



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:03 PM BST

PDB ID : 4ADX
EMDB ID: : EMD-2012
Title : The Cryo-EM Structure of the Archaeal 50S Ribosomal Subunit in Complex with Initiation Factor 6
Authors : Greber, B.J.; Boehringer, D.; Godinic-Mikulcic, V.; Crnkovic, A.; Ibba, M.; Weygand-Durasevic, I.; Ban, N.
Deposited on : 2012-01-04
Resolution : 6.60 Å(reported)
Based on PDB ID : 3CC2, 3O58, 4A17, 4A19

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

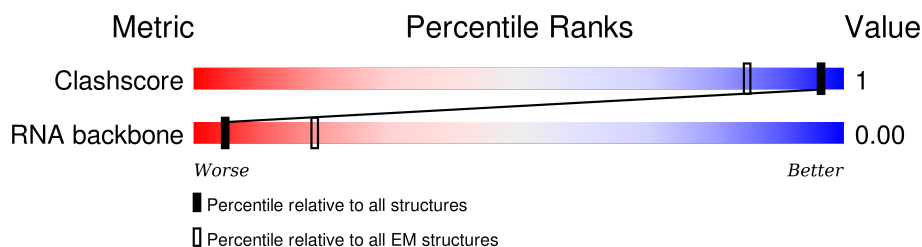
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 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.



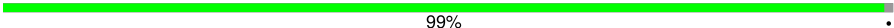
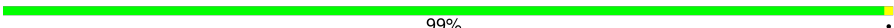
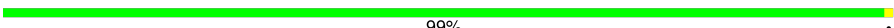










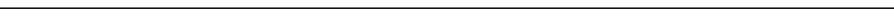

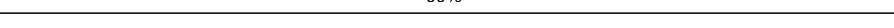
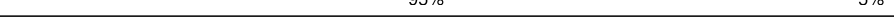
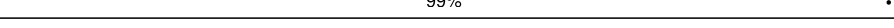
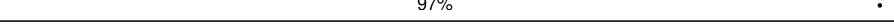
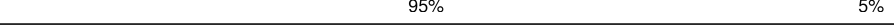
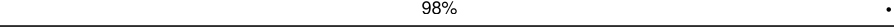


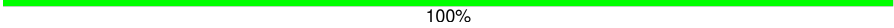

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
RNA backbone	3027	244

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	2923	92% 8%
2	1	57	98% .
3	2	50	92% 8%
4	3	92	100%
5	4	123	72% . 27%
6	5	129	39% 61%
7	6	104	91% . 8%
8	7	126	61% 39%
9	8	133	100%
10	9	122	99% .

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Mol	Chain	Length	Quality of chain
11	A	240	 99% .
12	B	338	 99% .
13	C	246	 99% .
14	D	177	 79% 21%
15	E	178	 97% .
16	F	120	 98% ..
17	G	78	 100%
18	H	177	 88% 12%
19	I	222	 99% .
20	J	145	 96% .
21	K	132	 100%
22	L	165	 85% 15%
23	M	196	 92% . 7%
24	N	187	 99% .
25	O	116	 99% .
26	P	149	 95% 5%
27	Q	96	 99% .
28	R	155	 97% .
29	S	85	 95% 5%
30	T	120	 98% .
31	U	67	 78% 22%
32	V	71	 90% 10%
33	W	154	 100%
34	X	92	 89% 11%
35	Y	241	 45% 55%

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Mol	Chain	Length	Quality of chain
36	Z	92	<div><div></div><div>79%</div><div>21%</div></div>

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 7164 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 23S rRNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	0	2688	Total	P	0	2688
			2688	2688		

- Molecule 2 is a protein called RPL37E.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	1	56	Total	C	0	56
			56	56		

- Molecule 3 is a protein called RPL39E.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	2	46	Total	C	0	46
			46	46		

- Molecule 4 is a protein called RPL44E.

Mol	Chain	Residues	Atoms		AltConf	Trace
4	3	92	Total	C	0	92
			92	92		

- Molecule 5 is a protein called RPL34E.

Mol	Chain	Residues	Atoms		AltConf	Trace
5	4	90	Total	C	0	90
			90	90		

- Molecule 6 is a protein called RPL40E.

Mol	Chain	Residues	Atoms		AltConf	Trace
6	5	50	Total	C	0	50
			50	50		

- Molecule 7 is a protein called RPL30E.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	6	96	Total C 96 96	0	96

- Molecule 8 is a protein called RPL14E.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	7	77	Total C 77 77	0	77

- Molecule 9 is a RNA chain called 23S RRNA EXPANSION SEGMENTS.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	8	133	Total P 133 133	0	133

- Molecule 10 is a RNA chain called 5S RRNA.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	9	121	Total P 121 121	0	121

- Molecule 11 is a protein called RPL2.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	A	237	Total C 237 237	0	237

- Molecule 12 is a protein called RPL3.

Mol	Chain	Residues	Atoms	AltConf	Trace
12	B	337	Total C 337 337	0	337

- Molecule 13 is a protein called RPL4.

Mol	Chain	Residues	Atoms	AltConf	Trace
13	C	246	Total C 246 246	0	246

- Molecule 14 is a protein called RPL5.

Mol	Chain	Residues	Atoms		AltConf	Trace
14	D	139	Total	C	0	139
			139	139		

- Molecule 15 is a protein called RPL6.

Mol	Chain	Residues	Atoms		AltConf	Trace
15	E	172	Total	C	0	172
			172	172		

- Molecule 16 is a protein called RPL7AE.

Mol	Chain	Residues	Atoms		AltConf	Trace
16	F	119	Total	C	0	119
			119	119		

- Molecule 17 is a protein called RPLX.

Mol	Chain	Residues	Atoms		AltConf	Trace
17	G	78	Total	C	0	78
			78	78		

- Molecule 18 is a protein called RPL10E.

Mol	Chain	Residues	Atoms		AltConf	Trace
18	H	156	Total	C	0	156
			156	156		

- Molecule 19 is a protein called AIF6.

Mol	Chain	Residues	Atoms		AltConf	Trace
19	I	220	Total	C	0	220
			220	220		

- Molecule 20 is a protein called RPL13.

Mol	Chain	Residues	Atoms		AltConf	Trace
20	J	139	Total	C	0	139
			139	139		

- Molecule 21 is a protein called RPL14.

Mol	Chain	Residues	Atoms		AltConf	Trace
21	K	132	Total	C	0	132
			132	132		

- Molecule 22 is a protein called RPL15.

Mol	Chain	Residues	Atoms		AltConf	Trace
22	L	140	Total	C	0	140
			140	140		

- Molecule 23 is a protein called RPL15E.

Mol	Chain	Residues	Atoms		AltConf	Trace
23	M	182	Total	C	0	182
			182	182		

- Molecule 24 is a protein called RPL18.

Mol	Chain	Residues	Atoms		AltConf	Trace
24	N	185	Total	C	0	185
			185	185		

- Molecule 25 is a protein called RPL18E.

Mol	Chain	Residues	Atoms		AltConf	Trace
25	O	115	Total	C	0	115
			115	115		

- Molecule 26 is a protein called RPL19E.

Mol	Chain	Residues	Atoms		AltConf	Trace
26	P	142	Total	C	0	142
			142	142		

- Molecule 27 is a protein called RPL21E.

Mol	Chain	Residues	Atoms		AltConf	Trace
27	Q	95	Total	C	0	95
			95	95		

- Molecule 28 is a protein called RPL22.

Mol	Chain	Residues	Atoms		AltConf	Trace
28	R	150	Total	C	0	150
			150	150		

- Molecule 29 is a protein called RPL23.

Mol	Chain	Residues	Atoms		AltConf	Trace
29	S	81	Total	C	0	81
			81	81		

- Molecule 30 is a protein called RPL24.

Mol	Chain	Residues	Atoms		AltConf	Trace
30	T	117	Total	C	0	117
			117	117		

- Molecule 31 is a protein called RPL24E.

Mol	Chain	Residues	Atoms		AltConf	Trace
31	U	52	Total	C	0	52
			52	52		

- Molecule 32 is a protein called RPL29.

Mol	Chain	Residues	Atoms		AltConf	Trace
32	V	64	Total	C	0	64
			64	64		

- Molecule 33 is a protein called RPL30.

Mol	Chain	Residues	Atoms		AltConf	Trace
33	W	154	Total	C	0	154
			154	154		

- Molecule 34 is a protein called RPL31E.

Mol	Chain	Residues	Atoms		AltConf	Trace
34	X	82	Total	C	0	82
			82	82		

- Molecule 35 is a protein called RPL32E.

Mol	Chain	Residues	Atoms		AltConf	Trace
35	Y	108	Total 108	C 108	0	108

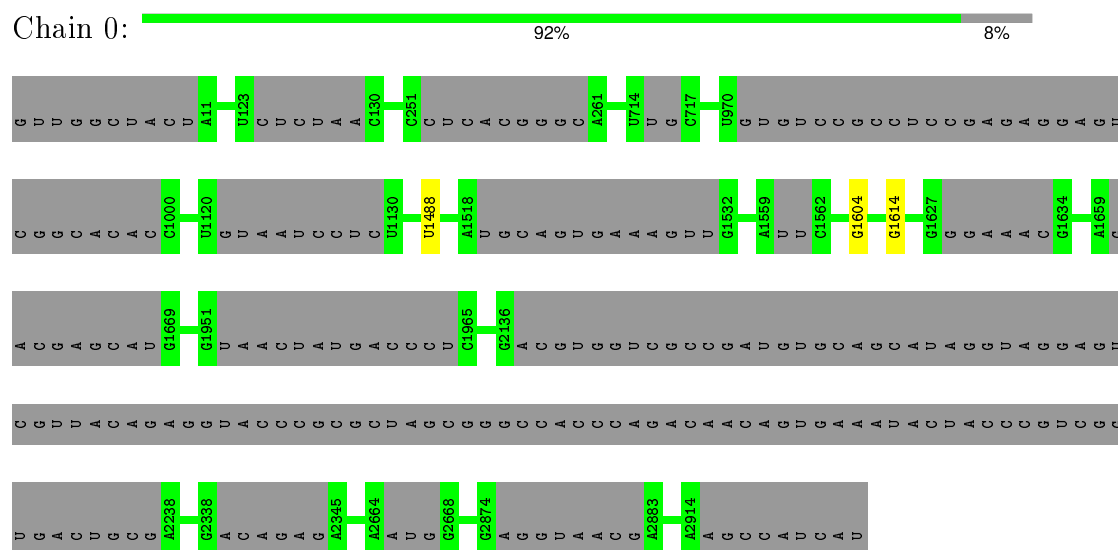
- Molecule 36 is a protein called RPL37AE.

Mol	Chain	Residues	Atoms		AltConf	Trace
36	Z	73	Total 73	C 73	0	73

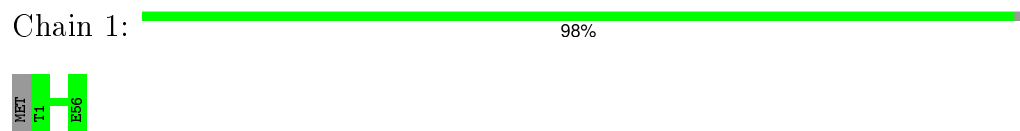
3 Residue-property plots [i](#)

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.

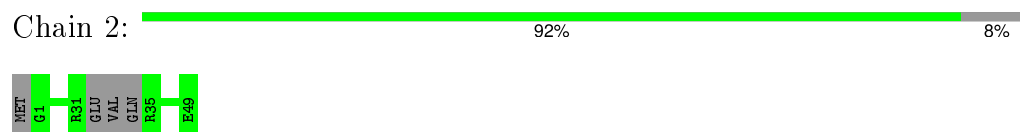
- Molecule 1: 23S rRNA



- Molecule 2: RPL37E



- Molecule 3: RPL39E



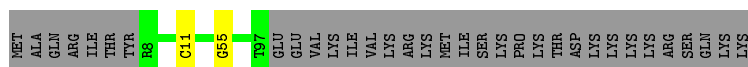
- Molecule 4: RPL44E



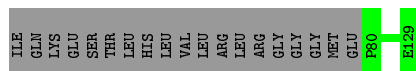
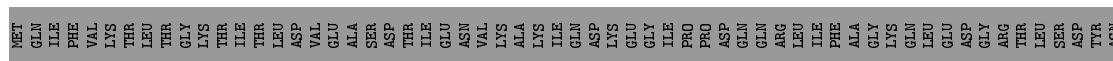
There are no outlier residues recorded for this chain.

- Molecule 5: RPL34E

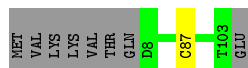




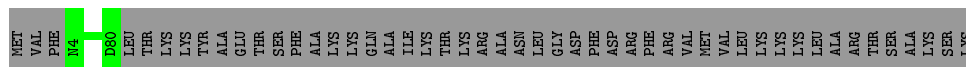
- Molecule 6: RPL40E



- Molecule 7: RPL30E



- Molecule 8: RPL14E



- Molecule 9: 23S rRNA EXPANSION SEGMENTS

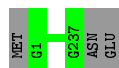


There are no outlier residues recorded for this chain.

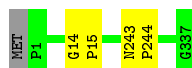
- Molecule 10: 5S rRNA



- Molecule 11: RPL2



- Molecule 12: RPL3




- Molecule 13: RPL4

Chain C:  99%



- Molecule 14: RPL5

Chain D:  79% 21%



- Molecule 15: RPL6

Chain E:  97%



- Molecule 16: RPL7AE

Chain F:  98%



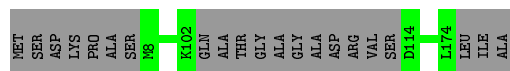
- Molecule 17: RPLX

Chain G:  100%

There are no outlier residues recorded for this chain.

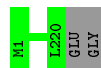
- Molecule 18: RPL10E

Chain H:  88% 12%



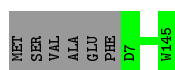
- Molecule 19: AIF6

Chain I:  99%



- Molecule 20: RPL13

Chain J:  96%



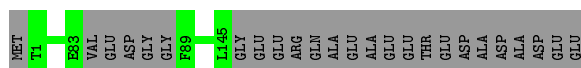
- Molecule 21: RPL14

Chain K: 100%

There are no outlier residues recorded for this chain.

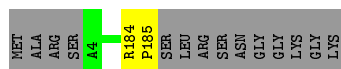
- Molecule 22: RPL15

Chain L: 85% 15%



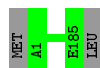
- Molecule 23: RPL15E

Chain M: 92% 7%



- Molecule 24: RPL18

Chain N: 99% 0%



- Molecule 25: RPL18E

Chain O: 99% 0%



- Molecule 26: RPL19E

Chain P: 95% 5%



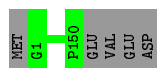
- Molecule 27: RPL21E

Chain Q: 99% 0%



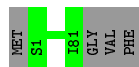
- Molecule 28: RPL22

Chain R:  97% .



- Molecule 29: RPL23

Chain S:  95% 5%




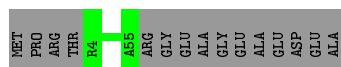
- Molecule 30: RPL24

Chain T:  98% .




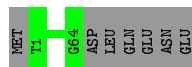
- Molecule 31: RPL24E

Chain U:  78% 22%



- Molecule 32: RPL29

Chain V:  90% 10%



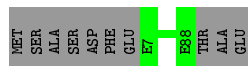
- Molecule 33: RPL30

Chain W:  100%

There are no outlier residues recorded for this chain.

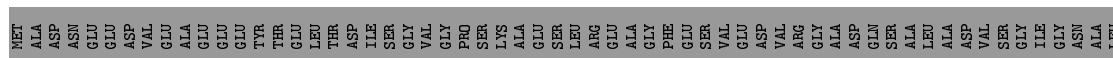
- Molecule 34: RPL31E

Chain X:  89% 11%



- Molecule 35: RPL32E

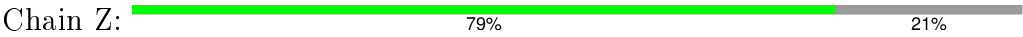
Chain Y:  45% 55%



ALA	ALA	ARG	ILE	LYS	ALA	ASP	VAL	GLY	GLY	LEU	GLU	VAL	GLU	SER	GLU	THR	GLU	ALA	GLU	VAL	GLU	GLU	GLY	GLY	GLU	GLU	ALA	PRO	ASP	GLU	ASP	VAL	GLU	THR	GLU	LEU	GLN	ALA	ARG	GLY	LEU	THR	GLU	LYS	THR	PRO	ASP	LEU	SER	ASP	ASP	ALA	ARG	LEU	THR	GLN
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ARG	HIS	VAL	GLY	K125	T232	TYR	VAL	GLU	VAL	GLU	VAL	SER	GLU
-----	-----	-----	-----	------	------	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 36: RPL37AE



MET	ALA	SER	LYS	SER	GLY	LYS	THR	GLY	S34	S106	ILE	ARG	ALA	ALA	LEU	SER	GLU	ASP	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

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	BY CCD FRAME	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1.2	Depositor
Maximum defocus (nm)	4.5	Depositor
Magnification	62000	Depositor
Image detector	GATAN US 4000 SPECIAL	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	0	2688	0	0	3	0
2	1	56	0	0	0	0
3	2	46	0	0	0	0
4	3	92	0	0	0	0
5	4	90	0	0	2	0
6	5	50	0	0	0	0
7	6	96	0	0	1	0
8	7	77	0	0	0	0
9	8	133	0	0	0	0
10	9	121	0	0	0	0
11	A	237	0	0	0	0
12	B	337	0	0	2	0
13	C	246	0	0	1	0
14	D	139	0	0	0	0
15	E	172	0	0	0	0
16	F	119	0	0	1	0
17	G	78	0	0	0	0
18	H	156	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	I	220	0	0	0	0
20	J	139	0	0	0	0
21	K	132	0	0	0	0
22	L	140	0	0	0	0
23	M	182	0	0	1	0
24	N	185	0	0	0	0
25	O	115	0	0	0	0
26	P	142	0	0	0	0
27	Q	95	0	0	0	0
28	R	150	0	0	0	0
29	S	81	0	0	0	0
30	T	117	0	0	0	0
31	U	52	0	0	0	0
32	V	64	0	0	0	0
33	W	154	0	0	0	0
34	X	82	0	0	0	0
35	Y	108	0	0	0	0
36	Z	73	0	0	0	0
All	All	7164	0	0	8	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 1.

All (8) 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)
1:0:1488:U:P	5:4:11:CYS:CA	2.82	0.67
1:0:1614:G:P	5:4:55:GLY:CA	2.88	0.61
12:B:14:GLY:CA	12:B:15:PRO:CA	2.80	0.59
1:0:1604:G:P	7:6:87:CYS:CA	2.92	0.58
12:B:243:ASN:CA	12:B:244:PRO:CA	2.93	0.47
23:M:184:ARG:CA	23:M:185:PRO:CA	2.94	0.46
16:F:55:GLN:CA	16:F:56:PRO:CA	2.96	0.44
13:C:136:VAL:CA	13:C:137:PRO:CA	2.99	0.41

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	0/2923	-	-
10	9	0/122	-	-
9	8	0/133	-	-
All	All	0/3178	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 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.