



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:45 PM UTC

PDB ID : 1FFK / pdb_00001ffk
Title : CRYSTAL STRUCTURE OF THE LARGE RIBOSOMAL SUBUNIT FROM HALOARCUA MARISMORTUI AT 2.4 ANGSTROM RESOLUTION
Authors : Ban, N.; Nissen, P.; Hansen, J.; Moore, P.B.; Steitz, T.A.
Deposited on : 2000-07-25
Resolution : 2.40 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

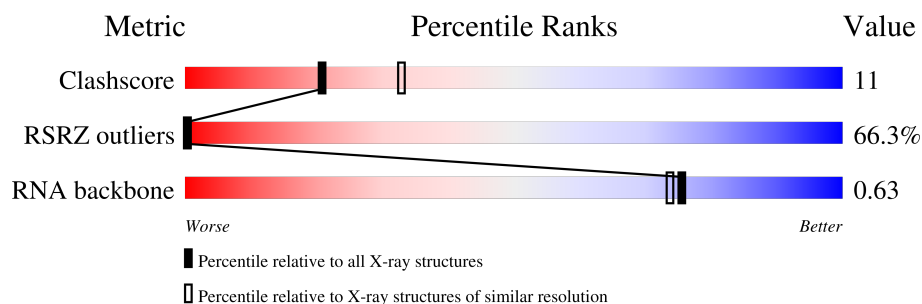
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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	0	2922	
2	9	122	
3	A	239	
4	B	337	
5	C	246	
6	D	176	
7	E	119	
8	F	157	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	G	145	98%
10	H	132	100%
11	I	194	100%
12	J	164	87%
13	K	186	100%
14	L	115	100%
15	M	148	96%
16	N	95	100%
17	O	154	97%
18	P	84	93%
19	Q	119	100%
20	R	66	80%
21	S	70	93%
22	T	154	100%
23	U	91	93%
24	V	143	99%
25	W	73	100%
26	X	56	100%
27	Y	49	63%
28	Z	92	100%
29	1	177	97%

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 64281 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 23S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2706	Total	C	N	O	P	0	0	0
			58012	25885	10685	18737	2705			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	conflict	GB 3377779

- Molecule 2 is a RNA chain called 5S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	A	237	Total	C	0	0	237
			237	237			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	B	337	Total	C	0	0	337
			337	337			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP P20279
B	311	PHE	-	insertion	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	C	246	Total C 246 246	0	0	246

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	conflict	UNP P12735

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	D	140	Total C 140 140	0	0	140

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	E	118	Total C 118 118	0	0	118

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	108	LEU	-	insertion	UNP P12743
E	109	GLU	-	insertion	UNP P12743
E	110	GLU	-	insertion	UNP P12743

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	F	157	Total C 157 157	0	0	157

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	G	142	Total C 142 142	0	0	142

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
10	H	132	Total	C	0	0	132
			132	132			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
11	I	194	Total	C	0	0	194
			194	194			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
12	J	143	Total	C	0	0	143
			143	143			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
13	K	186	Total	C	0	0	186
			186	186			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	186	LEU	-	insertion	UNP P14123

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
14	L	115	Total	C	0	0	115
			115	115			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
15	M	143	Total	C	0	0	143
			143	143			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	71	LYS	TYR	conflict	UNP P14119

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	N	95	Total C 95 95	0	0	95

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	O	150	Total C 150 150	0	0	150

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	P	78	Total C 78 78	0	0	78

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	Q	119	Total C 119 119	0	0	119

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L24E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	R	53	Total C 53 53	0	0	53

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	S	65	Total C 65 65	0	0	65

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	T	154	Total C 154 154	0	0	154

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L31E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	U	85	Total C 85 85	0	0	85

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	V	143	Total C 143 143	0	0	143

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	109	ASN	ALA	conflict	UNP P12736

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	W	73	Total C 73 73	0	0	73

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	X	56	Total C 56 56	0	0	56

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	Y	31	Total C 31 31	0	0	31

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	11	LYS	LEU	conflict	UNP P22452
Y	24	TYR	TRP	conflict	UNP P22452
Y	42	TRP	TYR	conflict	UNP P22452

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	Z	92	Total C 92 92	0	0	92

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	1	172	Total C 172 172	0	0	172

- Molecule 30 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	0	1	Total K 1 1	0	0

- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	0	2	Total Mg 2 2	0	0

- Molecule 32 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	R	1	Total Cd 1 1	0	0
32	W	1	Total Cd 1 1	0	0
32	X	1	Total Cd 1 1	0	0
32	Z	1	Total Cd 1 1	0	0

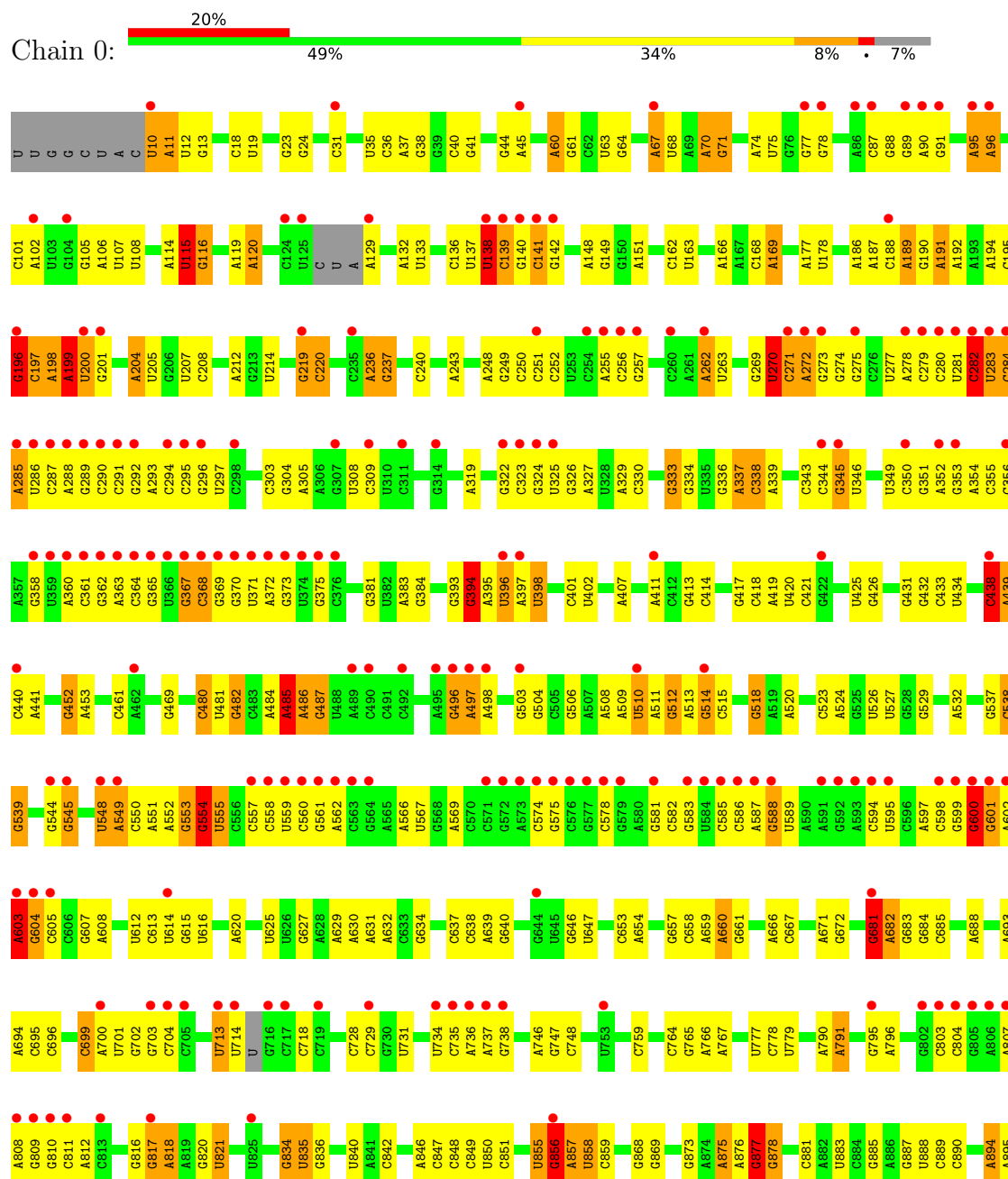
- Molecule 33 is water.

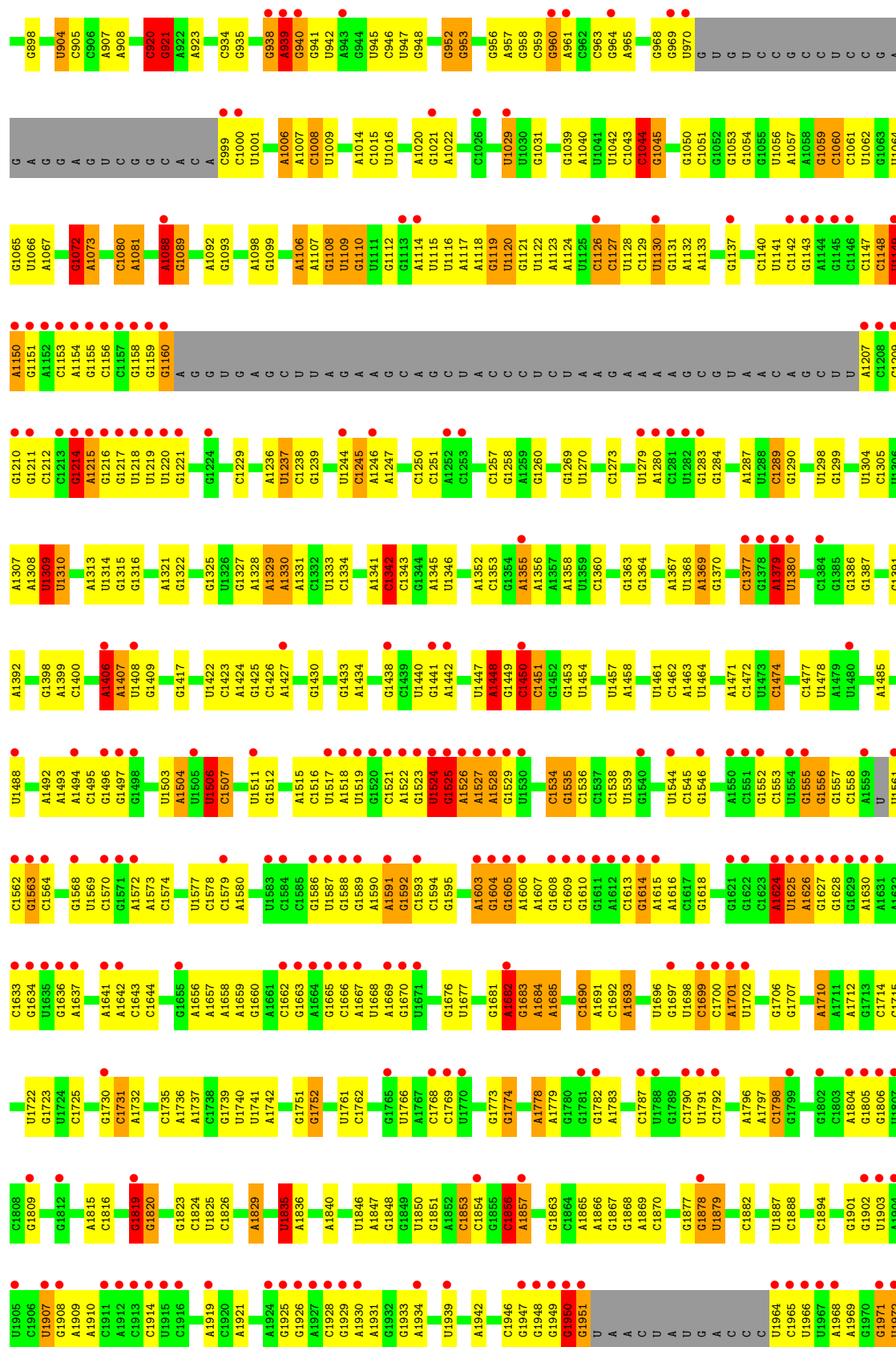
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	6	Total O 6 6	0	0

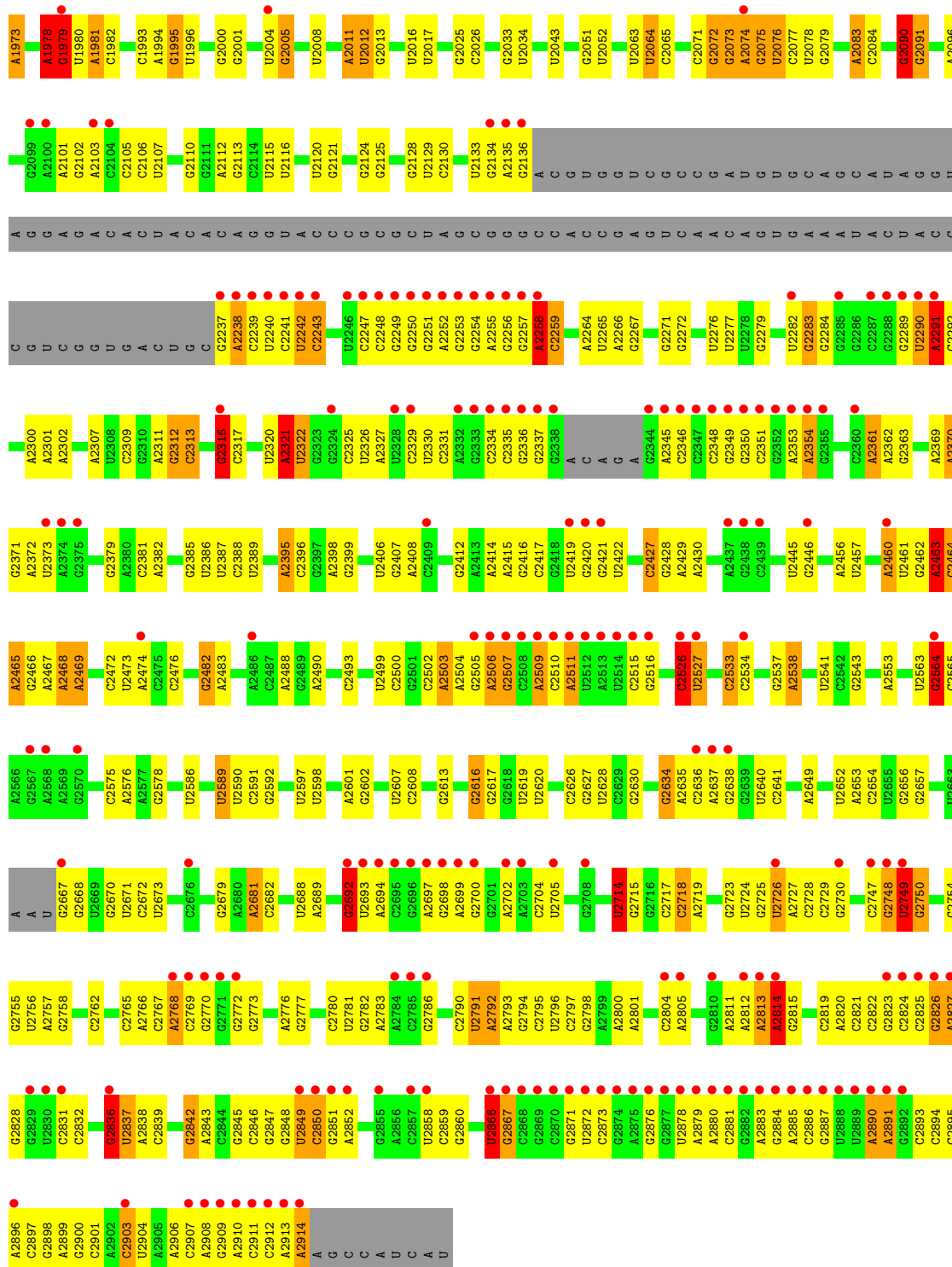
3 Residue-property plots

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: 23S rRNA



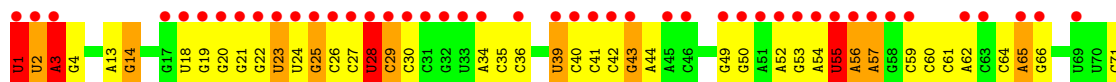


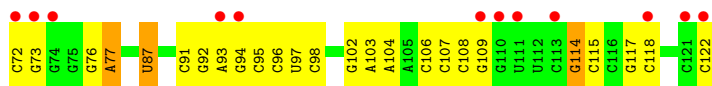


• Molecule 2: 5S rRNA

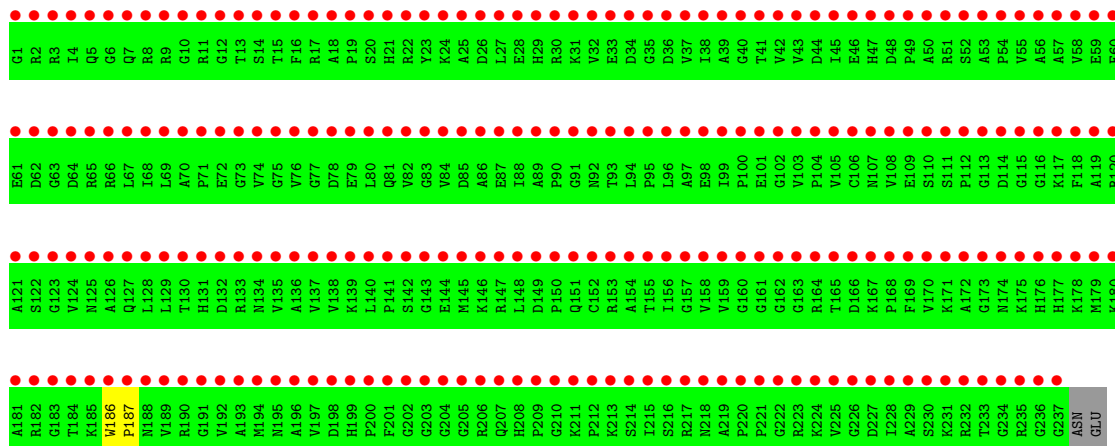


Chain 9:

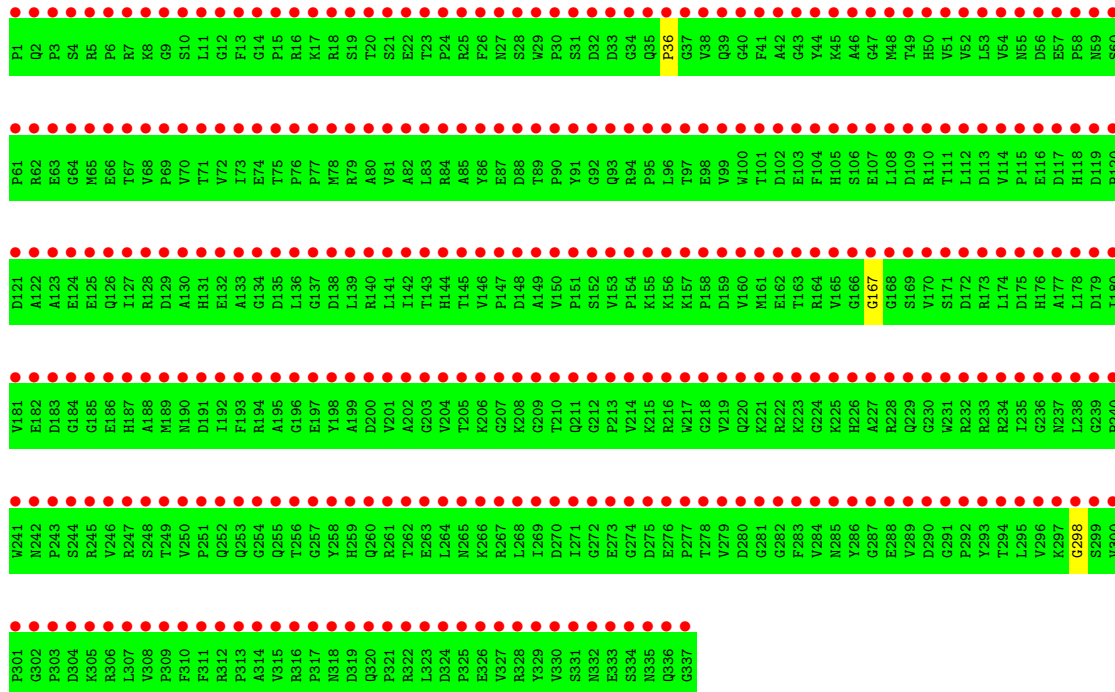




● Molecule 3: RIBOSOMAL PROTEIN L2

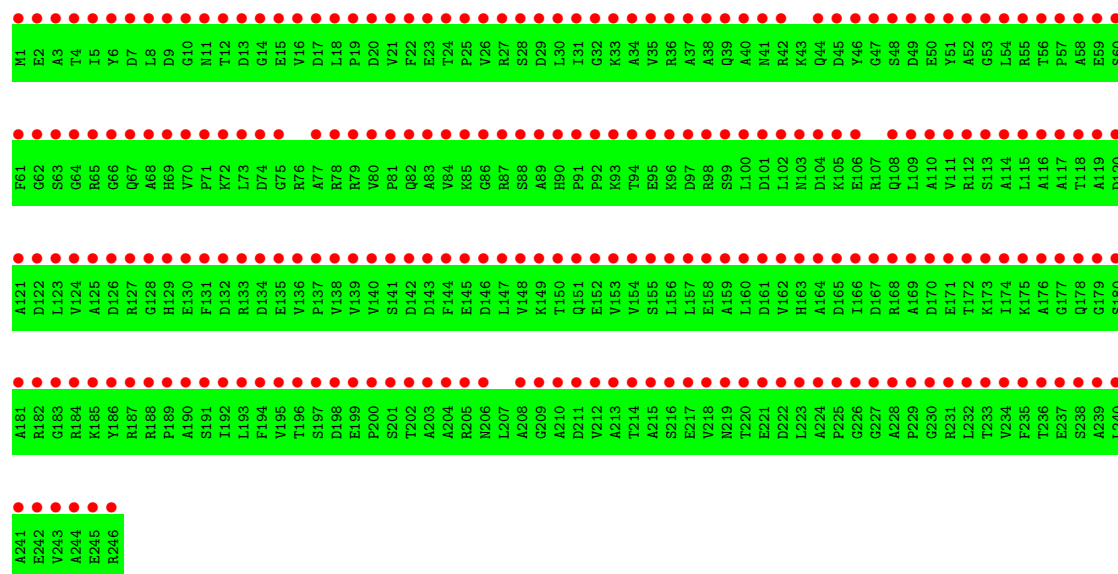


● Molecule 4: RIBOSOMAL PROTEIN L3

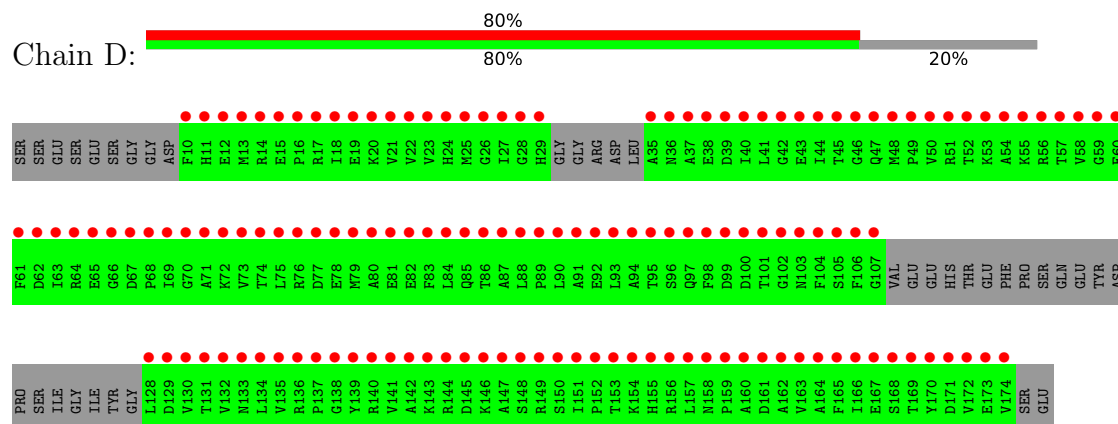


● Molecule 5: RIBOSOMAL PROTEIN L4

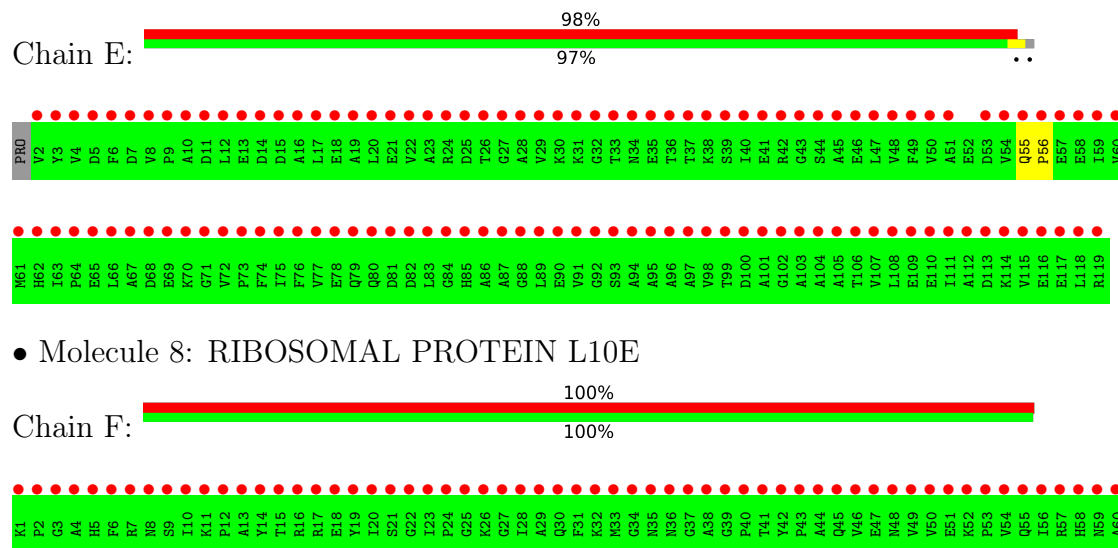




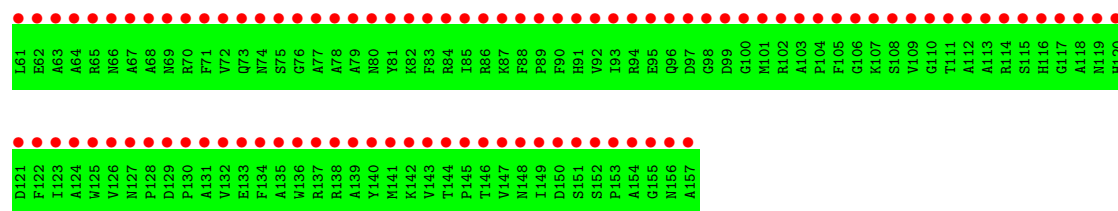
• Molecule 6: RIBOSOMAL PROTEIN L5



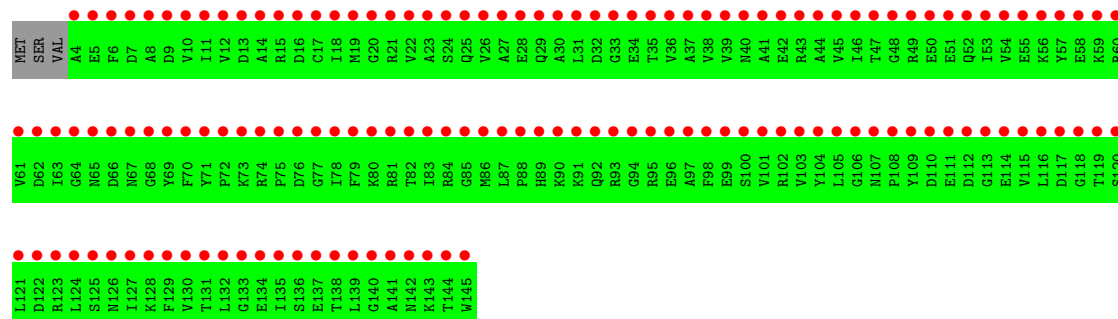
• Molecule 7: RIBOSOMAL PROTEIN L7AE



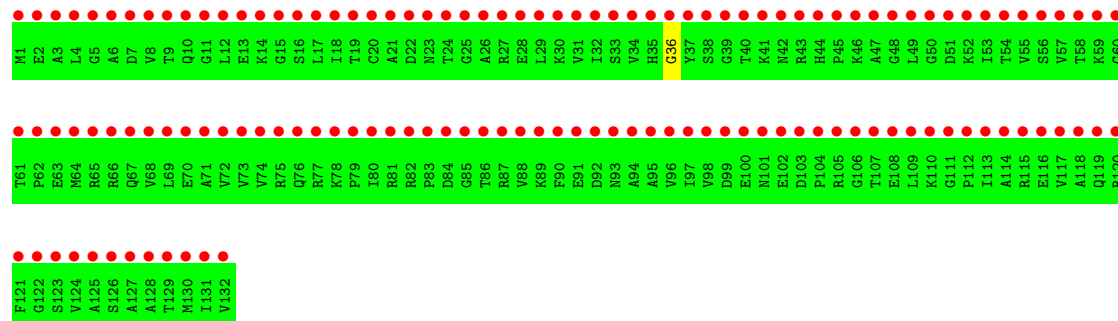
• Molecule 8: RIBOSOMAL PROTEIN L10E



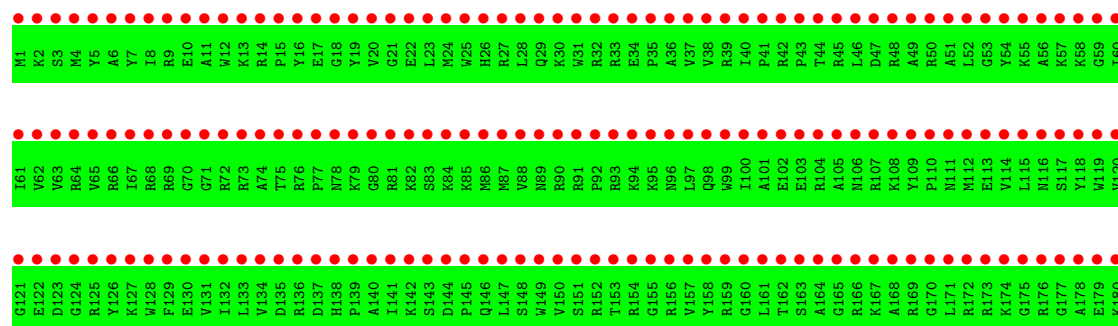
● Molecule 9: RIBOSOMAL PROTEIN L13



● Molecule 10: RIBOSOMAL PROTEIN L14



● Molecule 11: RIBOSOMAL PROTEIN L15E



V181
R182
P183
S184
L185
R186
A187
N188
F189
K190
K191
K192
R193
R194

• Molecule 12: RIBOSOMAL PROTEIN L15

Chain J:  87% 13%

T1 S2 K3 K4 I64 K5 R6 Q7 R8 G9 S10 D70 R11 R12 T12 H12 G14 G15 G16 G17 S17 H18 H19 N20 R21 R22 G23 G24 A24 G25 H26 R27 G28 G29 PHE R30 R31 G32 D32 A33 G34 R35 D36 K37 H38 E39 F40 H41 N42 N43 H44 E44 F45 Y105 V106 K107 K48 S49 G50 A111 F51 K52 R53 P54 Q55 H56 V57 Q58 T119 E59 E60

A61 A62 I64 I65 V66 R67 E68 I69 R130 D70 R131 N72 V73 V74 T74 G135 L76 A136 R137 A77 A78 D79 D80 E81 L82 E83 VAL G145 ASP GLY PHE Q150 ARG VAL D92 V93 R94 D95 V96 V97 E98 E99 A100 D101 A102 A103 D104 Y105 V106 K107 K109 G110 A111 G112 Q113 P114 Q115 H116 E117 L118 T119 E120

L121 A122 D123 D124 F125 S126 L127 G128 A129 R130 D131 K132 K133 E134 G135 A136 R137 G138 T138 S139 V140 E141 L142 T143 D144 L145 E147 E148 R149 Q150 A151 GLU ALA GLU GLU THR GLU ASP ALA ASP ASP GLU

• Molecule 13: RIBOSOMAL PROTEIN L18

Chain K:  100% 100%

A1 T2 G3 S4 R5 V6 K7 V8 P9 P10 R11 R12 R13 R14 E15 A16 R17 R18 T18 D19 V20 H21 Q22 R23 L24 R25 L26 L27 K28 S29 R30 G31 K31 P32 R33 L34 V35 A36 R37 R38 S39 K41 H42 V43 A44 A45 Q46 V48 V49 L50 G51 P52 N53 Q54 D55 T57 L58 A59 S60

A61 H62 S63 S64 D65 L66 A67 E68 Y69 G70 W71 E72 A73 P74 T75 G76 N77 N78 P79 S80 A81 Y82 L83 L84 T84 G85 L86 L87 A88 G89 L90 R91 A92 Q93 E94 A95 G96 V97 E98 E99 A100 V101 L102 D103 I104 G105 L106 N107 S108 P109 T110 P111 G112 S113 K114 Q115 F116 A117 T118 Q119 E120

G121 A122 I123 D124 A125 L126 L127 D128 I129 P130 H131 N132 D133 D134 V135 L136 A137 A138 V139 Q140 R141 T142 R143 A144 H146 I147 A148 E149 Y150 R151 E152 Q153 L154 E155 A156 P157 L158 Y159 S160 G161 D162 F163 D164 A165 A166 D167 L168 P169 E170 H171 F172 D173 E174 L175 E176 E177 T178 L179 L180

D181
G182
D183
I184
E185
L186

• Molecule 14: RIBOSOMAL PROTEIN L18E

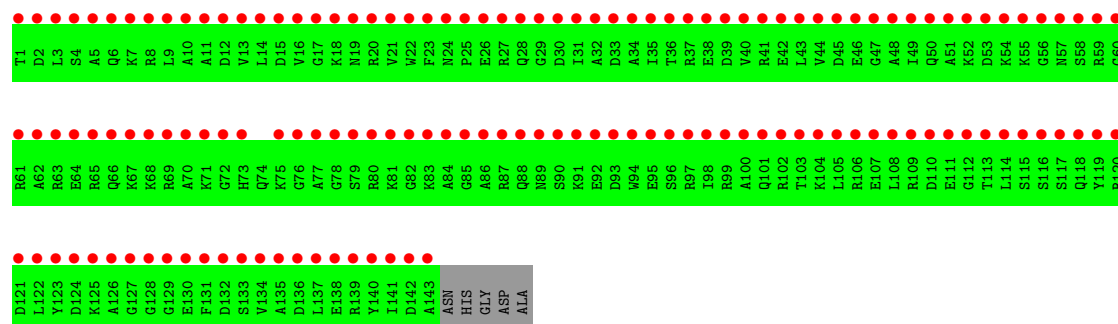
Chain L:  100% 100%

S1 K2 T3 N4 P5 R6 L7 S8 S9 L10 I11 A12 D13 L14 K15 S16 S17 A18 R19 R20 S21 G22 G23 A24 V25 W26 G27 D28 V29 R30 Q31 R32 L33 E34 K35 P36 R37 R38 T39 H40 A41 E42 V43 N44 L45 G46 E47 I48 S49 H50 Y51 A52 Q53 E54 I55 D56 T57 V58 V59 V60

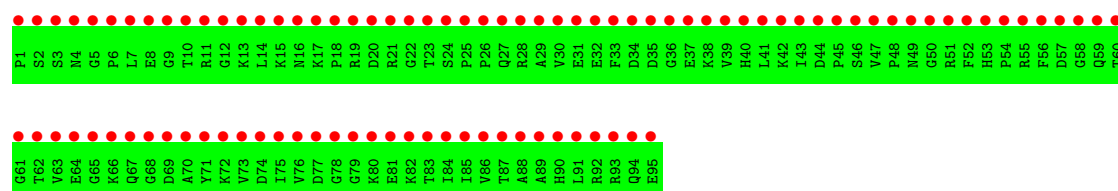
P61 G62 K63 V64 L65 G66 S67 G68 V69 L70 L71 L72 K73 D74 V75 V76 A77 A78 V79 D80 S81 S82 G83 G84 T84 A85 E86 T87 K88 I89 I90 D91 Q91 V92 G93 E94 A95 V96 S97 S98 L98 E99 Q100 A101 I102 E103 N104 N105 P106 E107 G108 S109 H110 V111 R112 Q113 I114 R115

• Molecule 15: RIBOSOMAL PROTEIN L19

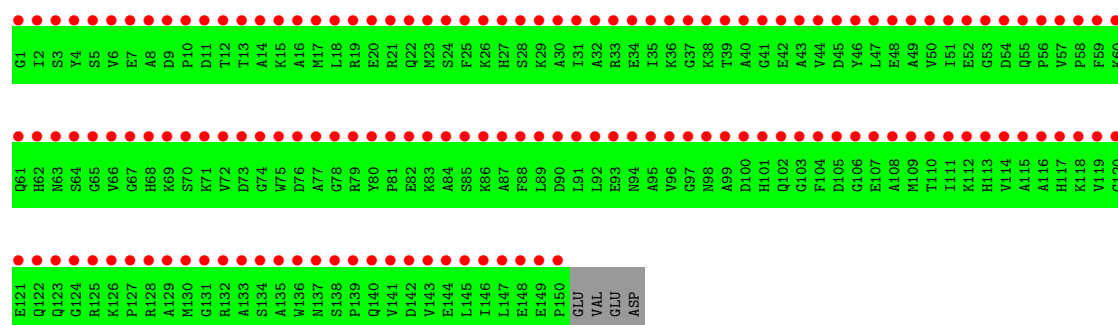
Chain M:  96% 97%



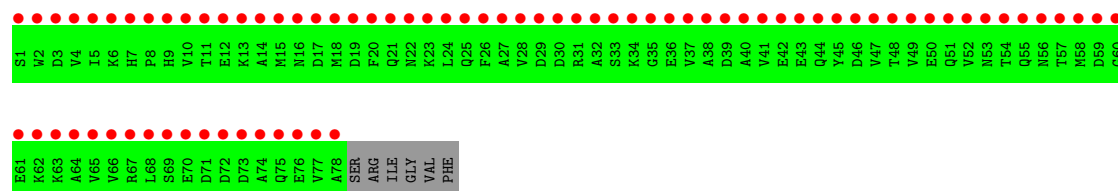
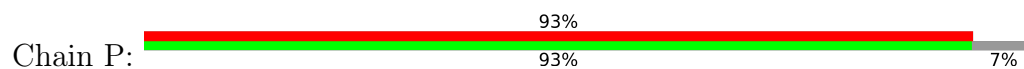
● Molecule 16: RIBOSOMAL PROTEIN L21E



● Molecule 17: RIBOSOMAL PROTEIN L22

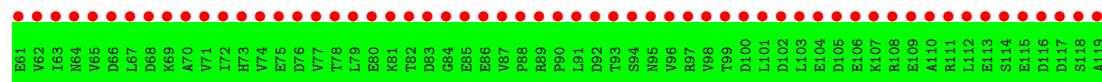
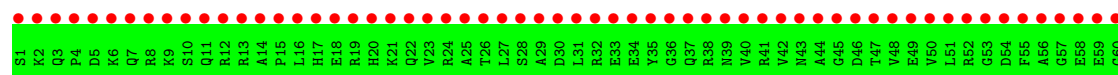


● Molecule 18: RIBOSOMAL PROTEIN L23

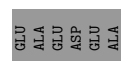
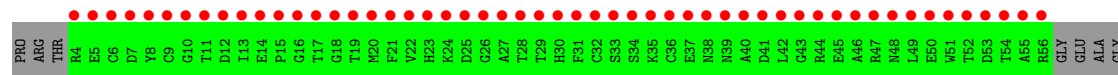
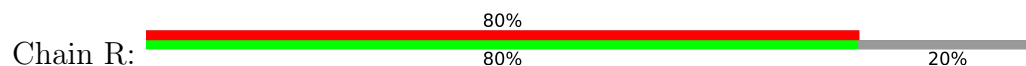


● Molecule 19: RIBOSOMAL PROTEIN L24

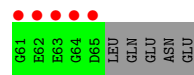
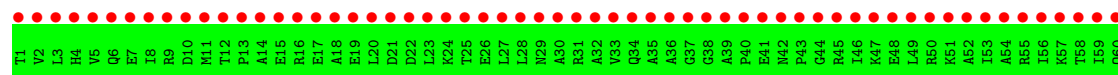




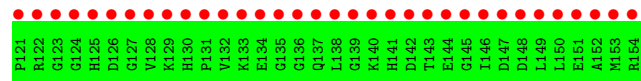
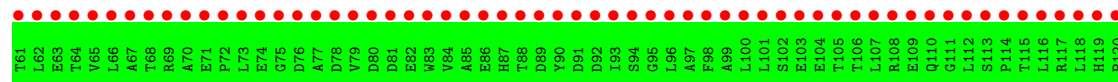
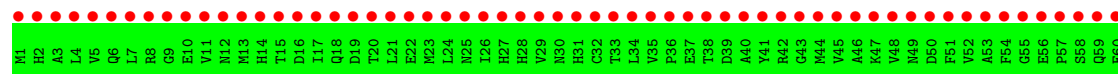
• Molecule 20: RIBOSOMAL PROTEIN L24E



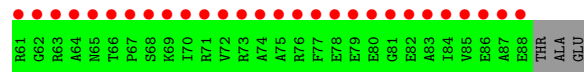
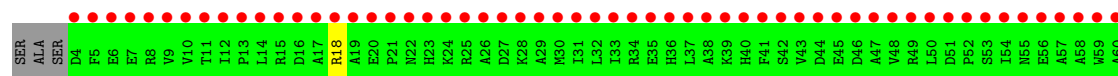
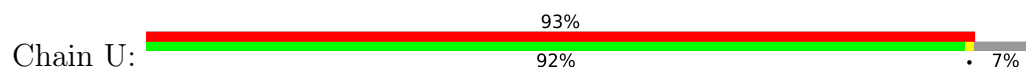
• Molecule 21: RIBOSOMAL PROTEIN L29



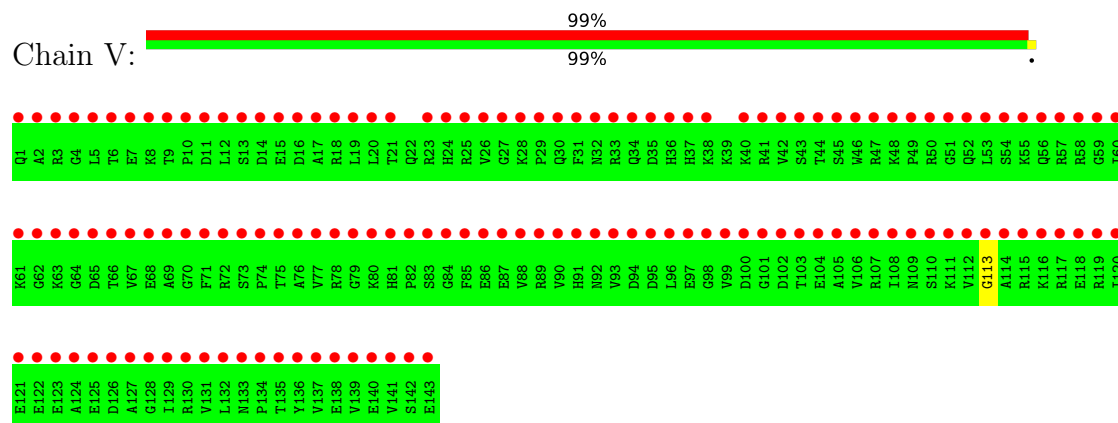
• Molecule 22: RIBOSOMAL PROTEIN L30



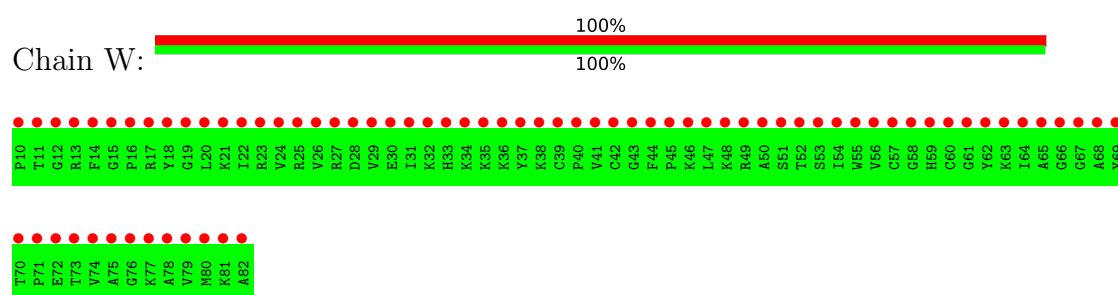
• Molecule 23: RIBOSOMAL PROTEIN L31E



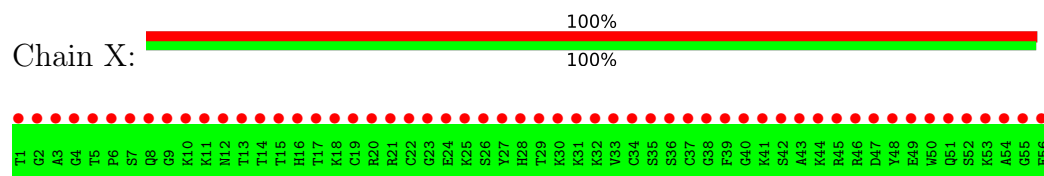
- Molecule 24: RIBOSOMAL PROTEIN L32E



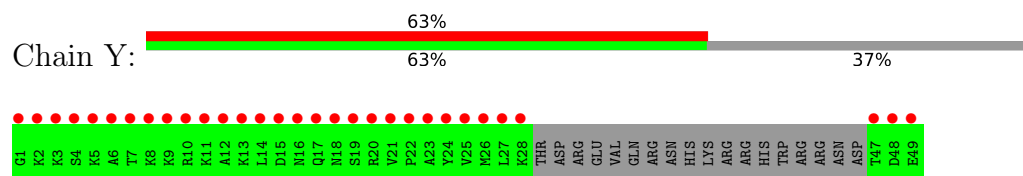
- Molecule 25: RIBOSOMAL PROTEIN L37AE



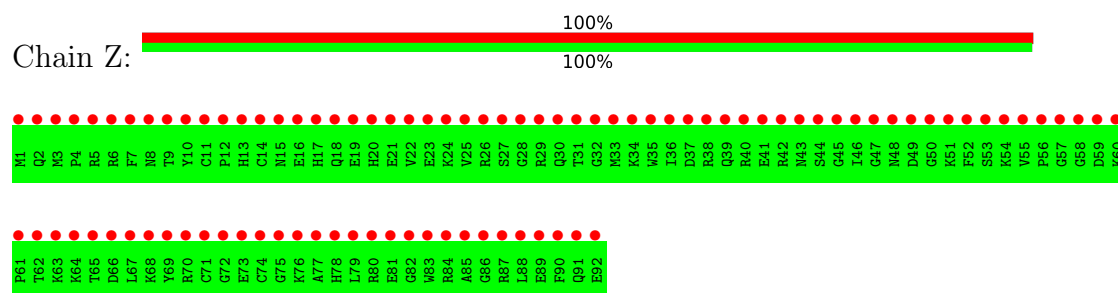
- Molecule 26: RIBOSOMAL PROTEIN L37E



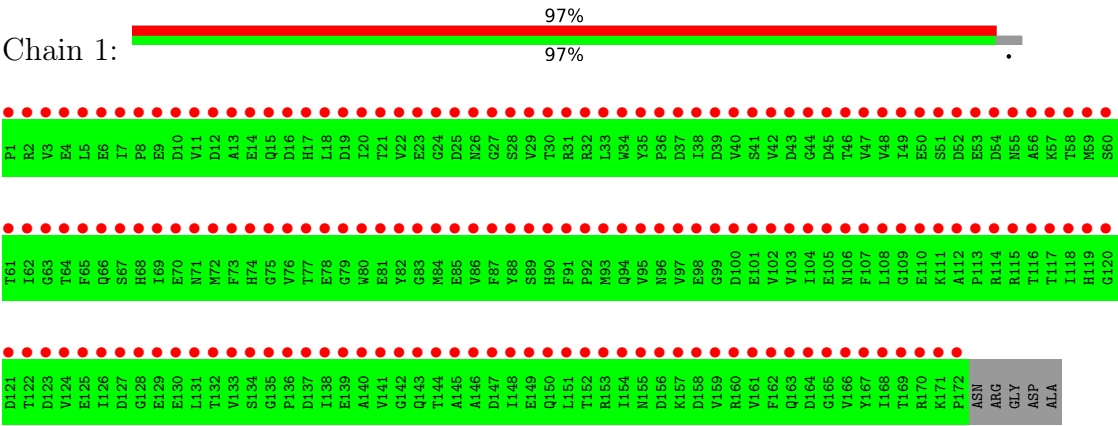
- Molecule 27: RIBOSOMAL PROTEIN L39E



- Molecule 28: RIBOSOMAL PROTEIN L44E



- Molecule 29: RIBOSOMAL PROTEIN L6



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.66Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.00 – 2.40 90.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	82.3 (90.00-2.40) 95.1 (90.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.40Å)	Xtriage
Refinement program	CNS, TNT & CNS	Depositor
R, R_{free}	0.252 , 0.261 0.346 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 276.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	64281	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, CD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.40	0/64945	0.66	119/101281 (0.1%)
2	9	0.36	0/2905	0.68	7/4528 (0.2%)
All	All	0.40	0/67850	0.66	126/105809 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	18	45
2	9	2	0
All	All	20	45

There are no bond length outliers.

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2749	U	C2'-C3'-O3'	16.23	133.85	109.50
1	0	904	U	C2'-C3'-O3'	15.24	132.35	109.50
1	0	1981	A	C2'-C3'-O3'	15.00	132.00	109.50
2	9	3	A	C2'-C3'-O3'	14.05	130.57	109.50
1	0	894	A	C2'-C3'-O3'	13.75	130.13	109.50
1	0	1059	G	C2'-C3'-O3'	12.98	128.97	109.50
1	0	713	U	C2'-C3'-O3'	12.77	128.66	109.50
1	0	191	A	C2'-C3'-O3'	12.67	128.51	109.50
1	0	2616	G	C2'-C3'-O3'	12.23	127.84	109.50
1	0	480	C	C2'-C3'-O3'	12.22	127.84	109.50
1	0	2482	G	C2'-C3'-O3'	12.10	127.66	109.50
1	0	1406	A	C2'-C3'-O3'	11.92	127.38	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2321	A	C2'-C3'-O3'	11.60	126.89	109.50
1	0	2370	A	C2'-C3'-O3'	11.15	126.22	109.50
1	0	1506	U	C2'-C3'-O3'	10.97	125.96	109.50
1	0	554	G	C2'-C3'-O3'	10.91	125.87	109.50
1	0	2813	A	C2'-C3'-O3'	10.62	125.43	109.50
1	0	1214	G	C4'-C3'-O3'	10.57	125.26	109.40
1	0	2283	G	C2'-C3'-O3'	10.51	125.26	109.50
1	0	191	A	C4'-C3'-O3'	10.33	124.89	109.40
1	0	1214	G	C2'-C3'-O3'	10.23	124.84	109.50
1	0	1379	A	C2'-C3'-O3'	10.16	124.74	109.50
1	0	1690	C	C2'-C3'-O3'	10.11	124.67	109.50
1	0	196	G	C2'-C3'-O3'	10.08	124.63	109.50
1	0	2692	G	N9-C1'-C2'	10.08	127.12	112.00
1	0	1979	G	C2'-C3'-O3'	10.01	124.51	109.50
1	0	1309	U	C2'-C3'-O3'	9.91	128.56	113.70
1	0	548	U	C2'-C3'-O3'	9.79	124.19	109.50
1	0	394	G	C2'-C3'-O3'	9.37	127.75	113.70
1	0	1126	C	C2'-C3'-O3'	9.33	123.50	109.50
1	0	2258	A	C2'-C3'-O3'	9.17	123.26	109.50
1	0	282	C	C2'-C3'-O3'	9.13	127.39	113.70
1	0	1835	U	C2'-C3'-O3'	9.09	127.34	113.70
1	0	894	A	C4'-C3'-O3'	9.08	123.01	109.40
1	0	2482	G	C4'-C3'-O3'	9.01	122.91	109.40
1	0	1907	U	C2'-C3'-O3'	9.00	127.20	113.70
1	0	600	G	C2'-C3'-O3'	8.92	127.08	113.70
1	0	1853	C	C2'-C3'-O3'	8.90	127.05	113.70
1	0	2714	U	C2'-C3'-O3'	8.89	127.04	113.70
1	0	1448	A	C2'-C3'-O3'	8.86	122.79	109.50
1	0	1108	G	C2'-C3'-O3'	8.65	122.48	109.50
1	0	1450	C	C2'-C3'-O3'	-8.64	100.75	113.70
1	0	2427	C	C2'-C3'-O3'	8.48	126.42	113.70
2	9	3	A	C4'-C3'-O3'	8.47	122.11	109.40
1	0	1699	C	C2'-C3'-O3'	8.46	126.39	113.70
1	0	452	G	C2'-C3'-O3'	8.45	122.18	109.50
1	0	1406	A	C4'-C3'-O3'	8.45	122.07	109.40
1	0	1683	G	C2'-C3'-O3'	8.42	122.13	109.50
1	0	2321	A	C4'-C3'-O3'	8.40	122.00	109.40
1	0	713	U	C4'-C3'-O3'	8.27	121.81	109.40
1	0	857	A	C2'-C3'-O3'	8.19	121.78	109.50
1	0	480	C	C4'-C3'-O3'	8.17	121.66	109.40
1	0	485	A	C2'-C3'-O3'	8.08	121.62	109.50
1	0	1981	A	C4'-C3'-O3'	8.06	121.49	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	28	U	C2'-C3'-O3'	7.92	125.58	113.70
1	0	2616	G	C4'-C3'-O3'	7.82	121.12	109.40
1	0	199	A	C2'-C3'-O3'	7.79	125.38	113.70
1	0	904	U	C4'-C3'-O3'	7.59	120.78	109.40
1	0	1059	G	C4'-C3'-O3'	7.33	120.40	109.40
1	0	438	C	C2'-C3'-O3'	7.18	120.28	109.50
1	0	856	G	N9-C1'-C2'	7.17	122.76	112.00
1	0	1072	G	C2'-C3'-O3'	7.08	120.12	109.50
1	0	600	G	C4'-C3'-O3'	7.07	123.60	113.00
1	0	681	G	C2'-C3'-O3'	6.98	119.97	109.50
1	0	1856	C	C2'-C3'-O3'	6.97	119.95	109.50
1	0	1907	U	C4'-C3'-O3'	6.94	123.41	113.00
1	0	1995	G	N9-C1'-C2'	6.91	122.37	112.00
1	0	2427	C	C4'-C3'-O3'	6.79	123.19	113.00
1	0	1835	U	C4'-C3'-O3'	6.76	123.13	113.00
1	0	2090	G	C2'-C3'-O3'	6.70	123.75	113.70
1	0	1682	A	N9-C1'-C2'	6.67	122.00	112.00
1	0	485	A	C4'-C3'-O3'	-6.58	99.53	109.40
1	0	603	A	C2'-C3'-O3'	6.58	119.37	109.50
1	0	2083	A	C2'-C3'-O3'	6.55	123.52	113.70
1	0	270	U	C2'-C3'-O3'	6.52	119.28	109.50
1	0	2395	A	C2'-C3'-O3'	6.52	123.48	113.70
1	0	1978	A	C2'-C3'-O3'	6.48	119.22	109.50
2	9	55	U	C2'-C3'-O3'	6.46	119.19	109.50
1	0	2749	U	C4'-C3'-O3'	6.42	119.03	109.40
1	0	834	G	C2'-C3'-O3'	-6.39	104.12	113.70
1	0	1504	A	C1'-C2'-O2'	-6.33	98.90	108.40
1	0	2814	A	C2'-C3'-O3'	6.32	118.98	109.50
2	9	39	U	N1-C1'-C2'	6.25	121.38	112.00
1	0	1120	U	C5'-C4'-C3'	-6.24	106.64	116.00
1	0	282	C	C4'-C3'-O3'	6.22	122.33	113.00
1	0	2463	A	C2'-C3'-O3'	6.04	118.57	109.50
1	0	452	G	N9-C1'-C2'	6.04	123.06	114.00
1	0	1699	C	C4'-C3'-O3'	6.01	122.02	113.00
1	0	877	G	C2'-C3'-O3'	-5.97	104.75	113.70
1	0	2866	U	C2'-C3'-O3'	5.96	118.44	109.50
1	0	1819	G	C5'-C4'-C3'	5.90	124.84	116.00
2	9	1	U	N1-C1'-C2'	5.89	120.84	112.00
1	0	1088	A	C4'-C3'-O3'	5.89	118.23	109.40
1	0	1995	G	C4'-C3'-O3'	-5.88	104.17	113.00
1	0	115	U	C2'-C3'-O3'	5.87	118.30	109.50
2	9	39	U	C4'-C3'-O3'	-5.84	104.24	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1379	A	C4'-C3'-O3'	5.83	118.15	109.40
1	0	2316	G	N9-C1'-C2'	5.82	120.73	112.00
1	0	1534	C	C2'-C3'-O3'	5.76	118.14	109.50
1	0	2465	A	C2'-C3'-O3'	5.72	118.08	109.50
1	0	2914	A	C2'-C3'-O3'	5.71	122.27	113.70
1	0	699	C	C2'-C3'-O3'	5.67	118.01	109.50
1	0	1072	G	N9-C1'-C2'	5.59	122.39	114.00
1	0	1524	U	N1-C1'-C2'	-5.54	105.69	114.00
1	0	2083	A	C4'-C3'-O3'	5.47	121.21	113.00
1	0	1615	A	C5'-C4'-C3'	5.46	124.18	116.00
1	0	2526	C	C2'-C3'-O3'	5.43	121.84	113.70
1	0	920	C	C2'-C3'-O3'	-5.42	105.57	113.70
1	0	938	G	N9-C1'-C2'	5.41	120.12	112.00
1	0	1214	G	C4'-C3'-C2'	5.30	107.90	102.60
1	0	1853	C	C4'-C3'-O3'	5.29	120.94	113.00
1	0	510	U	C4'-C3'-O3'	-5.25	105.13	113.00
1	0	718	C	C5'-C4'-C3'	-5.24	108.14	116.00
1	0	2836	G	C2'-C3'-O3'	5.23	117.34	109.50
1	0	939	A	C2'-C3'-O3'	5.22	117.33	109.50
1	0	938	G	C4'-C3'-O3'	-5.18	105.23	113.00
1	0	1149	U	C2'-C3'-O3'	5.18	117.26	109.50
1	0	921	G	N9-C1'-C2'	5.17	119.76	112.00
1	0	1504	A	C5'-C4'-C3'	5.16	123.74	116.00
1	0	1819	G	C2'-C3'-O3'	-5.15	105.97	113.70
1	0	1044	C	C2'-C3'-O3'	5.13	117.20	109.50
1	0	2316	G	C4'-C3'-O3'	-5.13	105.30	113.00
1	0	2460	A	N9-C1'-C2'	5.11	119.66	112.00
1	0	1624	A	N9-C1'-C2'	5.10	119.65	112.00
1	0	138	U	C2'-C3'-O3'	-5.10	106.06	113.70
1	0	2291	A	N9-C1'-C2'	5.09	119.64	112.00

All (20) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	191	A	C3'
1	0	282	C	C3'
1	0	600	G	C3'
1	0	894	A	C3'
1	0	904	U	C3'
1	0	1214	G	C3'
1	0	1309	U	C3'
1	0	1699	C	C3'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
1	0	1835	U	C3'
1	0	1853	C	C3'
1	0	1907	U	C3'
1	0	1981	A	C3'
1	0	2083	A	C3'
1	0	2427	C	C3'
1	0	2482	G	C3'
1	0	2692	G	C1'
1	0	2714	U	C3'
1	0	2749	U	C3'
2	9	1	U	C1'
2	9	3	A	C3'

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1122	U	Sidechain
1	0	1342	C	Sidechain
1	0	138	U	Sidechain
1	0	1417	G	Sidechain
1	0	1430	G	Sidechain
1	0	1524	U	Sidechain
1	0	1525	G	Sidechain
1	0	1555	G	Sidechain
1	0	1614	G	Sidechain
1	0	1682	A	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1848	G	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	189	A	Sidechain
1	0	1950	G	Sidechain
1	0	1972	U	Sidechain
1	0	1979	G	Sidechain
1	0	1995	G	Sidechain
1	0	2312	G	Sidechain
1	0	2313	C	Sidechain
1	0	2463	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2543	G	Sidechain
1	0	2564	G	Sidechain
1	0	2607	U	Sidechain
1	0	262	A	Sidechain
1	0	2630	G	Sidechain
1	0	270	U	Sidechain
1	0	2842	G	Sidechain
1	0	2866	U	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	469	G	Sidechain
1	0	482	G	Sidechain
1	0	485	A	Sidechain
1	0	518	G	Sidechain
1	0	529	G	Sidechain
1	0	791	A	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	58012	0	29282	980	0
2	9	2600	0	1326	62	0
3	A	237	0	0	1	0
4	B	337	0	0	2	0
5	C	246	0	0	0	0
6	D	140	0	0	0	0
7	E	118	0	0	1	0
8	F	157	0	0	0	0
9	G	142	0	0	0	0
10	H	132	0	0	1	0
11	I	194	0	0	0	0
12	J	143	0	0	0	0
13	K	186	0	0	0	0
14	L	115	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	M	143	0	0	0	0
16	N	95	0	0	0	0
17	O	150	0	0	0	0
18	P	78	0	0	0	0
19	Q	119	0	0	0	0
20	R	53	0	0	0	0
21	S	65	0	0	0	0
22	T	154	0	0	0	0
23	U	85	0	0	1	0
24	V	143	0	0	2	0
25	W	73	0	0	0	0
26	X	56	0	0	0	0
27	Y	31	0	0	0	0
28	Z	92	0	0	0	0
29	1	172	0	0	0	0
30	0	1	0	0	0	0
31	0	2	0	0	0	0
32	R	1	0	0	0	0
32	W	1	0	0	0	0
32	X	1	0	0	0	0
32	Z	1	0	0	0	0
33	0	6	0	0	0	0
All	All	64281	0	30608	1044	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1044) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:76:G:H3'	2:9:77:A:H5''	1.29	1.10
1:0:1682:A:H2	1:0:1696:U:H3	1.05	1.01
1:0:795:G:H2'	1:0:817:G:H22	1.25	1.00
1:0:326:G:H1	1:0:330:C:H5	1.03	1.00
1:0:1355:A:O2'	1:0:1356:A:H3'	1.60	1.00
2:9:56:A:H2'	2:9:57:A:H5''	1.44	0.99
1:0:337:A:H2	1:0:1314:U:HO2'	1.00	0.97
1:0:1147:C:H2'	1:0:1148:C:H5''	1.47	0.95
1:0:2768:A:H2'	1:0:2769:C:O4'	1.66	0.94
1:0:289:G:H22	1:0:363:A:H2	1.08	0.93
1:0:282:C:H1'	1:0:368:C:N4	1.82	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:C:C2'	1:0:2718:C:H5''	2.00	0.92
1:0:560:C:H42	1:0:597:A:H61	1.01	0.91
1:0:1751:G:H2'	1:0:1752:G:H5''	1.51	0.91
1:0:1116:U:HO2'	1:0:1118:A:H2	0.91	0.90
1:0:10:U:HO2'	1:0:11:A:H8	0.99	0.90
1:0:2890:A:H8	1:0:2890:A:H5''	1.37	0.90
1:0:1701:A:H4'	1:0:1702:U:H5''	1.54	0.90
1:0:1088:A:O2'	1:0:1089:G:H5''	1.71	0.90
1:0:45:A:H2	1:0:115:U:H3	0.94	0.89
1:0:199:A:O2'	1:0:200:U:H5''	1.72	0.88
1:0:2506:A:O2'	1:0:2507:G:H8	1.56	0.87
1:0:289:G:N2	1:0:363:A:H2	1.74	0.86
1:0:288:A:H61	1:0:364:C:H42	1.19	0.86
1:0:506:G:H22	1:0:509:A:H5'	1.43	0.84
1:0:2717:C:H2'	1:0:2718:C:H5''	1.57	0.84
1:0:1835:U:H5	1:0:1840:A:N7	1.77	0.82
1:0:283:U:H3'	1:0:284:C:C6	2.14	0.82
1:0:817:G:H4'	1:0:818:A:OP1	1.80	0.82
1:0:795:G:N2	1:0:817:G:H2'	1.94	0.81
1:0:795:G:H2'	1:0:817:G:N2	1.94	0.81
1:0:1147:C:C2'	1:0:1148:C:H5''	2.10	0.81
1:0:1106:A:H5'	1:0:1106:A:H8	1.46	0.81
1:0:371:U:H2'	1:0:372:A:C8	2.17	0.81
1:0:2812:A:H2	1:0:2814:A:H62	1.25	0.80
1:0:2090:G:H2'	1:0:2091:G:C8	2.17	0.79
1:0:2316:G:H4'	1:0:2316:G:OP1	1.81	0.79
2:9:29:C:H2'	2:9:30:C:H5'	1.65	0.79
2:9:56:A:C2'	2:9:57:A:H5''	2.13	0.78
1:0:2251:G:H2'	1:0:2252:A:C8	2.18	0.78
1:0:281:U:H2'	1:0:282:C:O4'	1.84	0.78
1:0:485:A:N3	1:0:487:G:H5''	1.98	0.78
1:0:1590:A:N6	1:0:1605:G:H1'	1.99	0.78
1:0:1148:C:H5'	1:0:1148:C:H6	1.49	0.77
1:0:2506:A:HO2'	1:0:2507:G:H8	0.79	0.77
1:0:45:A:H2	1:0:115:U:N3	1.77	0.77
1:0:506:G:H22	1:0:509:A:C5'	1.97	0.77
1:0:1088:A:H4'	1:0:1089:G:OP1	1.85	0.77
2:9:39:U:H1'	2:9:44:A:H61	1.50	0.76
1:0:1149:U:H5''	1:0:1151:G:O4'	1.84	0.76
1:0:2878:U:H2'	1:0:2879:A:O4'	1.86	0.76
1:0:796:A:N6	1:0:817:G:H1'	2.01	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:877:G:H5'	1:0:878:G:OP1	1.86	0.73
1:0:1438:G:N2	1:0:1685:A:H8	1.86	0.73
1:0:2103:A:H62	1:0:2538:A:H2	1.37	0.73
1:0:139:C:H4'	1:0:140:G:H5'	1.71	0.72
1:0:2866:U:H4'	1:0:2867:G:H5'	1.71	0.72
2:9:28:U:H2'	2:9:29:C:C6	2.24	0.72
1:0:1669:A:H2'	1:0:1670:G:C8	2.25	0.72
2:9:39:U:H1'	2:9:44:A:N6	2.05	0.72
1:0:2586:U:H3	1:0:2592:G:H22	1.37	0.71
1:0:2765:C:H4'	4:B:298:GLY:CA	2.20	0.71
1:0:544:G:H2'	1:0:545:G:H5''	1.72	0.71
2:9:76:G:C3'	2:9:77:A:H5''	2.16	0.71
1:0:1589:G:N2	1:0:1605:G:H2'	2.04	0.71
1:0:2851:G:O2'	1:0:2852:A:H5'	1.90	0.71
1:0:1972:U:H2'	1:0:1973:A:H5'	1.71	0.71
1:0:2903:C:H6	1:0:2903:C:H5'	1.54	0.71
1:0:2717:C:O2'	1:0:2718:C:H5''	1.89	0.71
1:0:2909:G:O2'	1:0:2910:A:H5'	1.91	0.71
1:0:138:U:H6	1:0:140:G:H1	1.39	0.71
1:0:371:U:H2'	1:0:372:A:H8	1.54	0.70
1:0:952:G:H4'	1:0:953:G:OP1	1.91	0.70
1:0:1441:G:O2'	1:0:1442:A:H5'	1.90	0.70
1:0:2866:U:H1'	1:0:2891:A:C4	2.25	0.70
1:0:67:A:OP2	1:0:108:U:H5'	1.91	0.70
1:0:2505:G:O2'	1:0:2506:A:H5'	1.91	0.70
1:0:1523:G:H2'	1:0:1524:U:C6	2.26	0.70
1:0:1119:G:N2	1:0:1246:A:C2	2.57	0.69
1:0:1751:G:C2'	1:0:1752:G:H5''	2.22	0.69
1:0:326:G:N1	1:0:330:C:H5	1.83	0.69
1:0:1681:G:H4'	1:0:1682:A:C8	2.27	0.69
1:0:2827:A:H2'	1:0:2828:G:O4'	1.92	0.69
1:0:362:G:H2'	1:0:363:A:H8	1.57	0.69
1:0:219:G:H3'	1:0:220:C:H5''	1.75	0.69
1:0:603:A:H4'	1:0:604:G:O5'	1.91	0.69
1:0:1209:C:H2'	1:0:1210:G:H8	1.57	0.69
1:0:1819:G:H2'	1:0:1820:G:H4'	1.74	0.69
1:0:2321:A:O2'	1:0:2322:U:H3'	1.93	0.69
1:0:1641:A:H2'	1:0:1642:A:H5'	1.75	0.69
1:0:2238:A:O2'	1:0:2239:C:H5'	1.93	0.68
1:0:1214:G:HO2'	1:0:1215:A:H8	1.39	0.68
2:9:14:G:H5'	2:9:14:G:H8	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:855:U:H4'	1:0:856:G:O5'	1.91	0.68
1:0:95:A:H5''	1:0:96:A:H3'	1.74	0.68
1:0:1380:U:H2'	1:0:1380:U:O2	1.92	0.68
1:0:2756:U:H3	1:0:2896:A:H2	1.41	0.68
1:0:12:U:H2'	1:0:13:G:H5'	1.75	0.68
1:0:1590:A:H61	1:0:1605:G:H1'	1.58	0.68
1:0:553:G:O2'	1:0:554:G:H5'	1.94	0.68
1:0:1666:C:H2'	1:0:1667:A:H8	1.59	0.68
1:0:2890:A:H5''	1:0:2890:A:C8	2.26	0.68
1:0:74:A:H2'	1:0:75:U:C6	2.28	0.68
1:0:1313:A:H5''	24:V:113:GLY:CA	2.23	0.67
1:0:1730:G:H5'	1:0:1731:C:C5	2.30	0.67
1:0:162:C:H2'	1:0:163:U:H5'	1.76	0.67
1:0:2250:G:H2'	1:0:2251:G:C8	2.29	0.67
1:0:284:C:H1'	1:0:285:A:OP2	1.94	0.67
1:0:1116:U:O2'	1:0:1118:A:H2	1.70	0.67
1:0:1561:U:H2'	1:0:1562:C:H6	1.60	0.67
2:9:49:G:O2'	2:9:50:G:H5'	1.95	0.67
1:0:545:G:H5'	1:0:545:G:H8	1.60	0.67
1:0:1118:A:H3'	1:0:1118:A:H8	1.60	0.67
1:0:1158:G:O2'	1:0:1159:G:H5'	1.95	0.67
1:0:2251:G:H2'	1:0:2252:A:H8	1.58	0.66
1:0:1684:A:O2'	1:0:1685:A:H5''	1.94	0.66
1:0:681:G:H4'	1:0:682:A:O5'	1.95	0.66
1:0:337:A:H2	1:0:1314:U:O2'	1.76	0.66
1:0:544:G:C2'	1:0:545:G:H5''	2.26	0.66
1:0:285:A:N6	1:0:367:G:H1'	2.11	0.66
1:0:1667:A:H2'	1:0:1668:U:C6	2.31	0.66
1:0:960:G:N3	1:0:960:G:H2'	2.11	0.66
1:0:1701:A:H5''	1:0:1702:U:H3'	1.77	0.66
1:0:1130:U:H2'	1:0:1131:G:O4'	1.96	0.65
1:0:1106:A:H5'	1:0:1106:A:C8	2.29	0.65
1:0:1448:A:H5'	1:0:1507:C:OP1	1.96	0.65
1:0:289:G:O2'	1:0:290:C:H5'	1.96	0.65
1:0:2894:C:O2'	1:0:2895:C:H5'	1.97	0.65
1:0:95:A:C5'	1:0:96:A:H3'	2.27	0.65
1:0:1613:C:H2'	1:0:1614:G:O4'	1.96	0.65
1:0:285:A:H62	1:0:367:G:H1'	1.61	0.64
1:0:601:G:O2'	1:0:602:A:H5'	1.96	0.64
2:9:29:C:C2'	2:9:30:C:H5'	2.26	0.64
1:0:2670:G:O2'	1:0:2671:U:H5'	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:10:U:H1'	1:0:532:A:H62	1.63	0.64
1:0:1579:C:H2'	1:0:1580:A:C8	2.33	0.64
1:0:2598:U:H5''	10:H:36:GLY:CA	2.28	0.64
1:0:1217:G:H2'	1:0:1218:U:C6	2.33	0.64
1:0:1355:A:H4'	1:0:1355:A:OP1	1.98	0.64
1:0:1438:G:N2	1:0:1684:A:HO2'	1.95	0.64
1:0:2253:G:H2'	1:0:2254:G:H8	1.63	0.64
1:0:420:U:H2'	1:0:421:C:C6	2.33	0.64
1:0:1766:U:O2	1:0:1778:A:H5'	1.98	0.64
1:0:1947:G:H2'	1:0:1948:G:H8	1.62	0.64
1:0:1778:A:H2'	1:0:1779:A:H5'	1.79	0.64
2:9:13:A:O2'	2:9:14:G:H5''	1.98	0.63
1:0:1149:U:O2'	1:0:1150:A:OP2	2.15	0.63
2:9:25:G:O2'	2:9:26:C:H5'	1.98	0.63
1:0:350:C:O2'	1:0:351:G:H5'	1.99	0.63
1:0:1118:A:H3'	1:0:1118:A:C8	2.32	0.63
1:0:349:U:O2'	1:0:350:C:H5'	1.98	0.63
1:0:362:G:H2'	1:0:363:A:C8	2.33	0.63
1:0:372:A:H2'	1:0:373:G:H8	1.64	0.63
1:0:582:C:H2'	1:0:583:G:H8	1.64	0.63
1:0:1947:G:H2'	1:0:1948:G:C8	2.34	0.63
1:0:2908:A:H2'	1:0:2909:G:O4'	1.98	0.63
1:0:795:G:H1'	1:0:818:A:N6	2.14	0.63
2:9:107:C:H2'	2:9:108:C:C6	2.34	0.63
1:0:646:G:H2'	1:0:647:U:C6	2.34	0.62
1:0:432:G:O2'	1:0:433:C:H5'	1.99	0.62
1:0:538:C:H5''	1:0:539:G:C8	2.34	0.62
1:0:1438:G:N2	1:0:1684:A:O2'	2.31	0.62
1:0:1525:G:H5'	1:0:1526:A:OP2	1.99	0.62
2:9:92:G:H2'	2:9:93:A:C8	2.33	0.62
1:0:2849:U:O2'	1:0:2850:C:OP2	2.17	0.62
2:9:55:U:H4'	2:9:56:A:O5'	1.99	0.62
1:0:613:C:H2'	1:0:614:U:H6	1.64	0.62
1:0:1211:G:O2'	1:0:1212:C:H5'	1.98	0.62
1:0:1450:C:O2'	1:0:1493:A:H2'	1.99	0.62
1:0:2266:A:H2'	1:0:2267:G:C8	2.35	0.62
1:0:2289:G:H21	1:0:2291:A:H2	1.47	0.62
1:0:2387:U:H2'	1:0:2388:C:C6	2.35	0.62
1:0:1474:C:H5'	1:0:1474:C:H6	1.65	0.62
1:0:702:G:O2'	1:0:703:G:H5'	2.00	0.62
1:0:2591:C:H2'	1:0:2592:G:O4'	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:20:G:O2'	2:9:21:G:H5'	1.99	0.62
1:0:999:C:H2'	1:0:1000:C:C6	2.35	0.61
1:0:2316:G:OP1	1:0:2316:G:C4'	2.47	0.61
1:0:671:A:O2'	1:0:672:G:H2'	2.00	0.61
1:0:625:U:H5''	1:0:1044:C:N4	2.15	0.61
1:0:2502:C:C2'	1:0:2503:A:H5'	2.30	0.61
1:0:1741:U:H5'	1:0:1742:A:OP1	2.01	0.61
2:9:22:G:O3'	2:9:23:U:H4'	2.01	0.61
1:0:968:G:O2'	1:0:969:G:H5'	2.00	0.61
1:0:2504:A:H2'	1:0:2505:G:O4'	2.01	0.61
1:0:283:U:C5	1:0:284:C:N4	2.68	0.61
1:0:2533:C:H6	1:0:2533:C:H5'	1.66	0.61
1:0:1120:U:H5'	1:0:1121:G:OP2	2.00	0.61
1:0:283:U:H3'	1:0:284:C:C5	2.35	0.60
1:0:1477:C:H5'	1:0:1868:G:C5'	2.31	0.60
1:0:1714:C:O2'	1:0:1715:C:H5'	2.00	0.60
1:0:255:A:H2'	1:0:256:C:C6	2.36	0.60
1:0:796:A:H62	1:0:817:G:H1'	1.64	0.60
1:0:2506:A:O2'	1:0:2507:G:C8	2.40	0.60
1:0:1528:A:H2'	1:0:1529:G:O4'	2.01	0.60
1:0:1377:C:H6	1:0:1377:C:H5'	1.66	0.60
1:0:1856:C:O2'	1:0:1857:A:OP2	2.19	0.60
1:0:2112:A:H2'	1:0:2113:G:C8	2.37	0.59
1:0:256:C:H2'	1:0:257:G:O4'	2.03	0.59
1:0:2240:U:O2'	1:0:2241:C:H5'	2.02	0.59
1:0:283:U:H5''	1:0:284:C:OP2	2.02	0.59
1:0:1557:G:O2'	1:0:1558:C:H5'	2.02	0.59
1:0:1636:G:O2'	1:0:1637:A:H5'	2.02	0.59
2:9:91:C:H2'	2:9:92:G:O4'	2.03	0.59
1:0:367:G:O2'	1:0:368:C:O5'	2.16	0.59
1:0:2488:A:H61	1:0:2534:C:H42	1.50	0.59
1:0:372:A:H2'	1:0:373:G:C8	2.38	0.59
1:0:599:G:O2'	1:0:600:G:H5'	2.03	0.59
1:0:795:G:C2'	1:0:817:G:N2	2.64	0.59
1:0:1506:U:H6	1:0:1506:U:H5'	1.67	0.59
1:0:2900:G:H2'	1:0:2901:C:O4'	2.02	0.59
1:0:1342:C:O2'	1:0:1343:C:H5'	2.03	0.59
1:0:1964:U:H2'	1:0:1965:C:C6	2.38	0.59
1:0:2507:G:H2'	1:0:2510:C:H42	1.67	0.59
1:0:1515:A:H2'	1:0:1516:C:C6	2.38	0.59
1:0:74:A:H2'	1:0:75:U:H6	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:290:C:O2'	1:0:291:C:H5'	2.03	0.59
1:0:820:G:H4'	1:0:856:G:H5'	1.84	0.59
1:0:2361:A:H2'	1:0:2362:A:C8	2.37	0.59
1:0:63:U:O2'	1:0:64:G:H5'	2.02	0.58
1:0:219:G:OP2	1:0:220:C:H5''	2.03	0.58
1:0:1280:A:H3'	1:0:1280:A:OP1	2.03	0.58
1:0:279:C:O2'	1:0:280:C:H5'	2.03	0.58
1:0:514:G:H3'	1:0:514:G:OP1	2.02	0.58
1:0:945:U:H2'	1:0:946:C:H6	1.69	0.58
1:0:2697:A:H2'	1:0:2698:G:O4'	2.03	0.58
1:0:1730:G:H5'	1:0:1731:C:C6	2.38	0.58
1:0:2635:A:O2'	1:0:2636:C:H5'	2.03	0.58
2:9:28:U:H5''	2:9:28:U:H6	1.68	0.58
1:0:1579:C:H2'	1:0:1580:A:H8	1.68	0.58
1:0:1701:A:H4'	1:0:1702:U:C5'	2.30	0.58
1:0:1804:A:H2'	1:0:1805:G:C8	2.39	0.58
1:0:1064:U:H2'	1:0:1065:G:C8	2.39	0.58
1:0:2907:C:H2'	1:0:2908:A:O4'	2.04	0.58
1:0:1497:G:H4'	1:0:1627:G:O2'	2.03	0.58
1:0:2866:U:H4'	1:0:2867:G:C5'	2.32	0.58
1:0:282:C:O2'	1:0:283:U:H4'	2.03	0.58
1:0:574:C:O2'	1:0:575:G:H5'	2.03	0.58
1:0:803:C:O2'	1:0:804:C:H5'	2.03	0.58
1:0:2679:G:H2'	1:0:2681:A:OP2	2.03	0.58
1:0:2819:C:H2'	1:0:2820:A:C8	2.38	0.58
1:0:945:U:H2'	1:0:946:C:C6	2.38	0.58
1:0:2780:C:H2'	1:0:2781:U:C6	2.38	0.58
2:9:22:G:O3'	2:9:23:U:C4'	2.52	0.58
1:0:795:G:C2'	1:0:817:G:H22	2.08	0.57
4:B:36:PRO:CA	4:B:167:GLY:CA	2.82	0.57
1:0:1477:C:O2'	1:0:1478:U:H5'	2.03	0.57
1:0:1522:A:O2'	1:0:1523:G:H5'	2.05	0.57
1:0:1805:G:H2'	1:0:1806:G:H8	1.68	0.57
1:0:195:C:H2'	1:0:196:G:H5'	1.84	0.57
1:0:703:G:O2'	1:0:704:C:H5'	2.04	0.57
1:0:2699:A:H2'	1:0:2700:G:O4'	2.05	0.57
1:0:1667:A:H2'	1:0:1668:U:H6	1.68	0.57
1:0:561:G:H2'	1:0:562:A:H8	1.67	0.57
1:0:807:A:H2'	1:0:808:A:O4'	2.03	0.57
1:0:1313:A:OP1	24:V:113:GLY:CA	2.53	0.57
1:0:2526:C:O2'	1:0:2527:U:H5'	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2748:G:O2'	1:0:2749:U:OP2	2.20	0.57
2:9:14:G:H5'	2:9:14:G:C8	2.39	0.57
1:0:1147:C:H2'	1:0:1148:C:C5'	2.26	0.57
1:0:1562:C:H3'	1:0:1563:G:C8	2.40	0.57
2:9:26:C:O2'	2:9:27:C:H5'	2.05	0.57
1:0:1304:U:H2'	1:0:1305:C:C6	2.40	0.57
2:9:29:C:H2'	2:9:30:C:C5'	2.34	0.57
1:0:396:U:O2'	1:0:418:C:H4'	2.05	0.56
1:0:660:A:H4'	1:0:661:G:O5'	2.04	0.56
1:0:1333:U:H2'	1:0:1334:C:C6	2.40	0.56
1:0:1950:G:O2'	1:0:1951:G:O5'	2.23	0.56
1:0:598:C:H2'	1:0:599:G:H8	1.70	0.56
1:0:2812:A:C2	1:0:2814:A:N6	2.69	0.56
1:0:566:A:H2'	1:0:567:U:O4'	2.06	0.56
1:0:1438:G:H21	1:0:1685:A:H8	1.52	0.56
1:0:1556:G:O2'	1:0:1557:G:H5'	2.05	0.56
1:0:1577:U:O2'	1:0:1578:C:H5'	2.05	0.56
1:0:2414:A:H2'	1:0:2415:A:C8	2.40	0.56
1:0:2825:C:H4'	1:0:2826:G:O5'	2.05	0.56
1:0:1056:U:H2'	1:0:1057:A:O4'	2.05	0.56
1:0:1682:A:H2	1:0:1696:U:N3	1.89	0.56
1:0:281:U:O2'	1:0:282:C:H5'	2.05	0.56
1:0:326:G:O2'	1:0:327:A:H5'	2.05	0.56
1:0:1586:G:O2'	1:0:1587:U:H5'	2.06	0.56
1:0:1641:A:C2'	1:0:1642:A:H5'	2.35	0.56
1:0:1666:C:H2'	1:0:1667:A:C8	2.41	0.56
1:0:2814:A:OP2	1:0:2814:A:H3'	2.05	0.56
1:0:1214:G:H4'	1:0:1215:A:OP1	2.06	0.56
1:0:1555:G:O2'	1:0:1556:G:P	2.64	0.56
1:0:1735:C:O2'	1:0:1736:A:H5'	2.06	0.56
1:0:560:C:O2'	1:0:561:G:H5'	2.06	0.55
1:0:1250:C:O2'	1:0:1251:C:H5'	2.05	0.55
1:0:2468:A:H4'	1:0:2469:A:OP1	2.06	0.55
1:0:1072:G:O2'	1:0:1073:A:H8	1.89	0.55
1:0:37:A:H2'	1:0:38:G:H8	1.70	0.55
1:0:1210:G:O2'	1:0:1211:G:H5'	2.06	0.55
1:0:1523:G:C6	1:0:1524:U:O4	2.60	0.55
2:9:59:C:H2'	2:9:60:C:C6	2.40	0.55
1:0:1289:C:O2'	1:0:1290:G:H5'	2.07	0.55
1:0:303:C:O2'	1:0:304:G:H5'	2.06	0.55
1:0:684:G:H2'	1:0:685:C:C6	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1438:G:N2	1:0:1685:A:C8	2.73	0.55
1:0:1515:A:H2'	1:0:1516:C:H6	1.69	0.55
1:0:1450:C:H4'	1:0:1451:C:OP2	2.06	0.55
1:0:1697:G:O2'	1:0:1698:U:H5'	2.05	0.55
1:0:137:U:H2'	1:0:139:C:C5	2.41	0.55
1:0:138:U:H6	1:0:140:G:N1	2.03	0.55
1:0:1909:A:H2'	1:0:1910:A:C8	2.42	0.55
1:0:2074:A:O2'	1:0:2076:U:OP2	2.24	0.55
1:0:1014:A:H2'	1:0:1015:C:H5'	1.88	0.55
1:0:1495:C:H2'	1:0:1496:G:C8	2.42	0.55
1:0:2072:G:C6	1:0:2533:C:H1'	2.42	0.55
1:0:370:G:O2'	1:0:371:U:H5'	2.07	0.54
1:0:817:G:O2'	1:0:818:A:H8	1.90	0.54
1:0:2692:G:H8	1:0:2693:U:C5	2.25	0.54
1:0:1450:C:O2'	1:0:1494:A:H5'	2.07	0.54
1:0:1761:U:H2'	1:0:1762:C:C6	2.42	0.54
1:0:2016:U:H2'	1:0:2017:U:C6	2.42	0.54
1:0:2237:G:H1'	1:0:2238:A:C8	2.42	0.54
1:0:2250:G:H2'	1:0:2251:G:H8	1.72	0.54
2:9:103:A:H2'	2:9:104:A:H8	1.71	0.54
1:0:1123:A:C2	1:0:1129:C:H4'	2.43	0.54
1:0:1367:A:H2'	1:0:1368:U:O4'	2.08	0.54
1:0:1804:A:H2'	1:0:1805:G:H8	1.71	0.54
1:0:2237:G:O2'	1:0:2238:A:C8	2.60	0.54
1:0:2769:C:H2'	1:0:2770:G:O4'	2.07	0.54
1:0:2795:C:O2'	1:0:2796:U:H5'	2.08	0.54
1:0:1088:A:H1'	1:0:1260:G:H21	1.72	0.54
1:0:1978:A:O2'	1:0:1979:G:OP1	2.24	0.54
1:0:2718:C:H5'	1:0:2718:C:H6	1.73	0.54
2:9:2:U:O5'	2:9:3:A:H5'	2.07	0.54
1:0:1730:G:C6	23:U:18:ARG:CA	2.90	0.54
1:0:2291:A:C8	1:0:2309:C:H5'	2.42	0.54
1:0:344:C:H2'	1:0:345:G:O4'	2.08	0.54
1:0:889:C:H2'	1:0:890:C:C6	2.43	0.54
1:0:1741:U:O2'	1:0:2723:G:H4'	2.08	0.54
1:0:2717:C:H2'	1:0:2718:C:C5'	2.32	0.54
1:0:37:A:H2'	1:0:38:G:C8	2.43	0.53
1:0:88:G:H2'	1:0:89:G:C8	2.43	0.53
1:0:1423:C:O2'	1:0:1424:A:H5'	2.08	0.53
1:0:1965:C:H6	1:0:1965:C:O5'	1.90	0.53
1:0:2681:A:N6	1:0:2714:U:H4'	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:597:A:O2'	1:0:598:C:H5'	2.09	0.53
1:0:1220:U:H2'	1:0:1221:G:H8	1.73	0.53
1:0:1327:G:N2	1:0:1329:A:H3'	2.23	0.53
1:0:1603:A:H5'	1:0:1605:G:O4'	2.07	0.53
1:0:1790:C:H2'	1:0:1791:U:H6	1.72	0.53
1:0:2463:A:O2'	1:0:2464:C:OP1	2.23	0.53
1:0:695:C:H2'	1:0:696:C:C6	2.43	0.53
1:0:1933:G:O2'	1:0:1934:A:H5'	2.08	0.53
1:0:1972:U:C2'	1:0:1973:A:H5'	2.37	0.53
1:0:2051:G:O2'	1:0:2052:U:H5'	2.08	0.53
1:0:2912:C:H2'	1:0:2913:A:O4'	2.09	0.53
1:0:367:G:H4'	1:0:368:C:OP1	2.07	0.53
1:0:1925:G:O2'	1:0:1926:G:H5'	2.09	0.53
1:0:881:C:OP1	1:0:883:U:H5	1.90	0.53
1:0:1245:C:H6	1:0:1245:C:O5'	1.90	0.53
1:0:790:A:H2'	1:0:791:A:O4'	2.09	0.53
1:0:1118:A:C8	1:0:1118:A:C3'	2.92	0.53
1:0:1218:U:H2'	1:0:1219:U:C6	2.44	0.53
1:0:1477:C:H5'	1:0:1868:G:H5''	1.90	0.53
1:0:2250:G:N2	1:0:2251:G:H1'	2.22	0.53
1:0:187:A:H3'	1:0:188:C:C6	2.43	0.53
1:0:646:G:H2'	1:0:647:U:H6	1.73	0.53
1:0:1116:U:O2'	1:0:1118:A:C2	2.46	0.53
1:0:413:G:H2'	1:0:414:C:C6	2.44	0.53
1:0:820:G:H5'	1:0:821:U:H5'	1.90	0.53
1:0:204:A:C2'	1:0:205:U:H5'	2.39	0.52
1:0:873:G:H21	1:0:876:A:H62	1.56	0.52
1:0:2692:G:C8	1:0:2693:U:H5	2.26	0.52
1:0:2866:U:O2'	1:0:2867:G:P	2.67	0.52
1:0:282:C:H1'	1:0:368:C:H42	1.68	0.52
1:0:1098:A:H2'	1:0:1099:G:O4'	2.10	0.52
1:0:1471:A:H2'	1:0:1472:C:C6	2.43	0.52
1:0:2858:U:H2'	1:0:2859:C:C6	2.44	0.52
1:0:236:A:H4'	1:0:237:G:OP1	2.10	0.52
1:0:282:C:O2'	1:0:283:U:C4'	2.57	0.52
1:0:1333:U:H2'	1:0:1334:C:H6	1.74	0.52
1:0:1588:G:C6	1:0:1589:G:N1	2.77	0.52
2:9:23:U:H3	2:9:54:A:H5''	1.74	0.52
1:0:503:G:H2'	1:0:504:G:H8	1.74	0.52
1:0:666:A:H2'	1:0:667:C:O4'	2.09	0.52
1:0:737:A:H2'	1:0:738:G:O4'	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1117:A:N1	1:0:1244:U:H2'	2.23	0.52
1:0:280:C:O2'	1:0:281:U:H5'	2.10	0.52
1:0:484:A:N1	1:0:506:G:H4'	2.24	0.52
1:0:1398:G:H2'	1:0:1399:A:C8	2.44	0.52
1:0:1589:G:H22	1:0:1605:G:H2'	1.73	0.52
1:0:282:C:H2'	1:0:283:U:O4'	2.09	0.52
1:0:1309:U:H2'	1:0:1310:U:C5'	2.40	0.52
1:0:1835:U:C5	1:0:1840:A:N7	2.69	0.52
1:0:2472:C:O2'	1:0:2634:G:H4'	2.10	0.52
1:0:2909:G:O2'	1:0:2910:A:C5'	2.56	0.52
1:0:1132:A:N6	1:0:1229:C:H2'	2.24	0.52
1:0:2768:A:C2'	1:0:2769:C:O4'	2.51	0.52
1:0:817:G:O2'	1:0:818:A:C8	2.62	0.52
1:0:1066:U:H2'	1:0:1067:A:C8	2.45	0.52
1:0:1591:A:H4'	1:0:1592:G:O5'	2.09	0.52
1:0:1950:G:HO2'	1:0:1951:G:C5'	2.23	0.52
1:0:2345:A:OP1	1:0:2346:C:H5	1.92	0.52
1:0:2597:U:H2'	1:0:2598:U:H5'	1.91	0.52
2:9:107:C:H2'	2:9:108:C:H6	1.75	0.52
1:0:2727:A:H2'	1:0:2728:C:H5'	1.92	0.51
1:0:1060:C:H2'	1:0:1061:C:H6	1.75	0.51
1:0:1561:U:H2'	1:0:1562:C:C6	2.44	0.51
1:0:2906:A:H5'	1:0:2907:C:O4'	2.10	0.51
1:0:249:G:O2'	1:0:250:C:H5'	2.11	0.51
1:0:2791:U:H1'	1:0:2792:A:H5''	1.92	0.51
1:0:289:G:N2	1:0:363:A:C2	2.61	0.51
1:0:612:U:H2'	1:0:613:C:C6	2.45	0.51
1:0:1616:A:H2'	1:0:1618:G:C8	2.46	0.51
1:0:2667:G:O2'	1:0:2668:G:H5'	2.10	0.51
1:0:842:C:O2	1:0:1693:A:H2'	2.11	0.51
1:0:2445:U:H2'	1:0:2446:G:C8	2.46	0.51
1:0:2509:A:OP2	1:0:2510:C:H5	1.92	0.51
1:0:272:A:C2	1:0:369:G:H5''	2.46	0.51
1:0:1042:U:O2'	1:0:1043:C:H5'	2.10	0.51
2:9:106:C:O2'	2:9:107:C:H5'	2.11	0.51
1:0:289:G:N1	1:0:363:A:C2	2.77	0.51
1:0:581:G:O2'	1:0:582:C:H5'	2.11	0.51
1:0:1008:C:H2'	1:0:1009:U:C6	2.45	0.51
1:0:1099:G:OP1	2:9:87:U:H2'	2.11	0.51
1:0:1790:C:H2'	1:0:1791:U:C6	2.45	0.51
1:0:1804:A:O2'	1:0:1805:G:H5'	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:114:G:H2'	2:9:115:C:C6	2.46	0.51
1:0:255:A:H2'	1:0:256:C:H6	1.73	0.51
1:0:559:U:O2'	1:0:560:C:H5'	2.10	0.51
1:0:1217:G:H2'	1:0:1218:U:H6	1.75	0.51
2:9:64:C:C2'	2:9:65:A:H5'	2.41	0.51
1:0:1386:G:O2'	1:0:1387:G:H5'	2.11	0.51
1:0:1909:A:N1	1:0:2128:G:H1'	2.26	0.51
1:0:2242:U:O2'	1:0:2243:C:O5'	2.29	0.51
1:0:834:G:H3'	1:0:835:U:H4'	1.92	0.50
1:0:2564:G:OP2	1:0:2565:C:H5''	2.11	0.50
1:0:939:A:H4'	1:0:940:G:O5'	2.11	0.50
1:0:1132:A:H2'	1:0:1133:A:C8	2.46	0.50
1:0:941:G:O2'	1:0:942:U:H5'	2.12	0.50
1:0:1006:A:H2'	1:0:1007:A:C8	2.47	0.50
1:0:1072:G:O2'	1:0:1073:A:P	2.69	0.50
1:0:553:G:C2'	1:0:554:G:H5'	2.42	0.50
1:0:2348:C:O2'	1:0:2349:G:H5'	2.11	0.50
2:9:103:A:O2'	2:9:104:A:H5'	2.10	0.50
1:0:2064:U:H5'	1:0:2652:U:O3'	2.12	0.50
1:0:2578:G:H5'	1:0:2578:G:H8	1.76	0.50
1:0:2766:A:O2'	1:0:2767:C:H5'	2.11	0.50
1:0:291:C:H2'	1:0:292:G:O4'	2.12	0.50
1:0:555:U:OP2	1:0:555:U:H6	1.95	0.50
1:0:1730:G:H4'	1:0:1731:C:O5'	2.12	0.50
1:0:2300:A:H4'	1:0:2301:A:O5'	2.12	0.50
1:0:1072:G:H1'	1:0:1088:A:N6	2.27	0.50
1:0:485:A:O2'	1:0:487:G:H5'	2.11	0.50
1:0:848:C:H2'	1:0:849:C:C6	2.46	0.50
1:0:1342:C:C2'	1:0:1343:C:H5'	2.41	0.50
1:0:2133:U:H4'	1:0:2134:G:H5'	1.93	0.50
2:9:52:A:O2'	2:9:53:G:H5'	2.12	0.50
1:0:2515:C:C2'	1:0:2516:G:H5'	2.43	0.49
1:0:2756:U:N3	1:0:2896:A:H2	2.09	0.49
2:9:25:G:H3'	2:9:25:G:OP1	2.12	0.49
1:0:195:C:C2'	1:0:196:G:H5'	2.42	0.49
1:0:1380:U:O2	1:0:1380:U:C2'	2.60	0.49
1:0:2242:U:O2'	1:0:2243:C:P	2.69	0.49
1:0:2726:U:O2	1:0:2749:U:O5'	2.30	0.49
1:0:969:G:H2'	1:0:970:U:C6	2.48	0.49
1:0:2502:C:H2'	1:0:2503:A:H5'	1.93	0.49
1:0:2681:A:C6	1:0:2714:U:H4'	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:10:U:O2'	1:0:11:A:P	2.69	0.49
1:0:496:G:H4'	1:0:497:A:OP1	2.12	0.49
1:0:1887:U:H2'	1:0:1888:C:C6	2.48	0.49
1:0:2290:U:H4'	1:0:2291:A:OP1	2.12	0.49
1:0:2656:G:O2'	1:0:2657:G:H5'	2.12	0.49
2:9:42:C:H5'	2:9:43:G:OP2	2.12	0.49
1:0:284:C:H1'	1:0:285:A:P	2.52	0.49
1:0:604:G:H4'	1:0:605:C:O5'	2.11	0.49
1:0:2381:C:H2'	1:0:2382:A:C8	2.48	0.49
1:0:2765:C:H2'	1:0:2766:A:C8	2.48	0.49
1:0:629:A:H2'	1:0:630:A:O4'	2.13	0.49
1:0:1461:U:H2'	1:0:1462:C:C6	2.48	0.49
1:0:2903:C:O2'	1:0:2904:U:H5'	2.12	0.49
1:0:44:G:H21	1:0:45:A:H62	1.60	0.49
1:0:639:A:H2'	1:0:640:G:C8	2.47	0.49
1:0:939:A:O2'	1:0:940:G:OP2	2.30	0.49
1:0:1309:U:C2'	1:0:1310:U:H5'	2.42	0.49
2:9:102:G:O2'	2:9:103:A:H5'	2.13	0.49
1:0:1477:C:C5'	1:0:1868:G:H5''	2.43	0.49
1:0:199:A:C2'	1:0:200:U:H5''	2.43	0.49
1:0:1511:U:O2'	1:0:1512:G:H5'	2.13	0.49
1:0:2011:A:H4'	1:0:2012:U:O5'	2.13	0.49
1:0:2242:U:O2'	1:0:2243:C:C6	2.63	0.49
1:0:2782:G:O6	1:0:2790:C:H5''	2.13	0.49
1:0:2842:G:H2'	1:0:2843:A:H5'	1.95	0.49
2:9:103:A:H2'	2:9:104:A:C8	2.48	0.49
1:0:1946:C:H2'	1:0:1971:G:C8	2.47	0.48
1:0:2883:A:H2'	1:0:2884:G:O4'	2.13	0.48
1:0:2912:C:O2'	1:0:2913:A:H5'	2.12	0.48
1:0:907:A:H2'	1:0:908:A:H8	1.77	0.48
1:0:1072:G:O2'	1:0:1073:A:C8	2.66	0.48
1:0:1669:A:H2'	1:0:1670:G:H8	1.72	0.48
1:0:2279:G:N2	1:0:2463:A:H1'	2.28	0.48
1:0:2329:C:O2'	1:0:2330:U:H5'	2.12	0.48
1:0:2804:C:H2'	1:0:2805:A:O4'	2.12	0.48
1:0:322:G:O2'	1:0:323:C:H5'	2.14	0.48
1:0:887:G:H2'	1:0:888:U:C6	2.48	0.48
1:0:1568:G:O2'	1:0:1569:U:H5'	2.12	0.48
1:0:2266:A:H2'	1:0:2267:G:H8	1.79	0.48
1:0:2473:U:O3'	1:0:2474:A:H3'	2.14	0.48
1:0:352:A:H2'	1:0:353:G:C8	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1000:C:H2'	1:0:1001:U:O4'	2.13	0.48
1:0:1140:C:O2'	1:0:1141:U:H5'	2.14	0.48
1:0:1209:C:O2'	1:0:1210:G:H5'	2.12	0.48
1:0:1214:G:O2'	1:0:1215:A:H8	1.96	0.48
1:0:1257:C:H2'	1:0:1258:G:O4'	2.14	0.48
1:0:1425:G:O2'	1:0:1426:C:H5'	2.13	0.48
1:0:1624:A:O2'	1:0:1625:U:P	2.71	0.48
1:0:1657:A:H2'	1:0:1658:A:C8	2.49	0.48
1:0:2103:A:N7	1:0:2538:A:N1	2.62	0.48
2:9:108:C:O2'	2:9:109:G:H5'	2.14	0.48
1:0:197:C:OP2	1:0:198:A:H8	1.97	0.48
1:0:938:G:HO2'	1:0:939:A:H8	1.54	0.48
1:0:1329:A:H2'	1:0:1330:A:C8	2.48	0.48
1:0:1773:G:N2	1:0:1774:G:C8	2.82	0.48
1:0:1950:G:O2'	1:0:1951:G:P	2.71	0.48
1:0:2387:U:H2'	1:0:2388:C:H6	1.77	0.48
1:0:1120:U:C6	1:0:1120:U:H5''	2.48	0.48
1:0:1503:U:H2'	1:0:1504:A:O4'	2.13	0.48
1:0:1662:C:H2'	1:0:1663:G:O4'	2.14	0.48
1:0:2886:C:O2'	1:0:2887:G:H5'	2.13	0.48
1:0:162:C:C2'	1:0:163:U:H5'	2.43	0.48
1:0:353:G:O2'	1:0:354:A:H5'	2.14	0.48
1:0:440:C:H2'	1:0:441:A:C8	2.48	0.48
1:0:555:U:OP2	1:0:555:U:C6	2.67	0.48
1:0:598:C:O2'	1:0:599:G:H5'	2.13	0.48
1:0:1805:G:H2'	1:0:1806:G:C8	2.47	0.48
1:0:2074:A:H4'	1:0:2075:G:OP1	2.13	0.48
1:0:116:G:H5'	1:0:129:A:H2'	1.94	0.48
1:0:557:C:O2'	1:0:558:C:H5'	2.14	0.48
1:0:1153:C:O2'	1:0:1154:A:H5'	2.14	0.48
1:0:1307:A:H2'	1:0:1308:A:C8	2.49	0.48
1:0:12:U:C2'	1:0:13:G:H5'	2.43	0.47
1:0:284:C:OP2	1:0:284:C:H6	1.95	0.47
1:0:1463:A:H2'	1:0:1464:U:C6	2.48	0.47
1:0:2252:A:H2'	1:0:2253:G:O4'	2.14	0.47
1:0:2353:A:H4'	1:0:2354:A:O5'	2.14	0.47
1:0:544:G:H2'	1:0:545:G:C5'	2.44	0.47
1:0:702:G:HO2'	1:0:703:G:H5'	1.79	0.47
1:0:958:G:H2'	1:0:959:C:C6	2.49	0.47
1:0:2257:G:H4'	1:0:2259:C:C2	2.49	0.47
1:0:2264:A:H2'	1:0:2265:U:C6	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2381:C:H2'	1:0:2382:A:H8	1.79	0.47
1:0:2836:G:H4'	1:0:2837:U:OP1	2.14	0.47
1:0:393:G:O2'	1:0:394:G:H5'	2.15	0.47
1:0:1119:G:N2	1:0:1246:A:N1	2.62	0.47
1:0:2692:G:H8	1:0:2693:U:H5	1.61	0.47
2:9:3:A:N7	2:9:25:G:N2	2.62	0.47
1:0:613:C:H2'	1:0:614:U:C6	2.48	0.47
1:0:2372:A:H2'	1:0:2373:U:C6	2.50	0.47
1:0:2748:G:H4'	1:0:2749:U:H5'	1.96	0.47
1:0:1791:U:O2'	1:0:1792:C:H5'	2.13	0.47
1:0:2320:U:H4'	1:0:2321:A:O4'	2.15	0.47
1:0:2385:G:H2'	1:0:2386:U:C6	2.50	0.47
1:0:2842:G:C2'	1:0:2843:A:H5'	2.45	0.47
1:0:2885:A:H2'	1:0:2886:C:H6	1.78	0.47
1:0:425:U:O2'	1:0:426:G:H5'	2.15	0.47
1:0:795:G:H21	1:0:817:G:H2'	1.78	0.47
1:0:952:G:N3	1:0:2302:A:H2'	2.30	0.47
1:0:1865:A:H2'	1:0:1866:A:C8	2.50	0.47
1:0:2238:A:C2'	1:0:2239:C:H5'	2.45	0.47
1:0:2415:A:H2'	1:0:2416:G:H5'	1.95	0.47
1:0:2697:A:H2'	1:0:2698:G:C8	2.50	0.47
1:0:35:U:H2'	1:0:36:C:C6	2.49	0.47
1:0:101:C:O2'	1:0:102:A:H5'	2.13	0.47
1:0:136:C:H2'	1:0:137:U:O4'	2.14	0.47
1:0:506:G:H22	1:0:509:A:H5''	1.80	0.47
1:0:817:G:HO2'	1:0:818:A:H8	1.49	0.47
1:0:940:G:O2'	1:0:941:G:H5'	2.15	0.47
1:0:1160:G:H21	1:0:1207:A:H62	1.63	0.47
1:0:1948:G:O2'	1:0:1949:G:H5'	2.14	0.47
1:0:2326:U:H2'	1:0:2327:A:C8	2.49	0.47
1:0:2672:C:H2'	1:0:2673:U:H6	1.79	0.47
2:9:96:C:H2'	2:9:97:U:C6	2.50	0.47
1:0:637:C:H2'	1:0:638:C:C6	2.50	0.47
1:0:1127:C:OP1	1:0:1128:U:H5	1.96	0.47
1:0:1355:A:OP1	1:0:1355:A:C4'	2.63	0.47
1:0:1605:G:C8	1:0:1605:G:H5''	2.50	0.47
1:0:1730:G:C5'	1:0:1731:C:C6	2.97	0.47
1:0:2511:A:H5'	1:0:2511:A:H8	1.80	0.47
1:0:2897:C:O2'	1:0:2898:G:H5'	2.15	0.47
1:0:197:C:OP2	1:0:198:A:C8	2.68	0.47
1:0:1447:U:H3'	1:0:1506:U:O2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1544:U:O2'	1:0:1545:C:H5'	2.15	0.47
1:0:2255:A:O2'	1:0:2256:G:H5'	2.14	0.47
1:0:2350:G:O2'	1:0:2351:C:H5'	2.14	0.47
1:0:2398:A:H2'	1:0:2399:G:O4'	2.14	0.47
1:0:550:C:O2'	1:0:551:A:H5'	2.14	0.47
1:0:1015:C:H2'	1:0:1016:U:C6	2.50	0.47
1:0:1218:U:H2'	1:0:1219:U:H6	1.80	0.47
1:0:1878:G:O2'	1:0:1879:U:OP2	2.32	0.47
1:0:438:C:O2'	1:0:439:A:OP1	2.30	0.46
1:0:90:A:H2'	1:0:91:G:O4'	2.14	0.46
1:0:284:C:C1'	1:0:285:A:OP2	2.61	0.46
1:0:506:G:N2	1:0:509:A:H5'	2.21	0.46
1:0:508:A:H2'	1:0:509:A:H5''	1.96	0.46
1:0:946:C:H2'	1:0:947:U:C6	2.51	0.46
1:0:1109:U:OP1	1:0:1110:G:H5''	2.15	0.46
1:0:1309:U:H2'	1:0:1310:U:H5'	1.96	0.46
1:0:1321:A:H2'	1:0:1322:G:C8	2.50	0.46
1:0:1552:G:H2'	1:0:1553:C:C6	2.49	0.46
1:0:1603:A:H4'	1:0:1604:G:OP2	2.14	0.46
1:0:2005:G:OP2	1:0:2005:G:H3'	2.14	0.46
1:0:2129:U:H2'	1:0:2130:C:C6	2.50	0.46
1:0:2589:U:H2'	1:0:2590:U:C6	2.50	0.46
1:0:293:A:O2'	1:0:294:C:H5'	2.16	0.46
1:0:681:G:O2'	1:0:682:A:OP2	2.29	0.46
1:0:2754:G:O2'	1:0:2755:G:H5'	2.15	0.46
1:0:1527:A:C2	1:0:1528:A:C5	3.03	0.46
1:0:2064:U:H5'	1:0:2652:U:H4'	1.98	0.46
1:0:1496:G:H5'	1:0:1572:A:H1'	1.98	0.46
1:0:2004:U:H6	1:0:2004:U:O5'	1.99	0.46
1:0:354:A:H2'	1:0:355:C:C6	2.51	0.46
1:0:657:G:H2'	1:0:658:C:C6	2.51	0.46
1:0:999:C:O2'	1:0:1000:C:H5'	2.15	0.46
1:0:1825:U:O2'	1:0:1826:C:H5'	2.16	0.46
1:0:2105:C:H2'	1:0:2106:C:C6	2.51	0.46
1:0:18:C:H2'	1:0:19:U:C6	2.51	0.46
1:0:939:A:O2'	1:0:940:G:P	2.74	0.46
1:0:1345:A:H2'	1:0:1346:U:C6	2.51	0.46
1:0:1730:G:H5'	1:0:1731:C:H5	1.80	0.46
1:0:1947:G:N2	1:0:1966:U:C2	2.84	0.46
1:0:2000:G:O2'	1:0:2001:G:H5'	2.16	0.46
1:0:2073:G:OP2	1:0:2490:A:H5'	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2251:G:C6	1:0:2252:A:C6	3.04	0.46
1:0:2430:A:N6	1:0:2460:A:H2	2.14	0.46
2:9:76:G:H3'	2:9:77:A:C5'	2.21	0.46
1:0:295:C:O2'	1:0:296:G:H5'	2.15	0.46
1:0:2866:U:O2'	1:0:2867:G:OP2	2.29	0.46
1:0:2911:C:O2'	1:0:2912:C:H5'	2.15	0.46
1:0:337:A:H2	1:0:1314:U:C2'	2.29	0.46
1:0:945:U:O2'	1:0:946:C:H5'	2.16	0.46
1:0:1114:A:H2'	1:0:1115:U:C6	2.51	0.46
1:0:1450:C:C4'	1:0:1451:C:OP2	2.64	0.46
1:0:2575:C:H2'	1:0:2576:A:O4'	2.16	0.46
1:0:2772:G:O2'	1:0:2773:G:H5'	2.15	0.46
1:0:2871:G:H2'	1:0:2872:U:C6	2.51	0.46
1:0:168:C:O2'	1:0:169:A:H5'	2.16	0.46
1:0:1114:A:H2'	1:0:1115:U:H6	1.80	0.46
1:0:1422:U:H2'	1:0:1423:C:C6	2.50	0.46
1:0:1607:A:H2'	1:0:1608:G:O4'	2.15	0.46
1:0:2831:C:H2'	1:0:2832:C:H5'	1.96	0.46
1:0:141:C:C2'	1:0:141:C:O2	2.63	0.45
1:0:279:C:H2'	1:0:280:C:H6	1.80	0.45
1:0:1080:C:O2'	1:0:1081:A:OP1	2.26	0.45
1:0:1586:G:H2'	1:0:1587:U:O4'	2.16	0.45
1:0:2255:A:H2'	1:0:2256:G:O4'	2.16	0.45
1:0:2456:A:H2'	1:0:2457:U:C6	2.51	0.45
1:0:2819:C:H2'	1:0:2820:A:H8	1.81	0.45
1:0:204:A:O2'	1:0:205:U:H5'	2.16	0.45
1:0:296:G:O2'	1:0:297:U:H5'	2.16	0.45
1:0:693:A:H2'	1:0:694:A:C8	2.51	0.45
1:0:1965:C:H2'	1:0:1966:U:C6	2.52	0.45
1:0:2653:A:H2'	1:0:2654:C:C6	2.51	0.45
1:0:2781:U:O2'	1:0:2782:G:H5'	2.16	0.45
1:0:2831:C:C2'	1:0:2832:C:H5'	2.46	0.45
1:0:40:C:O2'	1:0:41:G:H5'	2.16	0.45
1:0:747:G:H2'	1:0:748:C:C6	2.51	0.45
1:0:947:U:O2'	1:0:948:G:H5'	2.16	0.45
1:0:1315:G:H4'	1:0:1316:G:OP2	2.17	0.45
1:0:1573:A:H2'	1:0:1574:C:O4'	2.16	0.45
1:0:2074:A:O2'	1:0:2075:G:P	2.75	0.45
1:0:2416:G:H2'	1:0:2417:C:C6	2.52	0.45
1:0:2776:A:H2'	1:0:2777:G:O4'	2.16	0.45
1:0:2871:G:H2'	1:0:2872:U:H6	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:549:A:O2'	1:0:550:C:H5'	2.16	0.45
1:0:582:C:H2'	1:0:583:G:C8	2.48	0.45
1:0:683:G:O2'	1:0:684:G:H5'	2.16	0.45
1:0:696:C:O2'	1:0:731:U:OP1	2.34	0.45
1:0:728:C:H2'	1:0:729:C:H6	1.81	0.45
1:0:2251:G:C2	1:0:2252:A:C4	3.05	0.45
1:0:2429:A:H2'	1:0:2430:A:C8	2.51	0.45
1:0:274:G:O2'	1:0:275:G:H5'	2.17	0.45
1:0:1965:C:O2'	1:0:1966:U:H5'	2.16	0.45
1:0:2115:U:H2'	1:0:2116:U:C6	2.52	0.45
1:0:2242:U:H4'	1:0:2243:C:OP1	2.17	0.45
1:0:2729:C:O2'	1:0:2730:G:H5'	2.17	0.45
1:0:219:G:O2'	1:0:220:C:P	2.75	0.45
1:0:631:A:N3	1:0:2073:G:O2'	2.49	0.45
1:0:1535:G:H2'	1:0:1536:C:C6	2.52	0.45
1:0:1815:A:H2'	1:0:1816:C:O4'	2.17	0.45
1:0:2133:U:N3	1:0:2259:C:OP2	2.45	0.45
1:0:2499:U:O2'	1:0:2500:C:H5'	2.16	0.45
1:0:2765:C:H2'	1:0:2766:A:H8	1.82	0.45
1:0:2890:A:C2'	1:0:2891:A:OP2	2.65	0.45
2:9:55:U:O2'	2:9:56:A:OP2	2.26	0.45
1:0:695:C:H2'	1:0:696:C:H6	1.82	0.45
1:0:1526:A:H1'	1:0:1527:A:N7	2.32	0.45
1:0:1730:G:C5'	1:0:1731:C:H6	2.29	0.45
1:0:1928:C:H2'	1:0:1929:G:O4'	2.17	0.45
2:9:18:U:O2'	2:9:19:G:H5'	2.16	0.45
1:0:248:A:H5'	1:0:249:G:OP2	2.17	0.45
1:0:816:G:C6	1:0:817:G:N1	2.85	0.45
1:0:2112:A:H2'	1:0:2113:G:H8	1.79	0.45
1:0:2506:A:O2'	1:0:2507:G:O5'	2.34	0.45
2:9:95:C:O2'	2:9:96:C:H5'	2.17	0.45
1:0:305:A:C5	1:0:329:A:C2	3.05	0.45
1:0:956:G:H2'	1:0:957:A:O4'	2.17	0.45
1:0:1120:U:H5''	1:0:1120:U:H6	1.82	0.45
1:0:1283:G:O2'	1:0:1284:G:H5'	2.16	0.45
1:0:1406:A:H4'	1:0:1407:A:O5'	2.17	0.45
1:0:2672:C:O2'	1:0:2673:U:H5'	2.17	0.45
2:9:94:G:O2'	2:9:95:C:H5'	2.17	0.45
1:0:282:C:H3'	1:0:283:U:H5'	1.99	0.44
1:0:820:G:O2'	1:0:856:G:H4'	2.17	0.44
1:0:1116:U:H3	1:0:1246:A:H62	1.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1327:G:C2	1:0:1329:A:H3'	2.53	0.44
1:0:2419:U:H5''	1:0:2420:G:H5'	1.99	0.44
1:0:141:C:O2	1:0:141:C:H2'	2.17	0.44
1:0:438:C:O2'	1:0:439:A:P	2.75	0.44
1:0:638:C:H2'	1:0:639:A:C8	2.52	0.44
1:0:1118:A:H8	1:0:1119:G:H5''	1.83	0.44
1:0:1148:C:H6	1:0:1148:C:C5'	2.25	0.44
1:0:1433:G:O2'	1:0:1434:A:H5'	2.18	0.44
1:0:1496:G:H2'	1:0:1497:G:C8	2.52	0.44
1:0:1882:C:O2'	1:0:2012:U:OP2	2.33	0.44
1:0:2106:C:H2'	1:0:2107:U:C6	2.52	0.44
2:9:71:C:O2'	2:9:72:C:H5'	2.17	0.44
1:0:419:A:H1'	1:0:1921:A:C2	2.53	0.44
1:0:790:A:H1'	1:0:1710:A:H2'	1.99	0.44
1:0:920:C:H5''	1:0:921:G:O5'	2.17	0.44
1:0:1006:A:N1	1:0:2311:A:H1'	2.31	0.44
1:0:1902:G:H2'	1:0:1903:U:C6	2.51	0.44
1:0:1930:A:H2'	1:0:1931:A:C8	2.52	0.44
1:0:2688:U:O2'	1:0:2689:A:H5'	2.17	0.44
1:0:383:A:H2'	1:0:384:G:O4'	2.18	0.44
1:0:907:A:H2'	1:0:908:A:C8	2.51	0.44
1:0:1149:U:H4'	1:0:1150:A:H5''	1.98	0.44
1:0:1380:U:H5	1:0:2043:U:O2'	2.00	0.44
1:0:2388:C:O2'	1:0:2389:U:H5'	2.17	0.44
1:0:2515:C:H2'	1:0:2516:G:H5'	1.98	0.44
1:0:140:G:H3'	1:0:140:G:H8	1.83	0.44
1:0:324:G:O2'	1:0:325:U:H5'	2.18	0.44
1:0:2563:U:H2'	1:0:2565:C:O5'	2.16	0.44
1:0:270:U:O2'	1:0:271:C:P	2.75	0.44
1:0:319:A:H4'	1:0:338:C:C4	2.53	0.44
1:0:2279:G:C2	1:0:2463:A:H1'	2.53	0.44
2:9:35:C:H5'	2:9:36:C:OP2	2.18	0.44
2:9:52:A:C2'	2:9:53:G:H5'	2.48	0.44
1:0:766:A:O2'	1:0:767:A:H5''	2.18	0.44
1:0:1587:U:C4	1:0:1588:G:C6	3.06	0.44
1:0:2247:C:O2'	1:0:2248:C:H5'	2.18	0.44
1:0:2256:G:O2'	1:0:2257:G:H5'	2.17	0.44
1:0:2885:A:H2'	1:0:2886:C:C6	2.52	0.44
1:0:45:A:C8	1:0:45:A:H5'	2.53	0.44
1:0:212:A:O4'	1:0:214:U:C6	2.70	0.44
1:0:294:C:H2'	1:0:295:C:O4'	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:615:G:H2'	1:0:616:U:C6	2.52	0.44
1:0:858:U:H2'	1:0:859:C:H6	1.82	0.44
1:0:1517:U:O2'	1:0:1518:A:H5'	2.18	0.44
1:0:2846:C:H2'	1:0:2847:G:H8	1.82	0.44
1:0:95:A:H5''	1:0:96:A:C3'	2.45	0.44
1:0:105:G:O2'	1:0:106:A:H5'	2.18	0.44
1:0:243:A:H61	1:0:269:G:H1'	1.83	0.44
1:0:1589:G:N2	1:0:1605:G:C2'	2.80	0.44
1:0:1739:G:O2'	1:0:1740:U:H5'	2.18	0.44
2:9:61:C:H2'	2:9:62:A:H8	1.83	0.44
1:0:219:G:H3'	1:0:220:C:C5'	2.45	0.43
1:0:401:C:H2'	1:0:402:U:C6	2.52	0.43
1:0:1141:U:O2'	1:0:1142:C:H5'	2.18	0.43
1:0:2372:A:H2'	1:0:2373:U:H6	1.83	0.43
1:0:283:U:H5	1:0:284:C:H41	1.66	0.43
1:0:343:C:O2'	1:0:344:C:H5'	2.18	0.43
1:0:1524:U:O2'	1:0:1525:G:P	2.76	0.43
1:0:1609:C:H2'	1:0:1610:G:H8	1.83	0.43
1:0:1761:U:H2'	1:0:1762:C:H6	1.82	0.43
1:0:1878:G:O2'	1:0:1879:U:C6	2.66	0.43
1:0:2312:G:C2'	1:0:2313:C:H5'	2.48	0.43
1:0:2419:U:H5''	1:0:2420:G:C5'	2.48	0.43
1:0:2793:A:H2'	1:0:2794:G:H5'	1.99	0.43
1:0:737:A:O2'	1:0:738:G:H5'	2.18	0.43
1:0:1060:C:H2'	1:0:1061:C:C6	2.52	0.43
1:0:1399:A:H2'	1:0:1400:C:C6	2.54	0.43
1:0:1643:C:O2'	1:0:1644:C:H5'	2.18	0.43
1:0:1950:G:H4'	1:0:1951:G:OP1	2.17	0.43
1:0:2781:U:C2'	1:0:2782:G:H5'	2.48	0.43
1:0:2859:C:O2'	1:0:2860:G:H5'	2.18	0.43
1:0:45:A:H5'	1:0:45:A:H8	1.83	0.43
1:0:140:G:H3'	1:0:140:G:C8	2.53	0.43
1:0:735:C:C5	1:0:736:A:C5	3.06	0.43
1:0:875:A:H5'	1:0:876:A:C2	2.53	0.43
1:0:1246:A:O2'	1:0:1247:A:H3'	2.18	0.43
1:0:1968:A:H2'	1:0:1969:A:C8	2.53	0.43
1:0:2330:U:H4'	1:0:2331:C:OP1	2.19	0.43
1:0:2780:C:H2'	1:0:2781:U:H6	1.82	0.43
1:0:204:A:H2'	1:0:205:U:H5'	2.01	0.43
1:0:2460:A:O2'	1:0:2461:U:O4'	2.36	0.43
1:0:2756:U:N3	1:0:2896:A:C2	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:219:G:HO2'	1:0:220:C:P	2.42	0.43
1:0:1850:U:H2'	1:0:1851:G:H8	1.82	0.43
1:0:1901:G:O2'	1:0:1902:G:H5'	2.18	0.43
1:0:2619:U:H2'	1:0:2620:U:C6	2.53	0.43
1:0:95:A:H5'	1:0:96:A:H3'	1.99	0.43
1:0:588:G:O2'	1:0:589:U:P	2.77	0.43
1:0:631:A:C6	1:0:2074:A:H5'	2.53	0.43
1:0:963:C:H2'	1:0:964:G:C8	2.54	0.43
1:0:1768:C:H2'	1:0:1769:C:O4'	2.18	0.43
1:0:1823:G:O2'	1:0:1824:C:H5'	2.18	0.43
1:0:2312:G:H2'	1:0:2313:C:H5'	2.01	0.43
1:0:2694:A:C2	1:0:2702:A:C4	3.07	0.43
2:9:59:C:H2'	2:9:60:C:H6	1.82	0.43
1:0:728:C:H2'	1:0:729:C:C6	2.54	0.43
1:0:858:U:H2'	1:0:859:C:C6	2.53	0.43
1:0:1379:A:O2'	1:0:1380:U:H5''	2.19	0.43
1:0:1641:A:H2'	1:0:1642:A:C5'	2.46	0.43
1:0:1869:A:H2'	1:0:1870:C:O4'	2.19	0.43
1:0:2133:U:H4'	1:0:2134:G:C5'	2.48	0.43
1:0:2407:G:O2'	1:0:2408:A:H5'	2.18	0.43
1:0:485:A:H1'	1:0:486:A:H5'	2.00	0.43
1:0:1496:G:H2'	1:0:1497:G:H8	1.83	0.43
1:0:1730:G:N3	1:0:1730:G:H2'	2.34	0.43
1:0:2078:U:O2'	1:0:2079:G:H5'	2.19	0.43
1:0:2692:G:C8	1:0:2693:U:C5	3.02	0.43
1:0:2838:A:H2'	1:0:2839:C:C6	2.54	0.43
2:9:52:A:H2'	2:9:53:G:O4'	2.19	0.43
2:9:117:G:H2'	2:9:118:C:C6	2.54	0.43
1:0:288:A:N1	1:0:364:C:N3	2.67	0.43
1:0:1053:G:O2'	1:0:1054:G:H5'	2.19	0.43
1:0:1521:C:O2'	1:0:1522:A:H5'	2.19	0.43
1:0:1666:C:O2'	1:0:1667:A:H5'	2.19	0.43
1:0:1902:G:H2'	1:0:1903:U:O4'	2.18	0.43
1:0:2291:A:H5''	1:0:2292:C:C5'	2.49	0.43
1:0:2406:U:O2'	1:0:2407:G:H5'	2.19	0.43
1:0:364:C:H2'	1:0:365:G:O4'	2.18	0.42
1:0:603:A:O2'	1:0:604:G:OP2	2.36	0.42
1:0:807:A:N1	1:0:808:A:C2	2.87	0.42
1:0:1363:G:H2'	1:0:1364:G:C8	2.54	0.42
1:0:1518:A:H2'	1:0:1519:U:C6	2.54	0.42
1:0:1791:U:H2'	1:0:1792:C:C6	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1887:U:H2'	1:0:1888:C:H6	1.83	0.42
1:0:2511:A:H5'	1:0:2511:A:C8	2.53	0.42
1:0:2909:G:H2'	1:0:2910:A:H8	1.83	0.42
1:0:23:G:H1'	1:0:520:A:N6	2.35	0.42
1:0:653:C:H2'	1:0:654:A:C8	2.54	0.42
1:0:764:C:H2'	1:0:765:G:O4'	2.19	0.42
1:0:846:A:O2'	1:0:847:C:H5'	2.19	0.42
1:0:1021:G:O2'	1:0:1022:A:H5'	2.18	0.42
1:0:1369:A:H8	1:0:1369:A:OP1	2.01	0.42
1:0:1894:C:N4	1:0:1939:U:H2'	2.34	0.42
1:0:2134:G:O6	1:0:2258:A:H5''	2.18	0.42
1:0:2430:A:N6	1:0:2460:A:C2	2.87	0.42
1:0:2626:C:H2'	1:0:2627:G:C8	2.54	0.42
1:0:2899:A:O2'	1:0:2900:G:H5'	2.19	0.42
2:9:72:C:O2'	2:9:73:G:H5'	2.18	0.42
1:0:286:U:H2'	1:0:287:C:C6	2.54	0.42
1:0:369:G:C2	1:0:370:G:C8	3.08	0.42
1:0:947:U:H2'	1:0:948:G:C8	2.54	0.42
1:0:1072:G:O2'	1:0:1073:A:OP2	2.34	0.42
1:0:2301:A:H5''	1:0:2302:A:H5'	2.01	0.42
1:0:2748:G:H4'	1:0:2749:U:C5'	2.50	0.42
1:0:360:A:H2'	1:0:361:C:O4'	2.19	0.42
1:0:598:C:C4	1:0:599:G:N7	2.87	0.42
1:0:607:G:H2'	1:0:608:A:O4'	2.20	0.42
1:0:1092:A:H2'	1:0:1093:G:C8	2.54	0.42
1:0:1308:A:O2'	1:0:1309:U:H5'	2.20	0.42
1:0:1594:C:O2'	1:0:1595:G:H5'	2.18	0.42
1:0:2872:U:H2'	1:0:2873:C:H6	1.84	0.42
7:E:55:GLN:CA	7:E:56:PRO:CA	2.97	0.42
1:0:67:A:H5''	1:0:68:U:H3'	2.02	0.42
1:0:119:A:H2'	1:0:120:A:H5''	2.02	0.42
1:0:1088:A:O2'	1:0:1089:G:C5'	2.57	0.42
1:0:1142:C:O2'	1:0:1143:G:H5'	2.19	0.42
1:0:1462:C:H2'	1:0:1463:A:C8	2.55	0.42
1:0:1495:C:H2'	1:0:1496:G:H8	1.83	0.42
1:0:1526:A:O4'	1:0:1527:A:C5	2.72	0.42
1:0:1545:C:H2'	1:0:1546:G:O4'	2.20	0.42
1:0:1569:U:H3'	1:0:1570:C:H5'	2.00	0.42
1:0:2276:U:H2'	1:0:2277:U:C6	2.55	0.42
1:0:2335:C:H2'	1:0:2336:G:C8	2.55	0.42
1:0:2724:U:H2'	1:0:2725:G:O4'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2847:G:O2'	1:0:2848:G:H5'	2.19	0.42
1:0:2885:A:O2'	1:0:2886:C:H5'	2.19	0.42
1:0:60:A:O2'	1:0:61:G:H5'	2.19	0.42
1:0:70:A:H4'	1:0:71:G:O5'	2.18	0.42
1:0:766:A:HO2'	1:0:767:A:H5''	1.85	0.42
1:0:2415:A:C2'	1:0:2416:G:H5'	2.49	0.42
1:0:2563:U:O2'	1:0:2564:G:H3'	2.20	0.42
3:A:186:TRP:CA	3:A:187:PRO:CA	2.98	0.42
1:0:200:U:OP1	1:0:200:U:C6	2.73	0.42
1:0:1846:U:H2'	1:0:1847:A:C5	2.55	0.42
1:0:2253:G:O2'	1:0:2254:G:H5'	2.20	0.42
1:0:240:C:H5''	1:0:270:U:O4	2.20	0.42
1:0:333:G:O2'	1:0:334:G:H5'	2.20	0.42
1:0:850:U:H2'	1:0:851:C:O4'	2.19	0.42
1:0:1298:U:H2'	1:0:1299:G:C8	2.54	0.42
1:0:1516:C:H2'	1:0:1517:U:C6	2.54	0.42
1:0:1798:C:O2	1:0:1798:C:H2'	2.19	0.42
1:0:1850:U:H2'	1:0:1851:G:C8	2.54	0.42
1:0:2004:U:H2'	1:0:2005:G:OP1	2.20	0.42
2:9:3:A:H62	2:9:25:G:H1	1.66	0.42
1:0:345:G:H2'	1:0:346:U:H6	1.85	0.42
1:0:594:C:O2'	1:0:595:U:H5'	2.20	0.42
1:0:811:C:H2'	1:0:812:A:C8	2.54	0.42
1:0:1039:G:H2'	1:0:1040:A:O4'	2.20	0.42
1:0:1280:A:O5'	1:0:1280:A:H8	2.03	0.42
1:0:1457:U:O2'	1:0:1458:A:H5'	2.20	0.42
1:0:1626:A:H2'	1:0:1627:G:C5'	2.50	0.42
1:0:1805:G:O2'	1:0:1806:G:H5'	2.20	0.42
2:9:56:A:C3'	2:9:57:A:H5''	2.50	0.42
1:0:345:G:H2'	1:0:346:U:C6	2.55	0.42
1:0:375:G:C4	1:0:411:A:C6	3.08	0.42
1:0:778:C:H2'	1:0:779:U:O4'	2.20	0.42
1:0:1050:G:C6	1:0:1051:C:C4	3.08	0.42
1:0:1155:G:H2'	1:0:1156:C:C6	2.55	0.42
1:0:2025:G:O2'	1:0:2026:C:H5'	2.19	0.42
1:0:2325:C:H2'	1:0:2326:U:C6	2.55	0.42
1:0:2326:U:H4'	1:0:2412:G:C4'	2.50	0.42
1:0:2627:G:H2'	1:0:2628:U:C6	2.54	0.42
1:0:552:A:H3'	1:0:553:G:C5'	2.49	0.41
1:0:558:C:N3	1:0:600:G:C2	2.88	0.41
1:0:1735:C:H2'	1:0:1736:A:C8	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1787:C:H4'	1:0:2883:A:O4'	2.20	0.41
1:0:1878:G:O2'	1:0:1879:U:P	2.76	0.41
1:0:2242:U:O2'	1:0:2243:C:H2'	2.19	0.41
1:0:2335:C:H2'	1:0:2336:G:H8	1.84	0.41
1:0:364:C:H2'	1:0:365:G:C8	2.54	0.41
1:0:433:C:O2'	1:0:434:U:H5'	2.20	0.41
1:0:1044:C:O2'	1:0:1045:G:OP1	2.34	0.41
1:0:1555:G:H4'	1:0:1630:A:H2	1.85	0.41
1:0:2253:G:N3	1:0:2254:G:C8	2.88	0.41
1:0:2488:A:N6	1:0:2534:C:H42	2.16	0.41
1:0:2821:C:H2'	1:0:2822:C:C6	2.55	0.41
1:0:77:G:O2'	1:0:78:G:H5'	2.20	0.41
1:0:106:A:O2'	1:0:107:U:H5'	2.20	0.41
1:0:243:A:H61	1:0:269:G:C1'	2.33	0.41
1:0:281:U:O2	1:0:369:G:C2	2.73	0.41
1:0:659:A:N3	1:0:746:A:C2	2.89	0.41
1:0:694:A:H2'	1:0:695:C:H5'	2.03	0.41
1:0:810:G:O2'	1:0:811:C:H5'	2.21	0.41
1:0:1150:A:H4'	1:0:1151:G:OP2	2.19	0.41
1:0:1427:A:H61	1:0:1440:U:H1'	1.84	0.41
1:0:1706:G:H1'	1:0:1712:A:H61	1.85	0.41
1:0:2258:A:H1'	1:0:2259:C:OP2	2.19	0.41
2:9:97:U:H2'	2:9:98:C:C6	2.55	0.41
1:0:251:C:H2'	1:0:252:C:C6	2.56	0.41
1:0:281:U:C2'	1:0:282:C:O4'	2.60	0.41
1:0:553:G:O4'	1:0:1325:G:H5'	2.20	0.41
1:0:578:C:O2	1:0:1112:G:H4'	2.20	0.41
1:0:1020:A:H2'	1:0:1021:G:C8	2.55	0.41
1:0:1706:G:C6	1:0:1707:G:C6	3.08	0.41
1:0:1993:C:C4	1:0:1994:A:C6	3.08	0.41
1:0:2120:U:H2'	1:0:2121:G:O4'	2.21	0.41
1:0:2124:G:H2'	1:0:2125:G:H8	1.84	0.41
1:0:2820:A:H2'	1:0:2821:C:C6	2.54	0.41
1:0:23:G:C6	1:0:24:G:N1	2.89	0.41
1:0:95:A:H4'	1:0:96:A:O5'	2.20	0.41
1:0:877:G:C5'	1:0:878:G:OP1	2.65	0.41
1:0:1627:G:O2'	1:0:1628:G:H5'	2.20	0.41
1:0:1914:C:C2	1:0:1926:G:C2	3.08	0.41
1:0:2249:G:C2	1:0:2253:G:C6	3.09	0.41
1:0:2515:C:H2'	1:0:2516:G:C5'	2.50	0.41
1:0:2836:G:O2'	1:0:2837:U:P	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2893:C:O2'	1:0:2894:C:H5'	2.20	0.41
2:9:39:U:H3'	2:9:40:C:H5''	2.02	0.41
1:0:132:A:H2'	1:0:133:U:C6	2.55	0.41
1:0:569:A:H5''	1:0:587:A:N1	2.36	0.41
1:0:602:A:O2'	1:0:605:C:H4'	2.21	0.41
1:0:1029:U:H5'	1:0:1031:G:N7	2.36	0.41
1:0:1064:U:H2'	1:0:1065:G:H8	1.85	0.41
1:0:1269:G:H2'	1:0:1270:U:C6	2.56	0.41
1:0:1626:A:C2'	1:0:1627:G:H5'	2.50	0.41
1:0:2064:U:H2'	1:0:2065:C:C6	2.55	0.41
1:0:2640:U:H2'	1:0:2641:C:C6	2.56	0.41
1:0:2845:G:O2'	1:0:2846:C:H5'	2.20	0.41
2:9:76:G:C8	2:9:77:A:H2'	2.55	0.41
1:0:277:U:O2'	1:0:278:A:H5'	2.21	0.41
1:0:289:G:C2	1:0:363:A:H2	2.34	0.41
1:0:355:C:O2'	1:0:356:C:H5'	2.21	0.41
1:0:526:U:H2'	1:0:527:U:C6	2.56	0.41
1:0:1029:U:O2'	1:0:1273:C:OP1	2.30	0.41
1:0:1538:C:O2'	1:0:1539:U:H5'	2.21	0.41
1:0:1676:G:O2'	1:0:1677:U:H5'	2.20	0.41
1:0:2773:G:H22	1:0:2801:A:H2	1.69	0.41
1:0:255:A:O2'	1:0:256:C:H5'	2.20	0.41
1:0:512:G:O3'	1:0:513:A:H8	2.04	0.41
1:0:523:C:H2'	1:0:524:A:C8	2.56	0.41
1:0:836:G:O2'	1:0:1737:A:OP1	2.29	0.41
1:0:934:C:H2'	1:0:935:G:C8	2.56	0.41
1:0:1391:G:H2'	1:0:1392:A:H5'	2.01	0.41
1:0:1665:G:O2'	1:0:1666:C:H5'	2.20	0.41
1:0:2004:U:C2'	1:0:2005:G:OP1	2.69	0.41
1:0:2238:A:C2	1:0:2239:C:C6	3.09	0.41
1:0:2757:A:H2'	1:0:2758:G:O4'	2.21	0.41
1:0:24:G:N2	1:0:518:G:H1'	2.35	0.41
1:0:431:G:O2'	1:0:432:G:H5'	2.20	0.41
1:0:585:C:H2'	1:0:586:C:C6	2.56	0.41
1:0:627:G:H2'	1:0:2071:C:C4	2.56	0.41
1:0:1062:U:O2'	1:0:2307:A:N3	2.44	0.41
1:0:1209:C:H2'	1:0:1210:G:C8	2.45	0.41
1:0:1555:G:O2'	1:0:1556:G:H8	2.03	0.41
1:0:1659:A:H2'	1:0:1660:G:O4'	2.21	0.41
1:0:1964:U:O2'	1:0:1965:C:H5'	2.21	0.41
1:0:2135:A:O2'	1:0:2136:G:H5'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2336:G:O2'	1:0:2337:G:H5'	2.20	0.41
1:0:2823:G:O2'	1:0:2824:C:H5'	2.21	0.41
1:0:2824:C:O3'	1:0:2825:C:H6	2.04	0.41
1:0:2880:A:H2'	1:0:2881:C:O4'	2.21	0.41
2:9:1:U:O2'	2:9:3:A:OP1	2.38	0.41
1:0:394:G:H2'	1:0:398:U:C6	2.56	0.41
1:0:1474:C:H5'	1:0:1474:C:C6	2.49	0.41
1:0:2239:C:O2'	1:0:2240:U:H5'	2.21	0.41
1:0:2334:C:O2'	1:0:2335:C:H5'	2.21	0.41
1:0:282:C:C2'	1:0:283:U:C5'	2.99	0.40
1:0:634:G:O2'	1:0:1358:A:OP1	2.39	0.40
1:0:1236:A:H2'	1:0:1237:U:O4'	2.20	0.40
1:0:1782:G:O2'	1:0:1783:A:H5'	2.21	0.40
1:0:2362:A:H2'	1:0:2363:G:C8	2.55	0.40
1:0:2445:U:H2'	1:0:2446:G:H8	1.84	0.40
1:0:2823:G:C5'	1:0:2827:A:H5'	2.51	0.40
1:0:207:U:H2'	1:0:208:C:C6	2.56	0.40
1:0:272:A:N1	1:0:369:G:C5'	2.84	0.40
1:0:482:G:H4'	1:0:508:A:N1	2.36	0.40
1:0:598:C:H2'	1:0:599:G:C8	2.52	0.40
1:0:934:C:H2'	1:0:935:G:H8	1.87	0.40
1:0:1453:G:H2'	1:0:1454:U:O4'	2.20	0.40
1:0:1555:G:HO2'	1:0:1556:G:P	2.44	0.40
1:0:2597:U:C2'	1:0:2598:U:H5'	2.51	0.40
1:0:2825:C:C2	1:0:2826:G:C5	3.09	0.40
1:0:10:U:C2'	1:0:11:A:OP2	2.69	0.40
1:0:194:A:C2'	1:0:195:C:H5'	2.52	0.40
1:0:734:U:O2'	1:0:736:A:N7	2.50	0.40
1:0:735:C:C2'	1:0:736:A:H5'	2.50	0.40
1:0:2704:C:H2'	1:0:2705:U:O4'	2.21	0.40
1:0:148:A:O2'	1:0:149:G:H5'	2.22	0.40
1:0:189:A:H2'	1:0:190:G:O4'	2.22	0.40
1:0:270:U:O2'	1:0:271:C:OP2	2.33	0.40
1:0:284:C:H4'	1:0:285:A:C8	2.57	0.40
1:0:735:C:H2'	1:0:736:A:H5'	2.03	0.40
1:0:907:A:H4'	1:0:1328:A:C2	2.56	0.40
1:0:946:C:H2'	1:0:947:U:H6	1.85	0.40
1:0:1796:A:H2'	1:0:1797:A:C8	2.57	0.40
1:0:2265:U:H2'	1:0:2266:A:C8	2.56	0.40
1:0:140:G:C8	1:0:140:G:C3'	3.04	0.40
1:0:177:A:H2'	1:0:178:U:O4'	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:196:G:H1'	1:0:197:C:OP2	2.21	0.40
1:0:271:C:H4'	1:0:272:A:O5'	2.22	0.40
1:0:807:A:N1	1:0:808:A:N3	2.69	0.40
1:0:2252:A:H2'	1:0:2253:G:H5'	2.04	0.40
1:0:2252:A:H2'	1:0:2253:G:C5'	2.51	0.40
1:0:2750:G:O5'	1:0:2750:G:H8	2.05	0.40
1:0:2797:C:O2'	1:0:2798:G:H5'	2.22	0.40
2:9:64:C:O2'	2:9:65:A:H5'	2.22	0.40

There are no symmetry-related clashes.

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	0	2697/2922 (92%)	341 (12%)	107 (3%)
2	9	122/122 (100%)	17 (13%)	5 (4%)
All	All	2819/3044 (92%)	358 (12%)	112 (3%)

All (358) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	95	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	96	A
1	0	114	A
1	0	115	U
1	0	116	G
1	0	120	A
1	0	139	C
1	0	141	C
1	0	142	G
1	0	151	A
1	0	166	A
1	0	169	A
1	0	186	A
1	0	192	A
1	0	196	G
1	0	197	C
1	0	198	A
1	0	200	U
1	0	201	G
1	0	204	A
1	0	219	G
1	0	220	C
1	0	236	A
1	0	237	G
1	0	262	A
1	0	263	U
1	0	271	C
1	0	272	A
1	0	273	G
1	0	282	C
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	336	G
1	0	337	A
1	0	338	C
1	0	339	A
1	0	345	G
1	0	358	G
1	0	368	C
1	0	381	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	395	A
1	0	397	A
1	0	398	U
1	0	407	A
1	0	417	G
1	0	439	A
1	0	453	A
1	0	461	C
1	0	481	U
1	0	485	A
1	0	486	A
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	512	G
1	0	514	G
1	0	515	C
1	0	537	G
1	0	538	C
1	0	539	G
1	0	545	G
1	0	548	U
1	0	549	A
1	0	553	G
1	0	554	G
1	0	555	U
1	0	588	G
1	0	600	G
1	0	601	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	660	A
1	0	682	A
1	0	688	A
1	0	699	C
1	0	700	A
1	0	701	U
1	0	714	U
1	0	759	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	777	U
1	0	809	G
1	0	817	G
1	0	818	A
1	0	821	U
1	0	835	U
1	0	840	U
1	0	856	G
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	875	A
1	0	877	G
1	0	878	G
1	0	885	G
1	0	895	A
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	940	G
1	0	953	G
1	0	960	G
1	0	961	A
1	0	965	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1073	A
1	0	1081	A
1	0	1089	G
1	0	1106	A
1	0	1107	A
1	0	1108	G
1	0	1109	U
1	0	1110	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	1119	G
1	0	1124	A
1	0	1126	C
1	0	1127	C
1	0	1130	U
1	0	1137	G
1	0	1148	C
1	0	1149	U
1	0	1150	A
1	0	1160	G
1	0	1215	A
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1245	C
1	0	1279	U
1	0	1287	A
1	0	1289	C
1	0	1309	U
1	0	1310	U
1	0	1330	A
1	0	1331	A
1	0	1341	A
1	0	1342	C
1	0	1353	C
1	0	1355	A
1	0	1360	C
1	0	1369	A
1	0	1370	G
1	0	1377	C
1	0	1379	A
1	0	1380	U
1	0	1407	A
1	0	1409	G
1	0	1448	A
1	0	1449	G
1	0	1451	C
1	0	1474	C
1	0	1485	A
1	0	1488	U
1	0	1492	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	1506	U
1	0	1507	C
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1527	A
1	0	1528	A
1	0	1535	G
1	0	1556	G
1	0	1563	G
1	0	1564	C
1	0	1592	G
1	0	1593	C
1	0	1604	G
1	0	1605	G
1	0	1606	A
1	0	1624	A
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1682	A
1	0	1683	G
1	0	1684	A
1	0	1685	A
1	0	1690	C
1	0	1691	A
1	0	1692	C
1	0	1693	A
1	0	1699	C
1	0	1700	C
1	0	1701	A
1	0	1710	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1732	A
1	0	1752	G
1	0	1774	G
1	0	1778	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1835	U
1	0	1836	A
1	0	1853	C
1	0	1854	C
1	0	1857	A
1	0	1879	U
1	0	1907	U
1	0	1908	G
1	0	1919	A
1	0	1942	A
1	0	1951	G
1	0	1971	G
1	0	1973	A
1	0	1979	G
1	0	1980	U
1	0	1981	A
1	0	1982	C
1	0	1996	U
1	0	2005	G
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2063	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2075	G
1	0	2077	C
1	0	2083	A
1	0	2084	C
1	0	2091	G
1	0	2096	A
1	0	2101	A
1	0	2102	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2259	C
1	0	2271	G
1	0	2272	G
1	0	2283	G
1	0	2284	G
1	0	2291	A
1	0	2316	G
1	0	2317	C
1	0	2322	U
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2370	A
1	0	2371	G
1	0	2379	G
1	0	2396	C
1	0	2422	U
1	0	2427	C
1	0	2428	G
1	0	2462	G
1	0	2464	C
1	0	2466	G
1	0	2467	A
1	0	2469	A
1	0	2476	C
1	0	2482	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2527	U
1	0	2533	C
1	0	2537	G
1	0	2538	A
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2617	G
1	0	2634	G
1	0	2637	A
1	0	2638	G
1	0	2649	A
1	0	2681	A
1	0	2682	C
1	0	2714	U
1	0	2715	G
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2783	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2813	A
1	0	2814	A
1	0	2815	G
1	0	2826	G
1	0	2827	A
1	0	2837	U
1	0	2850	C
1	0	2867	G
1	0	2876	G
1	0	2890	A
1	0	2891	A
1	0	2903	C
1	0	2914	A
2	9	2	U
2	9	4	G
2	9	14	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	9	23	U
2	9	24	U
2	9	25	G
2	9	29	C
2	9	34	A
2	9	41	C
2	9	43	G
2	9	56	A
2	9	57	A
2	9	66	G
2	9	77	A
2	9	87	U
2	9	114	G
2	9	122	C

All (112) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U
1	0	95	A
1	0	115	U
1	0	191	A
1	0	196	G
1	0	199	A
1	0	270	U
1	0	282	C
1	0	283	U
1	0	284	C
1	0	338	C
1	0	367	G
1	0	394	G
1	0	438	C
1	0	452	G
1	0	480	C
1	0	485	A
1	0	496	G
1	0	514	G
1	0	548	U
1	0	554	G
1	0	600	G
1	0	603	A
1	0	681	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	699	C
1	0	713	U
1	0	817	G
1	0	855	U
1	0	857	A
1	0	877	G
1	0	894	A
1	0	904	U
1	0	939	A
1	0	952	G
1	0	1044	C
1	0	1059	G
1	0	1072	G
1	0	1080	C
1	0	1088	A
1	0	1106	A
1	0	1108	G
1	0	1126	C
1	0	1137	G
1	0	1149	U
1	0	1214	G
1	0	1237	U
1	0	1309	U
1	0	1329	A
1	0	1352	A
1	0	1369	A
1	0	1379	A
1	0	1406	A
1	0	1408	U
1	0	1448	A
1	0	1450	C
1	0	1506	U
1	0	1534	C
1	0	1591	A
1	0	1603	A
1	0	1605	G
1	0	1624	A
1	0	1683	G
1	0	1690	C
1	0	1699	C
1	0	1835	U
1	0	1853	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	1856	C
1	0	1907	U
1	0	1950	G
1	0	1978	A
1	0	1979	G
1	0	1981	A
1	0	2011	A
1	0	2074	A
1	0	2076	U
1	0	2083	A
1	0	2090	G
1	0	2242	U
1	0	2258	A
1	0	2282	U
1	0	2283	G
1	0	2290	U
1	0	2316	G
1	0	2321	A
1	0	2370	A
1	0	2395	A
1	0	2421	G
1	0	2427	C
1	0	2463	A
1	0	2465	A
1	0	2467	A
1	0	2468	A
1	0	2482	G
1	0	2526	C
1	0	2616	G
1	0	2692	G
1	0	2714	U
1	0	2718	C
1	0	2748	G
1	0	2749	U
1	0	2791	U
1	0	2813	A
1	0	2814	A
1	0	2836	G
1	0	2849	U
1	0	2866	U
1	0	2890	A
2	9	1	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	9	3	A
2	9	28	U
2	9	55	U
2	9	65	A

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 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	0	2706/2922 (92%)	1.36	593 (21%) 2 2	12, 29, 60, 87	0
2	9	122/122 (100%)	2.27	57 (46%) 0 0	22, 42, 67, 106	0
3	A	237/239 (99%)	7.71	237 (100%) 0 0	16, 35, 64, 78	0
4	B	337/337 (100%)	8.99	337 (100%) 0 0	18, 42, 65, 72	0
5	C	246/246 (100%)	7.23	242 (98%) 0 0	14, 31, 54, 76	0
6	D	140/176 (79%)	11.34	140 (100%) 0 0	49, 80, 90, 94	0
7	E	118/119 (99%)	8.39	117 (99%) 0 0	32, 51, 69, 72	0
8	F	157/157 (100%)	11.04	157 (100%) 0 0	33, 56, 81, 93	0
9	G	142/145 (97%)	7.95	142 (100%) 0 0	22, 38, 58, 68	0
10	H	132/132 (100%)	8.13	132 (100%) 0 0	20, 37, 55, 63	0
11	I	194/194 (100%)	9.04	194 (100%) 0 0	22, 36, 54, 66	0
12	J	143/164 (87%)	9.34	143 (100%) 0 0	21, 46, 73, 85	0
13	K	186/186 (100%)	11.32	186 (100%) 0 0	40, 65, 83, 87	0
14	L	115/115 (100%)	7.27	115 (100%) 0 0	28, 38, 55, 65	0
15	M	143/148 (96%)	7.40	142 (99%) 0 0	24, 38, 49, 58	0
16	N	95/95 (100%)	7.68	95 (100%) 0 0	20, 32, 53, 65	0
17	O	150/154 (97%)	6.95	150 (100%) 0 0	19, 31, 49, 58	0
18	P	78/84 (92%)	8.00	78 (100%) 0 0	27, 38, 63, 65	0
19	Q	119/119 (100%)	7.80	119 (100%) 0 0	28, 39, 56, 67	0
20	R	53/66 (80%)	8.02	53 (100%) 0 0	29, 43, 55, 58	0
21	S	65/70 (92%)	8.86	65 (100%) 0 0	35, 51, 77, 83	0
22	T	154/154 (100%)	7.75	154 (100%) 0 0	24, 35, 51, 56	0
23	U	85/91 (93%)	10.14	85 (100%) 0 0	29, 47, 73, 80	0
24	V	143/143 (100%)	8.04	141 (98%) 0 0	18, 33, 62, 76	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	73/73 (100%)	8.39	73 (100%) 0 0	36, 43, 57, 62	0
26	X	56/56 (100%)	8.33	56 (100%) 0 0	17, 27, 35, 41	0
27	Y	31/49 (63%)	7.48	31 (100%) 0 0	25, 33, 55, 61	0
28	Z	92/92 (100%)	8.41	92 (100%) 0 0	23, 40, 51, 63	0
29	1	172/177 (97%)	8.80	172 (100%) 0 0	31, 48, 64, 71	0
All	All	6484/6825 (95%)	5.45	4298 (66%) 0 0	12, 36, 70, 106	0

All (4298) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	80	GLU	56.9
10	H	61	THR	45.8
9	G	4	ALA	43.4
3	A	35	GLY	41.6
4	B	156	LYS	39.0
12	J	149	ARG	38.9
12	J	75	LEU	36.5
8	F	97	ASP	35.5
21	S	39	ALA	34.2
5	C	222	ASP	34.0
6	D	63	ILE	34.0
21	S	42	ASN	33.9
29	1	24	GLY	33.2
24	V	4	GLY	31.1
3	A	36	ASP	30.9
9	G	64	GLY	30.4
4	B	274	GLY	29.2
13	K	162	ASP	28.9
3	A	37	VAL	28.9
22	T	139	GLY	28.7
18	P	77	VAL	27.8
18	P	1	SER	26.7
11	I	187	ALA	26.5
4	B	134	GLY	26.0
19	Q	116	ASP	26.0
4	B	116	GLU	26.0
25	W	43	GLY	25.8
15	M	143	ALA	25.6
13	K	166	ALA	25.5
24	V	1	GLN	25.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	O	11	ASP	25.4
18	P	78	ALA	25.3
4	B	257	GLY	25.1
8	F	98	GLY	25.1
12	J	78	ALA	25.1
3	A	134	ASN	24.9
8	F	154	ALA	24.9
22	T	95	GLY	24.9
3	A	157	GLY	24.8
5	C	135	GLU	24.7
5	C	245	GLU	24.7
23	U	15	ARG	24.3
11	I	117	SER	24.1
19	Q	53	GLY	24.1
6	D	60	GLU	24.0
29	1	16	ASP	24.0
4	B	319	ASP	23.9
12	J	14	GLY	23.9
8	F	34	GLY	23.8
5	C	47	GLY	23.7
23	U	78	GLU	23.6
4	B	64	GLY	23.6
8	F	63	ALA	23.5
13	K	70	GLY	23.4
4	B	1	PRO	23.4
11	I	137	ASP	23.2
15	M	76	GLY	23.2
8	F	76	GLY	23.2
29	1	128	GLY	23.1
22	T	85	ALA	22.9
13	K	121	GLY	22.8
22	T	80	ASP	22.6
28	Z	45	GLY	22.6
19	Q	57	GLY	22.5
6	D	93	LEU	22.4
10	H	25	GLY	22.3
26	X	39	PHE	22.2
12	J	143	THR	22.2
4	B	185	GLY	22.2
23	U	5	PHE	22.1
28	Z	28	GLY	21.8
4	B	40	GLY	21.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	I	116	ASN	21.7
3	A	158	VAL	21.7
8	F	153	PRO	21.6
4	B	57	GLU	21.6
11	I	193	ARG	21.6
8	F	59	ASN	21.5
4	B	34	GLY	21.5
29	1	109	GLY	21.4
13	K	159	TYR	21.2
4	B	303	PRO	21.1
21	S	41	GLU	21.1
26	X	40	GLY	21.0
4	B	301	PRO	20.9
13	K	98	GLU	20.9
24	V	116	LYS	20.8
10	H	106	GLY	20.8
3	A	63	GLY	20.7
12	J	146	GLY	20.7
8	F	127	ASN	20.6
9	G	6	PHE	20.6
21	S	1	THR	20.6
4	B	169	SER	20.5
13	K	65	ASP	20.5
5	C	246	ARG	20.4
23	U	18	ARG	20.4
13	K	63	SER	20.4
8	F	117	GLY	20.3
5	C	132	ASP	20.3
5	C	209	GLY	20.3
8	F	155	GLY	20.2
6	D	138	GLY	20.1
3	A	237	GLY	20.1
8	F	35	ASN	20.0
4	B	290	ASP	19.9
23	U	81	GLY	19.8
6	D	85	GLN	19.8
11	I	70	GLY	19.7
6	D	49	PRO	19.6
7	E	84	GLY	19.6
29	1	63	GLY	19.6
11	I	185	LEU	19.6
4	B	300	VAL	19.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	K	165	ALA	19.4
13	K	76	GLY	19.4
6	D	81	GLU	19.4
9	G	68	GLY	19.4
22	T	91	ASP	19.3
3	A	34	ASP	19.3
13	K	185	GLU	19.2
8	F	79	ALA	19.2
8	F	157	ALA	19.1
5	C	243	VAL	19.1
29	1	121	ASP	19.1
29	1	165	GLY	19.0
6	D	86	THR	18.9
5	C	198	ASP	18.8
24	V	138	GLU	18.8
28	Z	14	CYS	18.8
8	F	106	GLY	18.5
4	B	32	ASP	18.4
5	C	10	GLY	18.4
6	D	70	GLY	18.4
11	I	18	GLY	18.3
8	F	78	ALA	18.3
10	H	128	ALA	18.2
23	U	16	ASP	18.2
21	S	44	GLY	18.2
14	L	69	VAL	18.1
26	X	1	THR	18.1
10	H	62	PRO	18.1
11	I	16	TYR	18.1
7	E	49	PHE	18.0
4	B	138	ASP	18.0
4	B	63	GLU	18.0
4	B	298	GLY	17.9
5	C	64	GLY	17.9
12	J	128	GLY	17.9
4	B	148	ASP	17.8
13	K	100	ALA	17.8
11	I	118	TYR	17.8
11	I	73	ARG	17.8
13	K	64	SER	17.7
13	K	161	GLY	17.7
12	J	145	LEU	17.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	G	113	GLY	17.5
24	V	3	ARG	17.4
7	E	101	ALA	17.4
10	H	23	ASN	17.4
21	S	18	ALA	17.4
5	C	139	VAL	17.4
3	A	77	GLY	17.3
25	W	80	MET	17.3
4	B	299	SER	17.3
19	Q	83	ASP	17.2
4	B	159	ASP	17.2
26	X	9	GLY	17.2
27	Y	24	TYR	17.1
11	I	35	PRO	17.1
29	1	100	ASP	17.0
3	A	236	GLY	17.0
4	B	62	ARG	17.0
4	B	272	GLY	17.0
25	W	19	GLY	17.0
4	B	149	ALA	16.9
21	S	38	GLY	16.9
5	C	32	GLY	16.8
17	O	53	GLY	16.8
17	O	149	GLU	16.8
4	B	167	GLY	16.7
7	E	119	ARG	16.7
11	I	157	VAL	16.7
13	K	134	ASP	16.6
8	F	125	TRP	16.6
13	K	6	TYR	16.5
19	Q	84	GLY	16.5
10	H	101	ASN	16.5
4	B	337	GLY	16.4
3	A	210	GLY	16.3
6	D	102	GLY	16.3
6	D	92	GLU	16.3
10	H	116	GLU	16.3
8	F	81	TYR	16.3
11	I	160	GLY	16.2
24	V	64	GLY	16.2
11	I	80	GLY	16.2
12	J	138	GLY	16.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	F	119	ASN	16.1
13	K	153	GLN	16.1
22	T	145	GLY	16.1
12	J	103	ALA	16.1
3	A	116	GLY	16.0
23	U	17	ALA	16.0
23	U	21	PRO	16.0
24	V	62	GLY	16.0
4	B	302	GLY	16.0
13	K	96	GLY	16.0
4	B	135	ASP	15.9
8	F	99	ASP	15.9
6	D	28	GLY	15.9
24	V	115	ARG	15.9
28	Z	74	CYS	15.9
13	K	71	TRP	15.8
23	U	75	ALA	15.8
6	D	101	THR	15.8
10	H	39	GLY	15.8
6	D	44	ILE	15.8
6	D	10	PHE	15.8
6	D	71	ALA	15.8
28	Z	29	ARG	15.7
7	E	71	GLY	15.7
24	V	59	GLY	15.7
13	K	50	LEU	15.7
14	L	108	GLY	15.7
11	I	38	VAL	15.7
4	B	304	ASP	15.7
28	Z	15	ASN	15.7
7	E	88	GLY	15.7
24	V	27	GLY	15.7
10	H	119	GLN	15.7
24	V	139	VAL	15.7
13	K	1	ALA	15.6
4	B	67	THR	15.6
5	C	230	GLY	15.6
20	R	26	GLY	15.6
13	K	154	LEU	15.6
6	D	69	ILE	15.6
6	D	132	VAL	15.6
7	E	100	ASP	15.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	I	165	GLY	15.5
13	K	68	GLU	15.5
4	B	56	ASP	15.4
16	N	79	GLY	15.4
4	B	106	SER	15.4
27	Y	49	GLU	15.4
9	G	117	ASP	15.4
5	C	1	MET	15.3
29	1	118	ILE	15.3
6	D	51	ARG	15.3
13	K	145	ALA	15.3
4	B	200	ASP	15.3
6	D	52	THR	15.3
29	1	89	SER	15.2
3	A	90	PRO	15.2
23	U	27	ASP	15.1
4	B	126	GLN	15.1
13	K	85	GLY	15.1
10	H	24	THR	15.1
14	L	70	LEU	15.1
5	C	237	GLU	15.1
6	D	134	LEU	15.1
13	K	126	GLY	15.1
13	K	88	ALA	15.1
29	1	68	HIS	15.0
9	G	33	GLY	15.0
12	J	92	ASP	15.0
24	V	11	ASP	15.0
4	B	256	THR	15.0
29	1	42	VAL	15.0
4	B	188	ALA	15.0
12	J	34	GLY	15.0
8	F	130	PRO	14.9
13	K	105	GLY	14.9
24	V	55	LYS	14.9
11	I	192	LYS	14.9
26	X	2	GLY	14.9
23	U	4	ASP	14.8
25	W	14	PHE	14.8
11	I	79	LYS	14.8
16	N	68	GLY	14.8
29	1	83	GLY	14.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	I	178	ALA	14.8
4	B	254	GLY	14.8
13	K	182	GLY	14.8
26	X	22	CYS	14.8
18	P	2	TRP	14.8
10	H	109	LEU	14.8
13	K	149	GLU	14.8
6	D	22	VAL	14.8
6	D	80	ALA	14.7
13	K	175	LEU	14.7
19	Q	1	SER	14.7
6	D	35	ALA	14.7
12	J	61	ALA	14.7
3	A	83	GLY	14.7
9	G	140	GLY	14.7
16	N	78	GLY	14.7
24	V	128	GLY	14.7
12	J	100	ALA	14.7
7	E	25	ASP	14.7
11	I	138	HIS	14.7
24	V	14	ASP	14.7
4	B	210	THR	14.7
24	V	101	GLY	14.6
8	F	152	SER	14.6
16	N	50	GLY	14.6
13	K	170	GLU	14.6
3	A	91	GLY	14.6
8	F	83	PHE	14.6
8	F	132	VAL	14.6
29	1	55	ASN	14.6
5	C	66	GLY	14.5
14	L	72	LYS	14.5
23	U	13	PRO	14.5
13	K	59	ALA	14.5
17	O	41	GLY	14.5
8	F	75	SER	14.5
6	D	72	LYS	14.5
9	G	8	ALA	14.5
3	A	114	ASP	14.5
3	A	234	GLY	14.4
4	B	196	GLY	14.4
6	D	94	ALA	14.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	Z	1	MET	14.3
13	K	73	ALA	14.3
19	Q	117	ASP	14.3
6	D	95	THR	14.3
29	1	86	VAL	14.3
23	U	26	ALA	14.3
8	F	150	ASP	14.3
11	I	124	GLY	14.3
29	1	172	PRO	14.2
15	M	118	GLN	14.2
7	E	29	VAL	14.2
8	F	118	ALA	14.2
8	F	135	ALA	14.2
9	G	40	ASN	14.2
3	A	44	ASP	14.2
8	F	93	ILE	14.2
28	Z	86	GLY	14.1
13	K	139	TRP	14.1
4	B	209	GLY	14.1
16	N	61	GLY	14.1
8	F	156	ASN	14.1
13	K	138	ASP	14.1
19	Q	36	GLY	14.1
4	B	103	GLU	14.0
12	J	15	GLY	14.0
20	R	10	GLY	14.0
12	J	60	GLU	14.0
4	B	59	ASN	13.9
4	B	207	GLY	13.9
16	N	65	GLY	13.9
25	W	45	PRO	13.9
7	E	27	GLY	13.9
12	J	137	GLY	13.9
19	Q	45	GLY	13.9
4	B	168	GLY	13.9
12	J	99	GLU	13.9
6	D	107	GLY	13.9
6	D	73	VAL	13.9
3	A	123	GLY	13.8
18	P	60	GLY	13.8
11	I	14	ARG	13.8
23	U	20	GLU	13.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	F	137	ARG	13.8
13	K	37	ARG	13.8
12	J	83	GLU	13.8
26	X	55	GLY	13.8
21	S	45	ARG	13.8
26	X	50	TRP	13.8
8	F	133	GLU	13.7
17	O	97	GLY	13.7
13	K	9	PRO	13.7
5	C	63	SER	13.7
7	E	32	GLY	13.7
5	C	9	ASP	13.7
12	J	57	VAL	13.7
8	F	85	ILE	13.7
24	V	8	LYS	13.7
13	K	99	GLU	13.6
10	H	127	ALA	13.6
12	J	112	GLY	13.6
3	A	135	VAL	13.6
6	D	50	VAL	13.6
12	J	139	SER	13.6
20	R	55	ALA	13.6
4	B	37	GLY	13.6
29	1	41	SER	13.6
4	B	43	GLY	13.6
4	B	33	ASP	13.6
14	L	68	GLY	13.5
4	B	150	VAL	13.5
16	N	22	GLY	13.5
20	R	43	GLY	13.5
26	X	38	GLY	13.5
19	Q	113	GLU	13.4
29	1	10	ASP	13.4
11	I	186	ARG	13.4
3	A	202	GLY	13.4
6	D	99	ASP	13.4
7	E	107	VAL	13.4
4	B	166	GLY	13.4
13	K	144	GLY	13.4
24	V	2	ALA	13.4
13	K	62	HIS	13.4
8	F	146	THR	13.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	J	81	VAL	13.4
13	K	164	ASP	13.4
11	I	119	TRP	13.4
9	G	94	GLY	13.4
13	K	112	GLY	13.4
13	K	152	GLU	13.4
7	E	75	ILE	13.3
8	F	33	MET	13.3
10	H	84	ASP	13.3
22	T	75	GLY	13.3
11	I	15	PRO	13.3
19	Q	82	THR	13.3
9	G	116	LEU	13.3
17	O	125	ARG	13.3
6	D	148	SER	13.2
29	1	43	ASP	13.2
19	Q	106	GLU	13.2
22	T	124	GLY	13.2
18	P	44	GLN	13.2
23	U	14	LEU	13.2
12	J	110	GLY	13.2
22	T	89	ASP	13.2
11	I	177	GLY	13.2
13	K	173	ASP	13.2
13	K	54	GLY	13.2
26	X	37	CYS	13.2
11	I	175	GLY	13.1
8	F	134	PHE	13.1
23	U	83	ALA	13.1
24	V	35	ASP	13.1
5	C	75	GLY	13.1
17	O	106	GLY	13.1
22	T	135	GLY	13.1
29	1	99	GLY	13.1
4	B	151	PRO	13.1
4	B	117	ASP	13.1
22	T	78	ASP	13.1
11	I	155	GLY	13.1
29	1	3	VAL	13.0
4	B	55	ASN	13.0
9	G	118	GLY	13.0
29	1	164	ASP	13.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	Z	72	GLY	13.0
25	W	79	VAL	13.0
11	I	30	LYS	13.0
8	F	28	ILE	12.9
14	L	78	ALA	12.9
8	F	71	PHE	12.9
12	J	80	ASP	12.9
13	K	89	GLY	12.9
19	Q	56	ALA	12.9
6	D	42	GLY	12.9
8	F	47	GLU	12.9
11	I	74	ALA	12.9
13	K	81	ALA	12.9
13	K	95	ALA	12.9
25	W	15	GLY	12.9
4	B	58	PRO	12.9
13	K	74	PRO	12.9
16	N	95	GLU	12.9
5	C	14	GLY	12.9
11	I	2	LYS	12.8
6	D	165	PHE	12.8
29	1	75	GLY	12.8
4	B	242	ASN	12.8
3	A	64	ASP	12.8
29	1	125	GLU	12.8
21	S	40	PRO	12.8
6	D	65	GLU	12.8
6	D	26	GLY	12.8
8	F	110	GLY	12.8
13	K	184	ILE	12.8
13	K	4	PRO	12.8
13	K	133	ASP	12.8
15	M	115	SER	12.7
11	I	150	VAL	12.7
13	K	186	LEU	12.7
29	1	105	GLU	12.7
8	F	36	ASN	12.7
27	Y	19	SER	12.6
13	K	5	ARG	12.6
6	D	91	ALA	12.6
13	K	67	ALA	12.6
16	N	66	LYS	12.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	6	GLY	12.6
25	W	76	GLY	12.6
23	U	73	ARG	12.6
6	D	83	PHE	12.6
10	H	108	GLU	12.6
19	Q	59	GLU	12.6
6	D	174	VAL	12.6
15	M	140	TYR	12.6
28	Z	50	GLY	12.6
11	I	10	GLU	12.6
23	U	86	GLU	12.6
11	I	123	ASP	12.5
18	P	72	ASP	12.5
13	K	39	SER	12.5
6	D	29	HIS	12.5
11	I	181	VAL	12.5
12	J	140	VAL	12.5
18	P	74	ALA	12.5
23	U	19	ALA	12.5
22	T	108	ARG	12.5
25	W	67	GLY	12.5
9	G	7	ASP	12.5
4	B	133	ALA	12.5
10	H	36	GLY	12.5
12	J	25	GLY	12.5
6	D	53	LYS	12.4
21	S	65	ASP	12.4
23	U	25	ARG	12.4
13	K	78	MET	12.4
12	J	142	LEU	12.4
6	D	68	PRO	12.4
3	A	1	GLY	12.4
4	B	12	GLY	12.4
29	1	11	VAL	12.4
12	J	82	ALA	12.4
22	T	77	ALA	12.4
3	A	65	ARG	12.4
5	C	161	ASP	12.4
4	B	153	VAL	12.4
8	F	74	ASN	12.4
19	Q	17	HIS	12.3
25	W	44	PHE	12.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	1	171	LYS	12.3
15	M	111	GLU	12.3
13	K	91	ARG	12.3
13	K	106	LEU	12.3
13	K	3	GLY	12.3
12	J	38	HIS	12.3
13	K	135	VAL	12.3
15	M	26	GLU	12.3
8	F	80	ASN	12.3
4	B	145	THR	12.3
4	B	173	ARG	12.3
7	E	10	ALA	12.2
17	O	74	GLY	12.2
6	D	153	THR	12.2
10	H	66	ARG	12.2
8	F	54	VAL	12.2
8	F	96	GLN	12.2
8	F	39	GLY	12.2
14	L	23	GLY	12.2
17	O	103	GLY	12.2
6	D	38	GLU	12.2
6	D	152	PRO	12.2
9	G	98	PHE	12.2
10	H	15	GLY	12.2
29	1	158	ASP	12.2
3	A	204	GLY	12.1
6	D	27	ILE	12.1
4	B	329	TYR	12.1
8	F	140	TYR	12.1
6	D	171	ASP	12.1
12	J	17	SER	12.1
29	1	15	GLN	12.1
3	A	40	GLY	12.1
5	C	179	GLY	12.1
6	D	66	GLY	12.1
13	K	176	ARG	12.1
13	K	58	LEU	12.0
15	M	112	GLY	12.0
9	G	129	PHE	12.0
23	U	82	GLU	12.0
8	F	40	PRO	12.0
16	N	18	PRO	12.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	U	47	ALA	12.0
3	A	162	GLY	12.0
12	J	16	GLY	12.0
6	D	161	ASP	12.0
29	1	119	HIS	12.0
15	M	47	GLY	12.0
16	N	5	GLY	12.0
13	K	53	ASN	12.0
4	B	28	SER	11.9
7	E	114	LYS	11.9
12	J	151	ALA	11.9
3	A	62	ASP	11.9
11	I	83	SER	11.9
6	D	78	GLU	11.9
11	I	71	GLY	11.9
17	O	78	GLY	11.9
6	D	16	PRO	11.9
10	H	121	PHE	11.9
7	E	24	ARG	11.9
15	M	15	ASP	11.9
3	A	14	SER	11.9
17	O	37	GLY	11.9
23	U	52	PRO	11.9
6	D	170	TYR	11.8
13	K	118	ILE	11.8
7	E	46	GLU	11.8
21	S	15	GLU	11.8
6	D	41	LEU	11.8
6	D	64	ARG	11.8
13	K	20	TYR	11.8
13	K	155	GLU	11.8
5	C	124	VAL	11.8
28	Z	58	GLY	11.8
15	M	110	ASP	11.7
17	O	1	GLY	11.7
8	F	103	ALA	11.7
22	T	39	ASP	11.7
8	F	100	GLY	11.7
14	L	85	ALA	11.7
18	P	75	GLN	11.7
14	L	104	ASN	11.7
28	Z	83	TRP	11.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	K	128	ASP	11.7
16	N	20	ASP	11.7
13	K	97	VAL	11.7
16	N	9	GLY	11.7
24	V	100	ASP	11.7
29	1	44	GLY	11.7
7	E	109	GLU	11.7
8	F	44	ALA	11.7
5	C	143	ASP	11.6
11	I	36	ALA	11.6
11	I	180	LYS	11.6
13	K	41	LYS	11.6
27	Y	47	THR	11.6
29	1	17	HIS	11.6
17	O	136	TRP	11.6
14	L	62	GLY	11.6
28	Z	82	GLY	11.6
28	Z	57	GLY	11.6
17	O	30	ALA	11.6
13	K	177	GLU	11.5
23	U	76	ARG	11.5
5	C	183	GLY	11.5
10	H	122	GLY	11.5
24	V	113	GLY	11.5
6	D	77	ASP	11.5
24	V	25	ARG	11.5
4	B	95	PRO	11.5
8	F	22	GLY	11.5
8	F	37	GLY	11.5
12	J	121	ILE	11.5
29	1	154	ILE	11.5
13	K	146	HIS	11.5
20	R	25	ASP	11.5
13	K	46	GLN	11.5
29	1	112	ALA	11.5
11	I	3	SER	11.5
18	P	3	ASP	11.5
3	A	113	GLY	11.5
10	H	110	LYS	11.5
8	F	113	ALA	11.5
12	J	24	ALA	11.5
4	B	60	SER	11.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	B	244	SER	11.4
22	T	86	GLU	11.4
29	1	25	ASP	11.4
11	I	145	PRO	11.4
12	J	144	ASP	11.4
29	1	45	ASP	11.4
8	F	32	LYS	11.4
4	B	230	GLY	11.4
13	K	51	GLY	11.4
4	B	170	VAL	11.4
6	D	25	MET	11.4
13	K	84	THR	11.4
21	S	6	GLN	11.4
23	U	28	LYS	11.4
15	M	17	GLY	11.4
4	B	181	VAL	11.4
6	D	150	SER	11.4
4	B	305	LYS	11.4
11	I	167	LYS	11.4
11	I	53	GLY	11.4
15	M	60	GLY	11.4
8	F	120	HIS	11.4
19	Q	10	SER	11.3
28	Z	8	ASN	11.3
12	J	104	ASP	11.3
16	N	19	ARG	11.3
8	F	147	VAL	11.3
11	I	69	ARG	11.3
10	H	60	GLY	11.3
29	1	97	VAL	11.3
13	K	77	ASN	11.3
11	I	121	GLY	11.3
4	B	186	GLU	11.3
8	F	95	GLU	11.3
10	H	125	ALA	11.3
13	K	36	ALA	11.3
24	V	52	GLN	11.3
4	B	19	SER	11.3
26	X	5	THR	11.3
13	K	107	ASN	11.3
4	B	275	ASP	11.3
13	K	172	PHE	11.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	M	116	SER	11.2
12	J	93	VAL	11.2
15	M	27	ARG	11.2
13	K	131	HIS	11.2
18	P	30	ASP	11.2
15	M	127	GLY	11.2
15	M	97	ARG	11.2
11	I	166	ARG	11.2
15	M	64	GLU	11.2
5	C	17	ASP	11.2
13	K	47	LEU	11.1
21	S	49	LEU	11.1
24	V	141	VAL	11.1
29	1	95	VAL	11.1
24	V	135	THR	11.1
13	K	124	ASP	11.1
15	M	128	GLY	11.1
22	T	55	GLY	11.1
22	T	148	ASP	11.1
17	O	16	ALA	11.1
20	R	11	THR	11.1
18	P	69	SER	11.1
11	I	72	ARG	11.1
8	F	131	ALA	11.1
16	N	70	ALA	11.1
4	B	132	GLU	11.1
14	L	110	HIS	11.1
8	F	144	THR	11.1
4	B	14	GLY	11.1
7	E	5	ASP	11.1
22	T	25	ASN	11.1
14	L	20	SER	11.1
28	Z	66	ASP	11.1
4	B	73	ILE	11.1
18	P	68	LEU	11.1
9	G	88	PRO	11.1
25	W	18	TYR	11.1
24	V	140	GLU	11.1
6	D	147	ALA	11.0
8	F	42	TYR	11.0
29	1	56	ALA	11.0
20	R	9	CYS	11.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	87	GLU	11.0
9	G	85	GLY	11.0
10	H	40	THR	11.0
25	W	66	GLY	11.0
28	Z	27	SER	11.0
8	F	67	ALA	11.0
24	V	137	VAL	11.0
12	J	98	GLU	11.0
9	G	77	GLY	11.0
12	J	28	GLY	11.0
8	F	149	ILE	11.0
4	B	187	HIS	11.0
20	R	36	CYS	11.0
10	H	50	GLY	11.0
19	Q	118	SER	11.0
8	F	139	ALA	11.0
8	F	25	GLY	11.0
17	O	127	PRO	10.9
26	X	36	SER	10.9
6	D	48	MET	10.9
15	M	120	ARG	10.9
7	E	103	ALA	10.9
24	V	114	ALA	10.9
12	J	58	GLN	10.9
15	M	141	ILE	10.9
8	F	104	PRO	10.9
12	J	97	VAL	10.9
24	V	90	VAL	10.9
25	W	69	TYR	10.9
4	B	93	GLN	10.9
25	W	30	GLU	10.9
4	B	152	SER	10.9
24	V	13	SER	10.9
8	F	105	PHE	10.9
3	A	13	THR	10.9
4	B	53	LEU	10.9
29	1	168	ILE	10.9
6	D	155	HIS	10.9
14	L	83	GLY	10.9
4	B	136	LEU	10.8
9	G	79	PHE	10.8
6	D	82	GLU	10.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	S	34	GLN	10.8
6	D	76	ARG	10.8
6	D	47	GLN	10.8
3	A	67	LEU	10.8
11	I	135	ASP	10.8
10	H	94	ALA	10.8
14	L	95	ALA	10.8
7	E	102	GLY	10.8
6	D	89	PRO	10.8
4	B	176	HIS	10.8
23	U	36	HIS	10.8
8	F	136	TRP	10.8
3	A	181	ALA	10.8
10	H	126	SER	10.8
13	K	60	SER	10.8
11	I	152	ARG	10.8
11	I	156	ARG	10.8
4	B	269	ILE	10.7
5	C	215	ALA	10.7
6	D	130	VAL	10.7
11	I	184	SER	10.7
13	K	113	SER	10.7
25	W	60	CYS	10.7
4	B	108	LEU	10.7
4	B	287	GLY	10.7
24	V	10	PRO	10.7
11	I	162	THR	10.7
29	1	155	ASN	10.7
3	A	56	ALA	10.7
13	K	122	ALA	10.7
20	R	5	GLU	10.7
19	Q	101	LEU	10.7
5	C	172	THR	10.7
13	K	142	THR	10.7
13	K	40	ASN	10.7
13	K	8	VAL	10.7
13	K	171	HIS	10.6
6	D	57	THR	10.6
28	Z	33	MET	10.6
24	V	143	GLU	10.6
15	M	62	ALA	10.6
6	D	159	PRO	10.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
22	T	32	CYS	10.6
4	B	82	ALA	10.6
13	K	61	ALA	10.6
6	D	13	MET	10.6
5	C	225	PRO	10.6
6	D	144	ARG	10.6
20	R	18	GLY	10.6
29	1	142	GLY	10.6
9	G	138	THR	10.6
25	W	39	CYS	10.6
13	K	109	PRO	10.6
17	O	120	GLY	10.5
17	O	12	THR	10.5
6	D	158	ASN	10.5
8	F	43	PRO	10.5
22	T	127	GLY	10.5
9	G	131	THR	10.5
10	H	21	ALA	10.5
11	I	114	VAL	10.5
22	T	43	GLY	10.5
24	V	109	ASN	10.5
24	V	5	LEU	10.5
25	W	42	CYS	10.5
9	G	120	SER	10.5
13	K	22	GLN	10.5
16	N	93	ARG	10.5
8	F	8	ASN	10.5
21	S	43	PRO	10.5
5	C	102	LEU	10.5
13	K	16	ALA	10.4
28	Z	22	VAL	10.4
5	C	65	ARG	10.4
5	C	134	ASP	10.4
8	F	116	HIS	10.4
8	F	50	VAL	10.4
16	N	63	VAL	10.4
18	P	4	VAL	10.4
14	L	22	GLY	10.4
6	D	97	GLN	10.4
29	1	122	THR	10.4
26	X	31	LYS	10.4
29	1	27	GLY	10.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	C	2	GLU	10.4
11	I	179	GLU	10.4
28	Z	87	ARG	10.4
17	O	80	TYR	10.4
13	K	178	THR	10.4
22	T	153	MET	10.4
13	K	168	LEU	10.4
29	1	108	LEU	10.4
9	G	20	GLY	10.4
14	L	46	GLY	10.4
18	P	5	ILE	10.4
11	I	27	ARG	10.4
22	T	90	TYR	10.4
22	T	66	LEU	10.4
23	U	22	ASN	10.3
6	D	19	GLU	10.3
19	Q	29	ALA	10.3
6	D	14	ARG	10.3
17	O	56	PRO	10.3
25	W	71	PRO	10.3
3	A	235	ARG	10.3
29	1	5	LEU	10.3
8	F	66	ASN	10.3
11	I	140	ALA	10.3
13	K	169	PRO	10.3
15	M	132	ASP	10.3
8	F	77	ALA	10.3
11	I	37	VAL	10.3
26	X	6	PRO	10.3
13	K	127	LEU	10.3
4	B	318	ASN	10.2
6	D	23	VAL	10.2
29	1	150	GLN	10.2
5	C	62	GLY	10.2
23	U	24	LYS	10.2
10	H	63	GLU	10.2
13	K	87	LEU	10.2
6	D	103	ASN	10.2
15	M	24	ASN	10.2
16	N	36	GLY	10.2
17	O	131	GLY	10.2
15	M	13	VAL	10.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
22	T	26	ILE	10.2
25	W	41	VAL	10.2
4	B	154	PRO	10.2
13	K	111	PRO	10.2
28	Z	26	ARG	10.2
6	D	43	GLU	10.2
3	A	85	ASP	10.2
16	N	34	ASP	10.2
16	N	35	ASP	10.2
25	W	55	TRP	10.2
4	B	155	LYS	10.2
3	A	12	GLY	10.2
7	E	92	GLY	10.2
28	Z	71	CYS	10.2
14	L	106	PRO	10.2
6	D	15	GLU	10.2
11	I	17	GLU	10.2
13	K	21	HIS	10.1
19	Q	25	ALA	10.1
13	K	147	ILE	10.1
29	1	8	PRO	10.1
16	N	23	THR	10.1
11	I	25	TRP	10.1
3	A	191	GLY	10.1
4	B	177	ALA	10.1
6	D	164	ALA	10.1
8	F	27	GLY	10.1
3	A	230	SER	10.1
6	D	67	ASP	10.1
13	K	140	GLN	10.1
6	D	136	ARG	10.1
11	I	149	TRP	10.1
8	F	10	ILE	10.1
13	K	101	VAL	10.1
28	Z	56	PRO	10.1
29	1	101	GLU	10.1
9	G	13	ASP	10.1
24	V	102	ASP	10.1
10	H	48	GLY	10.1
23	U	8	ARG	10.1
4	B	217	TRP	10.1
29	1	167	TYR	10.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	2637	A	10.0
6	D	100	ASP	10.0
22	T	147	ASP	10.0
8	F	115	SER	10.0
3	A	205	GLY	10.0
6	D	46	GLY	10.0
13	K	45	ALA	10.0
15	M	77	ALA	10.0
18	P	40	ALA	10.0
11	I	4	MET	10.0
5	C	163	HIS	10.0
11	I	169	ARG	10.0
6	D	168	SER	10.0
23	U	53	SER	10.0
8	F	122	PHE	10.0
16	N	12	GLY	10.0
19	Q	55	PHE	10.0
3	A	38	ILE	10.0
8	F	29	ALA	10.0
12	J	141	GLU	10.0
13	K	130	PRO	10.0
6	D	74	THR	10.0
6	D	169	THR	10.0
17	O	13	THR	10.0
29	1	21	THR	10.0
12	J	23	GLY	10.0
14	L	21	SER	10.0
22	T	9	GLY	10.0
9	G	70	PHE	10.0
29	1	9	GLU	10.0
13	K	129	ILE	10.0
14	L	54	GLU	9.9
28	Z	9	THR	9.9
24	V	51	GLY	9.9
4	B	142	ILE	9.9
8	F	53	PRO	9.9
13	K	55	ASP	9.9
29	1	156	ASP	9.9
3	A	183	GLY	9.9
6	D	139	TYR	9.9
12	J	77	ALA	9.9
16	N	4	ASN	9.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	G	143	LYS	9.9
13	K	66	LEU	9.9
7	E	78	GLU	9.9
9	G	5	GLU	9.9
11	I	126	TYR	9.9
13	K	150	TYR	9.9
22	T	94	SER	9.9
22	T	121	PRO	9.9
25	W	51	SER	9.9
11	I	67	ILE	9.9
13	K	116	PHE	9.9
13	K	158	LEU	9.9
15	M	30	ASP	9.8
3	A	212	PRO	9.8
15	M	129	GLY	9.8
25	W	12	GLY	9.8
23	U	12	ILE	9.8
5	C	241	ALA	9.8
29	1	51	SER	9.8
11	I	23	LEU	9.8
6	D	12	GLU	9.8
8	F	128	PRO	9.8
10	H	65	ARG	9.8
10	H	38	SER	9.8
12	J	126	SER	9.8
22	T	97	ALA	9.8
13	K	136	LEU	9.8
6	D	36	ASN	9.8
25	W	23	ARG	9.8
27	Y	20	ARG	9.8
5	C	13	ASP	9.8
29	1	127	ASP	9.8
4	B	236	GLY	9.8
8	F	41	THR	9.8
7	E	94	ALA	9.8
4	B	334	SER	9.8
22	T	96	LEU	9.8
3	A	102	GLY	9.8
10	H	103	ASP	9.8
11	I	189	PHE	9.8
21	S	36	ALA	9.8
7	E	44	SER	9.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	E	93	SER	9.8
8	F	9	SER	9.8
15	M	137	LEU	9.8
9	G	107	ASN	9.8
24	V	117	ARG	9.7
28	Z	80	ARG	9.7
6	D	137	PRO	9.7
20	R	15	PRO	9.7
11	I	59	GLY	9.7
26	X	4	GLY	9.7
11	I	153	THR	9.7
6	D	90	LEU	9.7
16	N	91	LEU	9.7
15	M	117	SER	9.7
29	1	170	ARG	9.7
3	A	163	GLY	9.7
6	D	106	PHE	9.7
13	K	163	PHE	9.7
28	Z	67	LEU	9.7
7	E	39	SER	9.7
9	G	136	SER	9.7
13	K	80	SER	9.7
16	N	76	VAL	9.7
17	O	96	VAL	9.7
4	B	281	GLY	9.7
12	J	50	GLY	9.7
21	S	61	GLY	9.7
23	U	62	GLY	9.7
3	A	170	VAL	9.7
5	C	57	PRO	9.7
7	E	9	PRO	9.7
3	A	101	GLU	9.7
13	K	72	GLU	9.7
11	I	39	ARG	9.7
20	R	56	ARG	9.7
17	O	10	PRO	9.6
7	E	43	GLY	9.6
6	D	145	ASP	9.6
5	C	171	GLU	9.6
4	B	65	MET	9.6
11	I	188	ASN	9.6
12	J	105	TYR	9.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	B	144	HIS	9.6
17	O	101	HIS	9.6
16	N	94	GLN	9.6
6	D	151	ILE	9.6
7	E	18	GLU	9.6
7	E	58	GLU	9.6
13	K	148	ALA	9.6
20	R	31	PHE	9.6
14	L	111	VAL	9.6
14	L	27	GLY	9.6
19	Q	60	GLY	9.6
19	Q	85	GLU	9.6
8	F	38	ALA	9.6
16	N	89	ALA	9.6
1	0	960	G	9.6
24	V	61	LYS	9.6
4	B	83	LEU	9.6
6	D	84	LEU	9.6
23	U	30	MET	9.6
4	B	314	ALA	9.6
7	E	112	ALA	9.6
8	F	64	ALA	9.6
22	T	3	ALA	9.6
25	W	65	ALA	9.6
25	W	32	LYS	9.5
5	C	19	PRO	9.5
8	F	148	ASN	9.5
25	W	54	ILE	9.5
13	K	86	LEU	9.5
19	Q	27	LEU	9.5
19	Q	78	THR	9.5
5	C	3	ALA	9.5
7	E	22	VAL	9.5
12	J	56	LYS	9.5
4	B	306	ARG	9.5
10	H	56	SER	9.5
17	O	98	ASN	9.5
7	E	13	GLU	9.5
13	K	120	GLU	9.5
4	B	184	GLY	9.5
11	I	54	TYR	9.5
3	A	95	PRO	9.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	E	41	GLU	9.5
29	1	50	GLU	9.5
6	D	87	ALA	9.5
4	B	72	VAL	9.5
5	C	144	PHE	9.5
11	I	33	ARG	9.5
15	M	94	TRP	9.5
28	Z	4	PRO	9.5
17	O	138	SER	9.5
29	1	96	ASN	9.5
15	M	105	LEU	9.5
8	F	142	LYS	9.5
7	E	37	THR	9.4
9	G	93	ARG	9.4
3	A	214	SER	9.4
6	D	55	LYS	9.4
13	K	114	LYS	9.4
6	D	75	LEU	9.4
4	B	158	PRO	9.4
6	D	135	VAL	9.4
6	D	141	VAL	9.4
7	E	6	PHE	9.4
23	U	77	PHE	9.4
25	W	29	VAL	9.4
12	J	59	GLU	9.4
3	A	106	CYS	9.4
25	W	25	ARG	9.4
29	1	102	VAL	9.4
29	1	157	LYS	9.4
19	Q	112	LEU	9.4
13	K	167	ASP	9.4
14	L	55	ASP	9.4
7	E	23	ALA	9.4
14	L	80	ASP	9.4
4	B	163	THR	9.3
16	N	64	GLU	9.3
13	K	48	VAL	9.3
4	B	91	TYR	9.3
5	C	73	LEU	9.3
15	M	99	ARG	9.3
24	V	54	SER	9.3
24	V	107	ARG	9.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	1	80	TRP	9.3
4	B	183	ASP	9.3
18	P	73	ASP	9.3
3	A	59	GLU	9.3
22	T	68	THR	9.3
11	I	120	VAL	9.3
21	S	2	VAL	9.3
12	J	42	ASN	9.3
15	M	63	ARG	9.3
11	I	147	LEU	9.3
22	T	136	GLY	9.3
9	G	63	ILE	9.3
10	H	104	PRO	9.3
10	H	118	ALA	9.3
13	K	49	THR	9.3
14	L	91	GLN	9.3
4	B	104	PHE	9.3
19	Q	35	TYR	9.3
2	9	23	U	9.3
22	T	102	SER	9.3
5	C	15	GLU	9.3
7	E	73	PRO	9.3
12	J	96	VAL	9.3
25	W	26	VAL	9.3
3	A	115	GLY	9.3
14	L	93	GLY	9.3
5	C	141	SER	9.3
6	D	24	HIS	9.2
16	N	90	HIS	9.2
8	F	101	MET	9.2
22	T	105	THR	9.2
5	C	227	GLY	9.2
7	E	68	ASP	9.2
11	I	154	ARG	9.2
4	B	284	VAL	9.2
3	A	27	LEU	9.2
7	E	117	GLU	9.2
10	H	102	GLU	9.2
18	P	43	GLU	9.2
2	9	1	U	9.2
17	O	105	ASP	9.2
29	1	13	ALA	9.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	J	119	THR	9.2
15	M	85	GLY	9.2
4	B	125	GLU	9.2
4	B	248	SER	9.2
11	I	91	ARG	9.2
15	M	136	ASP	9.2
27	Y	21	VAL	9.2
6	D	133	ASN	9.2
13	K	79	PRO	9.1
26	X	20	ARG	9.1
24	V	110	SER	9.1
5	C	74	ASP	9.1
6	D	62	ASP	9.1
9	G	32	ASP	9.1
22	T	76	ASP	9.1
14	L	77	ALA	9.1
15	M	84	ALA	9.1
4	B	20	THR	9.1
14	L	92	VAL	9.1
14	L	7	LEU	9.1
12	J	125	PHE	9.1
22	T	82	GLU	9.1
6	D	40	ILE	9.1
11	I	194	ARG	9.1
11	I	19	TYR	9.1
13	K	38	LYS	9.1
10	H	6	ALA	9.1
5	C	12	THR	9.1
25	W	11	THR	9.1
9	G	55	GLU	9.1
24	V	79	GLY	9.1
28	Z	7	PHE	9.1
28	Z	89	GLU	9.1
29	1	129	GLU	9.1
20	R	16	GLY	9.1
23	U	23	HIS	9.1
4	B	255	GLN	9.1
11	I	183	PRO	9.1
4	B	324	ASP	9.1
4	B	278	THR	9.1
3	A	148	LEU	9.1
15	M	114	LEU	9.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	N	14	LEU	9.1
29	1	107	PHE	9.1
13	K	132	ASN	9.1
8	F	107	LYS	9.1
20	R	32	CYS	9.1
13	K	29	SER	9.1
11	I	75	THR	9.1
4	B	54	VAL	9.1
27	Y	27	LEU	9.1
23	U	42	SER	9.0
13	K	110	THR	9.0
20	R	28	THR	9.0
22	T	143	THR	9.0
3	A	147	ARG	9.0
18	P	41	VAL	9.0
29	1	74	HIS	9.0
29	1	90	HIS	9.0
14	L	66	GLY	9.0
16	N	74	ASP	9.0
27	Y	48	ASP	9.0
3	A	145	MET	9.0
6	D	162	ALA	9.0
11	I	168	ALA	9.0
18	P	38	ALA	9.0
22	T	53	ALA	9.0
23	U	88	GLU	9.0
28	Z	3	MET	9.0
7	E	47	LEU	9.0
17	O	39	THR	9.0
20	R	42	LEU	9.0
22	T	149	LEU	9.0
4	B	160	VAL	9.0
5	C	137	PRO	9.0
13	K	52	PRO	9.0
24	V	120	ILE	9.0
4	B	113	ASP	9.0
18	P	59	ASP	9.0
6	D	17	ARG	9.0
17	O	5	SER	9.0
5	C	224	ALA	9.0
7	E	16	ALA	9.0
12	J	136	ALA	9.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
24	V	6	THR	9.0
5	C	133	ARG	9.0
8	F	51	GLU	9.0
25	W	72	GLU	9.0
13	K	31	LYS	9.0
13	K	2	THR	9.0
13	K	104	ILE	8.9
8	F	7	ARG	8.9
29	1	2	ARG	8.9
12	J	101	ASP	8.9
19	Q	61	GLU	8.9
19	Q	69	LYS	8.9
14	L	8	SER	8.9
28	Z	85	ALA	8.9
3	A	60	PHE	8.9
27	Y	3	LYS	8.9
19	Q	102	ASP	8.9
4	B	199	ALA	8.9
19	Q	79	LEU	8.9
14	L	75	THR	8.9
4	B	251	PRO	8.9
11	I	40	ILE	8.9
27	Y	18	ASN	8.9
8	F	58	HIS	8.9
8	F	129	ASP	8.9
11	I	151	SER	8.9
11	I	163	SER	8.9
15	M	56	GLY	8.9
29	1	7	ILE	8.9
13	K	69	TYR	8.9
8	F	82	LYS	8.9
6	D	79	MET	8.9
5	C	242	GLU	8.9
5	C	203	ALA	8.9
10	H	3	ALA	8.9
15	M	32	ALA	8.9
4	B	201	VAL	8.9
12	J	94	ARG	8.8
22	T	74	GLU	8.8
8	F	69	ASN	8.8
3	A	121	ALA	8.8
5	C	176	ALA	8.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	Q	119	ALA	8.8
11	I	41	PRO	8.8
5	C	226	GLY	8.8
14	L	32	ARG	8.8
16	N	37	GLU	8.8
7	E	3	TYR	8.8
10	H	99	ASP	8.8
13	K	103	ASP	8.8
17	O	9	ASP	8.8
29	1	120	GLY	8.8
10	H	100	GLU	8.8
17	O	48	GLU	8.8
9	G	145	TRP	8.8
28	Z	78	HIS	8.8
11	I	146	GLN	8.8
28	Z	18	GLN	8.8
4	B	122	ALA	8.8
13	K	92	ALA	8.8
13	K	143	ARG	8.8
13	K	157	PRO	8.8
17	O	108	ALA	8.8
9	G	119	THR	8.8
17	O	113	HIS	8.8
4	B	293	TYR	8.8
5	C	170	ASP	8.8
6	D	39	ASP	8.8
4	B	15	PRO	8.8
8	F	24	PRO	8.8
8	F	141	MET	8.8
16	N	3	SER	8.7
4	B	296	VAL	8.7
8	F	46	VAL	8.7
13	K	174	GLU	8.7
22	T	52	VAL	8.7
6	D	104	PHE	8.7
4	B	307	LEU	8.7
11	I	97	LEU	8.7
17	O	22	GLN	8.7
13	K	57	THR	8.7
23	U	7	GLU	8.7
9	G	46	ILE	8.7
28	Z	44	SER	8.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	R	23	HIS	8.7
13	K	25	ARG	8.7
8	F	45	GLN	8.7
18	P	46	ASP	8.7
22	T	92	ASP	8.7
19	Q	34	GLU	8.7
22	T	22	GLU	8.7
8	F	72	VAL	8.7
10	H	117	VAL	8.7
27	Y	2	LYS	8.7
13	K	119	GLN	8.7
5	C	92	PRO	8.7
18	P	71	ASP	8.7
4	B	107	GLU	8.7
6	D	167	GLU	8.7
5	C	150	THR	8.7
13	K	18	THR	8.7
11	I	76	ARG	8.7
14	L	53	GLN	8.7
8	F	14	TYR	8.7
19	Q	104	GLU	8.7
28	Z	92	GLU	8.7
3	A	66	ARG	8.6
13	K	44	ARG	8.6
14	L	37	ARG	8.6
8	F	6	PHE	8.6
13	K	93	GLN	8.6
29	1	26	ASN	8.6
29	1	19	ASP	8.6
4	B	263	GLU	8.6
11	I	34	GLU	8.6
18	P	76	GLU	8.6
28	Z	77	ALA	8.6
3	A	31	LYS	8.6
8	F	87	LYS	8.6
4	B	127	ILE	8.6
4	B	146	VAL	8.6
11	I	68	ARG	8.6
22	T	38	THR	8.6
5	C	88	SER	8.6
7	E	118	LEU	8.6
4	B	182	GLU	8.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	I	130	GLU	8.6
20	R	46	ALA	8.6
20	R	22	VAL	8.6
23	U	10	VAL	8.6
9	G	100	SER	8.6
13	K	108	SER	8.6
29	1	60	SER	8.6
7	E	12	LEU	8.6
11	I	1	MET	8.6
24	V	82	PRO	8.6
28	Z	12	PRO	8.6
28	Z	19	GLU	8.6
8	F	5	HIS	8.6
18	P	27	ALA	8.6
15	M	119	TYR	8.6
28	Z	55	VAL	8.6
11	I	12	TRP	8.6
5	C	155	SER	8.6
23	U	45	GLU	8.6
12	J	79	ASP	8.6
19	Q	76	ASP	8.6
17	O	65	GLY	8.5
21	S	46	ILE	8.5
8	F	126	VAL	8.5
14	L	84	THR	8.5
19	Q	50	VAL	8.5
26	X	33	VAL	8.5
29	1	132	THR	8.5
7	E	17	LEU	8.5
7	E	74	PHE	8.5
23	U	56	GLU	8.5
29	1	14	GLU	8.5
13	K	11	ARG	8.5
20	R	7	ASP	8.5
4	B	291	GLY	8.5
13	K	75	THR	8.5
9	G	69	TYR	8.5
9	G	59	LYS	8.5
21	S	47	LYS	8.5
6	D	140	ARG	8.5
9	G	15	ARG	8.5
28	Z	40	ARG	8.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	88	ILE	8.5
6	D	166	ILE	8.5
9	G	78	ILE	8.5
13	K	35	VAL	8.5
13	K	27	LEU	8.5
29	1	53	GLU	8.5
19	Q	5	ASP	8.5
4	B	80	ALA	8.5
13	K	10	MET	8.5
22	T	13	MET	8.5
4	B	208	LYS	8.5
12	J	74	THR	8.5
4	B	124	GLU	8.5
29	1	88	TYR	8.5
15	M	58	SER	8.5
29	1	87	PHE	8.5
28	Z	35	TRP	8.5
20	R	6	CYS	8.4
3	A	143	GLY	8.4
4	B	239	GLY	8.4
5	C	16	VAL	8.4
6	D	58	VAL	8.4
23	U	11	THR	8.4
3	A	72	GLU	8.4
10	H	28	GLU	8.4
13	K	156	GLU	8.4
29	1	78	GLU	8.4
4	B	323	LEU	8.4
20	R	44	ARG	8.4
13	K	82	TYR	8.4
7	E	113	ASP	8.4
29	1	54	ASP	8.4
4	B	157	LYS	8.4
6	D	143	LYS	8.4
3	A	97	ALA	8.4
5	C	34	ALA	8.4
7	E	28	ALA	8.4
12	J	150	GLN	8.4
9	G	43	ARG	8.4
6	D	88	LEU	8.4
6	D	128	LEU	8.4
3	A	142	SER	8.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	1	28	SER	8.4
4	B	29	TRP	8.4
4	B	100	TRP	8.4
10	H	1	MET	8.4
9	G	97	ALA	8.4
18	P	61	GLU	8.4
7	E	26	THR	8.4
12	J	51	PHE	8.4
25	W	81	LYS	8.4
11	I	87	MET	8.4
3	A	149	ASP	8.4
3	A	215	ILE	8.4
4	B	123	ALA	8.4
7	E	105	ALA	8.4
4	B	35	GLN	8.4
12	J	44	GLU	8.4
4	B	111	THR	8.4
29	1	67	SER	8.4
5	C	126	ASP	8.3
9	G	110	ASP	8.3
5	C	128	GLY	8.3
12	J	29	GLY	8.3
16	N	49	ASN	8.3
21	S	64	GLY	8.3
29	1	135	GLY	8.3
3	A	164	ARG	8.3
8	F	114	ARG	8.3
11	I	164	ALA	8.3
12	J	148	GLU	8.3
21	S	17	GLU	8.3
3	A	100	PRO	8.3
13	K	90	LEU	8.3
3	A	130	THR	8.3
4	B	249	THR	8.3
25	W	35	LYS	8.3
29	1	84	MET	8.3
8	F	90	PHE	8.3
18	P	45	TYR	8.3
6	D	59	GLY	8.3
17	O	54	ASP	8.3
17	O	67	GLY	8.3
19	Q	58	GLU	8.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	M	51	ALA	8.3
17	O	129	ALA	8.3
22	T	114	PRO	8.3
24	V	29	PRO	8.3
10	H	33	SER	8.3
8	F	30	GLN	8.3
13	K	30	GLY	8.3
9	G	44	ALA	8.3
4	B	292	PRO	8.3
3	A	131	HIS	8.3
9	G	12	VAL	8.3
22	T	35	VAL	8.3
4	B	21	SER	8.3
13	K	160	SER	8.3
4	B	282	GLY	8.3
7	E	14	ASP	8.3
17	O	124	GLY	8.3
6	D	18	ILE	8.3
8	F	19	TYR	8.3
11	I	89	ASN	8.3
17	O	8	ALA	8.3
23	U	64	ALA	8.3
15	M	54	LYS	8.3
4	B	89	THR	8.3
24	V	9	THR	8.3
8	F	138	ARG	8.3
20	R	4	ARG	8.3
19	Q	33	GLU	8.2
29	1	4	GLU	8.2
9	G	48	GLY	8.2
3	A	23	TYR	8.2
20	R	39	ASN	8.2
29	1	103	VAL	8.2
22	T	83	TRP	8.2
7	E	90	GLU	8.2
22	T	109	GLU	8.2
24	V	86	GLU	8.2
14	L	18	ALA	8.2
7	E	56	PRO	8.2
9	G	10	VAL	8.2
10	H	86	THR	8.2
12	J	127	GLU	8.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
22	T	144	GLU	8.2
4	B	171	SER	8.2
22	T	81	ASP	8.2
5	C	244	ALA	8.2
5	C	240	LEU	8.2
13	K	34	LEU	8.2
16	N	1	PRO	8.2
16	N	16	ASN	8.2
18	P	8	PRO	8.2
23	U	67	PRO	8.2
24	V	136	TYR	8.2
16	N	92	ARG	8.2
3	A	180	LYS	8.2
19	Q	22	GLN	8.2
24	V	46	TRP	8.2
1	O	1625	U	8.2
9	G	106	GLY	8.2
12	J	102	ASP	8.2
16	N	77	ASP	8.2
3	A	187	PRO	8.2
4	B	202	ALA	8.2
11	I	96	ASN	8.2
13	K	83	LEU	8.2
29	L	92	PRO	8.2
8	F	62	GLU	8.2
8	F	73	GLN	8.1
11	I	98	GLN	8.1
8	F	151	SER	8.1
5	C	142	ASP	8.1
9	G	66	ASP	8.1
22	T	62	LEU	8.1
22	T	107	LEU	8.1
22	T	152	ALA	8.1
11	I	5	TYR	8.1
10	H	2	GLU	8.1
20	R	54	THR	8.1
16	N	54	PRO	8.1
19	Q	68	ASP	8.1
22	T	93	ILE	8.1
4	B	141	LEU	8.1
10	H	26	ALA	8.1
13	K	117	ALA	8.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
18	P	16	ASN	8.1
24	V	133	ASN	8.1
20	R	52	THR	8.1
8	F	57	ARG	8.1
12	J	11	ARG	8.1
24	V	74	PRO	8.1
13	K	24	LEU	8.1
17	O	47	LEU	8.1
26	X	54	ALA	8.1
19	Q	9	LYS	8.1
4	B	327	VAL	8.1
15	M	103	THR	8.1
17	O	55	GLN	8.1
5	C	86	GLY	8.1
9	G	133	GLY	8.1
11	I	110	PRO	8.1
10	H	12	LEU	8.1
12	J	95	ASP	8.1
14	L	2	LYS	8.1
5	C	41	ASN	8.1
11	I	99	TRP	8.1
8	F	70	ARG	8.0
8	F	84	ARG	8.0
15	M	139	ARG	8.0
4	B	9	GLY	8.0
4	B	218	GLY	8.0
26	X	23	GLY	8.0
21	S	13	PRO	8.0
15	M	122	LEU	8.0
4	B	130	ALA	8.0
5	C	114	ALA	8.0
15	M	4	SER	8.0
5	C	145	GLU	8.0
15	M	113	THR	8.0
4	B	328	ARG	8.0
21	S	31	ARG	8.0
3	A	45	ILE	8.0
10	H	92	ASP	8.0
28	Z	59	ASP	8.0
4	B	335	ASN	8.0
14	L	26	TRP	8.0
4	B	143	THR	8.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	G	47	THR	8.0
13	K	12	ARG	8.0
26	X	29	THR	8.0
28	Z	47	GLY	8.0
18	P	20	PHE	8.0
23	U	6	GLU	8.0
7	E	19	ALA	8.0
19	Q	114	SER	8.0
22	T	45	VAL	8.0
22	T	117	ARG	8.0
18	P	18	MET	8.0
8	F	123	ILE	8.0
21	S	21	ASP	8.0
10	H	71	ALA	8.0
21	S	30	ALA	8.0
15	M	79	SER	8.0
26	X	52	SER	8.0
10	H	105	ARG	8.0
11	I	82	LYS	7.9
15	M	22	TRP	7.9
7	E	89	LEU	7.9
9	G	87	LEU	7.9
8	F	88	PHE	7.9
23	U	87	ALA	7.9
15	M	90	SER	7.9
29	1	111	LYS	7.9
7	E	36	THR	7.9
26	X	13	THR	7.9
29	1	131	LEU	7.9
8	F	124	ALA	7.9
14	L	6	ARG	7.9
15	M	96	SER	7.9
10	H	72	VAL	7.9
11	I	65	VAL	7.9
5	C	123	LEU	7.9
14	L	107	GLU	7.9
8	F	102	ARG	7.9
13	K	141	ARG	7.9
13	K	125	ALA	7.9
12	J	2	SER	7.9
8	F	109	VAL	7.9
4	B	23	THR	7.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	B	76	PRO	7.9
19	Q	49	GLU	7.9
17	O	100	ASP	7.9
7	E	45	ALA	7.9
10	H	47	ALA	7.9
28	Z	10	TYR	7.9
5	C	48	SER	7.8
18	P	33	SER	7.8
8	F	92	VAL	7.8
24	V	118	GLU	7.8
17	O	18	LEU	7.8
6	D	149	ARG	7.8
15	M	69	ARG	7.8
16	N	21	ARG	7.8
24	V	119	ARG	7.8
28	Z	5	ARG	7.8
28	Z	6	ARG	7.8
12	J	40	PHE	7.8
13	K	137	ALA	7.8
14	L	30	ALA	7.8
19	Q	43	ASN	7.8
7	E	110	GLU	7.8
22	T	63	GLU	7.8
29	1	6	GLU	7.8
10	H	111	GLY	7.8
26	X	53	LYS	7.8
17	O	31	ILE	7.8
4	B	2	GLN	7.8
12	J	13	HIS	7.8
25	W	37	TYR	7.8
29	1	35	TYR	7.8
4	B	332	ASN	7.8
5	C	28	SER	7.8
17	O	70	SER	7.8
8	F	143	VAL	7.8
29	1	23	GLU	7.8
4	B	49	THR	7.8
8	F	11	LYS	7.8
29	1	123	ASP	7.8
17	O	117	HIS	7.8
4	B	16	ARG	7.8
18	P	70	GLU	7.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	Q	111	ARG	7.8
14	L	33	LEU	7.8
14	L	65	LEU	7.8
29	1	49	ILE	7.8
19	Q	30	ASP	7.8
19	Q	54	ASP	7.8
4	B	273	GLU	7.7
4	B	322	ARG	7.7
28	Z	21	GLU	7.7
28	Z	41	GLU	7.7
29	1	70	GLU	7.7
7	E	72	VAL	7.7
5	C	146	ASP	7.7
22	T	28	HIS	7.7
24	V	65	ASP	7.7
14	L	24	ALA	7.7
27	Y	23	ALA	7.7
4	B	297	LYS	7.7
11	I	191	LYS	7.7
15	M	42	GLU	7.7
10	H	79	PRO	7.7
29	1	71	ASN	7.7
11	I	31	TRP	7.7
11	I	88	VAL	7.7
10	H	19	THR	7.7
12	J	107	LYS	7.7
11	I	6	ALA	7.7
11	I	125	ARG	7.7
12	J	21	ARG	7.7
15	M	126	ALA	7.7
4	B	240	PRO	7.7
8	F	145	PRO	7.7
9	G	45	VAL	7.7
9	G	125	SER	7.7
3	A	184	THR	7.7
4	B	212	GLY	7.7
12	J	43	HIS	7.7
9	G	51	GLU	7.7
7	E	48	VAL	7.7
23	U	31	ILE	7.7
22	T	87	HIS	7.7
26	X	21	ARG	7.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	G	111	GLU	7.6
6	D	160	ALA	7.6
4	B	36	PRO	7.6
4	B	213	PRO	7.6
22	T	88	THR	7.6
24	V	84	GLY	7.6
10	H	18	ILE	7.6
4	B	110	ARG	7.6
12	J	130	ARG	7.6
15	M	41	ARG	7.6
25	W	33	HIS	7.6
21	S	26	GLU	7.6
7	E	104	ALA	7.6
4	B	115	PRO	7.6
10	H	17	LEU	7.6
13	K	179	LEU	7.6
3	A	82	VAL	7.6
13	K	43	VAL	7.6
24	V	26	VAL	7.6
5	C	4	THR	7.6
19	Q	99	THR	7.6
21	S	60	GLN	7.6
22	T	59	GLN	7.6
24	V	36	HIS	7.6
17	O	116	ALA	7.6
22	T	131	PRO	7.6
6	D	146	LYS	7.6
6	D	154	LYS	7.6
8	F	52	LYS	7.6
18	P	53	ASN	7.6
8	F	111	THR	7.6
8	F	12	PRO	7.6
13	K	19	ASP	7.6
15	M	121	ASP	7.6
9	G	37	ALA	7.6
7	E	70	LYS	7.6
22	T	111	GLY	7.6
10	H	123	SER	7.6
13	K	123	ILE	7.6
10	H	91	GLU	7.6
8	F	31	PHE	7.5
29	1	33	LEU	7.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	U	49	ARG	7.5
5	C	153	VAL	7.5
22	T	30	ASN	7.5
29	1	166	VAL	7.5
12	J	18	HIS	7.5
11	I	24	MET	7.5
27	Y	11	LYS	7.5
22	T	67	ALA	7.5
6	D	61	PHE	7.5
9	G	49	ARG	7.5
4	B	308	VAL	7.5
8	F	108	SER	7.5
14	L	109	SER	7.5
21	S	10	ASP	7.5
11	I	136	ARG	7.5
19	Q	32	ARG	7.5
8	F	61	LEU	7.5
26	X	34	CYS	7.5
5	C	151	GLN	7.5
4	B	27	ASN	7.5
4	B	330	VAL	7.5
9	G	130	VAL	7.5
25	W	61	GLY	7.5
7	E	111	ILE	7.5
24	V	75	THR	7.5
21	S	11	MET	7.5
4	B	77	PRO	7.5
17	O	135	ALA	7.5
14	L	71	GLN	7.5
4	B	81	VAL	7.5
5	C	138	VAL	7.5
10	H	70	GLU	7.5
12	J	133	VAL	7.5
17	O	143	VAL	7.5
3	A	168	PRO	7.4
3	A	200	PRO	7.4
4	B	30	PRO	7.4
11	I	66	ARG	7.4
1	0	200	U	7.4
22	T	142	ASP	7.4
4	B	42	ALA	7.4
20	R	40	ALA	7.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	Z	39	GLN	7.4
5	C	11	ASN	7.4
17	O	6	VAL	7.4
22	T	1	MET	7.4
4	B	3	PRO	7.4
15	M	59	ARG	7.4
12	J	70	ASP	7.4
22	T	98	PHE	7.4
14	L	113	VAL	7.4
24	V	67	VAL	7.4
29	1	106	ASN	7.4
11	I	60	ILE	7.4
5	C	214	THR	7.4
25	W	70	THR	7.4
3	A	216	SER	7.4
13	K	32	PRO	7.4
5	C	147	LEU	7.4
19	Q	31	LEU	7.4
19	Q	37	GLN	7.4
4	B	74	GLU	7.4
5	C	46	TYR	7.4
15	M	81	LYS	7.4
21	S	7	GLU	7.4
22	T	151	GLU	7.4
10	H	5	GLY	7.4
21	S	37	GLY	7.4
3	A	133	ARG	7.4
24	V	89	ARG	7.4
17	O	81	PRO	7.4
5	C	8	LEU	7.4
15	M	124	ASP	7.4
24	V	12	LEU	7.4
12	J	132	LYS	7.4
5	C	6	TYR	7.4
9	G	57	TYR	7.4
11	I	129	PHE	7.4
28	Z	32	GLY	7.4
8	F	17	ARG	7.4
9	G	53	ILE	7.4
25	W	17	ARG	7.4
28	Z	36	ILE	7.4
5	C	189	PRO	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	E	66	LEU	7.3
11	I	47	ASP	7.3
15	M	9	LEU	7.3
17	O	147	LEU	7.3
23	U	37	LEU	7.3
19	Q	44	ALA	7.3
2	9	2	U	7.3
12	J	67	ARG	7.3
15	M	78	GLY	7.3
29	1	115	ARG	7.3
21	S	5	VAL	7.3
7	E	34	ASN	7.3
3	A	49	PRO	7.3
24	V	28	LYS	7.3
28	Z	16	GLU	7.3
4	B	92	GLY	7.3
5	C	22	PHE	7.3
19	Q	98	VAL	7.3
23	U	43	VAL	7.3
29	1	104	ILE	7.3
9	G	144	THR	7.3
24	V	21	THR	7.3
6	D	20	LYS	7.3
13	K	7	LYS	7.3
8	F	60	ALA	7.3
16	N	29	ALA	7.3
15	M	61	ARG	7.3
9	G	54	VAL	7.3
3	A	221	PRO	7.3
15	M	75	LYS	7.3
12	J	113	GLN	7.3
10	H	16	SER	7.3
14	L	1	SER	7.3
19	Q	103	LEU	7.3
4	B	102	ASP	7.3
4	B	119	ASP	7.3
12	J	9	GLY	7.3
17	O	150	PRO	7.3
13	K	15	GLU	7.2
18	P	21	GLN	7.2
24	V	7	GLU	7.2
14	L	67	SER	7.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	R	34	SER	7.2
25	W	20	LEU	7.2
15	M	20	ARG	7.2
24	V	98	GLY	7.2
25	W	21	LYS	7.2
4	B	204	VAL	7.2
18	P	47	VAL	7.2
3	A	21	HIS	7.2
18	P	48	THR	7.2
6	D	157	LEU	7.2
12	J	35	ARG	7.2
20	R	20	MET	7.2
7	E	7	ASP	7.2
14	L	52	ALA	7.2
4	B	114	VAL	7.2
4	B	147	PRO	7.2
16	N	25	PRO	7.2
19	Q	40	VAL	7.2
22	T	44	MET	7.2
25	W	52	THR	7.2
26	X	14	THR	7.2
3	A	129	LEU	7.2
12	J	10	SER	7.2
5	C	185	LYS	7.2
10	H	90	PHE	7.2
17	O	35	ILE	7.2
29	1	1	PRO	7.2
12	J	108	VAL	7.2
13	K	42	HIS	7.2
20	R	48	ASN	7.2
21	S	29	ASN	7.2
23	U	63	ARG	7.2
1	0	284	C	7.2
22	T	58	SER	7.2
26	X	18	LYS	7.2
28	Z	54	LYS	7.2
10	H	45	PRO	7.2
4	B	310	PHE	7.2
13	K	115	VAL	7.1
22	T	5	VAL	7.1
22	T	14	HIS	7.1
29	1	98	GLU	7.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	J	72	ASN	7.1
12	J	63	THR	7.1
22	T	106	THR	7.1
4	B	44	TYR	7.1
4	B	258	TYR	7.1
4	B	280	ASP	7.1
9	G	122	ASP	7.1
11	I	148	SER	7.1
3	A	19	PRO	7.1
4	B	120	PRO	7.1
4	B	222	ARG	7.1
11	I	172	ARG	7.1
16	N	28	ARG	7.1
20	R	51	TRP	7.1
23	U	85	VAL	7.1
24	V	112	VAL	7.1
4	B	206	LYS	7.1
6	D	45	THR	7.1
5	C	45	ASP	7.1
5	C	165	ASP	7.1
14	L	28	ASP	7.1
17	O	49	ALA	7.1
21	S	22	ASP	7.1
20	R	50	GLU	7.1
15	M	66	GLN	7.1
17	O	102	GLN	7.1
18	P	49	VAL	7.1
18	P	66	VAL	7.1
23	U	9	VAL	7.1
25	W	57	CYS	7.1
3	A	92	ASN	7.1
16	N	24	SER	7.1
1	O	283	U	7.1
4	B	233	ARG	7.1
9	G	114	GLU	7.1
9	G	52	GLN	7.1
5	C	169	ALA	7.1
17	O	134	SER	7.1
22	T	103	GLU	7.1
9	G	11	ILE	7.1
7	E	38	LYS	7.0
27	Y	9	LYS	7.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	B	311	PHE	7.0
5	C	61	PHE	7.0
15	M	131	PHE	7.0
24	V	71	PHE	7.0
29	1	40	VAL	7.0
3	A	69	LEU	7.0
1	0	2237	G	7.0
13	K	33	ARG	7.0
15	M	37	ARG	7.0
16	N	11	ARG	7.0
11	I	49	ALA	7.0
11	I	158	TYR	7.0
13	K	151	ASP	7.0
15	M	11	ALA	7.0
21	S	35	ALA	7.0
25	W	40	PRO	7.0
27	Y	22	PRO	7.0
29	1	93	MET	7.0
22	T	27	HIS	7.0
26	X	41	LYS	7.0
19	Q	7	GLN	7.0
4	B	52	VAL	7.0
5	C	148	VAL	7.0
4	B	285	ASN	7.0
5	C	202	THR	7.0
29	1	116	THR	7.0
3	A	98	GLU	7.0
15	M	107	GLU	7.0
22	T	56	GLU	7.0
3	A	73	GLY	7.0
16	N	58	GLY	7.0
4	B	165	VAL	7.0
6	D	163	VAL	7.0
6	D	156	ARG	7.0
8	F	15	THR	7.0
29	1	117	THR	7.0
5	C	93	LYS	7.0
11	I	113	GLU	7.0
12	J	134	GLU	7.0
17	O	7	GLU	7.0
20	R	45	GLU	7.0
3	A	154	ALA	7.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	G	76	ASP	7.0
14	L	101	ALA	7.0
5	C	238	SER	7.0
5	C	31	ILE	7.0
9	G	29	GLN	7.0
21	S	8	ILE	7.0
25	W	22	ILE	7.0
3	A	159	VAL	7.0
13	K	102	LEU	7.0
28	Z	88	LEU	7.0
29	1	151	LEU	7.0
3	A	120	ARG	7.0
14	L	3	THR	7.0
12	J	52	LYS	7.0
3	A	79	GLU	7.0
7	E	69	GLU	7.0
6	D	54	ALA	7.0
6	D	142	ALA	7.0
19	Q	14	ALA	7.0
23	U	74	ALA	7.0
10	H	97	ILE	6.9
11	I	141	ILE	6.9
29	1	134	SER	6.9
12	J	106	VAL	6.9
18	P	28	VAL	6.9
23	U	41	PHE	6.9
24	V	85	PHE	6.9
5	C	149	LYS	6.9
22	T	61	THR	6.9
1	0	282	C	6.9
19	Q	4	PRO	6.9
25	W	10	PRO	6.9
7	E	97	ALA	6.9
9	G	62	ASP	6.9
11	I	11	ALA	6.9
8	F	55	GLN	6.9
12	J	135	GLY	6.9
9	G	18	ILE	6.9
11	I	143	SER	6.9
3	A	32	VAL	6.9
4	B	178	LEU	6.9
7	E	115	VAL	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	Q	62	VAL	6.9
2	9	24	U	6.9
17	O	112	LYS	6.9
19	Q	21	LYS	6.9
26	X	32	LYS	6.9
11	I	78	ASN	6.9
4	B	22	GLU	6.9
3	A	112	PRO	6.9
19	Q	88	PRO	6.9
8	F	112	ALA	6.9
19	Q	46	ASP	6.9
22	T	99	ALA	6.9
25	W	68	ALA	6.9
9	G	81	ARG	6.9
9	G	109	TYR	6.9
4	B	279	VAL	6.9
5	C	21	VAL	6.9
15	M	55	LYS	6.9
16	N	81	GLU	6.9
17	O	52	GLU	6.9
6	D	131	THR	6.9
21	S	25	THR	6.9
22	T	20	THR	6.9
29	1	152	THR	6.9
8	F	121	ASP	6.9
9	G	16	ASP	6.9
12	J	36	ASP	6.9
25	W	31	ILE	6.9
28	Z	63	LYS	6.9
3	A	94	LEU	6.9
14	L	58	VAL	6.9
4	B	13	PHE	6.9
20	R	37	GLU	6.9
24	V	56	GLN	6.9
3	A	78	ASP	6.9
8	F	13	ALA	6.9
10	H	114	ALA	6.9
14	L	97	SER	6.8
15	M	14	LEU	6.8
6	D	172	VAL	6.8
14	L	51	TYR	6.8
10	H	112	PRO	6.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	J	1	THR	6.8
20	R	29	THR	6.8
4	B	260	GLN	6.8
7	E	87	ALA	6.8
4	B	4	SER	6.8
9	G	31	LEU	6.8
25	W	53	SER	6.8
6	D	21	VAL	6.8
21	S	63	GLU	6.8
6	D	98	PHE	6.8
12	J	41	HIS	6.8
17	O	68	HIS	6.8
28	Z	30	GLN	6.8
28	Z	64	LYS	6.8
9	G	9	ASP	6.8
12	J	46	LEU	6.8
3	A	71	PRO	6.8
8	F	48	ASN	6.8
26	X	44	LYS	6.8
26	X	51	GLN	6.8
6	D	129	ASP	6.8
8	F	68	ALA	6.8
11	I	144	ASP	6.8
15	M	142	ASP	6.8
24	V	105	ALA	6.8
14	L	102	ILE	6.8
10	H	132	VAL	6.8
5	C	33	LYS	6.8
3	A	127	GLN	6.8
4	B	7	ARG	6.8
4	B	86	TYR	6.8
16	N	71	TYR	6.8
3	A	75	GLY	6.7
12	J	31	GLY	6.7
4	B	270	ASP	6.7
7	E	51	ALA	6.7
26	X	43	ALA	6.7
29	1	12	ASP	6.7
12	J	118	LEU	6.7
15	M	43	LEU	6.7
16	N	7	LEU	6.7
29	1	149	GLU	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	190	ARG	6.7
8	F	2	PRO	6.7
28	Z	2	GLN	6.7
15	M	19	ASN	6.7
29	1	79	GLY	6.7
3	A	18	ALA	6.7
21	S	3	LEU	6.7
4	B	31	SER	6.7
17	O	3	SER	6.7
19	Q	71	VAL	6.7
22	T	113	SER	6.7
11	I	107	ARG	6.7
29	1	36	PRO	6.7
17	O	137	ASN	6.7
26	X	19	CYS	6.7
29	1	144	THR	6.7
18	P	15	MET	6.7
8	F	56	ILE	6.7
12	J	65	ASP	6.7
5	C	158	GLU	6.7
7	E	108	LEU	6.7
22	T	34	LEU	6.7
1	0	1130	U	6.7
11	I	32	ARG	6.7
10	H	68	VAL	6.7
22	T	6	GLN	6.7
5	C	103	ASN	6.7
12	J	12	THR	6.7
4	B	198	TYR	6.7
12	J	47	GLY	6.7
5	C	208	ALA	6.7
6	D	37	ALA	6.7
6	D	173	GLU	6.7
7	E	95	ALA	6.7
9	G	14	ALA	6.7
24	V	124	ALA	6.7
9	G	124	LEU	6.7
16	N	53	HIS	6.7
1	0	1929	G	6.7
15	M	21	VAL	6.7
17	O	72	VAL	6.7
25	W	56	VAL	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	L	100	GLN	6.7
18	P	25	GLN	6.7
28	Z	53	SER	6.7
5	C	190	ALA	6.6
7	E	40	ILE	6.6
11	I	115	LEU	6.6
16	N	15	LYS	6.6
18	P	64	ALA	6.6
19	Q	72	ILE	6.6
21	S	56	ILE	6.6
29	1	126	ILE	6.6
11	I	48	ARG	6.6
6	D	11	HIS	6.6
18	P	9	HIS	6.6
3	A	84	VAL	6.6
4	B	51	VAL	6.6
24	V	77	VAL	6.6
24	V	88	VAL	6.6
29	1	124	VAL	6.6
3	A	213	LYS	6.6
7	E	65	GLU	6.6
22	T	37	GLU	6.6
23	U	70	ILE	6.6
13	K	14	ARG	6.6
7	E	64	PRO	6.6
11	I	92	PRO	6.6
4	B	26	PHE	6.6
16	N	33	PHE	6.6
17	O	126	LYS	6.6
5	C	56	THR	6.6
9	G	126	ASN	6.6
18	P	42	GLU	6.6
20	R	38	ASN	6.6
3	A	30	ARG	6.6
4	B	245	ARG	6.6
5	C	223	LEU	6.6
14	L	45	LEU	6.6
15	M	34	ALA	6.6
4	B	88	ASP	6.6
24	V	126	ASP	6.6
1	0	2345	A	6.6
4	B	6	PRO	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	N	45	PRO	6.6
5	C	140	VAL	6.6
21	S	33	VAL	6.6
15	M	68	LYS	6.6
20	R	24	LYS	6.6
29	1	91	PHE	6.6
7	E	35	GLU	6.6
22	T	60	GLU	6.6
3	A	96	LEU	6.6
29	1	18	LEU	6.6
3	A	86	ALA	6.6
23	U	38	ALA	6.6
17	O	73	ASP	6.6
18	P	39	ASP	6.6
7	E	55	GLN	6.6
17	O	122	GLN	6.6
11	I	20	VAL	6.6
11	I	134	VAL	6.6
27	Y	28	LYS	6.6
3	A	201	PHE	6.6
14	L	94	GLU	6.6
16	N	8	GLU	6.6
17	O	59	PHE	6.6
24	V	125	GLU	6.6
1	0	2769	C	6.5
10	H	120	ARG	6.5
4	B	47	GLY	6.5
5	C	206	ASN	6.5
24	V	92	ASN	6.5
22	T	24	LEU	6.5
3	A	172	ALA	6.5
4	B	195	ALA	6.5
5	C	68	ALA	6.5
16	N	88	ALA	6.5
5	C	20	ASP	6.5
5	C	49	ASP	6.5
4	B	317	PRO	6.5
5	C	197	SER	6.5
10	H	77	ARG	6.5
18	P	35	GLY	6.5
28	Z	20	HIS	6.5
9	G	27	ALA	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	G	30	ALA	6.5
12	J	55	GLN	6.5
17	O	83	LYS	6.5
4	B	286	TYR	6.5
11	I	109	TYR	6.5
4	B	219	VAL	6.5
23	U	48	VAL	6.5
4	B	87	GLU	6.5
4	B	326	GLU	6.5
11	I	182	ARG	6.5
14	L	31	GLU	6.5
14	L	82	SER	6.5
16	N	2	SER	6.5
3	A	160	GLY	6.5
3	A	222	GLY	6.5
4	B	50	HIS	6.5
5	C	115	LEU	6.5
12	J	76	LEU	6.5
12	J	64	ILE	6.5
24	V	60	ILE	6.5
25	W	75	ALA	6.5
15	M	45	ASP	6.5
18	P	29	ASP	6.5
28	Z	42	ARG	6.5
1	0	2238	A	6.5
9	G	24	SER	6.5
9	G	121	LEU	6.5
14	L	40	HIS	6.5
20	R	13	ILE	6.5
20	R	17	THR	6.5
4	B	225	LYS	6.5
5	C	40	ALA	6.5
23	U	29	ALA	6.5
4	B	211	GLN	6.5
10	H	51	ASP	6.5
15	M	25	PRO	6.5
13	K	17	ARG	6.5
17	O	21	ARG	6.5
19	Q	8	ARG	6.5
7	E	21	GLU	6.5
8	F	18	GLU	6.5
9	G	42	GLU	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	108	VAL	6.5
15	M	44	VAL	6.5
18	P	10	VAL	6.5
22	T	84	VAL	6.5
14	L	81	PHE	6.4
3	A	176	HIS	6.4
5	C	156	LEU	6.4
11	I	21	GLY	6.4
10	H	41	LYS	6.4
23	U	66	THR	6.4
26	X	3	ALA	6.4
4	B	61	PRO	6.4
8	F	89	PRO	6.4
5	C	152	GLU	6.4
7	E	116	GLU	6.4
23	U	35	GLU	6.4
14	L	59	VAL	6.4
5	C	194	PHE	6.4
28	Z	90	PHE	6.4
4	B	174	LEU	6.4
23	U	55	ASN	6.4
15	M	5	ALA	6.4
16	N	27	GLN	6.4
14	L	73	ASP	6.4
19	Q	97	ARG	6.4
19	Q	100	ASP	6.4
19	Q	105	ASP	6.4
22	T	19	ASP	6.4
28	Z	37	ASP	6.4
19	Q	86	GLU	6.4
29	1	47	VAL	6.4
4	B	17	LYS	6.4
17	O	4	TYR	6.4
23	U	50	LEU	6.4
24	V	45	SER	6.4
4	B	229	GLN	6.4
12	J	62	ALA	6.4
24	V	47	ARG	6.4
29	1	153	ARG	6.4
5	C	50	GLU	6.4
12	J	147	GLU	6.4
18	P	37	VAL	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	80	LEU	6.4
5	C	160	LEU	6.4
20	R	8	TYR	6.4
17	O	2	ILE	6.4
24	V	142	SER	6.4
5	C	82	GLN	6.4
19	Q	11	GLN	6.4
9	G	67	ASN	6.4
9	G	75	PRO	6.4
15	M	89	ASN	6.4
22	T	49	ASN	6.4
19	Q	70	ALA	6.4
12	J	71	GLU	6.4
19	Q	18	GLU	6.4
3	A	225	VAL	6.4
14	L	25	VAL	6.4
19	Q	65	VAL	6.4
16	N	84	ILE	6.3
14	L	105	ASN	6.3
28	Z	23	GLU	6.3
29	1	39	ASP	6.3
3	A	29	HIS	6.3
10	H	69	LEU	6.3
15	M	108	LEU	6.3
5	C	25	PRO	6.3
11	I	101	ALA	6.3
12	J	4	LYS	6.3
3	A	226	GLY	6.3
8	F	3	GLY	6.3
5	C	186	TYR	6.3
22	T	41	TYR	6.3
4	B	237	ASN	6.3
7	E	96	ALA	6.3
17	O	43	ALA	6.3
25	W	38	LYS	6.3
22	T	125	HIS	6.3
9	G	123	ARG	6.3
4	B	39	GLN	6.3
7	E	31	LYS	6.3
24	V	48	LYS	6.3
28	Z	24	LYS	6.3
5	C	201	SER	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	H	54	THR	6.3
12	J	122	ALA	6.3
23	U	65	ASN	6.3
18	P	52	VAL	6.2
13	K	26	LEU	6.2
9	G	73	LYS	6.2
15	M	23	PHE	6.2
16	N	72	LYS	6.2
24	V	40	LYS	6.2
4	B	205	THR	6.2
6	D	105	SER	6.2
21	S	12	THR	6.2
11	I	106	ASN	6.2
15	M	57	ASN	6.2
4	B	129	ASP	6.2
4	B	172	ASP	6.2
5	C	232	LEU	6.2
14	L	98	LEU	6.2
27	Y	14	LEU	6.2
3	A	186	TRP	6.2
24	V	34	GLN	6.2
21	S	24	LYS	6.2
4	B	243	PRO	6.2
5	C	71	PRO	6.2
9	G	142	ASN	6.2
17	O	45	ASP	6.2
28	Z	13	HIS	6.2
28	Z	17	HIS	6.2
10	H	57	VAL	6.2
19	Q	77	VAL	6.2
25	W	36	LYS	6.2
27	Y	17	GLN	6.2
12	J	68	GLU	6.2
18	P	50	GLU	6.2
21	S	48	GLU	6.2
7	E	59	ILE	6.2
23	U	84	ILE	6.2
22	T	64	THR	6.2
5	C	55	ARG	6.2
8	F	94	ARG	6.2
17	O	14	ALA	6.2
22	T	31	HIS	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	U	40	HIS	6.2
23	U	32	LEU	6.2
3	A	58	VAL	6.2
1	0	1525	G	6.2
1	0	2136	G	6.2
3	A	54	PRO	6.2
28	Z	11	CYS	6.2
11	I	44	THR	6.2
14	L	87	THR	6.2
28	Z	48	ASN	6.2
3	A	166	ASP	6.2
3	A	198	ASP	6.2
7	E	53	ASP	6.2
16	N	69	ASP	6.2
20	R	12	ASP	6.2
20	R	53	ASP	6.2
11	I	28	LEU	6.1
10	H	13	GLU	6.1
11	I	29	GLN	6.1
29	1	133	VAL	6.1
5	C	177	GLY	6.1
28	Z	46	ILE	6.1
1	0	2748	G	6.1
23	U	34	ARG	6.1
10	H	58	THR	6.1
12	J	116	HIS	6.1
18	P	11	THR	6.1
22	T	2	HIS	6.1
24	V	24	HIS	6.1
5	C	29	ASP	6.1
11	I	85	LYS	6.1
23	U	51	ASP	6.1
4	B	220	GLN	6.1
4	B	252	GLN	6.1
5	C	130	GLU	6.1
17	O	107	GLU	6.1
17	O	123	GLN	6.1
22	T	21	LEU	6.1
22	T	138	LEU	6.1
24	V	97	GLU	6.1
28	Z	73	GLU	6.1
4	B	325	PRO	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	E	77	VAL	6.1
24	V	18	ARG	6.1
3	A	152	CYS	6.1
5	C	129	HIS	6.1
10	H	9	THR	6.1
26	X	25	LYS	6.1
10	H	93	ASN	6.1
24	V	43	SER	6.1
26	X	7	SER	6.1
1	O	2768	A	6.1
11	I	52	LEU	6.1
24	V	53	LEU	6.1
24	V	104	GLU	6.1
9	G	72	PRO	6.1
14	L	74	VAL	6.1
3	A	153	ARG	6.1
14	L	89	ILE	6.1
22	T	17	ILE	6.1
12	J	26	HIS	6.1
1	O	999	C	6.1
4	B	191	ASP	6.1
4	B	98	GLU	6.1
7	E	79	GLN	6.1
13	K	94	GLU	6.1
9	G	139	LEU	6.1
4	B	99	VAL	6.1
7	E	91	VAL	6.1
4	B	203	GLY	6.1
15	M	72	GLY	6.1
5	C	5	ILE	6.1
4	B	215	LYS	6.1
18	P	32	ALA	6.1
24	V	66	THR	6.1
3	A	227	ASP	6.1
16	N	67	GLN	6.0
17	O	89	LEU	6.0
3	A	192	VAL	6.0
7	E	98	VAL	6.0
27	Y	1	GLY	6.0
29	1	22	VAL	6.0
17	O	15	LYS	6.0
26	X	47	ASP	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	B	231	TRP	6.0
14	L	14	LEU	6.0
3	A	2	ARG	6.0
19	Q	13	ARG	6.0
5	C	136	VAL	6.0
22	T	129	LYS	6.0
1	0	497	A	6.0
22	T	115	THR	6.0
24	V	44	THR	6.0
29	1	81	GLU	6.0
29	1	140	ALA	6.0
13	K	181	ASP	6.0
27	Y	15	ASP	6.0
29	1	66	GLN	6.0
1	0	1913	C	6.0
3	A	161	GLY	6.0
4	B	48	MET	6.0
4	B	224	GLY	6.0
14	L	60	VAL	6.0
17	O	50	VAL	6.0
17	O	130	MET	6.0
5	C	166	ILE	6.0
11	I	100	ILE	6.0
17	O	82	GLU	6.0
12	J	123	ASP	6.0
13	K	13	ARG	6.0
22	T	154	ARG	6.0
23	U	46	ASP	6.0
4	B	277	PRO	6.0
11	I	142	LYS	6.0
11	I	86	MET	6.0
3	A	173	GLY	6.0
29	1	159	VAL	6.0
28	Z	69	TYR	6.0
11	I	22	GLU	6.0
4	B	194	ARG	6.0
1	0	809	G	6.0
1	0	2770	G	6.0
4	B	320	GLN	6.0
4	B	336	GLN	6.0
13	K	23	ARG	6.0
23	U	61	ARG	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	132	ASP	5.9
10	H	20	CYS	5.9
19	Q	19	ARG	5.9
3	A	39	ALA	5.9
3	A	70	ALA	5.9
3	A	211	LYS	5.9
5	C	236	THR	5.9
9	G	90	LYS	5.9
15	M	50	GLN	5.9
17	O	133	ALA	5.9
29	1	169	THR	5.9
9	G	132	LEU	5.9
22	T	101	LEU	5.9
5	C	84	VAL	5.9
9	G	115	VAL	5.9
29	1	69	ILE	5.9
23	U	79	GLU	5.9
3	A	151	GLN	5.9
3	A	231	LYS	5.9
4	B	193	PHE	5.9
22	T	51	PHE	5.9
3	A	50	ALA	5.9
4	B	227	ALA	5.9
21	S	32	ALA	5.9
5	C	193	LEU	5.9
4	B	189	MET	5.9
7	E	15	ASP	5.9
18	P	22	ASN	5.9
24	V	134	PRO	5.9
4	B	105	HIS	5.9
4	B	331	SER	5.9
5	C	99	SER	5.9
9	G	89	HIS	5.9
16	N	86	VAL	5.9
29	1	38	ILE	5.9
1	0	2004	U	5.9
5	C	127	ARG	5.9
9	G	134	GLU	5.9
11	I	190	ARG	5.9
5	C	91	PRO	5.9
14	L	61	PRO	5.9
29	1	52	ASP	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	C	53	GLY	5.9
3	A	232	ARG	5.9
16	N	13	LYS	5.9
1	0	970	U	5.9
5	C	108	GLN	5.9
25	W	78	ALA	5.8
26	X	48	TYR	5.8
16	N	48	PRO	5.8
22	T	36	PRO	5.8
12	J	32	ASP	5.8
23	U	44	ASP	5.8
7	E	62	HIS	5.8
24	V	73	SER	5.8
3	A	4	ILE	5.8
9	G	128	LYS	5.8
12	J	37	LYS	5.8
12	J	115	ARG	5.8
17	O	44	VAL	5.8
24	V	121	GLU	5.8
25	W	46	LYS	5.8
1	0	1950	G	5.8
17	O	75	TRP	5.8
7	E	106	THR	5.8
5	C	167	ASP	5.8
22	T	50	ASP	5.8
1	0	735	C	5.8
1	0	1000	C	5.8
28	Z	38	ARG	5.8
5	C	216	SER	5.8
19	Q	115	GLU	5.8
28	Z	81	GLU	5.8
1	0	285	A	5.8
7	E	11	ASP	5.8
7	E	81	ASP	5.8
24	V	94	ASP	5.8
4	B	79	ARG	5.8
4	B	232	ARG	5.8
11	I	61	ILE	5.8
5	C	218	VAL	5.8
14	L	76	VAL	5.8
18	P	65	VAL	5.8
22	T	110	GLN	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	Q	15	PRO	5.8
20	R	49	LEU	5.8
24	V	76	ALA	5.8
3	A	165	THR	5.8
5	C	24	THR	5.8
14	L	13	ASP	5.8
16	N	55	ARG	5.8
29	1	57	LYS	5.8
1	0	365	G	5.8
1	0	1634	G	5.8
14	L	4	ASN	5.8
15	M	95	GLU	5.8
4	B	137	GLY	5.8
15	M	98	ILE	5.8
25	W	74	VAL	5.8
1	0	2241	C	5.8
3	A	150	PRO	5.7
9	G	105	LEU	5.7
21	S	23	LEU	5.7
8	F	91	HIS	5.7
8	F	86	ARG	5.7
11	I	42	ARG	5.7
28	Z	84	ARG	5.7
1	0	1279	U	5.7
4	B	294	THR	5.7
16	N	83	THR	5.7
3	A	33	GLU	5.7
24	V	68	GLU	5.7
10	H	11	GLY	5.7
24	V	70	GLY	5.7
14	L	114	ILE	5.7
3	A	20	SER	5.7
4	B	10	SER	5.7
29	1	94	GLN	5.7
3	A	141	PRO	5.7
5	C	30	LEU	5.7
26	X	30	LYS	5.7
10	H	35	HIS	5.7
17	O	79	ARG	5.7
7	E	86	ALA	5.7
24	V	17	ALA	5.7
3	A	93	THR	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	H	107	THR	5.7
29	1	77	THR	5.7
19	Q	109	GLU	5.7
25	W	28	ASP	5.7
3	A	228	ILE	5.7
28	Z	25	VAL	5.7
29	1	76	VAL	5.7
11	I	13	LYS	5.7
29	1	136	PRO	5.7
29	1	85	GLU	5.7
4	B	109	ASP	5.7
13	K	56	ASP	5.7
25	W	64	ILE	5.7
29	1	20	ILE	5.7
17	O	28	SER	5.7
9	G	80	LYS	5.7
11	I	84	LYS	5.7
11	I	43	PRO	5.7
12	J	45	PRO	5.7
15	M	65	ARG	5.7
25	W	13	ARG	5.7
7	E	20	LEU	5.7
5	C	239	ALA	5.7
12	J	39	GLU	5.7
17	O	93	GLU	5.7
3	A	233	THR	5.7
9	G	35	THR	5.7
27	Y	16	ASN	5.7
8	F	23	ILE	5.7
15	M	101	GLN	5.7
22	T	65	VAL	5.7
29	1	48	VAL	5.7
5	C	205	ARG	5.7
10	H	43	ARG	5.7
11	I	81	ARG	5.7
3	A	177	HIS	5.6
4	B	90	PRO	5.7
7	E	83	LEU	5.6
25	W	16	PRO	5.7
4	B	333	GLU	5.6
17	O	121	GLU	5.6
26	X	24	GLU	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	L	12	ALA	5.6
4	B	175	ASP	5.6
11	I	108	LYS	5.6
16	N	17	LYS	5.6
17	O	38	LYS	5.6
25	W	63	LYS	5.6
19	Q	12	ARG	5.6
4	B	38	VAL	5.6
27	Y	25	VAL	5.6
5	C	191	SER	5.6
24	V	91	HIS	5.6
12	J	33	ALA	5.6
4	B	97	THR	5.6
29	1	58	THR	5.6
7	E	30	LYS	5.6
9	G	56	LYS	5.6
5	C	78	ARG	5.6
21	S	53	ILE	5.6
9	G	17	CYS	5.6
17	O	24	SER	5.6
5	C	159	ALA	5.6
15	M	71	LYS	5.6
18	P	6	LYS	5.6
22	T	33	THR	5.6
22	T	140	LYS	5.6
5	C	97	ASP	5.6
16	N	44	ASP	5.6
10	H	42	ASN	5.6
24	V	58	ARG	5.6
29	1	114	ARG	5.6
4	B	192	ILE	5.6
15	M	31	ILE	5.6
3	A	138	VAL	5.6
28	Z	61	PRO	5.6
12	J	131	GLU	5.6
16	N	80	LYS	5.6
4	B	283	PHE	5.6
16	N	52	PHE	5.6
18	P	57	THR	5.6
4	B	128	ARG	5.6
6	D	56	ARG	5.6
15	M	109	ARG	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	Q	108	ARG	5.6
10	H	80	ILE	5.6
29	1	62	ILE	5.6
14	L	29	VAL	5.6
1	0	290	C	5.5
1	0	368	C	5.5
4	B	288	GLU	5.5
3	A	52	SER	5.5
5	C	51	TYR	5.5
29	1	82	TYR	5.5
28	Z	34	LYS	5.5
19	Q	110	ALA	5.5
17	O	104	PHE	5.5
10	H	85	GLY	5.5
15	M	82	GLY	5.5
12	J	69	ILE	5.5
11	I	139	PRO	5.5
3	A	105	VAL	5.5
10	H	31	VAL	5.5
15	M	40	VAL	5.5
15	M	46	GLU	5.5
15	M	138	GLU	5.5
17	O	20	GLU	5.5
17	O	91	LEU	5.5
8	F	21	SER	5.5
10	H	75	ARG	5.5
11	I	50	ARG	5.5
12	J	129	ALA	5.5
19	Q	63	ILE	5.5
23	U	33	ILE	5.5
4	B	259	HIS	5.5
3	A	42	VAL	5.5
15	M	125	LYS	5.5
17	O	69	LYS	5.5
5	C	180	SER	5.5
26	X	42	SER	5.5
5	C	182	ARG	5.5
9	G	41	ALA	5.5
15	M	29	GLY	5.5
22	T	123	GLY	5.5
8	F	20	ILE	5.5
14	L	11	ILE	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	L	48	ILE	5.5
18	P	7	HIS	5.5
4	B	45	LYS	5.5
11	I	102	GLU	5.5
21	S	19	GLU	5.5
4	B	250	VAL	5.5
9	G	26	VAL	5.5
9	G	61	VAL	5.5
24	V	42	VAL	5.5
5	C	213	ALA	5.5
15	M	48	ALA	5.5
24	V	16	ASP	5.5
24	V	37	HIS	5.5
5	C	85	LYS	5.5
5	C	229	PRO	5.5
10	H	78	LYS	5.5
17	O	148	GLU	5.5
21	S	62	GLU	5.5
5	C	100	LEU	5.5
16	N	73	VAL	5.4
19	Q	42	VAL	5.4
19	Q	89	ARG	5.4
5	C	164	ALA	5.4
2	9	122	C	5.4
15	M	12	ASP	5.4
15	M	52	LYS	5.4
22	T	104	GLU	5.4
5	C	184	ARG	5.4
18	P	31	ARG	5.4
23	U	68	SER	5.4
27	Y	12	ALA	5.4
9	G	71	TYR	5.4
7	E	85	HIS	5.4
11	I	174	LYS	5.4
4	B	101	THR	5.4
5	C	94	THR	5.4
5	C	131	PHE	5.4
24	V	95	ASP	5.4
26	X	17	THR	5.4
16	N	85	ILE	5.4
17	O	139	PRO	5.4
3	A	128	LEU	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	J	6	ARG	5.4
9	G	38	VAL	5.4
10	H	98	VAL	5.4
11	I	63	VAL	5.4
3	A	25	ALA	5.4
8	F	4	ALA	5.4
14	L	56	GLU	5.4
5	C	118	THR	5.4
29	1	162	PHE	5.4
3	A	8	ARG	5.4
14	L	10	LEU	5.4
3	A	5	GLN	5.4
3	A	146	LYS	5.4
19	Q	81	LYS	5.4
27	Y	4	SER	5.4
4	B	118	HIS	5.4
23	U	57	ALA	5.4
24	V	81	HIS	5.4
4	B	71	THR	5.4
9	G	112	ASP	5.4
29	1	147	ASP	5.4
4	B	312	ARG	5.4
29	1	65	PHE	5.4
22	T	100	LEU	5.4
3	A	188	ASN	5.3
26	X	12	ASN	5.3
7	E	80	GLN	5.3
27	Y	13	LYS	5.3
12	J	8	ARG	5.3
17	O	33	ARG	5.3
17	O	109	MET	5.3
7	E	33	THR	5.3
16	N	75	ILE	5.3
24	V	129	ILE	5.3
21	S	28	LEU	5.3
19	Q	64	ASN	5.3
3	A	43	VAL	5.3
4	B	214	VAL	5.3
7	E	54	VAL	5.3
15	M	7	LYS	5.3
1	0	2239	C	5.3
19	Q	20	HIS	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	B	197	GLU	5.3
14	L	42	GLU	5.3
10	H	130	MET	5.3
10	H	7	ASP	5.3
29	1	64	THR	5.3
17	O	88	PHE	5.3
1	0	716	G	5.3
5	C	162	VAL	5.3
7	E	2	VAL	5.3
1	0	2910	A	5.3
3	A	206	ARG	5.3
17	O	115	ALA	5.3
15	M	36	THR	5.3
28	Z	60	LYS	5.3
28	Z	43	ASN	5.3
3	A	74	VAL	5.3
4	B	246	VAL	5.3
26	X	8	GLN	5.3
3	A	28	GLU	5.3
21	S	4	HIS	5.3
5	C	36	ARG	5.3
23	U	59	TRP	5.3
21	S	52	ALA	5.3
3	A	203	GLY	5.3
15	M	18	LYS	5.3
19	Q	39	ASN	5.2
11	I	131	VAL	5.2
1	0	2253	G	5.2
7	E	57	GLU	5.2
9	G	96	GLU	5.2
10	H	87	ARG	5.2
12	J	27	ARG	5.2
22	T	8	ARG	5.2
29	1	32	ARG	5.2
5	C	125	ALA	5.2
16	N	26	PRO	5.2
22	T	70	ALA	5.2
4	B	180	ILE	5.2
22	T	54	PHE	5.2
7	E	60	VAL	5.2
20	R	47	ARG	5.2
22	T	128	VAL	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	514	G	5.2
19	Q	2	LYS	5.2
9	G	22	VAL	5.2
12	J	114	VAL	5.2
17	O	141	VAL	5.2
20	R	30	HIS	5.2
26	X	56	GLU	5.2
11	I	77	PRO	5.2
24	V	49	PRO	5.2
1	0	2254	G	5.2
9	G	127	ILE	5.2
24	V	23	ARG	5.2
27	Y	10	ARG	5.2
14	L	79	VAL	5.2
3	A	104	PRO	5.2
17	O	145	LEU	5.2
29	1	138	ILE	5.2
4	B	262	THR	5.1
9	G	95	ARG	5.1
10	H	76	GLN	5.1
5	C	234	VAL	5.1
16	N	30	VAL	5.1
25	W	48	LYS	5.1
29	1	161	VAL	5.1
11	I	7	TYR	5.1
3	A	196	ALA	5.1
17	O	99	ALA	5.1
18	P	24	LEU	5.1
4	B	164	ARG	5.1
10	H	115	ARG	5.1
15	M	133	SER	5.1
26	X	35	SER	5.1
16	N	32	GLU	5.1
7	E	8	VAL	5.1
22	T	48	VAL	5.1
25	W	58	GLY	5.1
11	I	132	ILE	5.1
4	B	179	ASP	5.1
5	C	104	ASP	5.1
12	J	49	SER	5.1
20	R	41	ASP	5.1
4	B	75	THR	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	L	34	GLU	5.1
19	Q	95	ASN	5.1
22	T	12	ASN	5.1
1	0	1951	G	5.1
10	H	83	PRO	5.1
11	I	133	LEU	5.1
18	P	14	ALA	5.1
1	0	1524	U	5.1
3	A	207	GLN	5.1
12	J	7	GLN	5.1
11	I	122	GLU	5.1
10	H	129	THR	5.1
19	Q	47	THR	5.1
15	M	16	VAL	5.1
24	V	99	VAL	5.1
11	I	9	ARG	5.1
17	O	132	ARG	5.1
26	X	45	ARG	5.1
11	I	171	LEU	5.1
14	L	41	ALA	5.1
15	M	70	ALA	5.1
15	M	135	ALA	5.1
22	T	146	ILE	5.1
28	Z	91	GLN	5.0
29	1	143	GLN	5.0
1	0	10	U	5.0
9	G	28	GLU	5.0
12	J	117	GLU	5.0
4	B	226	HIS	5.0
5	C	211	ASP	5.0
15	M	39	ASP	5.0
24	V	83	SER	5.0
19	Q	87	VAL	5.0
11	I	173	ARG	5.0
9	G	104	TYR	5.0
10	H	67	GLN	5.0
15	M	33	ASP	5.0
19	Q	94	SER	5.0
4	B	309	PRO	5.0
5	C	72	LYS	5.0
5	C	52	ALA	5.0
22	T	18	GLN	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
22	T	137	GLN	5.0
19	Q	92	ASP	5.0
22	T	16	ASP	5.0
7	E	99	THR	5.0
4	B	234	ARG	5.0
12	J	22	ARG	5.0
8	F	26	LYS	5.0
15	M	91	LYS	5.0
1	O	1528	A	5.0
3	A	136	ALA	5.0
12	J	111	ALA	5.0
25	W	59	HIS	5.0
25	W	82	ALA	5.0
12	J	124	ASP	5.0
5	C	187	ARG	5.0
1	O	2870	C	5.0
1	O	1523	G	5.0
5	C	35	VAL	5.0
12	J	48	LYS	5.0
17	O	66	VAL	5.0
23	U	69	LYS	5.0
24	V	106	VAL	5.0
4	B	131	HIS	4.9
11	I	56	ALA	4.9
18	P	17	ASP	4.9
9	G	74	ARG	4.9
20	R	33	SER	4.9
26	X	11	LYS	4.9
1	O	2508	C	4.9
16	N	39	VAL	4.9
17	O	94	ASN	4.9
13	K	180	LEU	4.9
10	H	113	ILE	4.9
3	A	26	ASP	4.9
3	A	217	ARG	4.9
8	F	65	ARG	4.9
21	S	16	ARG	4.9
25	W	34	LYS	4.9
6	D	96	SER	4.9
19	Q	28	SER	4.9
19	Q	90	PRO	4.9
3	A	137	VAL	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	L	99	GLU	4.9
2	9	25	G	4.9
21	S	9	ARG	4.9
3	A	48	ASP	4.9
4	B	8	LYS	4.9
17	O	76	ASP	4.9
18	P	62	LYS	4.9
20	R	35	LYS	4.9
21	S	58	THR	4.9
17	O	46	TYR	4.9
3	A	61	GLU	4.9
24	V	15	GLU	4.9
24	V	20	LEU	4.9
7	E	63	ILE	4.9
10	H	131	ILE	4.9
3	A	229	ALA	4.9
12	J	53	ARG	4.9
29	1	145	ALA	4.9
1	0	2869	G	4.9
7	E	76	PHE	4.9
26	X	26	SER	4.9
9	G	50	GLU	4.9
23	U	72	VAL	4.9
4	B	271	ILE	4.8
15	M	86	ALA	4.8
29	1	37	ASP	4.8
1	0	2250	G	4.8
4	B	241	TRP	4.8
29	1	30	THR	4.8
1	0	1527	A	4.8
3	A	199	HIS	4.8
3	A	51	ARG	4.8
15	M	83	LYS	4.8
22	T	120	PRO	4.8
16	N	60	THR	4.8
22	T	118	LEU	4.8
11	I	45	ARG	4.8
24	V	111	LYS	4.8
3	A	89	ALA	4.8
5	C	210	ALA	4.8
1	0	804	C	4.8
4	B	66	GLU	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	X	49	GLU	4.8
11	I	26	HIS	4.8
15	M	6	GLN	4.8
10	H	73	VAL	4.8
11	I	62	VAL	4.8
21	S	20	LEU	4.8
22	T	11	VAL	4.8
1	0	2251	G	4.8
1	0	808	A	4.8
4	B	221	LYS	4.8
12	J	19	LYS	4.8
24	V	80	LYS	4.8
17	O	61	GLN	4.8
29	1	163	GLN	4.8
3	A	111	SER	4.8
1	0	810	G	4.7
17	O	32	ALA	4.7
27	Y	26	MET	4.7
14	L	86	GLU	4.7
24	V	87	GLU	4.7
12	J	5	LYS	4.7
3	A	41	THR	4.7
4	B	18	ARG	4.7
14	L	19	ARG	4.7
15	M	80	ARG	4.7
24	V	33	ARG	4.7
19	Q	48	VAL	4.7
4	B	85	ALA	4.7
7	E	61	MET	4.7
29	1	146	ALA	4.7
1	0	1966	U	4.7
3	A	109	GLU	4.7
4	B	276	GLU	4.7
18	P	36	GLU	4.7
28	Z	62	THR	4.7
5	C	157	LEU	4.7
9	G	39	VAL	4.7
17	O	57	VAL	4.7
3	A	174	ASN	4.7
3	A	68	ILE	4.7
26	X	27	TYR	4.7
29	1	59	MET	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	C	204	ALA	4.7
22	T	40	ALA	4.7
23	U	60	ALA	4.7
12	J	3	LYS	4.7
16	N	82	LYS	4.7
8	F	16	ARG	4.7
19	Q	52	ARG	4.7
1	0	1160	G	4.7
4	B	96	LEU	4.7
22	T	116	LEU	4.7
3	A	76	VAL	4.7
14	L	43	VAL	4.7
15	M	134	VAL	4.7
3	A	99	ILE	4.7
10	H	64	MET	4.7
4	B	316	ARG	4.7
14	L	115	ARG	4.7
1	0	510	U	4.7
24	V	96	LEU	4.7
15	M	67	LYS	4.6
28	Z	76	LYS	4.6
3	A	22	ARG	4.6
9	G	141	ALA	4.6
24	V	127	ALA	4.6
8	F	1	LYS	4.6
5	C	192	ILE	4.6
1	0	2256	G	4.6
1	0	2344	G	4.6
9	G	84	ARG	4.6
19	Q	80	GLU	4.6
3	A	53	ALA	4.6
23	U	58	ALA	4.6
5	C	122	ASP	4.6
11	I	46	LEU	4.6
7	E	4	VAL	4.6
12	J	66	VAL	4.6
17	O	114	VAL	4.6
22	T	29	VAL	4.6
22	T	42	ARG	4.6
3	A	218	ASN	4.6
17	O	40	ALA	4.6
16	N	57	ASP	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	9	40	C	4.6
3	A	178	LYS	4.6
9	G	91	LYS	4.6
19	Q	26	THR	4.6
22	T	15	THR	4.6
3	A	182	ARG	4.6
4	B	94	ARG	4.6
5	C	212	VAL	4.6
17	O	128	ARG	4.6
1	0	2914	A	4.6
15	M	38	GLU	4.6
22	T	10	GLU	4.6
24	V	122	GLU	4.6
16	N	6	PRO	4.6
17	O	84	ALA	4.6
29	1	137	ASP	4.6
5	C	109	LEU	4.6
10	H	59	LYS	4.6
11	I	55	LYS	4.6
13	K	28	LYS	4.6
16	N	62	THR	4.6
17	O	110	THR	4.6
11	I	159	ARG	4.5
15	M	87	ARG	4.5
15	M	106	ARG	4.5
9	G	34	GLU	4.5
22	T	134	GLU	4.5
1	0	363	A	4.5
15	M	88	GLN	4.5
7	E	82	ASP	4.5
17	O	23	MET	4.5
5	C	231	ARG	4.5
19	Q	93	THR	4.5
15	M	92	GLU	4.5
17	O	42	GLU	4.5
4	B	68	VAL	4.5
4	B	289	VAL	4.5
1	0	138	U	4.5
17	O	64	SER	4.5
3	A	193	ALA	4.5
5	C	117	ALA	4.5
5	C	101	ASP	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	B	25	ARG	4.5
27	Y	7	THR	4.5
15	M	130	GLU	4.5
18	P	12	GLU	4.5
11	I	170	GLY	4.5
4	B	41	PHE	4.5
29	1	141	VAL	4.5
9	G	108	PRO	4.5
22	T	72	PRO	4.5
1	0	2911	C	4.5
28	Z	68	LYS	4.5
11	I	51	ALA	4.5
14	L	50	ARG	4.5
24	V	57	ARG	4.5
14	L	103	GLU	4.5
10	H	14	LYS	4.5
17	O	60	LYS	4.5
3	A	81	GLN	4.5
1	0	280	C	4.5
1	0	2346	C	4.5
5	C	83	ALA	4.5
7	E	42	ARG	4.5
18	P	58	MET	4.5
10	H	29	LEU	4.5
29	1	130	GLU	4.5
15	M	1	THR	4.4
3	A	169	PHE	4.4
29	1	34	TRP	4.4
5	C	77	ALA	4.4
9	G	102	ARG	4.4
10	H	27	ARG	4.4
11	I	105	ALA	4.4
3	A	140	LEU	4.4
5	C	95	GLU	4.4
5	C	196	THR	4.4
3	A	24	LYS	4.4
14	L	15	LYS	4.4
3	A	156	ILE	4.4
11	I	8	ILE	4.4
16	N	40	HIS	4.4
5	C	235	PHE	4.4
17	O	63	ASN	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	B	46	ALA	4.4
5	C	38	ALA	4.4
5	C	116	ALA	4.4
1	0	289	G	4.4
1	0	2912	C	4.4
1	0	2252	A	4.4
19	Q	107	LYS	4.4
7	E	50	VAL	4.4
5	C	67	GLN	4.4
9	G	65	ASN	4.4
21	S	54	ALA	4.4
25	W	50	ALA	4.4
9	G	137	GLU	4.4
16	N	42	LYS	4.4
1	0	1948	G	4.4
14	L	57	THR	4.4
28	Z	65	THR	4.4
29	1	148	ILE	4.4
5	C	80	VAL	4.4
10	H	81	ARG	4.4
3	A	125	ASN	4.4
1	0	1965	C	4.3
10	H	32	ILE	4.3
1	0	601	G	4.3
1	0	604	G	4.3
1	0	2338	G	4.3
3	A	7	GLN	4.3
3	A	179	MET	4.3
3	A	189	VAL	4.3
3	A	57	ALA	4.3
22	T	150	LEU	4.3
18	P	54	THR	4.3
23	U	71	ARG	4.3
5	C	39	GLN	4.3
1	0	254	C	4.3
1	0	1208	C	4.3
16	N	47	VAL	4.3
4	B	267	ARG	4.3
1	0	1967	U	4.3
3	A	220	PRO	4.3
5	C	81	PRO	4.3
17	O	19	ARG	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	Z	31	THR	4.3
8	F	49	VAL	4.3
3	A	185	LYS	4.3
14	L	88	LYS	4.3
5	C	37	ALA	4.3
17	O	77	ALA	4.3
22	T	73	LEU	4.3
1	0	2700	G	4.3
17	O	85	SER	4.3
16	N	38	LYS	4.3
1	0	2248	C	4.3
12	J	109	LEU	4.3
4	B	261	ARG	4.3
12	J	30	ARG	4.3
18	P	67	ARG	4.3
3	A	47	HIS	4.2
1	0	370	G	4.2
3	A	194	MET	4.2
4	B	78	MET	4.2
9	G	82	THR	4.2
17	O	86	LYS	4.2
4	B	162	GLU	4.2
22	T	79	VAL	4.2
1	0	2526	C	4.2
22	T	130	HIS	4.2
15	M	53	ASP	4.2
1	0	1221	G	4.2
1	0	1605	G	4.2
1	0	2316	G	4.2
1	0	2909	G	4.2
17	O	119	VAL	4.2
5	C	18	LEU	4.2
16	N	46	SER	4.2
22	T	57	PRO	4.2
11	I	57	LYS	4.2
18	P	51	GLN	4.2
3	A	10	GLY	4.2
14	L	49	GLU	4.2
16	N	10	THR	4.2
29	1	46	THR	4.2
2	9	73	G	4.2
1	0	281	U	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	I	64	ARG	4.2
19	Q	24	ARG	4.2
17	O	87	ALA	4.2
17	O	58	PRO	4.2
4	B	121	ASP	4.2
15	M	28	GLN	4.2
1	0	288	A	4.2
1	0	361	C	4.2
9	G	36	VAL	4.2
19	Q	23	VAL	4.2
1	0	805	G	4.2
1	0	1216	G	4.2
1	0	2249	G	4.2
2	9	53	G	4.2
10	H	46	LYS	4.2
21	S	51	LYS	4.2
5	C	98	ARG	4.1
24	V	131	VAL	4.1
11	I	128	TRP	4.1
3	A	171	LYS	4.1
10	H	52	LYS	4.1
4	B	265	ASN	4.1
12	J	20	ASN	4.1
2	9	22	G	4.1
14	L	5	PRO	4.1
10	H	22	ASP	4.1
22	T	126	ASP	4.1
3	A	9	ARG	4.1
28	Z	70	ARG	4.1
10	H	124	VAL	4.1
10	H	95	ALA	4.1
17	O	95	ALA	4.1
4	B	190	ASN	4.1
1	0	1949	G	4.1
17	O	142	ASP	4.1
3	A	3	ARG	4.1
4	B	84	ARG	4.1
15	M	8	ARG	4.1
3	A	103	VAL	4.1
14	L	64	VAL	4.1
27	Y	8	LYS	4.1
19	Q	51	LEU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	807	A	4.1
1	0	2255	A	4.1
3	A	126	ALA	4.1
5	C	58	ALA	4.1
4	B	247	ARG	4.1
5	C	7	ASP	4.1
11	I	104	ARG	4.1
11	I	127	LYS	4.1
3	A	55	VAL	4.1
1	0	2509	A	4.1
18	P	26	PHE	4.1
4	B	264	LEU	4.0
4	B	295	LEU	4.0
19	Q	73	HIS	4.0
22	T	112	LEU	4.0
9	G	25	GLN	4.0
1	0	573	A	4.0
1	0	1701	A	4.0
1	0	1919	A	4.0
1	0	2291	A	4.0
22	T	46	ALA	4.0
1	0	2335	C	4.0
24	V	50	ARG	4.0
1	0	1561	U	4.0
28	Z	75	GLY	4.0
3	A	110	SER	4.0
5	C	113	SER	4.0
11	I	112	MET	4.0
3	A	15	THR	4.0
24	V	19	LEU	4.0
4	B	315	VAL	4.0
24	V	93	VAL	4.0
1	0	1159	G	4.0
1	0	1589	G	4.0
9	G	92	GLN	4.0
5	C	217	GLU	4.0
9	G	99	GLU	4.0
1	0	1562	C	4.0
22	T	7	LEU	4.0
26	X	28	HIS	4.0
10	H	55	VAL	4.0
10	H	74	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	N	56	PHE	4.0
19	Q	38	ARG	4.0
1	0	2771	G	4.0
1	0	1157	C	4.0
9	G	86	MET	4.0
1	0	1519	U	4.0
1	0	2247	C	4.0
5	C	60	SER	4.0
5	C	69	HIS	4.0
22	T	141	HIS	4.0
4	B	112	LEU	4.0
3	A	155	THR	4.0
14	L	39	THR	4.0
4	B	216	ARG	4.0
11	I	90	ARG	4.0
14	L	112	ARG	4.0
22	T	71	GLU	3.9
25	W	77	LYS	3.9
1	0	324	G	3.9
1	0	369	G	3.9
15	M	93	ASP	3.9
1	0	1927	A	3.9
1	0	2506	A	3.9
1	0	605	C	3.9
19	Q	67	LEU	3.9
11	I	93	ARG	3.9
5	C	178	GLN	3.9
10	H	44	HIS	3.9
10	H	53	ILE	3.9
1	0	806	A	3.9
1	0	1526	A	3.9
1	0	586	C	3.9
26	X	10	LYS	3.9
4	B	69	PRO	3.9
4	B	70	VAL	3.9
17	O	34	GLU	3.9
3	A	219	ALA	3.9
17	O	51	ILE	3.9
4	B	139	LEU	3.9
5	C	188	ARG	3.9
1	0	736	A	3.9
16	N	87	THR	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	362	G	3.9
12	J	73	VAL	3.9
17	O	17	MET	3.9
5	C	90	HIS	3.9
5	C	120	ASP	3.9
10	H	30	LYS	3.9
24	V	38	LYS	3.9
19	Q	75	GLU	3.9
4	B	313	PRO	3.9
1	0	2242	U	3.8
1	0	2890	A	3.9
1	0	575	G	3.8
2	9	32	G	3.8
2	9	41	C	3.8
15	M	73	HIS	3.8
14	L	96	VAL	3.8
1	0	2697	A	3.8
1	0	1806	G	3.8
1	0	2698	G	3.8
4	B	140	ARG	3.8
16	N	31	GLU	3.8
25	W	24	VAL	3.8
1	0	286	U	3.8
1	0	2419	U	3.8
1	0	737	A	3.8
2	9	57	A	3.8
5	C	181	ALA	3.8
14	L	35	LYS	3.8
24	V	72	ARG	3.8
4	B	235	ILE	3.8
1	0	373	G	3.8
1	0	599	G	3.8
1	0	969	G	3.8
1	0	1211	G	3.8
11	I	161	LEU	3.8
15	M	3	LEU	3.8
19	Q	16	LEU	3.8
3	A	224	LYS	3.8
14	L	63	LYS	3.8
1	0	2240	U	3.8
3	A	118	PHE	3.8
1	0	593	A	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
24	V	108	ILE	3.8
1	0	560	C	3.8
1	0	574	C	3.8
1	0	1666	C	3.8
14	L	9	SER	3.7
19	Q	96	VAL	3.7
21	S	55	ARG	3.7
5	C	228	ALA	3.7
1	0	1149	U	3.7
1	0	272	A	3.7
1	0	1912	A	3.7
3	A	195	ASN	3.7
5	C	54	LEU	3.7
1	0	279	C	3.7
11	I	176	ARG	3.7
24	V	41	ARG	3.7
5	C	89	ALA	3.7
9	G	23	ALA	3.7
1	0	1282	U	3.7
2	9	55	U	3.7
1	0	1355	A	3.7
1	0	1615	A	3.7
3	A	209	PRO	3.7
3	A	139	LYS	3.7
17	O	36	LYS	3.7
24	V	63	LYS	3.7
1	0	1579	C	3.7
1	0	2510	C	3.7
1	0	367	G	3.7
1	0	1137	G	3.7
1	0	1665	G	3.7
1	0	2826	G	3.7
5	C	121	ALA	3.7
3	A	16	PHE	3.7
25	W	47	LEU	3.7
4	B	24	PRO	3.7
14	L	90	ASP	3.7
5	C	96	LYS	3.7
1	0	1144	A	3.7
10	H	96	VAL	3.7
1	0	2243	C	3.7
1	0	1627	G	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	371	U	3.7
1	0	1219	U	3.7
1	0	262	A	3.6
9	G	101	VAL	3.6
24	V	123	GLU	3.6
29	1	110	GLU	3.6
1	0	1521	C	3.6
20	R	21	PHE	3.6
10	H	89	LYS	3.6
14	L	38	ARG	3.6
16	N	51	ARG	3.6
21	S	50	ARG	3.6
1	0	572	G	3.6
1	0	1158	G	3.6
1	0	1555	G	3.6
13	K	183	ASP	3.6
1	0	1964	U	3.6
25	W	62	TYR	3.6
1	0	2103	A	3.6
1	0	2437	A	3.6
5	C	233	THR	3.6
5	C	199	GLU	3.6
1	0	1914	C	3.6
1	0	1928	C	3.6
2	9	28	U	3.6
2	9	94	G	3.6
15	M	123	TYR	3.6
5	C	220	THR	3.6
3	A	46	GLU	3.6
1	0	1150	A	3.6
1	0	1522	A	3.6
11	I	95	LYS	3.6
12	J	54	PRO	3.6
14	L	36	PRO	3.6
22	T	119	HIS	3.6
1	0	1520	G	3.6
1	0	1611	G	3.6
1	0	2882	G	3.6
3	A	197	VAL	3.6
5	C	26	VAL	3.6
11	I	58	LYS	3.6
19	Q	74	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	1630	A	3.6
2	9	3	A	3.6
19	Q	3	GLN	3.6
28	Z	52	PHE	3.6
1	0	803	C	3.5
2	9	39	U	3.5
11	I	94	LYS	3.5
19	Q	6	LYS	3.5
1	0	738	G	3.5
4	B	321	PRO	3.5
1	0	811	C	3.5
1	0	1213	C	3.5
4	B	223	LYS	3.5
17	O	71	LYS	3.5
22	T	133	LYS	3.5
29	1	113	PRO	3.5
1	0	602	A	3.5
1	0	1628	G	3.5
1	0	2336	G	3.5
3	A	117	LYS	3.5
17	O	29	LYS	3.5
4	B	161	MET	3.5
9	G	19	MET	3.5
24	V	103	THR	3.5
16	N	43	ILE	3.5
23	U	54	ILE	3.5
1	0	1603	A	3.5
2	9	34	A	3.5
1	0	375	G	3.5
1	0	817	G	3.5
18	P	19	ASP	3.5
26	X	46	ARG	3.5
2	9	42	C	3.5
24	V	32	ASN	3.4
1	0	2880	A	3.4
5	C	168	ARG	3.4
4	B	268	LEU	3.4
10	H	4	LEU	3.4
1	0	31	C	3.4
1	0	2334	C	3.4
10	H	37	TYR	3.4
15	M	100	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	C	23	GLU	3.4
29	1	139	GLU	3.4
1	0	1626	A	3.4
2	9	56	A	3.4
1	0	2257	G	3.4
5	C	70	VAL	3.4
9	G	135	ILE	3.4
1	0	139	C	3.4
25	W	27	ARG	3.4
14	L	44	ASN	3.4
4	B	11	LEU	3.4
1	0	358	G	3.4
1	0	2446	G	3.4
2	9	109	G	3.4
26	X	16	HIS	3.4
1	0	2878	U	3.4
5	C	219	ASN	3.4
11	I	111	ASN	3.4
1	0	1207	A	3.4
20	R	19	THR	3.4
3	A	11	ARG	3.4
1	0	89	G	3.3
1	0	1610	G	3.3
1	0	1153	C	3.3
3	A	124	VAL	3.3
10	H	34	VAL	3.3
21	S	59	ILE	3.3
1	0	1915	U	3.3
1	0	1529	G	3.3
1	0	1636	G	3.3
2	9	110	G	3.3
28	Z	49	ASP	3.3
1	0	1570	C	3.3
1	0	1633	C	3.3
1	0	2825	C	3.3
15	M	2	ASP	3.3
1	0	125	U	3.3
10	H	10	GLN	3.3
1	0	1210	G	3.3
1	0	2871	G	3.3
1	0	287	C	3.3
4	B	5	ARG	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	1	160	ARG	3.3
1	0	2511	A	3.3
3	A	175	LYS	3.3
18	P	55	GLN	3.3
1	0	366	U	3.3
1	0	1530	U	3.3
1	0	2512	U	3.3
5	C	112	ARG	3.3
1	0	856	G	3.3
1	0	1283	G	3.3
1	0	1441	G	3.3
1	0	2516	G	3.3
5	C	59	GLU	3.3
1	0	1253	C	3.3
5	C	119	ALA	3.3
1	0	1804	A	3.2
1	0	2879	A	3.2
21	S	27	LEU	3.2
1	0	571	C	3.2
1	0	2505	G	3.2
14	L	16	SER	3.2
3	A	223	ARG	3.2
1	0	1671	U	3.2
18	P	23	LYS	3.2
3	A	119	ALA	3.2
1	0	557	C	3.2
1	0	2351	C	3.2
1	0	2638	G	3.2
17	O	90	ASP	3.2
1	0	2486	A	3.2
22	T	132	VAL	3.2
24	V	30	GLN	3.2
1	0	87	C	3.2
1	0	598	C	3.2
1	0	1551	C	3.2
1	0	2349	G	3.2
2	9	66	G	3.2
16	N	41	LEU	3.2
20	R	14	GLU	3.2
1	0	360	A	3.2
1	0	549	A	3.2
1	0	2513	A	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	2913	A	3.2
2	9	51	A	3.2
2	9	52	A	3.2
1	0	1788	U	3.2
10	H	82	ARG	3.1
1	0	1209	C	3.1
2	9	72	C	3.1
3	A	208	HIS	3.1
1	0	90	A	3.1
25	W	73	THR	3.1
17	O	27	HIS	3.1
1	0	717	C	3.1
1	0	2747	C	3.1
2	9	118	C	3.1
1	0	496	G	3.1
1	0	1143	G	3.1
1	0	2772	G	3.1
2	9	49	G	3.1
1	0	587	A	3.1
1	0	603	A	3.1
5	C	42	ARG	3.1
5	C	174	ILE	3.1
29	1	61	THR	3.1
29	1	73	PHE	3.1
3	A	107	ASN	3.1
1	0	364	C	3.1
1	0	1126	C	3.1
9	G	60	ARG	3.1
1	0	1280	A	3.1
1	0	1782	G	3.1
1	0	1925	G	3.1
1	0	2135	A	3.1
15	M	104	LYS	3.1
21	S	14	ALA	3.1
11	I	103	GLU	3.1
28	Z	79	LEU	3.1
5	C	87	ARG	3.1
1	0	256	C	3.1
1	0	291	C	3.1
1	0	1215	A	3.0
1	0	2908	A	3.0
2	9	33	U	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	2884	G	3.0
5	C	200	PRO	3.0
19	Q	41	ARG	3.0
5	C	154	VAL	3.0
10	H	88	VAL	3.0
1	0	295	C	3.0
1	0	585	C	3.0
1	0	2348	C	3.0
1	0	1664	A	3.0
1	0	579	G	3.0
2	9	20	G	3.0
22	T	47	LYS	3.0
26	X	15	THR	3.0
3	A	144	GLU	3.0
1	0	1156	C	3.0
1	0	2636	C	3.0
1	0	2852	A	3.0
1	0	2891	A	3.0
1	0	1608	G	3.0
2	9	17	G	3.0
5	C	44	GLN	3.0
5	C	195	VAL	3.0
14	L	17	ALA	3.0
20	R	27	ALA	3.0
5	C	79	ARG	3.0
2	9	29	C	3.0
22	T	4	LEU	3.0
24	V	132	LEU	3.0
1	0	372	A	3.0
1	0	1682	A	3.0
1	0	2896	A	3.0
1	0	600	G	2.9
19	Q	66	ASP	2.9
1	0	1380	U	2.9
1	0	1494	A	2.9
1	0	1572	A	2.9
2	9	65	A	2.9
1	0	2352	G	2.9
1	0	2438	G	2.9
2	9	50	G	2.9
15	M	102	ARG	2.9
1	0	1807	U	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	2849	U	2.9
2	9	31	C	2.9
1	0	1442	A	2.9
1	0	2814	A	2.9
17	O	92	LEU	2.9
1	0	1217	G	2.9
1	0	1438	G	2.9
1	0	1805	G	2.9
2	9	58	G	2.9
17	O	140	GLN	2.9
3	A	122	SER	2.9
9	G	58	GLU	2.9
1	0	1972	U	2.9
1	0	323	C	2.9
1	0	576	C	2.9
1	0	2804	C	2.9
1	0	2903	C	2.9
17	O	111	ILE	2.9
1	0	45	A	2.9
1	0	278	A	2.9
1	0	1088	A	2.9
1	0	1427	A	2.9
1	0	1612	A	2.9
14	L	47	ARG	2.9
1	0	581	G	2.9
1	0	1926	G	2.9
1	0	2877	G	2.9
4	B	253	GLN	2.9
29	1	31	ARG	2.8
1	0	255	A	2.8
1	0	2694	A	2.8
3	A	17	ARG	2.8
25	W	49	ARG	2.8
1	0	1819	G	2.8
1	0	2333	G	2.8
1	0	2692	G	2.8
1	0	2851	G	2.8
2	9	21	G	2.8
1	0	2830	U	2.8
1	0	309	C	2.8
1	0	2881	C	2.8
2	9	59	C	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	67	A	2.8
1	0	1968	A	2.8
1	0	2703	A	2.8
1	0	2827	A	2.8
22	T	23	MET	2.8
18	P	13	LYS	2.8
24	V	31	PHE	2.8
27	Y	5	LYS	2.8
1	0	296	G	2.8
1	0	588	G	2.8
1	0	1809	G	2.8
24	V	69	ALA	2.8
1	0	2868	C	2.8
1	0	86	A	2.8
1	0	397	A	2.8
1	0	1624	A	2.8
1	0	359	U	2.8
1	0	2527	U	2.8
1	0	583	G	2.8
1	0	1655	G	2.8
9	G	21	ARG	2.8
1	0	1154	A	2.8
1	0	1518	A	2.8
2	9	27	C	2.8
17	O	62	HIS	2.8
19	Q	91	LEU	2.7
1	0	559	U	2.7
1	0	964	G	2.7
1	0	1496	G	2.7
1	0	943	A	2.7
1	0	1550	A	2.7
1	0	2850	C	2.7
2	9	63	C	2.7
12	J	120	LEU	2.7
18	P	63	LYS	2.7
22	T	69	ARG	2.7
24	V	78	ARG	2.7
5	C	221	GLU	2.7
17	O	144	GLU	2.7
1	0	140	G	2.7
1	0	353	G	2.7
1	0	1151	G	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	1563	G	2.7
1	0	1614	G	2.7
1	0	1621	G	2.7
1	0	1670	G	2.7
1	0	1878	G	2.7
1	0	2289	G	2.7
1	0	294	C	2.7
1	0	591	A	2.7
1	0	704	C	2.7
1	0	1609	C	2.7
1	0	1642	A	2.7
1	0	2676	C	2.7
4	B	266	LYS	2.7
1	0	396	U	2.7
1	0	2866	U	2.7
1	0	2872	U	2.7
17	O	25	PHE	2.7
1	0	273	G	2.7
1	0	577	G	2.7
1	0	938	G	2.7
1	0	1552	G	2.7
1	0	1663	G	2.7
17	O	26	LYS	2.7
1	0	1635	U	2.7
1	0	2290	U	2.7
1	0	2100	A	2.6
1	0	196	G	2.6
1	0	1021	G	2.6
1	0	1214	G	2.6
1	0	1281	C	2.6
1	0	2360	C	2.6
1	0	2823	G	2.6
2	9	30	C	2.6
5	C	106	GLU	2.6
1	0	374	U	2.6
1	0	713	U	2.6
1	0	1587	U	2.6
1	0	2889	U	2.6
1	0	562	A	2.6
1	0	2258	A	2.6
2	9	54	A	2.6
1	0	1916	C	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	2104	C	2.6
2	9	26	C	2.6
2	9	121	C	2.6
1	0	104	G	2.6
1	0	219	G	2.6
1	0	1730	G	2.6
5	C	105	LYS	2.6
5	C	173	LYS	2.6
1	0	1244	U	2.6
1	0	2705	U	2.6
22	T	122	ARG	2.6
1	0	1930	A	2.6
1	0	2885	A	2.6
1	0	298	C	2.6
1	0	544	G	2.6
1	0	1498	G	2.6
1	0	2099	G	2.6
1	0	2134	G	2.6
1	0	2667	G	2.6
1	0	2887	G	2.6
24	V	130	ARG	2.6
1	0	1702	U	2.6
1	0	563	C	2.5
1	0	1142	C	2.5
1	0	681	G	2.5
1	0	1629	G	2.5
1	0	2867	G	2.5
1	0	1220	U	2.5
1	0	1903	U	2.5
2	9	18	U	2.5
5	C	111	VAL	2.5
27	Y	6	ALA	2.5
1	0	124	C	2.5
1	0	719	C	2.5
1	0	2515	C	2.5
1	0	322	G	2.5
1	0	1113	G	2.5
1	0	2337	G	2.5
1	0	2375	G	2.5
1	0	734	U	2.5
1	0	1905	U	2.5
1	0	95	A	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	1152	A	2.5
1	0	1669	A	2.5
21	S	57	LYS	2.5
1	0	584	U	2.5
1	0	753	U	2.5
1	0	825	U	2.5
1	0	2246	U	2.5
1	0	2876	G	2.5
1	0	495	A	2.5
1	0	2883	A	2.5
1	0	558	C	2.5
1	0	2347	C	2.5
1	0	2824	C	2.5
1	0	2873	C	2.5
1	0	1511	U	2.5
1	0	1568	G	2.5
1	0	1586	G	2.5
1	0	1947	G	2.5
1	0	2350	G	2.5
1	0	2421	G	2.5
1	0	2507	G	2.5
2	9	19	G	2.5
29	1	72	MET	2.5
1	0	1934	A	2.4
1	0	578	C	2.4
29	1	29	VAL	2.4
1	0	1544	U	2.4
1	0	1546	G	2.4
1	0	1604	G	2.4
1	0	2730	G	2.4
1	0	498	A	2.4
1	0	438	C	2.4
1	0	492	C	2.4
1	0	2695	C	2.4
1	0	2831	C	2.4
2	9	113	C	2.4
15	M	10	ALA	2.4
1	0	2282	U	2.4
1	0	2888	U	2.4
15	M	49	ILE	2.4
1	0	307	G	2.4
1	0	1497	G	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	2836	G	2.4
5	C	27	ARG	2.4
1	0	2332	A	2.4
2	9	62	A	2.4
23	U	39	LYS	2.4
1	0	251	C	2.4
1	0	729	C	2.4
1	0	1517	U	2.4
1	0	1584	C	2.4
1	0	2693	U	2.4
2	9	111	U	2.4
4	B	238	LEU	2.4
1	0	201	G	2.4
1	0	257	G	2.4
1	0	1622	G	2.4
1	0	1799	G	2.4
1	0	2570	G	2.4
1	0	2829	G	2.4
1	0	96	A	2.4
1	0	1631	A	2.4
1	0	1641	A	2.4
1	0	1667	A	2.4
1	0	2784	A	2.4
1	0	1554	U	2.3
17	O	118	LYS	2.3
1	0	1902	G	2.3
1	0	2355	G	2.3
1	0	2696	G	2.3
18	P	56	ASN	2.3
1	0	1637	A	2.3
1	0	2812	A	2.3
1	0	1029	U	2.3
1	0	1480	U	2.3
1	0	705	C	2.3
1	0	1911	C	2.3
1	0	2534	C	2.3
10	H	8	VAL	2.3
1	0	561	G	2.3
1	0	802	G	2.3
1	0	1908	G	2.3
1	0	2810	G	2.3
1	0	2892	G	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	102	A	2.3
1	0	1406	A	2.3
16	N	59	GLN	2.3
1	0	714	U	2.3
1	0	1218	U	2.3
1	0	1564	C	2.3
1	0	2287	C	2.3
1	0	2786	G	2.3
1	0	2074	A	2.3
9	G	83	ILE	2.3
1	0	260	C	2.3
1	0	344	C	2.3
1	0	813	C	2.3
1	0	1699	C	2.3
18	P	34	LYS	2.2
1	0	1252	A	2.2
1	0	1379	A	2.2
1	0	2460	A	2.2
1	0	314	G	2.2
1	0	592	G	2.2
1	0	940	G	2.2
1	0	1802	G	2.2
1	0	2420	G	2.2
1	0	1939	U	2.2
1	0	271	C	2.2
1	0	1026	C	2.2
1	0	1790	C	2.2
2	9	46	C	2.2
7	E	67	ALA	2.2
5	C	175	LYS	2.2
28	Z	51	LYS	2.2
1	0	352	A	2.2
1	0	961	A	2.2
1	0	1114	A	2.2
1	0	2353	A	2.2
1	0	595	U	2.2
1	0	1488	U	2.2
1	0	2726	U	2.2
1	0	2749	U	2.2
1	0	78	G	2.2
1	0	91	G	2.2
1	0	275	G	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	1155	G	2.2
1	0	2855	G	2.2
1	0	311	C	2.2
1	0	1854	C	2.2
2	9	36	C	2.2
10	H	49	LEU	2.2
17	O	146	ILE	2.2
1	0	462	A	2.2
1	0	614	U	2.2
1	0	1770	U	2.2
1	0	2374	A	2.2
1	0	2805	A	2.2
1	0	77	G	2.2
1	0	1378	G	2.2
1	0	1540	G	2.2
1	0	1697	G	2.2
1	0	2564	G	2.2
2	9	43	G	2.2
1	0	594	C	2.2
1	0	1450	C	2.2
1	0	1700	C	2.2
1	0	2886	C	2.2
1	0	411	A	2.1
1	0	489	A	2.1
1	0	1246	A	2.1
1	0	1559	A	2.1
1	0	1791	U	2.2
1	0	2875	A	2.1
1	0	422	G	2.1
1	0	644	G	2.1
1	0	2285	G	2.1
1	0	2288	G	2.1
15	M	35	ILE	2.1
1	0	1768	C	2.1
1	0	2785	C	2.1
1	0	2857	C	2.1
4	B	228	ARG	2.1
3	A	167	LYS	2.1
1	0	325	U	2.1
1	0	2328	U	2.1
1	0	129	A	2.1
1	0	939	A	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	2474	A	2.1
1	0	2813	A	2.1
2	9	45	A	2.1
2	9	93	A	2.1
1	0	1588	G	2.1
1	0	350	C	2.1
1	0	356	C	2.1
1	0	1146	C	2.1
1	0	1613	C	2.1
1	0	1792	C	2.1
2	9	69	U	2.1
1	0	700	A	2.1
1	0	2354	A	2.1
1	0	292	G	2.1
1	0	503	G	2.1
1	0	1145	G	2.1
1	0	1765	G	2.1
1	0	1812	G	2.1
1	0	1979	G	2.1
1	0	2324	G	2.1
1	0	2708	G	2.1
1	0	2874	G	2.1
1	0	188	C	2.1
1	0	376	C	2.1
1	0	440	C	2.1
1	0	1377	C	2.1
1	0	2329	C	2.1
1	0	2439	C	2.1
9	G	103	VAL	2.1
1	0	1505	U	2.1
1	0	2514	U	2.1
1	0	1591	A	2.1
1	0	2568	A	2.1
1	0	141	C	2.1
1	0	142	G	2.0
1	0	545	G	2.0
1	0	703	G	2.0
1	0	1384	C	2.1
1	0	1571	G	2.0
1	0	1662	C	2.1
1	0	1781	G	2.0
1	0	1787	C	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	9	74	G	2.0
5	C	110	ALA	2.0
1	0	548	U	2.0
1	0	1408	U	2.0
1	0	1583	U	2.0
1	0	1907	U	2.0
1	0	2373	U	2.0
1	0	1606	A	2.0
1	0	1857	A	2.0
1	0	2702	A	2.0
1	0	235	C	2.0
1	0	490	C	2.0
1	0	1593	C	2.0
1	0	1769	C	2.0
1	0	2409	C	2.0
1	0	2907	C	2.0
1	0	345	G	2.0
1	0	564	G	2.0
1	0	795	G	2.0
1	0	1224	G	2.0
1	0	1971	G	2.0
1	0	2567	G	2.0
1	0	2858	U	2.0
1	0	1904	A	2.0
1	0	1924	A	2.0
1	0	2699	A	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
32	CD	X	102	1/1	0.82	0.11	48,48,48,48	0
30	K	0	2924	1/1	0.87	0.24	30,30,30,30	0
31	MG	0	2926	1/1	0.94	0.09	30,30,30,30	0
32	CD	R	101	1/1	0.96	0.06	39,39,39,39	0
32	CD	W	103	1/1	0.96	0.05	30,30,30,30	0
31	MG	0	2925	1/1	0.96	0.07	30,30,30,30	0
32	CD	Z	104	1/1	0.97	0.16	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.