



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:08 PM UTC

PDB ID : 7U44 / pdb_00007u44
Title : [F344] Self-assembling tensegrity triangle with three turns, four 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 : 8.46 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

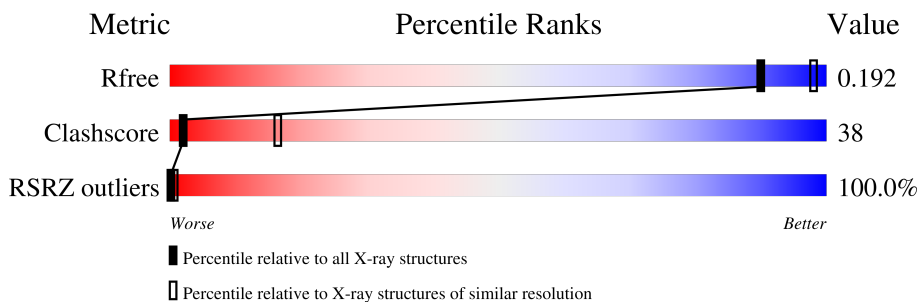
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.46 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}	180053	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
RSRZ outliers	180081	1162 (11.50-4.00)

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 ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	42	100% 5% 95%
2	E	24	100% 21% 79%
3	D	35	100% 29% 71%
4	B	42	100% 33% 67%
5	F	35	100% 23% 71% 6%
6	C	31	100% 6% 90% .
7	M	21	100% 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4712 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 (42-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	42	Total	C	N	O	P	0	0	0
			863	408	165	248	42			

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*TP*TP*AP*GP*CP*AP*TP*AP*GP*GP*CP*AP*GP*TP*CP*GP*TP*GP*GP*CP*TP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	24	Total	C	N	O	P	0	0	0
			495	235	89	147	24			

- Molecule 3 is a DNA chain called DNA (35-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	35	Total	C	N	O	P	0	0	0
			718	341	127	215	35			

- 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
			860	408	159	251	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	136	211	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	31	Total	C	N	O	P	0	0	0
			629	300	117	182	30			

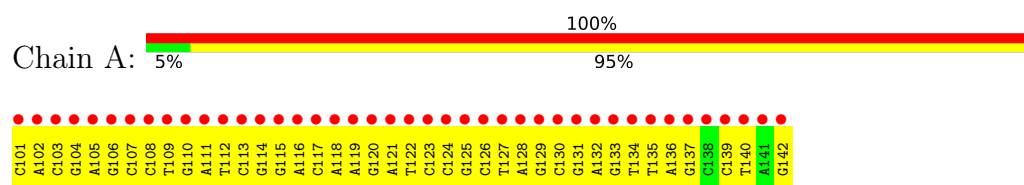
- Molecule 7 is a DNA chain called DNA (5'-D(P*CP*AP*CP*CP*GP*AP*TP*CP*AP*CP*CP*TP*GP*CP*CP*AP*CP*CP*GP*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	M	21	Total	C	N	O	P	0	0	0
			421	200	76	124	21			

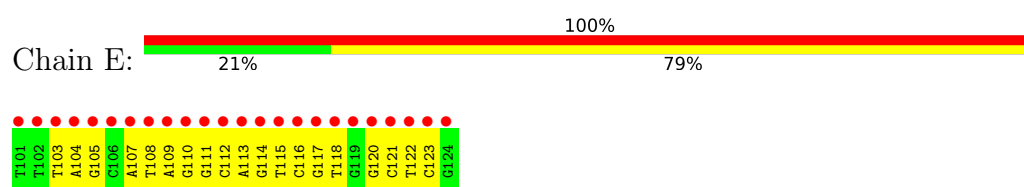
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

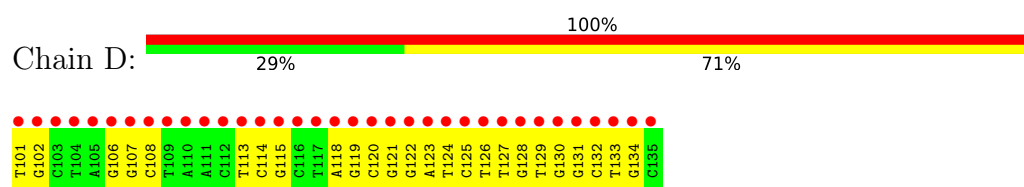
- Molecule 1: DNA (42-MER)



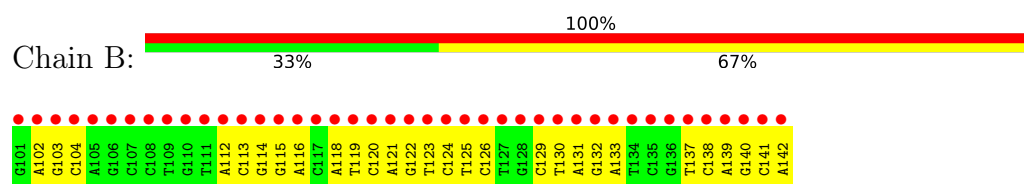
- Molecule 2: DNA (5'-D(P*TP*TP*TP*AP*GP*CP*AP*TP*AP*GP*GP*CP*AP*GP*TP*C P*GP*TP*GP*GP*CP*TP*CP*G)-3')



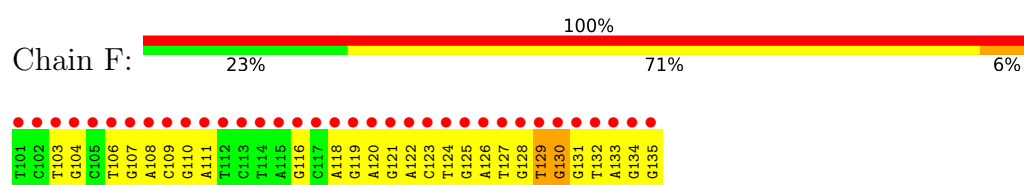
- Molecule 3: DNA (35-MER)



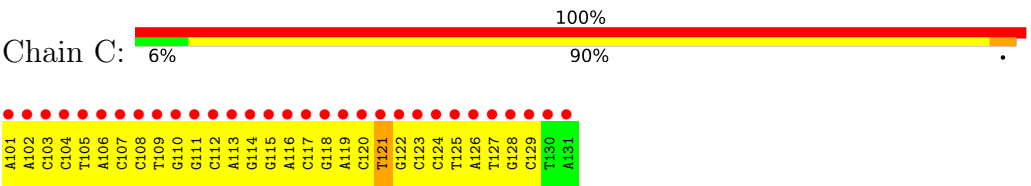
- Molecule 4: DNA (42-MER)



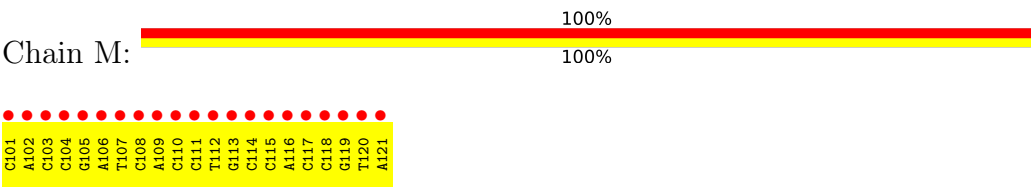
- Molecule 5: DNA (35-MER)



● Molecule 6: DNA (31-MER)



● Molecule 7: DNA (5'-D(P*CP*AP*CP*CP*GP*AP*TP*CP*AP*CP*CP*TP*GP*CP*CP*AP*CP*CP*GP*TP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	100.42Å 135.34Å 135.19Å 99.31° 95.66° 106.50°	Depositor
Resolution (Å)	38.27 – 8.46 38.27 – 8.46	Depositor EDS
% Data completeness (in resolution range)	58.4 (38.27-8.46) 49.2 (38.27-8.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.54 (at 8.42Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.160 , 0.192 0.161 , 0.192	Depositor DCC
R_{free} test set	185 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	337.7	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	1.16 , 576.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4712	wwPDB-VP
Average B, all atoms (Å ²)	1274.0	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 37.04 % 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 4.5549e-04.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.50	0/969	0.71	0/1493
2	E	0.61	0/554	0.83	0/854
3	D	0.44	0/803	0.67	0/1238
4	B	0.47	0/964	0.67	0/1485
5	F	0.60	1/815 (0.1%)	0.78	1/1258 (0.1%)
6	C	0.57	0/705	0.86	2/1085 (0.2%)
7	M	0.80	0/470	1.12	1/720 (0.1%)
All	All	0.56	1/5280 (0.0%)	0.79	4/8133 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	130	DG	O5'-C5'	5.81	1.60	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	121	DT	P-O3'-C3'	-8.19	107.92	120.20
6	C	121	DT	O3'-P-O5'	7.04	114.56	104.00
7	M	109	DA	C3'-C2'-C1'	-5.94	92.69	101.60
5	F	129	DT	O3'-P-O5'	5.78	112.67	104.00

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	863	0	470	59	1
2	E	495	0	272	35	0
3	D	718	0	396	34	0
4	B	860	0	472	40	0
5	F	726	0	395	54	0
6	C	629	0	349	47	0
7	M	421	0	235	45	0
All	All	4712	0	2589	274	1

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 38.

All (274) 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:118:DT:H2'	7:M:111:DC:H4'	1.42	1.01
1:A:108:DC:H2'	1:A:109:DT:H71	1.51	0.93
5:F:107:DG:H2''	5:F:108:DA:H5''	1.55	0.88
5:F:130:DG:C8	7:M:117:DC:H5''	2.09	0.87
1:A:114:DG:H2''	1:A:115:DG:C8	2.10	0.86
6:C:110:DG:H2'	6:C:111:DG:H4'	1.57	0.85
7:M:113:DG:H1'	7:M:114:DC:H5'	1.60	0.83
1:A:112:DT:H2'	1:A:113:DC:C6	2.18	0.79
5:F:133:DA:H2'	5:F:134:DG:H8	1.47	0.78
6:C:111:DG:H2''	6:C:112:DC:OP1	1.80	0.78
6:C:112:DC:H2'	6:C:113:DA:C8	2.20	0.76
5:F:119:DG:H2'	5:F:120:DA:C8	2.21	0.76
3:D:130:DG:H3'	3:D:131:DG:C8	2.22	0.75
3:D:130:DG:H3'	3:D:131:DG:H8	1.52	0.75
6:C:103:DC:H2''	6:C:104:DC:H5''	1.68	0.74
2:E:107:DA:N1	6:C:128:DG:N2	2.36	0.74
5:F:130:DG:P	7:M:118:DC:H2''	2.29	0.72
4:B:112:DA:H2''	4:B:113:DC:H5'	1.71	0.72
7:M:102:DA:H4'	7:M:103:DC:OP2	1.90	0.72
1:A:140:DT:O2	3:D:106:DG:N2	2.24	0.70
2:E:108:DT:H2'	2:E:109:DA:H8	1.56	0.70
5:F:129:DT:H3'	7:M:118:DC:C2	2.26	0.70
6:C:124:DC:H2''	6:C:125:DT:H5''	1.74	0.70
1:A:112:DT:H2'	1:A:113:DC:H6	1.57	0.69
6:C:117:DC:H2''	6:C:118:DG:C8	2.26	0.69
3:D:128:DG:H2''	3:D:129:DT:H5''	1.73	0.69
3:D:133:DT:H2'	3:D:134:DG:H8	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:115:DG:H4'	4:B:116:DA:O5'	1.92	0.69
5:F:129:DT:O3'	7:M:118:DC:H2''	1.92	0.69
2:E:117:DG:H2''	2:E:118:DT:H5''	1.74	0.69
2:E:108:DT:H2''	2:E:109:DA:H5'	1.74	0.68
4:B:130:DT:H2''	4:B:131:DA:C8	2.29	0.67
4:B:103:DG:H2''	4:B:104:DC:H5''	1.74	0.67
2:E:103:DT:H2''	2:E:104:DA:C8	2.30	0.67
4:B:123:DT:H2''	4:B:124:DC:H2'	1.77	0.67
1:A:115:DG:H4'	1:A:116:DA:H5'	1.77	0.66
5:F:129:DT:H2''	7:M:119:DG:O4'	1.95	0.66
3:D:133:DT:H2'	3:D:134:DG:C8	2.30	0.66
7:M:114:DC:H2''	7:M:115:DC:O4'	1.96	0.65
6:C:110:DG:H5'	6:C:110:DG:H8	1.61	0.65
1:A:104:DG:H2''	1:A:105:DA:C8	2.31	0.65
2:E:109:DA:H1'	2:E:110:DG:H5'	1.79	0.64
5:F:108:DA:H3'	5:F:109:DC:H4'	1.79	0.64
1:A:101:DC:H3'	1:A:102:DA:H4'	1.80	0.64
1:A:115:DG:H1'	1:A:116:DA:C8	2.33	0.63
1:A:129:DG:H2''	1:A:130:DC:O4'	2.00	0.62
5:F:133:DA:H2'	5:F:134:DG:C8	2.32	0.62
5:F:129:DT:H3'	7:M:118:DC:O2	1.99	0.61
3:D:130:DG:N3	3:D:130:DG:H2'	2.16	0.61
7:M:116:DA:H2''	7:M:117:DC:O5'	2.01	0.61
2:E:107:DA:C6	6:C:128:DG:N2	2.69	0.60
5:F:129:DT:H3'	7:M:118:DC:H1'	1.83	0.60
7:M:116:DA:H2''	7:M:117:DC:C5'	2.30	0.60
1:A:109:DT:H2''	1:A:110:DG:N7	2.16	0.60
5:F:110:DG:H2''	5:F:111:DA:C8	2.36	0.60
6:C:110:DG:H5'	6:C:110:DG:C8	2.36	0.60
7:M:120:DT:C2	7:M:121:DA:H1'	2.37	0.60
5:F:130:DG:O5'	7:M:118:DC:H2''	2.01	0.60
1:A:131:DG:H2'	1:A:132:DA:C8	2.37	0.59
2:E:108:DT:H2'	2:E:109:DA:C8	2.36	0.59
3:D:129:DT:H3'	7:M:104:DC:OP1	2.02	0.59
4:B:129:DC:H5''	4:B:129:DC:H6	1.68	0.59
1:A:123:DC:H42	3:D:122:DG:H22	1.51	0.58
1:A:139:DC:N3	3:D:107:DG:N2	2.51	0.58
3:D:107:DG:H2''	3:D:108:DC:H5''	1.85	0.58
5:F:122:DA:H2'	5:F:123:DC:C6	2.38	0.58
6:C:115:DG:H4'	6:C:116:DA:H5'	1.85	0.58
6:C:128:DG:H1'	6:C:129:DC:O4'	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:DG:H2''	1:A:126:DC:C6	2.39	0.58
6:C:102:DA:H1'	6:C:103:DC:OP2	2.04	0.58
1:A:106:DG:OP2	1:A:106:DG:H3'	2.03	0.58
2:E:107:DA:C2	2:E:108:DT:H1'	2.40	0.57
5:F:129:DT:H4'	7:M:118:DC:O3'	2.04	0.57
1:A:104:DG:H2''	1:A:105:DA:H8	1.68	0.57
2:E:110:DG:H2''	2:E:111:DG:C8	2.40	0.57
2:E:104:DA:H2''	2:E:105:DG:O5'	2.05	0.56
6:C:108:DC:H2'	6:C:109:DT:O4'	2.04	0.56
6:C:123:DC:H1'	6:C:124:DC:OP2	2.05	0.56
4:B:133:DA:H8	4:B:133:DA:OP1	1.88	0.56
7:M:104:DC:H5''	7:M:104:DC:C6	2.40	0.56
1:A:111:DA:H2''	1:A:112:DT:OP2	2.06	0.56
2:E:108:DT:H2''	2:E:109:DA:C5'	2.35	0.56
4:B:141:DC:H1'	4:B:142:DA:H5'	1.88	0.56
2:E:105:DG:H8	2:E:105:DG:H5''	1.71	0.55
3:D:122:DG:H2''	3:D:123:DA:N7	2.22	0.55
4:B:113:DC:H2''	4:B:114:DG:N7	2.20	0.55
5:F:119:DG:H2'	5:F:120:DA:H8	1.66	0.55
5:F:129:DT:H5'	7:M:118:DC:O2	2.05	0.55
2:E:103:DT:H2''	2:E:104:DA:N7	2.20	0.55
4:B:121:DA:H2''	4:B:122:DG:C8	2.41	0.55
1:A:117:DC:H2''	1:A:118:DA:C8	2.41	0.55
2:E:122:DT:H2''	2:E:123:DC:O5'	2.07	0.55
5:F:124:DT:H2''	5:F:125:DG:H8	1.73	0.54
2:E:112:DC:H1'	2:E:113:DA:OP2	2.07	0.54
2:E:109:DA:C2	6:C:126:DA:C2	2.95	0.54
1:A:112:DT:H2''	1:A:113:DC:H5'	1.89	0.53
4:B:130:DT:H2''	4:B:131:DA:N7	2.23	0.53
5:F:129:DT:OP1	7:M:118:DC:H4'	2.08	0.53
7:M:104:DC:OP1	7:M:104:DC:H4'	2.09	0.53
5:F:130:DG:H8	7:M:117:DC:H5''	1.67	0.53
1:A:107:DC:H2''	1:A:108:DC:H6	1.73	0.53
7:M:120:DT:N3	7:M:121:DA:H1'	2.25	0.52
5:F:133:DA:H2''	5:F:134:DG:C5'	2.39	0.52
1:A:103:DC:H2''	1:A:104:DG:H5''	1.91	0.52
4:B:119:DT:H2''	4:B:120:DC:O5'	2.08	0.52
5:F:129:DT:C3'	7:M:118:DC:H1'	2.39	0.52
7:M:104:DC:H5''	7:M:104:DC:H6	1.74	0.52
2:E:112:DC:H2''	2:E:113:DA:OP1	2.09	0.52
5:F:127:DT:H2''	5:F:128:DG:H8	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:DT:H2''	1:A:113:DC:C5'	2.38	0.52
1:A:130:DC:C2	1:A:131:DG:C8	2.98	0.52
4:B:112:DA:H2''	4:B:113:DC:C5'	2.38	0.52
5:F:123:DC:H1'	5:F:124:DT:OP2	2.10	0.52
1:A:118:DA:H2''	1:A:119:DA:C8	2.45	0.51
5:F:118:DA:H2''	5:F:119:DG:O4'	2.11	0.51
5:F:132:DT:H2''	5:F:133:DA:O5'	2.09	0.51
1:A:111:DA:C4	1:A:112:DT:H72	2.45	0.51
2:E:114:DG:H1'	2:E:115:DT:C5	2.45	0.51
3:D:124:DT:H2''	3:D:125:DC:C5	2.45	0.51
4:B:139:DA:H2''	4:B:140:DG:C8	2.46	0.51
5:F:134:DG:H1'	5:F:135:DG:H5'	1.93	0.51
1:A:134:DT:H2''	1:A:135:DT:H72	1.92	0.51
1:A:131:DG:C2	3:D:115:DG:C2	2.98	0.50
3:D:124:DT:H2''	3:D:125:DC:C6	2.46	0.50
1:A:128:DA:H2''	1:A:129:DG:C8	2.46	0.50
3:D:113:DT:H2''	3:D:114:DC:C5	2.46	0.50
3:D:128:DG:H2''	3:D:129:DT:H6	1.76	0.50
4:B:133:DA:H8	4:B:133:DA:P	2.35	0.50
1:A:112:DT:P	1:A:112:DT:O4'	2.70	0.50
5:F:131:DG:N2	5:F:132:DT:C4	2.79	0.50
1:A:121:DA:H2'	1:A:122:DT:H72	1.93	0.50
6:C:122:DG:H2''	6:C:123:DC:O4'	2.12	0.49
6:C:113:DA:H1'	6:C:114:DG:N7	2.27	0.49
6:C:120:DC:H2''	6:C:121:DT:H72	1.93	0.49
1:A:118:DA:H2''	1:A:119:DA:H8	1.76	0.49
2:E:116:DC:H1'	2:E:117:DG:C5	2.48	0.49
6:C:127:DT:H2''	6:C:128:DG:H2'	1.94	0.49
7:M:115:DC:H2''	7:M:116:DA:H5'	1.94	0.49
2:E:112:DC:H1'	2:E:113:DA:P	2.52	0.49
4:B:137:DT:C4	4:B:138:DC:C4	3.00	0.49
3:D:127:DT:H1'	3:D:128:DG:O4'	2.13	0.49
6:C:101:DA:N3	6:C:101:DA:H2'	2.28	0.49
2:E:116:DC:H1'	2:E:117:DG:N7	2.28	0.48
3:D:118:DA:H4'	3:D:119:DG:OP1	2.12	0.48
3:D:130:DG:O4'	7:M:104:DC:O5'	2.32	0.48
6:C:126:DA:H2''	6:C:127:DT:O4'	2.13	0.48
6:C:104:DC:H2''	6:C:105:DT:H5'	1.96	0.48
7:M:105:DG:C2	7:M:106:DA:C4	3.02	0.48
3:D:129:DT:H72	7:M:103:DC:C2	2.48	0.48
4:B:132:DG:H2''	4:B:133:DA:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:128:DG:H2'	3:D:129:DT:H71	1.95	0.48
3:D:122:DG:H2''	3:D:123:DA:C8	2.49	0.47
1:A:135:DT:C2	1:A:136:DA:C8	3.02	0.47
1:A:106:DG:C2	1:A:107:DC:C2	3.03	0.47
1:A:129:DG:C2	1:A:130:DC:C2	3.02	0.47
4:B:113:DC:H1'	4:B:114:DG:C8	2.49	0.47
5:F:129:DT:P	7:M:118:DC:H4'	2.54	0.47
6:C:118:DG:C2	6:C:119:DA:C2	3.03	0.47
7:M:113:DG:N3	7:M:114:DC:O4'	2.47	0.47
2:E:107:DA:H2''	2:E:108:DT:O5'	2.15	0.47
1:A:103:DC:H2'	1:A:104:DG:C8	2.50	0.47
3:D:132:DC:H2'	3:D:133:DT:H71	1.96	0.47
5:F:125:DG:H4'	5:F:126:DA:OP1	2.14	0.47
6:C:116:DA:C5	6:C:117:DC:C4	3.03	0.47
3:D:121:DG:O6	3:D:122:DG:N2	2.48	0.47
4:B:125:DT:H2''	4:B:126:DC:H5'	1.96	0.47
1:A:120:DG:H2''	1:A:121:DA:C8	2.50	0.47
5:F:132:DT:H2'	5:F:132:DT:OP1	2.15	0.46
5:F:129:DT:N1	5:F:129:DT:H5''	2.30	0.46
5:F:134:DG:N2	6:C:105:DT:C2	2.83	0.46
4:B:118:DA:C4	5:F:128:DG:N2	2.83	0.46
5:F:134:DG:N2	6:C:105:DT:O2	2.49	0.46
5:F:134:DG:C6	5:F:135:DG:C5	3.04	0.46
7:M:106:DA:H1'	7:M:107:DT:O5'	2.16	0.46
5:F:116:DG:C8	5:F:116:DG:H5''	2.51	0.46
6:C:106:DA:H1'	6:C:107:DC:H5'	1.98	0.46
1:A:112:DT:H2''	1:A:113:DC:O5'	2.15	0.46
4:B:138:DC:C2	4:B:139:DA:C8	3.04	0.45
2:E:117:DG:C8	2:E:118:DT:H72	2.51	0.45
6:C:115:DG:N2	6:C:116:DA:C6	2.85	0.45
2:E:105:DG:H5''	2:E:105:DG:C8	2.51	0.45
2:E:113:DA:H2''	2:E:114:DG:C8	2.51	0.45
1:A:114:DG:N2	1:A:115:DG:C2	2.84	0.45
3:D:119:DG:H2''	3:D:120:DC:O5'	2.17	0.45
6:C:124:DC:H2''	6:C:125:DT:O4'	2.16	0.45
6:C:126:DA:C2	6:C:127:DT:C2	3.05	0.45
1:A:106:DG:C4	1:A:107:DC:C6	3.05	0.45
4:B:114:DG:C2	7:M:119:DG:N2	2.85	0.45
4:B:124:DC:H2''	4:B:125:DT:H71	1.98	0.45
7:M:101:DC:H1'	7:M:102:DA:H5'	1.99	0.45
5:F:127:DT:H2''	5:F:128:DG:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:DC:H2''	1:A:104:DG:O4'	2.17	0.44
5:F:133:DA:H2''	5:F:134:DG:H5'	1.99	0.44
6:C:110:DG:H8	6:C:110:DG:C5'	2.28	0.44
1:A:107:DC:C2	1:A:108:DC:C6	3.05	0.44
1:A:118:DA:C6	1:A:119:DA:C6	3.05	0.44
4:B:112:DA:C2'	4:B:113:DC:H5'	2.44	0.44
4:B:102:DA:H2''	4:B:103:DG:OP2	2.17	0.44
5:F:120:DA:C6	5:F:121:DG:C6	3.05	0.44
6:C:117:DC:C2	6:C:118:DG:C2	3.05	0.44
1:A:129:DG:C4	1:A:130:DC:C6	3.05	0.44
4:B:114:DG:N2	7:M:119:DG:H21	2.15	0.44
4:B:123:DT:C4	4:B:124:DC:C5	3.06	0.44
2:E:114:DG:H2''	2:E:115:DT:C7	2.48	0.44
5:F:120:DA:H2''	5:F:121:DG:H8	1.82	0.44
6:C:116:DA:C2	6:C:117:DC:C2	3.05	0.44
5:F:108:DA:C3'	5:F:109:DC:H4'	2.47	0.44
1:A:112:DT:C2	1:A:113:DC:C5	3.06	0.44
4:B:125:DT:C2	4:B:126:DC:C5	3.06	0.44
5:F:124:DT:H2''	5:F:125:DG:C8	2.51	0.43
7:M:120:DT:C4	7:M:121:DA:H1'	2.53	0.43
1:A:123:DC:C2	1:A:124:DC:N4	2.86	0.43
5:F:120:DA:H2''	5:F:121:DG:C8	2.53	0.43
1:A:123:DC:H42	3:D:122:DG:N2	2.15	0.43
3:D:101:DT:H2'	3:D:102:DG:C8	2.54	0.43
3:D:132:DC:H2''	3:D:133:DT:O5'	2.19	0.43
4:B:118:DA:C2	5:F:128:DG:C2	3.07	0.43
5:F:116:DG:H5''	5:F:116:DG:H8	1.82	0.43
6:C:128:DG:C2	6:C:129:DC:C2	3.07	0.43
7:M:111:DC:H2''	7:M:112:DT:O4'	2.19	0.43
3:D:119:DG:H2''	3:D:120:DC:C5'	2.47	0.43
4:B:114:DG:H2''	4:B:115:DG:O4'	2.18	0.43
2:E:121:DC:H4'	2:E:122:DT:OP1	2.18	0.42
6:C:127:DT:H2''	6:C:128:DG:O5'	2.19	0.42
7:M:110:DC:H2''	7:M:111:DC:OP1	2.17	0.42
1:A:119:DA:C6	1:A:120:DG:C6	3.07	0.42
5:F:130:DG:H3'	5:F:131:DG:H5''	2.01	0.42
7:M:107:DT:C2	7:M:108:DC:C6	3.07	0.42
1:A:110:DG:H8	1:A:110:DG:P	2.41	0.42
1:A:115:DG:C2'	1:A:116:DA:H8	2.32	0.42
6:C:105:DT:C2	6:C:106:DA:C2	3.07	0.42
1:A:132:DA:H1'	1:A:133:DG:OP2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:103:DC:C2	6:C:104:DC:C5	3.08	0.42
1:A:118:DA:C2	3:D:128:DG:N2	2.88	0.42
6:C:122:DG:H5''	6:C:122:DG:H8	1.85	0.42
7:M:103:DC:H2''	7:M:104:DC:C5	2.54	0.42
4:B:123:DT:C5	4:B:124:DC:H5	2.37	0.42
4:B:139:DA:H2''	4:B:140:DG:H8	1.84	0.42
4:B:140:DG:N2	5:F:106:DT:O2	2.53	0.42
5:F:129:DT:H2''	7:M:119:DG:C1'	2.50	0.42
6:C:105:DT:H2''	6:C:106:DA:C8	2.54	0.42
4:B:112:DA:N6	7:M:121:DA:C2	2.88	0.42
6:C:107:DC:H2''	6:C:108:DC:O4'	2.20	0.42
5:F:130:DG:C2	5:F:131:DG:C4	3.08	0.41
3:D:125:DC:H4'	3:D:126:DT:OP1	2.18	0.41
2:E:113:DA:H2''	2:E:114:DG:H8	1.85	0.41
2:E:117:DG:N2	6:C:118:DG:H21	2.18	0.41
3:D:133:DT:H2''	3:D:134:DG:C5'	2.50	0.41
3:D:133:DT:H2''	3:D:134:DG:H5'	2.03	0.41
4:B:113:DC:H2''	4:B:114:DG:C8	2.56	0.41
1:A:114:DG:C2'	1:A:115:DG:C8	2.95	0.41
4:B:114:DG:N2	7:M:119:DG:N2	2.69	0.41
4:B:137:DT:C2	4:B:138:DC:C6	3.08	0.41
2:E:117:DG:N2	6:C:118:DG:N2	2.68	0.41
4:B:115:DG:C2	4:B:116:DA:C6	3.08	0.41
1:A:105:DA:C6	1:A:106:DG:C6	3.09	0.41
1:A:127:DT:C4	1:A:128:DA:C6	3.09	0.41
2:E:116:DC:H6	2:E:116:DC:H2'	1.73	0.41
4:B:115:DG:N2	4:B:116:DA:C6	2.88	0.41
4:B:139:DA:C6	4:B:140:DG:C6	3.09	0.41
6:C:113:DA:H1'	6:C:114:DG:C5	2.56	0.41
6:C:114:DG:H8	6:C:114:DG:O5'	2.03	0.41
6:C:124:DC:H4'	6:C:125:DT:OP1	2.21	0.41
2:E:107:DA:H1'	2:E:108:DT:P	2.61	0.41
5:F:118:DA:H2''	5:F:119:DG:O5'	2.19	0.41
1:A:115:DG:H2''	1:A:116:DA:H8	1.85	0.40
1:A:136:DA:H2'	1:A:137:DG:C8	2.56	0.40
5:F:103:DT:H1'	5:F:104:DG:OP1	2.22	0.40
7:M:104:DC:H2''	7:M:105:DG:O4'	2.20	0.40
1:A:108:DC:C2	2:E:120:DG:N2	2.90	0.40
7:M:103:DC:H2''	7:M:104:DC:C6	2.56	0.40
1:A:116:DA:C6	1:A:117:DC:N3	2.89	0.40
5:F:103:DT:H2''	5:F:104:DG:O5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:113:DA:O3'	6:C:114:DG:C8	2.75	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:DC:OP1	1:A:142:DG:N2[1_556]	2.14	0.06

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 oligosaccharides 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	42/42 (100%)	6.52	42 (100%)	0 1	1013, 1265, 1450, 1500	0
2	E	24/24 (100%)	6.71	24 (100%)	0 1	1075, 1308, 1382, 1413	0
3	D	35/35 (100%)	6.26	35 (100%)	0 1	1122, 1345, 1469, 1495	0
4	B	42/42 (100%)	6.55	42 (100%)	0 1	947, 1319, 1535, 1547	0
5	F	35/35 (100%)	6.48	35 (100%)	0 1	1030, 1341, 1594, 1620	0
6	C	31/31 (100%)	6.58	31 (100%)	0 1	1033, 1185, 1288, 1312	0
7	M	21/21 (100%)	5.86	21 (100%)	0 1	939, 1084, 1157, 1231	0
All	All	230/230 (100%)	6.45	230 (100%)	0 1	939, 1271, 1502, 1620	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	111	DA	10.3
6	C	106	DA	9.9
3	D	110	DA	9.8
6	C	111	DG	9.6
1	A	111	DA	9.3
5	F	111	DA	9.1
4	B	112	DA	9.0
5	F	120	DA	8.9
5	F	121	DG	8.9
3	D	122	DG	8.8
5	F	126	DA	8.8
5	F	108	DA	8.7
4	B	102	DA	8.6
2	E	112	DC	8.5
6	C	113	DA	8.4
2	E	105	DG	8.4
7	M	102	DA	8.4

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Mol	Chain	Res	Type	RSRZ
1	A	112	DT	8.3
7	M	105	DG	8.3
2	E	107	DA	8.2
3	D	127	DT	8.2
2	E	110	DG	8.2
1	A	121	DA	8.1
4	B	111	DT	8.1
1	A	119	DA	8.0
4	B	110	DG	8.0
1	A	113	DC	8.0
5	F	117	DC	8.0
2	E	108	DT	7.9
4	B	123	DT	7.9
1	A	118	DA	7.9
3	D	112	DC	7.9
6	C	123	DC	7.8
1	A	136	DA	7.8
1	A	134	DT	7.8
4	B	105	DA	7.8
5	F	127	DT	7.8
6	C	114	DG	7.8
5	F	109	DC	7.7
5	F	122	DA	7.7
2	E	122	DT	7.7
4	B	115	DG	7.7
6	C	119	DA	7.7
4	B	106	DG	7.6
1	A	114	DG	7.6
3	D	126	DT	7.6
1	A	102	DA	7.6
5	F	119	DG	7.6
1	A	135	DT	7.5
1	A	133	DG	7.5
4	B	139	DA	7.5
1	A	120	DG	7.4
2	E	123	DC	7.4
4	B	114	DG	7.3
4	B	136	DG	7.3
3	D	109	DT	7.3
3	D	108	DC	7.3
2	E	124	DG	7.3
4	B	135	DC	7.3

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Mol	Chain	Res	Type	RSRZ
4	B	133	DA	7.3
7	M	121	DA	7.3
1	A	125	DG	7.3
1	A	140	DT	7.3
1	A	141	DA	7.2
4	B	125	DT	7.2
1	A	110	DG	7.2
6	C	115	DG	7.2
4	B	121	DA	7.2
3	D	128	DG	7.2
1	A	105	DA	7.2
4	B	122	DG	7.2
6	C	112	DC	7.2
2	E	120	DG	7.2
3	D	131	DG	7.1
5	F	131	DG	7.1
3	D	117	DT	7.1
1	A	115	DG	7.1
4	B	124	DC	7.1
1	A	122	DT	7.1
6	C	102	DA	7.1
6	C	126	DA	7.0
4	B	113	DC	7.0
5	F	115	DA	7.0
1	A	126	DC	7.0
4	B	104	DC	7.0
1	A	127	DT	6.9
6	C	105	DT	6.9
4	B	140	DG	6.9
2	E	106	DC	6.9
2	E	113	DA	6.9
1	A	132	DA	6.8
5	F	110	DG	6.8
5	F	112	DT	6.8
2	E	116	DC	6.8
2	E	111	DG	6.8
6	C	129	DC	6.8
6	C	116	DA	6.8
7	M	108	DC	6.8
2	E	109	DA	6.8
5	F	105	DC	6.7
2	E	115	DT	6.7

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Mol	Chain	Res	Type	RSRZ
7	M	109	DA	6.7
4	B	126	DC	6.7
4	B	103	DG	6.7
4	B	127	DT	6.7
4	B	107	DC	6.7
4	B	138	DC	6.7
7	M	101	DC	6.7
2	E	117	DG	6.7
4	B	132	DG	6.7
6	C	124	DC	6.7
1	A	106	DG	6.7
7	M	106	DA	6.7
3	D	107	DG	6.7
4	B	120	DC	6.7
6	C	107	DC	6.6
6	C	120	DC	6.6
4	B	119	DT	6.6
5	F	118	DA	6.6
6	C	104	DC	6.6
6	C	127	DT	6.6
7	M	119	DG	6.6
6	C	125	DT	6.6
1	A	139	DC	6.6
6	C	121	DT	6.5
5	F	116	DG	6.5
2	E	104	DA	6.5
5	F	128	DG	6.5
7	M	112	DT	6.5
3	D	118	DA	6.5
3	D	114	DC	6.5
1	A	137	DG	6.4
4	B	137	DT	6.4
5	F	107	DG	6.4
3	D	113	DT	6.4
5	F	133	DA	6.4
1	A	104	DG	6.4
3	D	101	DT	6.3
5	F	114	DT	6.3
7	M	115	DC	6.3
3	D	121	DG	6.2
7	M	116	DA	6.2
4	B	118	DA	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	124	DC	6.2
2	E	121	DC	6.2
5	F	132	DT	6.1
3	D	115	DG	6.1
5	F	106	DT	6.1
7	M	117	DC	6.0
2	E	102	DT	5.9
6	C	118	DG	5.9
6	C	103	DC	5.8
5	F	104	DG	5.8
2	E	101	DT	5.8
3	D	134	DG	5.8
5	F	124	DT	5.7
3	D	123	DA	5.7
3	D	132	DC	5.7
3	D	119	DG	5.7
5	F	125	DG	5.7
4	B	134	DT	5.7
7	M	107	DT	5.7
4	B	116	DA	5.6
1	A	117	DC	5.6
3	D	135	DC	5.6
6	C	110	DG	5.6
5	F	113	DC	5.6
6	C	122	DG	5.6
6	C	131	DA	5.6
3	D	133	DT	5.5
6	C	109	DT	5.5
7	M	114	DC	5.5
5	F	135	DG	5.5
1	A	138	DC	5.5
4	B	142	DA	5.4
5	F	102	DC	5.4
1	A	107	DC	5.4
1	A	129	DG	5.3
1	A	128	DA	5.3
7	M	113	DG	5.3
4	B	130	DT	5.2
1	A	142	DG	5.2
3	D	116	DC	5.1
6	C	108	DC	5.1
4	B	101	DG	5.0

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Mol	Chain	Res	Type	RSRZ
3	D	124	DT	4.9
6	C	130	DT	4.9
3	D	105	DA	4.9
3	D	125	DC	4.9
3	D	120	DC	4.8
1	A	123	DC	4.8
4	B	128	DG	4.8
3	D	103	DC	4.8
1	A	131	DG	4.8
3	D	130	DG	4.8
5	F	123	DC	4.7
5	F	101	DT	4.7
3	D	129	DT	4.7
4	B	108	DC	4.7
7	M	103	DC	4.7
2	E	119	DG	4.7
2	E	118	DT	4.6
5	F	134	DG	4.6
6	C	101	DA	4.6
2	E	103	DT	4.6
6	C	117	DC	4.6
1	A	116	DA	4.5
4	B	117	DC	4.5
4	B	129	DC	4.5
1	A	108	DC	4.5
3	D	102	DG	4.5
2	E	114	DG	4.4
1	A	103	DC	4.4
4	B	141	DC	4.4
3	D	106	DG	4.4
1	A	130	DC	4.3
7	M	118	DC	4.3
4	B	109	DT	4.3
7	M	120	DT	4.3
5	F	130	DG	4.3
6	C	128	DG	4.3
1	A	109	DT	4.2
7	M	104	DC	4.0
4	B	131	DA	4.0
3	D	104	DT	3.8
1	A	101	DC	3.8
7	M	110	DC	3.8

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Mol	Chain	Res	Type	RSRZ
5	F	129	DT	3.4
7	M	111	DC	3.2
5	F	103	DT	3.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.