



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 05:10 am BST

PDB ID : 3PQY
Title : Crystal Structure of 6218 TCR in complex with the H2Db-PA224
Authors : Gras, S.; Guillonneau, C.; Turner, S.J.; Rossjohn, J.
Deposited on : 2010-11-28
Resolution : 3.19 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

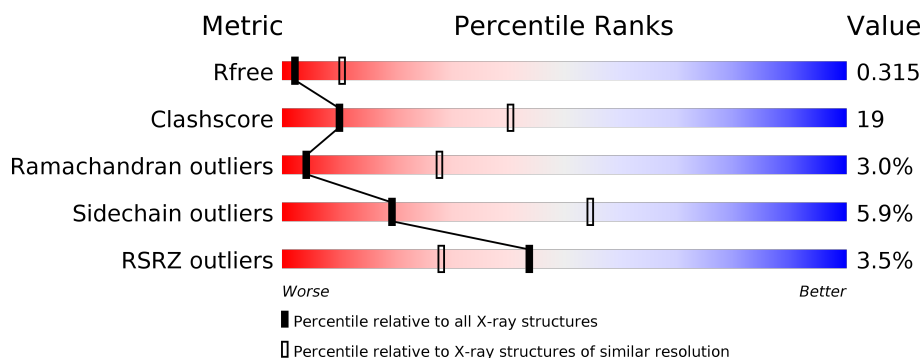
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	275	
1	F	275	
1	K	275	
1	P	275	
2	B	99	
2	G	99	

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Mol	Chain	Length	Quality of chain
2	L	99	
2	Q	99	
3	C	10	
3	H	10	
3	M	10	
3	R	10	
4	D	195	
4	I	195	
4	N	195	
4	S	195	
5	E	240	
5	J	240	
5	O	240	
5	T	240	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25956 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	1	0	0
			2260	1428	399	424	9			
1	F	267	Total	C	N	O	S	1	0	0
			2198	1391	389	409	9			
1	K	275	Total	C	N	O	S	0	0	0
			2260	1428	399	424	9			
1	P	273	Total	C	N	O	S	1	0	0
			2244	1418	397	420	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			
2	G	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			
2	L	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			
2	Q	98	Total	C	N	O	S	0	0	0
			813	518	137	151	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ASP	ALA	variant	UNP P01887
G	85	ASP	ALA	variant	UNP P01887
L	85	ASP	ALA	variant	UNP P01887
Q	85	ASP	ALA	variant	UNP P01887

- Molecule 3 is a protein called 10-mer peptide from RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			84	53	14	17			
3	H	10	Total	C	N	O	0	0	0
			84	53	14	17			
3	M	10	Total	C	N	O	0	0	0
			84	53	14	17			
3	R	10	Total	C	N	O	0	0	0
			84	53	14	17			

- Molecule 4 is a protein called T cell receptor alpha variable 21-DV12,T-cell receptor, sp3.4 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	189	Total	C	N	O	S	0	0	0
			1464	916	244	295	9			
4	I	188	Total	C	N	O	S	0	0	0
			1464	918	243	294	9			
4	N	174	Total	C	N	O	S	0	0	0
			1350	846	226	269	9			
4	S	174	Total	C	N	O	S	0	0	0
			1348	845	225	269	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	107	SER	-	linker	UNP A0A075B6C4
D	108	GLY	-	linker	UNP A0A075B6C4
D	109	GLY	-	linker	UNP A0A075B6C4
D	110	SER	-	linker	UNP A0A075B6C4
D	111	ASN	-	linker	UNP A0A075B6C4
D	112	TYR	-	linker	UNP A0A075B6C4
D	113	LYS	-	linker	UNP A0A075B6C4
D	114	LEU	-	linker	UNP A0A075B6C4
D	115	THR	-	linker	UNP A0A075B6C4
D	116	PHE	-	linker	UNP A0A075B6C4
D	117	GLY	-	linker	UNP A0A075B6C4
D	118	LYS	-	linker	UNP A0A075B6C4
D	119	GLY	-	linker	UNP A0A075B6C4
D	120	THR	-	linker	UNP A0A075B6C4
D	121	LEU	-	linker	UNP A0A075B6C4
D	122	LEU	-	linker	UNP A0A075B6C4
D	123	THR	-	linker	UNP A0A075B6C4
D	124	VAL	-	linker	UNP A0A075B6C4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	125	THR	-	linker	UNP A0A075B6C4
D	126	PRO	-	linker	UNP A0A075B6C4
I	107	SER	-	linker	UNP A0A075B6C4
I	108	GLY	-	linker	UNP A0A075B6C4
I	109	GLY	-	linker	UNP A0A075B6C4
I	110	SER	-	linker	UNP A0A075B6C4
I	111	ASN	-	linker	UNP A0A075B6C4
I	112	TYR	-	linker	UNP A0A075B6C4
I	113	LYS	-	linker	UNP A0A075B6C4
I	114	LEU	-	linker	UNP A0A075B6C4
I	115	THR	-	linker	UNP A0A075B6C4
I	116	PHE	-	linker	UNP A0A075B6C4
I	117	GLY	-	linker	UNP A0A075B6C4
I	118	LYS	-	linker	UNP A0A075B6C4
I	119	GLY	-	linker	UNP A0A075B6C4
I	120	THR	-	linker	UNP A0A075B6C4
I	121	LEU	-	linker	UNP A0A075B6C4
I	122	LEU	-	linker	UNP A0A075B6C4
I	123	THR	-	linker	UNP A0A075B6C4
I	124	VAL	-	linker	UNP A0A075B6C4
I	125	THR	-	linker	UNP A0A075B6C4
I	126	PRO	-	linker	UNP A0A075B6C4
N	107	SER	-	linker	UNP A0A075B6C4
N	108	GLY	-	linker	UNP A0A075B6C4
N	109	GLY	-	linker	UNP A0A075B6C4
N	110	SER	-	linker	UNP A0A075B6C4
N	111	ASN	-	linker	UNP A0A075B6C4
N	112	TYR	-	linker	UNP A0A075B6C4
N	113	LYS	-	linker	UNP A0A075B6C4
N	114	LEU	-	linker	UNP A0A075B6C4
N	115	THR	-	linker	UNP A0A075B6C4
N	116	PHE	-	linker	UNP A0A075B6C4
N	117	GLY	-	linker	UNP A0A075B6C4
N	118	LYS	-	linker	UNP A0A075B6C4
N	119	GLY	-	linker	UNP A0A075B6C4
N	120	THR	-	linker	UNP A0A075B6C4
N	121	LEU	-	linker	UNP A0A075B6C4
N	122	LEU	-	linker	UNP A0A075B6C4
N	123	THR	-	linker	UNP A0A075B6C4
N	124	VAL	-	linker	UNP A0A075B6C4
N	125	THR	-	linker	UNP A0A075B6C4
N	126	PRO	-	linker	UNP A0A075B6C4

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Chain	Residue	Modelled	Actual	Comment	Reference
S	107	SER	-	linker	UNP A0A075B6C4
S	108	GLY	-	linker	UNP A0A075B6C4
S	109	GLY	-	linker	UNP A0A075B6C4
S	110	SER	-	linker	UNP A0A075B6C4
S	111	ASN	-	linker	UNP A0A075B6C4
S	112	TYR	-	linker	UNP A0A075B6C4
S	113	LYS	-	linker	UNP A0A075B6C4
S	114	LEU	-	linker	UNP A0A075B6C4
S	115	THR	-	linker	UNP A0A075B6C4
S	116	PHE	-	linker	UNP A0A075B6C4
S	117	GLY	-	linker	UNP A0A075B6C4
S	118	LYS	-	linker	UNP A0A075B6C4
S	119	GLY	-	linker	UNP A0A075B6C4
S	120	THR	-	linker	UNP A0A075B6C4
S	121	LEU	-	linker	UNP A0A075B6C4
S	122	LEU	-	linker	UNP A0A075B6C4
S	123	THR	-	linker	UNP A0A075B6C4
S	124	VAL	-	linker	UNP A0A075B6C4
S	125	THR	-	linker	UNP A0A075B6C4
S	126	PRO	-	linker	UNP A0A075B6C4

- Molecule 5 is a protein called T cell receptor beta, variable 29,Human nkt tcr beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	240	Total	C	N	O	S	0	0	0
			1941	1224	337	370	10			
5	J	240	Total	C	N	O	S	0	0	0
			1941	1224	337	370	10			
5	O	240	Total	C	N	O	S	0	0	0
			1941	1224	337	370	10			
5	T	240	Total	C	N	O	S	0	0	0
			1941	1224	337	370	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	108	PHE	-	linker	UNP A0A0G2LB96
E	109	GLY	-	linker	UNP A0A0G2LB96
E	110	ARG	-	linker	UNP A0A0G2LB96
E	123	LEU	THR	conflict	UNP K7N5M4
J	108	PHE	-	linker	UNP A0A0G2LB96
J	109	GLY	-	linker	UNP A0A0G2LB96

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Chain	Residue	Modelled	Actual	Comment	Reference
J	110	ARG	-	linker	UNP A0A0G2LB96
J	123	LEU	THR	conflict	UNP K7N5M4
O	108	PHE	-	linker	UNP A0A0G2LB96
O	109	GLY	-	linker	UNP A0A0G2LB96
O	110	ARG	-	linker	UNP A0A0G2LB96
O	123	LEU	THR	conflict	UNP K7N5M4
T	108	PHE	-	linker	UNP A0A0G2LB96
T	109	GLY	-	linker	UNP A0A0G2LB96
T	110	ARG	-	linker	UNP A0A0G2LB96
T	123	LEU	THR	conflict	UNP K7N5M4

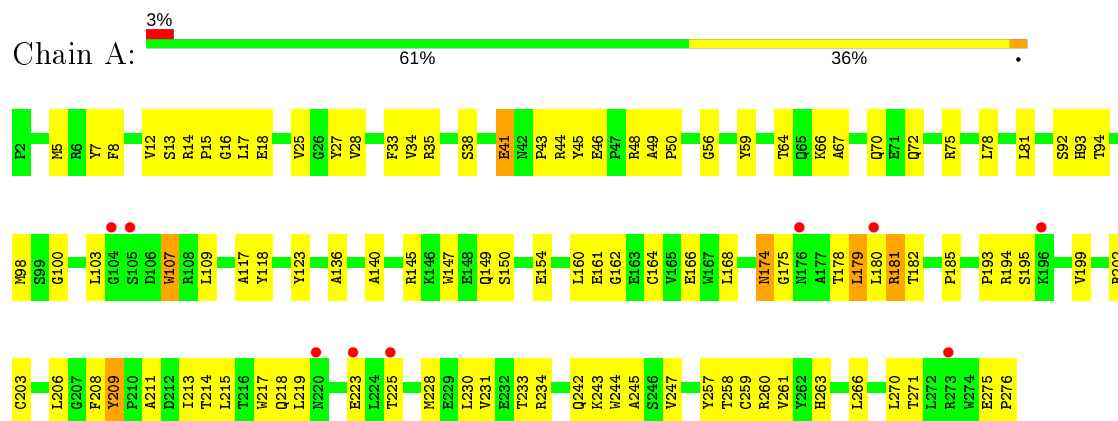
- Molecule 6 is water.

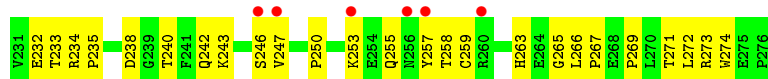
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total O 2 2	0	0
6	B	2	Total O 2 2	0	0
6	D	1	Total O 1 1	0	0
6	E	2	Total O 2 2	0	0
6	J	1	Total O 1 1	0	0
6	K	1	Total O 1 1	0	0
6	N	1	Total O 1 1	0	0
6	O	2	Total O 2 2	0	0
6	P	2	Total O 2 2	0	0
6	R	1	Total O 1 1	0	0
6	S	1	Total O 1 1	0	0

3 Residue-property plots [i](#)

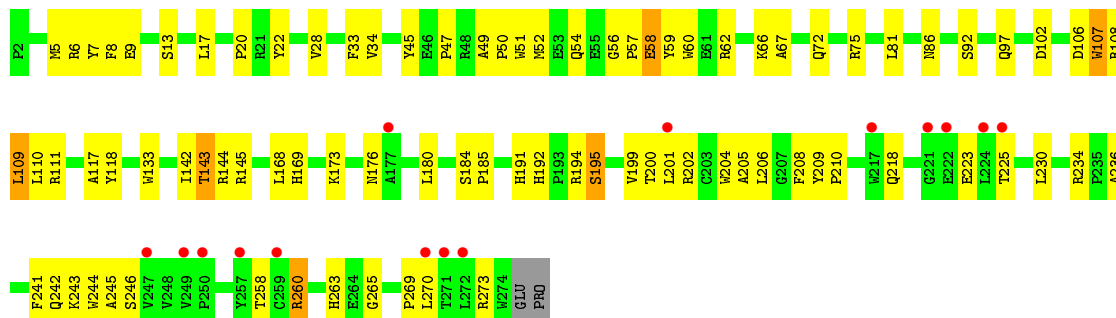
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: H-2 class I histocompatibility antigen, D-B alpha chain





- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



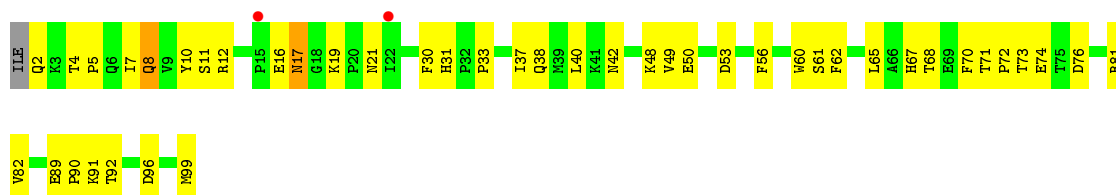
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

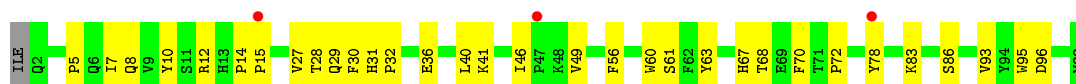


- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin





- Molecule 3: 10-mer peptide from RNA-directed RNA polymerase



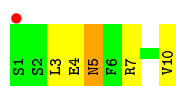
- Molecule 3: 10-mer peptide from RNA-directed RNA polymerase



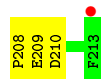
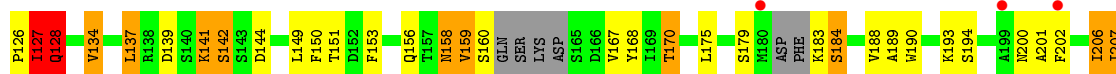
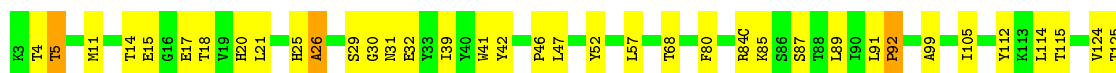
- Molecule 3: 10-mer peptide from RNA-directed RNA polymerase



- Molecule 3: 10-mer peptide from RNA-directed RNA polymerase

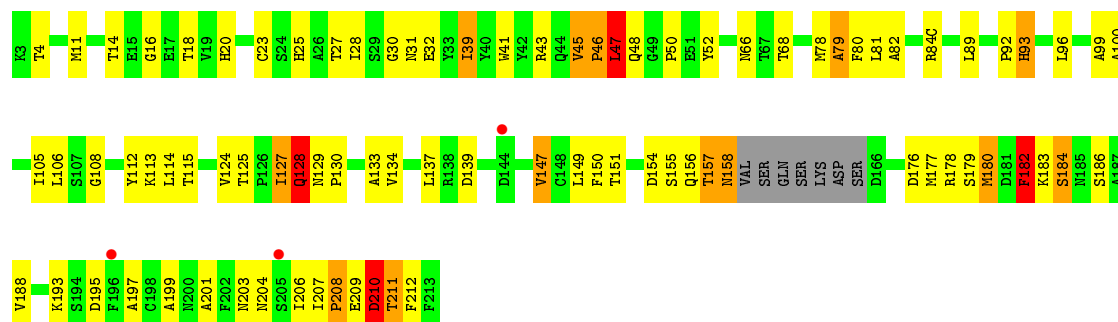


- Molecule 4: T cell receptor alpha variable 21-DV12,T-cell receptor, sp3.4 alpha chain

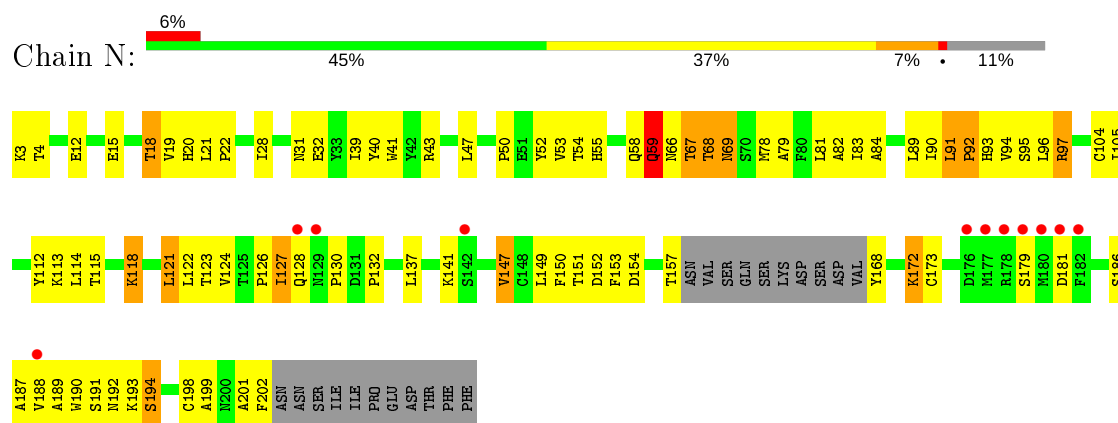


- Molecule 4: T cell receptor alpha variable 21-DV12,T-cell receptor, sp3.4 alpha chain

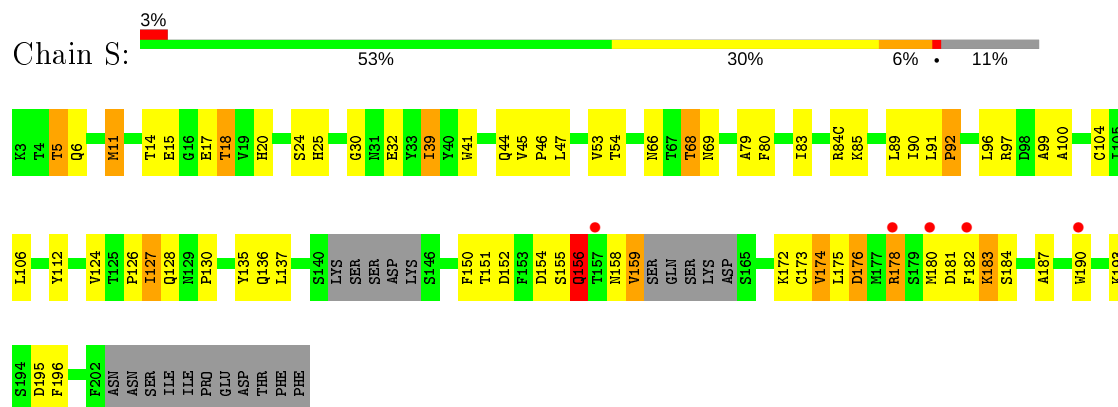




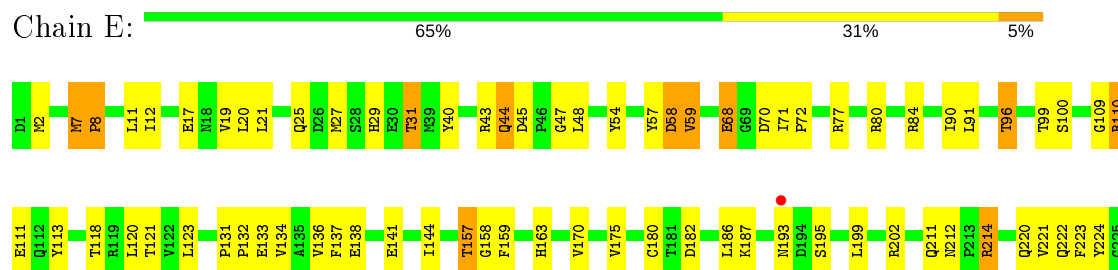
- Molecule 4: T cell receptor alpha variable 21-DV12, T-cell receptor, sp3.4 alpha chain



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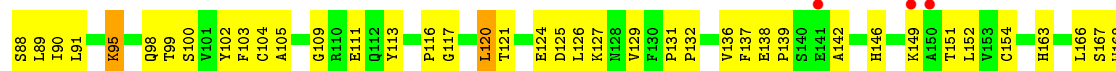


- Molecule 5: T cell receptor beta, variable 29, Human nkt tcr beta chain





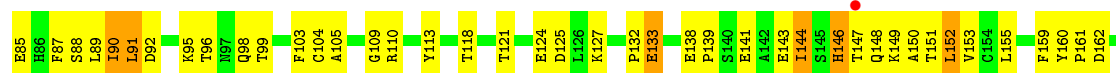
- Molecule 5: T cell receptor beta, variable 29, Human nkt tcr beta chain



- Molecule 5: T cell receptor beta, variable 29, Human nkt tcr beta chain



- Molecule 5: T cell receptor beta, variable 29, Human nkt tcr beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.89Å 199.06Å 202.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.61 – 3.19 49.61 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.61-3.19) 97.4 (49.61-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 3.19Å)	Xtriage
Refinement program	REFMAC, PHENIX 1.6.1_357	Depositor
R, R_{free}	0.246 , 0.316 0.242 , 0.315	Depositor DCC
R_{free} test set	3545 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	25956	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2923e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.21	0/2327	0.37	0/3160
1	F	0.20	0/2264	0.36	0/3073
1	K	0.21	0/2327	0.36	0/3160
1	P	0.20	0/2310	0.37	0/3136
2	B	0.21	0/839	0.40	0/1137
2	G	0.21	0/839	0.38	0/1137
2	L	0.21	0/839	0.40	0/1137
2	Q	0.20	0/839	0.39	0/1137
3	C	0.25	0/85	0.40	0/112
3	H	0.23	0/85	0.34	0/112
3	M	0.23	0/85	0.40	0/112
3	R	0.24	0/85	0.36	0/112
4	D	0.22	0/1495	0.41	0/2032
4	I	0.22	0/1497	0.43	0/2036
4	N	0.22	0/1380	0.42	0/1875
4	S	0.22	0/1377	0.41	0/1873
5	E	0.22	0/1992	0.39	0/2702
5	J	0.22	0/1992	0.39	0/2702
5	O	0.22	0/1992	0.38	0/2702
5	T	0.22	0/1992	0.39	0/2702
All	All	0.21	0/26641	0.39	0/36149

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2260	0	2131	73	0
1	F	2198	0	2072	66	0
1	K	2260	0	2133	74	0
1	P	2244	0	2118	66	0
2	B	813	0	782	26	0
2	G	813	0	782	33	0
2	L	813	0	782	35	0
2	Q	813	0	782	21	0
3	C	84	0	80	8	0
3	H	84	0	80	3	0
3	M	84	0	80	2	0
3	R	84	0	80	5	0
4	D	1464	0	1399	73	0
4	I	1464	0	1394	98	0
4	N	1350	0	1294	83	0
4	S	1348	0	1286	64	0
5	E	1941	0	1857	63	0
5	J	1941	0	1857	96	0
5	O	1941	0	1857	71	0
5	T	1941	0	1857	102	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	D	1	0	0	0	0
6	E	2	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	N	1	0	0	0	0
6	O	2	0	0	0	0
6	P	2	0	0	0	0
6	R	1	0	0	0	0
6	S	1	0	0	0	0
All	All	25956	0	24703	956	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 19.

The worst 5 of 956 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)
4:S:183:LYS:HB2	4:S:184:SER:HB2	1.38	1.03
4:S:30:GLY:HA2	4:S:84(C):ARG:HH12	1.22	1.02
5:E:7:MET:HB3	5:E:8:PRO:HD2	1.43	1.00
5:J:59:VAL:HG13	5:J:60:ASP:H	1.30	0.96
5:T:7:MET:HB3	5:T:8:PRO:HD2	1.45	0.95

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	273/275 (99%)	244 (89%)	26 (10%)	3 (1%)	14	51
1	F	263/275 (96%)	222 (84%)	39 (15%)	2 (1%)	19	58
1	K	273/275 (99%)	235 (86%)	30 (11%)	8 (3%)	4	28
1	P	271/275 (98%)	244 (90%)	25 (9%)	2 (1%)	22	61
2	B	96/99 (97%)	87 (91%)	7 (7%)	2 (2%)	7	37
2	G	96/99 (97%)	82 (85%)	11 (12%)	3 (3%)	4	26
2	L	96/99 (97%)	81 (84%)	13 (14%)	2 (2%)	7	37
2	Q	96/99 (97%)	87 (91%)	9 (9%)	0	100	100
3	C	8/10 (80%)	5 (62%)	2 (25%)	1 (12%)	0	1
3	H	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	M	8/10 (80%)	7 (88%)	0	1 (12%)	0	1
3	R	8/10 (80%)	7 (88%)	0	1 (12%)	0	1
4	D	183/195 (94%)	132 (72%)	37 (20%)	14 (8%)	1	6
4	I	184/195 (94%)	128 (70%)	45 (24%)	11 (6%)	1	12
4	N	170/195 (87%)	119 (70%)	40 (24%)	11 (6%)	1	10
4	S	168/195 (86%)	132 (79%)	31 (18%)	5 (3%)	4	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	238/240 (99%)	206 (87%)	24 (10%)	8 (3%)	3	24
5	J	238/240 (99%)	200 (84%)	30 (13%)	8 (3%)	3	24
5	O	238/240 (99%)	207 (87%)	25 (10%)	6 (2%)	5	32
5	T	238/240 (99%)	197 (83%)	34 (14%)	7 (3%)	4	28
All	All	3153/3276 (96%)	2629 (83%)	429 (14%)	95 (3%)	4	28

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	5	ASN
4	D	92	PRO
4	D	179	SER
5	E	8	PRO
5	E	68	GLU

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	234/234 (100%)	225 (96%)	9 (4%)	33	67
1	F	227/234 (97%)	220 (97%)	7 (3%)	40	72
1	K	234/234 (100%)	222 (95%)	12 (5%)	24	60
1	P	232/234 (99%)	222 (96%)	10 (4%)	29	64
2	B	93/94 (99%)	90 (97%)	3 (3%)	39	71
2	G	93/94 (99%)	86 (92%)	7 (8%)	13	45
2	L	93/94 (99%)	88 (95%)	5 (5%)	22	58
2	Q	93/94 (99%)	92 (99%)	1 (1%)	73	88
3	C	9/9 (100%)	9 (100%)	0	100	100
3	H	9/9 (100%)	9 (100%)	0	100	100
3	M	9/9 (100%)	9 (100%)	0	100	100
3	R	9/9 (100%)	9 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	169/175 (97%)	158 (94%)	11 (6%)	17	51
4	I	168/175 (96%)	150 (89%)	18 (11%)	6	27
4	N	154/175 (88%)	140 (91%)	14 (9%)	9	34
4	S	154/175 (88%)	140 (91%)	14 (9%)	9	34
5	E	213/213 (100%)	199 (93%)	14 (7%)	16	51
5	J	213/213 (100%)	199 (93%)	14 (7%)	16	51
5	O	213/213 (100%)	202 (95%)	11 (5%)	23	59
5	T	213/213 (100%)	197 (92%)	16 (8%)	13	45
All	All	2832/2900 (98%)	2666 (94%)	166 (6%)	19	54

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	J	87	PHE
1	K	217	TRP
5	T	54	TYR
5	J	120	LEU
1	K	45	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
5	J	146	HIS
2	L	31	HIS
5	T	6	GLN
5	J	171	ASN
1	K	188	HIS

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 [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	275/275 (100%)	0.18	9 (3%) 46 30	27, 74, 122, 148	1 (0%)
1	F	267/275 (97%)	0.45	23 (8%) 10 5	37, 100, 168, 201	1 (0%)
1	K	275/275 (100%)	0.50	24 (8%) 10 5	29, 95, 177, 194	0
1	P	273/275 (99%)	0.44	15 (5%) 25 14	38, 90, 152, 165	1 (0%)
2	B	98/99 (98%)	-0.02	0 100 100	42, 68, 103, 112	0
2	G	98/99 (98%)	0.29	3 (3%) 49 32	54, 104, 152, 156	0
2	L	98/99 (98%)	0.29	2 (2%) 65 51	53, 100, 144, 151	0
2	Q	98/99 (98%)	0.32	3 (3%) 49 32	58, 97, 129, 145	0
3	C	10/10 (100%)	-0.05	0 100 100	31, 38, 66, 70	0
3	H	10/10 (100%)	-0.09	0 100 100	40, 49, 81, 88	0
3	M	10/10 (100%)	0.03	0 100 100	37, 44, 71, 83	0
3	R	10/10 (100%)	0.18	1 (10%) 7 4	42, 49, 80, 86	0
4	D	189/195 (96%)	0.33	4 (2%) 63 49	32, 79, 149, 169	0
4	I	188/195 (96%)	0.21	3 (1%) 72 59	40, 85, 146, 163	0
4	N	174/195 (89%)	0.41	11 (6%) 20 11	37, 79, 162, 179	0
4	S	174/195 (89%)	0.33	5 (2%) 51 36	40, 85, 150, 197	0
5	E	240/240 (100%)	0.04	1 (0%) 92 89	32, 69, 120, 135	0
5	J	240/240 (100%)	0.07	4 (1%) 70 57	32, 69, 128, 152	0
5	O	240/240 (100%)	0.11	2 (0%) 86 78	31, 69, 113, 149	0
5	T	240/240 (100%)	0.24	1 (0%) 92 89	40, 90, 135, 155	0
All	All	3207/3276 (97%)	0.27	111 (3%) 44 28	27, 82, 152, 201	3 (0%)

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	179	LEU	5.6
1	K	223	GLU	5.1
1	F	180	LEU	5.1
1	K	215	LEU	4.8
4	D	213	PHE	4.8

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.