Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:03 PM GMT

PDB ID   :   2IZM
Title   :   MS2-RNA HAIRPIN (C-10) COMPLEX
Authors   :   Helgstrand, C.; Grahn, E.; Moss, T.; Stonehouse, N.J.; Tars, K.; Stockley, P.G.; Liljas, L.
Deposited on :   2006-07-25
Resolution :   2.70 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.70 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	Percentile Ranks	Value
Rfree		0.588
Clashscore		11
Ramachandran outliers		0.3%
Sidechain outliers		4.1%
RSRZ outliers		39.7%
RNA backbone		0.50

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
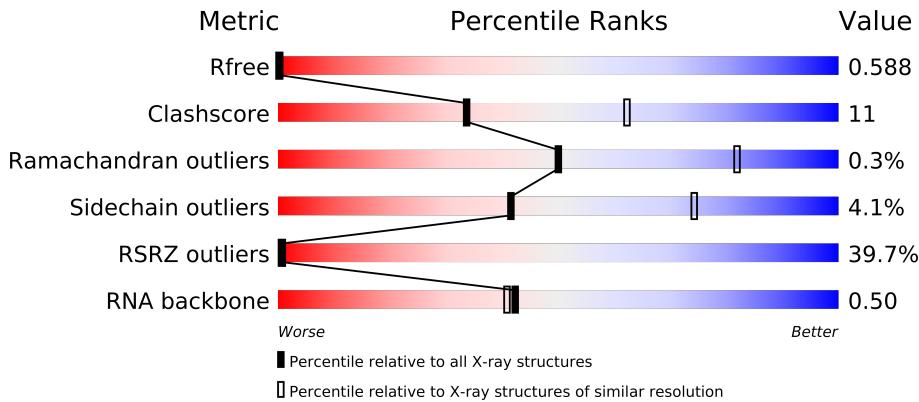
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)
RNA backbone	1838	1042 (3.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	129	
1	B	129	
1	C	129	
2	R	19	
2	S	19	
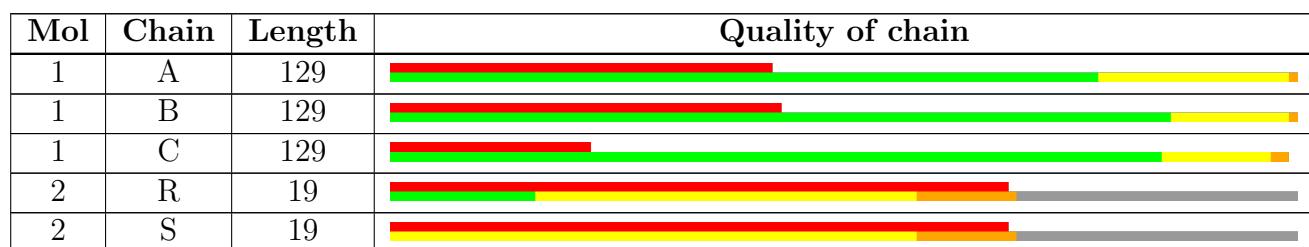
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3591 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MS2 COAT PROTEIN.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			965	606	165	190	4			
1	B	129	Total	C	N	O	S	0	0	0
			965	606	165	190	4			
1	C	129	Total	C	N	O	S	0	0	0
			965	606	165	190	4			

- Molecule 2 is a RNA chain called 5'-R(*AP*CP*AP*UP*GP*CP*GP*GP*AP*UP*CP*AP*CP*CP*CP*AP*UP*GP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	13	Total	C	N	O	P	0	0	0
			272	123	49	88	12			
2	S	13	Total	C	N	O	P	0	0	0
			272	123	49	88	12			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total	O	0	0
			51	51		
3	B	60	Total	O	0	0
			60	60		
3	C	39	Total	O	0	0
			39	39		
3	R	2	Total	O	0	0
			2	2		

3 Residue-property plots ⓘ

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

- Molecule 1: MS2 COAT PROTEIN

Chain A:
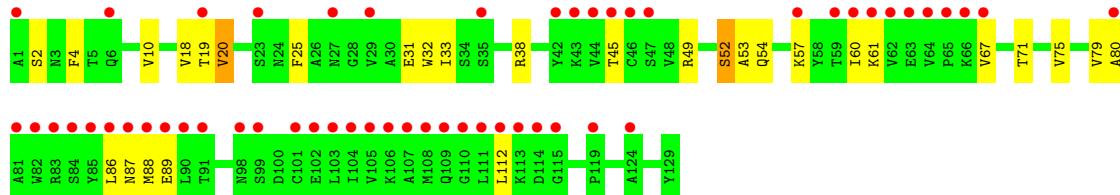
- Molecule 1: MS2 COAT PROTEIN

Chain B:
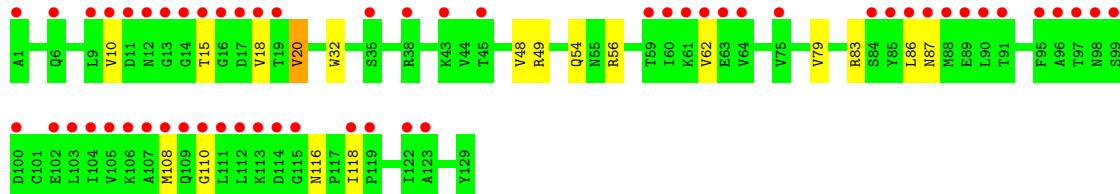
- Molecule 1: MS2 COAT PROTEIN

Chain C:
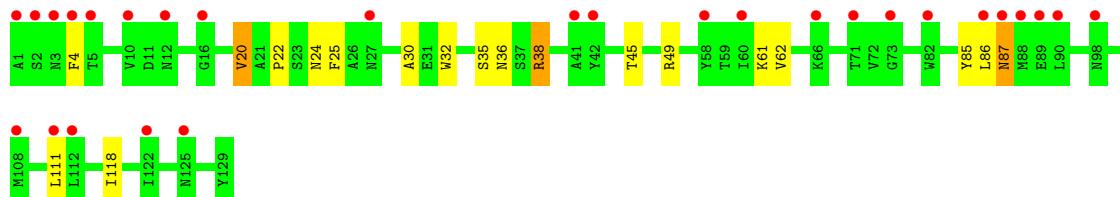
- Molecule 2: 5'-R(*AP*CP*AP*UP*GP*CP*GP*GP*AP*UP*CP*AP*CP*CP*CP*AP*UP*GP*U)-3'

Chain R:
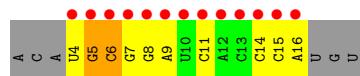
- Molecule 2: 5'-R(*AP*CP*AP*UP*GP*CP*GP*GP*AP*UP*CP*AP*CP*CP*CP*AP*UP*GP*U)-3'

Chain S:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	288.00Å 288.00Å 653.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.24 – 2.70 94.27 – 6.65	Depositor EDS
% Data completeness (in resolution range)	48.3 (38.24-2.70) 57.9 (94.27-6.65)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	6.66 (at 6.72Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.246 , 0.243 0.615 , 0.588	Depositor DCC
R_{free} test set	516 reflections (4.61%)	DCC
Wilson B-factor (Å^2)	213.2	Xtriage
Anisotropy	0.951	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 3710.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$<|L|> = 0.49, <L^2> = 0.33$	Xtriage
Outliers	0 of 12186 reflections	Xtriage
F_o,F_c correlation	0.62	EDS
Total number of atoms	3591	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.42	0/982	0.68	0/1337
1	B	0.42	0/982	0.67	0/1337
1	C	0.42	0/982	0.68	0/1337
2	R	0.41	0/303	0.68	0/470
2	S	0.51	0/303	0.70	0/470
All	All	0.43	0/3552	0.68	0/4951

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	965	0	964	23	0
1	B	965	0	964	16	0
1	C	965	0	964	14	0
2	R	272	0	143	11	0
2	S	272	0	143	15	0
3	A	51	0	0	3	0
3	B	60	0	0	3	0
3	C	39	0	0	1	0
3	R	2	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3591	0	3178	73	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (73) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:20:VAL:HG13	1:C:32:TRP:HB3	1.38	1.05
1:A:20:VAL:HG13	1:A:32:TRP:HB3	1.52	0.91
1:A:79:VAL:HG22	1:A:80:ALA:H	1.43	0.83
1:C:20:VAL:CG1	1:C:32:TRP:HB3	2.12	0.77
1:C:111:LEU:HD11	1:C:118:ILE:HD12	1.69	0.73
2:R:4:U:H2'	2:R:5:G:C5'	2.23	0.69
2:R:4:U:H2'	2:R:5:G:H5"	1.75	0.69
1:B:20:VAL:HG13	1:B:32:TRP:HB3	1.79	0.63
1:A:79:VAL:HG22	1:A:80:ALA:N	2.14	0.63
2:R:4:U:C2'	2:R:5:G:H5"	2.29	0.62
1:B:10:VAL:HB	1:B:18:VAL:HB	1.82	0.61
1:C:61:LYS:HE2	1:C:87:ASN:HD21	1.63	0.61
2:S:6:C:H5'	2:S:7:G:H5"	1.82	0.61
2:S:4:U:C2'	2:S:5:G:H5"	2.32	0.59
1:A:61:LYS:HG2	1:A:87:ASN:ND2	2.18	0.59
2:S:4:U:H2'	2:S:5:G:C5'	2.34	0.58
2:S:4:U:H2'	2:S:5:G:H5"	1.86	0.56
1:A:60:ILE:HB	1:A:88:MET:HG3	1.87	0.56
1:B:15:THR:HG23	1:B:15:THR:O	2.08	0.54
1:B:83:ARG:HD2	3:B:2016:HOH:O	2.07	0.54
1:A:19:THR:HG22	3:A:2006:HOH:O	2.08	0.53
2:R:4:U:H2'	2:R:5:G:H5'	1.90	0.53
1:C:61:LYS:HD2	2:S:12:A:N7	2.24	0.53
1:A:20:VAL:CG1	1:A:32:TRP:HB3	2.33	0.53
2:S:6:C:H5'	2:S:7:G:C5'	2.38	0.52
2:R:15:C:H2'	2:R:16:A:C8	2.44	0.52
1:A:52:SER:OG	1:A:53:ALA:N	2.43	0.52
1:A:10:VAL:HB	1:A:18:VAL:HB	1.92	0.51
2:S:15:C:H2'	2:S:16:A:H8	1.75	0.50
2:R:8:G:O2'	2:R:9:A:H5'	2.11	0.50
1:B:62:VAL:HB	1:B:86:LEU:HB3	1.93	0.49
2:R:6:C:H5'	2:R:7:G:C5'	2.42	0.49
2:R:15:C:H2'	2:R:16:A:H8	1.76	0.49
1:A:112:LEU:HD13	1:B:108:MET:HB3	1.95	0.48
1:C:4:PHE:CZ	1:C:22:PRO:HB3	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:49:ARG:NE	3:R:2001:HOH:O	2.46	0.48
1:B:49:ARG:CD	3:R:2001:HOH:O	2.62	0.48
1:B:83:ARG:HG2	1:B:83:ARG:HH11	1.79	0.47
2:R:6:C:H5'	2:R:7:G:H5"	1.96	0.46
1:A:33:ILE:HD13	1:A:38:ARG:NH1	2.31	0.46
2:R:4:U:C2'	2:R:5:G:C5'	2.90	0.46
2:S:9:A:HO2'	2:S:10:U:H6	1.63	0.46
2:S:13:C:H2'	2:S:14:C:C6	2.52	0.45
1:A:57:LYS:HE3	1:A:89:GLU:HB3	1.98	0.45
1:A:88:MET:HA	1:B:87:ASN:O	2.17	0.45
1:C:49:ARG:HG2	1:C:49:ARG:HH11	1.81	0.45
2:R:14:C:O2'	2:R:15:C:H5'	2.16	0.44
1:B:56:ARG:NH2	3:B:2021:HOH:O	2.46	0.44
2:S:15:C:H2'	2:S:16:A:C8	2.52	0.44
1:C:35:SER:O	1:C:36:ASN:HB2	2.16	0.44
1:A:45:THR:OG1	1:A:61:LYS:HB2	2.18	0.44
2:S:4:U:O2'	2:S:5:G:H5"	2.17	0.43
2:S:8:G:O2'	2:S:9:A:H5'	2.18	0.43
1:C:62:VAL:HB	1:C:86:LEU:HB3	2.00	0.43
2:S:4:U:H2'	2:S:5:G:H5'	2.00	0.43
1:C:49:ARG:NH1	1:C:49:ARG:HG2	2.33	0.43
1:C:85:TYR:CE2	2:S:11:C:H2'	2.54	0.43
1:B:79:VAL:HG13	3:B:2016:HOH:O	2.18	0.42
1:A:67:VAL:HG22	3:A:2029:HOH:O	2.19	0.42
2:S:4:U:C2'	2:S:5:G:C5'	2.97	0.42
1:A:49:ARG:HB2	3:A:2021:HOH:O	2.19	0.42
1:C:38:ARG:NH1	3:C:2016:HOH:O	2.53	0.42
1:B:83:ARG:HG2	1:B:83:ARG:NH1	2.35	0.42
1:A:61:LYS:HE2	1:A:61:LYS:HB3	1.73	0.42
1:B:110:GLY:O	1:B:116:ASN:ND2	2.53	0.41
1:A:57:LYS:CE	1:A:89:GLU:HB3	2.50	0.41
1:A:60:ILE:HD13	1:B:118:ILE:HG21	2.02	0.41
1:C:30:ALA:O	1:C:45:THR:HA	2.21	0.41
1:C:111:LEU:CD1	1:C:118:ILE:HD12	2.45	0.40
1:A:86:LEU:HD22	1:B:108:MET:HG2	2.03	0.40
1:A:31:GLU:HG2	1:A:32:TRP:N	2.36	0.40
1:A:60:ILE:HB	1:A:88:MET:CG	2.51	0.40
1:A:71:THR:HA	1:A:75:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	27	58
1	B	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	C	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
All	All	381/387 (98%)	363 (95%)	17 (4%)	1 (0%)	50	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	106/106 (100%)	101 (95%)	5 (5%)	36	69
1	B	106/106 (100%)	103 (97%)	3 (3%)	56	86
1	C	106/106 (100%)	101 (95%)	5 (5%)	36	69
All	All	318/318 (100%)	305 (96%)	13 (4%)	41	74

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	20	VAL
1	A	25	PHE
1	A	52	SER
1	A	54	GLN

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Mol	Chain	Res	Type
1	B	20	VAL
1	B	48	VAL
1	B	54	GLN
1	C	20	VAL
1	C	24	ASN
1	C	25	PHE
1	C	38	ARG
1	C	87	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	87	ASN
1	B	54	GLN
1	B	87	ASN
1	C	24	ASN
1	C	87	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	12/19 (63%)	3 (25%)	0
2	S	12/19 (63%)	2 (16%)	0
All	All	24/38 (63%)	5 (20%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	5	G
2	R	6	C
2	R	11	C
2	S	5	G
2	S	6	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	129/129 (100%)	5.55	54 (41%)	1	0	26, 38, 60, 75	0
1	B	129/129 (100%)	4.31	56 (43%)	1	0	27, 34, 57, 75	0
1	C	129/129 (100%)	1.58	28 (21%)	1	2	30, 40, 59, 82	0
2	R	13/19 (68%)	28.22	13 (100%)	0	0	17, 40, 65, 75	13 (100%)
2	S	13/19 (68%)	19.35	13 (100%)	0	0	47, 62, 98, 116	13 (100%)
All	All	413/425 (97%)	5.07	164 (39%)	1	0	17, 38, 66, 116	26 (6%)

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	ASN	73.9
1	A	88	MET	73.3
1	A	86	LEU	71.5
1	B	87	ASN	57.7
1	B	86	LEU	57.4
1	A	108	MET	47.9
2	R	11	C	46.2
2	R	7	G	46.0
1	B	88	MET	43.8
2	R	12	A	39.0
2	S	9	A	38.8
1	A	60	ILE	38.6
2	R	5	G	37.3
2	S	13	C	36.9
1	A	62	VAL	35.7
2	S	14	C	33.0
1	B	62	VAL	32.5
1	A	61	LYS	31.8
2	R	13	C	31.0
2	S	8	G	30.2

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Mol	Chain	Res	Type	RSRZ
2	R	14	C	29.7
2	R	16	A	26.2
1	A	112	LEU	24.8
1	A	89	GLU	24.2
1	B	108	MET	23.9
2	R	6	C	23.4
1	B	89	GLU	22.3
2	S	6	C	22.1
2	R	15	C	21.1
1	C	2	SER	20.5
1	B	61	LYS	19.2
2	R	4	U	19.2
1	B	85	TYR	19.0
1	A	85	TYR	18.8
1	B	112	LEU	18.7
1	A	105	VAL	17.9
1	B	111	LEU	17.3
2	R	8	G	17.3
1	A	109	GLN	17.2
1	B	60	ILE	17.1
1	C	3	ASN	16.3
2	S	10	U	16.3
2	R	9	A	15.8
1	A	59	THR	15.5
1	C	88	MET	15.5
1	A	106	LYS	14.7
2	R	10	U	14.6
2	S	5	G	14.1
1	B	114	ASP	13.8
1	A	111	LEU	13.5
2	S	4	U	12.7
1	B	63	GLU	12.4
1	A	63	GLU	11.7
2	S	15	C	11.7
1	A	107	ALA	11.7
1	A	81	ALA	11.3
1	B	12	ASN	11.2
1	A	104	ILE	11.0
1	B	15	THR	10.8
2	S	11	C	10.6
1	B	107	ALA	10.4
1	A	90	LEU	10.2

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Mol	Chain	Res	Type	RSRZ
1	C	89	GLU	10.1
1	B	16	GLY	10.1
2	S	7	G	9.9
2	S	12	A	9.7
1	A	35	SER	9.6
1	B	109	GLN	9.2
1	C	87	ASN	9.1
1	A	64	VAL	9.0
1	C	1	ALA	9.0
1	A	45	THR	8.5
1	A	84	SER	8.3
1	A	110	GLY	8.2
1	A	102	GLU	7.9
1	A	114	ASP	7.8
1	B	95	PHE	7.4
1	B	119	PRO	7.2
1	B	1	ALA	7.1
1	C	90	LEU	7.0
1	A	103	LEU	6.7
1	B	118	ILE	6.5
1	B	11	ASP	6.5
1	B	13	GLY	6.3
1	B	99	SER	6.2
1	B	104	ILE	6.2
1	B	90	LEU	6.0
1	B	35	SER	5.9
1	B	105	VAL	5.9
1	B	64	VAL	5.6
1	C	86	LEU	5.4
2	S	16	A	5.4
1	A	82	TRP	5.4
1	A	43	LYS	5.2
1	A	113	LYS	5.2
1	A	66	LYS	5.2
1	B	115	GLY	5.1
1	B	84	SER	4.9
1	C	27	ASN	4.9
1	C	58	TYR	4.9
1	C	12	ASN	4.8
1	B	113	LYS	4.8
1	C	125	ASN	4.7
1	B	97	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	46	CYS	4.5
1	B	122	ILE	4.5
1	C	16	GLY	4.1
1	A	91	THR	4.1
1	A	44	VAL	4.1
1	C	108	MET	4.0
1	C	122	ILE	3.9
1	B	19	THR	3.9
1	A	42	TYR	3.9
1	B	110	GLY	3.9
1	B	17	ASP	3.8
1	C	5	THR	3.8
1	A	65	PRO	3.7
1	B	103	LEU	3.7
1	B	59	THR	3.7
1	A	99	SER	3.7
1	B	98	ASN	3.6
1	A	67	VAL	3.6
1	B	43	LYS	3.6
1	B	6	GLN	3.5
1	A	23	SER	3.5
1	A	1	ALA	3.4
1	B	10	VAL	3.4
1	C	82	TRP	3.4
1	A	83	ARG	3.4
1	C	112	LEU	3.2
1	A	27	ASN	3.2
1	A	115	GLY	3.1
1	C	60	ILE	3.1
1	B	102	GLU	2.9
1	C	4	PHE	2.9
1	B	106	LYS	2.9
1	C	111	LEU	2.8
1	C	42	TYR	2.8
1	A	80	ALA	2.8
1	C	66	LYS	2.7
1	B	14	GLY	2.6
1	B	91	THR	2.6
1	B	18	VAL	2.5
1	B	45	THR	2.5
1	A	124	ALA	2.5
1	B	100	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	119	PRO	2.5
1	C	10	VAL	2.5
1	A	101	CYS	2.4
1	C	98	ASN	2.3
1	C	71	THR	2.3
1	B	96	ALA	2.3
1	A	6	GLN	2.3
1	B	123	ALA	2.2
1	B	38	ARG	2.2
1	B	9	LEU	2.1
1	A	19	THR	2.1
1	C	73	GLY	2.1
1	A	98	ASN	2.1
1	A	47	SER	2.0
1	A	57	LYS	2.0
1	B	75	VAL	2.0
1	C	41	ALA	2.0
1	A	29	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.