



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2022 – 04:02 PM EDT

PDB ID : 7U41  
Title : [F234] Self-assembling tensegrity triangle with two turns, three turns and four turns of DNA per axis by extension with P1 symmetry  
Authors : Woloszyn, K.; Vecchioni, S.; Seeman, N.C.; Sha, R.; Ohayon, Y.P.  
Deposited on : 2022-02-28  
Resolution : 7.24 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

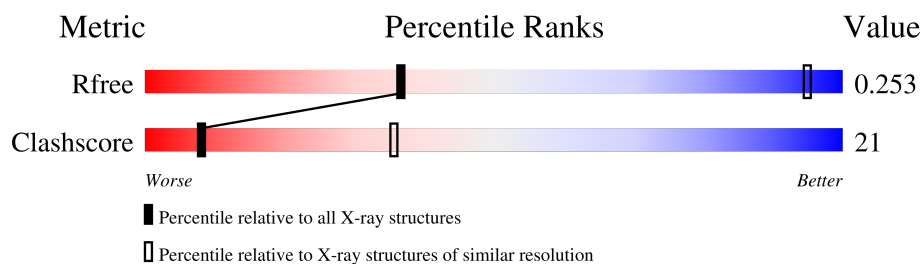
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 7.24 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	21	
2	E	24	
3	D	14	
4	B	42	
5	F	35	
6	C	31	
7	M	21	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3843 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA chain called DNA (5'-D(P\*CP\*AP\*AP\*GP\*AP\*GP\*CP\*CP\*TP\*GP\*AP\*TP\*CP\*GP\*GP\*AP\*CP\*AP\*AP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	P	0	0	0
			433	204	87	121	21			

- Molecule 2 is a DNA chain called DNA (5'-D(P\*TP\*CP\*AP\*CP\*TP\*CP\*AP\*GP\*CP\*AP\*TP\*GP\*TP\*GP\*AP\*TP\*GP\*TP\*GP\*GP\*CP\*TP\*CP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	24	Total	C	N	O	P	0	0	0
			490	234	84	148	24			

- Molecule 3 is a DNA chain called DNA (5'-D(P\*TP\*CP\*GP\*CP\*TP\*TP\*GP\*TP\*GP\*GP\*TP\*AP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			291	138	51	88	14			

- Molecule 4 is a DNA chain called DNA (42-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	42	Total	C	N	O	P	0	0	0
			853	405	156	250	42			

- Molecule 5 is a DNA chain called DNA (35-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	35	Total	C	N	O	P	0	0	0
			726	344	133	214	35			

- Molecule 6 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	31	Total 632	C 301	N 119	O 182	P 30	0	0	0

- Molecule 7 is a DNA chain called DNA (5'-D(\*GP\*CP\*CP\*AP\*CP\*CP\*GP\*AP\*TP\*CP\*AP\*CP\*CP\*GP\*AP\*TP\*CP\*AP\*CP\*CP\*T)-3').

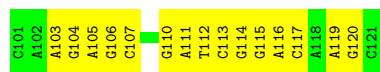
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	M	21	Total 418	C 200	N 76	O 122	P 20	0	0	0

### 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.

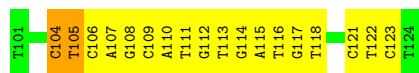
- Molecule 1: DNA (5'-D(P\*CP\*AP\*AP\*GP\*AP\*GP\*CP\*CP\*TP\*GP\*AP\*TP\*CP\*GP\*GP\*AP\*CP\*AP\*AP\*GP\*C)-3')

Chain A: 



- Molecule 2: DNA (5'-D(P\*TP\*CP\*AP\*CP\*TP\*CP\*AP\*GP\*CP\*AP\*TP\*GP\*TP\*GP\*AP\*T\*P\*GP\*TP\*GP\*GP\*CP\*TP\*CP\*T)-3')

Chain E: 



- Molecule 3: DNA (5'-D(P\*TP\*CP\*GP\*CP\*TP\*TP\*GP\*TP\*GP\*GP\*TP\*AP\*GP\*G)-3')

Chain D: 



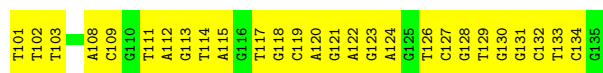
- Molecule 4: DNA (42-MER)

Chain B: 



- Molecule 5: DNA (35-MER)

Chain F: 



- Molecule 6: DNA (31-MER)

Chain C:  32% 65%



- Molecule 7: DNA (5'-D(\*GP\*CP\*CP\*AP\*CP\*CP\*GP\*AP\*TP\*CP\*AP\*CP\*CP\*GP\*AP\*TP\*CP\*AP\*CP\*CP\*T)-3')

Chain M:  33% 62% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.12Å 100.81Å 134.24Å 108.50° 98.10° 100.93°	Depositor
Resolution (Å)	36.19 – 7.24 92.57 – 7.20	Depositor EDS
% Data completeness (in resolution range)	38.3 (36.19-7.24) 31.7 (92.57-7.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.64 (at 7.43Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.241 , 0.257 0.238 , 0.253	Depositor DCC
$R_{free}$ test set	103 reflections (5.44%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.9	Xtriage
Anisotropy	1.724	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 500.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.286 for -h,-k,h+k+l	Xtriage
$F_o, F_c$ correlation	0.54	EDS
Total number of atoms	3843	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	823.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0998e-03.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.65	0/487	0.89	0/749
2	E	0.71	0/547	1.10	2/842 (0.2%)
3	D	0.61	0/325	1.09	1/501 (0.2%)
4	B	0.72	0/955	1.00	2/1469 (0.1%)
5	F	0.65	0/814	1.02	0/1257
6	C	0.71	0/709	0.97	1/1092 (0.1%)
7	M	0.60	0/467	1.01	1/716 (0.1%)
All	All	0.68	0/4304	1.01	7/6626 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
7	M	108	DA	P-O3'-C3'	-10.80	106.74	119.70
2	E	104	DC	P-O3'-C3'	-8.84	109.09	119.70
4	B	132	DC	O4'-C1'-N1	6.40	112.48	108.00
2	E	105	DT	P-O3'-C3'	-6.37	112.05	119.70
6	C	121	DA	C1'-O4'-C4'	-5.34	104.76	110.10
3	D	110	DG	O4'-C1'-N9	5.25	111.68	108.00
4	B	122	DC	O4'-C1'-N1	5.16	111.61	108.00

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	A	433	0	234	16	0
2	E	490	0	273	23	0
3	D	291	0	160	6	0
4	B	853	0	471	25	0
5	F	726	0	396	28	0
6	C	632	0	349	26	0
7	M	418	0	236	9	0
All	All	3843	0	2119	124	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 21.

All (124) 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)
2:E:104:DC:H4'	2:E:105:DT:OP1	1.29	1.03
2:E:104:DC:C4'	2:E:105:DT:OP1	2.01	1.03
4:B:133:DT:H2'	4:B:134:DA:C8	2.15	0.81
3:D:113:DG:N1	4:B:104:DC:N3	2.29	0.80
3:D:113:DG:N2	4:B:104:DC:O2	2.13	0.79
7:M:113:DC:H2''	7:M:114:DG:C8	2.19	0.77
2:E:111:DT:H2'	2:E:112:DG:C8	2.20	0.76
5:F:108:DA:H2'	5:F:109:DC:H4'	1.68	0.75
1:A:103:DA:H2''	1:A:104:DG:H5''	1.72	0.72
2:E:117:DG:H2''	2:E:118:DT:H5''	1.72	0.70
5:F:132:DC:H42	6:C:106:DG:H22	1.43	0.67
5:F:113:DG:H2'	5:F:114:DT:C5	2.30	0.67
5:F:101:DT:H2''	5:F:102:DT:C5	2.32	0.65
5:F:130:DG:N3	5:F:130:DG:H2'	2.11	0.65
4:B:128:DA:H2''	4:B:129:DC:C5	2.32	0.64
5:F:111:DT:H2'	5:F:112:DA:N7	2.14	0.63
2:E:106:DC:H1'	2:E:107:DA:OP2	1.99	0.62
2:E:105:DT:H3	6:C:129:DA:H61	1.47	0.61
4:B:120:DC:H2''	4:B:121:DT:H5''	1.82	0.61
7:M:104:DA:OP1	7:M:105:DC:N4	2.34	0.61
7:M:107:DG:H2''	7:M:108:DA:O5'	2.01	0.60
4:B:120:DC:H2'	4:B:121:DT:H71	1.82	0.60
6:C:118:DA:H2''	6:C:119:DT:H71	1.83	0.60
2:E:110:DA:H2'	2:E:111:DT:O4'	2.02	0.58
5:F:128:DG:H2''	5:F:129:DT:H5''	1.86	0.58
4:B:110:DG:H2'	4:B:111:DG:C8	2.40	0.57
2:E:104:DC:H2''	2:E:105:DT:C5	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:113:DG:O6	4:B:104:DC:N4	2.33	0.56
4:B:119:DA:H2''	4:B:120:DC:O5'	2.06	0.56
3:D:107:DG:H2''	3:D:108:DT:H5''	1.87	0.56
1:A:105:DA:H8	1:A:105:DA:H5'	1.72	0.55
6:C:121:DA:H3'	6:C:122:DC:H2'	1.88	0.55
6:C:120:DC:O2	6:C:121:DA:H1'	2.07	0.55
1:A:113:DC:H1'	1:A:114:DG:C5	2.43	0.53
6:C:122:DC:H1'	6:C:123:DA:C8	2.44	0.53
7:M:102:DC:H2''	7:M:103:DC:C5	2.43	0.53
2:E:122:DT:H2'	2:E:123:DC:C6	2.43	0.53
1:A:110:DG:H2''	1:A:111:DA:H8	1.74	0.53
6:C:129:DA:H2''	6:C:130:DG:C8	2.44	0.53
1:A:110:DG:H2''	1:A:111:DA:C8	2.43	0.52
6:C:108:DC:C2	6:C:109:DT:H73	2.44	0.52
4:B:132:DC:H2''	4:B:133:DT:OP1	2.08	0.52
3:D:106:DT:H2''	3:D:107:DG:C8	2.45	0.52
2:E:113:DT:C2	2:E:114:DG:C8	2.98	0.51
4:B:130:DT:H4'	4:B:131:DA:OP1	2.10	0.51
5:F:122:DA:H2''	5:F:123:DG:C8	2.45	0.51
4:B:140:DG:H4'	4:B:141:DC:OP1	2.10	0.51
6:C:120:DC:C2	6:C:121:DA:H1'	2.45	0.51
6:C:103:DC:H2'	6:C:103:DC:OP1	2.10	0.51
6:C:109:DT:H2'	6:C:110:DG:C8	2.46	0.51
5:F:113:DG:H2'	5:F:114:DT:C6	2.45	0.51
5:F:122:DA:H2''	5:F:123:DG:H8	1.76	0.51
1:A:119:DA:H4'	1:A:120:DG:OP1	2.09	0.50
5:F:120:DA:H2''	5:F:121:DG:C8	2.46	0.50
7:M:109:DT:H2''	7:M:110:DC:O4'	2.11	0.50
4:B:136:DG:H4'	4:B:137:DT:OP1	2.10	0.50
6:C:105:DA:H2''	6:C:106:DG:C8	2.47	0.50
4:B:129:DC:H6	4:B:129:DC:H5''	1.76	0.50
2:E:116:DT:C2	2:E:117:DG:C6	3.00	0.49
2:E:112:DG:C6	6:C:121:DA:N6	2.81	0.49
1:A:106:DG:H2''	1:A:107:DC:O5'	2.12	0.49
2:E:115:DA:H2''	2:E:116:DT:H71	1.94	0.48
2:E:121:DC:H2''	2:E:122:DT:O5'	2.13	0.48
5:F:112:DA:H1'	5:F:113:DG:H5'	1.95	0.48
2:E:105:DT:H3	6:C:129:DA:N6	2.11	0.48
4:B:129:DC:C6	4:B:130:DT:H72	2.48	0.48
6:C:121:DA:H2'	6:C:122:DC:C6	2.48	0.48
1:A:111:DA:H2''	1:A:112:DT:H71	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:DA:H5'	1:A:105:DA:C8	2.50	0.47
5:F:132:DC:C4	5:F:133:DT:C4	3.03	0.47
7:M:101:DG:H5'	7:M:121:DT:H1'	1.98	0.47
4:B:108:DC:H2'	4:B:109:DT:C6	2.49	0.46
4:B:121:DT:H2''	4:B:122:DC:O4'	2.15	0.46
6:C:122:DC:C2	6:C:123:DA:N7	2.84	0.46
1:A:117:DC:C6	1:A:117:DC:H5'	2.51	0.46
2:E:105:DT:H2'	2:E:106:DC:C4	2.50	0.46
7:M:120:DC:H2''	7:M:121:DT:C5	2.51	0.46
1:A:117:DC:H5'	1:A:117:DC:H6	1.81	0.46
2:E:114:DG:H2''	2:E:115:DA:C8	2.51	0.46
2:E:118:DT:H2''	7:M:112:DC:O4'	2.15	0.46
3:D:104:DC:H1'	3:D:105:DT:H5'	1.97	0.46
2:E:104:DC:H2''	2:E:105:DT:C7	2.46	0.45
5:F:132:DC:H2''	5:F:133:DT:O5'	2.16	0.45
6:C:121:DA:H2'	6:C:122:DC:N1	2.32	0.45
1:A:119:DA:H2''	1:A:120:DG:H5''	1.98	0.45
5:F:118:DG:H2''	5:F:119:DC:O5'	2.15	0.45
5:F:123:DG:H1'	5:F:124:DA:OP2	2.16	0.45
5:F:130:DG:C2	5:F:131:DG:C4	3.04	0.45
5:F:133:DT:H2''	5:F:134:DC:O5'	2.17	0.45
6:C:122:DC:H4'	6:C:123:DA:OP1	2.15	0.45
2:E:104:DC:C1'	2:E:105:DT:OP1	2.64	0.45
5:F:108:DA:H5'	5:F:108:DA:H8	1.82	0.45
5:F:117:DT:H2''	5:F:118:DG:OP1	2.17	0.44
6:C:128:DG:H2''	6:C:129:DA:C8	2.53	0.44
4:B:112:DC:H2''	4:B:113:DA:O5'	2.18	0.44
5:F:132:DC:H42	6:C:106:DG:N2	2.14	0.44
5:F:102:DT:H2'	5:F:103:DT:H71	1.99	0.44
5:F:127:DC:H2''	5:F:128:DG:C8	2.53	0.44
6:C:103:DC:H1'	6:C:104:DG:C8	2.53	0.44
2:E:108:DG:H2''	2:E:109:DC:O5'	2.18	0.44
1:A:104:DG:C2	1:A:105:DA:C5	3.06	0.43
4:B:115:DG:H2''	4:B:116:DA:H8	1.84	0.43
5:F:131:DG:N2	5:F:132:DC:C4	2.85	0.43
1:A:115:DG:C2	1:A:116:DA:C6	3.07	0.43
4:B:114:DG:H1'	4:B:115:DG:C8	2.55	0.42
4:B:115:DG:H1'	4:B:116:DA:O5'	2.18	0.42
4:B:113:DA:H1'	4:B:114:DG:N7	2.35	0.42
4:B:132:DC:H2''	4:B:133:DT:H71	2.02	0.42
4:B:132:DC:H1'	4:B:133:DT:OP2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:114:DG:H2''	6:C:115:DG:C8	2.55	0.41
5:F:126:DT:H6	5:F:126:DT:H2'	1.64	0.41
2:E:113:DT:N3	2:E:114:DG:N7	2.68	0.41
6:C:102:DA:H2''	6:C:103:DC:C5	2.55	0.41
1:A:112:DT:H2''	1:A:113:DC:O5'	2.20	0.41
4:B:128:DA:H2''	4:B:129:DC:H5	1.82	0.41
6:C:106:DG:C2	6:C:107:DC:C2	3.09	0.41
6:C:117:DC:H2''	6:C:118:DA:C8	2.55	0.41
6:C:120:DC:C4	6:C:121:DA:C8	3.09	0.41
2:E:105:DT:H2'	2:E:106:DC:C5	2.56	0.41
5:F:114:DT:H2''	5:F:115:DA:C8	2.56	0.41
5:F:130:DG:C6	5:F:131:DG:C6	3.08	0.41
5:F:112:DA:C4	5:F:113:DG:C8	3.09	0.41
7:M:104:DA:O5'	7:M:105:DC:H5	2.03	0.40
1:A:110:DG:C2	1:A:111:DA:C5	3.09	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 monosaccharides 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.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.