



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 24, 2018 – 09:15 PM EST

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/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

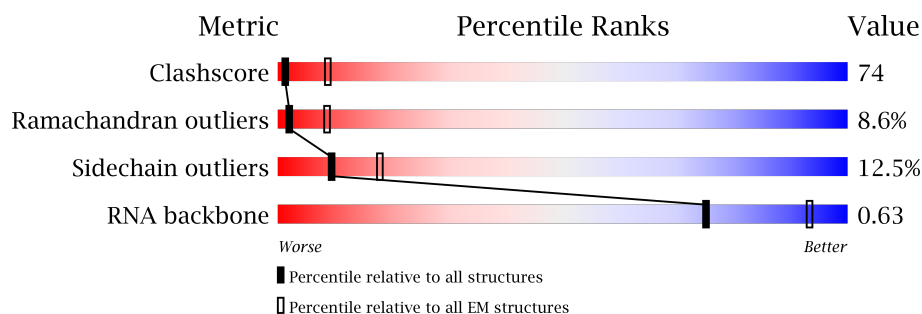
1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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 $\leq 5\%$

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 [i](#)

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
1	4	81	Total	C	N	O	S	0	0
			652	423	108	119	2		

- Molecule 2 is a protein called RIBOSOMAL PROTEIN L35.

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L31.

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

- Molecule 4 is a RNA chain called SRP RNA.

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

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

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

- Molecule 6 is a protein called SIGNAL SEQUENCE.

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

- 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		

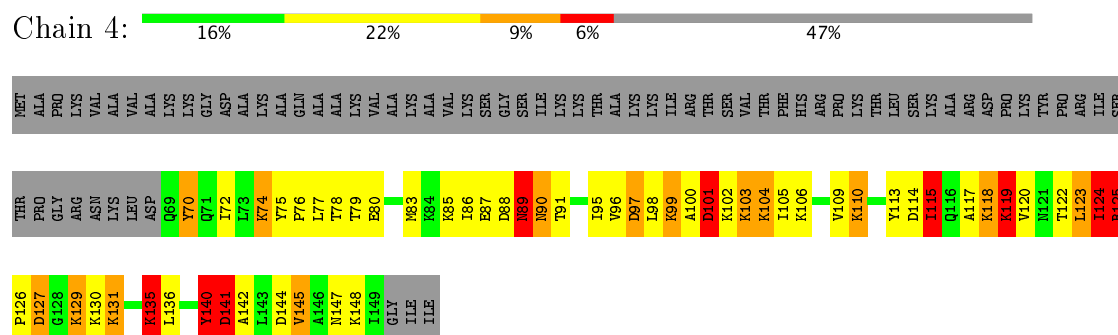
- Molecule 8 is a RNA chain called RIBOSOMAL RNA.

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

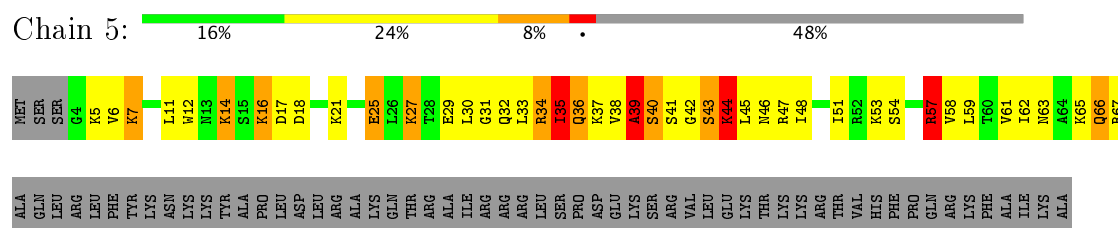
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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.

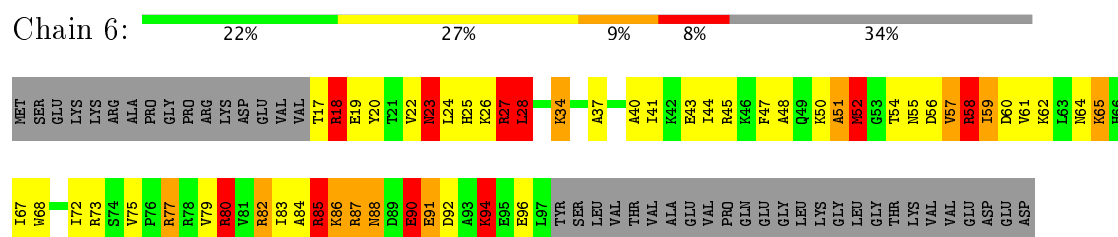
• Molecule 1: 60S RIBOSOMAL PROTEIN L23



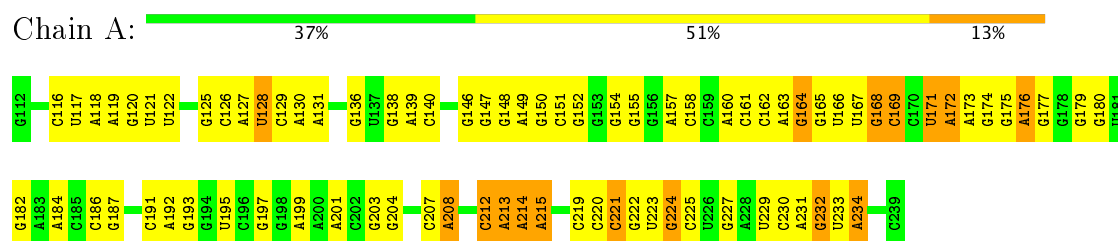
- Molecule 2: RIBOSOMAL PROTEIN L35



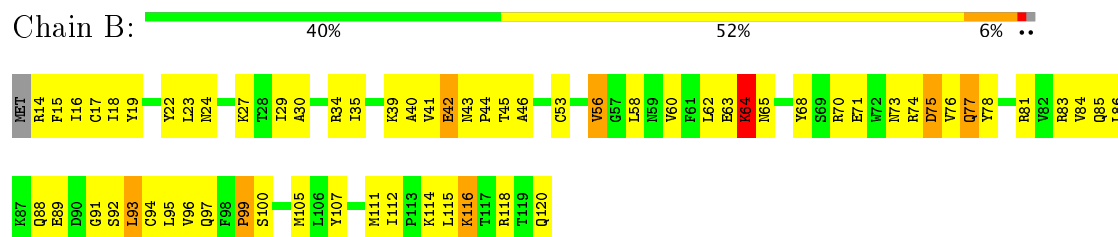
- Molecule 3: RIBOSOMAL PROTEIN L31



- Molecule 4: SRP RNA



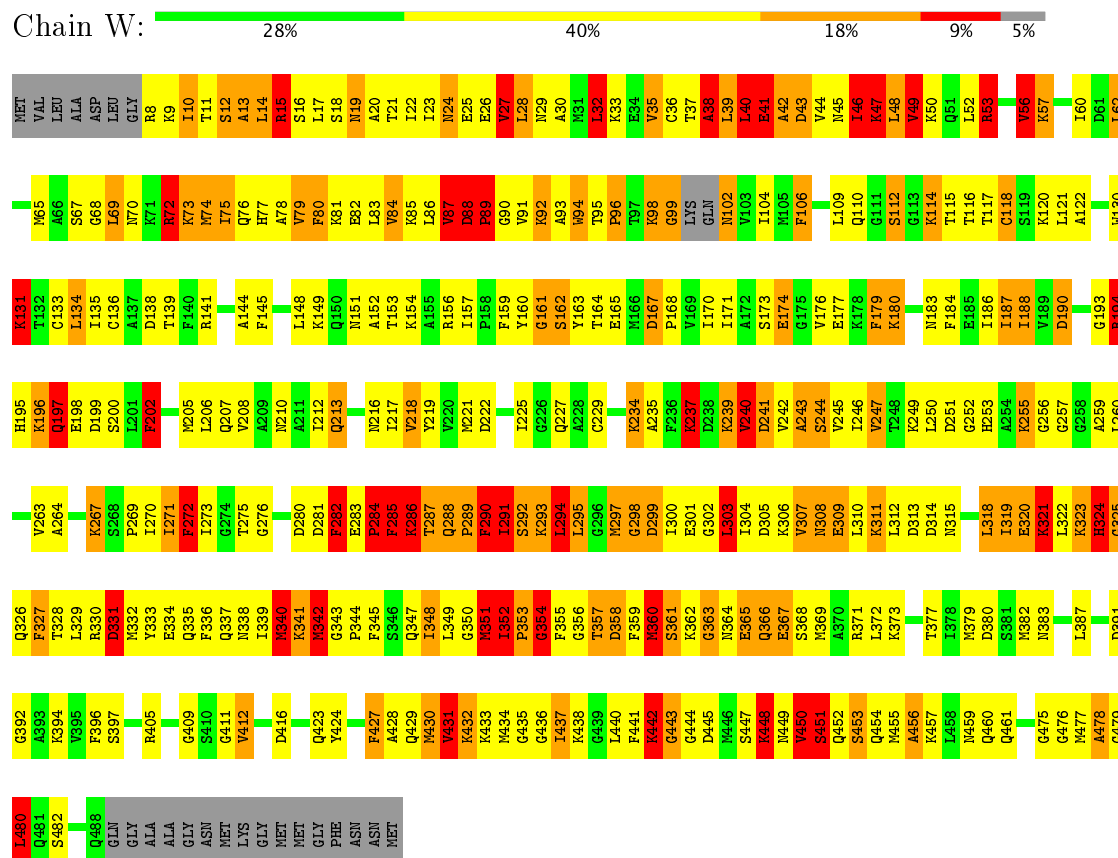
• Molecule 5: SIGNAL RECOGNITION PARTICLE 19 KDA PROTEIN (SRP19)



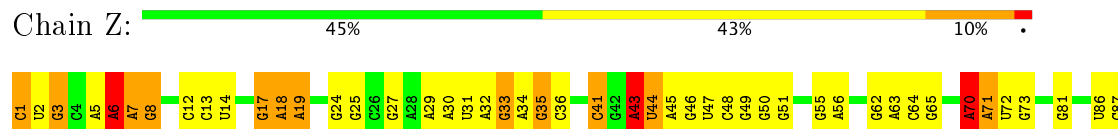
• Molecule 6: SIGNAL SEQUENCE



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



• Molecule 8: RIBOSOMAL RNA



A255	U175	A88
A256	G176	G89
C257		C90
G258	A179	A91
	C180	
A264	G181	G94
U265	G182	
A266		G97
G267	U185	A98
	C186	
A270	G187	U104
		G105
C273	G193	A106
G274	C194	
U275	U195	G109
G276	G196	U110
A277	A197	U111
	G198	A112
G280	C199	G113
	A200	C114
	U201	C115
	C202	G116
	G203	G117
	C204	U118
	G208	U121
	U209	A122
	C210	
	G211	U125
	A212	C126
	A213	A127
	C214	U128
	U217	A135
	C218	C136
	C219	U137
	A220	C138
	G226	C141
	U227	U142
	G228	
	G229	
	A230	A149
	A231	U152
	G232	
	C233	A156
	C234	A157
	G235	A158
		C159
	A243	G160
	G244	G161
	G245	
	A246	U167
	A247	A168
	G248	U169
	C249	U170
	G250	C171
		G172
	C253	C173
	G254	G174

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	Depositor
Image detector	KODAK SO-163 FILM	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(°)	Ideal(°)
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	21
2	5	62/124 (50%)	54 (87%)	3 (5%)	5 (8%)	1	16
3	6	79/123 (64%)	66 (84%)	10 (13%)	3 (4%)	4	32
5	B	105/108 (97%)	87 (83%)	12 (11%)	6 (6%)	2	24
6	S	15/17 (88%)	13 (87%)	2 (13%)	0	100	100
7	W	442/504 (88%)	338 (76%)	56 (13%)	48 (11%)	0	10
All	All	778/1028 (76%)	624 (80%)	87 (11%)	67 (9%)	2	15

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 ⓘ

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	5
2	5	55/109 (50%)	45 (82%)	10 (18%)	2	12
3	6	72/108 (67%)	51 (71%)	21 (29%)	0	3
5	B	96/97 (99%)	92 (96%)	4 (4%)	34	64
6	S	16/16 (100%)	16 (100%)	0	100	100
7	W	360/420 (86%)	329 (91%)	31 (9%)	12	42
All	All	671/878 (76%)	587 (88%)	84 (12%)	9	26

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	W	35
8	Z	5
1	4	2
2	5	1

The worst 5 of 43 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	37:A	O3'	38:C	P	52.59
1	Z	180:C	O3'	181:G	P	51.07
1	Z	200:A	O3'	201:U	P	4.54
1	W	432:LYS	C	433:LYS	N	3.98
1	4	98:LEU	C	99:LYS	N	3.96