



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 08:30 pm GMT

PDB ID : 2QKV  
Title : Crystal Structure of the C645S Mutant of the 5th PDZ Domain of InaD  
Authors : Ranganathan, R.; Socolich, M.  
Deposited on : 2007-07-11  
Resolution : 1.55 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

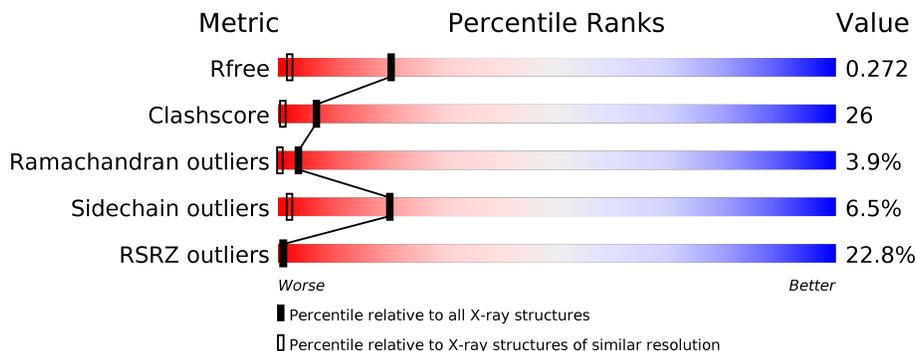
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 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))
$R_{free}$	100719	1088 (1.56-1.56)
Clashscore	112137	1132 (1.56-1.56)
Ramachandran outliers	110173	1110 (1.56-1.56)
Sidechain outliers	110143	1108 (1.56-1.56)
RSRZ outliers	101464	1089 (1.56-1.56)

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	96	
1	B	96	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1547 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 Inactivation-no-after-potential D protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	92	702	446	119	134	3	0	0	0
1	B	92	702	446	119	134	3	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	574	GLY	-	EXPRESSION TAG	UNP Q24008
A	575	ILE	-	EXPRESSION TAG	UNP Q24008
A	576	PRO	-	EXPRESSION TAG	UNP Q24008
A	577	ARG	-	EXPRESSION TAG	UNP Q24008
A	578	ASN	-	EXPRESSION TAG	UNP Q24008
A	579	SER	-	EXPRESSION TAG	UNP Q24008
A	645	SER	CYS	ENGINEERED	UNP Q24008
A	666	ALA	-	EXPRESSION TAG	UNP Q24008
A	667	ALA	-	EXPRESSION TAG	UNP Q24008
A	668	ALA	-	EXPRESSION TAG	UNP Q24008
A	669	SER	-	EXPRESSION TAG	UNP Q24008
B	574	GLY	-	EXPRESSION TAG	UNP Q24008
B	575	ILE	-	EXPRESSION TAG	UNP Q24008
B	576	PRO	-	EXPRESSION TAG	UNP Q24008
B	577	ARG	-	EXPRESSION TAG	UNP Q24008
B	578	ASN	-	EXPRESSION TAG	UNP Q24008
B	579	SER	-	EXPRESSION TAG	UNP Q24008
B	645	SER	CYS	ENGINEERED	UNP Q24008
B	666	ALA	-	EXPRESSION TAG	UNP Q24008
B	667	ALA	-	EXPRESSION TAG	UNP Q24008
B	668	ALA	-	EXPRESSION TAG	UNP Q24008
B	669	SER	-	EXPRESSION TAG	UNP Q24008

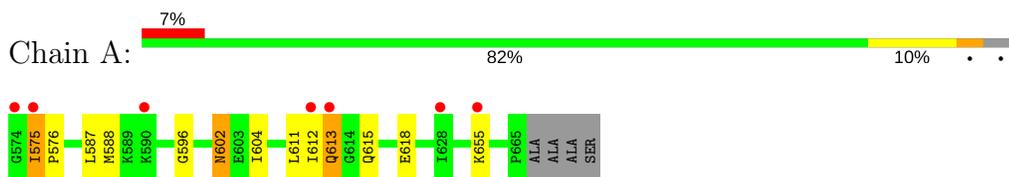
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	94	Total O 94 94	0	0
2	B	49	Total O 49 49	0	0

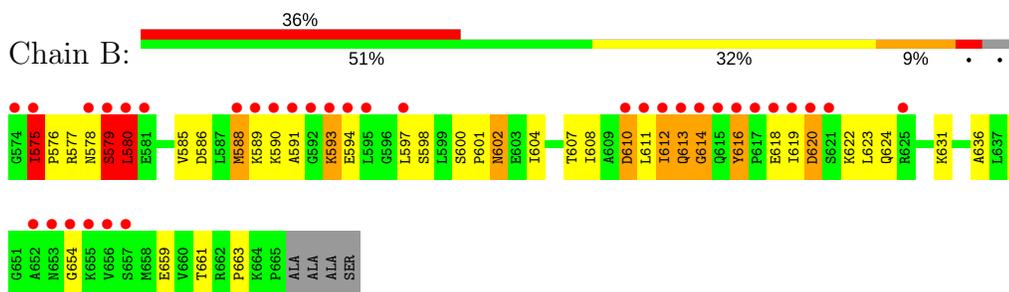
### 3 Residue-property plots [i](#)

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: Inactivation-no-after-potential D protein



- Molecule 1: Inactivation-no-after-potential D protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.04Å 112.04Å 112.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.55 37.35 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-1.55) 94.3 (37.35-1.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.50 (at 1.55Å)	Xtrriage
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.248 , 0.267 0.248 , 0.272	Depositor DCC
$R_{free}$ test set	3324 reflections (9.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.8	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	1547	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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, 0.333 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	0.39	0/713	0.70	0/958
1	B	0.33	0/713	0.79	3/958 (0.3%)
All	All	0.36	0/1426	0.74	3/1916 (0.2%)

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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	579	SER	N-CA-C	5.97	127.13	111.00
1	B	580	LEU	N-CA-C	-5.78	95.38	111.00
1	B	594	GLU	N-CA-C	-5.10	97.24	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	616	TYR	Sidechain

### 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	702	0	721	13	0
1	B	702	0	721	60	0
2	A	94	0	0	0	0
2	B	49	0	0	4	0
All	All	1547	0	1442	73	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 26.

All (73) 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:B:593:LYS:HG3	1:B:616:TYR:OH	1.56	1.05
1:A:587:LEU:HB3	1:A:618:GLU:HG3	1.37	1.04
1:B:589:LYS:HA	1:B:593:LYS:HZ1	1.23	1.02
1:B:597:LEU:HD23	1:B:611:LEU:HD21	1.38	1.00
1:B:586:ASP:O	1:B:618:GLU:HG3	1.66	0.94
1:B:597:LEU:HD23	1:B:611:LEU:CD2	2.02	0.90
1:B:578:ASN:ND2	1:B:579:SER:H	1.71	0.88
1:B:589:LYS:HA	1:B:593:LYS:NZ	1.89	0.87
1:B:593:LYS:NZ	1:B:616:TYR:OH	2.10	0.85
1:B:589:LYS:HD2	1:B:593:LYS:HE3	1.63	0.80
1:B:643:GLN:HG3	2:B:23:HOH:O	1.83	0.78
1:B:575:ILE:HG22	1:B:576:PRO:HD3	1.67	0.75
1:B:577:ARG:NH2	2:B:64:HOH:O	2.18	0.75
1:B:575:ILE:HG22	1:B:576:PRO:CD	2.17	0.75
1:A:587:LEU:HB3	1:A:618:GLU:CG	2.16	0.74
1:B:602:ASN:HD22	1:B:604:ILE:H	1.35	0.74
1:B:590:LYS:H	1:B:593:LYS:HZ3	1.32	0.73
1:B:589:LYS:HA	1:B:593:LYS:CE	2.18	0.72
1:B:597:LEU:CD2	1:B:611:LEU:HD21	2.20	0.71
1:B:590:LYS:N	1:B:593:LYS:HZ3	1.88	0.71
1:B:589:LYS:CA	1:B:593:LYS:HZ1	2.03	0.67
1:B:579:SER:O	1:B:580:LEU:HB2	1.94	0.66
1:B:590:LYS:N	1:B:593:LYS:NZ	2.42	0.66
1:B:590:LYS:H	1:B:593:LYS:NZ	1.93	0.66
1:B:600:SER:HB3	1:B:607:THR:HB	1.78	0.66
1:B:589:LYS:HD2	1:B:593:LYS:CE	2.26	0.66
1:B:590:LYS:O	1:B:593:LYS:HD2	1.96	0.65
1:B:575:ILE:HG22	1:B:576:PRO:N	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:636:ALA:HB1	1:B:638:GLU:OE2	2.00	0.62
1:B:608:ILE:HG21	1:B:611:LEU:HG	1.84	0.60
1:B:593:LYS:HG3	1:B:616:TYR:HH	1.68	0.59
1:B:602:ASN:ND2	1:B:604:ILE:H	2.00	0.59
1:A:596:GLY:HA3	1:A:612:ILE:HG12	1.84	0.58
1:B:593:LYS:HG2	1:B:593:LYS:O	2.03	0.58
1:B:589:LYS:HB3	1:B:654:GLY:H	1.69	0.57
1:B:608:ILE:CG2	1:B:611:LEU:HG	2.36	0.56
1:A:602:ASN:HD22	1:A:604:ILE:H	1.54	0.55
1:B:618:GLU:O	1:B:622:LYS:HB2	2.07	0.54
1:B:612:ILE:O	1:B:613:GLN:C	2.45	0.54
1:A:612:ILE:O	1:A:612:ILE:HG13	2.07	0.53
1:A:575:ILE:HG22	1:A:576:PRO:CD	2.38	0.53
1:B:608:ILE:HG21	1:B:611:LEU:CG	2.40	0.52
1:B:589:LYS:CA	1:B:593:LYS:NZ	2.69	0.52
1:B:661:THR:O	1:B:663:PRO:HD3	2.11	0.50
1:B:589:LYS:C	1:B:593:LYS:HE2	2.31	0.50
1:B:575:ILE:CG2	1:B:576:PRO:N	2.74	0.50
1:B:589:LYS:CA	1:B:593:LYS:HE2	2.41	0.50
1:A:612:ILE:HG13	1:A:615:GLN:HG2	1.95	0.49
1:B:601:PRO:HB3	1:B:642:PHE:CD1	2.47	0.49
1:B:578:ASN:ND2	1:B:579:SER:N	2.51	0.49
1:A:575:ILE:HG22	1:A:576:PRO:N	2.27	0.48
1:B:589:LYS:CA	1:B:593:LYS:CE	2.91	0.48
1:B:579:SER:O	1:B:580:LEU:CB	2.60	0.48
1:B:619:ILE:HG23	1:B:623:LEU:HD12	1.96	0.48
1:B:600:SER:HB2	2:B:92:HOH:O	2.12	0.48
1:B:593:LYS:CG	1:B:616:TYR:OH	2.44	0.48
1:B:586:ASP:O	1:B:618:GLU:CG	2.53	0.46
1:B:578:ASN:HB3	2:B:81:HOH:O	2.14	0.46
1:A:596:GLY:O	1:A:611:LEU:HA	2.15	0.46
1:A:613:GLN:N	1:A:613:GLN:OE1	2.49	0.45
1:B:631:LYS:HB3	1:B:659:GLU:HB2	1.97	0.45
1:B:598:SER:HB3	1:B:610:ASP:H	1.81	0.45
1:A:575:ILE:HG22	1:A:576:PRO:HD3	1.99	0.44
1:B:578:ASN:HD22	1:B:579:SER:H	1.57	0.44
1:A:588:MET:CE	1:A:655:LYS:HE2	2.48	0.43
1:B:598:SER:HB3	1:B:610:ASP:N	2.34	0.43
1:B:614:GLY:HA3	1:B:620:ASP:OD1	2.20	0.42
1:B:602:ASN:HD21	1:B:604:ILE:HG12	1.83	0.42
1:B:593:LYS:CE	1:B:616:TYR:OH	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:LYS:CG	1:B:593:LYS:HE2	2.50	0.41
1:A:611:LEU:HG	1:A:613:GLN:OE1	2.20	0.41
1:B:585:VAL:HG13	1:B:618:GLU:HB3	2.02	0.41
1:B:588:MET:O	1:B:593:LYS:NZ	2.52	0.41

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 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	90/96 (94%)	88 (98%)	2 (2%)	0	100	100
1	B	90/96 (94%)	80 (89%)	3 (3%)	7 (8%)	1	0
All	All	180/192 (94%)	168 (93%)	5 (3%)	7 (4%)	3	0

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	575	ILE
1	B	579	SER
1	B	591	ALA
1	B	612	ILE
1	B	613	GLN
1	B	614	GLY
1	B	580	LEU

### 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 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	77/78 (99%)	74 (96%)	3 (4%)	37	7
1	B	77/78 (99%)	70 (91%)	7 (9%)	11	1
All	All	154/156 (99%)	144 (94%)	10 (6%)	20	2

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	575	ILE
1	A	602	ASN
1	A	613	GLN
1	B	575	ILE
1	B	588	MET
1	B	593	LYS
1	B	602	ASN
1	B	610	ASP
1	B	620	ASP
1	B	624	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	602	ASN
1	B	578	ASN
1	B	602	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](#)

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, 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	92/96 (95%)	0.56	7 (7%) 15 17	7, 14, 28, 32	0
1	B	92/96 (95%)	2.47	35 (38%) 0 0	9, 32, 53, 56	0
All	All	184/192 (95%)	1.52	42 (22%) 1 1	7, 21, 51, 56	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	614	GLY	20.6
1	B	611	LEU	13.9
1	B	617	PRO	13.6
1	B	613	GLN	9.8
1	B	612	ILE	8.1
1	B	590	LYS	7.8
1	B	591	ALA	7.7
1	B	616	TYR	7.6
1	B	593	LYS	6.3
1	B	578	ASN	6.0
1	B	653	ASN	5.9
1	B	594	GLU	5.9
1	B	592	GLY	5.3
1	B	655	LYS	5.2
1	B	579	SER	4.6
1	B	597	LEU	4.4
1	B	610	ASP	4.3
1	A	575	ILE	4.1
1	B	581	GLU	4.0
1	A	574	GLY	3.6
1	B	595	LEU	3.4
1	B	588	MET	3.4
1	B	574	GLY	3.2
1	B	621	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	580	LEU	3.2
1	A	613	GLN	3.0
1	B	620	ASP	3.0
1	B	615	GLN	3.0
1	B	656	VAL	3.0
1	B	575	ILE	2.9
1	B	618	GLU	2.8
1	B	589	LYS	2.7
1	B	619	ILE	2.7
1	B	654	GLY	2.7
1	B	625	ARG	2.6
1	A	612	ILE	2.6
1	A	655	LYS	2.4
1	B	657	SER	2.4
1	B	650	LYS	2.3
1	A	590	LYS	2.3
1	B	652	ALA	2.2
1	A	628	ILE	2.1

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.