAL	6.9
3	J	635	ASP	6.9
9	7	522	GLU	6.9
1	V	8	C	6.9
7	W	244	GLU	6.9
4	N	410	LEU	6.9
3	I	471	LEU	6.9
1	V	101	C	6.9
4	M	275	PRO	6.9
1	w	427	U	6.9
6	Z	225	TRP	6.9
10	l	659	GLN	6.9
7	W	223	ARG	6.9
2	T	460	GLN	6.8
4	N	469	ILE	6.8
8	3	229	GLY	6.8
5	P	249	ASN	6.8
5	R	669	ASN	6.8
4	O	671	PRO	6.8
9	8	617	ASP	6.8
8	3	242	ILE	6.8
8	4	461	VAL	6.8
7	Y	670	SER	6.8
1	w	563	U	6.8
7	Y	659	ASP	6.8
9	7	545	GLY	6.8
9	6	340	SER	6.8
7	X	448	ILE	6.8
7	E	21	ILE	6.8
5	C	30	SER	6.8
9	7	580	ARG	6.8
9	8	622	LEU	6.8
7	W	290	VAL	6.8
10	L	21	ARG	6.8
7	X	478	MET	6.8
7	X	483	ASN	6.8

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Mol	Chain	Res	Type	RSRZ
6	1	448	GLU	6.8
4	O	615	VAL	6.8
5	P	271	LYS	6.8
9	7	520	ARG	6.7
2	D	79	ASN	6.7
3	J	634	PHE	6.7
2	D	74	PRO	6.7
3	H	221	LEU	6.7
7	X	475	GLY	6.7
6	1	472	ILE	6.7
5	P	274	TRP	6.7
9	8	671	ARG	6.7
8	5	626	HIS	6.7
9	7	554	GLU	6.7
3	H	244	ASP	6.7
5	R	699	MET	6.7
7	X	420	LEU	6.7
3	H	212	HIS	6.7
2	S	254	ARG	6.7
7	W	261	ALA	6.7
5	Q	411	MET	6.7
6	1	430	LYS	6.7
8	5	633	GLY	6.7
3	J	670	VAL	6.7
2	U	679	ASN	6.7
9	K	141	GLY	6.7
7	E	18	ILE	6.7
1	v	255	G	6.7
5	C	101	LEU	6.7
5	Q	416	LEU	6.7
6	F	52	ASP	6.7
5	R	666	VAL	6.7
2	T	481	PRO	6.7
9	7	546	TYR	6.7
6	2	673	ARG	6.7
7	W	227	ASN	6.6
7	X	487	LEU	6.6
2	S	209	VAL	6.6
4	M	228	THR	6.6
3	A	25	ARG	6.6
7	Y	648	ILE	6.6
9	8	721	ARG	6.6

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Mol	Chain	Res	Type	RSRZ
9	8	623	PRO	6.6
1	v	216	G	6.6
3	J	613	ILE	6.6
5	P	252	LEU	6.6
9	K	136	TYR	6.6
9	6	313	ASP	6.6
8	5	613	MET	6.6
2	D	16	HIS	6.6
4	M	202	LYS	6.6
4	M	252	PRO	6.6
9	6	335	VAL	6.6
5	Q	446	CYS	6.6
8	5	635	ASP	6.6
3	A	78	VAL	6.6
3	A	71	LEU	6.6
5	Q	438	ASN	6.6
1	x	720	U	6.6
5	Q	414	GLU	6.6
7	Y	689	SER	6.6
7	Y	632	GLN	6.6
10	0	405	TYR	6.6
9	6	323	PHE	6.6
10	L	5	TYR	6.6
6	2	630	LYS	6.6
1	v	325	A	6.6
5	P	294	ARG	6.5
7	Y	639	VAL	6.5
9	K	150	GLU	6.5
5	Q	428	PRO	6.5
2	U	664	ARG	6.5
5	Q	423	GLU	6.5
6	Z	219	VAL	6.5
3	H	278	VAL	6.5
5	Q	447	ARG	6.5
9	8	717	SER	6.5
1	w	552	G	6.5
5	R	650	LYS	6.5
3	H	287	PRO	6.5
1	w	535	A	6.5
8	3	222	ASN	6.5
8	4	475	ARG	6.5
5	Q	476	GLU	6.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	R	709	VAL	6.5
8	4	423	GLY	6.5
4	M	213	GLU	6.5
9	7	419	ILE	6.5
7	Y	630	ARG	6.5
10	0	415	HIS	6.5
5	R	621	GLU	6.5
10	9	222	LYS	6.5
10	l	617	SER	6.4
7	E	20	LEU	6.4
1	x	738	G	6.4
1	v	226	A	6.4
2	D	58	LEU	6.4
2	T	413	ALA	6.4
9	7	544	ARG	6.4
5	C	15	GLU	6.4
6	2	653	GLY	6.4
6	F	22	LYS	6.4
8	4	434	PHE	6.4
9	7	412	LEU	6.4
2	D	66	CYS	6.4
2	T	409	VAL	6.4
1	w	553	C	6.4
5	C	20	GLU	6.4
5	C	55	ARG	6.4
7	W	252	GLU	6.4
2	S	278	LYS	6.4
6	Z	218	PRO	6.4
1	x	758	U	6.4
7	Y	620	LEU	6.4
5	Q	442	VAL	6.4
4	M	227	GLY	6.3
4	O	678	THR	6.3
9	K	125	VAL	6.3
10	9	219	SER	6.3
9	K	168	LYS	6.3
4	B	3	LEU	6.3
10	0	436	ASP	6.3
10	9	230	HIS	6.3
1	v	308	G	6.3
3	A	38	MET	6.3
6	1	440	MET	6.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	2	679	GLU	6.3
2	U	616	HIS	6.3
7	E	67	LYS	6.3
7	E	33	VAL	6.3
4	N	412	HIS	6.3
9	K	176	VAL	6.3
1	v	299	C	6.3
4	N	404	VAL	6.3
2	S	264	ARG	6.3
5	Q	426	THR	6.3
7	X	462	GLU	6.3
8	G	19	LEU	6.3
8	5	652	GLY	6.3
9	8	768	LYS	6.2
9	8	618	PRO	6.2
4	M	222	GLY	6.2
4	M	232	VAL	6.2
5	C	105	SER	6.2
3	A	31	PHE	6.2
4	M	210	LEU	6.2
1	w	437	G	6.2
4	O	657	THR	6.2
1	V	147	C	6.2
7	E	56	LEU	6.2
3	I	475	GLU	6.2
5	P	238	ASN	6.2
4	M	225	VAL	6.2
9	6	380	ARG	6.2
3	I	418	CYS	6.2
2	T	473	LEU	6.1
8	3	253	GLN	6.1
9	8	704	THR	6.1
9	8	762	LYS	6.1
2	D	7	ILE	6.1
6	2	643	GLN	6.1
10	9	259	GLN	6.1
4	M	273	SER	6.1
3	A	23	ASP	6.1
9	7	565	ASP	6.1
5	C	97	SER	6.1
4	N	418	GLU	6.1
6	F	31	GLY	6.1

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Mol	Chain	Res	Type	RSRZ
7	W	250	PHE	6.1
4	M	269	ILE	6.1
7	Y	646	CYS	6.1
5	P	299	MET	6.1
3	I	465	ARG	6.1
9	8	670	LYS	6.1
8	G	66	SER	6.1
8	5	661	VAL	6.1
10	l	620	VAL	6.1
3	H	277	LEU	6.1
7	E	89	SER	6.1
5	Q	445	ASN	6.1
4	N	426	HIS	6.1
7	E	86	LEU	6.1
2	T	451	ARG	6.1
1	v	300	C	6.1
6	F	63	LEU	6.1
8	3	218	SER	6.1
9	7	421	TYR	6.1
6	Z	223	LEU	6.0
6	Z	236	VAL	6.0
9	K	81	GLU	6.0
9	6	305	LEU	6.0
2	U	673	LEU	6.0
2	T	470	PHE	6.0
4	M	242	ALA	6.0
1	V	51	G	6.0
2	T	455	VAL	6.0
3	H	286	PRO	6.0
9	7	529	ILE	6.0
10	L	35	LYS	6.0
1	V	107	U	6.0
8	3	207	PRO	6.0
8	3	255	ASN	6.0
9	7	530	LYS	6.0
2	T	464	ARG	6.0
9	K	22	LEU	6.0
7	E	55	ASN	6.0
5	C	47	ARG	6.0
9	K	68	GLU	6.0
4	M	239	HIS	6.0
8	4	453	GLN	6.0

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Mol	Chain	Res	Type	RSRZ
7	X	444	GLU	6.0
1	v	329	U	6.0
2	T	441	CYS	6.0
2	U	608	LYS	6.0
5	P	262	HIS	6.0
9	6	223	PRO	6.0
2	U	613	ALA	6.0
3	H	231	PHE	6.0
9	K	79	GLN	5.9
9	7	527	GLY	5.9
2	T	475	ASP	5.9
3	H	236	LYS	5.9
9	7	510	VAL	5.9
9	7	517	SER	5.9
6	Z	232	TYR	5.9
8	5	657	ILE	5.9
9	K	126	TYR	5.9
10	l	609	CYS	5.9
9	8	720	ARG	5.9
1	v	306	G	5.9
8	3	211	LYS	5.9
4	B	12	HIS	5.9
6	F	26	GLY	5.9
7	Y	641	MET	5.9
7	W	229	SER	5.9
9	7	579	GLU	5.9
4	N	450	ARG	5.9
6	Z	252	ASP	5.9
6	1	450	TYR	5.9
6	2	670	LEU	5.9
7	W	278	MET	5.9
1	v	309	G	5.9
8	G	53	GLN	5.9
8	G	33	GLY	5.9
8	G	75	ARG	5.9
4	B	55	LEU	5.9
1	V	33	C	5.8
5	C	28	PRO	5.8
9	K	160	ALA	5.8
5	Q	469	ASN	5.8
7	E	31	ILE	5.8
4	B	56	GLU	5.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	7	533	HIS	5.8
4	M	267	TYR	5.8
4	O	663	ASN	5.8
6	F	78	GLU	5.8
7	W	220	LEU	5.8
1	V	92	C	5.8
8	G	24	GLY	5.8
5	R	618	LYS	5.8
7	Y	651	ASP	5.8
9	K	77	ARG	5.8
9	7	534	MET	5.8
1	x	724	U	5.8
1	V	156	U	5.8
2	D	41	CYS	5.8
5	Q	501	LEU	5.8
3	J	623	ASP	5.8
8	G	63	ARG	5.8
9	K	73	GLU	5.8
3	A	10	LEU	5.8
4	O	664	ASN	5.8
4	M	212	HIS	5.8
2	S	266	CYS	5.8
10	L	37	TYR	5.8
1	w	543	A	5.7
2	S	252	ASP	5.7
7	E	62	GLU	5.7
7	W	242	ARG	5.7
2	D	30	GLY	5.7
2	T	480	ALA	5.7
7	X	480	LYS	5.7
6	Z	254	ALA	5.7
2	S	211	HIS	5.7
7	Y	624	TYR	5.7
5	P	269	ASN	5.7
2	S	256	ALA	5.7
2	U	680	ALA	5.7
7	Y	652	GLU	5.7
9	K	13	PHE	5.7
10	L	22	LYS	5.7
5	R	611	MET	5.7
6	Z	237	ASP	5.7
6	Z	268	ASN	5.7

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Mol	Chain	Res	Type	RSRZ
4	B	46	THR	5.7
9	7	488	MET	5.7
1	V	40	G	5.7
4	N	411	SER	5.7
8	G	52	GLY	5.7
9	K	179	GLU	5.7
1	x	603	A	5.7
6	2	612	ASN	5.7
5	C	11	MET	5.7
6	2	666	CYS	5.7
5	R	712	ASN	5.7
6	F	46	ASN	5.6
7	W	291	SER	5.6
2	U	650	TYR	5.6
2	D	20	CYS	5.6
9	K	66	ARG	5.6
5	R	701	LEU	5.6
10	0	430	HIS	5.6
6	2	626	GLY	5.6
2	T	462	TYR	5.6
1	V	120	U	5.6
5	P	213	PRO	5.6
2	D	54	ARG	5.6
5	Q	436	VAL	5.6
5	P	298	LYS	5.6
5	P	297	SER	5.6
5	R	673	MET	5.6
2	T	463	ILE	5.6
10	0	416	ASP	5.6
1	v	349	U	5.6
1	x	704	A	5.6
3	H	279	SER	5.6
4	N	477	ASP	5.6
8	G	15	LYS	5.6
2	U	609	VAL	5.6
4	N	455	LEU	5.6
1	w	492	C	5.5
3	J	629	GLY	5.5
9	7	571	GLY	5.5
7	W	274	LEU	5.5
8	G	41	VAL	5.5
4	N	414	THR	5.5

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Mol	Chain	Res	Type	RSRZ
9	8	685	GLU	5.5
10	L	45	GLN	5.5
10	0	408	TYR	5.5
2	T	412	GLU	5.5
7	X	433	VAL	5.5
4	M	241	LYS	5.5
8	4	417	LEU	5.5
6	Z	263	LEU	5.5
4	M	218	GLU	5.5
10	l	610	ASP	5.5
4	O	668	PHE	5.5
7	X	427	ASN	5.5
7	E	32	GLN	5.5
2	S	227	VAL	5.5
7	E	64	ILE	5.5
8	4	476	VAL	5.5
2	S	228	TYR	5.5
10	0	454	THR	5.5
6	F	36	VAL	5.5
8	G	64	GLY	5.5
8	G	32	ARG	5.5
4	B	6	PHE	5.5
5	Q	475	THR	5.4
9	7	577	ASP	5.4
7	E	60	ASP	5.4
5	C	37	LYS	5.4
8	4	425	ARG	5.4
9	6	304	THR	5.4
3	A	22	GLN	5.4
2	U	620	CYS	5.4
8	5	656	ASN	5.4
9	7	524	GLU	5.4
6	Z	250	TYR	5.4
7	W	262	GLU	5.4
6	Z	212	ASN	5.4
1	x	647	C	5.4
6	1	432	TYR	5.4
9	K	132	ILE	5.4
3	I	436	HIS	5.3
5	C	72	GLU	5.3
4	B	36	MET	5.3
5	C	31	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
2	D	55	VAL	5.3
3	H	241	ILE	5.3
6	2	637	ASP	5.3
7	X	463	GLU	5.3
8	3	243	ASP	5.3
3	J	608	LYS	5.3
4	M	268	PHE	5.3
9	7	482	VAL	5.3
4	N	428	THR	5.3
7	E	38	GLN	5.3
9	8	747	ALA	5.3
10	0	429	LYS	5.3
2	U	666	CYS	5.3
3	A	37	HIS	5.3
2	S	249	THR	5.3
9	K	109	ARG	5.3
10	L	20	VAL	5.3
1	V	50	G	5.3
5	R	627	GLY	5.3
4	B	13	GLU	5.3
7	X	434	TRP	5.3
4	N	421	ASN	5.3
7	X	441	MET	5.3
3	H	246	ASP	5.3
2	S	263	ILE	5.3
8	5	668	ILE	5.3
8	G	27	VAL	5.3
8	4	427	VAL	5.3
9	K	71	ARG	5.3
5	R	713	PRO	5.3
3	J	665	ARG	5.3
5	Q	511	ARG	5.3
8	G	37	PHE	5.3
2	T	433	ILE	5.3
1	w	523	A	5.3
1	x	756	U	5.2
2	T	453	GLY	5.2
9	K	107	VAL	5.2
7	W	279	LEU	5.2
9	K	162	LYS	5.2
4	N	419	LEU	5.2
6	Z	269	VAL	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	Y	647	ILE	5.2
7	E	69	LYS	5.2
1	v	363	U	5.2
9	K	114	THR	5.2
4	O	612	HIS	5.2
6	2	614	LEU	5.2
9	K	127	GLY	5.2
9	7	475	ILE	5.2
8	3	241	VAL	5.2
4	M	244	LYS	5.2
9	8	733	HIS	5.2
6	F	34	VAL	5.2
4	M	214	THR	5.2
6	1	426	GLY	5.2
4	M	221	ASN	5.2
4	N	454	GLN	5.2
9	6	315	THR	5.2
4	B	30	THR	5.2
2	D	10	LEU	5.2
4	O	602	LYS	5.2
5	P	267	LEU	5.2
4	O	626	HIS	5.2
4	O	666	ARG	5.2
5	R	707	ILE	5.2
6	1	431	GLY	5.2
4	B	11	SER	5.2
5	P	312	ASN	5.2
4	M	247	LEU	5.2
3	I	414	TYR	5.1
1	v	341	G	5.1
9	6	336	TYR	5.1
8	5	616	LYS	5.1
9	6	212	LEU	5.1
3	I	480	MET	5.1
9	8	758	HIS	5.1
8	5	647	GLU	5.1
10	9	220	VAL	5.1
4	O	628	THR	5.1
3	I	443	ASP	5.1
5	R	642	VAL	5.1
3	I	487	PRO	5.1
2	T	443	MET	5.1

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Mol	Chain	Res	Type	RSRZ
2	U	617	ILE	5.1
1	v	316	C	5.1
8	4	437	PHE	5.1
10	l	644	GLU	5.1
9	K	106	PHE	5.1
5	C	36	VAL	5.1
6	F	69	VAL	5.1
3	I	476	ASN	5.1
1	v	246	C	5.1
3	I	419	ILE	5.1
6	Z	273	ARG	5.1
10	l	634	VAL	5.1
4	N	475	PRO	5.1
2	S	241	CYS	5.1
4	B	39	HIS	5.1
1	w	418	G	5.1
8	3	228	GLN	5.1
2	S	219	THR	5.1
8	4	433	GLY	5.1
10	L	16	ASP	5.1
9	8	679	GLN	5.1
2	S	246	ILE	5.1
2	T	423	ASN	5.1
3	I	411	HIS	5.1
6	1	420	MET	5.1
2	U	662	TYR	5.0
5	R	643	LEU	5.0
7	X	479	LEU	5.0
8	4	438	MET	5.0
6	Z	274	GLY	5.0
8	5	664	GLY	5.0
1	V	116	C	5.0
2	U	649	THR	5.0
8	5	662	ILE	5.0
5	P	302	ARG	5.0
8	3	249	ALA	5.0
4	B	76	LEU	5.0
5	C	25	ASN	5.0
9	K	180	ARG	5.0
3	I	486	PRO	5.0
8	5	672	ALA	5.0
8	5	608	GLU	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	M	276	LEU	5.0
7	W	268	THR	5.0
1	V	22	U	4.9
10	9	232	GLU	4.9
5	C	50	LYS	4.9
7	X	443	ILE	4.9
1	V	89	C	4.9
7	E	59	ASP	4.9
4	N	457	THR	4.9
7	E	23	ARG	4.9
9	7	466	ARG	4.9
1	v	345	U	4.9
5	C	49	ASN	4.9
3	H	238	MET	4.9
5	P	222	GLU	4.9
6	Z	272	ILE	4.9
9	K	88	MET	4.9
6	1	424	LYS	4.9
7	Y	682	ASP	4.9
1	V	145	U	4.9
1	x	714	C	4.9
8	5	625	ARG	4.9
7	W	271	ARG	4.9
3	A	27	PHE	4.9
7	X	491	SER	4.9
1	V	136	G	4.9
9	8	723	PHE	4.9
7	W	246	CYS	4.9
1	w	447	C	4.9
9	7	409	LEU	4.9
5	Q	508	VAL	4.9
8	5	640	LEU	4.9
7	X	456	LEU	4.9
2	S	220	CYS	4.8
4	O	629	ILE	4.8
9	6	377	ASP	4.8
9	7	575	LEU	4.8
5	R	708	VAL	4.8
5	C	54	GLY	4.8
4	O	639	HIS	4.8
2	U	667	LYS	4.8
8	5	615	LYS	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	E	53	TYR	4.8
10	9	252	LYS	4.8
9	K	112	TYR	4.8
9	6	280	GLN	4.8
6	1	439	TYR	4.8
10	L	31	LYS	4.8
8	3	237	PHE	4.8
5	Q	448	ASN	4.8
7	E	71	ARG	4.8
4	M	223	THR	4.8
6	2	663	LEU	4.8
3	A	33	ALA	4.8
1	w	421	A	4.8
5	P	229	LEU	4.7
3	J	632	LYS	4.7
3	I	422	ASP	4.7
10	9	205	TYR	4.7
9	6	339	ARG	4.7
8	3	264	GLY	4.7
8	3	276	VAL	4.7
4	N	424	GLN	4.7
9	6	209	LEU	4.7
2	D	37	ASP	4.7
5	Q	493	ASP	4.7
9	7	572	ARG	4.7
2	T	457	GLN	4.7
4	B	29	ILE	4.7
4	O	676	LEU	4.7
9	8	735	VAL	4.7
9	6	369	ILE	4.7
8	G	76	VAL	4.7
9	K	103	LYS	4.7
3	A	20	ILE	4.7
9	6	341	GLY	4.7
9	7	559	SER	4.7
6	2	623	LEU	4.7
9	8	674	LYS	4.7
10	0	419	SER	4.7
9	7	512	TYR	4.7
3	A	72	LEU	4.7
6	F	79	GLU	4.6
2	U	631	LYS	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	N	463	ASN	4.6
6	F	42	MET	4.6
6	Z	234	VAL	4.6
4	N	422	GLY	4.6
10	0	441	TRP	4.6
9	8	714	THR	4.6
8	3	262	ILE	4.6
1	V	93	G	4.6
6	1	461	GLU	4.6
7	Y	673	GLN	4.6
5	C	56	VAL	4.6
2	U	645	ASN	4.6
1	v	247	C	4.6
8	4	467	ILE	4.6
3	I	442	CYS	4.6
7	Y	678	MET	4.6
9	K	155	ARG	4.6
3	H	283	GLU	4.6
9	8	752	GLU	4.6
9	8	708	ALA	4.6
9	8	777	ASP	4.6
9	6	319	LEU	4.6
9	6	342	LYS	4.6
9	8	664	GLU	4.6
2	U	644	SER	4.6
7	Y	677	ILE	4.5
7	Y	629	SER	4.5
4	O	607	LEU	4.5
4	O	635	SER	4.5
8	3	224	GLY	4.5
4	N	402	LYS	4.5
7	W	258	LEU	4.5
4	O	645	MET	4.5
9	8	609	LEU	4.5
9	7	576	VAL	4.5
6	1	478	GLU	4.5
10	0	414	THR	4.5
7	E	63	GLU	4.5
5	Q	470	VAL	4.5
5	C	13	PRO	4.5
7	X	477	ILE	4.5
2	U	619	THR	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
8	4	406	PRO	4.5
8	3	256	ASN	4.5
8	3	261	VAL	4.5
8	4	443	ASP	4.5
8	5	649	ALA	4.5
8	4	415	LYS	4.5
9	K	89	TRP	4.5
10	l	660	GLY	4.5
7	W	292	ASN	4.5
5	C	103	GLY	4.5
9	6	264	GLU	4.5
4	B	44	LYS	4.5
8	4	473	LEU	4.5
10	l	613	LEU	4.5
2	D	11	HIS	4.5
10	L	39	CYS	4.5
4	O	621	ASN	4.5
5	C	62	HIS	4.4
7	W	235	LEU	4.4
8	4	426	HIS	4.4
8	G	36	PRO	4.4
2	U	671	LEU	4.4
5	P	217	GLN	4.4
1	V	26	A	4.4
7	W	230	ARG	4.4
4	O	673	SER	4.4
7	X	439	VAL	4.4
1	w	542	G	4.4
5	Q	444	ILE	4.4
10	L	41	TRP	4.4
6	Z	209	PRO	4.4
9	K	121	ARG	4.4
5	R	693	ASP	4.4
9	7	519	LEU	4.4
6	F	66	CYS	4.4
7	W	238	GLN	4.4
4	N	436	MET	4.4
9	7	543	PRO	4.4
1	x	734	U	4.4
5	R	630	SER	4.3
9	8	766	GLY	4.3
6	1	471	TYR	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	A	28	ILE	4.3
3	I	433	PHE	4.3
1	w	558	U	4.3
5	C	73	MET	4.3
6	Z	267	ASN	4.3
5	Q	452	LEU	4.3
8	G	31	LEU	4.3
9	K	63	ARG	4.3
2	T	447	THR	4.3
3	A	65	ARG	4.3
4	M	240	LEU	4.3
5	Q	499	MET	4.3
1	v	293	G	4.3
7	W	255	ASN	4.3
7	X	469	LYS	4.3
9	8	676	GLU	4.3
9	8	681	GLU	4.3
7	E	43	ILE	4.3
5	Q	425	ASN	4.3
5	P	224	PHE	4.3
5	Q	441	GLN	4.3
3	I	408	MET	4.3
6	F	70	LEU	4.3
1	w	529	U	4.3
3	H	218	ARG	4.3
6	F	57	GLY	4.3
7	X	418	ILE	4.3
8	4	408	GLU	4.3
9	6	263	ARG	4.3
1	V	45	U	4.3
9	6	326	TYR	4.3
10	l	604	PHE	4.2
8	4	429	GLY	4.2
4	M	216	THR	4.2
9	K	175	LEU	4.2
9	K	15	PRO	4.2
5	C	108	VAL	4.2
5	C	112	ASN	4.2
9	8	710	VAL	4.2
1	w	455	G	4.2
2	D	46	ILE	4.2
4	B	69	ILE	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	R	667	LEU	4.2
6	2	632	TYR	4.2
8	4	422	ASN	4.2
9	8	663	ARG	4.2
6	F	61	GLU	4.2
9	K	9	LEU	4.2
4	M	255	LEU	4.2
1	x	639	U	4.1
5	P	272	GLU	4.1
4	N	456	GLU	4.1
5	R	671	LYS	4.1
10	9	251	ASP	4.1
10	9	204	PHE	4.1
2	U	656	ALA	4.1
9	6	338	LYS	4.1
4	O	640	LEU	4.1
2	S	261	VAL	4.1
2	U	606	PRO	4.1
9	6	343	PRO	4.1
7	E	75	GLY	4.1
10	9	261	LYS	4.1
9	K	130	LYS	4.1
4	O	604	VAL	4.1
4	O	623	THR	4.1
6	F	81	ASP	4.1
9	6	322	GLU	4.1
4	O	655	LEU	4.1
5	C	94	ARG	4.1
7	Y	674	LEU	4.1
1	x	719	C	4.1
2	T	440	ASN	4.1
2	S	274	PRO	4.1
9	6	210	LEU	4.1
3	H	217	MET	4.1
9	6	306	PHE	4.0
8	G	38	MET	4.0
1	x	745	U	4.0
4	B	16	THR	4.0
2	D	44	SER	4.0
2	U	633	ILE	4.0
6	2	645	ALA	4.0
9	7	528	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
10	l	656	ALA	4.0
3	I	479	SER	4.0
8	3	238	MET	4.0
7	E	48	ILE	4.0
10	0	446	ALA	4.0
5	R	706	VAL	4.0
6	2	671	TYR	4.0
2	S	225	GLY	4.0
8	G	9	LEU	4.0
10	l	628	ARG	4.0
2	S	244	SER	4.0
8	3	245	CYS	4.0
4	M	236	MET	4.0
2	D	18	VAL	4.0
4	O	653	VAL	4.0
7	Y	645	GLY	4.0
8	5	638	MET	4.0
8	3	223	GLY	3.9
1	v	334	U	3.9
7	W	280	LYS	3.9
10	0	404	PHE	3.9
6	2	674	GLY	3.9
9	8	682	VAL	3.9
7	W	218	ILE	3.9
7	X	442	ARG	3.9
7	Y	628	ARG	3.9
1	v	359	C	3.9
2	U	660	GLN	3.9
7	E	81	GLY	3.9
7	W	289	SER	3.9
6	F	16	GLY	3.9
2	T	459	GLU	3.9
4	B	42	ALA	3.9
4	O	636	MET	3.9
10	0	426	SER	3.9
10	9	246	ALA	3.9
8	G	8	GLU	3.9
3	H	210	LEU	3.9
5	Q	512	ASN	3.9
5	R	623	GLU	3.9
2	T	430	GLY	3.9
6	Z	233	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
10	I	612	TYR	3.9
9	8	673	GLU	3.9
4	M	226	HIS	3.9
6	Z	242	MET	3.9
8	5	630	ILE	3.9
6	Z	249	GLU	3.9
3	I	430	PHE	3.9
7	X	419	ASN	3.9
4	M	243	VAL	3.9
8	G	68	ILE	3.9
7	W	225	LEU	3.9
6	2	608	LYS	3.9
5	R	635	SER	3.9
4	M	264	ASN	3.9
3	J	666	VAL	3.9
6	2	677	GLU	3.9
7	X	421	ILE	3.9
8	3	220	LYS	3.8
8	3	239	ASN	3.8
5	P	255	ARG	3.8
5	P	261	ARG	3.8
3	I	412	ILE	3.8
5	C	60	ASP	3.8
6	1	425	TRP	3.8
7	Y	675	GLY	3.8
8	4	447	GLU	3.8
1	V	158	U	3.8
9	7	516	GLU	3.8
10	0	422	LYS	3.8
6	Z	275	VAL	3.8
3	I	425	ILE	3.8
3	A	82	VAL	3.8
2	U	641	CYS	3.8
8	G	28	GLN	3.8
2	D	32	LEU	3.8
3	H	280	MET	3.8
5	Q	419	ARG	3.8
9	6	309	ARG	3.8
4	N	476	LEU	3.7
10	I	648	SER	3.7
5	C	110	LEU	3.7
6	Z	256	SER	3.7

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Mol	Chain	Res	Type	RSRZ
10	9	253	THR	3.7
2	S	232	LEU	3.7
8	3	209	LEU	3.7
7	W	221	ILE	3.7
9	8	711	ASN	3.7
2	T	456	ALA	3.7
8	4	439	ASN	3.7
6	F	27	MET	3.7
8	5	611	LYS	3.7
3	I	478	VAL	3.7
3	H	209	MET	3.7
4	M	277	ASP	3.7
5	C	69	ASN	3.7
4	M	207	LEU	3.7
2	U	629	ARG	3.6
3	H	215	TYR	3.6
3	I	439	LEU	3.6
3	J	639	ASN	3.6
7	Y	687	LEU	3.6
8	G	60	VAL	3.6
10	L	15	HIS	3.6
10	L	18	PRO	3.6
3	H	226	ILE	3.6
4	M	229	ILE	3.6
3	H	208	LYS	3.6
5	R	633	THR	3.6
3	J	609	MET	3.6
4	O	652	PRO	3.6
10	L	53	THR	3.6
9	7	540	SER	3.6
5	R	641	GLN	3.6
9	K	10	LEU	3.6
10	L	55	ALA	3.6
6	F	25	TRP	3.6
1	v	320	U	3.6
2	D	34	GLU	3.6
2	S	237	ASP	3.6
6	2	665	ARG	3.6
6	Z	215	THR	3.6
7	E	65	HIS	3.6
2	D	76	MET	3.6
7	Y	644	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
5	C	21	GLU	3.6
6	Z	210	PHE	3.6
8	3	268	ILE	3.6
8	5	617	LEU	3.6
3	H	219	CYS	3.6
9	6	289	TRP	3.6
4	O	613	GLU	3.6
8	4	456	ASN	3.5
5	P	236	VAL	3.5
3	H	273	ARG	3.5
5	R	652	LEU	3.5
10	L	50	ILE	3.5
8	3	272	ALA	3.5
3	A	18	ARG	3.5
6	1	469	VAL	3.5
7	W	257	VAL	3.5
2	D	23	ASN	3.5
9	7	555	ARG	3.5
5	R	672	GLU	3.5
10	9	229	LYS	3.5
5	Q	431	VAL	3.5
9	8	734	MET	3.5
4	N	403	LEU	3.5
5	Q	463	CYS	3.5
8	3	273	LEU	3.5
10	L	34	VAL	3.5
7	E	26	GLN	3.5
9	7	508	ALA	3.5
9	7	570	ASP	3.5
3	H	269	LEU	3.5
5	P	228	PRO	3.5
3	J	610	LEU	3.5
3	I	440	ILE	3.5
8	3	263	ARG	3.5
5	C	35	SER	3.5
6	Z	220	MET	3.5
9	6	286	LEU	3.5
5	P	226	THR	3.4
9	6	211	ALA	3.4
5	P	253	LEU	3.4
6	2	649	GLU	3.4
4	B	67	TYR	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	1	443	GLN	3.4
6	F	49	GLU	3.4
6	Z	261	GLU	3.4
8	G	17	LEU	3.4
6	F	23	LEU	3.4
7	X	437	GLU	3.4
7	X	460	ASP	3.4
9	6	284	THR	3.4
8	5	648	MET	3.4
6	F	13	GLY	3.4
7	E	27	ASN	3.4
6	F	44	LEU	3.4
5	Q	502	ARG	3.4
5	R	654	GLY	3.4
2	D	47	THR	3.4
2	U	621	GLU	3.4
5	P	254	GLY	3.4
6	1	419	VAL	3.4
4	O	641	LYS	3.4
5	R	624	PHE	3.4
5	R	668	GLU	3.4
8	4	452	GLY	3.4
3	J	640	LEU	3.4
4	O	647	LEU	3.4
3	I	483	GLU	3.4
8	5	607	PRO	3.4
6	2	631	GLY	3.3
4	N	468	PHE	3.3
7	X	432	GLN	3.3
4	N	434	VAL	3.3
5	R	644	ILE	3.3
6	Z	229	TYR	3.3
3	I	473	ARG	3.3
9	8	744	ARG	3.3
7	E	34	TRP	3.3
5	P	273	MET	3.3
6	F	37	ASP	3.3
7	Y	657	VAL	3.3
8	3	210	LYS	3.3
8	4	472	ALA	3.3
8	3	269	MET	3.3
5	R	697	SER	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	W	231	ILE	3.3
2	T	408	LYS	3.3
8	3	227	VAL	3.3
10	9	221	ARG	3.3
9	7	503	LYS	3.3
4	N	465	ILE	3.3
4	B	22	GLY	3.3
8	3	226	HIS	3.3
10	9	227	GLY	3.2
2	S	233	ILE	3.2
4	N	449	ASN	3.2
7	W	222	PHE	3.2
5	P	293	ASP	3.2
5	P	234	GLN	3.2
5	P	310	LEU	3.2
9	8	770	ASP	3.2
3	A	86	PRO	3.2
4	B	26	HIS	3.2
8	5	676	VAL	3.2
6	1	415	THR	3.2
4	B	24	GLN	3.2
8	5	621	LEU	3.2
8	4	412	PHE	3.2
10	9	243	GLU	3.2
1	x	613	C	3.2
2	S	258	LEU	3.2
5	R	702	ARG	3.2
4	B	70	LEU	3.2
5	C	24	PHE	3.2
10	l	652	LYS	3.2
8	4	459	MET	3.2
6	Z	238	GLY	3.2
9	8	709	ARG	3.2
2	S	281	PRO	3.2
9	K	138	LYS	3.1
3	I	435	LYS	3.1
9	K	12	LEU	3.1
8	5	644	GLU	3.1
5	P	259	PHE	3.1
8	4	471	GLU	3.1
4	O	617	ILE	3.1
8	3	234	PHE	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	T	415	GLY	3.1
7	X	468	THR	3.1
4	M	203	LEU	3.1
9	7	521	ARG	3.1
8	5	618	SER	3.1
9	7	463	ARG	3.1
6	2	638	GLY	3.1
6	1	422	LYS	3.1
5	C	22	GLU	3.0
3	J	612	HIS	3.0
10	9	225	CYS	3.0
6	Z	259	LEU	3.0
6	1	436	VAL	3.0
7	Y	655	ASN	3.0
6	2	620	MET	3.0
10	0	409	CYS	3.0
9	6	288	MET	3.0
5	C	16	LEU	3.0
8	3	205	HIS	3.0
2	S	259	GLU	3.0
10	9	206	CYS	3.0
9	6	320	ARG	3.0
3	J	679	SER	3.0
4	O	661	ARG	3.0
5	C	14	GLU	3.0
6	1	456	SER	3.0
4	B	7	LEU	3.0
5	R	692	LYS	3.0
10	9	214	THR	3.0
6	Z	260	GLY	3.0
10	1	642	MET	3.0
9	K	154	GLU	3.0
9	6	303	LYS	3.0
10	1	639	CYS	3.0
5	C	98	LYS	3.0
8	5	641	VAL	3.0
8	5	609	LEU	3.0
4	O	619	LEU	3.0
9	8	774	VAL	3.0
10	1	646	ALA	2.9
3	J	674	GLY	2.9
5	C	95	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	U	670	PHE	2.9
8	G	20	LYS	2.9
4	B	23	THR	2.9
8	4	462	ILE	2.9
9	K	82	VAL	2.9
4	N	413	GLU	2.9
6	Z	230	LYS	2.9
9	K	134	MET	2.9
9	6	282	VAL	2.9
3	I	472	LEU	2.9
5	C	46	CYS	2.9
7	Y	649	GLY	2.9
3	I	434	ASP	2.9
4	O	618	GLU	2.9
5	P	292	LYS	2.9
5	Q	465	MET	2.9
9	6	368	LYS	2.9
9	7	556	ASP	2.9
4	N	467	TYR	2.9
6	1	459	LEU	2.9
9	8	707	VAL	2.9
4	M	234	VAL	2.9
9	K	105	LEU	2.9
5	R	659	PHE	2.9
6	Z	207	PRO	2.9
9	8	672	ARG	2.9
2	D	64	ARG	2.9
7	Y	667	LYS	2.9
9	K	178	VAL	2.9
5	R	617	GLN	2.8
7	Y	626	GLN	2.8
6	1	423	LEU	2.8
7	E	77	ILE	2.8
5	C	61	ARG	2.8
6	2	634	VAL	2.8
8	G	14	ASP	2.8
7	Y	662	GLU	2.8
9	K	148	PHE	2.8
5	P	244	ILE	2.8
4	B	57	THR	2.8
6	F	62	VAL	2.8
9	6	371	GLY	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	9	249	LEU	2.8
4	M	249	ASN	2.8
5	C	39	ASN	2.8
9	K	17	ASP	2.8
9	7	518	LYS	2.8
4	N	472	ASP	2.8
5	C	111	ARG	2.8
6	2	657	GLY	2.8
7	X	425	LEU	2.8
9	K	124	GLU	2.8
6	F	7	PRO	2.8
9	8	610	LEU	2.8
9	8	751	TYR	2.8
4	B	25	VAL	2.8
5	P	258	ALA	2.8
2	T	446	ILE	2.8
10	I	645	GLN	2.7
10	L	13	LEU	2.7
4	B	32	VAL	2.7
5	P	268	GLU	2.7
9	8	667	MET	2.7
10	9	241	TRP	2.7
9	7	465	GLU	2.7
9	8	612	LEU	2.7
10	9	248	SER	2.7
4	B	41	LYS	2.7
9	6	337	SER	2.7
3	A	21	LEU	2.7
1	x	746	G	2.7
4	M	251	GLU	2.7
6	1	413	GLY	2.7
2	D	36	GLU	2.7
10	L	17	SER	2.7
9	7	486	LEU	2.7
6	1	462	VAL	2.7
5	Q	434	GLN	2.7
10	9	213	LEU	2.7
3	A	9	MET	2.7
7	W	281	GLY	2.7
6	F	29	TYR	2.7
2	T	421	GLU	2.6
4	M	266	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
8	5	631	LEU	2.6
10	L	57	PHE	2.6
9	7	472	ARG	2.6
9	6	318	LYS	2.6
4	M	217	ILE	2.6
8	3	271	GLU	2.6
8	5	628	GLN	2.6
5	R	626	THR	2.6
10	0	439	CYS	2.6
6	1	414	LEU	2.6
8	4	469	MET	2.6
7	E	25	LEU	2.6
2	D	51	ARG	2.6
3	J	618	ARG	2.6
9	7	476	GLU	2.6
2	D	43	MET	2.6
8	4	448	MET	2.6
5	C	45	ASN	2.6
3	A	70	VAL	2.6
7	X	449	GLY	2.6
2	U	614	GLU	2.6
10	I	647	GLN	2.5
6	F	40	MET	2.5
4	B	68	PHE	2.5
2	T	476	MET	2.5
4	O	620	LYS	2.5
6	1	410	PHE	2.5
3	H	234	PHE	2.5
8	G	6	PRO	2.5
4	N	464	ASN	2.5
7	W	285	THR	2.5
3	J	682	VAL	2.5
3	H	216	ARG	2.5
9	6	321	ARG	2.5
7	X	446	CYS	2.5
4	B	37	ASN	2.5
2	U	661	VAL	2.5
5	C	51	LYS	2.5
5	C	93	ASP	2.5
9	K	156	ASP	2.5
7	W	275	GLY	2.5
2	D	56	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
8	5	673	LEU	2.4
1	V	14	A	2.4
2	S	270	PHE	2.4
4	O	622	GLY	2.4
1	x	735	A	2.4
5	Q	462	HIS	2.4
8	G	43	ASP	2.4
6	2	660	GLY	2.4
5	C	92	LYS	2.4
8	G	42	ILE	2.4
2	U	678	LYS	2.4
3	I	409	LEU	2.4
7	Y	638	GLN	2.4
10	0	447	GLN	2.4
6	1	460	GLY	2.4
7	E	57	VAL	2.4
10	l	658	GLN	2.4
3	I	470	VAL	2.4
3	H	270	VAL	2.4
7	X	461	ALA	2.4
2	S	222	THR	2.4
9	7	541	GLY	2.3
3	A	26	ILE	2.3
9	6	266	ARG	2.3
7	Y	634	TRP	2.3
5	Q	429	LEU	2.3
8	G	5	HIS	2.3
3	H	235	ASP	2.3
8	3	206	PRO	2.3
7	W	249	GLY	2.3
4	M	204	VAL	2.3
8	G	61	VAL	2.3
3	I	474	GLY	2.3
7	X	450	PHE	2.3
4	B	34	VAL	2.3
1	v	213	C	2.3
8	5	606	PRO	2.3
8	G	21	LEU	2.3
4	N	461	ARG	2.3
4	B	14	THR	2.3
5	P	250	LYS	2.3
9	6	347	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
9	6	274	LYS	2.2
7	W	254	MET	2.2
9	6	348	PHE	2.2
5	R	651	LYS	2.2
2	T	461	VAL	2.2
5	P	230	SER	2.2
2	U	655	VAL	2.2
5	R	634	GLN	2.2
5	C	67	LEU	2.2
6	2	616	GLY	2.2
6	Z	239	TYR	2.2
9	7	464	GLU	2.2
1	v	297	U	2.2
9	8	763	HIS	2.2
6	1	463	LEU	2.2
4	M	262	GLY	2.2
8	5	620	LYS	2.2
9	8	731	ARG	2.2
9	8	736	TYR	2.2
5	C	53	LEU	2.2
3	A	44	ASP	2.2
6	F	12	ASN	2.2
6	2	636	VAL	2.2
3	H	237	HIS	2.2
10	l	649	LEU	2.2
5	P	218	LYS	2.2
2	S	215	GLY	2.2
6	Z	266	CYS	2.2
9	6	359	SER	2.2
9	8	737	SER	2.2
5	C	34	GLN	2.2
7	W	265	HIS	2.2
7	W	224	TYR	2.1
9	6	349	ILE	2.1
7	W	269	LYS	2.1
4	B	64	ASN	2.1
5	Q	430	SER	2.1
4	O	642	ALA	2.1
9	6	327	GLY	2.1
9	8	669	ARG	2.1
5	Q	471	LYS	2.1
2	U	632	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
6	Z	216	GLY	2.1
10	I	630	HIS	2.1
6	F	10	PHE	2.1
9	8	684	THR	2.1
3	H	222	GLN	2.1
9	7	507	VAL	2.1
7	Y	669	LYS	2.1
7	X	486	LEU	2.1
4	O	627	GLY	2.0
2	T	472	ILE	2.0
9	6	316	GLU	2.0
5	Q	497	SER	2.0
8	3	233	GLY	2.0
9	7	481	GLU	2.0
2	D	31	LYS	2.0
5	C	65	MET	2.0
4	B	62	GLY	2.0
7	W	287	LEU	2.0
5	Q	461	ARG	2.0
5	Q	466	VAL	2.0
4	N	474	LEU	2.0
6	1	421	VAL	2.0

## 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( $\text{\AA}^2$ )	Q<0.9
11	ZN	9	278	1/1	0.22	0.95	-	231,231,231,231	0
11	ZN	L	78	1/1	-0.10	0.74	-	231,231,231,231	0
11	ZN	1	678	1/1	-0.02	0.78	-	231,231,231,231	0
11	ZN	0	478	1/1	0.25	2.12	-	231,231,231,231	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.