



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:07 am GMT

PDB ID : 1RY1
EMDB ID: : EMD-1063
Title : Structure of the signal recognition particle interacting with the elongation-arrested ribosome
Authors : Halic, M.; Becker, T.; Pool, M.R.; Spahn, C.M.; Grassucci, R.A.; Frank, J.; Beckmann, R.
Deposited on : 2003-12-19
Resolution : 12.00 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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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) : recalc29047

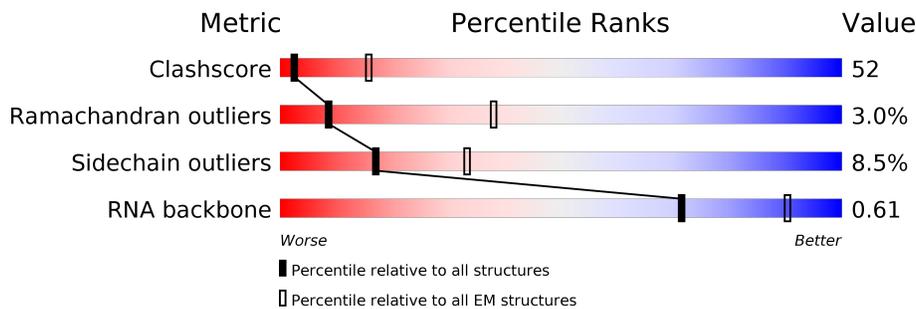
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 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	E	50	22% (green), 56% (yellow), 14% (orange), 6% (red), 2% (grey)
2	A	128	37% (green), 52% (yellow), 12% (orange)
3	M	27	15% (green), 48% (yellow), 26% (orange), 11% (red)
4	N	31	45% (yellow), 35% (orange), 16% (red)
5	O	24	25% (green), 58% (yellow), 8% (orange), 8% (red)
6	P	20	10% (green), 60% (yellow), 25% (orange), 5% (grey)
7	Q	12	8% (green), 33% (yellow), 50% (orange), 8% (red)
8	R	12	25% (yellow), 67% (orange), 8% (red)

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Mol	Chain	Length	Quality of chain
9	C	85	
10	D	106	
11	B	108	
12	U	296	
13	W	109	
14	S	18	

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 11794 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 RNA chain called ALU DOMAIN (RNA FRAGMENTS).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	E	49	1051	466	190	346	49	0	0

- Molecule 2 is a RNA chain called ALU DOMAIN (SRP9, SRP14 + RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	A	128	2751	1226	511	886	128	0	0

- Molecule 3 is a RNA chain called fragment of 7S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	M	27	585	260	110	188	27	0	0

- Molecule 4 is a RNA chain called RNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	N	31	649	291	109	218	31	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	O	24	511	227	86	174	24	0	0

- Molecule 6 is a RNA chain called RNA (5'-R(*CP*AP*AP*UP*AP*GP*CP*CP*AP*CP*UP*GP*CP*AP*CP*UP*CP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	P	19	401	180	72	130	19	0	0

- Molecule 7 is a RNA chain called RNA (5'-R(P*CP*GP*AP*UP*CP*GP*GP*GP*UP*GP*UP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	Q	12	257	114	45	86	12	0	0

- Molecule 8 is a RNA chain called RNA (5'-R(P*AP*UP*CP*GP*CP*GP*CP*CP*UP*GP*UP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	R	12	254	113	43	86	12	0	0

- Molecule 9 is a protein called PROTEIN (Signal recognition particle 9 kDa protein).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	C	71	580	369	101	105	5	0	0

- Molecule 10 is a protein called PROTEIN (Signal recognition particle 14 kDa protein).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	D	76	604	382	105	113	4	0	0

- Molecule 11 is a protein called PROTEIN (Signal recognition particle 19 kDa protein).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	B	107	870	549	159	156	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	MET	-	INITIATING METHIONINE	UNP P09132

- Molecule 12 is a protein called Signal recognition particle protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	U	294	2266	1424	413	423	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	1	MET	-	INITIATING METHIONINE	UNP O07347

- Molecule 13 is a protein called Signal recognition particle 54 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	W	109	865	540	150	164	11	0	0

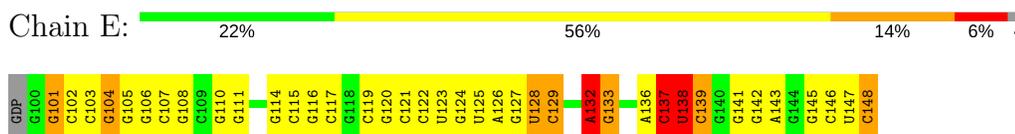
- Molecule 14 is a protein called Rhodopsin.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	S	18	150	103	24	23	0	0

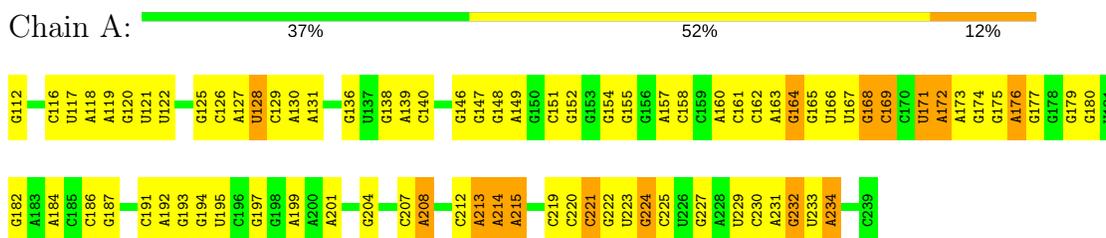
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

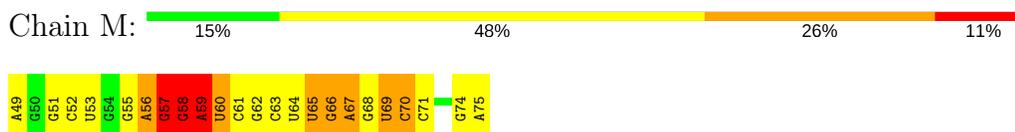
- Molecule 1: ALU DOMAIN (RNA FRAGMENTS)



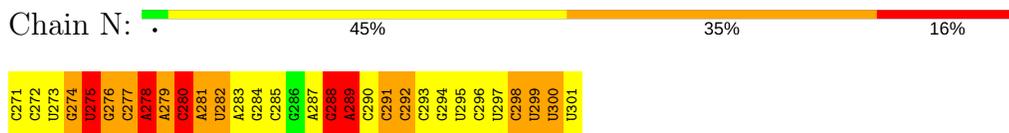
- Molecule 2: ALU DOMAIN (SRP9, SRP14 + RNA)



- Molecule 3: fragment of 7S RNA



- Molecule 4: RNA (31-MER)



- Molecule 5: RNA (5'-R(P*GP*UP*UP*CP*UP*GP*GP*GP*CP*UP*GP*UP*AP*GP*UP*GP*CP*GP*CP*UP*AP*UP*GP*C)-3')



- Molecule 6: RNA (5'-R(*CP*AP*AP*UP*AP*GP*CP*CP*AP*CP*UP*GP*CP*AP*CP*UP*CP*CP*AP*G)-3')

Chain P: 



- Molecule 7: RNA (5'-R(P*CP*GP*AP*UP*CP*GP*GP*GP*UP*GP*UP*C)-3')

Chain Q: 

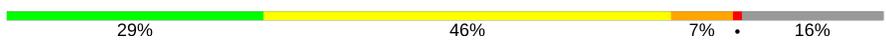


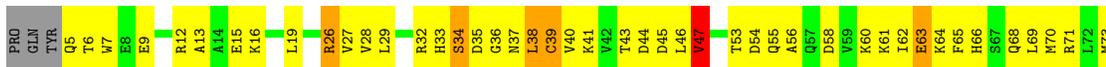
- Molecule 8: RNA (5'-R(P*AP*UP*CP*GP*CP*GP*CP*CP*UP*GP*UP*G)-3')

Chain R: 



- Molecule 9: PROTEIN (Signal recognition particle 9 kDa protein)

Chain C: 



- Molecule 10: PROTEIN (Signal recognition particle 14 kDa protein)

Chain D: 

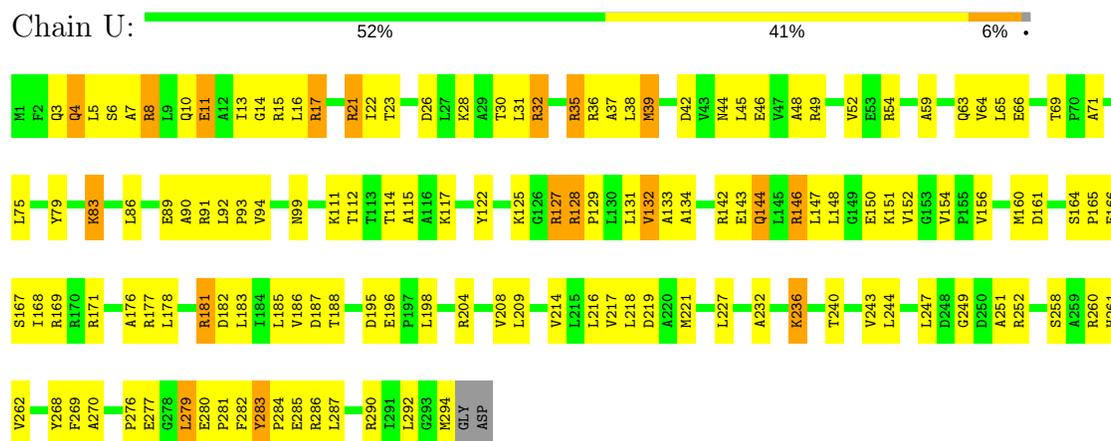


- Molecule 11: PROTEIN (Signal recognition particle 19 kDa protein)

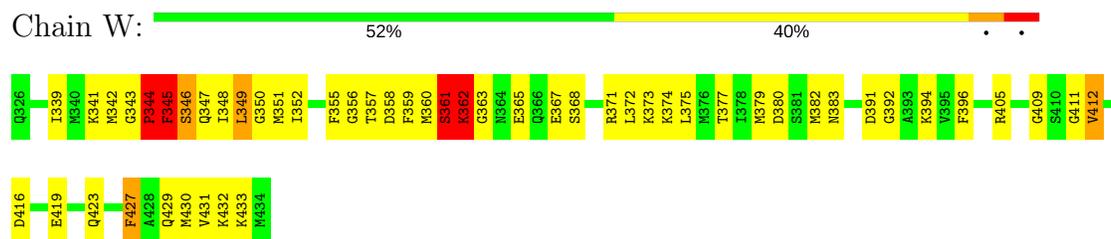
Chain B: 



- Molecule 12: Signal recognition particle protein



- Molecule 13: Signal recognition particle 54 kDa protein



- Molecule 14: Rhodopsin



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1000	Depositor
Minimum defocus (nm)	10000	Depositor
Maximum defocus (nm)	45000	Depositor
Magnification	52000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	E	0.57	0/1173	0.81	3/1829 (0.2%)
10	D	0.39	0/608	0.66	0/809
11	B	0.46	0/884	0.69	0/1188
12	U	0.27	0/2291	0.50	0/3086
13	W	0.95	2/876 (0.2%)	1.26	8/1165 (0.7%)
14	S	0.55	0/154	0.72	0/208
2	A	0.45	0/3055	0.70	0/4766
3	M	1.23	2/651 (0.3%)	2.01	12/1005 (1.2%)
4	N	2.23	4/721 (0.6%)	2.65	18/1116 (1.6%)
5	O	0.85	0/567	2.75	6/877 (0.7%)
6	P	0.91	0/446	2.33	5/689 (0.7%)
7	Q	2.50	2/284 (0.7%)	3.20	10/436 (2.3%)
8	R	1.31	1/282 (0.4%)	2.53	9/437 (2.1%)
9	C	0.42	0/589	0.66	0/791
All	All	0.89	11/12581 (0.1%)	1.42	71/18402 (0.4%)

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
13	W	0	5
2	A	0	3
All	All	0	8

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	288	G	O3'-P	40.60	2.09	1.61
7	Q	110	U	O3'-P	38.67	2.07	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	292	C	O3'-P	34.73	2.02	1.61
3	M	74	G	O3'-P	19.79	1.84	1.61
13	W	345	PHE	C-N	-18.39	0.91	1.34

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	92	C	P-O3'-C3'	-65.35	41.28	119.70
4	N	280	C	P-O3'-C3'	-57.26	50.99	119.70
6	P	252	A	P-O3'-C3'	-45.34	65.29	119.70
7	Q	101	G	P-O3'-C3'	-40.29	71.36	119.70
3	M	69	U	O3'-P-O5'	-36.27	35.09	104.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	197	G	Sidechain
2	A	201	A	Sidechain
2	A	208	A	Sidechain
13	W	344	PRO	Mainchain,Peptide
13	W	361	SER	Mainchain

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	E	1051	0	528	84	0
2	A	2751	0	1387	96	0
3	M	585	0	289	99	0
4	N	649	0	330	150	0
5	O	511	0	258	25	0
6	P	401	0	208	108	0
7	Q	257	0	129	83	0
8	R	254	0	128	75	0
9	C	580	0	594	85	0
10	D	604	0	638	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	870	0	901	80	0
12	U	2266	0	2367	226	0
13	W	865	0	865	233	0
14	S	150	0	158	64	0
All	All	11794	0	8780	1071	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 52.

The worst 5 of 1071 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)
6:P:252:A:C2	8:R:250:U:H2'	1.25	1.63
12:U:281:PRO:CB	13:W:347:GLN:HG3	1.15	1.61
4:N:274:G:H2'	4:N:275:U:C5	1.11	1.59
12:U:283:TYR:CZ	13:W:360:MET:HE2	1.34	1.58
12:U:283:TYR:CE1	13:W:360:MET:HB2	1.05	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	
9	C	69/85 (81%)	57 (83%)	9 (13%)	3 (4%)	3	29
10	D	72/106 (68%)	63 (88%)	5 (7%)	4 (6%)	2	25
11	B	105/108 (97%)	87 (83%)	11 (10%)	7 (7%)	1	21
12	U	292/296 (99%)	273 (94%)	18 (6%)	1 (0%)	44	81
13	W	107/109 (98%)	100 (94%)	2 (2%)	5 (5%)	3	28
14	S	16/18 (89%)	14 (88%)	2 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	661/722 (92%)	594 (90%)	47 (7%)	20 (3%)	9	37

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	34	SER
9	C	47	VAL
10	D	6	SER
11	B	42	GLU
11	B	75	ASP

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	
9	C	64/77 (83%)	58 (91%)	6 (9%)	10	36
10	D	69/96 (72%)	66 (96%)	3 (4%)	33	64
11	B	96/97 (99%)	92 (96%)	4 (4%)	34	64
12	U	233/234 (100%)	202 (87%)	31 (13%)	4	24
13	W	96/96 (100%)	91 (95%)	5 (5%)	27	59
14	S	17/17 (100%)	17 (100%)	0	100	100
All	All	575/617 (93%)	526 (92%)	49 (8%)	17	42

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	U	45	LEU
12	U	99	ASN
13	W	365	GLU
12	U	63	GLN
12	U	127	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
11	B	73	ASN
11	B	88	GLN
13	W	385	GLN
11	B	65	ASN
13	W	383	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	48/50 (96%)	11 (22%)	0
2	A	127/128 (99%)	22 (17%)	0
3	M	22/27 (81%)	8 (36%)	0
4	N	28/31 (90%)	12 (42%)	0
5	O	21/24 (87%)	4 (19%)	0
6	P	17/20 (85%)	2 (11%)	0
7	Q	9/12 (75%)	4 (44%)	0
8	R	11/12 (91%)	6 (54%)	0
All	All	283/304 (93%)	69 (24%)	0

5 of 69 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	101	G
1	E	104	G
1	E	128	U
1	E	129	C
1	E	132	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CCC	A	239	8,2	16,25,26	0.93	0	19,38,41	3.51	5 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CCC	A	239	8,2	-	0/3/35/36	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	239	CCC	O3'-PC-O1C	-7.07	97.11	115.76
2	A	239	CCC	O2'-PC-O1C	-5.43	101.44	115.76
2	A	239	CCC	O3'-C3'-C2'	3.24	111.24	105.13
2	A	239	CCC	O2'-C2'-C3'	4.07	112.79	105.13
2	A	239	CCC	O2C-PC-O1C	11.05	145.57	109.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

There are no chain breaks in this entry.