



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 13, 2016 – 01:53 PM EDT

PDB ID : 5E6I
Title : Crystal structure of TCR PF8 in complex with flu MP(58-66) epitope presented by HLA-A2
Authors : Gao, M.; Mariuzza, R.
Deposited on : 2015-10-09
Resolution : 4.00 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:

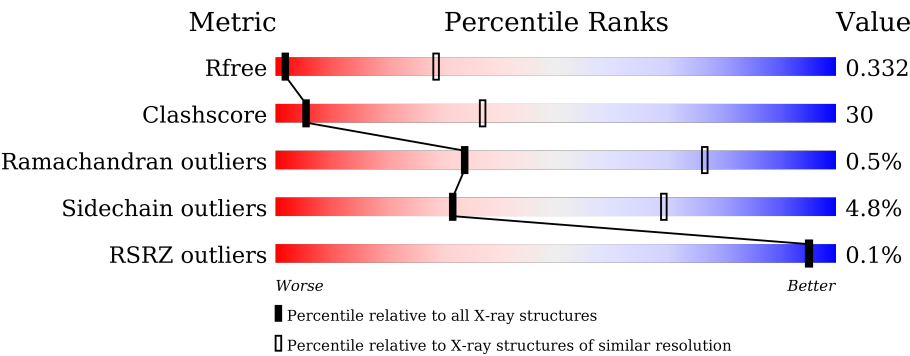
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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 ≥ 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	208	<div><div></div><div>57%34%6%</div></div>
1	F	208	<div><div></div><div>57%35%5%</div></div>
1	G	208	<div><div></div><div>62%30%5%</div></div>
1	P	208	<div><div></div><div>57%32%8%</div></div>
2	B	243	<div><div></div><div>60%36%...</div></div>
2	H	243	<div><div></div><div>58%38%..</div></div>

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Mol	Chain	Length	Quality of chain
2	L	243	 61% 36% .
2	Q	243	 59% 35% . .
3	C	276	 57% 34% . 7%
3	I	276	 38% 51% 5% 5%
3	M	276	 50% 43% . .
3	R	276	 51% 38% . 9%
4	D	100	 % 44% 42% 11% .
4	J	100	 36% 50% 9% . .
4	N	100	 54% 33% 5% 8%
4	U	100	 49% 44% 6% .
5	E	9	 56% 44%
5	K	9	 33% 56% 11%
5	O	9	 67% 33%
5	T	9	 67% 22% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24882 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 TCR alpha chain,Human nkt tcr alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	201	Total	C	N	O	S	0	0	0
			1535	961	252	313	9			
1	A	196	Total	C	N	O	S	0	0	0
			1459	910	241	300	8			
1	F	198	Total	C	N	O	S	0	0	0
			1486	930	243	304	9			
1	P	191	Total	C	N	O	S	0	0	0
			1426	895	232	292	7			

- Molecule 2 is a protein called T-cell receptor beta-2 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	239	Total	C	N	O	S	0	0	0
			1878	1189	320	361	8			
2	B	241	Total	C	N	O	S	0	0	0
			1870	1179	316	367	8			
2	L	242	Total	C	N	O	S	0	0	0
			1891	1199	314	370	8			
2	Q	238	Total	C	N	O	S	0	0	0
			1840	1164	312	356	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	0	MET	LEU	conflict	UNP A0A087WZ08
H	18	GLU	LYS	conflict	UNP A0A087WZ08
H	?	-	SER	deletion	UNP A0A087WZ08
H	96	ILE	THR	conflict	UNP A0A087WZ08
H	97	TYR	VAL	conflict	UNP A0A087WZ08
H	98	PRO	LEU	conflict	UNP A0A087WZ08
H	99	GLY	HIS	conflict	UNP A0A087WZ08
H	100	GLU	SER	conflict	UNP A0A087WZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
H	101	LEU	GLN	conflict	UNP A0A087WZ08
H	102	PHE	TYR	conflict	UNP A0A087WZ08
H	105	GLU	PRO	conflict	UNP A0A087WZ08
H	107	SER	THR	conflict	UNP A0A087WZ08
H	110	THR	LEU	conflict	UNP A0A087WZ08
H	122	GLU	LYS	conflict	UNP A0A087WZ08
H	169	CYS	SER	conflict	UNP A0A087WZ08
H	187	ALA	CYS	conflict	UNP A0A087WZ08
B	0	MET	LEU	conflict	UNP A0A087WZ08
B	18	GLU	LYS	conflict	UNP A0A087WZ08
B	?	-	SER	deletion	UNP A0A087WZ08
B	96	ILE	THR	conflict	UNP A0A087WZ08
B	97	TYR	VAL	conflict	UNP A0A087WZ08
B	98	PRO	LEU	conflict	UNP A0A087WZ08
B	99	GLY	HIS	conflict	UNP A0A087WZ08
B	100	GLU	SER	conflict	UNP A0A087WZ08
B	101	LEU	GLN	conflict	UNP A0A087WZ08
B	102	PHE	TYR	conflict	UNP A0A087WZ08
B	105	GLU	PRO	conflict	UNP A0A087WZ08
B	107	SER	THR	conflict	UNP A0A087WZ08
B	110	THR	LEU	conflict	UNP A0A087WZ08
B	122	GLU	LYS	conflict	UNP A0A087WZ08
B	169	CYS	SER	conflict	UNP A0A087WZ08
B	187	ALA	CYS	conflict	UNP A0A087WZ08
L	0	MET	LEU	conflict	UNP A0A087WZ08
L	18	GLU	LYS	conflict	UNP A0A087WZ08
L	?	-	SER	deletion	UNP A0A087WZ08
L	96	ILE	THR	conflict	UNP A0A087WZ08
L	97	TYR	VAL	conflict	UNP A0A087WZ08
L	98	PRO	LEU	conflict	UNP A0A087WZ08
L	99	GLY	HIS	conflict	UNP A0A087WZ08
L	100	GLU	SER	conflict	UNP A0A087WZ08
L	101	LEU	GLN	conflict	UNP A0A087WZ08
L	102	PHE	TYR	conflict	UNP A0A087WZ08
L	105	GLU	PRO	conflict	UNP A0A087WZ08
L	107	SER	THR	conflict	UNP A0A087WZ08
L	110	THR	LEU	conflict	UNP A0A087WZ08
L	122	GLU	LYS	conflict	UNP A0A087WZ08
L	169	CYS	SER	conflict	UNP A0A087WZ08
L	187	ALA	CYS	conflict	UNP A0A087WZ08
Q	0	MET	LEU	conflict	UNP A0A087WZ08
Q	18	GLU	LYS	conflict	UNP A0A087WZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	SER	deletion	UNP A0A087WZ08
Q	96	ILE	THR	conflict	UNP A0A087WZ08
Q	97	TYR	VAL	conflict	UNP A0A087WZ08
Q	98	PRO	LEU	conflict	UNP A0A087WZ08
Q	99	GLY	HIS	conflict	UNP A0A087WZ08
Q	100	GLU	SER	conflict	UNP A0A087WZ08
Q	101	LEU	GLN	conflict	UNP A0A087WZ08
Q	102	PHE	TYR	conflict	UNP A0A087WZ08
Q	105	GLU	PRO	conflict	UNP A0A087WZ08
Q	107	SER	THR	conflict	UNP A0A087WZ08
Q	110	THR	LEU	conflict	UNP A0A087WZ08
Q	122	GLU	LYS	conflict	UNP A0A087WZ08
Q	169	CYS	SER	conflict	UNP A0A087WZ08
Q	187	ALA	CYS	conflict	UNP A0A087WZ08

- Molecule 3 is a protein called HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	261	Total	C	N	O	S	0	0	0
			2072	1297	378	388	9			
3	C	258	Total	C	N	O	S	0	0	0
			2034	1273	363	389	9			
3	M	268	Total	C	N	O	S	0	0	0
			2076	1294	375	399	8			
3	R	251	Total	C	N	O	S	0	0	0
			1994	1249	360	376	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	0	MET	-	initiating methionine	UNP P01892
C	0	MET	-	initiating methionine	UNP P01892
M	0	MET	-	initiating methionine	UNP P01892
R	0	MET	-	initiating methionine	UNP P01892

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	96	Total	C	N	O	S	0	0	0
			772	489	131	149	3			
4	D	97	Total	C	N	O	S	0	0	0
			787	503	131	150	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	92	Total	C	N	O	S	0	0	0
			697	440	123	132	2			
4	U	99	Total	C	N	O	S	0	0	0
			793	504	133	153	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769
N	0	MET	-	initiating methionine	UNP P61769
U	0	MET	-	initiating methionine	UNP P61769

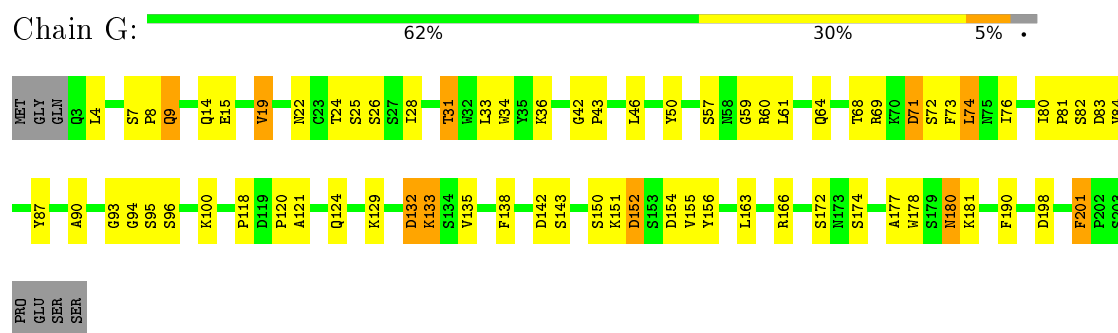
- Molecule 5 is a protein called Matrix protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	9	Total	C	N	O	0	0	0
			68	49	9	10			
5	E	9	Total	C	N	O	0	0	0
			68	49	9	10			
5	O	9	Total	C	N	O	0	0	0
			68	49	9	10			
5	T	9	Total	C	N	O	0	0	0
			68	49	9	10			

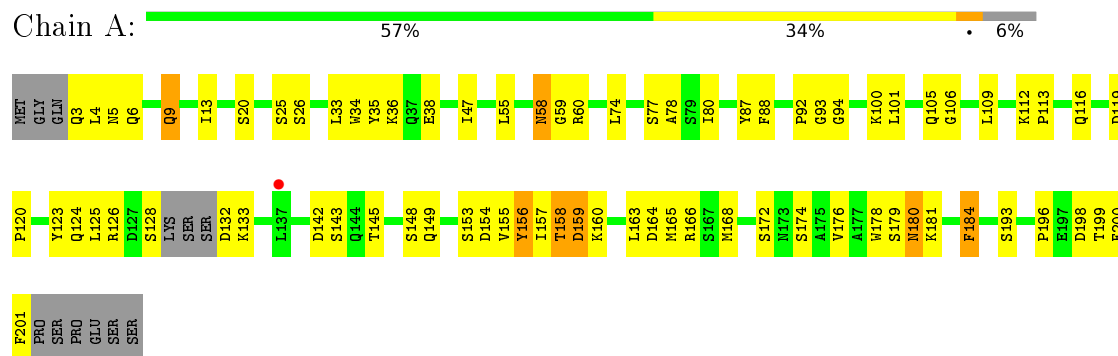
3 Residue-property plots [i](#)

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

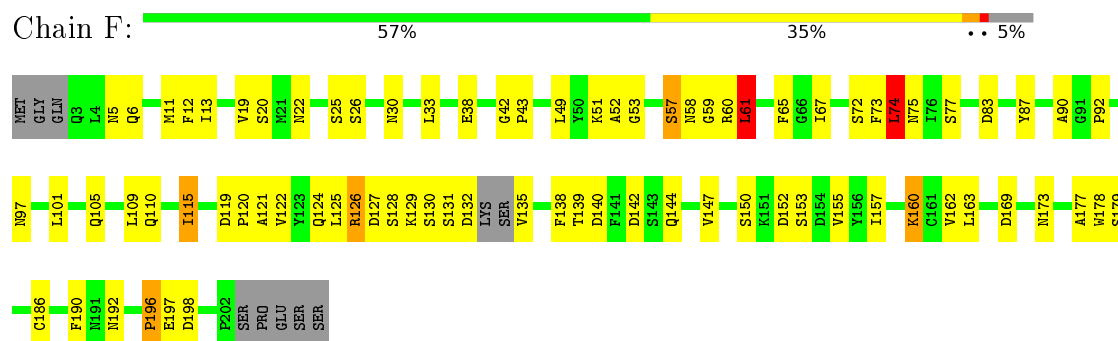
- Molecule 1: TCR alpha chain,Human nkt tcr alpha chain



- Molecule 1: TCR alpha chain,Human nkt tcr alpha chain

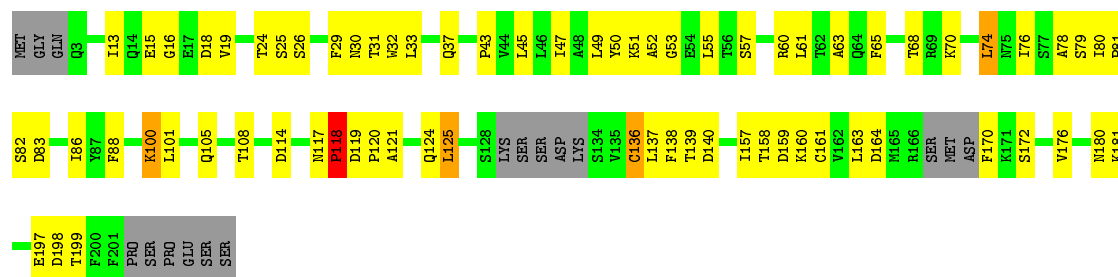


- Molecule 1: TCR alpha chain,Human nkt tcr alpha chain



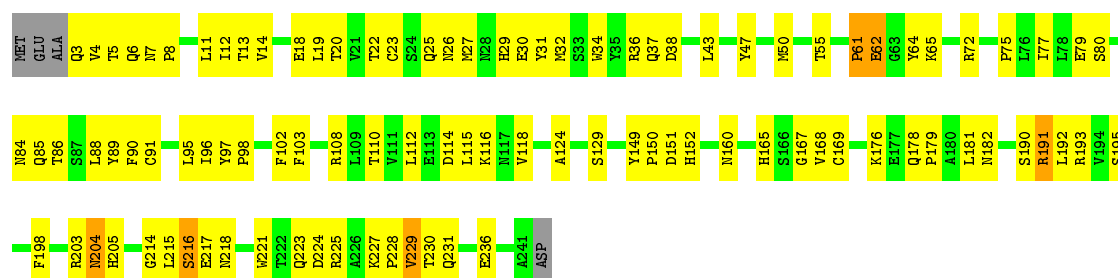
- Molecule 1: TCR alpha chain,Human nkt tcr alpha chain

Chain P:  57% 32% 8%



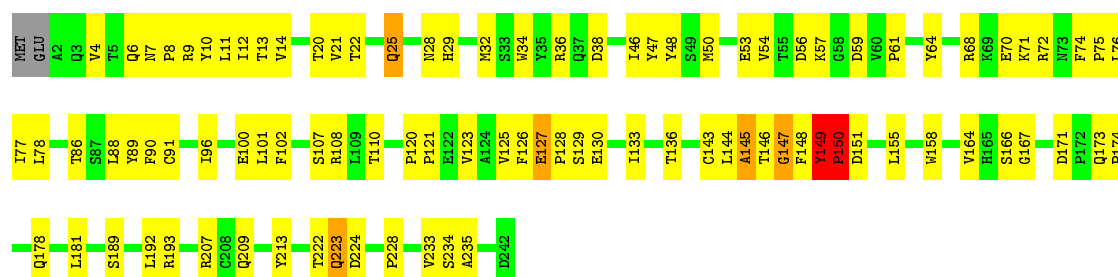
- Molecule 2: T-cell receptor beta-2 chain C region

Chain H:  58% 38% 2%



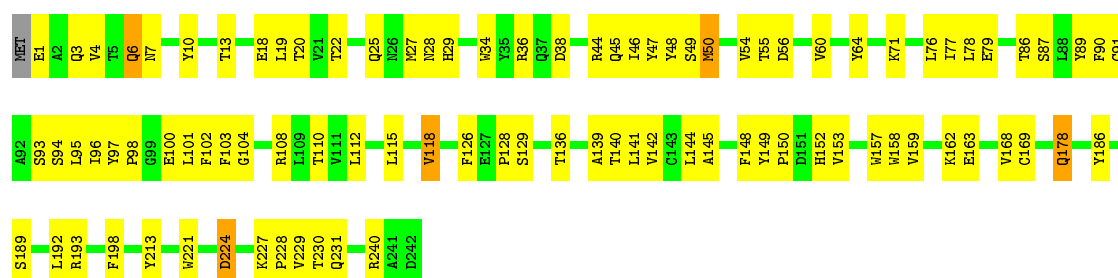
- Molecule 2: T-cell receptor beta-2 chain C region

Chain B:  60% 36% 2%

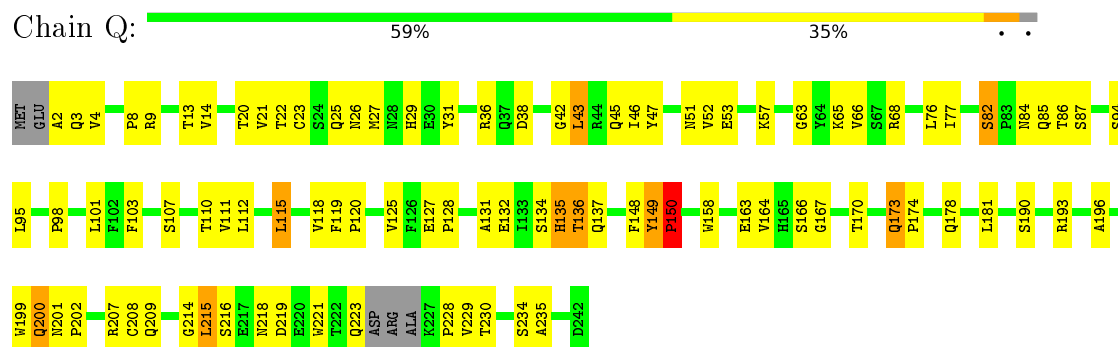


- Molecule 2: T-cell receptor beta-2 chain C region

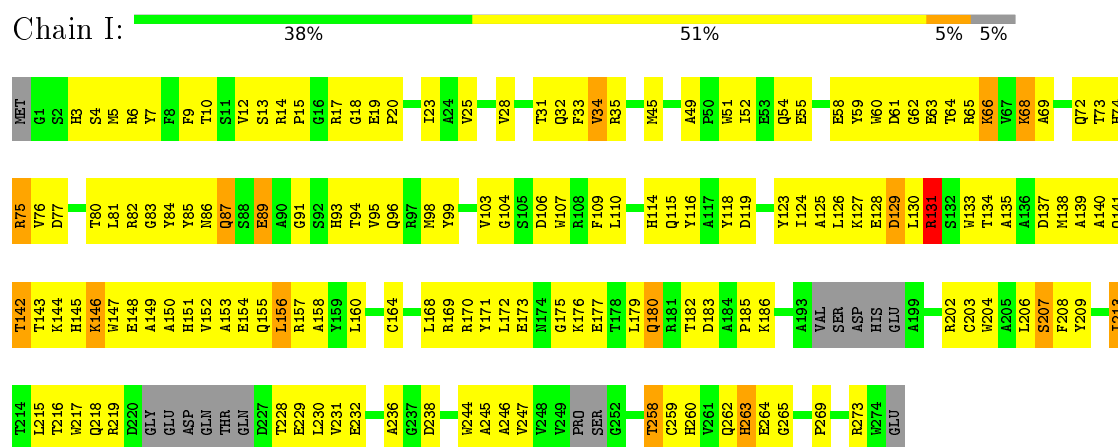
Chain L:  61% 36% 2%



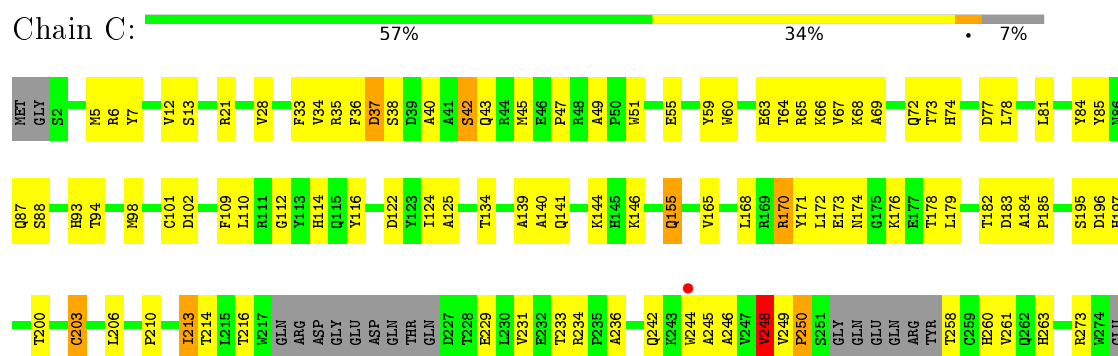
- Molecule 2: T-cell receptor beta-2 chain C region



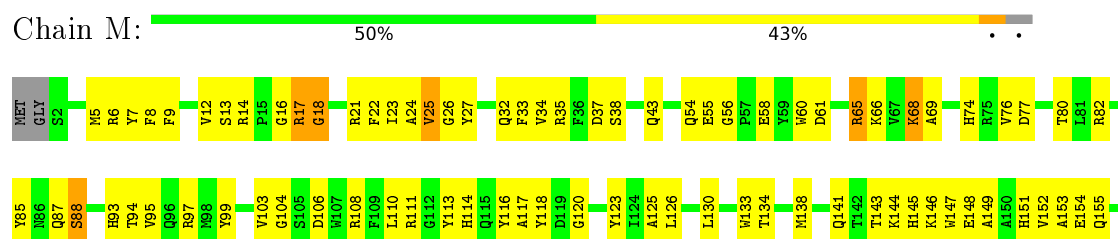
- Molecule 3: HLA class I histocompatibility antigen, A-2 alpha chain

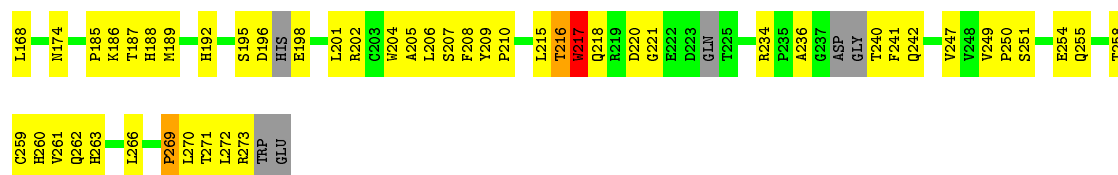


- Molecule 3: HLA class I histocompatibility antigen, A-2 alpha chain



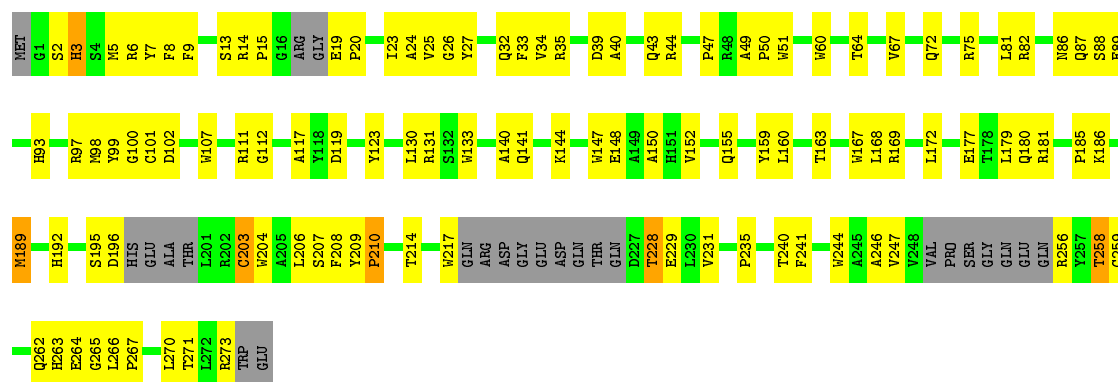
- Molecule 3: HLA class I histocompatibility antigen, A-2 alpha chain





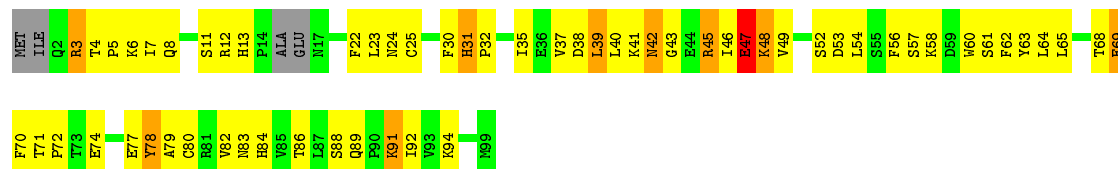
• Molecule 3: HLA class I histocompatibility antigen, A-2 alpha chain

Chain R: 51% 38% 9%



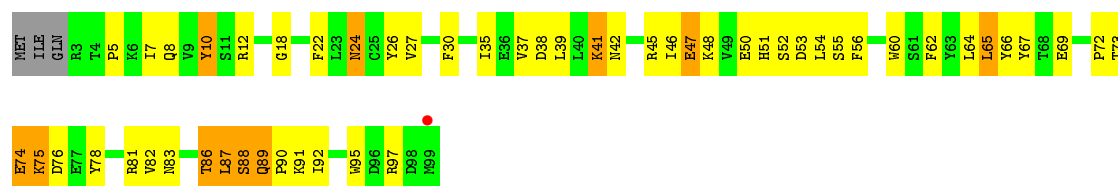
• Molecule 4: Beta-2-microglobulin

Chain J: 36% 50% 9%



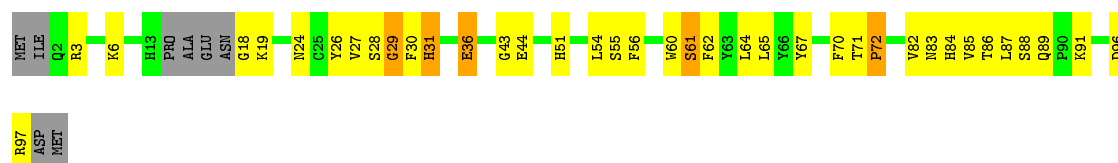
• Molecule 4: Beta-2-microglobulin

Chain D: 44% 42% 11%

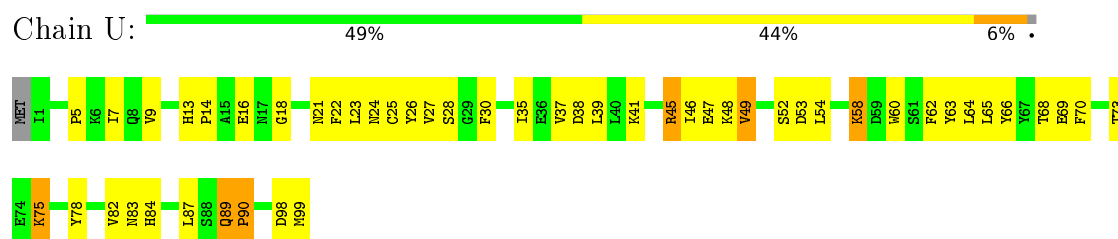


• Molecule 4: Beta-2-microglobulin

Chain N: 54% 33% 5% 8%



- Molecule 4: Beta-2-microglobulin



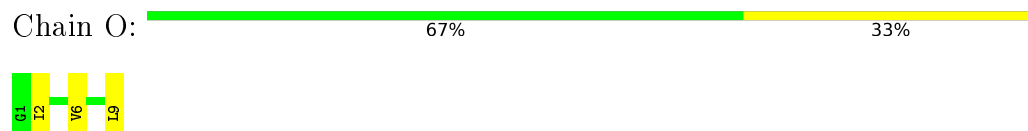
- Molecule 5: Matrix protein 1



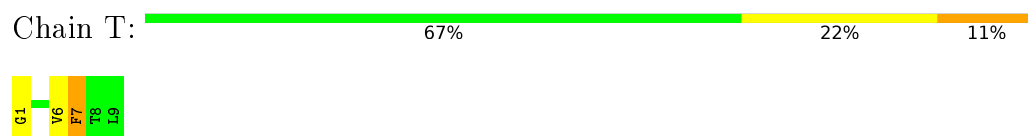
- Molecule 5: Matrix protein 1



- Molecule 5: Matrix protein 1



- Molecule 5: Matrix protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.85Å 123.61Å 139.04Å 83.66° 74.87° 73.17°	Depositor
Resolution (Å)	36.56 – 4.00 46.15 – 4.00	Depositor EDS
% Data completeness (in resolution range)	91.0 (36.56-4.00) 79.4 (46.15-4.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 4.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.259 , 0.338 0.258 , 0.332	Depositor DCC
R_{free} test set	1442 reflections (4.80%)	DCC
Wilson B-factor (Å ²)	97.3	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , -11.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.247 for h,h-k,h-l 0.000 for -h,-h+k,-l 0.000 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	24882	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 ⓘ

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	0.39	0/1486	0.67	1/2013 (0.0%)
1	F	0.40	0/1517	0.70	5/2060 (0.2%)
1	G	0.38	0/1567	0.63	3/2125 (0.1%)
1	P	0.39	0/1454	0.66	4/1977 (0.2%)
2	B	0.39	1/1917 (0.1%)	0.63	2/2616 (0.1%)
2	H	0.35	0/1930	0.63	1/2635 (0.0%)
2	L	0.36	0/1944	0.59	0/2659
2	Q	0.38	0/1891	0.66	2/2583 (0.1%)
3	C	0.42	2/2091 (0.1%)	0.72	3/2841 (0.1%)
3	I	0.48	0/2129	0.77	3/2887 (0.1%)
3	M	0.44	0/2130	0.73	4/2890 (0.1%)
3	R	0.38	0/2048	0.61	0/2777
4	D	0.45	0/809	0.76	2/1098 (0.2%)
4	J	0.38	0/793	0.76	4/1075 (0.4%)
4	N	0.51	0/715	0.85	2/962 (0.2%)
4	U	0.46	1/815 (0.1%)	0.80	2/1104 (0.2%)
5	E	0.31	0/69	0.50	0/92
5	K	0.56	0/69	0.83	1/92 (1.1%)
5	O	0.28	0/69	0.48	0/92
5	T	0.33	0/69	0.52	0/92
All	All	0.41	4/25512 (0.0%)	0.69	39/34670 (0.1%)

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	A	0	1
1	F	0	1
1	P	0	1
2	Q	0	1
3	C	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	1
3	M	0	2
3	R	0	2
4	D	0	1
4	J	0	2
4	N	0	1
All	All	0	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	150	PRO	N-CD	5.22	1.55	1.47
3	C	248	VAL	CB-CG2	-5.20	1.42	1.52
3	C	250	PRO	N-CD	5.10	1.54	1.47
4	U	90	PRO	N-CD	5.04	1.54	1.47

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	179	LEU	CA-CB-CG	9.22	136.52	115.30
2	H	231	GLN	N-CA-CB	9.00	126.79	110.60
4	N	19	LYS	N-CA-C	-8.43	88.24	111.00
3	I	203	CYS	CA-CB-SG	8.22	128.80	114.00
1	F	196	PRO	CA-N-CD	-8.14	100.10	111.50

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	THR	Peptide
3	C	178	THR	Peptide
3	I	131	ARG	Peptide
4	J	47	GLU	Peptide
4	J	68	THR	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	1459	0	1369	65	0
1	F	1486	0	1377	72	0
1	G	1535	0	1459	86	0
1	P	1426	0	1324	72	0
2	B	1870	0	1737	107	0
2	H	1878	0	1760	101	0
2	L	1891	0	1754	109	0
2	Q	1840	0	1701	88	0
3	C	2034	0	1862	109	0
3	I	2072	0	1914	210	0
3	M	2076	0	1865	138	0
3	R	1994	0	1836	116	0
4	D	787	0	736	79	0
4	J	772	0	706	80	0
4	N	697	0	612	51	0
4	U	793	0	732	68	0
5	E	68	0	75	6	0
5	K	68	0	75	17	0
5	O	68	0	75	6	0
5	T	68	0	75	4	0
All	All	24882	0	23044	1434	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 30.

The worst 5 of 1434 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:G:133:LYS:CB	1:G:180:ASN:HD21	1.15	1.51
1:P:47:ILE:CD1	1:P:57:SER:HB2	1.37	1.50
1:G:59:GLY:CA	1:G:61:LEU:H	1.24	1.50
1:G:59:GLY:HA3	1:G:61:LEU:N	1.32	1.44
1:G:133:LYS:CB	1:G:180:ASN:ND2	1.89	1.33

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	192/208 (92%)	161 (84%)	31 (16%)	0	100	100
1	F	194/208 (93%)	173 (89%)	20 (10%)	1 (0%)	34	76
1	G	199/208 (96%)	176 (88%)	23 (12%)	0	100	100
1	P	185/208 (89%)	151 (82%)	32 (17%)	2 (1%)	17	64
2	B	239/243 (98%)	212 (89%)	26 (11%)	1 (0%)	39	79
2	H	237/243 (98%)	201 (85%)	32 (14%)	4 (2%)	11	56
2	L	240/243 (99%)	213 (89%)	27 (11%)	0	100	100
2	Q	234/243 (96%)	211 (90%)	21 (9%)	2 (1%)	21	66
3	C	252/276 (91%)	223 (88%)	29 (12%)	0	100	100
3	I	253/276 (92%)	218 (86%)	34 (13%)	1 (0%)	39	79
3	M	260/276 (94%)	225 (86%)	33 (13%)	2 (1%)	24	69
3	R	241/276 (87%)	210 (87%)	31 (13%)	0	100	100
4	D	95/100 (95%)	82 (86%)	13 (14%)	0	100	100
4	J	92/100 (92%)	86 (94%)	6 (6%)	0	100	100
4	N	88/100 (88%)	76 (86%)	10 (11%)	2 (2%)	8	51
4	U	97/100 (97%)	82 (84%)	14 (14%)	1 (1%)	19	65
5	E	7/9 (78%)	7 (100%)	0	0	100	100
5	K	7/9 (78%)	7 (100%)	0	0	100	100
5	O	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
5	T	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
All	All	3126/3344 (94%)	2724 (87%)	386 (12%)	16 (0%)	34	76

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	156	LEU

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Mol	Chain	Res	Type
4	N	26	TYR
4	N	72	PRO
2	Q	136	THR
2	H	61	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	162/183 (88%)	156 (96%)	6 (4%)	41	75
1	F	165/183 (90%)	158 (96%)	7 (4%)	36	72
1	G	175/183 (96%)	165 (94%)	10 (6%)	25	65
1	P	157/183 (86%)	151 (96%)	6 (4%)	40	74
2	B	201/217 (93%)	192 (96%)	9 (4%)	34	71
2	H	204/217 (94%)	198 (97%)	6 (3%)	50	79
2	L	205/217 (94%)	198 (97%)	7 (3%)	44	77
2	Q	198/217 (91%)	191 (96%)	7 (4%)	43	76
3	C	205/232 (88%)	198 (97%)	7 (3%)	44	77
3	I	206/232 (89%)	189 (92%)	17 (8%)	14	51
3	M	203/232 (88%)	194 (96%)	9 (4%)	35	71
3	R	201/232 (87%)	194 (96%)	7 (4%)	43	76
4	D	87/95 (92%)	78 (90%)	9 (10%)	9	40
4	J	85/95 (90%)	75 (88%)	10 (12%)	6	35
4	N	70/95 (74%)	65 (93%)	5 (7%)	18	58
4	U	87/95 (92%)	83 (95%)	4 (5%)	33	70
5	E	7/7 (100%)	7 (100%)	0	100	100
5	K	7/7 (100%)	7 (100%)	0	100	100
5	O	7/7 (100%)	7 (100%)	0	100	100
5	T	7/7 (100%)	6 (86%)	1 (14%)	4	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2639/2936 (90%)	2512 (95%)	127 (5%)	31 69

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	224	ASP
4	D	75	LYS
3	R	189	MET
3	C	155	GLN
3	C	248	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
2	B	7	ASN
4	N	84	HIS
4	J	89	GLN
1	A	9	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [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	196/208 (94%)	-0.62	1 (0%) 91 88	57, 111, 150, 165	0
1	F	198/208 (95%)	-0.76	0 100 100	57, 94, 135, 145	0
1	G	201/208 (96%)	-0.79	0 100 100	50, 92, 133, 156	0
1	P	191/208 (91%)	-0.65	0 100 100	60, 101, 146, 158	0
2	B	241/243 (99%)	-0.77	0 100 100	61, 99, 139, 160	0
2	H	239/243 (98%)	-0.72	0 100 100	65, 92, 132, 144	0
2	L	242/243 (99%)	-0.76	0 100 100	70, 91, 131, 165	0
2	Q	238/243 (97%)	-0.69	0 100 100	77, 102, 130, 151	0
3	C	258/276 (93%)	-0.66	1 (0%) 93 90	74, 110, 154, 176	0
3	I	261/276 (94%)	-0.69	0 100 100	91, 119, 150, 182	0
3	M	268/276 (97%)	-0.67	0 100 100	83, 122, 159, 176	0
3	R	251/276 (90%)	-0.68	0 100 100	72, 106, 145, 152	0
4	D	97/100 (97%)	-0.59	1 (1%) 84 77	84, 127, 157, 167	0
4	J	96/100 (96%)	-0.74	0 100 100	106, 135, 164, 170	0
4	N	92/100 (92%)	-0.68	0 100 100	100, 136, 168, 174	0
4	U	99/100 (99%)	-0.78	0 100 100	79, 130, 151, 174	0
5	E	9/9 (100%)	-0.71	0 100 100	80, 83, 89, 92	0
5	K	9/9 (100%)	-0.57	0 100 100	91, 97, 103, 106	0
5	O	9/9 (100%)	-0.42	0 100 100	87, 104, 113, 114	0
5	T	9/9 (100%)	-0.52	0 100 100	78, 83, 90, 91	0
All	All	3204/3344 (95%)	-0.70	3 (0%) 95 95	50, 107, 149, 182	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	244	TRP	2.2
4	D	99	MET	2.2
1	A	137	LEU	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.