



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 09:38 am BST

PDB ID : 6CFN
Title : Crystal Structure of the DNA-free Glucocorticoid Receptor DNA Binding Domain
Authors : Frank, F.; Okafor, C.D.; Ortlund, E.A.
Deposited on : 2018-02-15
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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	:	2.11
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)	:	2.11

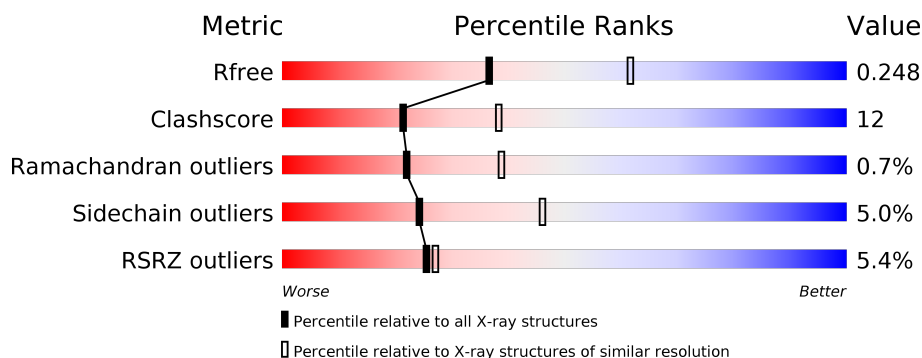
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 ≥ 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	90	<div> <div>8%</div> <div> <div></div> <div>66%</div> <div>23%</div> <div>11%</div> </div> </div>
1	B	90	<div> <div>%</div> <div> <div></div> <div>51%</div> <div>23%</div> <div>••</div> <div>22%</div> </div> </div>
1	C	90	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>•</div> <div>10%</div> </div> </div>
1	D	90	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>14%</div> <div>•</div> <div>24%</div> </div> </div>
1	E	90	<div> <div>6%</div> <div> <div></div> <div>54%</div> <div>30%</div> <div>••</div> <div>12%</div> </div> </div>
1	F	90	<div> <div>8%</div> <div> <div></div> <div>62%</div> <div>21%</div> <div>••</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	90	<div><div>%</div><div><div></div><div>66%</div><div>12%</div><div>22%</div></div></div>
1	H	90	<div><div>4%</div><div><div></div><div>61%</div><div>16%</div><div>23%</div></div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4643 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 protein called Glucocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	80	Total	C	N	O	S	0	0	0
			624	385	122	106	11			
1	B	70	Total	C	N	O	S	0	0	0
			539	331	104	93	11			
1	C	81	Total	C	N	O	S	0	0	0
			627	387	122	107	11			
1	D	68	Total	C	N	O	S	0	0	0
			522	319	101	91	11			
1	E	79	Total	C	N	O	S	0	0	0
			615	379	120	105	11			
1	F	78	Total	C	N	O	S	0	0	0
			605	372	118	104	11			
1	G	70	Total	C	N	O	S	0	0	0
			538	330	104	93	11			
1	H	69	Total	C	N	O	S	0	0	0
			531	325	103	92	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	SER	-	expression tag	UNP P04150
B	417	SER	-	expression tag	UNP P04150
C	417	SER	-	expression tag	UNP P04150
D	417	SER	-	expression tag	UNP P04150
E	417	SER	-	expression tag	UNP P04150
F	417	SER	-	expression tag	UNP P04150
G	417	SER	-	expression tag	UNP P04150
H	417	SER	-	expression tag	UNP P04150

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	B	3	Total O 3 3	0	0
3	C	4	Total O 4 4	0	0
3	D	6	Total O 6 6	0	0
3	E	3	Total O 3 3	0	0
3	F	1	Total O 1 1	0	0
3	G	2	Total O 2 2	0	0
3	H	3	Total O 3 3	0	0

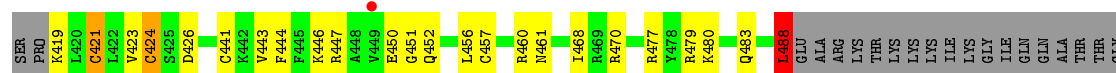
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Glucocorticoid receptor



- Molecule 1: Glucocorticoid receptor



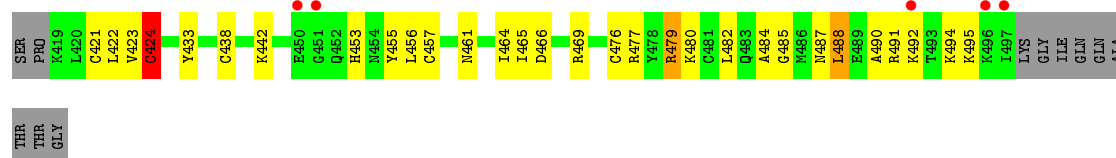
- Molecule 1: Glucocorticoid receptor



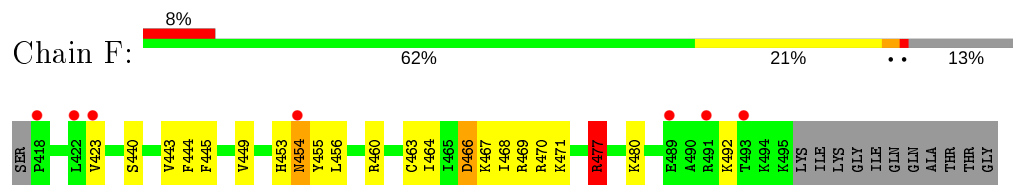
- Molecule 1: Glucocorticoid receptor



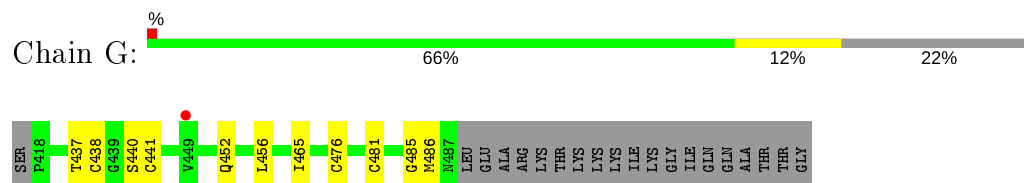
- Molecule 1: Glucocorticoid receptor



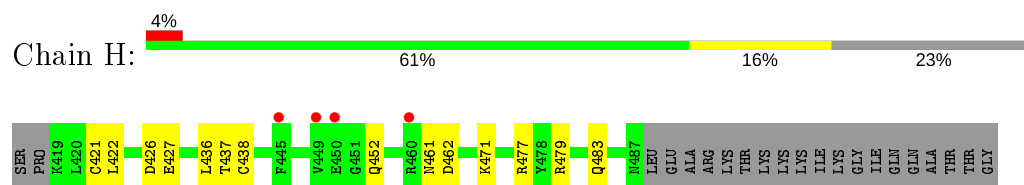
- Molecule 1: Glucocorticoid receptor



- Molecule 1: Glucocorticoid receptor



- Molecule 1: Glucocorticoid receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.80Å 65.43Å 72.66Å 71.27° 84.96° 68.44°	Depositor
Resolution (Å)	36.04 – 2.50 36.04 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.5 (36.04-2.50) 89.5 (36.04-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.195 , 0.248 0.195 , 0.248	Depositor DCC
R_{free} test set	1654 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4643	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

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

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	0.52	0/631	0.63	0/837
1	B	0.49	0/546	0.76	1/728 (0.1%)
1	C	0.53	0/634	0.68	0/842
1	D	0.45	0/529	0.70	0/706
1	E	0.54	1/622 (0.2%)	0.76	1/826 (0.1%)
1	F	0.52	1/613 (0.2%)	0.76	1/815 (0.1%)
1	G	0.44	0/546	0.58	0/728
1	H	0.47	0/538	0.61	0/717
All	All	0.50	2/4659 (0.0%)	0.69	3/6199 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	424	CYS	CB-SG	-6.56	1.71	1.82
1	F	463	CYS	CB-SG	5.00	1.90	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	456	LEU	CA-CB-CG	-5.73	102.13	115.30
1	B	488	LEU	CA-CB-CG	5.54	128.04	115.30
1	F	477	ARG	NE-CZ-NH1	-5.21	117.69	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	492	LYS	Peptide

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	624	0	642	26	0
1	B	539	0	535	15	0
1	C	627	0	643	18	1
1	D	522	0	511	12	0
1	E	615	0	629	17	1
1	F	605	0	613	12	0
1	G	538	0	532	6	0
1	H	531	0	524	7	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	4	0	0	0	0
3	B	3	0	0	1	0
3	C	4	0	0	1	0
3	D	6	0	0	0	0
3	E	3	0	0	1	0
3	F	1	0	0	0	0
3	G	2	0	0	1	0
3	H	3	0	0	0	0
All	All	4643	0	4629	111	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 12.

The worst 5 of 111 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:446:LYS:NZ	1:A:491:ARG:HH12	1.63	0.95
1:A:446:LYS:HZ3	1:A:491:ARG:HH12	1.20	0.89
1:C:435:VAL:HG11	1:C:486:MET:HG2	1.58	0.85
1:A:467:LYS:HG3	1:A:470:ARG:NH2	1.92	0.85
1:C:491:ARG:HG2	1:C:495:LYS:HE3	1.61	0.83

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:C:479:ARG:NH1	1:E:457:CYS:O[1_545]	2.10	0.10

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	78/90 (87%)	77 (99%)	1 (1%)	0	100	100
1	B	68/90 (76%)	66 (97%)	1 (2%)	1 (2%)	10	18
1	C	79/90 (88%)	75 (95%)	4 (5%)	0	100	100
1	D	66/90 (73%)	65 (98%)	1 (2%)	0	100	100
1	E	77/90 (86%)	72 (94%)	5 (6%)	0	100	100
1	F	76/90 (84%)	67 (88%)	7 (9%)	2 (3%)	5	8
1	G	68/90 (76%)	66 (97%)	2 (3%)	0	100	100
1	H	67/90 (74%)	64 (96%)	2 (3%)	1 (2%)	10	18
All	All	579/720 (80%)	552 (95%)	23 (4%)	4 (1%)	22	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	454	ASN
1	B	451	GLY
1	F	492	LYS
1	H	452	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	68/75 (91%)	66 (97%)	2 (3%)	42	69
1	B	59/75 (79%)	54 (92%)	5 (8%)	10	21
1	C	68/75 (91%)	64 (94%)	4 (6%)	19	37
1	D	57/75 (76%)	55 (96%)	2 (4%)	36	62
1	E	67/75 (89%)	62 (92%)	5 (8%)	13	26
1	F	66/75 (88%)	63 (96%)	3 (4%)	27	51
1	G	59/75 (79%)	57 (97%)	2 (3%)	37	63
1	H	58/75 (77%)	56 (97%)	2 (3%)	37	63
All	All	502/600 (84%)	477 (95%)	25 (5%)	24	46

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	446	LYS
1	E	424	CYS
1	H	421	CYS
1	D	487	ASN
1	E	442	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	472	ASN
1	D	487	ASN

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Mol	Chain	Res	Type
1	E	461	ASN
1	B	483	GLN
1	E	454	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - 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 [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	80/90 (88%)	0.55	7 (8%) 10 10	44, 67, 112, 138	0
1	B	70/90 (77%)	0.07	1 (1%) 75 77	47, 66, 98, 111	0
1	C	81/90 (90%)	0.41	5 (6%) 20 21	40, 72, 112, 138	0
1	D	68/90 (75%)	-0.14	2 (2%) 51 55	45, 65, 94, 105	0
1	E	79/90 (87%)	0.52	5 (6%) 20 21	38, 71, 127, 150	0
1	F	78/90 (86%)	0.54	7 (8%) 9 9	43, 77, 121, 142	0
1	G	70/90 (77%)	-0.00	1 (1%) 75 77	48, 71, 93, 113	0
1	H	69/90 (76%)	0.12	4 (5%) 23 24	54, 73, 101, 130	0
All	All	595/720 (82%)	0.28	32 (5%) 25 27	38, 70, 112, 150	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	492	LYS	5.2
1	H	450	GLU	5.0
1	B	449	VAL	4.2
1	A	497	ILE	3.9
1	F	423	VAL	3.7

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
2	ZN	H	601	1/1	0.97	0.12	65,65,65,65	0
2	ZN	H	602	1/1	0.98	0.13	58,58,58,58	0
2	ZN	A	601	1/1	0.99	0.16	51,51,51,51	0
2	ZN	G	602	1/1	0.99	0.17	51,51,51,51	0
2	ZN	D	602	1/1	0.99	0.16	47,47,47,47	0
2	ZN	F	602	1/1	0.99	0.16	47,47,47,47	0
2	ZN	C	602	1/1	0.99	0.14	48,48,48,48	0
2	ZN	E	602	1/1	0.99	0.16	45,45,45,45	0
2	ZN	B	602	1/1	0.99	0.15	45,45,45,45	0
2	ZN	A	602	1/1	0.99	0.18	47,47,47,47	0
2	ZN	E	601	1/1	0.99	0.15	53,53,53,53	0
2	ZN	F	601	1/1	0.99	0.12	62,62,62,62	0
2	ZN	B	601	1/1	0.99	0.15	62,62,62,62	0
2	ZN	C	601	1/1	0.99	0.15	54,54,54,54	0
2	ZN	G	601	1/1	0.99	0.15	61,61,61,61	0
2	ZN	D	601	1/1	1.00	0.12	58,58,58,58	0

6.5 Other polymers

There are no such residues in this entry.