



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 04:59 AM UTC

PDB ID : 6VR1 / pdb\_00006vr1  
Title : Complex of HLA-A2, a class I MHC, with a p53 peptide  
Authors : Wu, D.; Pierce, B.G.; Gallagher, D.T.; Mariuzza, R.A.  
Deposited on : 2020-02-06  
Resolution : 2.37 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](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 : 4-5-2 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

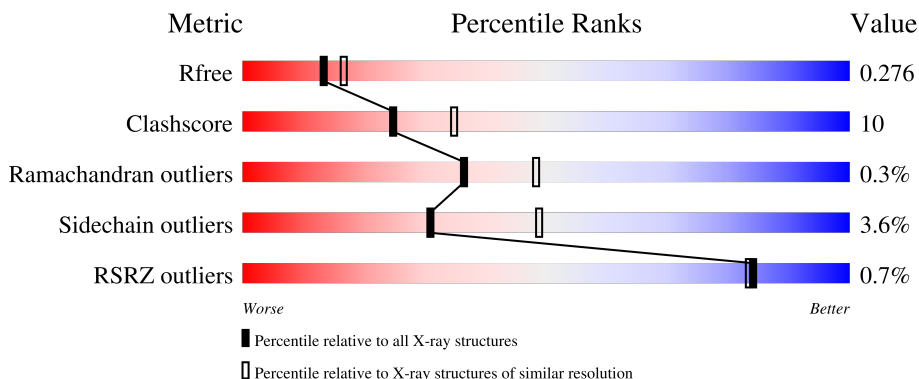
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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  $\leq 5\%$ . 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	293	 73% 19% 6%
1	D	293	 73% 18% 6%
2	B	100	 79% 20%
2	E	100	 78% 22%
3	P	9	 11% 56% 44%

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Mol	Chain	Length	Quality of chain
3	Q	9	 33% 67%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6514 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	2219	1389	402	419	9	0	0	0
1	D	275	2184	1371	388	416	9	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q861F7
A	276	GLY	-	expression tag	UNP Q861F7
A	277	GLY	-	expression tag	UNP Q861F7
A	278	GLY	-	expression tag	UNP Q861F7
A	279	LEU	-	expression tag	UNP Q861F7
A	280	ASN	-	expression tag	UNP Q861F7
A	281	ASP	-	expression tag	UNP Q861F7
A	282	ILE	-	expression tag	UNP Q861F7
A	283	PHE	-	expression tag	UNP Q861F7
A	284	GLU	-	expression tag	UNP Q861F7
A	285	ALA	-	expression tag	UNP Q861F7
A	286	GLN	-	expression tag	UNP Q861F7
A	287	LYS	-	expression tag	UNP Q861F7
A	288	ILE	-	expression tag	UNP Q861F7
A	289	GLU	-	expression tag	UNP Q861F7
A	290	TRP	-	expression tag	UNP Q861F7
A	291	HIS	-	expression tag	UNP Q861F7
A	292	GLU	-	expression tag	UNP Q861F7
D	0	MET	-	initiating methionine	UNP Q861F7
D	276	GLY	-	expression tag	UNP Q861F7
D	277	GLY	-	expression tag	UNP Q861F7
D	278	GLY	-	expression tag	UNP Q861F7
D	279	LEU	-	expression tag	UNP Q861F7
D	280	ASN	-	expression tag	UNP Q861F7
D	281	ASP	-	expression tag	UNP Q861F7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	282	ILE	-	expression tag	UNP Q861F7
D	283	PHE	-	expression tag	UNP Q861F7
D	284	GLU	-	expression tag	UNP Q861F7
D	285	ALA	-	expression tag	UNP Q861F7
D	286	GLN	-	expression tag	UNP Q861F7
D	287	LYS	-	expression tag	UNP Q861F7
D	288	ILE	-	expression tag	UNP Q861F7
D	289	GLU	-	expression tag	UNP Q861F7
D	290	TRP	-	expression tag	UNP Q861F7
D	291	HIS	-	expression tag	UNP Q861F7
D	292	GLU	-	expression tag	UNP Q861F7

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			801	511	137	150	3			
2	E	100	Total	C	N	O	S	0	0	0
			806	516	137	149	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P61769
E	1	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Cellular tumor antigen p53 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	S	0	0	0
			77	45	17	13	2			
3	Q	9	Total	C	N	O	S	0	0	0
			77	45	17	13	2			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	28	Total	O	0	0
			28	28		

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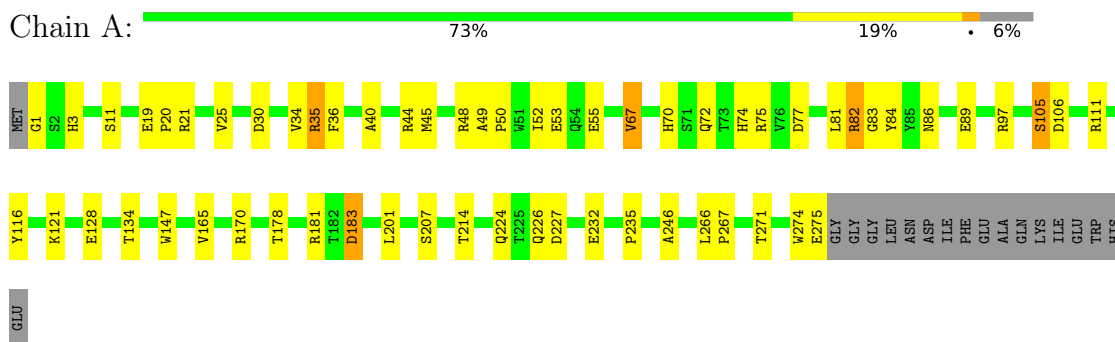
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	D	95	Total 95	O 95	0	0
4	E	52	Total 52	O 52	0	0
4	P	10	Total 10	O 10	0	0
4	Q	4	Total 4	O 4	0	0

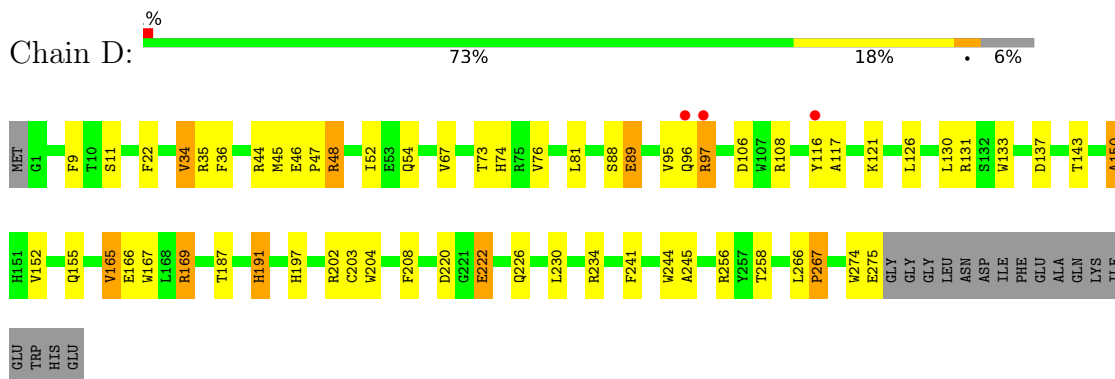
### 3 Residue-property plots [i](#)

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 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.

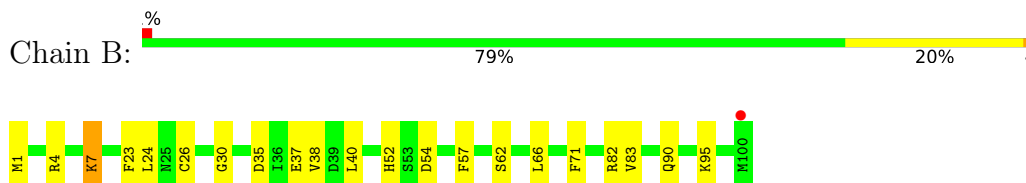
- Molecule 1: MHC class I antigen



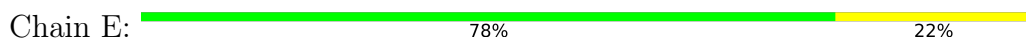
- Molecule 1: MHC class I antigen

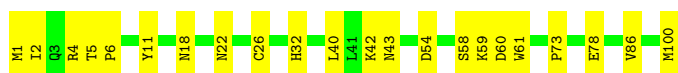


- Molecule 2: Beta-2-microglobulin

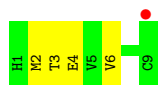


- Molecule 2: Beta-2-microglobulin

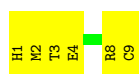




- Molecule 3: Cellular tumor antigen p53 peptide



- Molecule 3: Cellular tumor antigen p53 peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.33Å 79.73Å 85.85Å 90.00° 101.68° 90.00°	Depositor
Resolution (Å)	20.00 – 2.37 20.00 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.37) 99.6 (20.00-2.37)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.37Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.217 , 0.274 0.217 , 0.276	Depositor DCC
$R_{free}$ test set	1879 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtrriage
Anisotropy	0.620	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6514	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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	0.84	1/2283 (0.0%)	1.38	14/3102 (0.5%)
1	D	0.91	6/2249 (0.3%)	1.40	16/3064 (0.5%)
2	B	0.76	0/824	1.25	3/1123 (0.3%)
2	E	0.86	1/829 (0.1%)	1.33	1/1127 (0.1%)
3	P	1.13	0/77	2.00	2/100 (2.0%)
3	Q	0.72	0/77	1.10	0/100
All	All	0.86	8/6339 (0.1%)	1.37	36/8616 (0.4%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	97	ARG	N-CA	-18.51	1.22	1.46
1	D	150	ALA	CA-CB	-9.95	1.36	1.53
1	D	95	VAL	C-N	-7.57	1.23	1.33
2	E	32	HIS	CE1-NE2	7.17	1.39	1.32
1	D	197	HIS	CE1-NE2	6.67	1.39	1.32

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	95	VAL	CA-C-O	-8.06	112.48	121.92
1	D	258	THR	CA-CB-OG1	-7.04	99.03	109.60
1	D	96	GLN	CB-CG-CD	7.03	124.56	112.60
1	A	235	PRO	CA-C-N	6.83	130.69	120.31
1	A	235	PRO	C-N-CA	6.83	130.69	120.31

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	2219	0	2060	37	0
1	D	2184	0	1990	54	0
2	B	801	0	736	15	0
2	E	806	0	752	16	0
3	P	77	0	80	4	0
3	Q	77	0	80	11	0
4	A	161	0	0	6	1
4	B	28	0	0	2	0
4	D	95	0	0	7	2
4	E	52	0	0	2	0
4	P	10	0	0	1	1
4	Q	4	0	0	0	0
All	All	6514	0	5698	116	2

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 10.

The worst 5 of 116 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:D:208:PHE:O	4:D:302:HOH:O	1.67	1.13
1:D:67:VAL:HB	3:Q:2:MET:HE1	1.27	1.13
1:D:34:VAL:HG13	1:D:45:MET:HE3	1.48	0.94
2:E:60:ASP:O	4:E:201:HOH:O	2.00	0.80
1:D:34:VAL:CG1	1:D:45:MET:HE3	2.13	0.78

All (2) 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)
4:D:383:HOH:O	4:P:103:HOH:O[1_556]	1.56	0.64
4:A:441:HOH:O	4:D:373:HOH:O[1_554]	1.99	0.21

## 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	273/293 (93%)	264 (97%)	9 (3%)	0	100	100
1	D	273/293 (93%)	262 (96%)	9 (3%)	2 (1%)	18	26
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	E	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	P	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	Q	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	756/804 (94%)	729 (96%)	25 (3%)	2 (0%)	36	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	54	GLN
1	D	267	PRO

### 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	225/245 (92%)	216 (96%)	9 (4%)	28	44
1	D	218/245 (89%)	210 (96%)	8 (4%)	30	47
2	B	86/95 (90%)	83 (96%)	3 (4%)	32	50
2	E	87/95 (92%)	85 (98%)	2 (2%)	44	64
3	P	9/9 (100%)	8 (89%)	1 (11%)	6	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	9/9 (100%)	9 (100%)	0	100	100
All	All	634/698 (91%)	611 (96%)	23 (4%)	31	49

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	89	GLU
1	D	166	GLU
1	D	165	VAL
1	D	169	ARG
1	A	105	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	188	HIS
2	B	14	HIS
2	E	18	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 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 [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	275/293 (93%)	0.03	0 <a href="#">100</a>   <a href="#">100</a>	19, 34, 56, 85	0
1	D	275/293 (93%)	0.31	3 (1%) <a href="#">78</a>   <a href="#">77</a>	21, 43, 64, 165	0
2	B	100/100 (100%)	0.31	1 (1%) <a href="#">79</a>   <a href="#">78</a>	22, 44, 69, 103	0
2	E	100/100 (100%)	0.21	0 <a href="#">100</a>   <a href="#">100</a>	21, 38, 60, 68	0
3	P	9/9 (100%)	0.13	1 (11%) <a href="#">10</a>   <a href="#">9</a>	11, 25, 30, 31	0
3	Q	9/9 (100%)	0.36	0 <a href="#">100</a>   <a href="#">100</a>	40, 55, 63, 74	0
All	All	768/804 (95%)	0.19	5 (0%) <a href="#">84</a>   <a href="#">83</a>	11, 39, 65, 165	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	96	GLN	9.0
3	P	9	CYS	3.5
1	D	97	ARG	2.4
2	B	100	MET	2.3
1	D	116	TYR	2.3

### 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.