wwPDB EM Validation Summary Report

Feb 24, 2025 – 12:06 pm GMT

PDB ID	:	8Q86
EMDB ID	:	EMD-18248
Title	:	Trimer of the dimeric SaPI2 Stl transcriptional regulator
Authors	:	Qiao, C.; Debiasi-Anders, G.; Mir-Sanchis, I.
Deposited on	:	2023-08-18
Resolution	:	3.69 Å(reported)
Based on initial model	:	.

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

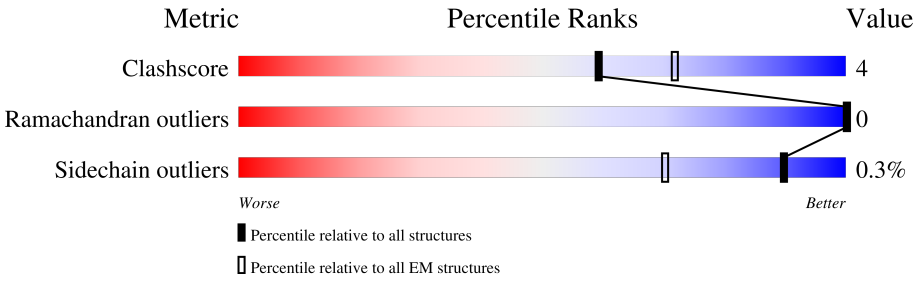
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 3.69 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	A	232	7% · 91%
1	B	232	18% 6% 77%
1	C	232	62% 9% 30%
1	D	232	81% 9% 11%
1	E	232	82% 12% 6%
1	F	232	88% 7% 6%
1	G	232	75% 11% 14%
1	H	232	69% 6% 26%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10351 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 Helix-turn-helix XRE family protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	21	Total C N O S 167 108 29 29 1	0	0
1	B	54	Total C N O 463 308 70 85	0	0
1	C	163	Total C N O S 1330 844 227 255 4	0	0
1	D	207	Total C N O S 1701 1083 281 333 4	0	0
1	E	219	Total C N O S 1797 1142 296 355 4	0	0
1	F	219	Total C N O S 1797 1142 296 355 4	0	0
1	G	199	Total C N O S 1635 1040 270 321 4	0	0
1	H	172	Total C N O S 1401 890 239 268 4	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	LEU	-	expression tag	UNP A0FIL5
A	226	GLU	-	expression tag	UNP A0FIL5
A	227	HIS	-	expression tag	UNP A0FIL5
A	228	HIS	-	expression tag	UNP A0FIL5
A	229	HIS	-	expression tag	UNP A0FIL5
A	230	HIS	-	expression tag	UNP A0FIL5
A	231	HIS	-	expression tag	UNP A0FIL5
A	232	HIS	-	expression tag	UNP A0FIL5
B	225	LEU	-	expression tag	UNP A0FIL5
B	226	GLU	-	expression tag	UNP A0FIL5
B	227	HIS	-	expression tag	UNP A0FIL5
B	228	HIS	-	expression tag	UNP A0FIL5
B	229	HIS	-	expression tag	UNP A0FIL5
B	230	HIS	-	expression tag	UNP A0FIL5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	231	HIS	-	expression tag	UNP A0FIL5
B	232	HIS	-	expression tag	UNP A0FIL5
C	225	LEU	-	expression tag	UNP A0FIL5
C	226	GLU	-	expression tag	UNP A0FIL5
C	227	HIS	-	expression tag	UNP A0FIL5
C	228	HIS	-	expression tag	UNP A0FIL5
C	229	HIS	-	expression tag	UNP A0FIL5
C	230	HIS	-	expression tag	UNP A0FIL5
C	231	HIS	-	expression tag	UNP A0FIL5
C	232	HIS	-	expression tag	UNP A0FIL5
D	225	LEU	-	expression tag	UNP A0FIL5
D	226	GLU	-	expression tag	UNP A0FIL5
D	227	HIS	-	expression tag	UNP A0FIL5
D	228	HIS	-	expression tag	UNP A0FIL5
D	229	HIS	-	expression tag	UNP A0FIL5
D	230	HIS	-	expression tag	UNP A0FIL5
D	231	HIS	-	expression tag	UNP A0FIL5
D	232	HIS	-	expression tag	UNP A0FIL5
E	225	LEU	-	expression tag	UNP A0FIL5
E	226	GLU	-	expression tag	UNP A0FIL5
E	227	HIS	-	expression tag	UNP A0FIL5
E	228	HIS	-	expression tag	UNP A0FIL5
E	229	HIS	-	expression tag	UNP A0FIL5
E	230	HIS	-	expression tag	UNP A0FIL5
E	231	HIS	-	expression tag	UNP A0FIL5
E	232	HIS	-	expression tag	UNP A0FIL5
F	225	LEU	-	expression tag	UNP A0FIL5
F	226	GLU	-	expression tag	UNP A0FIL5
F	227	HIS	-	expression tag	UNP A0FIL5
F	228	HIS	-	expression tag	UNP A0FIL5
F	229	HIS	-	expression tag	UNP A0FIL5
F	230	HIS	-	expression tag	UNP A0FIL5
F	231	HIS	-	expression tag	UNP A0FIL5
F	232	HIS	-	expression tag	UNP A0FIL5
G	225	LEU	-	expression tag	UNP A0FIL5
G	226	GLU	-	expression tag	UNP A0FIL5
G	227	HIS	-	expression tag	UNP A0FIL5
G	228	HIS	-	expression tag	UNP A0FIL5
G	229	HIS	-	expression tag	UNP A0FIL5
G	230	HIS	-	expression tag	UNP A0FIL5
G	231	HIS	-	expression tag	UNP A0FIL5
G	232	HIS	-	expression tag	UNP A0FIL5

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Chain	Residue	Modelled	Actual	Comment	Reference
H	225	LEU	-	expression tag	UNP A0FIL5
H	226	GLU	-	expression tag	UNP A0FIL5
H	227	HIS	-	expression tag	UNP A0FIL5
H	228	HIS	-	expression tag	UNP A0FIL5
H	229	HIS	-	expression tag	UNP A0FIL5
H	230	HIS	-	expression tag	UNP A0FIL5
H	231	HIS	-	expression tag	UNP A0FIL5
H	232	HIS	-	expression tag	UNP A0FIL5

- Molecule 2 is water.

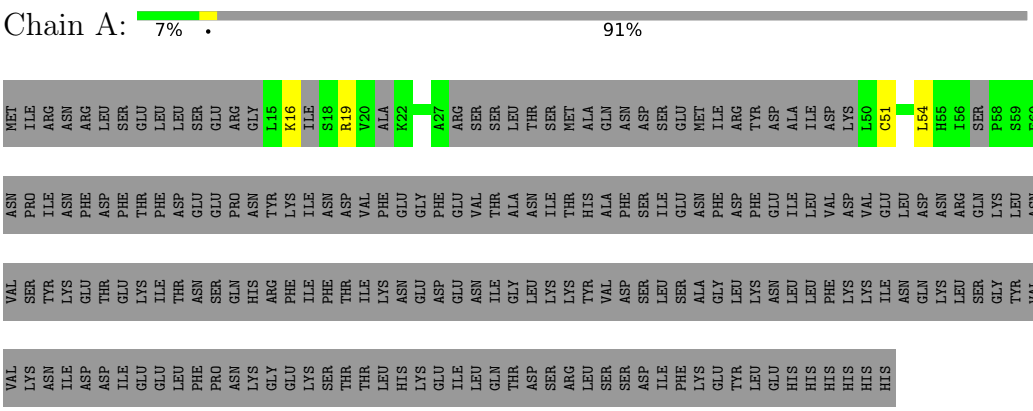
Mol	Chain	Residues	Atoms	AltConf
2	A	3	Total O 3 3	0
2	B	9	Total O 9 9	0
2	C	10	Total O 10 10	0
2	D	15	Total O 15 15	0
2	E	3	Total O 3 3	0
2	F	1	Total O 1 1	0
2	G	8	Total O 8 8	0
2	H	11	Total O 11 11	0

3 Residue-property plots (i)

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

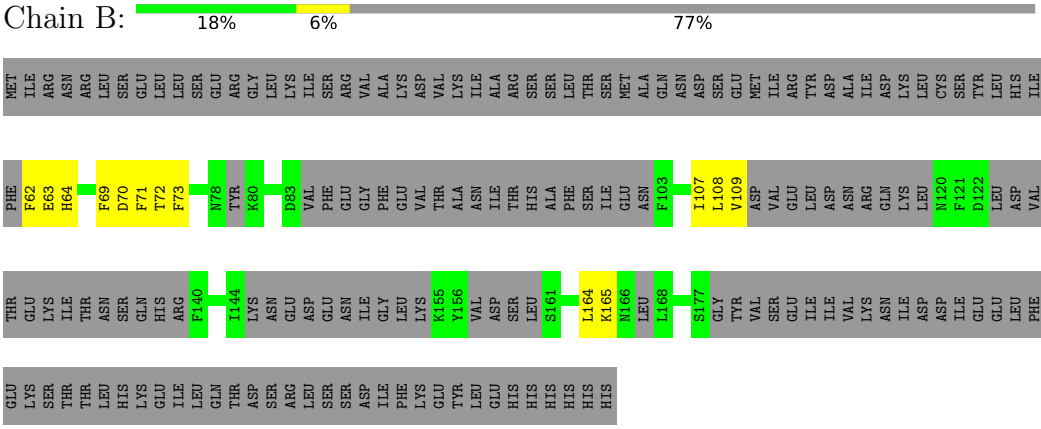
• Molecule 1: Helix-turn-helix XRE family protein

Chain A:



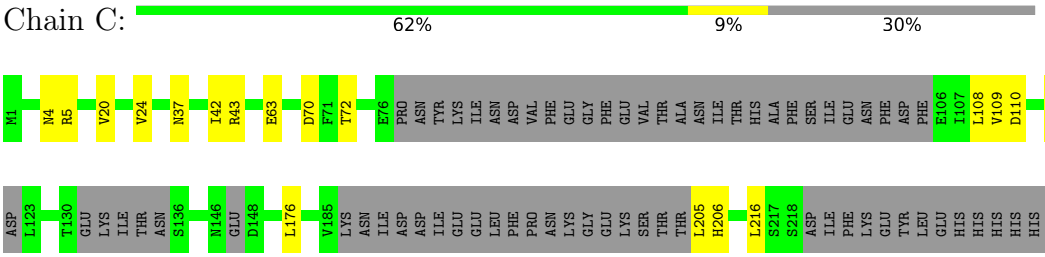
• Molecule 1: Helix-turn-helix XRE family protein

Chain B:



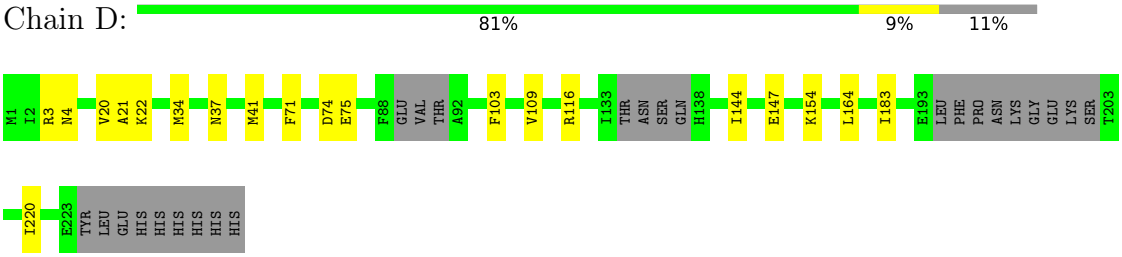
• Molecule 1: Helix-turn-helix XRE family protein

Chain C:



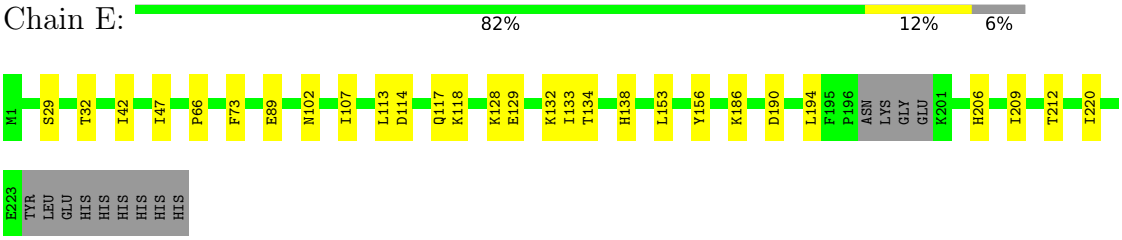
• Molecule 1: Helix-turn-helix XRE family protein

Chain D:



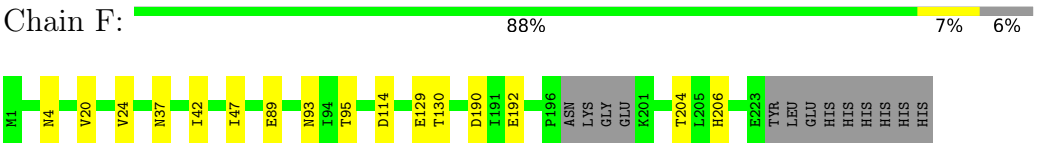
• Molecule 1: Helix-turn-helix XRE family protein

Chain E:



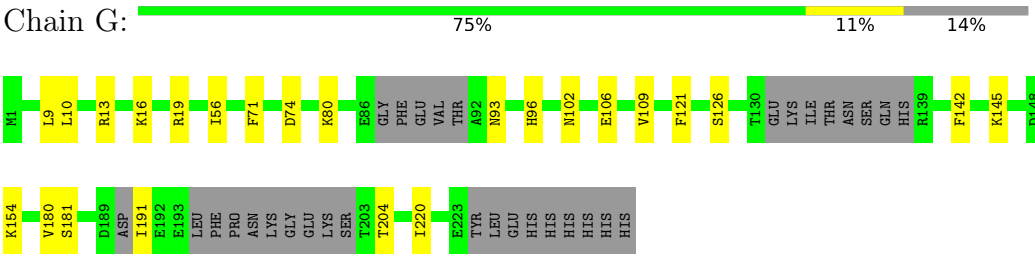
• Molecule 1: Helix-turn-helix XRE family protein

Chain F:



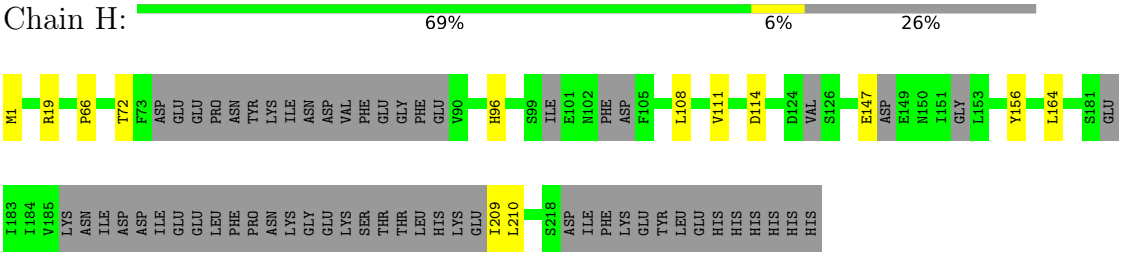
• Molecule 1: Helix-turn-helix XRE family protein

Chain G:



• Molecule 1: Helix-turn-helix XRE family protein

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	594605	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Estimate and correct for full-frame motion (eg. stage drift) as well as sample deformation (local motion) by Cryosparc Patch Motion Correction.	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	190000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.65	0/165	0.63	0/213
1	B	0.60	0/469	0.54	0/619
1	C	0.57	0/1344	0.57	0/1794
1	D	0.58	0/1726	0.58	0/2314
1	E	0.46	0/1826	0.55	0/2455
1	F	0.47	0/1826	0.54	0/2455
1	G	0.61	0/1656	0.58	0/2219
1	H	0.51	0/1414	0.55	0/1887
All	All	0.54	0/10426	0.56	0/13956

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

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	A	167	0	179	5	0
1	B	463	0	435	8	0
1	C	1330	0	1346	13	0
1	D	1701	0	1685	15	0
1	E	1797	0	1780	17	0
1	F	1797	0	1780	11	0
1	G	1635	0	1624	17	0
1	H	1401	0	1413	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3	0	0	2	0
2	B	9	0	0	0	0
2	C	10	0	0	1	0
2	D	15	0	0	1	0
2	E	3	0	0	0	0
2	F	1	0	0	0	0
2	G	8	0	0	2	0
2	H	11	0	0	2	0
All	All	10351	0	10242	91	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 4.

The worst 5 of 91 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:D:103:PHE:HZ	1:D:183:ILE:HG21	1.54	0.73
1:D:22:LYS:NZ	2:D:301:HOH:O	2.22	0.72
1:F:129:GLU:HG2	1:F:130:THR:H	1.56	0.70
1:F:129:GLU:HG2	1:F:130:THR:N	2.07	0.69
1:H:19:ARG:NH2	2:H:301:HOH:O	2.29	0.64

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	A	11/232 (5%)	10 (91%)	1 (9%)	0	100	100
1	B	38/232 (16%)	37 (97%)	1 (3%)	0	100	100
1	C	151/232 (65%)	141 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	199/232 (86%)	191 (96%)	8 (4%)	0	100	100
1	E	215/232 (93%)	210 (98%)	5 (2%)	0	100	100
1	F	215/232 (93%)	206 (96%)	9 (4%)	0	100	100
1	G	187/232 (81%)	177 (95%)	10 (5%)	0	100	100
1	H	154/232 (66%)	150 (97%)	4 (3%)	0	100	100
All	All	1170/1856 (63%)	1122 (96%)	48 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	A	20/219 (9%)	20 (100%)	0	100	100
1	B	52/219 (24%)	52 (100%)	0	100	100
1	C	154/219 (70%)	153 (99%)	1 (1%)	84	90
1	D	195/219 (89%)	195 (100%)	0	100	100
1	E	207/219 (94%)	206 (100%)	1 (0%)	86	92
1	F	207/219 (94%)	206 (100%)	1 (0%)	86	92
1	G	188/219 (86%)	188 (100%)	0	100	100
1	H	162/219 (74%)	162 (100%)	0	100	100
All	All	1185/1752 (68%)	1182 (100%)	3 (0%)	90	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4	ASN
1	E	102	ASN
1	F	89	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes.

such sidechains are listed below:

Mol	Chain	Res	Type
1	E	138	HIS
1	F	37	ASN
1	H	96	HIS
1	G	120	ASN
1	D	96	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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 oligosaccharides 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.