



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:43 PM GMT

PDB ID : 1QCU  
Title : CRYSTAL STRUCTURE OF AN 18 BASE PAIR COPY CONTROL RELATED RNA DUPLEX  
Authors : Klosterman, P.S.; Shah, S.A.; Steitz, T.A.  
Deposited on : 1999-05-14  
Resolution : 1.20 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

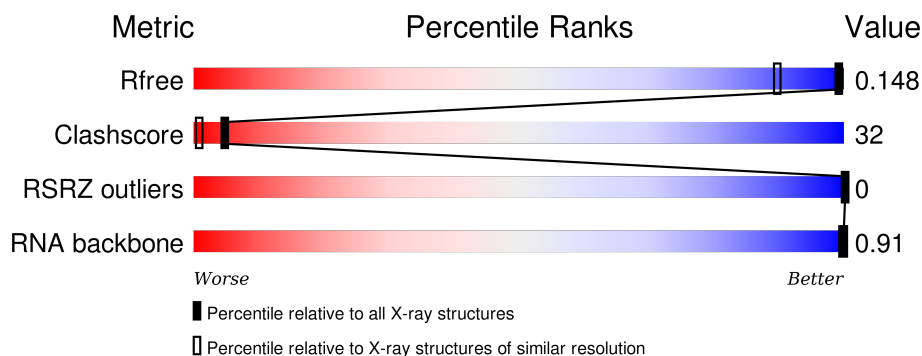
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.20 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))
$R_{free}$	91344	1495 (1.26-1.14)
Clashscore	102246	1607 (1.26-1.14)
RSRZ outliers	91569	1500 (1.26-1.14)
RNA backbone	2183	1046 (2.70-0.62)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	11	<div> <div></div> <div>27%</div> <div>73%</div> </div>
1	D	11	<div> <div></div> <div>45%</div> <div>55%</div> </div>
2	B	11	<div> <div></div> <div>36%</div> <div>55%</div> <div>9%</div> </div>
2	C	11	<div> <div></div> <div>18%</div> <div>55%</div> <div>27%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1614 atoms, of which 469 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.

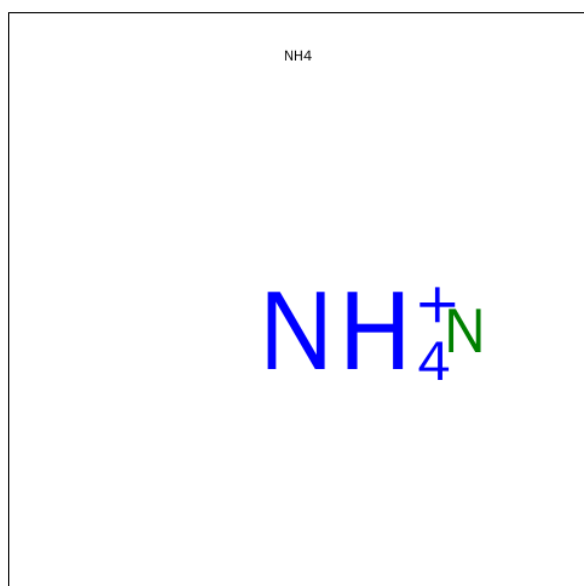
- Molecule 1 is a RNA chain called 5'-R(P\*GP\*GP\*GP\*GP\*GP\*GP\*GP\*GP\*GP\*G)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	11	Total	C	H	N	O	P	0	0	0
			371	110	118	55	77	11			
1	D	11	Total	C	H	N	O	P	0	0	0
			370	110	117	55	77	11			

- Molecule 2 is a RNA chain called 5'-R(P\*CP\*CP\*CP\*CP\*CP\*CP\*CP\*CP\*CP\*C)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	11	Total	C	H	N	O	P	0	0	0
			338	99	118	33	77	11			
2	C	11	Total	C	H	N	O	P	0	0	0
			336	99	116	33	77	11			

- Molecule 3 is AMMONIUM ION (three-letter code: NH4) (formula: H<sub>4</sub>N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total N 1 1	0	0
3	A	1	Total N 1 1	0	0
3	A	1	Total N 1 1	0	0
3	B	1	Total N 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	78	Total O 78 78	0	0
4	B	89	Total O 89 89	0	0
4	C	26	Total O 26 26	0	0
4	D	2	Total O 2 2	0	0

### 3 Residue-property plots

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 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: 5'-R(P\*GP\*GP\*GP\*GP\*GP\*GP\*GP\*GP\*GP\*G)-3'

Chain A: 



- Molecule 1: 5'-R(P\*GP\*GP\*GP\*GP\*GP\*GP\*GP\*GP\*GP\*G)-3'

Chain D: 



- Molecule 2: 5'-R(P\*CP\*CP\*CP\*CP\*CP\*CP\*CP\*CP\*CP\*C)-3'

Chain B: 



- Molecule 2: 5'-R(P\*CP\*CP\*CP\*CP\*CP\*CP\*CP\*CP\*CP\*C)-3'

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.81Å 43.81Å 29.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.20 23.12 – 1.20	Depositor EDS
% Data completeness (in resolution range)	92.5 (30.00-1.20) 88.8 (23.12-1.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.21 (at 1.20Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.117 , 0.150 0.122 , 0.148	Depositor DCC
$R_{free}$ test set	907 reflections (5.48%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.2	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 101.1	EDS
Estimated twinning fraction	0.027 for -h,-k,l 0.469 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	0 of 18266 reflections	Xtriage
$F_o, F_c$ correlation	0.99	EDS
Total number of atoms	1614	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH4

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	1.25	6/285 (2.1%)	2.27	21/447 (4.7%)
1	D	1.23	3/285 (1.1%)	2.51	29/447 (6.5%)
2	B	0.79	0/241	1.77	5/370 (1.4%)
2	C	0.78	0/241	1.84	8/370 (2.2%)
All	All	1.06	9/1052 (0.9%)	2.15	63/1634 (3.9%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	114	G	C6-O6	6.35	1.29	1.24
1	A	3	G	C6-O6	6.18	1.29	1.24
1	D	121	G	C6-O6	5.67	1.29	1.24
1	A	5	G	C6-O6	5.61	1.29	1.24
1	D	116	G	C6-O6	5.50	1.29	1.24
1	A	10	G	C6-O6	5.26	1.28	1.24
1	A	7	G	C6-O6	5.26	1.28	1.24
1	A	9	G	C6-O6	5.14	1.28	1.24
1	A	11	G	C6-O6	5.11	1.28	1.24

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	G	C5-C6-O6	-11.39	121.77	128.60
1	D	119	G	C5-C6-O6	-10.49	122.31	128.60
1	A	10	G	C5-C6-O6	-9.66	122.80	128.60
1	D	113	G	C5-C6-N1	9.13	116.07	111.50
1	A	2	G	C4-C5-C6	-8.94	113.44	118.80
1	D	119	G	N3-C2-N2	-8.81	113.73	119.90
1	D	118	G	N1-C6-O6	-8.23	114.96	119.90
1	A	2	G	C5-C6-O6	-8.20	123.68	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	121	G	C5-C6-O6	-8.00	123.80	128.60
1	D	120	G	C8-N9-C4	-7.96	103.22	106.40
1	A	2	G	C6-C5-N7	7.77	135.06	130.40
1	A	8	G	N3-C2-N2	-7.60	114.58	119.90
1	D	113	G	C4-C5-C6	-7.51	114.29	118.80
1	D	121	G	C5-C6-N1	7.47	115.23	111.50
1	D	115	G	C5-C6-N1	7.45	115.22	111.50
1	A	2	G	C5-C6-N1	7.29	115.14	111.50
2	C	110	C	C2-N3-C4	7.07	123.44	119.90
1	A	9	G	N1-C6-O6	-7.03	115.68	119.90
1	D	116	G	C5-C6-N1	6.92	114.96	111.50
1	D	119	G	N1-C2-N2	6.81	122.33	116.20
1	D	121	G	O4'-C1'-N9	6.75	113.60	108.20
1	D	121	G	C2-N3-C4	6.68	115.24	111.90
1	D	115	G	C2-N3-C4	6.36	115.08	111.90
1	D	119	G	N1-C6-O6	6.36	123.71	119.90
1	D	116	G	C8-N9-C4	-6.29	103.88	106.40
2	B	17	C	C6-N1-C2	-6.24	117.81	120.30
1	A	4	G	C5-C6-N1	6.21	114.60	111.50
1	D	120	G	N1-C6-O6	-6.19	116.18	119.90
1	A	2	G	N3-C4-C5	6.18	131.69	128.60
1	A	2	G	N1-C2-N2	6.14	121.72	116.20
2	C	109	C	N1-C2-O2	-6.09	115.25	118.90
1	A	5	G	C5-C6-N1	6.05	114.52	111.50
1	A	9	G	N7-C8-N9	6.04	116.12	113.10
1	A	9	G	C5-C6-N1	5.99	114.49	111.50
1	D	120	G	N9-C4-C5	5.97	107.79	105.40
1	D	113	G	C4-C5-N7	5.89	113.16	110.80
2	B	21	C	N3-C4-C5	-5.82	119.57	121.90
1	A	4	G	C2-N3-C4	5.75	114.77	111.90
2	B	20	C	N1-C2-O2	-5.73	115.46	118.90
1	D	116	G	C6-N1-C2	-5.69	121.69	125.10
1	D	121	G	N3-C2-N2	-5.66	115.94	119.90
1	A	2	G	N3-C4-N9	-5.66	122.60	126.00
2	C	106	C	C6-N1-C2	-5.60	118.06	120.30
1	A	4	G	C5-C6-O6	-5.56	125.26	128.60
1	A	5	G	C2-N3-C4	5.55	114.68	111.90
1	D	118	G	C5-C6-O6	5.53	131.92	128.60
1	D	115	G	O4'-C1'-N9	5.47	112.58	108.20
2	C	107	C	C2-N3-C4	5.39	122.60	119.90
2	C	110	C	N1-C2-N3	-5.25	115.53	119.20
1	A	11	G	C5-C6-O6	-5.23	125.46	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	121	G	N1-C2-N3	-5.21	120.77	123.90
1	A	9	G	C8-N9-C4	-5.21	104.31	106.40
1	D	121	G	C6-N1-C2	-5.21	121.97	125.10
2	B	17	C	C5-C4-N4	5.21	123.84	120.20
1	A	1	G	C6-N1-C2	-5.20	121.98	125.10
2	C	107	C	C5-C6-N1	5.20	123.60	121.00
1	D	115	G	C5-C6-O6	-5.16	125.50	128.60
2	B	19	C	C5-C6-N1	5.12	123.56	121.00
1	A	7	G	C8-N9-C4	-5.09	104.36	106.40
1	D	114	G	N1-C6-O6	-5.09	116.85	119.90
2	C	110	C	C6-N1-C2	5.07	122.33	120.30
1	D	114	G	C8-N9-C4	-5.04	104.38	106.40
2	C	110	C	N1-C2-O2	5.02	121.91	118.90

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	253	118	89	26	0
1	D	253	117	90	27	0
2	B	220	118	99	6	0
2	C	220	116	99	10	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	78	0	0	1	0
4	B	89	0	0	5	0
4	C	26	0	0	9	0
4	D	2	0	0	0	0
All	All	1145	469	377	42	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 32.

All (42) 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:A:2:G:O6	1:D:121:G:O6	1.55	1.24
1:A:10:G:O6	1:D:113:G:O6	1.62	1.17
1:A:7:G:O6	1:D:116:G:O6	1.59	1.17
1:A:8:G:O6	1:D:115:G:O6	1.63	1.17
1:A:4:G:O6	1:D:119:G:O6	1.64	1.16
1:A:5:G:O6	1:D:118:G:O6	1.62	1.15
1:A:6:G:O6	1:D:117:G:O6	1.67	1.12
1:A:1:G:O6	1:D:122:G:O6	1.71	1.09
2:B:15:C:N4	1:D:115:G:O6	1.56	1.08
1:A:11:G:O6	1:D:112:G:O6	1.71	1.07
4:A:390:HOH:O	2:C:102:C:H5	1.48	0.94
1:A:2:G:O6	1:D:121:G:C6	2.28	0.84
1:A:10:G:C6	1:D:113:G:O6	2.28	0.83
1:A:8:G:C6	1:D:115:G:O6	2.34	0.79
2:C:108:C:N4	4:C:397:HOH:O	2.11	0.78
1:A:7:G:O6	1:D:116:G:C6	2.40	0.74
1:A:4:G:O6	1:D:119:G:C6	2.41	0.73
1:A:5:G:C6	1:D:118:G:O6	2.42	0.73
1:A:4:G:C6	1:D:119:G:O6	2.40	0.71
1:A:7:G:C6	1:D:116:G:O6	2.44	0.69
1:A:5:G:O6	1:D:118:G:C6	2.46	0.68
2:C:104:C:H5	4:C:357:HOH:O	1.76	0.67
1:A:2:G:C6	1:D:121:G:O6	2.43	0.67
1:A:6:G:C6	1:D:117:G:O6	2.49	0.66
1:A:1:G:C6	1:D:122:G:O6	2.49	0.66
1:A:1:G:O6	1:D:122:G:C6	2.49	0.65
1:A:8:G:O6	1:D:115:G:C6	2.46	0.65
1:A:11:G:O6	1:D:112:G:C6	2.49	0.65
1:A:6:G:O6	1:D:117:G:C6	2.49	0.63
1:A:11:G:C6	1:D:112:G:O6	2.51	0.63
2:C:105:C:H5	4:C:282:HOH:O	1.85	0.58
2:B:15:C:H5	4:B:358:HOH:O	1.86	0.58
2:C:107:C:N4	4:C:389:HOH:O	2.37	0.58
2:C:111:C:H5	4:C:354:HOH:O	1.87	0.57
2:B:16:C:H5	4:B:359:HOH:O	1.87	0.57
2:C:106:C:N4	4:C:364:HOH:O	2.38	0.54
2:C:108:C:H5	4:C:355:HOH:O	1.94	0.50
2:B:14:C:H5	4:B:382:HOH:O	1.98	0.47
2:C:109:C:H5	4:C:350:HOH:O	1.98	0.47
2:B:15:C:N4	4:B:358:HOH:O	2.37	0.46
2:B:20:C:N4	4:B:343:HOH:O	2.30	0.43
2:C:104:C:N4	4:C:351:HOH:O	2.40	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](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	10/11 (90%)	0	0
1	D	10/11 (90%)	0	0
2	B	10/11 (90%)	0	0
2	C	10/11 (90%)	0	0
All	All	40/44 (90%)	0	0

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](#)

Of 4 ligands modelled in this entry, 4 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	11/11 (100%)	-0.85	0 100 100	16, 20, 22, 25	11 (100%)
1	D	11/11 (100%)	-0.83	0 100 100	16, 20, 22, 25	11 (100%)
2	B	11/11 (100%)	-0.87	0 100 100	17, 21, 23, 25	11 (100%)
2	C	11/11 (100%)	-0.88	0 100 100	17, 21, 22, 25	11 (100%)
All	All	44/44 (100%)	-0.86	0 100 100	16, 21, 25, 25	44 (100%)

There are no RSRZ outliers to report.

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NH4	B	204	1/1	0.99	0.12	-	16,16,16,16	1
3	NH4	B	201	1/1	0.99	0.11	-	19,19,19,19	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NH4	A	202	1/1	1.00	0.09	-	19,19,19,19	1
3	NH4	A	203	1/1	0.99	0.04	-	19,19,19,19	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.