



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:41 PM UTC

PDB ID : 3CW1 / pdb_00003cw1
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

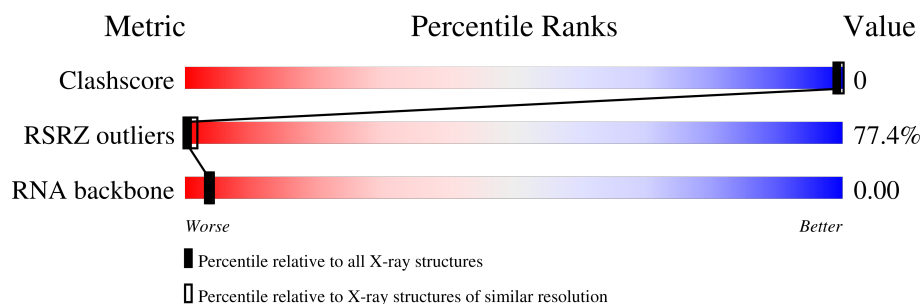
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1147 (7.00-4.00)
RSRZ outliers	180081	1081 (7.00-4.00)
RNA backbone	3983	1052 (7.80-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	V	138	100% 100%
1	v	138	99% 99%
1	w	138	100% 100%
1	x	138	97% 100%
2	D	126	56% 60% 40%
2	S	126	44% 60% 40%
2	T	126	33% 60% 40%
2	U	126	44% 60% 40%

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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	
9	8	216	
9	K	216	
10	0	77	
10	9	77	
10	L	77	
10	l	77	

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
11	ZN	0	478	-	-	-	X
11	ZN	9	278	-	-	-	X
11	ZN	L	78	-	-	-	X
11	ZN	l	678	-	-	-	X

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	0	0	138
			138	138			
1	v	138	Total	P	0	0	138
			138	138			
1	w	138	Total	P	0	0	138
			138	138			
1	x	138	Total	P	0	0	138
			138	138			

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

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

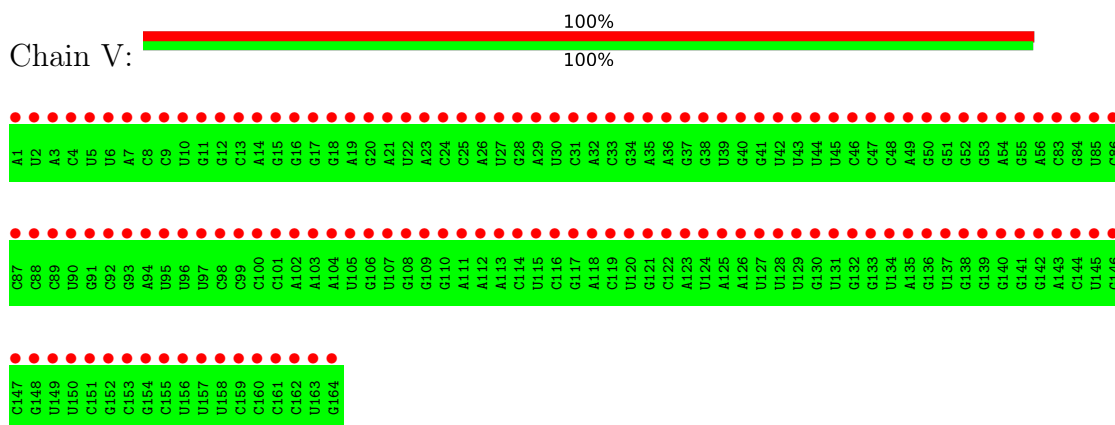
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

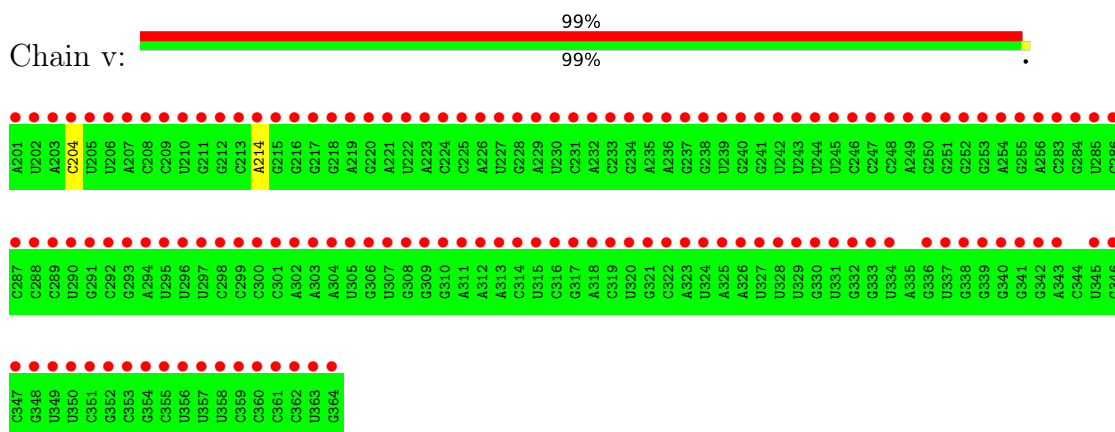
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

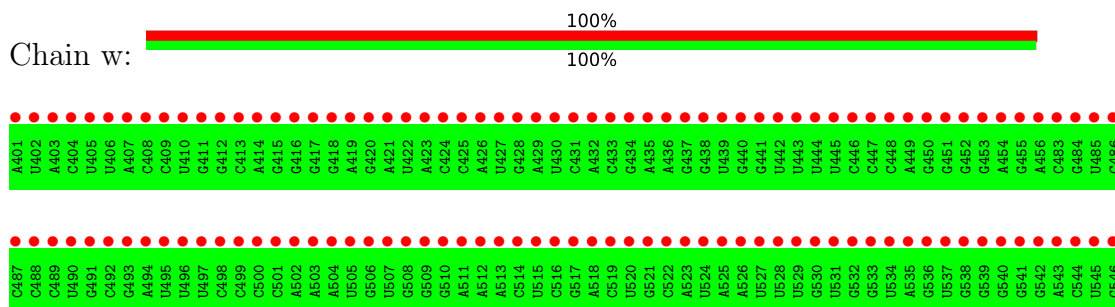
- Molecule 1: U1 snRNA

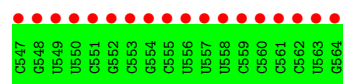


- Molecule 1: U1 snRNA

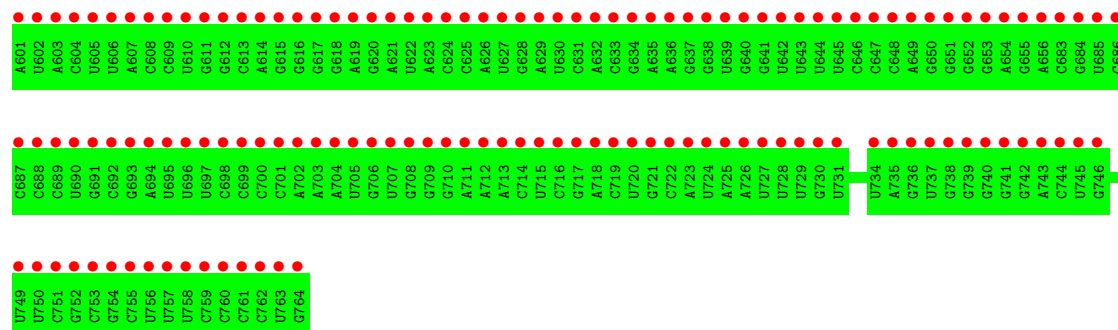


- Molecule 1: U1 snRNA

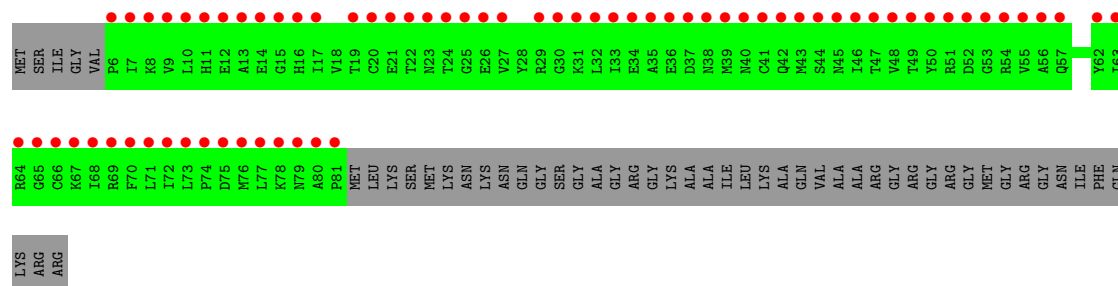




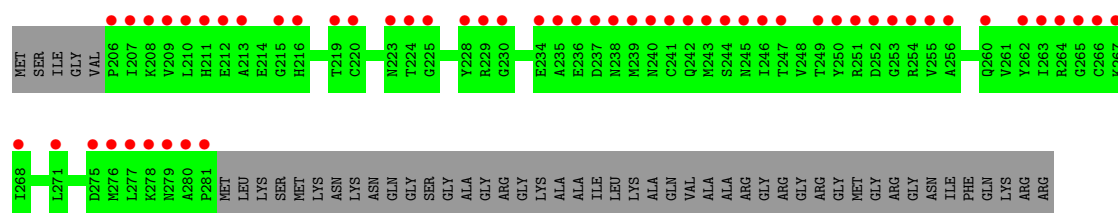
• Molecule 1: U1 snRNA



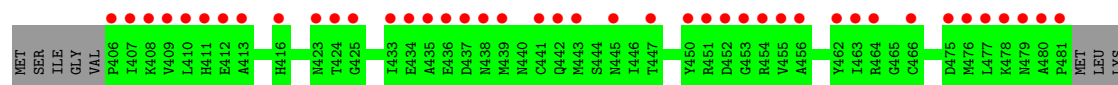
• Molecule 2: Small nuclear ribonucleoprotein Sm D3



• Molecule 2: Small nuclear ribonucleoprotein Sm D3

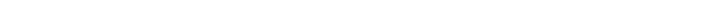


• Molecule 2: Small nuclear ribonucleoprotein Sm D3



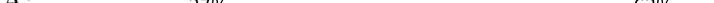
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- Molecule 2: Small nuclear ribonucleoprotein Sm D3

Chain U:  44% 60% 40%

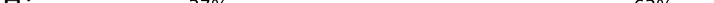
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- Molecule 3: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain A:  26% 37% 63%

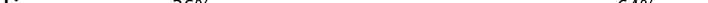
[illegible]

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

Chain H:  23% 37% 63%

[illegible]

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

Chain I: 

P4837	LYS	THR	ASP	VAL	THR	GLY	GLY	ILE	ALA	ARG	ARG	R407	R408	R409	Q410	ALA	GLY	ALA	ALA	ALA	GLY	GLY	GLY	GLY	GLY	PRO	PRO	GLY	ILE	R431	R432	R433	F433	D434	R435	R436	R437	ILE	PRO	ALA	ALA	GLY	VAL	E446	PHE	ARG	LYS	ILE	LYS	PRO	PRO	LYS	ASN	SER	LYS	GLN	ALA	GLU	ARG	GLY	VAL	GLY	LYS	R465	G468	L469	E475	S479	R485	GLN	PRO	THR	THR	MET
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ARG
GLY
THR
THR
VAL
GLY
ALA
ALA
ALA
ALA
ALA
ALA
ALA
THR
THR
SER
ILE
ILE
GLY
ALA
ALA
PRO
THR
THR
GLN
TYR
PRO
PRO
GLY
ARG
GLY

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

Chain J:

MET THR VAL VAL LYS SER S607 S608 M609 M610 Q611 Q612 I613 C619 I620 Q622 D623 G624 I626 K632 A633 F634 D635 K636 H637 M638 M639 I640 I641 L642 C643 D644 C645 D646 E647 PHE ARG LYS ILE LYS PRO LYS ASN SER LYS GLN ALA GLU ARG GLU LYS R665 V666 L667 G668

L669 V670 L671 L672 R673 R674 E675 R676 L677 V678 S679 S683 G684 P686 PRO LYS ASP THR GLY ILE ALA ARG VAL PRO LEU ALA GLY ALA PRO ILE GLY ARG ALA ARG ARG ILE PRO ALA GLY ILE PRO ALA GLY VAL PRO MET PRO GLN ALA PRO GLU ALA PRO ALA GLY LEU ALA PRO VAL ARG GLY THR VAL ALA ALA ALA ALA ALA ALA THR THR ALA ILE SER ALA ILE GLY THR VAL THR ARG GLY GLN MET PRO THR THR VAL VAL ARG GLY VAL ARG GLY GLY GLY

VAL ARG GLY VAL GLY GLY PRO SER GLN VAL MET PRO GLN THR PRO GLN ARG GLY THR VAL ALA ALA ALA ALA ALA ALA VAL PRO LEU ALA THR ALA ALA SER ILE ALA GLY PRO GLY THR TYR PRO PRO GLY ARG GLY GLY

- Molecule 4: Small nuclear ribonucleoprotein Sm D1

Chain B:

MET K2 L3 V4 R5 R6 L7 R8 R9 R10 L11 S11 H12 H13 T14 V15 T16 I17 I18 E19 L19 K20 N21 G22 G23 T23 Q24 Q25 H26 D27 T28 I29 T30 T31 G31 V32 D33 V34 S35 S36 M36 N37 N38 T38 H39 L40 K41 A42 V43 L47 K48 M49 R50 R51 P52 V53 Q54 L55 E56 T57 L58 S59 I60 R61 Q62

N63 N64 I65 R66 Y67 F68 I69 L70 M71 D72 S73 L74 P75 L76 D77 T78 LEU LEU VAL ASP VAL N221 G222 T223 Q224 V225 H226 S227 T228 I229 T230 T231 G231 V232 D233 V234 S235 S236 M236 N237 N238 T238 H239 L240 K241 A242 V243 L244 M245 T246 L247 K248 M249 R250 R251 P252 V253 Q254 L255 E256 T257 L258 S259 I260 R261 Q262

N63 N64 I65 R66 Y67 F68 I69 L70 M71 D72 S73 L74 P75 L76 D77 T78 LEU LEU VAL ASP VAL N221 G222 T223 Q224 V225 H226 S227 T228 I229 T230 T231 G231 V232 D233 V234 S235 S236 M236 N237 N238 T238 H239 L240 K241 A242 V243 L244 M245 T246 L247 K248 M249 R250 R251 P252 V253 Q254 L255 E256 T257 L258 S259 I260 R261 Q262

- Molecule 4: Small nuclear ribonucleoprotein Sm D1

Chain M:

MET K202 L203 V204 R205 R206 L207 M208 K209 L210 S211 H212 H213 T214 V215 T216 I217 I218 E219 L219 K220 N221 G222 T223 Q224 V225 H226 S227 T228 I229 T230 T231 G231 V232 D233 V234 S235 S236 M236 N237 N238 T238 H239 L240 K241 A242 V243 L244 M245 T246 L247 K248 M249 R250 R251 P252 V253 Q254 L255 E256 T257 L258 S259 I260 R261 Q262

R261 G262 N263 N264 I265 R266 Y267 F268 I269 L270 M271 D272 S273 L274 P275 L276 D277 T278 LEU LEU VAL ASP VAL N221 G222 T223 Q224 V225 H226 S227 T228 I229 T230 T231 G231 V232 D233 V234 S235 S236 M236 N237 N238 T238 H239 L240 K241 A242 V243 L244 M245 T246 L247 K248 M249 R250 R251 P252 V253 Q254 L255 E256 T257 L258 S259 I260 R261 Q262

R261 G262 N263 N264 I265 R266 Y267 F268 I269 L270 M271 D272 S273 L274 P275 L276 D277 T278 LEU LEU VAL ASP VAL N221 G222 T223 Q224 V225 H226 S227 T228 I229 T230 T231 G231 V232 D233 V234 S235 S236 M236 N237 N238 T238 H239 L240 K241 A242 V243 L244 M245 T246 L247 K248 M249 R250 R251 P252 V253 Q254 L255 E256 T257 L258 S259 I260 R261 Q262

- Molecule 4: Small nuclear ribonucleoprotein Sm D1

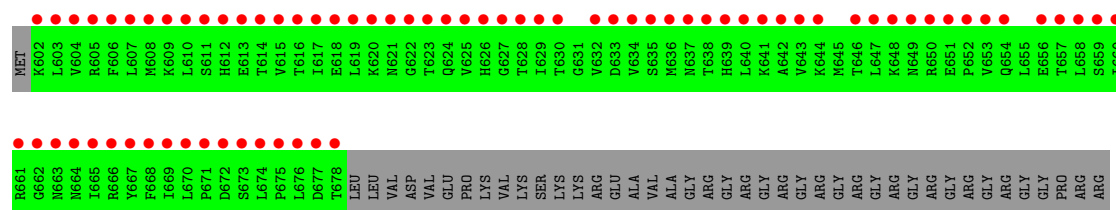
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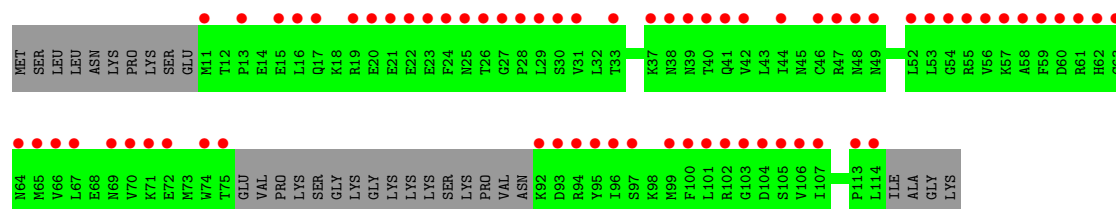
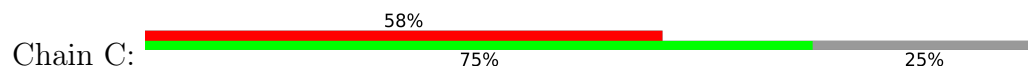
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K462 N463 N464 I465 R466 Y467 F468 I469 L470 M471 D472 S473 L474 P475 L476 D477 LEU LEU VAL ASP VAL N421 G422 T423 Q424 V425 H426 S427 T428 I429 T430 T431 G431 V432 D433 V434 S435 S436 M436 N437 N438 T438 H439 L440 K441 A442 V443 L444 M445 T446 L447 K448 M449 R450 R451 P452 V453 Q454 L455 E456 T457 L458 S459 I460 R461

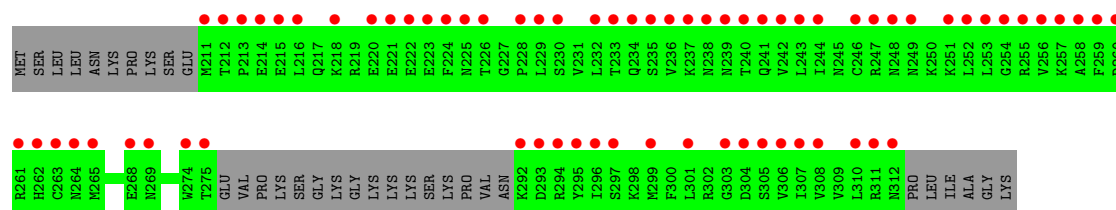
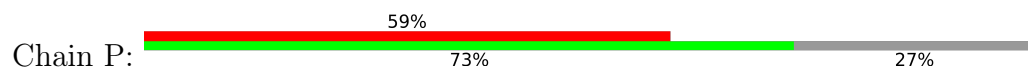
- Molecule 4: Small nuclear ribonucleoprotein Sm D1



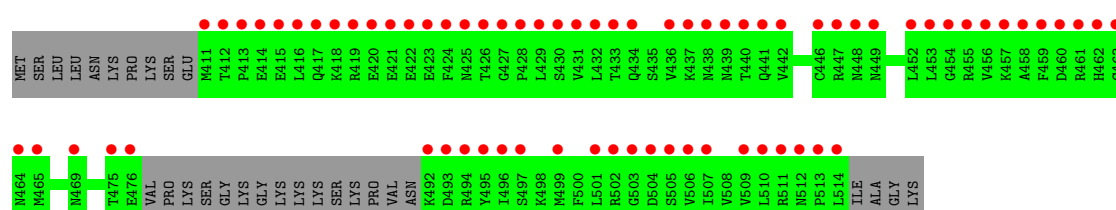
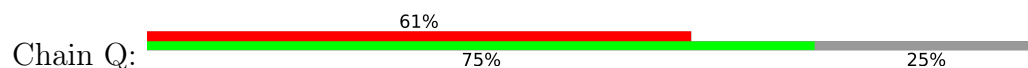
• Molecule 5: Small nuclear ribonucleoprotein Sm D2



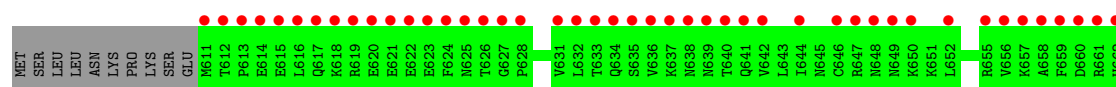
• Molecule 5: Small nuclear ribonucleoprotein Sm D2

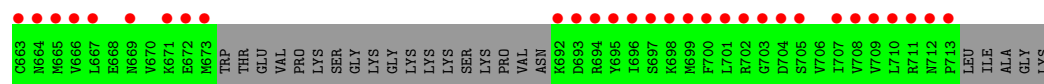


• Molecule 5: Small nuclear ribonucleoprotein Sm D2

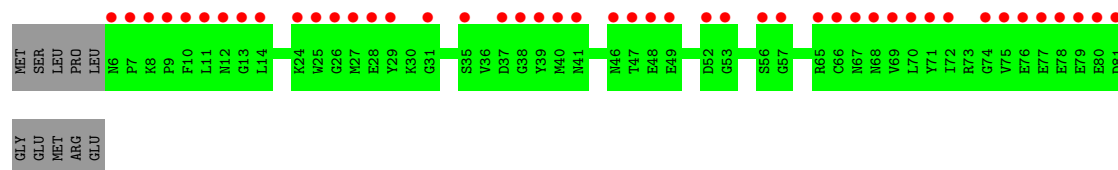
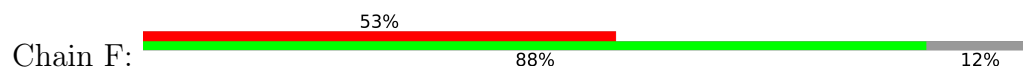


• Molecule 5: Small nuclear ribonucleoprotein Sm D2

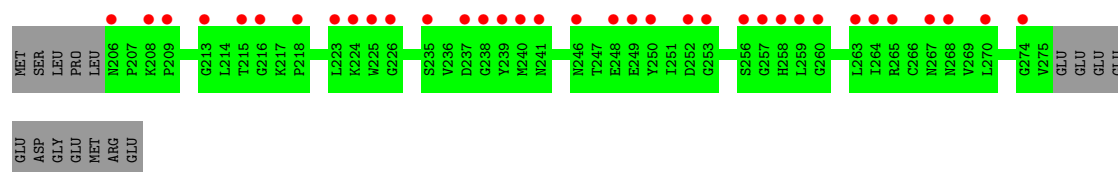
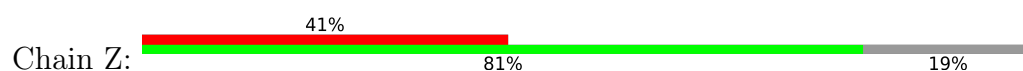




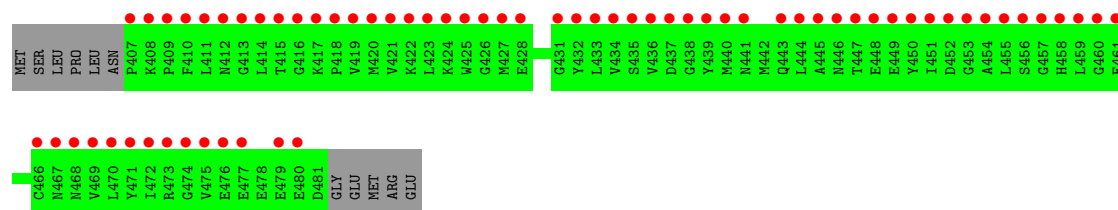
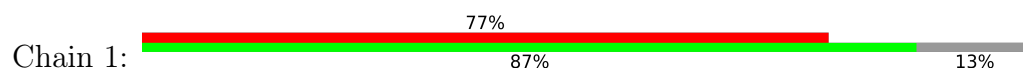
• Molecule 6: Small nuclear ribonucleoprotein F



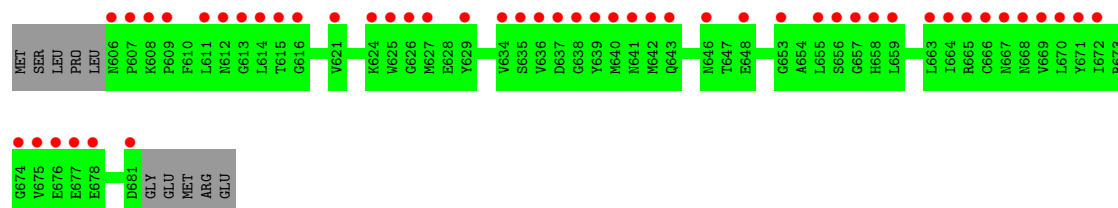
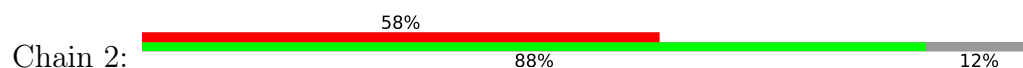
• Molecule 6: Small nuclear ribonucleoprotein F



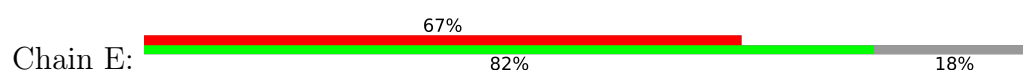
• Molecule 6: Small nuclear ribonucleoprotein F

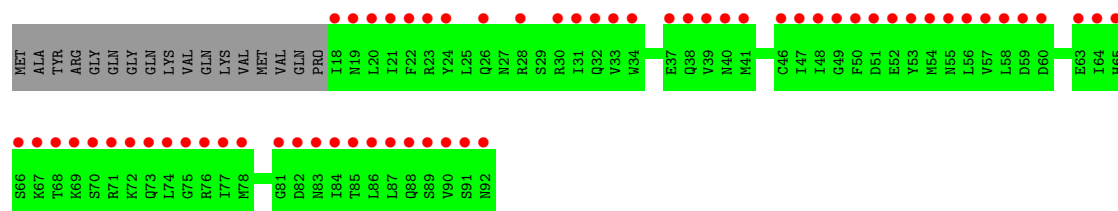


• Molecule 6: Small nuclear ribonucleoprotein F

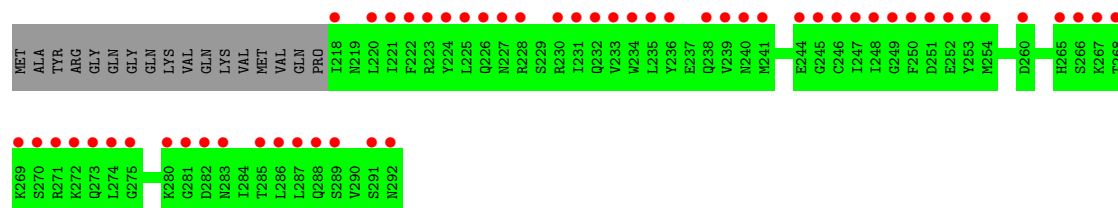
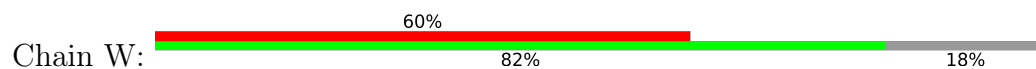


• Molecule 7: Small nuclear ribonucleoprotein E

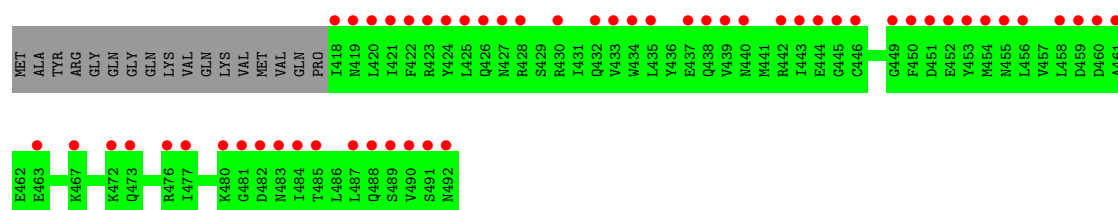
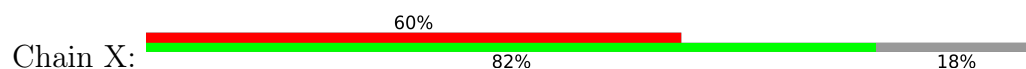




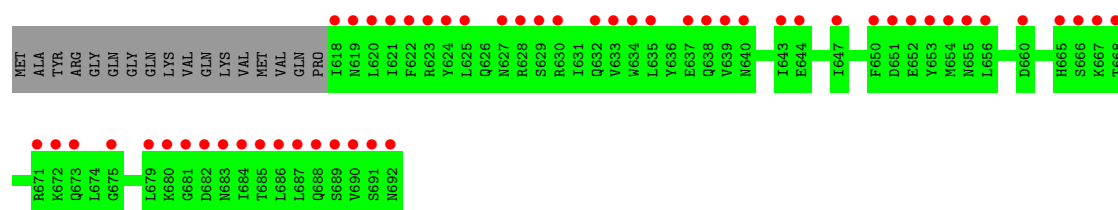
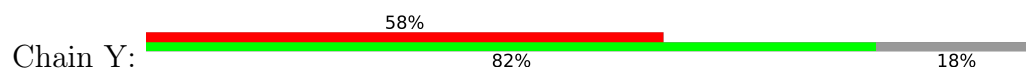
• Molecule 7: Small nuclear ribonucleoprotein E



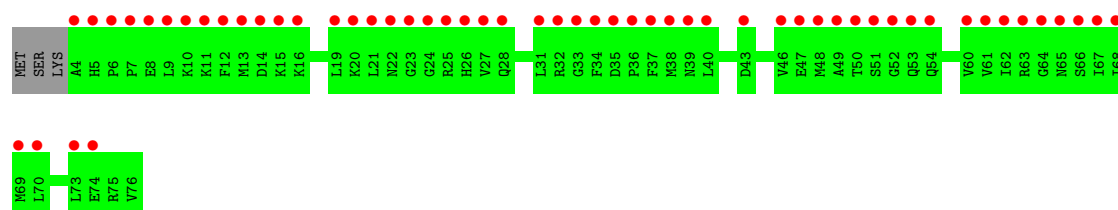
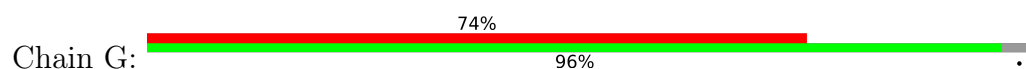
• Molecule 7: Small nuclear ribonucleoprotein E



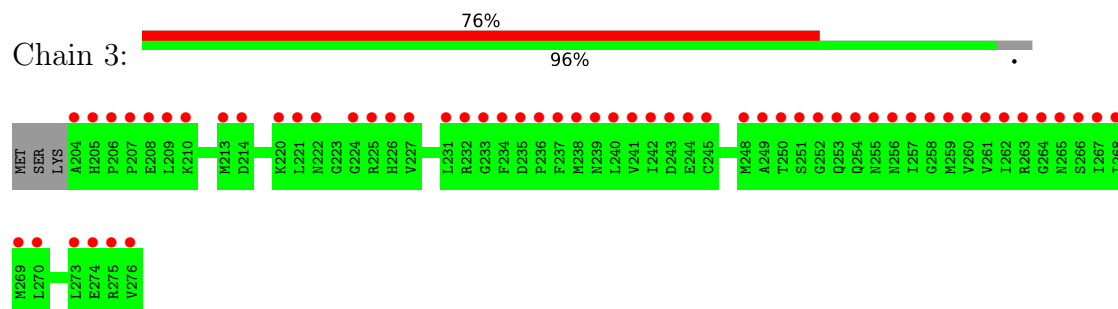
• Molecule 7: Small nuclear ribonucleoprotein E



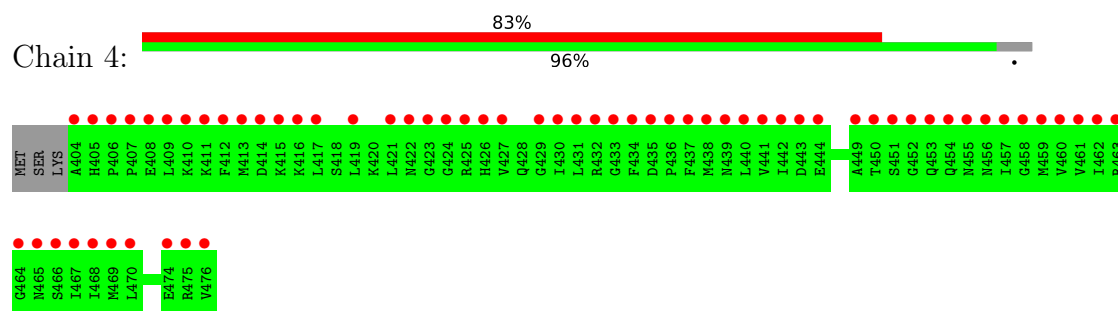
• Molecule 8: Small nuclear ribonucleoprotein G



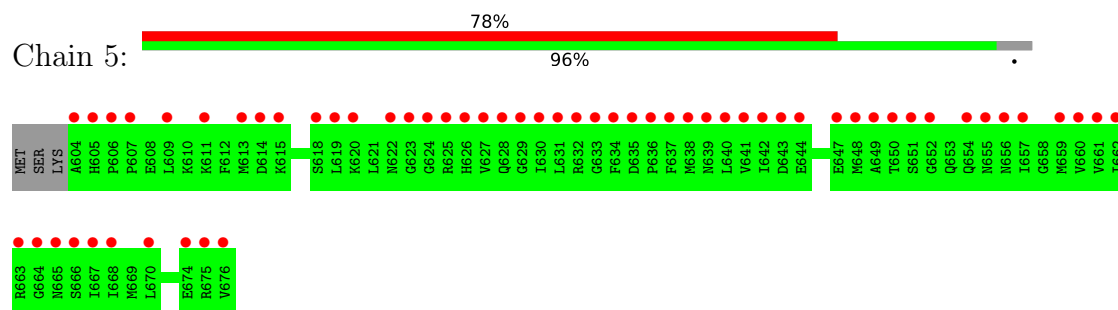
- Molecule 8: Small nuclear ribonucleoprotein G



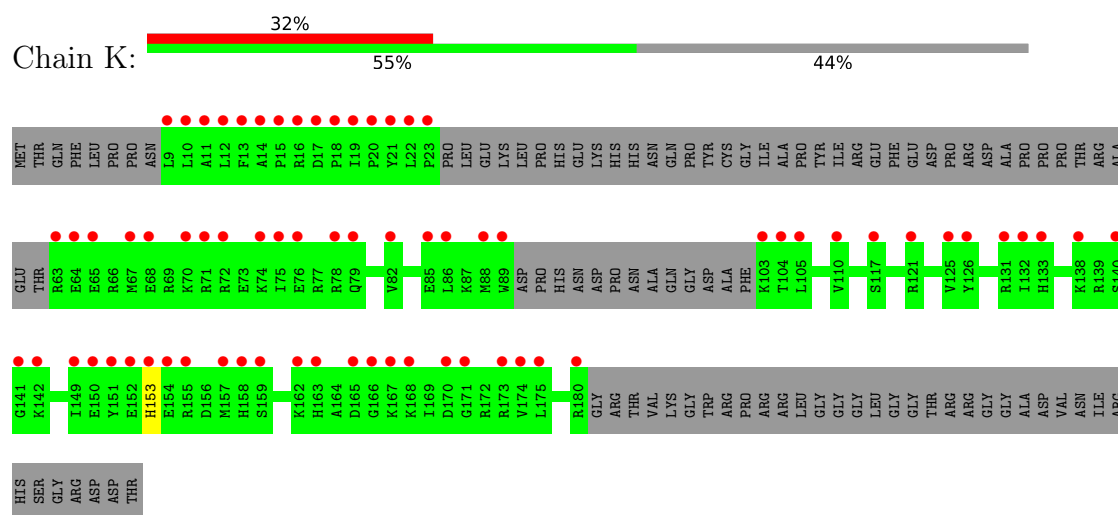
- Molecule 8: Small nuclear ribonucleoprotein G



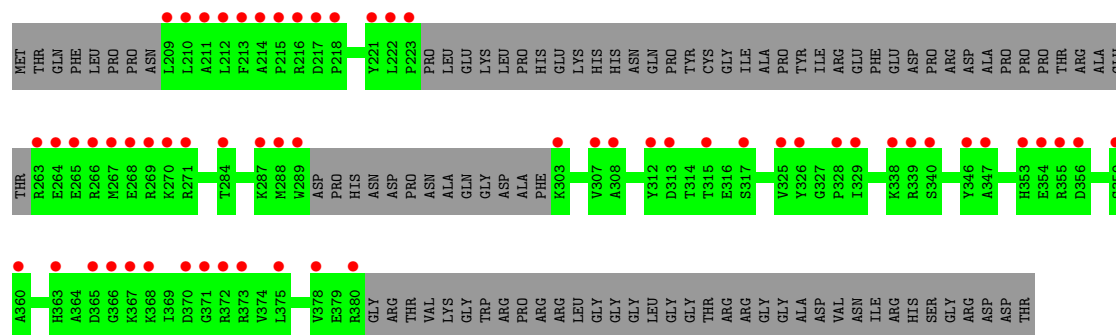
- Molecule 8: Small nuclear ribonucleoprotein G



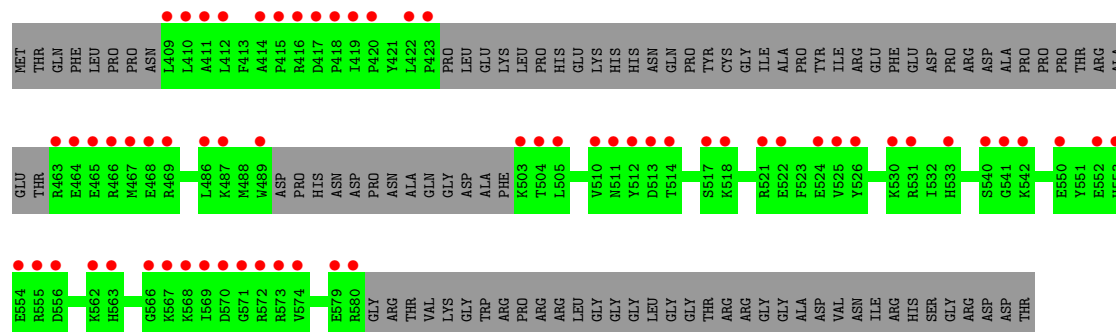
- Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa



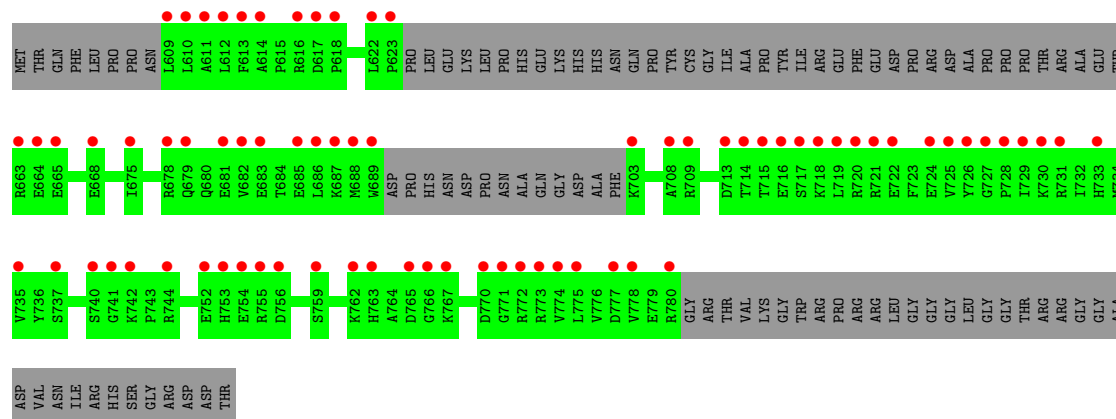
- Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa



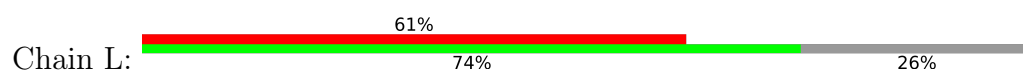
• Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa

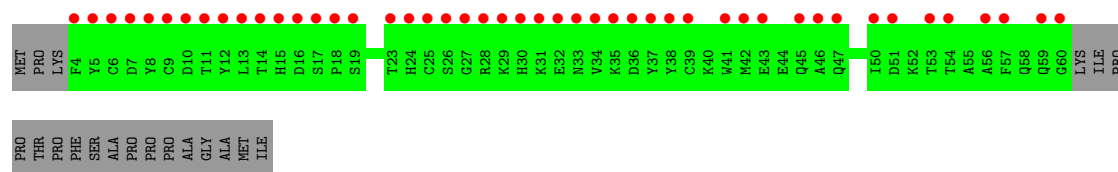


• Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa

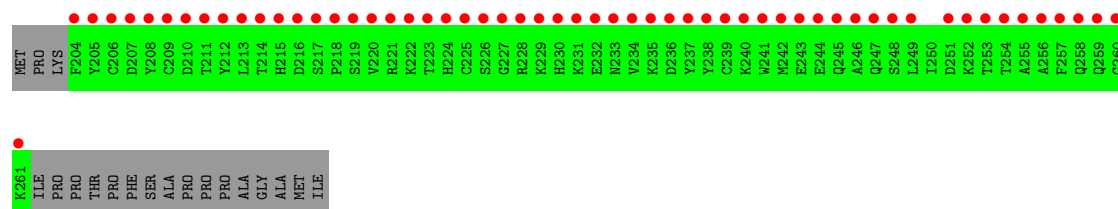
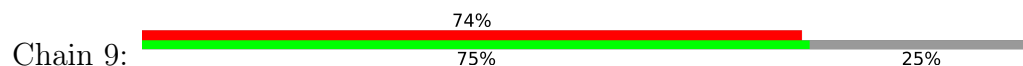


• Molecule 10: U1 small nuclear ribonucleoprotein C

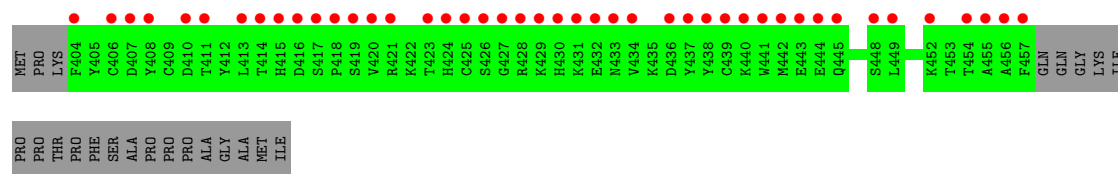




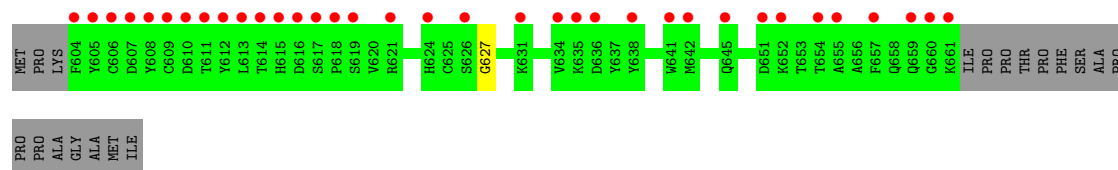
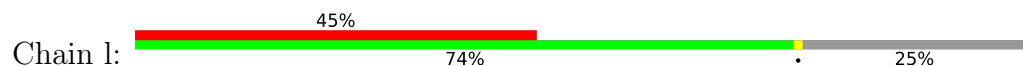
- Molecule 10: U1 small nuclear ribonucleoprotein C



- 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, α , β , γ	126.47Å 127.08Å 152.02Å 95.42° 105.92° 101.80°	Depositor
Resolution (Å)	123.09 – 5.49 123.09 – 5.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (123.09-5.49) 99.0 (123.09-5.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 5.42Å)	Xtriage
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available) 0.477 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	251.7	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	4.52 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	3365	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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	1	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	1	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	1	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.

All (1) 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)
1:v:204:C:P	10:l:627:GLY:CA	2.48	1.02

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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	V	138/138 (100%)	12.79	138 (100%) 0 0	232, 232, 232, 232	0
1	v	138/138 (100%)	14.88	136 (98%) 0 1	232, 232, 232, 232	0
1	w	138/138 (100%)	13.19	138 (100%) 0 0	232, 232, 232, 232	0
1	x	138/138 (100%)	11.98	134 (97%) 0 1	232, 232, 232, 232	0
2	D	76/126 (60%)	11.50	70 (92%) 0 1	232, 232, 232, 232	0
2	S	76/126 (60%)	9.95	56 (73%) 0 1	232, 232, 232, 232	0
2	T	76/126 (60%)	6.62	42 (55%) 0 2	232, 232, 232, 232	0
2	U	76/126 (60%)	8.17	55 (72%) 0 1	232, 232, 232, 232	0
3	A	64/174 (36%)	5.94	45 (70%) 0 2	232, 232, 232, 232	0
3	H	64/174 (36%)	6.27	40 (62%) 0 2	232, 232, 232, 232	0
3	I	63/174 (36%)	3.05	26 (41%) 0 3	232, 232, 232, 232	0
3	J	63/174 (36%)	5.39	45 (71%) 0 2	232, 232, 232, 232	0
4	B	77/119 (64%)	8.41	73 (94%) 0 1	232, 232, 232, 232	0
4	M	77/119 (64%)	8.06	70 (90%) 0 1	232, 232, 232, 232	0
4	N	76/119 (63%)	8.21	67 (88%) 0 1	232, 232, 232, 232	0
4	O	77/119 (64%)	8.31	74 (96%) 0 1	232, 232, 232, 232	0
5	C	88/118 (74%)	7.27	69 (78%) 0 1	232, 232, 232, 232	0
5	P	86/118 (72%)	8.33	70 (81%) 0 1	232, 232, 232, 232	0
5	Q	89/118 (75%)	8.39	72 (80%) 0 1	232, 232, 232, 232	0
5	R	85/118 (72%)	6.51	75 (88%) 0 1	232, 232, 232, 232	0
6	1	75/86 (87%)	8.81	66 (88%) 0 1	232, 232, 232, 232	0
6	2	76/86 (88%)	4.45	50 (65%) 0 2	232, 232, 232, 232	0
6	F	76/86 (88%)	6.96	46 (60%) 0 2	232, 232, 232, 232	0
6	Z	70/86 (81%)	3.93	35 (50%) 0 3	232, 232, 232, 232	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
7	E	75/92 (81%)	6.32	62 (82%) 0 1	232, 232, 232, 232	0
7	W	75/92 (81%)	5.81	55 (73%) 0 1	232, 232, 232, 232	0
7	X	75/92 (81%)	6.24	55 (73%) 0 1	232, 232, 232, 232	0
7	Y	75/92 (81%)	5.82	53 (70%) 0 2	232, 232, 232, 232	0
8	3	73/76 (96%)	6.51	58 (79%) 0 1	232, 232, 232, 232	0
8	4	73/76 (96%)	8.25	63 (86%) 0 1	232, 232, 232, 232	0
8	5	73/76 (96%)	6.57	59 (80%) 0 1	232, 232, 232, 232	0
8	G	73/76 (96%)	8.01	56 (76%) 0 1	232, 232, 232, 232	0
9	6	120/216 (55%)	4.26	60 (50%) 0 3	232, 232, 232, 232	0
9	7	120/216 (55%)	5.33	63 (52%) 0 3	232, 232, 232, 232	0
9	8	120/216 (55%)	5.42	74 (61%) 0 2	232, 232, 232, 232	0
9	K	120/216 (55%)	5.40	70 (58%) 0 2	232, 232, 232, 232	0
10	0	54/77 (70%)	6.18	44 (81%) 0 1	232, 232, 232, 232	0
10	9	58/77 (75%)	8.62	57 (98%) 0 1	232, 232, 232, 232	0
10	L	57/77 (74%)	6.19	47 (82%) 0 1	232, 232, 232, 232	0
10	l	58/77 (75%)	3.89	35 (60%) 0 2	232, 232, 232, 232	0
All	All	3361/4888 (68%)	7.79	2603 (77%) 0 1	232, 232, 232, 232	0

All (2603) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	81	ASP	54.8
2	S	206	PRO	53.4
2	D	6	PRO	53.2
8	G	67	ILE	53.0
2	T	481	PRO	50.4
5	C	106	VAL	48.0
8	4	463	ARG	47.7
1	x	764	G	46.3
1	x	754	G	45.8
5	P	240	THR	44.1
6	2	676	GLU	44.0
6	1	472	ILE	43.8
1	v	306	G	43.7
8	4	464	GLY	43.3
2	D	81	PRO	42.8

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Mol	Chain	Res	Type	RSRZ
6	F	80	GLU	41.7
2	S	209	VAL	41.2
6	F	76	GLU	40.6
2	D	70	PHE	40.5
2	D	69	ARG	40.5
2	S	265	GLY	40.3
1	w	554	G	39.8
6	1	452	ASP	39.5
1	w	526	A	39.4
1	v	364	G	39.3
1	v	353	C	38.6
1	w	541	G	38.5
5	P	239	ASN	38.4
2	D	71	LEU	37.7
1	V	161	C	37.6
2	D	72	ILE	37.6
1	v	218	G	37.5
1	x	753	C	37.5
6	F	78	GLU	37.5
1	v	307	U	37.0
4	O	672	ASP	36.4
2	D	20	CYS	36.4
5	P	305	SER	36.2
5	C	105	SER	35.8
2	D	21	GLU	35.7
6	1	453	GLY	35.5
1	v	347	C	35.3
2	T	475	ASP	35.2
4	B	65	ILE	35.1
5	Q	512	ASN	35.0
1	v	343	A	35.0
6	F	79	GLU	34.7
2	T	479	ASN	34.5
1	V	102	A	34.1
1	w	504	A	34.0
10	9	218	PRO	33.9
1	V	37	G	33.8
9	K	166	GLY	33.6
2	T	437	ASP	33.0
7	W	254	MET	33.0
1	v	348	G	32.9
1	w	542	G	32.9

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Mol	Chain	Res	Type	RSRZ
3	H	243	CYS	32.8
1	v	304	A	32.7
2	U	606	PRO	32.5
8	3	205	HIS	32.3
10	9	204	PHE	32.0
1	v	201	A	31.9
1	v	302	A	31.8
8	G	68	ILE	31.7
2	U	679	ASN	31.6
2	S	210	LEU	31.5
3	H	233	ALA	31.3
7	W	251	ASP	31.3
5	P	233	THR	31.1
2	D	68	ILE	30.9
5	R	656	VAL	30.9
2	S	277	LEU	30.5
8	4	462	ILE	30.3
1	V	104	A	30.3
2	S	280	ALA	30.3
5	Q	433	THR	30.1
1	v	248	C	30.1
2	U	639	MET	30.0
1	v	342	G	29.8
1	v	299	C	29.7
1	v	216	G	29.7
1	v	346	G	29.4
1	x	755	C	29.3
5	Q	439	ASN	29.1
8	G	64	GLY	29.1
2	U	668	ILE	29.1
2	S	275	ASP	29.0
7	Y	628	ARG	29.0
10	9	217	SER	28.9
9	8	766	GLY	28.8
2	T	477	LEU	28.8
2	S	237	ASP	28.8
8	5	676	VAL	28.7
5	Q	505	SER	28.7
5	Q	438	ASN	28.7
1	w	540	G	28.6
4	O	674	LEU	28.6
2	U	608	LYS	28.3

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Mol	Chain	Res	Type	RSRZ
6	1	468	ASN	28.2
4	O	676	LEU	28.2
2	U	610	LEU	28.1
7	E	59	ASP	28.0
4	B	64	ASN	28.0
5	P	238	ASN	28.0
2	S	208	LYS	27.8
5	R	657	LYS	27.8
1	w	501	C	27.7
5	Q	414	GLU	27.6
3	A	66	VAL	27.6
5	P	306	VAL	27.5
5	Q	415	GLU	27.4
2	U	607	ILE	27.3
10	0	414	THR	27.3
7	X	459	ASP	27.2
1	v	219	A	27.1
3	H	241	ILE	27.1
1	w	401	A	27.1
8	5	638	MET	27.0
9	7	570	ASP	26.9
10	9	255	ALA	26.7
8	G	66	SER	26.7
1	v	354	G	26.6
6	1	426	GLY	26.6
1	v	217	G	26.6
10	9	216	ASP	26.5
2	S	207	ILE	26.4
1	V	162	C	26.4
9	K	21	TYR	26.3
8	3	238	MET	26.3
9	7	511	ASN	26.2
5	P	241	GLN	26.2
8	3	235	ASP	26.1
7	W	271	ARG	26.1
7	X	454	MET	26.1
8	4	405	HIS	26.1
9	7	569	ILE	26.1
1	v	303	A	26.0
1	V	100	C	26.0
1	w	525	A	25.9
9	7	572	ARG	25.9

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Mol	Chain	Res	Type	RSRZ
4	O	664	ASN	25.9
7	Y	686	LEU	25.9
5	Q	412	THR	25.8
1	x	707	U	25.8
10	0	416	ASP	25.8
2	D	65	GLY	25.8
2	D	78	LYS	25.5
4	N	472	ASP	25.5
2	U	676	MET	25.5
1	V	99	C	25.3
4	O	673	SER	25.3
2	D	37	ASP	25.3
8	4	439	ASN	24.9
3	A	65	ARG	24.9
1	V	49	A	24.8
2	S	279	ASN	24.6
2	U	609	VAL	24.6
1	V	18	G	24.6
2	S	239	MET	24.5
8	4	435	ASP	24.5
9	8	612	LEU	24.5
5	P	236	VAL	24.5
2	D	76	MET	24.4
5	C	46	CYS	24.4
3	J	674	GLY	24.3
1	w	450	G	24.3
1	x	742	G	24.3
4	M	251	GLU	24.3
9	8	613	PHE	24.3
9	K	64	GLU	24.2
8	G	35	ASP	24.2
1	w	416	G	24.1
7	X	492	ASN	24.1
4	M	254	GLN	24.0
8	4	438	MET	24.0
1	V	101	C	23.9
4	N	421	ASN	23.9
3	I	422	ASP	23.8
8	3	206	PRO	23.7
10	0	417	SER	23.7
1	x	704	A	23.6
9	6	366	GLY	23.6

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Mol	Chain	Res	Type	RSRZ
9	K	19	ILE	23.5
4	N	420	LYS	23.5
9	6	371	GLY	23.5
5	P	247	ARG	23.4
4	O	671	PRO	23.4
8	5	647	GLU	23.3
1	V	147	C	23.3
9	7	465	GLU	23.2
1	v	341	G	23.1
5	C	47	ARG	23.1
6	1	407	PRO	23.1
9	K	20	PRO	23.0
4	O	675	PRO	23.0
1	V	98	C	23.0
2	T	478	LYS	23.0
1	x	618	G	23.0
1	v	247	C	22.9
1	x	699	C	22.9
7	Y	654	MET	22.9
9	7	411	ALA	22.9
2	S	281	PRO	22.8
1	v	313	A	22.8
1	x	741	G	22.8
1	x	702	A	22.7
1	w	500	C	22.7
1	v	324	U	22.7
2	T	410	LEU	22.7
1	v	238	G	22.7
1	x	721	G	22.7
9	8	728	PRO	22.6
8	5	662	ILE	22.6
2	S	264	ARG	22.5
6	F	77	GLU	22.4
9	8	611	ALA	22.4
4	M	272	ASP	22.4
4	B	72	ASP	22.3
5	R	637	LYS	22.2
9	7	464	GLU	22.2
2	S	266	CYS	22.2
5	Q	437	LYS	22.2
1	V	45	U	22.1
1	x	648	C	22.0

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Mol	Chain	Res	Type	RSRZ
3	J	637	HIS	22.0
4	N	451	GLU	21.8
5	P	297	SER	21.8
2	U	678	LYS	21.8
6	1	473	ARG	21.7
7	X	483	ASN	21.6
2	U	637	ASP	21.6
10	L	17	SER	21.6
9	6	264	GLU	21.5
8	5	663	ARG	21.4
1	w	449	A	21.3
1	v	321	G	21.3
6	Z	224	LYS	21.3
2	T	407	ILE	21.3
1	V	88	C	21.2
5	Q	413	PRO	21.2
8	4	466	SER	21.2
2	D	67	LYS	21.2
9	6	263	ARG	21.2
5	Q	513	PRO	21.1
4	B	71	PRO	21.0
9	K	63	ARG	21.0
6	Z	226	GLY	20.9
6	F	10	PHE	20.9
4	N	422	GLY	20.9
5	C	56	VAL	20.8
9	8	727	GLY	20.8
6	1	424	LYS	20.8
4	B	51	GLU	20.8
4	M	250	ARG	20.8
10	L	6	CYS	20.8
4	M	253	VAL	20.8
7	X	446	CYS	20.8
4	B	74	LEU	20.7
1	w	498	C	20.7
7	X	482	ASP	20.7
9	7	466	ARG	20.7
1	w	553	C	20.7
2	S	267	LYS	20.6
4	M	220	LYS	20.6
2	T	480	ALA	20.6
9	8	682	VAL	20.5

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Mol	Chain	Res	Type	RSRZ
1	x	760	C	20.5
6	1	425	TRP	20.5
1	V	121	G	20.4
4	N	476	LEU	20.4
4	M	276	LEU	20.4
3	H	235	ASP	20.3
1	V	84	G	20.3
6	1	474	GLY	20.3
1	w	524	U	20.3
4	M	271	PRO	20.3
8	5	635	ASP	20.2
4	O	677	ASP	20.1
1	w	513	A	20.1
2	S	238	ASN	20.1
5	P	307	ILE	20.1
5	P	237	LYS	20.0
1	V	48	C	20.0
3	A	68	GLY	19.9
8	G	38	MET	19.9
4	N	454	GLN	19.8
4	O	619	LEU	19.8
10	0	415	HIS	19.8
9	K	18	PRO	19.7
9	6	373	ARG	19.7
8	4	476	VAL	19.7
1	V	106	G	19.6
7	E	75	GLY	19.6
1	x	715	U	19.6
2	S	278	LYS	19.6
7	X	450	PHE	19.6
9	6	217	ASP	19.6
9	8	773	ARG	19.6
3	H	236	LYS	19.5
9	K	89	TRP	19.5
2	T	476	MET	19.4
1	w	499	C	19.4
1	w	514	C	19.4
4	O	670	LEU	19.4
2	D	10	LEU	19.4
3	A	67	LEU	19.4
2	U	671	LEU	19.3
5	Q	447	ARG	19.3

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Mol	Chain	Res	Type	RSRZ
1	w	418	G	19.3
1	V	107	U	19.3
10	L	38	TYR	19.2
1	v	305	U	19.2
1	w	417	G	19.2
1	v	312	A	19.1
2	D	39	MET	19.1
6	F	13	GLY	19.1
9	6	218	PRO	19.0
1	V	87	C	19.0
1	V	16	G	19.0
5	C	16	LEU	18.9
2	U	638	ASN	18.9
4	M	274	LEU	18.9
2	U	666	CYS	18.8
1	w	556	U	18.8
9	K	12	LEU	18.8
1	x	761	C	18.7
1	x	716	C	18.7
4	N	442	ALA	18.7
8	G	63	ARG	18.6
1	x	619	A	18.6
1	x	646	C	18.6
1	w	422	U	18.6
8	3	264	GLY	18.6
9	7	571	GLY	18.6
8	5	605	HIS	18.5
1	v	301	C	18.5
8	4	467	ILE	18.5
3	H	232	LYS	18.5
4	B	69	ILE	18.4
4	N	430	THR	18.4
7	W	283	ASN	18.4
4	M	249	ASN	18.3
1	V	89	C	18.3
2	T	439	MET	18.3
8	G	21	LEU	18.3
1	v	293	G	18.3
5	Q	434	GLN	18.3
1	x	638	G	18.2
10	L	19	SER	18.2
10	9	252	LYS	18.2

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Mol	Chain	Res	Type	RSRZ
1	x	628	G	18.2
1	x	714	C	18.2
6	Z	225	TRP	18.1
7	Y	687	LEU	18.1
9	7	463	ARG	18.1
4	M	277	ASP	18.1
1	v	322	C	18.0
10	9	245	GLN	18.0
9	8	610	LEU	18.0
1	V	46	C	18.0
2	T	438	ASN	18.0
9	6	211	ALA	17.9
4	N	473	SER	17.9
1	V	38	G	17.9
1	w	505	U	17.9
7	E	60	ASP	17.8
3	J	675	GLU	17.8
1	x	706	G	17.8
4	M	264	ASN	17.8
7	X	481	GLY	17.8
1	w	519	C	17.8
2	U	677	LEU	17.7
1	w	523	A	17.7
6	2	677	GLU	17.7
8	5	648	MET	17.7
10	L	35	LYS	17.7
4	M	273	SER	17.7
8	4	465	ASN	17.7
4	B	20	LYS	17.7
1	x	617	G	17.6
9	K	17	ASP	17.6
1	V	105	U	17.6
4	O	665	ILE	17.6
7	E	83	ASN	17.6
9	7	573	ARG	17.6
1	v	323	A	17.6
5	P	256	VAL	17.6
1	V	36	A	17.5
4	N	474	LEU	17.5
1	w	521	G	17.5
7	X	451	ASP	17.5
1	v	345	U	17.5

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Mol	Chain	Res	Type	RSRZ
5	C	104	ASP	17.5
7	W	282	ASP	17.5
1	v	363	U	17.4
3	J	676	ASN	17.4
5	P	269	ASN	17.4
5	C	103	GLY	17.4
1	v	316	C	17.4
8	G	5	HIS	17.4
1	x	698	C	17.3
1	v	359	C	17.3
5	R	713	PRO	17.3
8	5	606	PRO	17.3
1	w	555	C	17.3
1	x	700	C	17.2
1	x	615	G	17.2
1	v	298	C	17.2
4	N	452	PRO	17.2
6	F	24	LYS	17.1
4	B	75	PRO	17.1
9	8	775	LEU	17.0
10	L	16	ASP	17.0
6	1	469	VAL	16.9
4	B	21	ASN	16.9
7	W	253	TYR	16.9
5	R	666	VAL	16.9
1	w	502	A	16.9
1	V	141	G	16.8
1	v	249	A	16.8
9	6	212	LEU	16.8
1	v	253	G	16.8
8	3	204	ALA	16.8
6	Z	268	ASN	16.8
3	A	22	GLN	16.8
7	W	252	GLU	16.8
2	U	665	GLY	16.8
2	D	7	ILE	16.7
1	v	300	C	16.6
5	R	658	ALA	16.6
6	1	470	LEU	16.6
1	V	53	G	16.6
8	3	236	PRO	16.6
2	U	681	PRO	16.5

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Mol	Chain	Res	Type	RSRZ
4	O	618	GLU	16.5
1	v	360	C	16.5
1	x	718	A	16.5
1	v	223	A	16.5
1	w	557	U	16.5
8	3	276	VAL	16.5
2	S	276	MET	16.5
9	6	380	ARG	16.5
9	7	513	ASP	16.4
9	8	609	LEU	16.4
4	N	412	HIS	16.4
1	v	297	U	16.3
10	L	37	TYR	16.3
1	w	491	G	16.3
1	w	452	G	16.3
1	V	111	A	16.2
1	v	286	C	16.2
1	w	497	U	16.1
4	B	76	LEU	16.1
6	1	409	PRO	16.1
1	v	221	A	16.1
4	B	66	ARG	16.1
9	K	167	LYS	16.1
6	1	467	ASN	16.0
4	B	73	SER	16.0
5	Q	449	ASN	16.0
10	9	219	SER	16.0
7	E	87	LEU	16.0
9	7	568	LYS	16.0
2	S	236	GLU	16.0
9	K	16	ARG	16.0
1	v	308	G	15.9
4	M	263	ASN	15.9
8	4	436	PRO	15.9
9	6	267	MET	15.9
1	w	421	A	15.8
1	v	245	U	15.8
3	J	622	GLN	15.8
5	P	255	ARG	15.8
2	D	25	GLY	15.7
7	Y	682	ASP	15.7
7	E	54	MET	15.7

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Mol	Chain	Res	Type	RSRZ
1	w	510	G	15.7
1	w	511	A	15.7
1	V	17	G	15.7
1	x	701	C	15.7
5	C	48	ASN	15.7
1	V	52	G	15.7
5	R	697	SER	15.6
9	8	686	LEU	15.6
1	w	522	C	15.6
1	V	21	A	15.6
5	Q	514	LEU	15.6
1	w	550	U	15.6
1	w	483	C	15.6
5	C	95	TYR	15.6
1	x	756	U	15.5
1	V	116	C	15.5
3	I	435	LYS	15.5
4	N	449	ASN	15.5
8	3	237	PHE	15.5
10	l	604	PHE	15.5
1	V	113	A	15.5
9	K	65	GLU	15.5
1	V	8	C	15.5
1	v	288	C	15.5
9	7	489	TRP	15.5
7	E	76	ARG	15.5
6	1	471	TYR	15.4
7	Y	629	SER	15.4
5	C	99	MET	15.4
1	w	512	A	15.4
10	0	413	LEU	15.4
1	w	456	A	15.3
9	7	418	PRO	15.3
6	Z	239	TYR	15.3
1	v	310	G	15.3
3	A	43	CYS	15.3
4	M	275	PRO	15.3
1	V	119	C	15.3
2	D	77	LEU	15.3
3	A	24	GLY	15.2
5	Q	440	THR	15.2
1	V	22	U	15.2

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Mol	Chain	Res	Type	RSRZ
2	U	669	ARG	15.2
1	v	251	G	15.2
1	v	244	U	15.2
3	H	223	ASP	15.2
1	V	118	A	15.1
1	x	743	A	15.1
10	9	249	LEU	15.1
9	7	566	GLY	15.1
2	D	75	ASP	15.1
3	I	421	GLN	15.1
1	V	85	U	15.1
1	v	355	C	15.1
2	D	66	CYS	15.1
4	M	248	LYS	15.0
4	B	63	ASN	15.0
1	w	485	U	15.0
8	5	604	ALA	15.0
9	K	11	ALA	15.0
4	B	77	ASP	15.0
10	l	606	CYS	15.0
8	4	475	ARG	15.0
1	w	455	G	14.9
9	K	67	MET	14.9
1	w	520	U	14.9
1	x	717	G	14.9
8	G	69	MET	14.9
1	w	426	A	14.9
1	w	433	C	14.8
5	Q	448	ASN	14.8
4	B	68	PHE	14.8
1	x	705	U	14.7
7	W	239	VAL	14.7
10	9	206	CYS	14.7
4	O	667	TYR	14.7
1	x	623	A	14.7
1	w	446	C	14.7
1	w	492	C	14.7
9	6	289	TRP	14.7
1	V	86	C	14.6
1	w	448	C	14.6
1	x	637	G	14.6
1	V	157	U	14.6

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Mol	Chain	Res	Type	RSRZ
1	V	112	A	14.6
6	Z	253	GLY	14.6
5	Q	441	GLN	14.6
1	V	91	G	14.6
1	v	289	C	14.6
1	v	362	C	14.6
1	x	763	U	14.6
1	V	20	G	14.6
9	6	265	GLU	14.6
4	M	221	ASN	14.6
8	G	62	ILE	14.6
4	N	475	PRO	14.5
1	w	431	C	14.5
1	v	252	G	14.5
1	w	453	G	14.5
1	x	740	G	14.5
7	Y	627	ASN	14.5
5	C	94	ARG	14.4
1	w	515	U	14.4
2	D	38	ASN	14.4
5	R	648	ASN	14.4
6	l	480	GLU	14.4
3	H	224	GLY	14.4
1	V	10	U	14.4
1	v	250	G	14.4
8	G	27	VAL	14.4
1	w	509	G	14.4
4	N	448	LYS	14.4
1	V	103	A	14.3
5	Q	511	ARG	14.3
10	l	617	SER	14.3
8	G	36	PRO	14.3
1	V	123	A	14.2
3	A	69	LEU	14.2
1	w	438	G	14.2
1	V	5	U	14.2
1	V	117	G	14.2
5	C	93	ASP	14.2
1	v	202	U	14.1
9	K	75	ILE	14.1
1	V	2	U	14.1
1	w	432	A	14.1

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Mol	Chain	Res	Type	RSRZ
4	B	19	LEU	14.1
1	V	109	G	14.1
1	v	361	C	14.1
1	v	285	U	14.1
1	w	517	G	14.1
4	N	413	GLU	14.0
1	V	9	C	14.0
1	V	4	C	14.0
9	7	467	MET	14.0
7	E	82	ASP	14.0
7	Y	681	GLY	14.0
1	v	287	C	14.0
4	M	252	PRO	14.0
3	H	244	ASP	13.9
7	X	439	VAL	13.9
3	J	638	MET	13.9
2	U	670	PHE	13.9
4	N	471	PRO	13.9
6	F	25	TRP	13.9
7	Y	630	ARG	13.9
4	M	256	GLU	13.9
1	x	692	C	13.9
1	w	489	C	13.8
7	E	86	LEU	13.8
1	V	51	G	13.8
1	x	640	G	13.8
6	2	608	LYS	13.8
8	4	469	MET	13.8
2	D	19	THR	13.8
9	8	663	ARG	13.8
8	4	437	PHE	13.8
5	R	636	VAL	13.7
1	x	650	G	13.7
8	G	39	ASN	13.7
1	w	516	C	13.7
1	x	711	A	13.7
4	B	49	ASN	13.7
1	V	1	A	13.7
9	8	752	GLU	13.7
1	V	92	C	13.6
1	V	120	U	13.6
5	Q	430	SER	13.6

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Mol	Chain	Res	Type	RSRZ
1	w	434	G	13.6
1	x	649	A	13.6
1	x	647	C	13.6
1	v	315	U	13.6
2	D	80	ALA	13.6
4	N	477	ASP	13.5
3	J	636	LYS	13.5
1	x	691	G	13.5
1	V	15	G	13.5
8	4	404	ALA	13.5
10	0	455	ALA	13.5
1	x	686	C	13.4
5	R	633	THR	13.4
1	x	626	A	13.4
1	V	110	G	13.4
1	V	90	U	13.4
6	1	438	GLY	13.4
1	x	696	U	13.4
9	K	9	LEU	13.4
1	w	420	G	13.4
9	8	623	PRO	13.4
1	w	490	U	13.4
2	T	409	VAL	13.4
1	x	653	G	13.3
1	x	746	G	13.3
10	0	404	PHE	13.3
1	w	486	C	13.3
5	Q	411	MET	13.3
8	G	24	GLY	13.3
1	x	601	A	13.3
1	x	709	G	13.3
1	x	641	G	13.2
1	V	156	U	13.2
9	8	688	MET	13.2
6	2	609	PRO	13.2
4	B	78	THR	13.1
4	B	22	GLY	13.1
1	w	454	A	13.1
2	U	624	THR	13.1
4	B	10	LEU	13.1
1	v	208	C	13.1
1	x	651	G	13.1

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Mol	Chain	Res	Type	RSRZ
4	N	453	VAL	13.1
1	w	408	C	13.0
1	x	634	G	13.0
1	v	284	G	13.0
1	V	19	A	13.0
5	R	638	ASN	13.0
1	V	97	U	13.0
1	v	317	G	13.0
1	w	496	U	13.0
8	4	458	GLY	13.0
6	1	454	ALA	13.0
8	5	636	PRO	13.0
2	S	268	ILE	12.9
1	v	358	U	12.9
9	8	777	ASP	12.9
6	2	606	ASN	12.9
8	3	265	ASN	12.9
1	w	558	U	12.9
1	v	246	C	12.9
1	V	108	G	12.8
1	v	222	U	12.8
1	v	212	G	12.8
1	w	410	U	12.7
9	7	417	ASP	12.7
6	Z	270	LEU	12.7
1	v	254	A	12.7
1	V	33	C	12.7
1	V	47	C	12.7
1	w	451	G	12.7
1	x	687	C	12.7
1	V	12	G	12.7
7	X	453	TYR	12.7
10	l	641	TRP	12.7
1	V	50	G	12.7
1	x	713	A	12.7
1	w	436	A	12.6
1	v	220	G	12.6
1	x	655	G	12.6
8	G	65	ASN	12.6
5	Q	436	VAL	12.6
1	x	720	U	12.6
5	P	232	LEU	12.6

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Mol	Chain	Res	Type	RSRZ
1	V	140	G	12.6
2	S	224	THR	12.6
4	M	222	GLY	12.6
1	V	142	G	12.5
1	v	340	G	12.5
1	x	654	A	12.5
7	X	460	ASP	12.5
9	K	171	GLY	12.4
4	M	278	THR	12.4
10	0	441	TRP	12.4
3	J	624	GLY	12.3
1	V	114	C	12.3
5	R	699	MET	12.3
7	E	39	VAL	12.3
1	w	495	U	12.3
7	W	267	LYS	12.3
1	V	54	A	12.3
1	v	226	A	12.3
1	v	236	A	12.3
5	P	312	ASN	12.2
1	x	712	A	12.2
4	O	678	THR	12.2
7	X	452	GLU	12.2
10	9	205	TYR	12.2
2	D	73	LEU	12.2
8	3	207	PRO	12.2
1	V	115	U	12.2
1	v	314	C	12.2
1	x	639	U	12.2
3	A	33	ALA	12.2
4	N	466	ARG	12.2
4	M	266	ARG	12.2
2	D	79	ASN	12.2
1	v	233	C	12.2
10	9	251	ASP	12.1
1	V	93	G	12.1
1	v	309	G	12.1
1	x	652	G	12.1
3	A	23	ASP	12.1
1	v	320	U	12.1
1	w	518	A	12.1
8	G	37	PHE	12.0

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Mol	Chain	Res	Type	RSRZ
3	A	86	PRO	12.0
7	Y	683	ASN	12.0
6	1	413	GLY	12.0
1	x	625	C	12.0
1	x	719	C	12.0
7	E	73	GLN	12.0
1	x	739	G	11.9
1	v	294	A	11.9
1	w	435	A	11.9
1	v	291	G	11.9
7	E	51	ASP	11.9
4	B	67	TYR	11.9
6	Z	264	ILE	11.9
1	w	559	C	11.9
1	x	708	G	11.9
10	l	616	ASP	11.9
3	I	423	GLY	11.9
1	x	609	C	11.9
3	J	623	ASP	11.9
7	X	491	SER	11.8
1	w	508	G	11.8
1	x	622	U	11.8
8	G	47	GLU	11.8
9	8	678	ARG	11.7
1	v	211	G	11.7
9	K	141	GLY	11.7
2	D	64	ARG	11.7
2	D	22	THR	11.7
7	E	40	ASN	11.7
5	C	96	ILE	11.7
1	V	139	G	11.7
1	v	296	U	11.7
1	x	633	C	11.7
1	w	402	U	11.7
10	0	448	SER	11.7
1	w	493	G	11.6
1	w	447	C	11.6
10	L	32	GLU	11.6
2	D	9	VAL	11.6
1	w	562	C	11.6
5	C	57	LYS	11.5
8	4	454	GLN	11.5

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Mol	Chain	Res	Type	RSRZ
2	U	675	ASP	11.5
1	v	243	U	11.5
1	V	28	G	11.5
5	C	61	ARG	11.5
9	8	687	LYS	11.5
7	Y	624	TYR	11.5
7	E	72	LYS	11.4
1	x	631	C	11.4
1	v	255	G	11.4
6	2	678	GLU	11.4
1	x	697	U	11.4
1	x	694	A	11.4
1	V	26	A	11.3
1	V	55	G	11.3
1	w	494	A	11.3
3	H	242	LEU	11.3
5	C	60	ASP	11.3
10	9	248	SER	11.3
1	w	411	G	11.3
1	w	424	C	11.2
6	1	450	TYR	11.2
1	v	234	G	11.2
1	v	240	G	11.2
9	7	533	HIS	11.2
8	G	70	LEU	11.2
1	V	96	U	11.1
1	v	224	C	11.1
1	v	210	U	11.1
1	v	225	C	11.1
1	V	164	G	11.1
5	P	235	SER	11.1
2	S	235	ALA	11.1
9	8	689	TRP	11.1
1	x	695	U	11.0
2	T	424	THR	11.0
8	5	637	PHE	11.0
1	w	488	C	11.0
6	F	40	MET	11.0
1	w	563	U	11.0
7	W	270	SER	11.0
9	6	270	LYS	10.9
3	H	286	PRO	10.9

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Mol	Chain	Res	Type	RSRZ
1	V	11	G	10.9
1	v	242	U	10.9
1	V	27	U	10.9
9	6	266	ARG	10.9
7	E	48	ILE	10.9
9	K	82	VAL	10.9
9	8	679	GLN	10.9
5	C	63	CYS	10.8
1	w	539	G	10.8
4	N	428	THR	10.8
9	7	409	LEU	10.8
1	v	357	U	10.8
4	O	653	VAL	10.8
1	w	425	C	10.7
7	X	425	LEU	10.7
6	1	408	LYS	10.7
8	3	274	GLU	10.7
1	V	41	G	10.7
5	C	92	LYS	10.7
1	V	163	U	10.7
3	H	269	LEU	10.7
1	x	710	G	10.7
9	8	730	LYS	10.7
1	V	39	U	10.7
1	w	412	G	10.6
5	P	243	LEU	10.6
1	v	241	G	10.6
6	F	26	GLY	10.6
1	x	621	A	10.6
1	v	350	U	10.6
5	R	647	ARG	10.6
1	x	689	C	10.5
4	B	50	ARG	10.5
5	Q	455	ARG	10.5
1	v	356	U	10.5
10	l	614	THR	10.5
1	w	487	C	10.5
1	v	295	U	10.5
5	C	114	LEU	10.5
9	6	209	LEU	10.4
4	O	663	ASN	10.4
4	N	456	GLU	10.4

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Mol	Chain	Res	Type	RSRZ
1	v	290	U	10.4
1	V	95	U	10.4
1	w	429	A	10.4
9	7	541	GLY	10.4
1	V	83	C	10.4
4	O	622	GLY	10.4
2	T	464	ARG	10.3
7	W	268	THR	10.3
10	9	258	GLN	10.3
1	V	32	A	10.3
1	v	227	U	10.3
10	0	418	PRO	10.3
3	A	7	SER	10.3
9	K	68	GLU	10.3
1	V	94	A	10.3
1	x	643	U	10.3
1	v	228	G	10.3
5	C	11	MET	10.2
5	P	248	ASN	10.2
8	4	422	ASN	10.2
10	9	254	THR	10.2
1	v	231	C	10.2
1	v	213	C	10.2
1	w	409	C	10.2
1	v	256	A	10.2
1	V	155	C	10.2
4	O	614	THR	10.2
7	Y	651	ASP	10.1
2	D	27	VAL	10.1
1	v	311	A	10.1
3	H	234	PHE	10.1
6	F	53	GLY	10.1
1	x	684	G	10.1
1	V	158	U	10.1
4	M	210	LEU	10.1
1	v	215	G	10.1
3	H	287	PRO	10.0
8	5	670	LEU	10.0
4	N	450	ARG	10.0
7	Y	673	GLN	10.0
9	7	567	LYS	10.0
7	E	58	LEU	10.0

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Mol	Chain	Res	Type	RSRZ
1	V	42	U	10.0
8	G	51	SER	10.0
9	8	665	GLU	10.0
9	K	173	ARG	9.9
9	K	10	LEU	9.9
1	V	24	C	9.9
5	P	261	ARG	9.9
1	v	319	C	9.9
3	I	442	CYS	9.9
4	O	654	GLN	9.9
1	w	430	U	9.9
1	x	762	C	9.9
10	L	41	TRP	9.9
3	I	486	PRO	9.9
8	G	50	THR	9.9
8	3	250	THR	9.9
1	v	232	A	9.9
10	9	213	LEU	9.9
8	G	46	VAL	9.8
1	V	44	U	9.8
8	3	268	ILE	9.8
9	7	468	GLU	9.8
7	W	250	PHE	9.8
10	L	18	PRO	9.8
1	x	602	U	9.8
3	H	268	GLY	9.8
1	w	428	G	9.8
1	x	683	C	9.8
1	w	442	U	9.7
3	H	285	PRO	9.7
1	v	339	G	9.7
1	V	25	C	9.7
7	Y	691	SER	9.7
2	S	212	GLU	9.7
1	w	543	A	9.7
6	F	14	LEU	9.7
1	w	560	C	9.7
2	T	452	ASP	9.7
4	O	613	GLU	9.7
5	P	246	CYS	9.7
1	V	13	C	9.6
4	O	612	HIS	9.6

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Mol	Chain	Res	Type	RSRZ
7	E	68	THR	9.6
7	Y	672	LYS	9.6
7	W	292	ASN	9.6
1	x	616	G	9.6
3	J	673	ARG	9.6
1	v	318	A	9.6
1	w	441	G	9.5
1	V	40	G	9.5
1	w	403	A	9.5
1	v	239	U	9.5
1	v	207	A	9.5
4	M	247	LEU	9.5
9	7	419	ILE	9.5
5	R	640	THR	9.4
5	R	692	LYS	9.4
5	R	641	GLN	9.4
1	x	611	G	9.4
6	2	672	ILE	9.4
7	W	225	LEU	9.4
1	V	122	C	9.4
1	v	209	C	9.4
1	x	642	U	9.3
9	K	170	ASP	9.3
8	3	275	ARG	9.3
4	M	242	ALA	9.3
8	3	262	ILE	9.3
8	G	20	LYS	9.3
1	x	636	A	9.2
7	E	81	GLY	9.2
5	P	262	HIS	9.2
5	C	71	LYS	9.2
7	W	291	SER	9.2
5	C	101	LEU	9.2
1	x	644	U	9.2
1	w	546	G	9.1
2	D	23	ASN	9.1
7	E	53	TYR	9.1
6	F	8	LYS	9.1
9	K	72	ARG	9.1
1	v	235	A	9.1
8	3	251	SER	9.1
1	w	561	C	9.1

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Mol	Chain	Res	Type	RSRZ
9	K	78	ARG	9.1
1	w	443	U	9.0
8	G	4	ALA	9.0
9	8	774	VAL	9.0
1	x	632	A	9.0
10	9	241	TRP	9.0
6	2	639	TYR	9.0
10	9	236	ASP	9.0
5	R	649	ASN	9.0
1	x	635	A	9.0
8	5	624	GLY	9.0
9	6	210	LEU	9.0
9	7	542	LYS	9.0
6	2	675	VAL	8.9
5	Q	461	ARG	8.9
9	7	412	LEU	8.9
4	M	202	LYS	8.9
1	w	419	A	8.9
5	Q	460	ASP	8.9
1	x	620	G	8.9
4	B	35	SER	8.9
6	F	9	PRO	8.9
1	x	608	C	8.8
6	1	421	VAL	8.8
6	F	70	LEU	8.8
6	Z	252	ASP	8.8
7	E	38	GLN	8.8
7	Y	621	ILE	8.8
5	P	212	THR	8.8
10	0	445	GLN	8.8
9	6	271	ARG	8.8
1	V	56	A	8.8
1	x	693	G	8.8
4	N	435	SER	8.7
4	B	13	GLU	8.7
2	S	211	HIS	8.7
5	R	616	LEU	8.7
5	R	611	MET	8.7
9	8	778	VAL	8.7
10	L	36	ASP	8.7
1	V	23	A	8.7
8	5	654	GLN	8.7

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Mol	Chain	Res	Type	RSRZ
2	T	445	ASN	8.7
5	P	211	MET	8.7
4	O	642	ALA	8.7
4	B	18	GLU	8.7
8	3	239	ASN	8.7
9	6	328	PRO	8.6
3	J	643	CYS	8.6
5	P	242	VAL	8.6
4	O	669	ILE	8.6
1	x	624	C	8.6
8	5	664	GLY	8.6
8	5	675	ARG	8.6
1	x	627	U	8.6
9	7	530	LYS	8.6
3	H	240	LEU	8.6
1	V	148	G	8.6
5	Q	418	LYS	8.6
3	A	85	PRO	8.5
1	w	437	G	8.5
2	S	225	GLY	8.5
1	w	484	G	8.5
8	3	221	LEU	8.4
1	v	292	C	8.4
3	J	641	ILE	8.4
6	2	624	LYS	8.4
1	x	738	G	8.4
5	P	304	ASP	8.4
5	C	17	GLN	8.4
8	4	451	SER	8.4
10	L	4	PHE	8.4
6	1	446	ASN	8.4
9	K	15	PRO	8.4
7	Y	653	TYR	8.4
1	V	160	C	8.4
7	W	220	LEU	8.4
1	x	703	A	8.4
1	x	688	C	8.3
5	R	696	ILE	8.3
1	x	629	A	8.3
2	U	627	VAL	8.3
1	v	338	G	8.3
8	4	450	THR	8.3

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Mol	Chain	Res	Type	RSRZ
1	V	125	A	8.3
9	K	13	PHE	8.3
8	5	639	ASN	8.3
1	x	610	U	8.3
5	C	97	SER	8.3
6	1	410	PHE	8.3
7	X	443	ILE	8.3
8	5	665	ASN	8.3
10	L	33	ASN	8.3
5	Q	475	THR	8.3
4	B	48	LYS	8.2
7	X	449	GLY	8.2
5	R	660	ASP	8.2
4	M	205	ARG	8.2
4	O	605	ARG	8.2
1	x	603	A	8.2
4	B	2	LYS	8.2
10	L	34	VAL	8.2
5	R	693	ASP	8.2
3	A	32	LYS	8.2
1	v	237	G	8.2
9	K	71	ARG	8.2
5	P	258	ALA	8.2
5	R	612	THR	8.2
1	V	138	G	8.2
1	w	407	A	8.1
10	L	15	HIS	8.1
4	B	52	PRO	8.1
1	w	427	U	8.1
10	L	13	LEU	8.1
5	Q	463	CYS	8.1
10	9	233	ASN	8.1
5	C	62	HIS	8.1
6	1	437	ASP	8.1
6	2	670	LEU	8.0
5	P	253	LEU	8.0
7	W	265	HIS	8.0
4	N	441	LYS	8.0
8	5	649	ALA	8.0
6	1	423	LEU	8.0
5	P	263	CYS	8.0
7	E	52	GLU	8.0

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Mol	Chain	Res	Type	RSRZ
5	Q	462	HIS	7.9
3	I	485	PRO	7.9
8	5	622	ASN	7.9
6	Z	267	ASN	7.9
1	v	206	U	7.9
9	8	753	HIS	7.9
5	C	58	ALA	7.9
9	7	410	LEU	7.9
3	H	207	SER	7.9
5	Q	423	GLU	7.9
10	l	610	ASP	7.8
10	l	611	THR	7.8
4	O	656	GLU	7.8
7	E	32	GLN	7.8
10	9	232	GLU	7.8
10	L	42	MET	7.8
1	w	423	A	7.8
5	R	613	PRO	7.7
1	w	530	G	7.7
7	W	269	LYS	7.7
1	v	203	A	7.7
3	J	607	SER	7.7
2	S	252	ASP	7.7
1	x	656	A	7.7
8	G	22	ASN	7.7
5	P	260	ASP	7.7
2	S	223	ASN	7.7
6	Z	265	ARG	7.7
1	w	538	G	7.7
6	Z	206	ASN	7.7
6	F	71	TYR	7.7
4	B	70	LEU	7.7
4	N	431	GLY	7.7
3	A	87	PRO	7.7
4	O	651	GLU	7.7
9	7	552	GLU	7.7
1	x	613	C	7.6
5	R	704	ASP	7.6
8	3	208	GLU	7.6
4	O	649	ASN	7.6
9	7	580	ARG	7.6
3	I	437	MET	7.6

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Mol	Chain	Res	Type	RSRZ
6	1	466	CYS	7.6
10	9	247	GLN	7.6
1	V	145	U	7.6
5	R	634	GLN	7.6
4	B	9	LYS	7.5
3	I	431	LYS	7.5
5	C	33	THR	7.5
4	O	628	THR	7.5
10	L	24	HIS	7.5
3	J	625	ARG	7.5
1	V	132	G	7.5
1	x	614	A	7.5
3	I	436	HIS	7.5
4	N	463	ASN	7.5
8	3	225	ARG	7.5
3	I	487	PRO	7.5
1	w	439	U	7.5
4	O	610	LEU	7.5
5	C	67	LEU	7.5
1	w	503	A	7.5
7	X	445	GLY	7.5
9	6	367	LYS	7.4
1	w	444	U	7.4
1	V	14	A	7.4
5	C	15	GLU	7.4
4	N	409	LYS	7.4
8	5	623	GLY	7.4
5	Q	501	LEU	7.4
10	L	26	SER	7.4
3	J	678	VAL	7.4
4	B	6	PHE	7.4
9	6	347	ALA	7.4
1	V	151	C	7.4
10	9	259	GLN	7.4
2	S	240	ASN	7.4
5	R	663	CYS	7.4
4	O	606	PHE	7.3
5	C	49	ASN	7.3
6	F	12	ASN	7.3
1	v	328	U	7.3
8	G	52	GLY	7.3
5	Q	426	THR	7.3

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Mol	Chain	Res	Type	RSRZ
1	v	330	G	7.3
2	U	636	GLU	7.3
9	6	223	PRO	7.3
7	W	221	ILE	7.3
9	8	759	SER	7.3
4	N	405	ARG	7.3
9	7	510	VAL	7.3
5	P	292	LYS	7.3
10	9	211	THR	7.3
5	R	700	PHE	7.3
8	G	34	PHE	7.3
5	P	234	GLN	7.3
1	v	283	C	7.3
3	A	46	ASP	7.3
5	Q	459	PHE	7.3
10	9	207	ASP	7.3
2	T	453	GLY	7.3
9	6	372	ARG	7.3
4	M	267	TYR	7.2
1	w	547	C	7.2
3	J	672	LEU	7.2
1	v	333	G	7.2
6	1	439	TYR	7.2
4	B	12	HIS	7.2
4	O	635	SER	7.2
5	C	59	PHE	7.2
9	K	174	VAL	7.2
4	B	23	THR	7.2
8	3	234	PHE	7.2
9	8	616	ARG	7.2
7	Y	620	LEU	7.2
5	Q	476	GLU	7.2
7	W	236	TYR	7.2
4	B	34	VAL	7.2
8	5	661	VAL	7.2
3	A	9	MET	7.2
9	8	683	GLU	7.2
9	K	175	LEU	7.1
9	K	79	GLN	7.1
8	5	660	VAL	7.1
1	x	690	U	7.1
1	V	34	G	7.1

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Mol	Chain	Res	Type	RSRZ
1	w	536	G	7.1
6	F	57	GLY	7.1
8	3	270	LEU	7.1
1	V	43	U	7.1
1	w	545	U	7.1
7	X	421	ILE	7.1
1	x	604	C	7.1
1	V	3	A	7.1
1	x	685	U	7.1
10	l	605	TYR	7.1
10	9	246	ALA	7.1
4	O	630	THR	7.1
8	4	470	LEU	7.1
4	M	235	SER	7.1
3	A	44	ASP	7.0
8	5	643	ASP	7.0
8	4	474	GLU	7.0
5	Q	422	GLU	7.0
2	T	466	CYS	7.0
6	1	427	MET	7.0
4	M	206	PHE	7.0
9	8	765	ASP	7.0
1	v	214	A	7.0
4	O	602	LYS	7.0
1	x	612	G	7.0
3	A	36	LYS	7.0
6	F	52	ASP	6.9
4	B	7	LEU	6.9
6	2	655	LEU	6.9
5	C	23	GLU	6.9
8	5	633	GLY	6.9
6	1	435	SER	6.9
1	V	7	A	6.9
8	G	23	GLY	6.9
5	R	659	PHE	6.9
4	N	406	PHE	6.9
1	w	415	G	6.9
10	L	5	TYR	6.9
10	0	432	GLU	6.9
3	J	647	GLU	6.8
6	Z	240	MET	6.8
7	Y	680	LYS	6.8

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Mol	Chain	Res	Type	RSRZ
1	V	126	A	6.8
8	G	74	GLU	6.8
4	B	5	ARG	6.8
7	E	90	VAL	6.8
8	G	19	LEU	6.8
2	D	53	GLY	6.8
8	3	254	GLN	6.8
5	Q	469	ASN	6.8
1	w	506	G	6.8
7	X	435	LEU	6.8
2	U	620	CYS	6.8
4	O	668	PHE	6.8
7	Y	638	GLN	6.7
7	X	419	ASN	6.7
6	2	667	ASN	6.7
9	7	512	TYR	6.7
1	x	645	U	6.7
6	Z	223	LEU	6.7
4	M	209	LYS	6.7
5	Q	504	ASP	6.7
9	8	618	PRO	6.7
2	U	621	GLU	6.7
9	8	741	GLY	6.7
8	G	25	ARG	6.7
1	V	29	A	6.7
9	6	368	LYS	6.7
2	D	42	GLN	6.7
5	Q	464	ASN	6.7
7	W	224	TYR	6.7
10	0	430	HIS	6.6
2	D	54	ARG	6.6
7	Y	671	ARG	6.6
9	6	346	TYR	6.6
10	L	60	GLY	6.6
1	w	537	U	6.6
6	1	416	GLY	6.6
10	l	645	GLN	6.6
4	N	437	ASN	6.6
1	V	31	C	6.6
1	x	607	A	6.6
6	2	635	SER	6.6
9	8	767	LYS	6.6

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Mol	Chain	Res	Type	RSRZ
8	5	632	ARG	6.6
1	w	440	G	6.5
5	C	26	THR	6.5
4	N	408	MET	6.5
7	Y	652	GLU	6.5
5	R	635	SER	6.5
7	W	232	GLN	6.5
9	8	762	LYS	6.5
10	9	214	THR	6.5
3	J	609	MET	6.5
8	G	53	GLN	6.5
10	9	260	GLY	6.5
1	x	630	U	6.5
3	J	611	GLN	6.5
7	X	438	GLN	6.5
10	9	230	HIS	6.4
8	4	432	ARG	6.4
3	H	238	MET	6.4
5	Q	428	PRO	6.4
1	w	529	U	6.4
8	5	614	ASP	6.4
9	K	165	ASP	6.4
5	P	301	LEU	6.4
1	v	329	U	6.4
1	v	327	U	6.4
1	V	153	C	6.4
8	4	433	GLY	6.4
5	P	294	ARG	6.4
10	l	631	LYS	6.3
3	A	75	GLU	6.3
5	P	222	GLU	6.3
3	A	25	ARG	6.3
1	w	413	C	6.3
3	A	11	GLN	6.3
8	4	455	ASN	6.3
2	T	425	GLY	6.3
10	0	437	TYR	6.3
1	V	144	C	6.3
3	H	211	GLN	6.3
6	2	665	ARG	6.3
7	W	289	SER	6.2
10	9	209	CYS	6.2

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Mol	Chain	Res	Type	RSRZ
4	N	407	LEU	6.2
4	N	464	ASN	6.2
1	V	152	G	6.2
6	1	447	THR	6.2
9	7	554	GLU	6.2
1	x	723	A	6.2
3	A	37	HIS	6.2
2	T	451	ARG	6.2
10	0	410	ASP	6.2
2	D	41	CYS	6.2
1	x	745	U	6.2
3	H	221	LEU	6.2
7	X	424	TYR	6.2
1	x	722	C	6.2
4	M	270	LEU	6.1
6	Z	238	GLY	6.1
6	2	640	MET	6.1
9	7	503	LYS	6.1
5	R	626	THR	6.1
2	S	251	ARG	6.1
8	4	457	ILE	6.1
2	U	625	GLY	6.1
8	5	651	SER	6.1
8	4	414	ASP	6.1
5	R	712	ASN	6.1
9	7	423	PRO	6.1
7	X	422	PHE	6.1
1	w	414	A	6.1
7	X	423	ARG	6.1
6	1	458	HIS	6.1
8	3	227	VAL	6.1
7	E	50	PHE	6.1
2	D	52	ASP	6.1
1	v	229	A	6.1
7	X	489	SER	6.1
7	Y	635	LEU	6.1
3	A	72	LEU	6.0
5	C	22	GLU	6.0
8	3	269	MET	6.0
4	B	37	ASN	6.0
6	1	412	ASN	6.0
4	B	36	MET	6.0

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Mol	Chain	Res	Type	RSRZ
10	l	635	LYS	6.0
7	Y	660	ASP	6.0
4	O	621	ASN	6.0
9	6	268	GLU	6.0
4	N	402	LYS	6.0
6	F	69	VAL	6.0
8	3	259	MET	6.0
3	J	621	LEU	6.0
7	E	92	ASN	6.0
6	2	656	SER	6.0
9	7	525	VAL	6.0
4	M	208	MET	6.0
6	F	11	LEU	5.9
3	H	225	ARG	5.9
6	2	638	GLY	5.9
2	T	406	PRO	5.9
6	F	67	ASN	5.9
9	K	153	HIS	5.9
4	N	436	MET	5.9
1	V	136	G	5.9
9	6	216	ARG	5.9
8	G	26	HIS	5.9
7	X	476	ARG	5.9
1	x	751	C	5.9
5	P	213	PRO	5.9
6	2	637	ASP	5.9
5	Q	425	ASN	5.9
8	G	49	ALA	5.9
4	O	620	LYS	5.9
7	E	69	LYS	5.8
4	M	237	ASN	5.8
9	K	88	MET	5.8
5	Q	446	CYS	5.8
7	W	288	GLN	5.8
10	0	424	HIS	5.8
1	x	744	C	5.8
4	N	427	GLY	5.8
4	M	207	LEU	5.7
4	M	204	VAL	5.7
7	Y	640	ASN	5.7
1	x	757	U	5.7
2	T	454	ARG	5.7

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Mol	Chain	Res	Type	RSRZ
7	E	21	ILE	5.7
5	R	694	ARG	5.7
7	X	488	GLN	5.7
4	M	234	VAL	5.7
7	W	272	LYS	5.7
2	T	442	GLN	5.7
2	U	611	HIS	5.7
5	C	75	THR	5.7
1	x	736	G	5.7
10	0	436	ASP	5.7
5	Q	420	GLU	5.7
10	9	239	CYS	5.7
7	E	67	LYS	5.7
3	H	209	MET	5.6
5	C	13	PRO	5.6
3	J	610	LEU	5.6
1	w	548	G	5.6
7	Y	690	VAL	5.6
3	H	237	HIS	5.6
9	6	378	VAL	5.6
5	R	639	ASN	5.6
4	M	213	GLU	5.6
8	4	444	GLU	5.6
7	E	70	SER	5.6
4	N	416	THR	5.6
2	T	412	GLU	5.6
5	C	55	ARG	5.6
3	I	407	LYS	5.6
5	P	254	GLY	5.6
6	1	434	VAL	5.6
7	X	420	LEU	5.6
5	R	661	ARG	5.6
4	N	444	LYS	5.6
1	v	331	U	5.6
7	X	418	ILE	5.6
5	C	54	GLY	5.5
10	L	11	THR	5.5
10	0	438	TYR	5.5
6	F	38	GLY	5.5
6	2	657	GLY	5.5
7	Y	622	PHE	5.5
7	Y	632	GLN	5.5

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Mol	Chain	Res	Type	RSRZ
4	B	33	ASP	5.5
10	l	659	GLN	5.5
1	V	146	G	5.5
5	Q	494	ARG	5.5
1	v	205	U	5.5
4	O	604	VAL	5.5
4	O	634	VAL	5.5
8	4	427	VAL	5.5
6	1	436	VAL	5.5
4	N	410	LEU	5.4
7	Y	684	ILE	5.4
1	v	336	G	5.4
9	6	325	VAL	5.4
9	K	14	ALA	5.4
9	8	717	SER	5.4
5	C	24	PHE	5.4
3	J	608	LYS	5.4
3	H	222	GLN	5.4
1	v	230	U	5.4
1	w	532	G	5.4
5	C	28	PRO	5.4
10	l	638	TYR	5.4
4	N	467	TYR	5.4
9	K	162	LYS	5.4
1	v	325	A	5.4
1	V	128	U	5.4
5	C	52	LEU	5.4
6	F	75	VAL	5.4
5	C	25	ASN	5.4
10	l	642	MET	5.4
6	2	615	THR	5.4
10	L	23	THR	5.4
10	0	433	ASN	5.4
10	9	225	CYS	5.3
3	H	208	LYS	5.3
3	A	12	HIS	5.3
4	M	255	LEU	5.3
5	P	221	GLU	5.3
5	P	223	GLU	5.3
10	9	234	VAL	5.3
10	9	231	LYS	5.3
2	S	244	SER	5.3

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Mol	Chain	Res	Type	RSRZ
9	K	154	GLU	5.3
7	E	85	THR	5.3
3	A	10	LEU	5.3
4	B	4	VAL	5.3
5	Q	506	VAL	5.3
10	9	242	MET	5.3
1	x	727	U	5.3
7	W	218	ILE	5.3
9	K	22	LEU	5.3
8	G	14	ASP	5.3
6	1	456	SER	5.3
7	X	455	ASN	5.3
8	3	260	VAL	5.3
9	7	531	ARG	5.3
3	A	73	ARG	5.3
10	9	221	ARG	5.3
6	1	460	GLY	5.3
7	E	91	SER	5.3
9	8	729	ILE	5.3
4	O	623	THR	5.2
3	A	8	LYS	5.2
1	V	159	C	5.2
10	9	226	SER	5.2
4	N	433	ASP	5.2
5	P	296	ILE	5.2
7	Y	666	SER	5.2
10	0	428	ARG	5.2
8	4	410	LYS	5.2
10	l	655	ALA	5.2
1	x	737	U	5.2
8	G	6	PRO	5.2
3	A	47	GLU	5.2
10	l	607	ASP	5.2
4	N	434	VAL	5.2
8	3	252	GLY	5.2
1	w	535	A	5.2
3	H	247	GLU	5.2
8	5	625	ARG	5.2
9	8	780	ARG	5.2
6	1	455	LEU	5.2
7	Y	656	LEU	5.2
5	C	64	ASN	5.2

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Mol	Chain	Res	Type	RSRZ
8	3	267	ILE	5.2
7	E	71	ARG	5.2
8	4	413	MET	5.2
9	8	713	ASP	5.2
6	Z	248	GLU	5.1
4	O	627	GLY	5.1
7	Y	618	ILE	5.1
9	8	756	ASP	5.1
1	v	351	C	5.1
4	M	236	MET	5.1
5	C	69	ASN	5.1
3	I	475	GLU	5.1
8	G	7	PRO	5.1
9	8	725	VAL	5.1
5	R	711	ARG	5.1
2	U	623	ASN	5.1
6	1	415	THR	5.1
10	9	235	LYS	5.1
10	0	431	LYS	5.1
1	w	406	U	5.1
9	K	85	GLU	5.1
7	E	78	MET	5.1
1	w	404	C	5.0
10	0	452	LYS	5.0
5	C	19	ARG	5.0
7	Y	655	ASN	5.0
2	S	253	GLY	5.0
10	0	419	SER	5.0
1	w	564	G	5.0
5	C	20	GLU	5.0
6	2	612	ASN	5.0
4	O	638	THR	5.0
5	Q	424	PHE	5.0
1	x	750	U	5.0
5	C	27	GLY	5.0
2	D	34	GLU	5.0
9	K	76	GLU	5.0
5	P	226	THR	5.0
1	V	129	U	5.0
10	0	444	GLU	5.0
1	x	725	A	5.0
3	A	76	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
4	M	265	ILE	5.0
3	I	446	GLU	5.0
9	8	685	GLU	5.0
10	0	406	CYS	5.0
6	Z	218	PRO	4.9
1	V	30	U	4.9
7	E	28	ARG	4.9
7	Y	623	ARG	4.9
9	6	339	ARG	4.9
9	8	721	ARG	4.9
8	3	249	ALA	4.9
5	R	617	GLN	4.9
6	2	636	VAL	4.9
2	U	667	LYS	4.9
10	L	59	GLN	4.9
3	A	41	ILE	4.9
4	O	608	MET	4.9
7	X	456	LEU	4.9
8	4	419	LEU	4.9
2	D	44	SER	4.9
2	D	43	MET	4.9
2	U	642	GLN	4.9
7	E	88	GLN	4.9
1	V	135	A	4.9
5	C	21	GLU	4.9
2	D	56	ALA	4.9
4	N	404	VAL	4.9
10	l	626	SER	4.9
5	C	100	PHE	4.9
8	4	434	PHE	4.9
5	C	37	LYS	4.9
6	2	625	TRP	4.9
5	Q	458	ALA	4.9
6	2	659	LEU	4.9
9	7	517	SER	4.9
7	Y	692	ASN	4.9
6	2	653	GLY	4.9
1	V	124	U	4.9
1	v	352	G	4.9
9	6	370	ASP	4.9
5	R	664	ASN	4.9
5	R	646	CYS	4.8

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Mol	Chain	Res	Type	RSRZ
9	6	353	HIS	4.8
7	E	66	SER	4.8
6	1	432	TYR	4.8
4	O	637	ASN	4.8
5	P	244	ILE	4.8
6	F	74	GLY	4.8
9	8	709	ARG	4.8
7	E	20	LEU	4.8
7	E	74	LEU	4.8
9	6	222	LEU	4.8
6	F	39	TYR	4.8
8	G	10	LYS	4.8
5	R	667	LEU	4.8
4	B	53	VAL	4.8
4	B	14	THR	4.8
8	G	33	GLY	4.8
2	S	242	GLN	4.8
9	6	288	MET	4.8
2	T	447	THR	4.8
3	H	265	ARG	4.8
5	R	710	LEU	4.8
1	x	758	U	4.8
6	F	72	ILE	4.8
8	5	613	MET	4.8
9	6	313	ASP	4.8
5	P	252	LEU	4.8
7	E	18	ILE	4.8
4	N	411	SER	4.8
7	E	89	SER	4.8
5	Q	452	LEU	4.8
8	5	650	THR	4.8
9	7	416	ARG	4.8
7	E	77	ILE	4.7
8	G	13	MET	4.7
4	B	3	LEU	4.7
4	B	56	GLU	4.7
6	2	658	HIS	4.7
7	Y	619	ASN	4.7
2	T	423	ASN	4.7
6	F	7	PRO	4.7
8	4	431	LEU	4.7
2	S	215	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
10	I	651	ASP	4.7
1	V	134	U	4.7
8	4	406	PRO	4.7
5	Q	431	VAL	4.6
2	S	243	MET	4.6
9	7	487	LYS	4.6
10	L	10	ASP	4.6
3	J	632	LYS	4.6
9	6	355	ARG	4.6
3	A	35	ASP	4.6
5	Q	454	GLY	4.6
3	J	671	LEU	4.6
4	M	214	THR	4.6
7	X	485	THR	4.6
7	W	230	ARG	4.6
3	J	685	PRO	4.6
2	U	647	THR	4.6
4	O	657	THR	4.6
2	S	213	ALA	4.6
7	W	233	VAL	4.6
9	8	771	GLY	4.6
1	V	137	U	4.6
10	9	212	TYR	4.6
2	D	40	ASN	4.6
5	R	628	PRO	4.6
5	P	214	GLU	4.6
10	L	43	GLU	4.6
3	J	635	ASP	4.6
7	W	223	ARG	4.6
2	D	55	VAL	4.6
3	J	669	LEU	4.6
4	O	607	LEU	4.6
4	O	652	PRO	4.6
5	R	627	GLY	4.6
1	x	724	U	4.6
2	D	16	HIS	4.6
3	J	683	GLU	4.6
4	N	426	HIS	4.6
7	W	246	CYS	4.6
8	4	421	LEU	4.5
6	F	46	ASN	4.5
6	2	671	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
5	Q	457	LYS	4.5
7	X	458	LEU	4.5
5	Q	427	GLY	4.5
6	Z	216	GLY	4.5
1	w	531	U	4.5
2	U	635	ALA	4.5
1	V	131	U	4.5
5	Q	493	ASP	4.5
10	9	210	ASP	4.5
4	O	650	ARG	4.5
5	R	655	ARG	4.5
9	7	579	GLU	4.5
9	6	359	SER	4.5
3	H	210	LEU	4.5
7	Y	625	LEU	4.5
6	1	440	MET	4.5
6	1	445	ALA	4.5
3	A	71	LEU	4.5
4	O	647	LEU	4.5
8	G	32	ARG	4.5
2	U	641	CYS	4.5
6	2	616	GLY	4.5
4	M	238	THR	4.4
5	R	709	VAL	4.4
1	w	544	C	4.4
7	Y	667	LYS	4.4
10	9	237	TYR	4.4
4	B	55	LEU	4.4
4	N	469	ILE	4.4
8	4	449	ALA	4.4
5	R	619	ARG	4.4
5	P	264	ASN	4.4
5	Q	507	ILE	4.4
5	Q	421	GLU	4.4
7	W	227	ASN	4.4
7	W	226	GLN	4.4
7	X	472	LYS	4.4
9	6	317	SER	4.3
5	P	293	ASP	4.3
6	1	476	GLU	4.3
4	B	27	GLY	4.3
4	B	62	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
2	S	241	CYS	4.3
3	J	686	PRO	4.3
5	P	275	THR	4.3
8	3	243	ASP	4.3
4	N	418	GLU	4.3
7	Y	685	THR	4.3
1	V	133	G	4.3
2	U	656	ALA	4.3
5	R	702	ARG	4.3
5	C	65	MET	4.3
7	Y	675	GLY	4.3
8	3	233	GLY	4.3
2	D	26	GLU	4.3
4	B	42	ALA	4.3
10	L	50	ILE	4.3
7	Y	639	VAL	4.3
8	G	54	GLN	4.3
4	N	462	GLY	4.3
6	1	457	GLY	4.3
8	4	423	GLY	4.3
8	3	244	GLU	4.3
8	4	468	ILE	4.3
5	C	29	LEU	4.3
6	Z	246	ASN	4.3
8	3	263	ARG	4.3
4	M	216	THR	4.3
10	l	613	LEU	4.3
6	Z	208	LYS	4.3
2	S	245	ASN	4.3
2	D	33	ILE	4.2
2	S	254	ARG	4.2
9	K	125	VAL	4.2
7	W	273	GLN	4.2
4	O	615	VAL	4.2
8	5	626	HIS	4.2
6	Z	256	SER	4.2
8	5	634	PHE	4.2
4	B	16	THR	4.2
4	B	28	THR	4.2
6	2	663	LEU	4.2
4	O	636	MET	4.2
4	O	648	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
6	2	666	CYS	4.2
9	8	763	HIS	4.2
1	w	528	U	4.2
4	M	233	ASP	4.2
8	5	607	PRO	4.2
9	K	155	ARG	4.2
10	L	12	TYR	4.2
6	2	674	GLY	4.2
7	W	245	GLY	4.2
8	3	222	ASN	4.1
7	W	228	ARG	4.1
8	3	253	GLN	4.1
10	0	423	THR	4.1
4	O	639	HIS	4.1
4	M	203	LEU	4.1
7	E	47	ILE	4.1
2	D	8	LYS	4.1
9	8	720	ARG	4.1
6	2	681	ASP	4.1
2	S	230	GLY	4.1
6	Z	263	LEU	4.1
8	3	226	HIS	4.1
5	R	621	GLU	4.1
8	4	459	MET	4.1
6	Z	260	GLY	4.1
6	1	422	LYS	4.1
9	6	287	LYS	4.1
7	E	57	VAL	4.1
10	l	615	HIS	4.1
1	v	349	U	4.1
3	J	665	ARG	4.1
5	R	708	VAL	4.1
4	O	626	HIS	4.1
10	L	46	ALA	4.1
6	1	459	LEU	4.1
7	W	248	ILE	4.1
3	A	81	THR	4.1
6	2	613	GLY	4.1
10	L	54	THR	4.1
1	w	551	C	4.1
6	1	420	MET	4.1
9	7	553	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
2	U	612	GLU	4.1
6	F	6	ASN	4.1
5	P	311	ARG	4.0
5	Q	419	ARG	4.0
1	w	445	U	4.0
3	H	281	THR	4.0
6	F	37	ASP	4.0
10	l	660	GLY	4.0
10	0	443	GLU	4.0
5	P	225	ASN	4.0
7	E	49	GLY	4.0
7	Y	689	SER	4.0
4	N	423	THR	4.0
5	R	671	LYS	4.0
5	C	107	ILE	4.0
9	7	521	ARG	4.0
3	A	78	VAL	4.0
7	X	473	GLN	4.0
9	8	622	LEU	4.0
4	N	414	THR	4.0
9	6	213	PHE	4.0
6	Z	213	GLY	4.0
5	C	39	ASN	4.0
6	2	664	ILE	4.0
3	J	633	ALA	4.0
3	J	679	SER	4.0
7	E	23	ARG	4.0
1	V	127	U	4.0
1	w	534	U	4.0
5	P	308	VAL	4.0
1	V	154	G	4.0
5	Q	465	MET	4.0
4	N	403	LEU	3.9
2	U	652	ASP	3.9
8	4	411	LYS	3.9
8	5	667	ILE	3.9
2	U	651	ARG	3.9
2	T	441	CYS	3.9
4	B	43	VAL	3.9
1	v	326	A	3.9
2	S	216	HIS	3.9
7	X	444	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
10	0	429	LYS	3.9
6	2	641	ASN	3.9
4	B	31	GLY	3.9
5	R	662	HIS	3.9
10	0	425	CYS	3.9
5	R	615	GLU	3.9
2	D	49	THR	3.9
9	6	221	TYR	3.9
4	N	415	VAL	3.9
4	O	617	ILE	3.9
5	R	705	SER	3.9
9	7	563	HIS	3.9
10	0	411	THR	3.9
10	0	442	MET	3.9
5	R	620	GLU	3.9
5	Q	492	LYS	3.9
3	J	640	LEU	3.9
5	R	614	GLU	3.9
5	R	642	VAL	3.9
4	O	662	GLY	3.8
4	M	212	HIS	3.8
8	5	640	LEU	3.8
7	X	430	ARG	3.8
2	D	47	THR	3.8
4	B	24	GLN	3.8
5	Q	417	GLN	3.8
7	Y	643	ILE	3.8
7	Y	634	TRP	3.8
9	7	420	PRO	3.8
8	3	232	ARG	3.8
8	4	443	ASP	3.8
4	N	461	ARG	3.8
10	l	612	TYR	3.8
7	W	247	ILE	3.8
9	K	23	PRO	3.8
1	w	507	U	3.8
1	x	606	U	3.8
9	8	733	HIS	3.8
3	J	613	ILE	3.8
8	3	266	SER	3.8
9	K	168	LYS	3.8
2	D	63	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
6	1	475	VAL	3.7
10	1	661	LYS	3.7
8	4	408	GLU	3.7
3	J	684	GLY	3.7
3	A	19	CYS	3.7
6	1	451	ILE	3.7
5	R	622	GLU	3.7
6	1	448	GLU	3.7
8	3	209	LEU	3.7
2	S	255	VAL	3.7
10	L	57	PHE	3.7
8	G	11	LYS	3.7
8	G	60	VAL	3.7
9	K	131	ARG	3.7
3	J	612	HIS	3.7
1	w	549	U	3.7
2	S	271	LEU	3.7
10	L	31	LYS	3.7
10	9	261	LYS	3.7
5	R	673	MET	3.7
1	x	728	U	3.7
8	3	245	CYS	3.7
8	4	452	GLY	3.7
5	R	672	GLU	3.7
7	E	37	GLU	3.7
8	G	43	ASP	3.7
3	A	70	VAL	3.6
8	5	655	ASN	3.6
8	5	656	ASN	3.6
9	K	159	SER	3.6
2	U	653	GLY	3.6
3	I	469	LEU	3.6
5	Q	429	LEU	3.6
5	Q	510	LEU	3.6
10	L	39	CYS	3.6
8	3	220	LYS	3.6
7	E	24	TYR	3.6
9	8	708	ALA	3.6
5	P	303	GLY	3.6
10	0	426	SER	3.6
8	G	8	GLU	3.6
6	2	669	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
7	W	286	LEU	3.6
1	w	552	G	3.6
2	D	36	GLU	3.6
8	G	73	LEU	3.6
4	O	629	ILE	3.6
7	W	275	GLY	3.6
8	3	242	ILE	3.6
6	1	449	GLU	3.6
7	W	222	PHE	3.6
9	7	469	ARG	3.6
10	L	27	GLY	3.6
7	E	84	ILE	3.6
1	x	605	U	3.6
5	C	102	ARG	3.6
9	8	772	ARG	3.6
5	R	625	ASN	3.6
4	B	38	THR	3.6
7	W	244	GLU	3.6
4	B	41	LYS	3.6
8	4	453	GLN	3.6
10	L	47	GLN	3.6
3	J	644	ASP	3.5
4	N	425	VAL	3.5
8	G	61	VAL	3.5
2	S	247	THR	3.5
6	2	626	GLY	3.5
1	w	405	U	3.5
2	U	643	MET	3.5
7	X	461	ALA	3.5
6	F	47	THR	3.5
9	6	375	LEU	3.5
5	Q	509	VAL	3.5
10	0	421	ARG	3.5
4	N	438	THR	3.5
6	Z	241	ASN	3.5
8	3	256	ASN	3.5
8	4	456	ASN	3.5
5	Q	453	LEU	3.5
7	X	426	GLN	3.5
6	Z	209	PRO	3.5
8	4	407	PRO	3.5
3	I	413	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
4	O	633	ASP	3.5
5	Q	503	GLY	3.5
4	M	257	THR	3.5
7	E	22	PHE	3.5
2	S	250	TYR	3.5
5	P	295	TYR	3.5
2	U	654	ARG	3.5
5	P	259	PHE	3.5
6	F	56	SER	3.5
8	3	241	VAL	3.5
4	O	660	ILE	3.5
3	H	277	LEU	3.5
4	B	26	HIS	3.5
5	Q	432	LEU	3.5
5	R	701	LEU	3.5
8	3	231	LEU	3.5
5	R	703	GLY	3.5
10	L	7	ASP	3.5
9	K	150	GLU	3.5
4	O	611	SER	3.5
5	P	249	ASN	3.5
2	D	50	TYR	3.5
2	U	662	TYR	3.5
2	D	35	ALA	3.4
2	S	249	THR	3.4
4	B	57	THR	3.4
4	O	616	THR	3.4
10	L	56	ALA	3.4
10	9	228	ARG	3.4
3	I	408	MET	3.4
9	8	770	ASP	3.4
10	0	407	ASP	3.4
10	9	208	TYR	3.4
2	U	655	VAL	3.4
4	M	227	GLY	3.4
4	M	244	LYS	3.4
6	2	642	MET	3.4
7	X	477	ILE	3.4
6	Z	250	TYR	3.4
7	X	428	ARG	3.4
8	G	48	MET	3.4
2	D	14	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
10	9	244	GLU	3.4
6	F	68	ASN	3.4
7	Y	650	PHE	3.4
6	Z	257	GLY	3.4
10	l	609	CYS	3.4
9	6	340	SER	3.4
7	W	241	MET	3.4
2	D	15	GLY	3.4
4	O	640	LEU	3.4
9	8	737	SER	3.4
4	O	646	THR	3.4
7	W	285	THR	3.4
1	V	130	G	3.3
5	R	695	TYR	3.3
5	R	707	ILE	3.3
2	T	408	LYS	3.3
9	8	703	LYS	3.3
9	8	718	LYS	3.3
10	l	618	PRO	3.3
1	v	332	G	3.3
1	V	6	U	3.3
4	M	230	THR	3.3
5	R	618	LYS	3.3
9	8	754	GLU	3.3
7	E	46	CYS	3.3
2	T	456	ALA	3.3
9	K	180	ARG	3.3
9	6	363	HIS	3.3
2	T	450	TYR	3.3
8	3	273	LEU	3.3
9	8	726	TYR	3.3
7	E	63	GLU	3.3
1	w	533	G	3.3
5	R	624	PHE	3.3
8	3	261	VAL	3.3
10	9	223	THR	3.3
8	4	430	ILE	3.3
3	I	410	GLN	3.3
6	1	431	GLY	3.3
8	4	441	VAL	3.3
8	5	627	VAL	3.3
10	l	624	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
4	M	218	GLU	3.3
3	I	424	ARG	3.3
9	8	731	ARG	3.3
8	5	631	LEU	3.3
3	J	626	ILE	3.3
7	E	31	ILE	3.3
5	Q	495	TYR	3.3
2	D	45	ASN	3.2
3	J	619	CYS	3.2
10	9	215	HIS	3.2
6	F	49	GLU	3.2
9	8	681	GLU	3.2
10	9	227	GLY	3.2
4	N	424	GLN	3.2
9	8	744	ARG	3.2
7	W	231	ILE	3.2
9	7	556	ASP	3.2
2	D	24	THR	3.2
6	F	35	SER	3.2
7	E	55	ASN	3.2
4	M	224	GLN	3.2
9	K	104	THR	3.2
9	6	354	GLU	3.2
9	7	562	LYS	3.2
8	3	224	GLY	3.2
4	B	40	LEU	3.2
6	F	28	GLU	3.2
10	L	9	CYS	3.2
7	Y	665	HIS	3.2
4	O	659	SER	3.2
5	P	220	GLU	3.2
2	D	57	GLN	3.2
7	X	432	GLN	3.2
1	v	204	C	3.2
4	B	15	VAL	3.2
1	V	143	A	3.1
9	8	735	VAL	3.1
10	0	427	GLY	3.1
5	R	650	LYS	3.1
5	R	698	LYS	3.1
9	8	617	ASP	3.1
6	Z	259	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
9	7	422	LEU	3.1
1	x	759	C	3.1
5	C	42	VAL	3.1
8	3	258	GLY	3.1
2	D	11	HIS	3.1
9	6	315	THR	3.1
2	U	640	ASN	3.1
7	E	33	VAL	3.1
7	W	280	LYS	3.1
8	3	257	ILE	3.1
2	D	32	LEU	3.1
5	Q	416	LEU	3.1
8	5	618	SER	3.1
9	7	540	SER	3.1
8	3	255	ASN	3.1
4	B	47	LEU	3.1
6	Z	258	HIS	3.1
10	l	634	VAL	3.1
5	P	218	LYS	3.1
9	6	303	LYS	3.1
7	E	19	ASN	3.1
4	O	661	ARG	3.1
5	R	623	GLU	3.1
2	D	30	GLY	3.1
7	Y	668	THR	3.1
8	4	429	GLY	3.1
4	N	470	LEU	3.1
2	D	51	ARG	3.1
4	O	625	VAL	3.1
8	4	425	ARG	3.1
5	Q	496	ILE	3.1
8	G	28	GLN	3.0
8	5	629	GLY	3.0
10	0	457	PHE	3.0
9	8	742	LYS	3.0
10	9	224	HIS	3.0
4	B	54	GLN	3.0
6	1	433	LEU	3.0
5	Q	502	ARG	3.0
7	X	467	LYS	3.0
5	C	113	PRO	3.0
2	S	246	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
7	E	41	MET	3.0
1	V	35	A	3.0
4	M	239	HIS	3.0
3	J	668	GLY	3.0
2	D	12	GLU	3.0
7	W	240	ASN	3.0
4	O	609	LYS	3.0
7	E	34	TRP	3.0
9	6	356	ASP	3.0
9	7	504	THR	3.0
9	K	163	HIS	3.0
6	2	634	VAL	3.0
8	4	461	VAL	3.0
5	R	644	ILE	3.0
7	Y	647	ILE	3.0
2	D	13	ALA	3.0
8	5	644	GLU	3.0
8	5	674	GLU	3.0
9	K	152	GLU	3.0
4	N	417	ILE	2.9
7	E	64	ILE	2.9
6	1	414	LEU	2.9
8	3	210	LYS	2.9
4	N	432	VAL	2.9
5	R	652	LEU	2.9
7	W	249	GLY	2.9
9	K	121	ARG	2.9
3	A	39	ASN	2.9
1	x	726	A	2.9
4	N	459	SER	2.9
6	2	643	GLN	2.9
5	C	74	TRP	2.9
10	l	657	PHE	2.9
2	D	62	TYR	2.9
6	F	29	TYR	2.9
8	3	240	LEU	2.9
7	X	490	VAL	2.9
10	L	51	ASP	2.9
4	N	468	PHE	2.9
4	B	17	ILE	2.9
6	1	419	VAL	2.9
10	l	621	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
2	T	443	MET	2.9
3	J	645	CYS	2.9
5	C	30	SER	2.9
5	Q	497	SER	2.9
9	K	133	HIS	2.9
9	8	715	THR	2.9
10	L	30	HIS	2.9
5	P	310	LEU	2.9
4	B	29	ILE	2.8
4	B	32	VAL	2.8
5	C	31	VAL	2.8
5	C	44	ILE	2.8
9	6	215	PRO	2.8
9	7	526	TYR	2.8
2	U	616	HIS	2.8
9	K	117	SER	2.8
4	N	455	LEU	2.8
8	4	409	LEU	2.8
8	4	412	PHE	2.8
8	5	628	GLN	2.8
4	M	232	VAL	2.8
8	4	415	LYS	2.8
8	4	440	LEU	2.8
3	I	434	ASP	2.8
6	Z	249	GLU	2.8
9	8	755	ARG	2.8
6	F	66	CYS	2.8
7	X	440	ASN	2.8
2	U	661	VAL	2.8
6	2	621	VAL	2.8
3	A	38	MET	2.8
4	M	259	SER	2.8
3	I	432	ALA	2.8
2	S	229	ARG	2.8
10	9	222	LYS	2.8
10	L	8	TYR	2.8
9	7	415	PRO	2.8
3	H	219	CYS	2.8
3	H	274	GLY	2.8
3	I	468	GLY	2.8
6	1	428	GLU	2.8
6	2	614	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
8	5	630	ILE	2.7
2	U	615	GLY	2.7
9	8	664	GLU	2.7
3	A	14	ASP	2.7
9	8	614	ALA	2.7
2	U	657	GLN	2.7
9	8	724	GLU	2.7
6	F	27	MET	2.7
10	l	652	LYS	2.7
5	P	229	LEU	2.7
6	F	41	ASN	2.7
3	H	212	HIS	2.7
10	9	238	TYR	2.7
9	K	142	LYS	2.7
7	W	287	LEU	2.7
5	P	224	PHE	2.7
7	X	434	TRP	2.7
8	5	642	ILE	2.7
10	0	439	CYS	2.7
9	7	518	LYS	2.7
9	7	574	VAL	2.7
4	N	446	THR	2.7
1	x	730	G	2.7
8	G	9	LEU	2.7
4	M	268	PHE	2.7
10	9	256	ALA	2.7
9	K	151	TYR	2.7
5	P	257	LYS	2.7
8	G	31	LEU	2.7
10	9	253	THR	2.7
1	V	149	U	2.7
1	x	735	A	2.7
2	D	74	PRO	2.7
7	X	484	ILE	2.7
9	6	329	ILE	2.7
4	B	8	MET	2.7
9	8	716	GLU	2.7
8	4	442	ILE	2.6
9	K	132	ILE	2.6
10	L	28	ARG	2.6
8	4	417	LEU	2.6
6	Z	235	SER	2.6

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Mol	Chain	Res	Type	RSRZ
9	7	414	ALA	2.6
2	S	263	ILE	2.6
8	5	615	LYS	2.6
7	E	65	HIS	2.6
9	K	105	LEU	2.6
5	C	38	ASN	2.6
6	1	477	GLU	2.6
9	8	722	GLU	2.6
7	X	480	LYS	2.6
10	9	220	VAL	2.6
4	M	260	ILE	2.6
8	5	611	LYS	2.6
2	S	219	THR	2.6
2	S	228	TYR	2.6
4	M	240	LEU	2.6
7	X	433	VAL	2.6
5	P	230	SER	2.6
5	Q	499	MET	2.6
2	T	411	HIS	2.6
10	l	636	ASP	2.6
3	H	276	ASN	2.6
6	Z	274	GLY	2.6
9	7	486	LEU	2.6
10	L	14	THR	2.6
3	I	443	ASP	2.6
7	W	281	GLY	2.6
9	7	522	GLU	2.6
9	6	326	TYR	2.6
4	B	11	SER	2.6
6	1	417	LYS	2.6
7	W	260	ASP	2.6
2	S	234	GLU	2.6
3	A	13	ILE	2.6
5	C	41	GLN	2.6
5	C	53	LEU	2.6
2	T	435	ALA	2.6
10	L	53	THR	2.6
9	K	86	LEU	2.5
7	W	238	GLN	2.5
9	6	214	ALA	2.5
1	w	527	U	2.5
1	x	729	U	2.5

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Mol	Chain	Res	Type	RSRZ
2	U	650	TYR	2.5
9	7	514	THR	2.5
7	W	235	LEU	2.5
8	5	659	MET	2.5
10	L	45	GLN	2.5
1	x	731	U	2.5
4	O	641	LYS	2.5
1	x	752	G	2.5
2	D	46	ILE	2.5
10	0	449	LEU	2.5
1	v	337	U	2.5
9	K	70	LYS	2.5
7	X	487	LEU	2.5
4	O	643	VAL	2.5
9	6	307	VAL	2.5
6	2	627	MET	2.5
10	9	229	LYS	2.5
4	M	215	VAL	2.5
2	U	680	ALA	2.5
8	5	666	SER	2.5
7	Y	679	LEU	2.5
2	U	646	ILE	2.5
2	D	48	VAL	2.5
2	D	31	LYS	2.5
7	E	56	LEU	2.5
10	9	257	PHE	2.5
2	U	663	ILE	2.5
4	O	666	ARG	2.5
4	M	262	GLY	2.5
4	M	226	HIS	2.5
6	2	629	TYR	2.4
6	Z	215	THR	2.4
9	8	714	THR	2.4
9	6	269	ARG	2.4
10	0	420	VAL	2.4
3	J	646	ASP	2.4
8	G	16	LYS	2.4
10	L	29	LYS	2.4
2	U	673	LEU	2.4
10	l	608	TYR	2.4
5	C	40	THR	2.4
7	Y	633	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
9	8	668	GLU	2.4
9	6	338	LYS	2.4
3	J	667	LEU	2.4
9	6	365	ASP	2.4
9	6	312	TYR	2.4
4	M	228	THR	2.4
5	R	665	MET	2.4
6	2	607	PRO	2.4
6	2	648	GLU	2.4
9	K	157	MET	2.4
10	0	454	THR	2.4
3	A	79	SER	2.4
3	I	479	SER	2.4
6	2	668	ASN	2.4
5	P	228	PRO	2.4
10	9	243	GLU	2.4
10	1	619	SER	2.4
2	T	462	TYR	2.4
9	7	555	ARG	2.4
7	E	26	GLN	2.4
4	B	30	THR	2.4
9	7	524	GLU	2.4
7	W	234	TRP	2.4
8	3	213	MET	2.4
2	T	416	HIS	2.4
4	B	39	HIS	2.4
9	K	74	LYS	2.4
2	U	626	GLU	2.3
6	F	31	GLY	2.3
3	H	279	SER	2.3
9	K	110	VAL	2.3
7	X	442	ARG	2.3
10	9	240	LYS	2.3
8	G	40	LEU	2.3
2	S	220	CYS	2.3
4	B	60	ILE	2.3
4	M	269	ILE	2.3
4	O	624	GLN	2.3
6	1	441	ASN	2.3
5	C	66	VAL	2.3
6	1	411	LEU	2.3
8	5	609	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
4	M	231	GLY	2.3
7	Y	637	GLU	2.3
5	C	70	VAL	2.3
5	P	216	LEU	2.3
9	8	719	LEU	2.3
9	K	126	TYR	2.3
4	M	245	MET	2.3
2	D	17	ILE	2.3
3	H	270	VAL	2.3
3	H	272	LEU	2.3
5	P	215	GLU	2.3
10	0	408	TYR	2.3
3	A	84	GLY	2.3
8	5	619	LEU	2.3
9	K	158	HIS	2.3
3	H	218	ARG	2.3
6	1	443	GLN	2.3
4	M	229	ILE	2.2
4	N	460	ILE	2.2
4	O	603	LEU	2.2
6	2	611	LEU	2.2
5	C	72	GLU	2.2
4	B	58	LEU	2.2
4	M	219	LEU	2.2
2	T	413	ALA	2.2
3	J	666	VAL	2.2
5	R	631	VAL	2.2
10	0	434	VAL	2.2
6	F	48	GLU	2.2
7	X	437	GLU	2.2
8	G	15	LYS	2.2
9	K	138	LYS	2.2
3	I	465	ARG	2.2
4	N	457	THR	2.2
1	v	334	U	2.2
6	1	479	GLU	2.2
6	1	444	LEU	2.2
4	O	632	VAL	2.2
5	R	669	ASN	2.2
8	5	652	GLY	2.2
4	M	223	THR	2.2
10	L	25	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
8	G	12	PHE	2.2
9	K	149	ILE	2.2
9	8	675	ILE	2.2
8	4	416	LYS	2.2
7	X	463	GLU	2.2
8	3	214	ASP	2.2
2	T	455	VAL	2.2
5	Q	456	VAL	2.2
4	B	59	SER	2.2
10	0	440	LYS	2.2
6	F	65	ARG	2.2
6	1	418	PRO	2.2
10	0	456	ALA	2.2
9	K	140	SER	2.2
5	P	299	MET	2.2
1	x	749	U	2.1
9	K	103	LYS	2.1
9	7	505	LEU	2.1
9	6	284	THR	2.1
7	E	30	ARG	2.1
8	4	424	GLY	2.1
2	T	433	ILE	2.1
4	O	644	LYS	2.1
5	R	632	LEU	2.1
10	l	654	THR	2.1
9	8	740	SER	2.1
2	S	260	GLN	2.1
5	P	268	GLU	2.1
9	6	308	ALA	2.1
8	4	460	VAL	2.1
8	5	641	VAL	2.1
2	D	29	ARG	2.1
8	4	426	HIS	2.1
3	I	425	ILE	2.1
4	O	658	LEU	2.1
6	Z	237	ASP	2.1
3	A	82	VAL	2.1
8	5	620	LYS	2.1
2	T	463	ILE	2.1
7	Y	644	GLU	2.1
8	5	668	ILE	2.1
5	Q	442	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	V	150	U	2.1
6	2	646	ASN	2.1
7	Y	688	GLN	2.1
5	P	251	LYS	2.1
7	X	427	ASN	2.1
8	5	657	ILE	2.1
2	U	649	THR	2.1
3	H	230	THR	2.1
7	W	266	SER	2.1
4	M	243	VAL	2.1
8	3	248	MET	2.0
3	J	677	LEU	2.0
7	W	274	LEU	2.0
2	S	256	ALA	2.0
2	T	434	GLU	2.0
2	T	436	GLU	2.0
6	1	461	GLU	2.0
1	x	734	U	2.0
4	B	61	ARG	2.0
9	6	360	ALA	2.0
5	P	274	TRP	2.0
9	7	550	GLU	2.0
2	S	262	TYR	2.0
2	U	617	ILE	2.0
3	A	74	GLY	2.0
5	P	265	MET	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	ZN	9	278	1/1	0.24	0.55	231,231,231,231	0
11	ZN	0	478	1/1	0.29	0.42	231,231,231,231	0
11	ZN	1	678	1/1	0.33	0.84	231,231,231,231	0
11	ZN	L	78	1/1	0.43	1.69	231,231,231,231	0

6.5 Other polymers [i](#)

There are no such residues in this entry.