



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 11:27 PM GMT

PDB ID : 3C60
Title : Crystal structure of mouse MHC class II I-Ab/3K peptide complexed with mouse TCR YAc62
Authors : Dai, S.
Deposited on : 2008-02-01
Resolution : 3.05 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

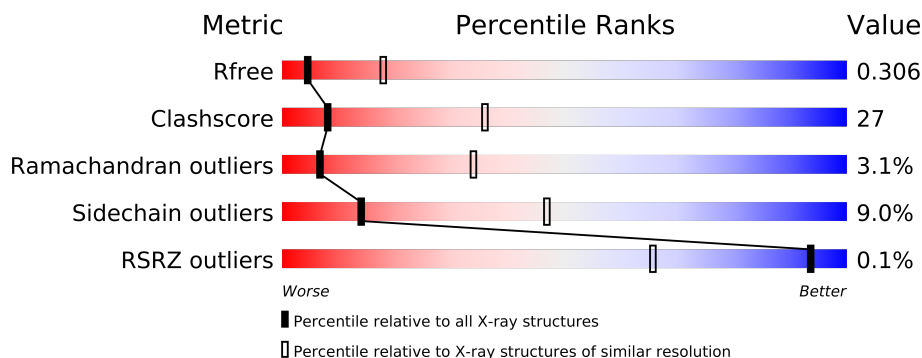
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.05 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}	66092	2079 (3.12-3.00)
Clashscore	79885	2629 (3.12-3.00)
Ramachandran outliers	78287	2536 (3.12-3.00)
Sidechain outliers	78261	2539 (3.12-3.00)
RSRZ outliers	66119	2081 (3.12-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	199	
1	E	199	
2	B	236	
2	F	236	
3	C	182	
3	G	182	
4	D	217	
4	H	217	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13102 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TCR YAc62 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1554	971	252	323	8			
1	E	199	Total	C	N	O	S	0	0	0
			1554	971	252	323	8			

- Molecule 2 is a protein called TCR YAc62 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	0
			1869	1177	325	361	6			
2	F	236	Total	C	N	O	S	0	0	0
			1869	1177	325	361	6			

- Molecule 3 is a protein called H-2 class II histocompatibility antigen, A-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	182	Total	C	N	O	S	0	0	0
			1459	944	230	282	3			
3	G	182	Total	C	N	O	S	0	0	0
			1459	944	230	282	3			

- Molecule 4 is a protein called 3K peptide, Linker, and H-2 class II histocompatibility antigen (A beta chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	201	Total	C	N	O	S	0	0	0
			1669	1045	303	314	7			
4	H	201	Total	C	N	O	S	0	0	0
			1669	1045	303	314	7			

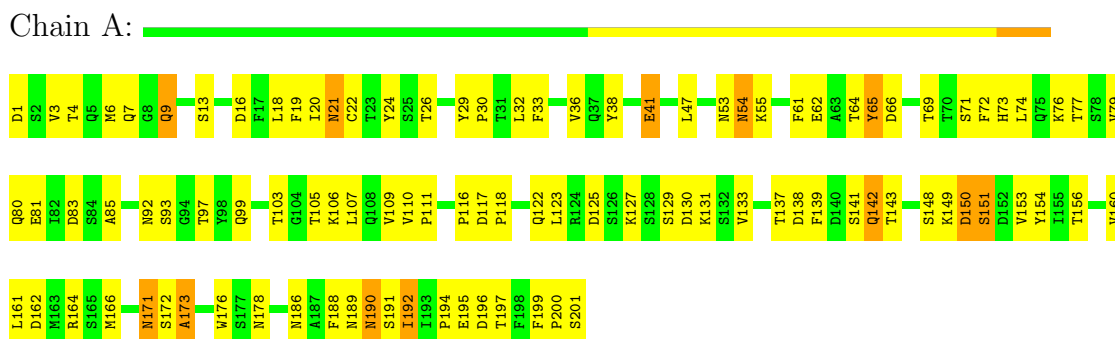
There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	14	GLY	-	LINKER	UNP P14483
D	15	GLY	-	LINKER	UNP P14483
D	16	GLY	-	LINKER	UNP P14483
D	17	GLY	-	LINKER	UNP P14483
D	18	SER	-	LINKER	UNP P14483
D	19	LEU	-	LINKER	UNP P14483
D	20	VAL	-	LINKER	UNP P14483
D	21	PRO	-	LINKER	UNP P14483
D	22	ARG	-	LINKER	UNP P14483
D	23	GLY	-	LINKER	UNP P14483
D	24	SER	-	LINKER	UNP P14483
D	25	GLY	-	LINKER	UNP P14483
D	26	GLY	-	LINKER	UNP P14483
D	27	GLY	-	LINKER	UNP P14483
D	28	GLY	-	LINKER	UNP P14483
D	216	LYS	ARG	ENGINEERED	UNP P14483
H	14	GLY	-	LINKER	UNP P14483
H	15	GLY	-	LINKER	UNP P14483
H	16	GLY	-	LINKER	UNP P14483
H	17	GLY	-	LINKER	UNP P14483
H	18	SER	-	LINKER	UNP P14483
H	19	LEU	-	LINKER	UNP P14483
H	20	VAL	-	LINKER	UNP P14483
H	21	PRO	-	LINKER	UNP P14483
H	22	ARG	-	LINKER	UNP P14483
H	23	GLY	-	LINKER	UNP P14483
H	24	SER	-	LINKER	UNP P14483
H	25	GLY	-	LINKER	UNP P14483
H	26	GLY	-	LINKER	UNP P14483
H	27	GLY	-	LINKER	UNP P14483
H	28	GLY	-	LINKER	UNP P14483
H	216	LYS	ARG	ENGINEERED	UNP P14483

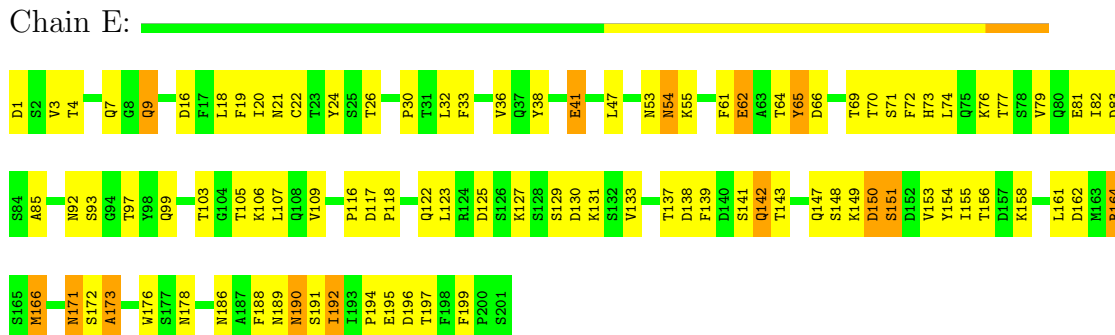
3 Residue-property plots

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: TCR YAE62 alpha chain



- Molecule 1: TCR YAE62 alpha chain

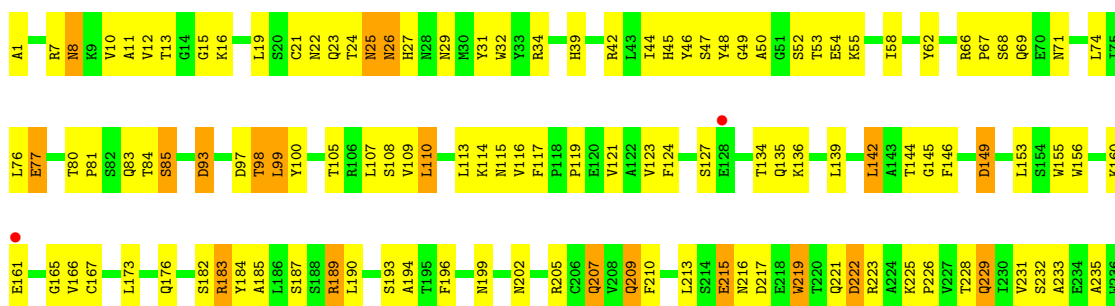


- Molecule 2: TCR YAE62 beta chain



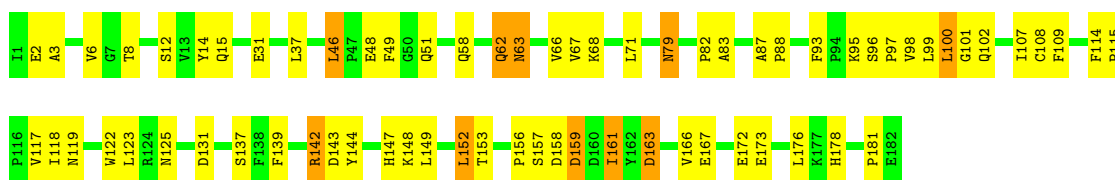
- Molecule 2: TCR YAE62 beta chain





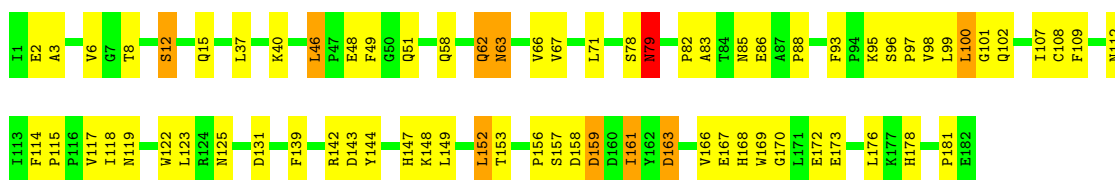
- Molecule 3: H-2 class II histocompatibility antigen, A-B alpha chain

Chain C:



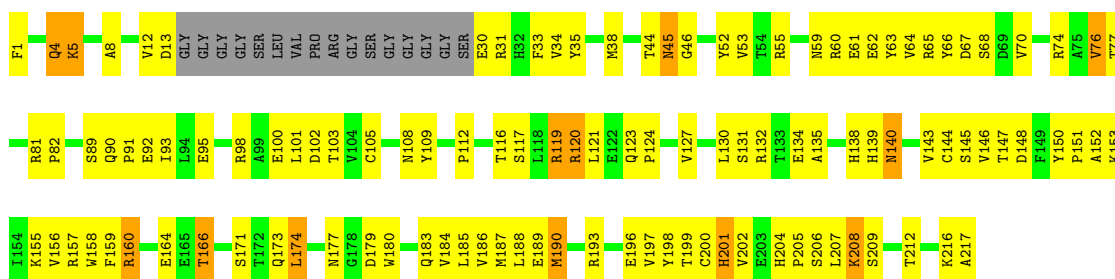
- Molecule 3: H-2 class II histocompatibility antigen, A-B alpha chain

Chain G:



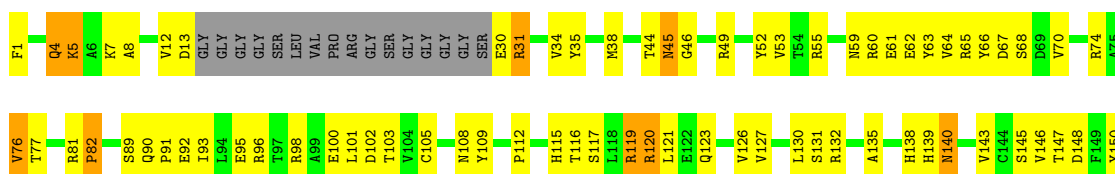
- Molecule 4: 3K peptide, Linker, and H-2 class II histocompatibility antigen (A beta chain)

Chain D:



- Molecule 4: 3K peptide, Linker, and H-2 class II histocompatibility antigen (A beta chain)

Chain H:



P151	A152	K153	I154	K155	V156	R157	V158	F159	R160	E164	E165	T166	V167	G168	S171	L174	N177	G178	D179	M180	Q183	V184	L185	V186	M187	L188	E189	M190	R193	E196	V197	Y198	T199	C200	H201	V202	E203	H204	P205	S206	L207	K208	S209	T212	K216	A217
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.06Å 126.17Å 277.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.92 – 3.05 40.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.6 (40.92-3.05) 90.7 (40.91-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.267 , 0.309 0.266 , 0.306	Depositor DCC
R_{free} test set	2085 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 47352 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13102	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.45	0/1588	0.61	0/2157
1	E	0.47	0/1588	0.61	0/2157
2	B	0.42	0/1922	0.57	0/2620
2	F	0.43	0/1922	0.57	0/2620
3	C	0.56	0/1504	0.67	0/2054
3	G	0.55	0/1504	0.67	0/2054
4	D	0.50	0/1709	0.62	0/2316
4	H	0.49	0/1709	0.64	0/2316
All	All	0.48	0/13446	0.62	0/18294

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
3	C	0	1
3	G	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	144	TYR	Sidechain
3	G	144	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1554	0	1454	79	0
1	E	1554	0	1454	75	0
2	B	1869	0	1763	99	0
2	F	1869	0	1763	117	0
3	C	1459	0	1386	63	0
3	G	1459	0	1386	64	0
4	D	1669	0	1600	119	0
4	H	1669	0	1600	119	0
All	All	13102	0	12406	682	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

The worst 5 of 682 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:208:LYS:HE3	4:D:208:LYS:H	1.14	1.12
4:H:208:LYS:HE3	4:H:208:LYS:H	1.18	1.09
4:D:174:LEU:H	4:D:174:LEU:HD13	1.34	0.93
2:F:48:TYR:CE1	3:G:62:GLN:HG2	2.05	0.91
2:F:16:LYS:HD2	2:F:77:GLU:HA	1.51	0.90

There are no symmetry-related clashes.

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	197/199 (99%)	159 (81%)	27 (14%)	11 (6%)	3	17
1	E	197/199 (99%)	160 (81%)	25 (13%)	12 (6%)	2	14
2	B	234/236 (99%)	192 (82%)	33 (14%)	9 (4%)	5	28
2	F	234/236 (99%)	193 (82%)	33 (14%)	8 (3%)	6	31
3	C	180/182 (99%)	162 (90%)	17 (9%)	1 (1%)	33	79
3	G	180/182 (99%)	161 (89%)	18 (10%)	1 (1%)	33	79
4	D	197/217 (91%)	166 (84%)	27 (14%)	4 (2%)	11	48
4	H	197/217 (91%)	166 (84%)	27 (14%)	4 (2%)	11	48
All	All	1616/1668 (97%)	1359 (84%)	207 (13%)	50 (3%)	7	34

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	E	142	GLN
2	F	215	GLU
1	A	150	ASP
1	A	151	SER

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	178/178 (100%)	167 (94%)	11 (6%)	26	66
1	E	178/178 (100%)	167 (94%)	11 (6%)	26	66
2	B	203/203 (100%)	185 (91%)	18 (9%)	14	47
2	F	203/203 (100%)	186 (92%)	17 (8%)	16	51
3	C	163/163 (100%)	147 (90%)	16 (10%)	12	41
3	G	163/163 (100%)	147 (90%)	16 (10%)	12	41
4	D	182/189 (96%)	162 (89%)	20 (11%)	9	34
4	H	182/189 (96%)	161 (88%)	21 (12%)	8	32
All	All	1452/1466 (99%)	1322 (91%)	130 (9%)	14	47

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	140	ASN
1	E	103	THR
4	H	119	ARG
4	D	174	LEU
1	E	21	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	183	GLN
1	E	190	ASN
4	H	138	HIS
4	D	201	HIS
1	E	54	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

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	199/199 (100%)	-0.08	0	100	100	29, 84, 130, 140	0
1	E	199/199 (100%)	0.03	0	100	100	29, 85, 131, 140	0
2	B	236/236 (100%)	-0.01	0	100	100	26, 89, 139, 159	0
2	F	236/236 (100%)	0.04	2 (0%)	83	27	29, 90, 139, 158	0
3	C	182/182 (100%)	-0.22	0	100	100	23, 55, 107, 128	0
3	G	182/182 (100%)	-0.21	0	100	100	26, 56, 106, 130	0
4	D	201/217 (92%)	-0.10	0	100	100	26, 72, 113, 128	0
4	H	201/217 (92%)	-0.13	0	100	100	30, 72, 112, 127	0
All	All	1636/1668 (98%)	-0.08	2 (0%)	93	65	23, 74, 129, 159	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	128	GLU	2.3
2	F	161	GLU	2.2

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.