



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2016 – 08:36 AM EDT

PDB ID : 5IRO
Title : Crystal structure of a complex between the Human adenovirus type 4 E3-19K protein and MHC class molecule HLA-A2/TAX
Authors : Li, L.; Bouvier, M.
Deposited on : 2016-03-14
Resolution : 2.64 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

<http://wwpdb.org/validation/2016/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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

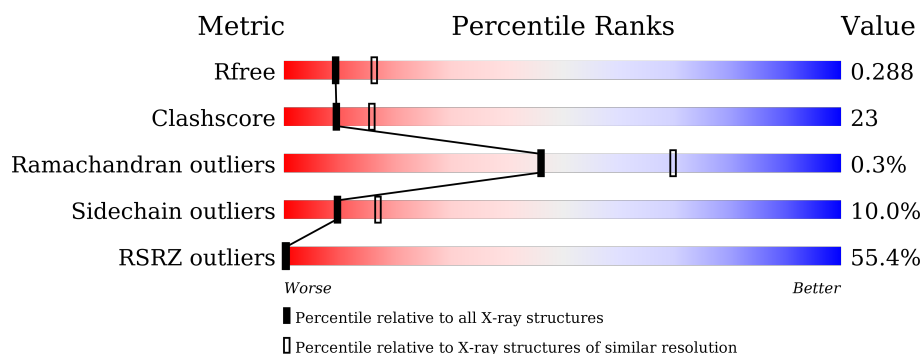
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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. 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	275	<div> <div>43%</div> <div> <div>46%</div> <div>44%</div> <div>6%</div> <div>.</div> </div> </div>
1	E	275	<div> <div>48%</div> <div> <div>51%</div> <div>41%</div> <div>5%</div> <div>.</div> </div> </div>
1	I	275	<div> <div>38%</div> <div> <div>52%</div> <div>35%</div> <div>5%</div> <div>8%</div> </div> </div>
1	M	275	<div> <div>48%</div> <div> <div>46%</div> <div>44%</div> <div>6%</div> <div>.</div> </div> </div>
1	Q	275	<div> <div>76%</div> <div> <div>44%</div> <div>43%</div> <div>7%</div> <div>6%</div> </div> </div>
1	U	275	<div> <div>72%</div> <div> <div>46%</div> <div>37%</div> <div>6%</div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	B	9	
2	F	9	
2	J	9	
2	N	9	
2	R	9	
2	V	9	
3	C	100	
3	G	100	
3	K	100	
3	O	100	
3	S	100	
3	W	100	
4	D	108	
4	H	108	
4	L	108	
4	P	108	
4	T	108	
4	X	108	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23039 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2144	1338	389	408	9			
1	E	268	Total	C	N	O	S	0	0	0
			2183	1363	398	413	9			
1	I	252	Total	C	N	O	S	0	0	0
			2053	1282	376	386	9			
1	M	265	Total	C	N	O	S	0	0	0
			2160	1351	392	408	9			
1	Q	259	Total	C	N	O	S	0	0	0
			2111	1315	385	402	9			
1	U	246	Total	C	N	O	S	0	0	0
			2007	1259	363	376	9			

- Molecule 2 is a protein called TAX protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			76	56	9	11			
2	F	9	Total	C	N	O	0	0	0
			76	56	9	11			
2	J	9	Total	C	N	O	0	0	0
			76	56	9	11			
2	N	9	Total	C	N	O	0	0	0
			76	56	9	11			
2	R	9	Total	C	N	O	0	0	0
			76	56	9	11			
2	V	9	Total	C	N	O	0	0	0
			76	56	9	11			

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	96	Total	C	N	O	S	0	0	0
			802	513	136	150	3			
3	G	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	K	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	O	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	S	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	W	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769
K	0	MET	-	initiating methionine	UNP P61769
O	0	MET	-	initiating methionine	UNP P61769
S	0	MET	-	initiating methionine	UNP P61769
W	0	MET	-	initiating methionine	UNP P61769

- Molecule 4 is a protein called E3 19 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			823	520	144	149	10			
4	H	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	L	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	P	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	T	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	X	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			

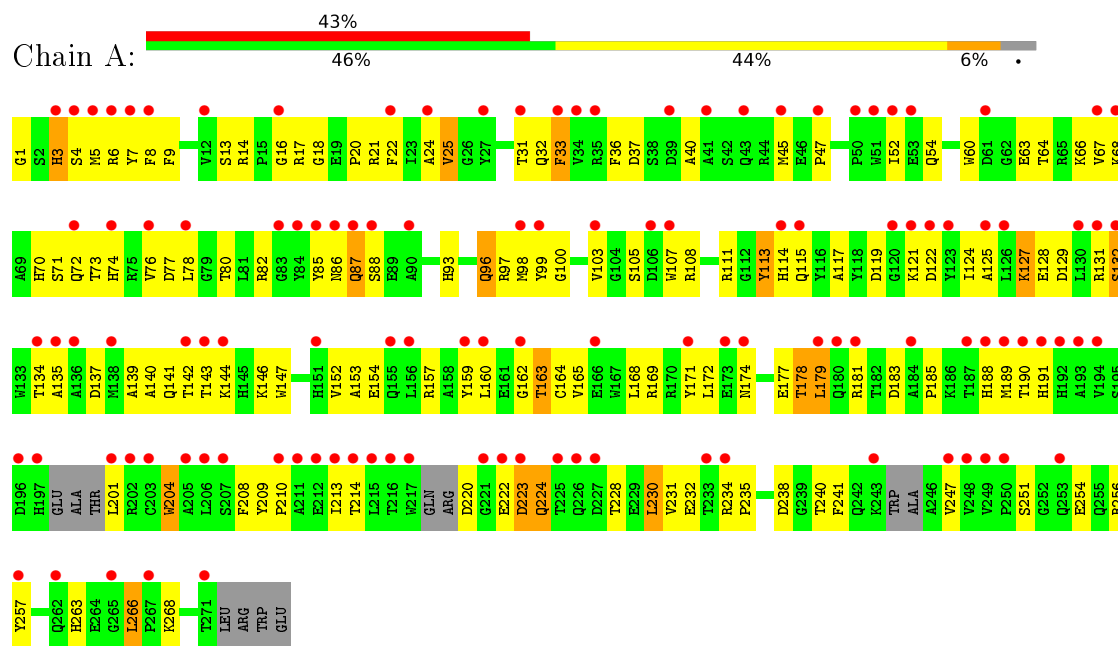
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0
5	D	2	Total O 2 2	0	0
5	E	3	Total O 3 3	0	0
5	G	1	Total O 1 1	0	0
5	I	5	Total O 5 5	0	0
5	J	1	Total O 1 1	0	0
5	K	2	Total O 2 2	0	0
5	L	1	Total O 1 1	0	0
5	M	4	Total O 4 4	0	0
5	O	2	Total O 2 2	0	0
5	P	3	Total O 3 3	0	0
5	Q	3	Total O 3 3	0	0
5	S	3	Total O 3 3	0	0
5	T	3	Total O 3 3	0	0
5	U	3	Total O 3 3	0	0
5	W	1	Total O 1 1	0	0

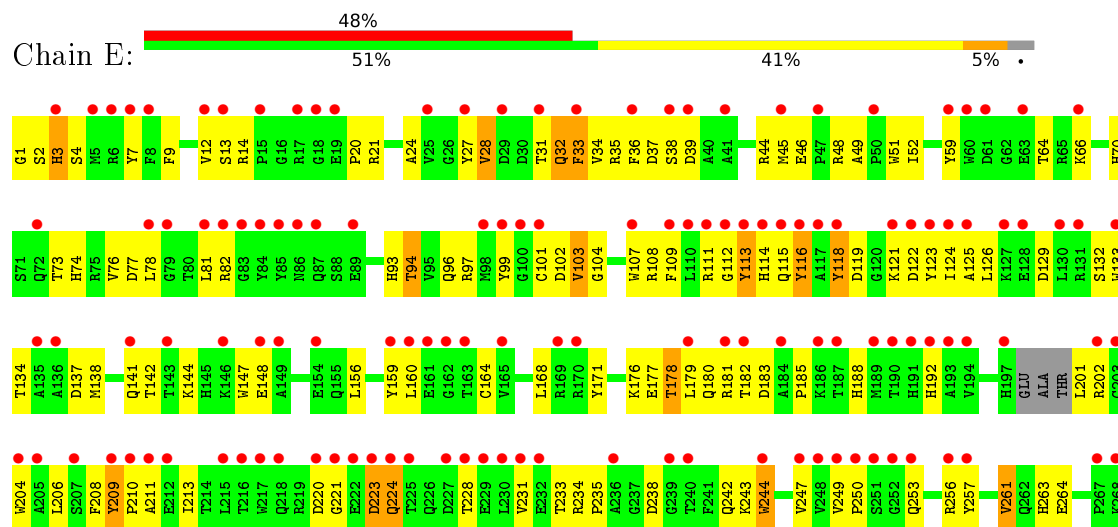
3 Residue-property plots

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: HLA class I histocompatibility antigen, A-2 alpha chain

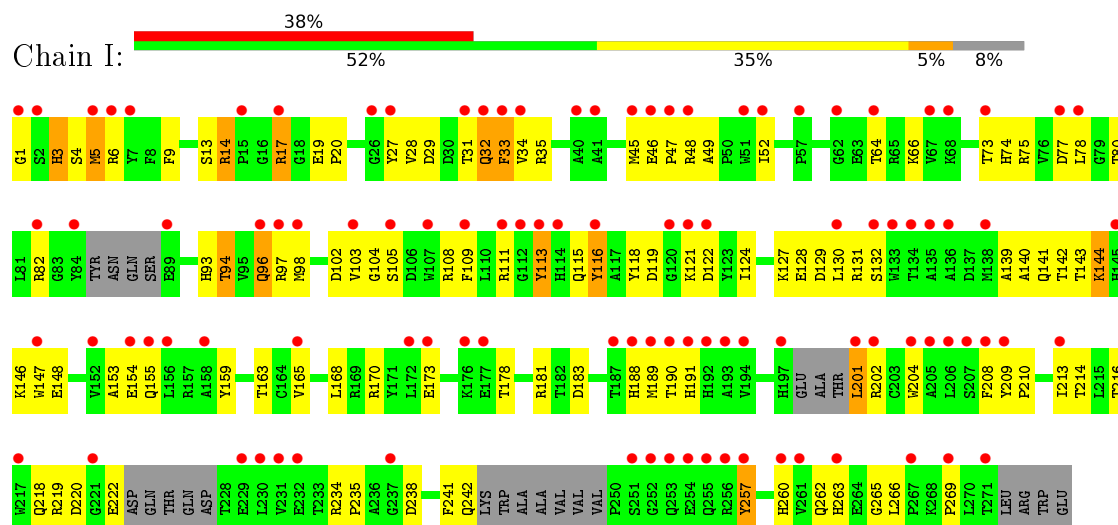


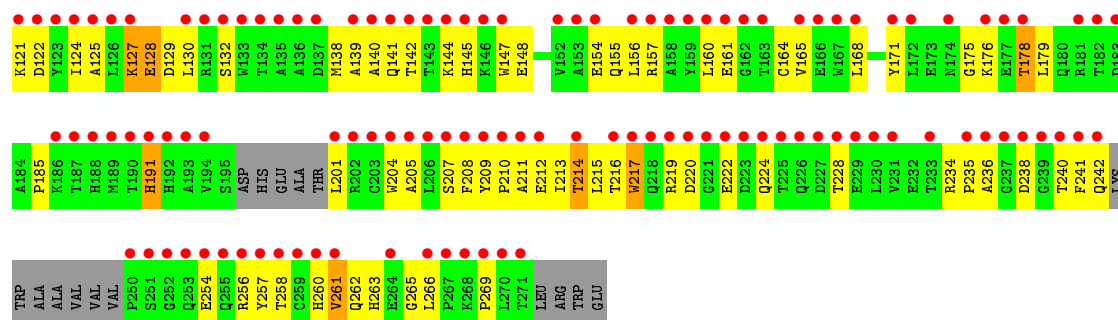
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



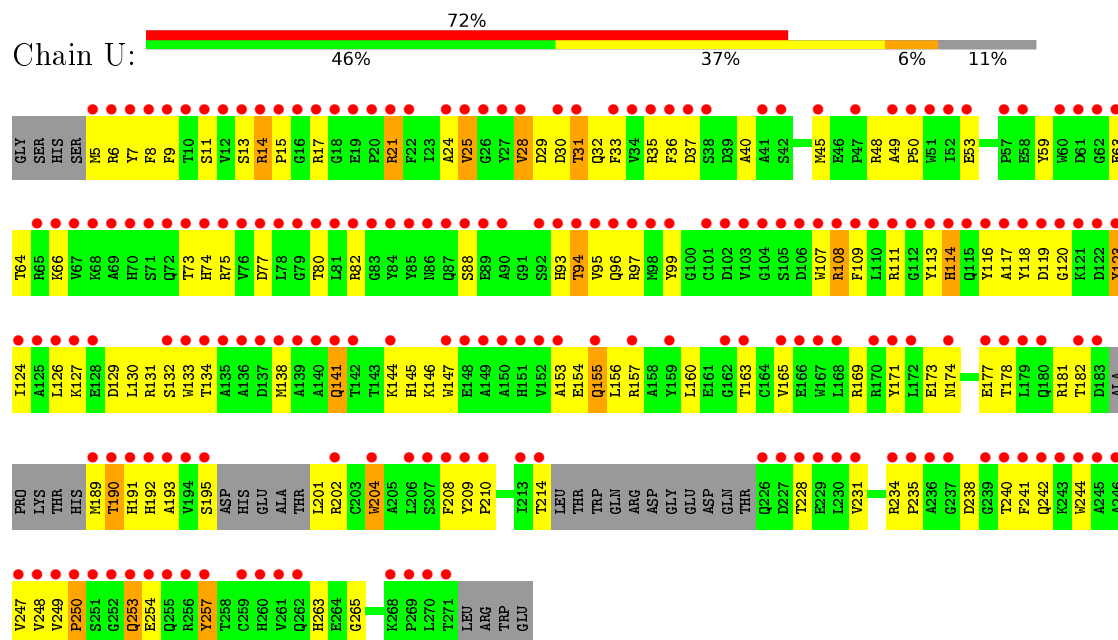


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain





- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



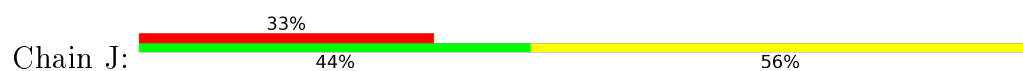
- Molecule 2: TAX protein



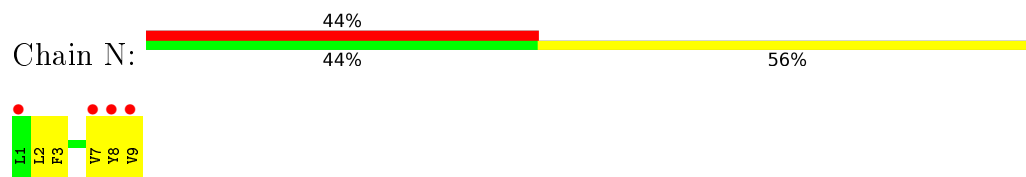
- Molecule 2: TAX protein



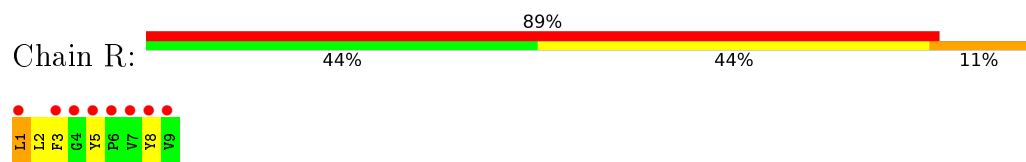
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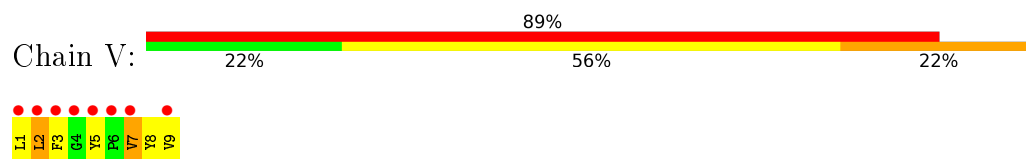
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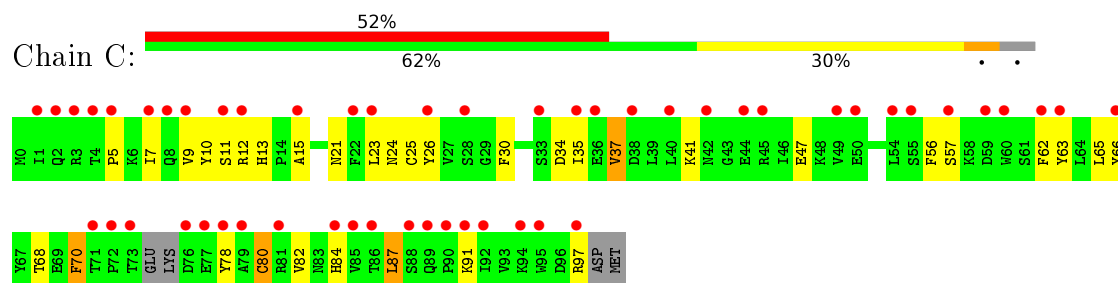
- Molecule 2: TAX protein



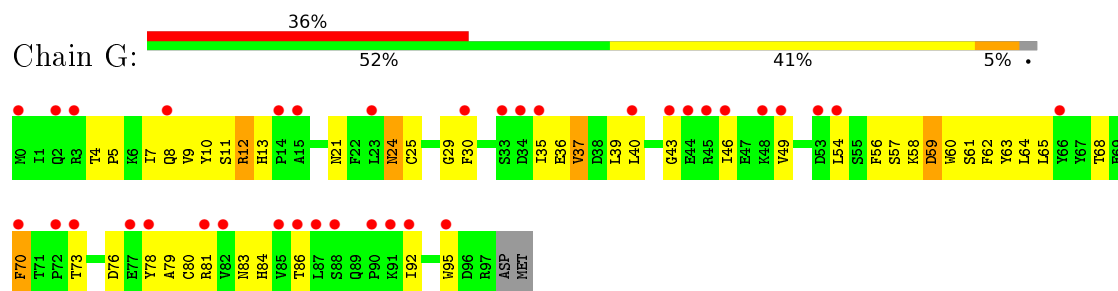
- Molecule 2: TAX protein



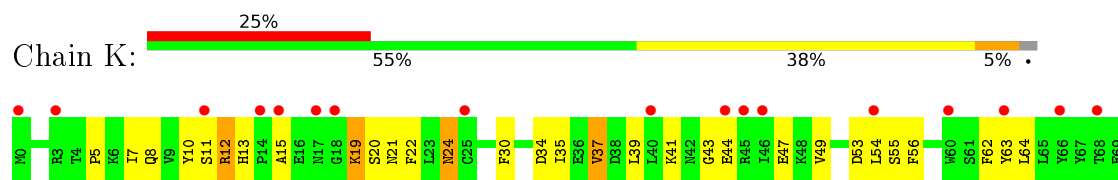
- Molecule 3: Beta-2-microglobulin



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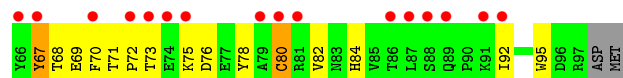
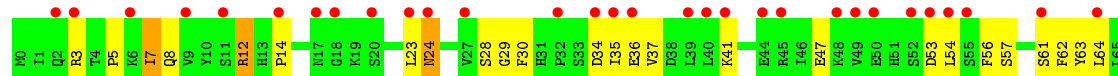


- Molecule 3: Beta-2-microglobulin

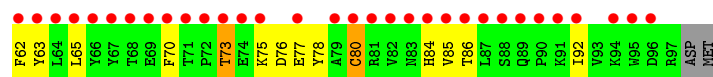
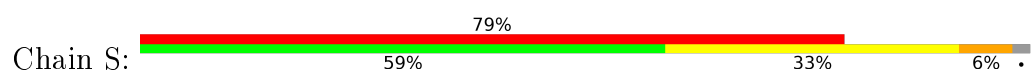




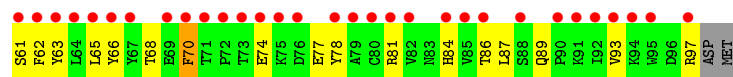
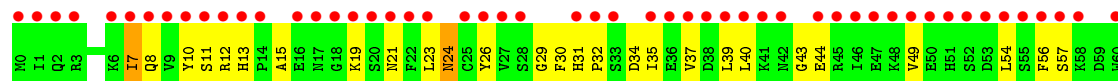
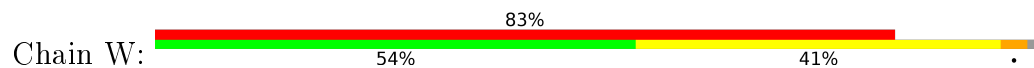
• Molecule 3: Beta-2-microglobulin



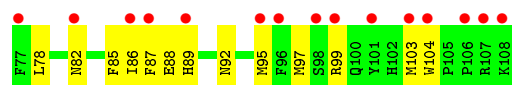
• Molecule 3: Beta-2-microglobulin



• Molecule 3: Beta-2-microglobulin

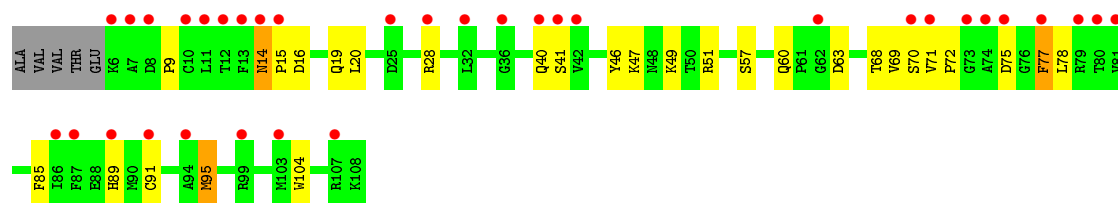


• Molecule 4: E3 19 kDa protein

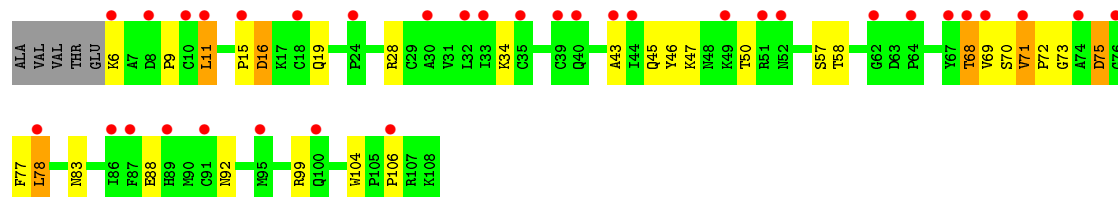


• Molecule 4: E3 19 kDa protein

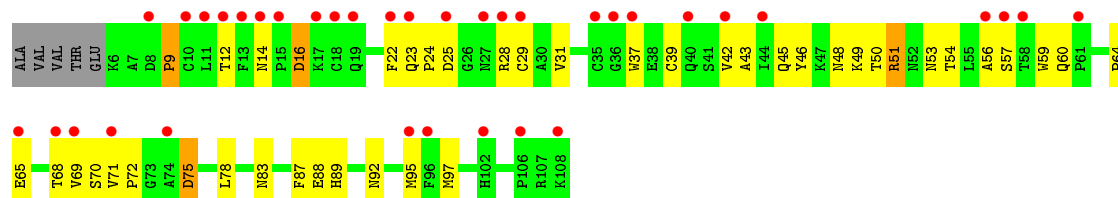




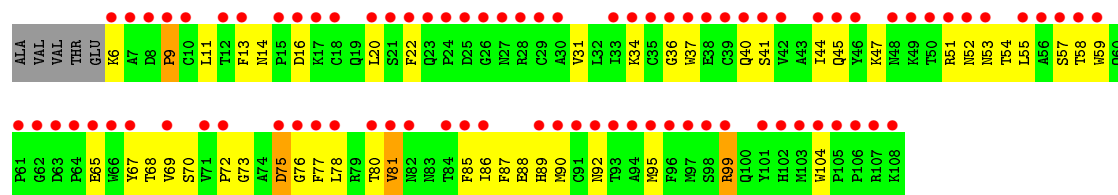
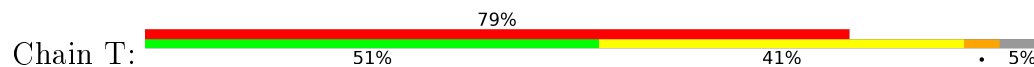
• Molecule 4: E3 19 kDa protein



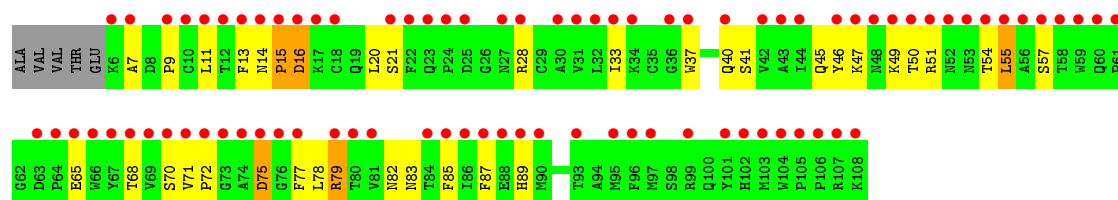
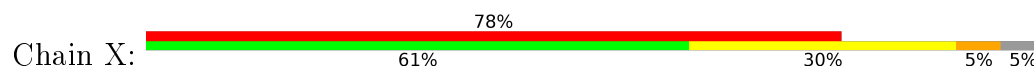
• Molecule 4: E3 19 kDa protein



• Molecule 4: E3 19 kDa protein



• Molecule 4: E3 19 kDa protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	165.73Å 165.73Å 122.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.62 – 2.64 49.62 – 2.64	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.62-2.64) 99.3 (49.62-2.64)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.257 , 0.288 0.256 , 0.288	Depositor DCC
R_{free} test set	1970 reflections (1.79%)	DCC
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	0.359 for -h,-k,l 0.389 for h,-h-k,-l 0.337 for -k,-h,-l	Xtriage
Reported twinning fraction	0.470 for -h,-k,l	Depositor
Outliers	0 of 110879 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	23039	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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 [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	0.38	1/2202 (0.0%)	0.60	0/2983
1	E	0.32	0/2245	0.59	0/3045
1	I	0.29	0/2109	0.57	0/2852
1	M	0.39	0/2221	0.75	3/3012 (0.1%)
1	Q	0.36	0/2169	0.69	1/2937 (0.0%)
1	U	0.34	0/2061	0.62	0/2791
2	B	0.46	0/79	0.66	0/108
2	F	0.48	0/79	0.79	0/108
2	J	0.32	0/79	0.47	0/108
2	N	0.37	0/79	0.45	0/108
2	R	0.33	0/79	0.48	0/108
2	V	0.47	0/79	0.89	1/108 (0.9%)
3	C	0.31	0/824	0.57	0/1115
3	G	0.28	0/843	0.57	0/1141
3	K	0.28	0/843	0.52	0/1141
3	O	0.28	0/843	0.54	0/1141
3	S	0.28	0/843	0.56	0/1141
3	W	0.30	0/843	0.59	0/1141
4	D	0.28	0/849	0.56	0/1154
4	H	0.34	0/858	0.63	0/1165
4	L	0.27	0/858	0.58	0/1165
4	P	0.31	0/858	0.57	0/1165
4	T	0.28	0/858	0.55	0/1165
4	X	0.29	0/858	0.64	1/1165 (0.1%)
All	All	0.33	1/23659 (0.0%)	0.61	6/32067 (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	M	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	SER	CB-OG	-7.13	1.32	1.42

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	202	ARG	NE-CZ-NH2	-17.95	111.33	120.30
1	M	202	ARG	NE-CZ-NH1	8.67	124.64	120.30
2	V	2	LEU	CA-CB-CG	-5.83	101.89	115.30
1	Q	27	TYR	CA-CB-CG	5.74	124.31	113.40
1	M	190	THR	OG1-CB-CG2	-5.69	96.91	110.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	189	MET	Peptide

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	2144	0	1999	131	1
1	E	2183	0	2037	105	0
1	I	2053	0	1916	103	0
1	M	2160	0	2016	150	0
1	Q	2111	0	1966	114	0
1	U	2007	0	1881	112	0
2	B	76	0	79	12	0
2	F	76	0	79	9	0
2	J	76	0	79	6	0
2	N	76	0	79	10	0
2	R	76	0	79	8	0
2	V	76	0	79	8	0
3	C	802	0	770	27	0
3	G	820	0	790	37	0
3	K	820	0	790	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	820	0	790	32	0
3	S	820	0	790	36	0
3	W	820	0	790	41	0
4	D	823	0	773	27	0
4	H	832	0	786	16	0
4	L	832	0	786	22	0
4	P	832	0	786	26	0
4	T	832	0	786	39	0
4	X	832	0	786	29	0
5	A	3	0	0	0	0
5	D	2	0	0	0	0
5	E	3	0	0	0	0
5	G	1	0	0	0	0
5	I	5	0	0	0	0
5	J	1	0	0	0	0
5	K	2	0	0	0	0
5	L	1	0	0	0	0
5	M	4	0	0	0	0
5	O	2	0	0	1	0
5	P	3	0	0	0	0
5	Q	3	0	0	0	0
5	S	3	0	0	0	0
5	T	3	0	0	0	0
5	U	3	0	0	0	0
5	W	1	0	0	0	0
All	All	23039	0	21712	1015	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 23.

The worst 5 of 1015 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:I:32:GLN:HB2	1:I:48:ARG:HH12	1.24	1.01
1:M:205:ALA:HB3	1:M:243:LYS:HE2	1.45	0.99
1:Q:5:MET:HG3	1:Q:6:ARG:HG3	1.47	0.96
1:U:250:PRO:O	1:U:253:GLN:NE2	2.01	0.93
1:E:59:TYR:HH	1:E:171:TYR:HH	1.12	0.91

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:A:105:SER:OG	1:A:129:ASP:OD1[3_555]	2.13	0.07

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	256/275 (93%)	229 (90%)	27 (10%)	0	100	100
1	E	264/275 (96%)	233 (88%)	31 (12%)	0	100	100
1	I	242/275 (88%)	216 (89%)	26 (11%)	0	100	100
1	M	259/275 (94%)	230 (89%)	29 (11%)	0	100	100
1	Q	253/275 (92%)	225 (89%)	27 (11%)	1 (0%)	39	63
1	U	238/275 (86%)	214 (90%)	23 (10%)	1 (0%)	39	63
2	B	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	J	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	N	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	V	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	C	92/100 (92%)	82 (89%)	10 (11%)	0	100	100
3	G	96/100 (96%)	85 (88%)	11 (12%)	0	100	100
3	K	96/100 (96%)	84 (88%)	12 (12%)	0	100	100
3	O	96/100 (96%)	86 (90%)	10 (10%)	0	100	100
3	S	96/100 (96%)	86 (90%)	10 (10%)	0	100	100
3	W	96/100 (96%)	85 (88%)	11 (12%)	0	100	100
4	D	100/108 (93%)	88 (88%)	11 (11%)	1 (1%)	19	37
4	H	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	19	37
4	L	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	19	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	P	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	19	37
4	T	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	19	37
4	X	101/108 (94%)	89 (88%)	10 (10%)	2 (2%)	9	16
All	All	2731/2952 (92%)	2424 (89%)	298 (11%)	9 (0%)	46	70

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	9	PRO
4	P	9	PRO
4	X	9	PRO
4	H	9	PRO
4	T	9	PRO

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	222/231 (96%)	199 (90%)	23 (10%)	9	15
1	E	225/231 (97%)	200 (89%)	25 (11%)	8	13
1	I	211/231 (91%)	188 (89%)	23 (11%)	8	13
1	M	223/231 (96%)	200 (90%)	23 (10%)	9	15
1	Q	218/231 (94%)	188 (86%)	30 (14%)	4	7
1	U	206/231 (89%)	179 (87%)	27 (13%)	5	8
2	B	8/8 (100%)	6 (75%)	2 (25%)	1	1
2	F	8/8 (100%)	5 (62%)	3 (38%)	0	0
2	J	8/8 (100%)	8 (100%)	0	100	100
2	N	8/8 (100%)	8 (100%)	0	100	100
2	R	8/8 (100%)	7 (88%)	1 (12%)	6	10
2	V	8/8 (100%)	6 (75%)	2 (25%)	1	1
3	C	91/95 (96%)	86 (94%)	5 (6%)	27	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	93/95 (98%)	84 (90%)	9 (10%)	10	18
3	K	93/95 (98%)	83 (89%)	10 (11%)	8	14
3	O	93/95 (98%)	85 (91%)	8 (9%)	13	24
3	S	93/95 (98%)	84 (90%)	9 (10%)	10	18
3	W	93/95 (98%)	88 (95%)	5 (5%)	27	50
4	D	91/96 (95%)	87 (96%)	4 (4%)	35	61
4	H	92/96 (96%)	85 (92%)	7 (8%)	16	30
4	L	92/96 (96%)	84 (91%)	8 (9%)	13	23
4	P	92/96 (96%)	83 (90%)	9 (10%)	10	18
4	T	92/96 (96%)	87 (95%)	5 (5%)	27	50
4	X	92/96 (96%)	84 (91%)	8 (9%)	13	23
All	All	2460/2580 (95%)	2214 (90%)	246 (10%)	9	17

5 of 246 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	11	LEU
1	M	188	HIS
1	U	228	THR
4	L	68	THR
1	M	27	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	96	GLN
3	O	8	GLN
3	W	31	HIS
1	M	253	GLN
4	P	92	ASN

5.3.3 RNA ⓘ

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, 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	264/275 (96%)	2.18	118 (44%) 0 0	20, 49, 98, 218	0
1	E	268/275 (97%)	2.51	133 (49%) 0 0	18, 49, 126, 173	0
1	I	252/275 (91%)	2.06	104 (41%) 0 0	14, 41, 85, 176	0
1	M	265/275 (96%)	2.55	132 (49%) 0 0	18, 51, 117, 161	0
1	Q	259/275 (94%)	4.72	210 (81%) 0 0	22, 61, 134, 238	0
1	U	246/275 (89%)	4.95	199 (80%) 0 0	27, 59, 131, 224	0
2	B	9/9 (100%)	2.16	2 (22%) 1 0	29, 33, 52, 58	0
2	F	9/9 (100%)	2.19	4 (44%) 0 0	34, 53, 82, 85	0
2	J	9/9 (100%)	2.06	3 (33%) 0 0	22, 33, 49, 83	0
2	N	9/9 (100%)	2.16	4 (44%) 0 0	20, 39, 61, 77	0
2	R	9/9 (100%)	4.52	8 (88%) 0 0	33, 41, 70, 75	0
2	V	9/9 (100%)	4.30	8 (88%) 0 0	41, 51, 77, 80	0
3	C	96/100 (96%)	2.31	52 (54%) 0 0	30, 54, 130, 166	0
3	G	98/100 (98%)	1.97	36 (36%) 0 0	16, 42, 73, 218	0
3	K	98/100 (98%)	1.62	25 (25%) 1 0	15, 40, 74, 180	0
3	O	98/100 (98%)	2.28	46 (46%) 0 0	26, 48, 121, 147	0
3	S	98/100 (98%)	5.05	79 (80%) 0 0	23, 57, 142, 203	0
3	W	98/100 (98%)	4.93	83 (84%) 0 0	20, 57, 115, 187	0
4	D	102/108 (94%)	1.87	38 (37%) 0 0	15, 42, 79, 193	0
4	H	103/108 (95%)	1.95	34 (33%) 0 0	22, 38, 76, 132	0
4	L	103/108 (95%)	1.77	34 (33%) 0 0	17, 36, 81, 129	0
4	P	103/108 (95%)	1.99	36 (34%) 0 0	16, 44, 115, 147	0
4	T	103/108 (95%)	4.48	85 (82%) 0 0	19, 54, 114, 160	0
4	X	103/108 (95%)	3.98	84 (81%) 0 0	18, 49, 92, 186	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	2811/2952 (95%)	3.01	1557 (55%) 0 0	14, 49, 118, 238	0

The worst 5 of 1557 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	33	PHE	22.2
1	E	227	ASP	22.0
3	W	9	VAL	21.8
3	W	93	VAL	20.9
1	U	83	GLY	19.9

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.