wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:39 PM BST

PDB ID	:	2J37
EMDB ID:	:	EMD-1264
Title	:	MODEL OF MAMMALIAN SRP BOUND TO 80S RNCS
Authors	:	Halic, M.; Blau, M.; Becker, T.; Mielke, T.; Pool, M.R.; Wild, K.; Sinning, I.; Beckmann, R.
Deposited on	:	2006-08-18
Resolution	:	8.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

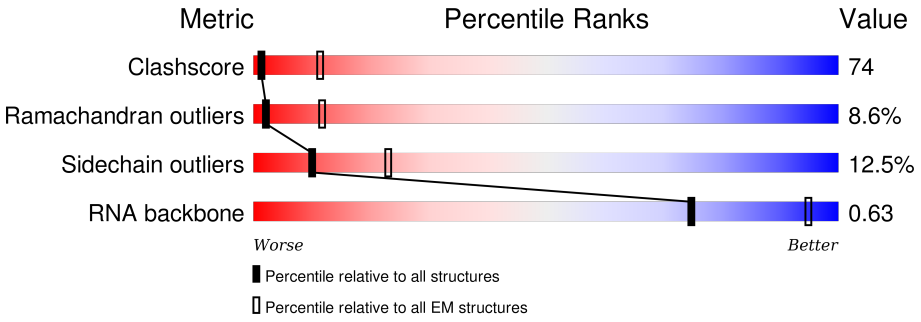
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	4	152	16% 22% 9% 6% 47%
2	5	124	16% 24% 8% • 48%
3	6	123	22% 27% 9% 8% 34%
4	A	128	37% 51% 13%
5	B	108	40% 52% 6% ••
6	S	17	18% 82%
7	W	504	28% 40% 18% 9% 5%
8	Z	280	45% 43% 10% •

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15110 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 60S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	4	81	652	423	108	119	2	0	0

- Molecule 2 is a protein called RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	5	64	504	314	99	91	0	0

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	6	81	671	416	138	115	2	0	0

- Molecule 4 is a RNA chain called SRP RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	A	128	2748	1226	511	884	127	0	0

- Molecule 5 is a protein called SIGNAL RECOGNITION PARTICLE 19 KDA PROTEIN (SRP19).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	107	869	549	159	155	6	0	0

- Molecule 6 is a protein called SIGNAL SEQUENCE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	S	17	141	97	22	22	0	0

- Molecule 7 is a protein called SIGNAL RECOGNITION PARTICLE 54 KDA PROTEIN (SRP54).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	479	Total	C	N	O	S	0	0
			3517	2196	614	683	24		

- Molecule 8 is a RNA chain called RIBOSOMAL RNA.

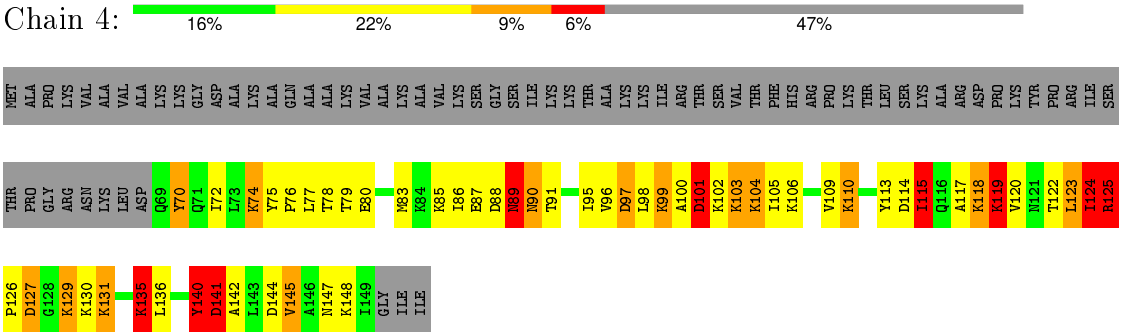
Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	280	Total	C	N	O	P	0	0
			6008	2681	1115	1932	280		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

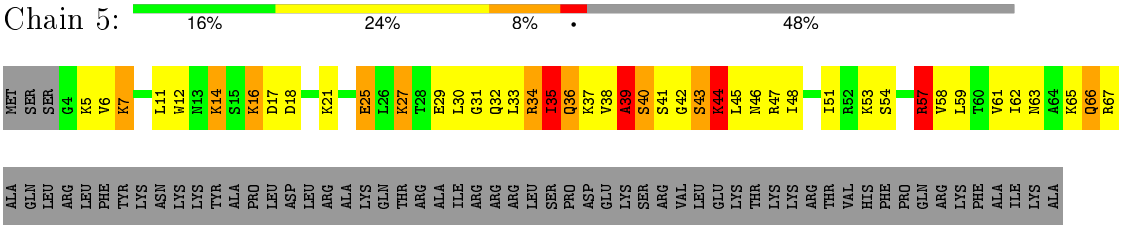
- Molecule 1: 60S RIBOSOMAL PROTEIN L23

Chain 4:



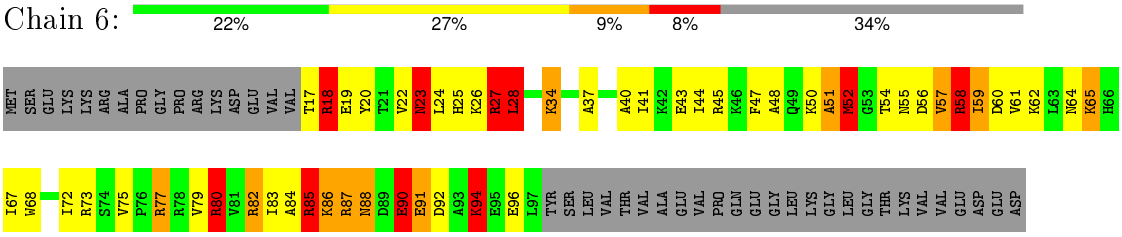
- Molecule 2: RIBOSOMAL PROTEIN L35

Chain 5:



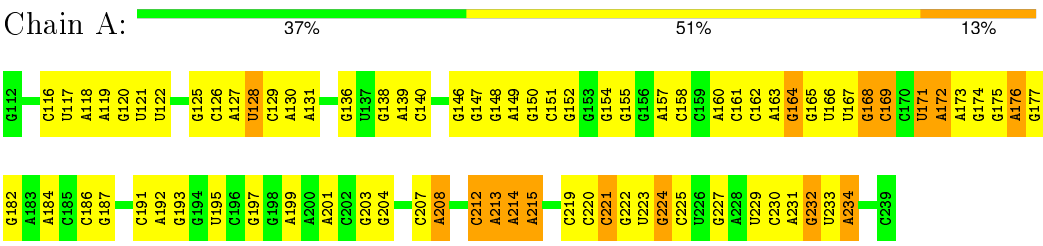
- Molecule 3: RIBOSOMAL PROTEIN L31

Chain 6:



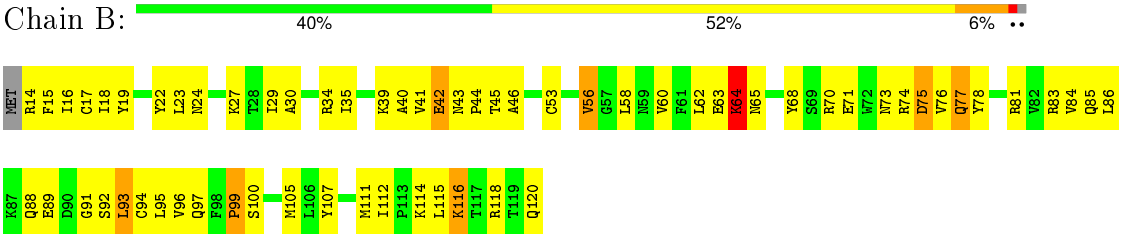
- Molecule 4: SRP RNA

Chain A:



• Molecule 5: SIGNAL RECOGNITION PARTICLE 19 KDA PROTEIN (SRP19)

Chain B:

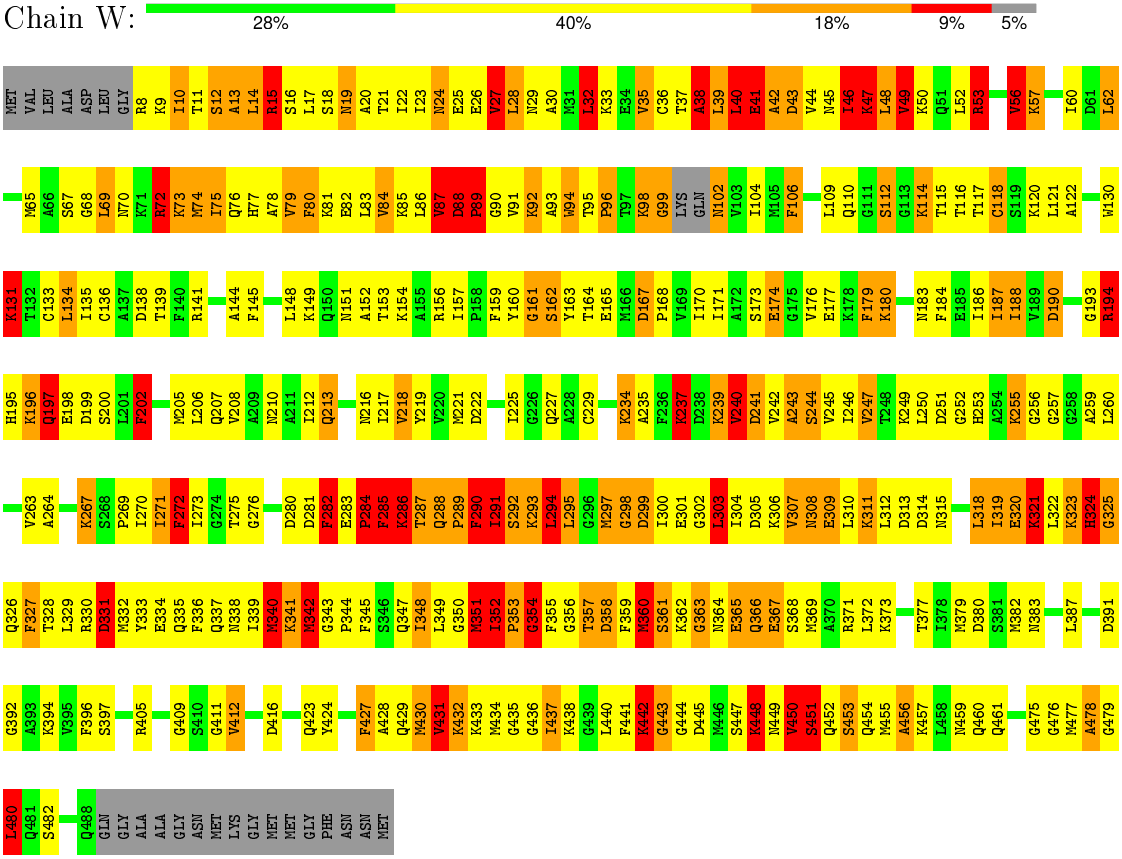


• Molecule 6: SIGNAL SEQUENCE

Chain S:

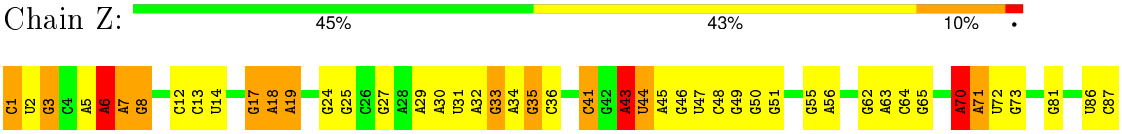
• Molecule 7: SIGNAL RECOGNITION PARTICLE 54 KDA PROTEIN (SRP54)

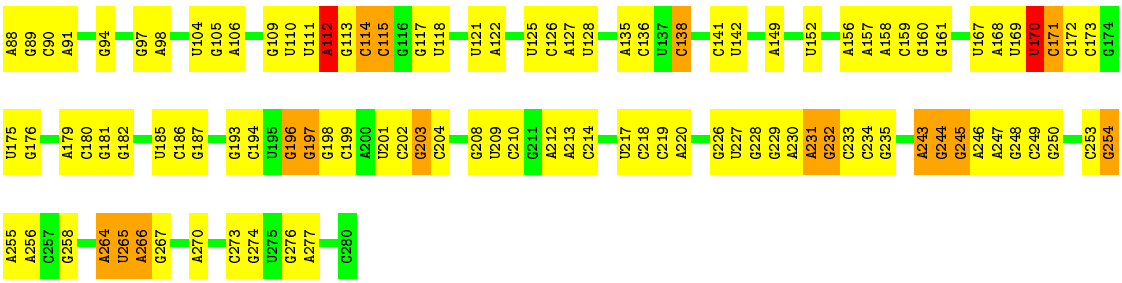
Chain W:



• Molecule 8: RIBOSOMAL RNA

Chain Z:




A88 G89 C90 A91
G94
G97 A98
U104 G105 A106
G109 U110 U111 A112 G113 C114 C115 G116 G117 U118
U121 A122
U125 C126 A127 U128
A135 C136 U137 C138
C141 U142
A149
U152
A156 A157 A158 C159 G160 G161
U167 A168 U169 U170 C171 C172 C173 G174
U175 G176
A179 C180 G181 G182
U185 C186 G187
G193 C194 U195 G196 G197 G198 C199 A200 U201 C202 G203 C204
G208 U209 C210 G211 A212 A213 C214
U217 C218 C219 A220
G226 U227 G228 G229 A230 A231 G232 C233 C234 G235
A243 G244 G245 A246 A247 G248 C249 G250
C253 G254
A255 A256 C257 G258
A264 U265 A266 G267
A270
C273 G274 U275 G276 A277 C280

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	4	1.34	7/658 (1.1%)	3.28	37/879 (4.2%)
2	5	1.39	4/506 (0.8%)	2.45	20/673 (3.0%)
3	6	1.35	3/680 (0.4%)	1.95	24/906 (2.6%)
4	A	0.46	0/3077	0.71	0/4800
5	B	0.46	0/883	0.70	0/1188
6	S	0.54	0/145	0.72	0/197
7	W	4.09	89/3545 (2.5%)	3.39	180/4707 (3.8%)
8	Z	0.45	0/6723	0.73	6/10473 (0.1%)
All	All	2.00	103/16217 (0.6%)	1.83	267/23823 (1.1%)

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	4	2	7
2	5	0	4
3	6	0	11
4	A	0	3
7	W	3	38
8	Z	0	6
All	All	5	69

The worst 5 of 103 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	W	284	PRO	N-CD	139.54	3.43	1.47
7	W	92	LYS	CB-CG	66.27	3.31	1.52
7	W	294	LEU	CB-CG	61.58	3.31	1.52
7	W	331	ASP	CB-CG	57.69	2.72	1.51
7	W	286	LYS	CB-CG	55.40	3.02	1.52

The worst 5 of 267 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	W	285	PHE	CB-CG-CD1	-73.05	69.66	120.80
1	4	125	ARG	NE-CZ-NH2	-72.81	83.89	120.30
7	W	285	PHE	CB-CG-CD2	66.74	167.52	120.80
7	W	352	ILE	C-N-CD	-49.65	11.38	120.60
7	W	284	PRO	CA-N-CD	-43.64	50.41	111.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	4	125	ARG	CA
1	4	141	ASP	CA
7	W	40	LEU	CA
7	W	285	PHE	CA
7	W	287	THR	CB

5 of 69 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	4	101	ASP	Mainchain,Peptide
1	4	124	ILE	Peptide
1	4	125	ARG	Sidechain
1	4	140	TYR	Sidechain
1	4	89	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4	652	0	703	156	0
2	5	504	0	550	95	0
3	6	671	0	704	117	0
4	A	2748	0	1389	87	0
5	B	869	0	901	80	0
6	S	141	0	146	107	0
7	W	3517	0	3388	1251	0
8	Z	6008	0	3033	302	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15110	0	10814	1922	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 74.

The worst 5 of 1922 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)
7:W:432:LYS:HA	7:W:436:GLY:CA	1.16	1.63
1:4:89:ASN:CB	8:Z:172:C:C5'	1.80	1.60
7:W:52:LEU:CD1	7:W:86:LEU:HD21	1.18	1.57
7:W:87:VAL:HG22	7:W:257:GLY:CA	1.19	1.56
3:6:65:LYS:HD2	8:Z:64:C:C2'	1.23	1.56

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	4	75/152 (49%)	66 (88%)	4 (5%)	5 (7%)	1 24
2	5	62/124 (50%)	54 (87%)	3 (5%)	5 (8%)	1 19
3	6	79/123 (64%)	66 (84%)	10 (13%)	3 (4%)	4 37
5	B	105/108 (97%)	87 (83%)	12 (11%)	6 (6%)	2 28
6	S	15/17 (88%)	13 (87%)	2 (13%)	0	100 100
7	W	442/504 (88%)	338 (76%)	56 (13%)	48 (11%)	0 11
All	All	778/1028 (76%)	624 (80%)	87 (11%)	67 (9%)	2 17

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	4	101	ASP
1	4	125	ARG
2	5	35	ILE
2	5	36	GLN
2	5	40	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	4	72/128 (56%)	54 (75%)	18 (25%)	1 6
2	5	55/109 (50%)	45 (82%)	10 (18%)	2 15
3	6	72/108 (67%)	51 (71%)	21 (29%)	0 3
5	B	96/97 (99%)	92 (96%)	4 (4%)	36 70
6	S	16/16 (100%)	16 (100%)	0	100 100
7	W	360/420 (86%)	329 (91%)	31 (9%)	13 47
All	All	671/878 (76%)	587 (88%)	84 (12%)	10 30

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	6	62	LYS
3	6	91	GLU
7	W	294	LEU
3	6	73	ARG
3	6	85	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	65	ASN
7	W	51	GLN
7	W	385	GLN
5	B	73	ASN

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Mol	Chain	Res	Type
5	B	88	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	A	127/128 (99%)	22 (17%)	1 (0%)
8	Z	274/280 (97%)	35 (12%)	13 (4%)
All	All	401/408 (98%)	57 (14%)	14 (3%)

5 of 57 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	A	128	U
4	A	129	C
4	A	164	G
4	A	168	G
4	A	169	C

5 of 14 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	Z	72	U
8	Z	112	A
8	Z	243	A
8	Z	70	A
8	Z	231	A

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.