Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:09 pm BST

PDB ID	:	4MNH
Title	:	Structure of the DP10.7 TCR
Authors	:	Luoma, A.M.; Adams, E.J.
Deposited on	:	2013-09-10
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ①) were used in the production of this report:

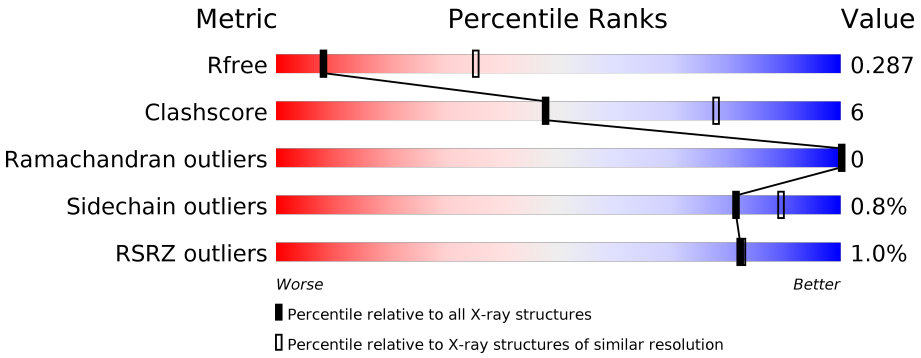
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	259	73% 16% 11%
1	C	259	77% 14% 9%
2	B	226	72% 15% 13%
2	D	226	77% 11% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6440 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 T-cell receptor gamma chain V region PT-gamma-1/2, Human nkt tcr beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1751	1118	301	326	6			
1	C	236	Total	C	N	O	S	0	0	0
			1803	1147	308	342	6			

- Molecule 2 is a protein called Human nkt tcr alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	197	Total	C	N	O	S	0	0	0
			1449	927	243	270	9			
2	D	199	Total	C	N	O	S	0	0	0
			1437	917	240	271	9			

There are 262 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ALA	-	expression tag	UNP Q6PJ56
B	-1	ASP	-	expression tag	UNP Q6PJ56
B	0	PRO	-	expression tag	UNP Q6PJ56
B	96	PRO	SER	conflict	UNP Q6PJ56
B	97	SER	PHE	conflict	UNP Q6PJ56
B	98	TYR	LEU	conflict	UNP Q6PJ56
B	99	TRP	PRO	conflict	UNP Q6PJ56
B	100	GLY	PHE	conflict	UNP Q6PJ56
B	101	PHE	ARG	conflict	UNP Q6PJ56
B	102	PRO	GLY	conflict	UNP Q6PJ56
B	103	ARG	ASN	conflict	UNP Q6PJ56
B	104	THR	PHE	conflict	UNP Q6PJ56
B	105	THR	HIS	conflict	UNP Q6PJ56
B	106	ARG	TYR	conflict	UNP Q6PJ56
B	107	VAL	-	linker	UNP Q6PJ56
B	108	ILE	-	linker	UNP Q6PJ56

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Chain	Residue	Modelled	Actual	Comment	Reference
B	109	PHE	-	linker	UNP Q6PJ56
B	110	GLY	-	linker	UNP Q6PJ56
B	111	LYS	-	linker	UNP Q6PJ56
B	112	GLY	-	expression tag	UNP Q6PJ56
B	113	THR	-	expression tag	UNP Q6PJ56
B	114	ARG	-	expression tag	UNP Q6PJ56
B	115	VAL	-	expression tag	UNP Q6PJ56
B	116	THR	-	expression tag	UNP Q6PJ56
B	117	VAL	-	expression tag	UNP Q6PJ56
B	118	GLU	-	expression tag	UNP Q6PJ56
B	119	PRO	-	expression tag	UNP Q6PJ56
B	120	ASN	-	expression tag	UNP Q6PJ56
B	121	ILE	-	expression tag	UNP Q6PJ56
B	122	GLN	-	expression tag	UNP Q6PJ56
B	123	ASN	-	expression tag	UNP Q6PJ56
B	124	PRO	-	expression tag	UNP Q6PJ56
B	125	ASP	-	expression tag	UNP Q6PJ56
B	126	PRO	-	expression tag	UNP Q6PJ56
B	127	ALA	-	expression tag	UNP Q6PJ56
B	128	VAL	-	expression tag	UNP Q6PJ56
B	129	TYR	-	expression tag	UNP Q6PJ56
B	130	GLN	-	expression tag	UNP Q6PJ56
B	131	LEU	-	expression tag	UNP Q6PJ56
B	132	ARG	-	expression tag	UNP Q6PJ56
B	133	ASP	-	expression tag	UNP Q6PJ56
B	134	SER	-	expression tag	UNP Q6PJ56
B	135	LYS	-	expression tag	UNP Q6PJ56
B	136	SER	-	expression tag	UNP Q6PJ56
B	137	SER	-	expression tag	UNP Q6PJ56
B	138	ASP	-	expression tag	UNP Q6PJ56
B	139	LYS	-	expression tag	UNP Q6PJ56
B	140	SER	-	expression tag	UNP Q6PJ56
B	141	VAL	-	expression tag	UNP Q6PJ56
B	142	CYS	-	expression tag	UNP Q6PJ56
B	143	LEU	-	expression tag	UNP Q6PJ56
B	144	PHE	-	expression tag	UNP Q6PJ56
B	145	THR	-	expression tag	UNP Q6PJ56
B	146	ASP	-	expression tag	UNP Q6PJ56
B	147	PHE	-	expression tag	UNP Q6PJ56
B	148	ASP	-	expression tag	UNP Q6PJ56
B	149	SER	-	expression tag	UNP Q6PJ56
B	150	GLN	-	expression tag	UNP Q6PJ56

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Chain	Residue	Modelled	Actual	Comment	Reference
B	151	THR	-	expression tag	UNP Q6PJ56
B	152	ASN	-	expression tag	UNP Q6PJ56
B	153	VAL	-	expression tag	UNP Q6PJ56
B	154	SER	-	expression tag	UNP Q6PJ56
B	155	GLN	-	expression tag	UNP Q6PJ56
B	156	SER	-	expression tag	UNP Q6PJ56
B	157	LYS	-	expression tag	UNP Q6PJ56
B	158	ASP	-	expression tag	UNP Q6PJ56
B	159	SER	-	expression tag	UNP Q6PJ56
B	160	ASP	-	expression tag	UNP Q6PJ56
B	161	VAL	-	expression tag	UNP Q6PJ56
B	162	TYR	-	expression tag	UNP Q6PJ56
B	163	ILE	-	expression tag	UNP Q6PJ56
B	164	THR	-	expression tag	UNP Q6PJ56
B	165	ASP	-	expression tag	UNP Q6PJ56
B	166	LYS	-	expression tag	UNP Q6PJ56
B	167	CYS	-	expression tag	UNP Q6PJ56
B	168	VAL	-	expression tag	UNP Q6PJ56
B	169	LEU	-	expression tag	UNP Q6PJ56
B	170	ASP	-	expression tag	UNP Q6PJ56
B	171	MET	-	expression tag	UNP Q6PJ56
B	172	ARG	-	expression tag	UNP Q6PJ56
B	173	SER	-	expression tag	UNP Q6PJ56
B	174	MET	-	expression tag	UNP Q6PJ56
B	175	ASP	-	expression tag	UNP Q6PJ56
B	176	PHE	-	expression tag	UNP Q6PJ56
B	177	LYS	-	expression tag	UNP Q6PJ56
B	178	SER	-	expression tag	UNP Q6PJ56
B	179	ASN	-	expression tag	UNP Q6PJ56
B	180	SER	-	expression tag	UNP Q6PJ56
B	181	ALA	-	expression tag	UNP Q6PJ56
B	182	VAL	-	expression tag	UNP Q6PJ56
B	183	ALA	-	expression tag	UNP Q6PJ56
B	184	TRP	-	expression tag	UNP Q6PJ56
B	185	SER	-	expression tag	UNP Q6PJ56
B	186	ASN	-	expression tag	UNP Q6PJ56
B	187	LYS	-	expression tag	UNP Q6PJ56
B	188	SER	-	expression tag	UNP Q6PJ56
B	189	ASP	-	expression tag	UNP Q6PJ56
B	190	PHE	-	expression tag	UNP Q6PJ56
B	191	ALA	-	expression tag	UNP Q6PJ56
B	192	CYS	-	expression tag	UNP Q6PJ56

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Chain	Residue	Modelled	Actual	Comment	Reference
B	193	ALA	-	expression tag	UNP Q6PJ56
B	194	ASN	-	expression tag	UNP Q6PJ56
B	195	ALA	-	expression tag	UNP Q6PJ56
B	196	PHE	-	expression tag	UNP Q6PJ56
B	197	ASN	-	expression tag	UNP Q6PJ56
B	198	ASN	-	expression tag	UNP Q6PJ56
B	199	SER	-	expression tag	UNP Q6PJ56
B	200	ILE	-	expression tag	UNP Q6PJ56
B	201	ILE	-	expression tag	UNP Q6PJ56
B	202	PRO	-	expression tag	UNP Q6PJ56
B	203	GLU	-	expression tag	UNP Q6PJ56
B	204	ASP	-	expression tag	UNP Q6PJ56
B	205	THR	-	expression tag	UNP Q6PJ56
B	206	PHE	-	expression tag	UNP Q6PJ56
B	207	PHE	-	expression tag	UNP Q6PJ56
B	208	PRO	-	expression tag	UNP Q6PJ56
B	209	SER	-	expression tag	UNP Q6PJ56
B	210	PRO	-	expression tag	UNP Q6PJ56
B	211	GLU	-	expression tag	UNP Q6PJ56
B	212	SER	-	expression tag	UNP Q6PJ56
B	213	SER	-	expression tag	UNP Q6PJ56
B	214	SER	-	expression tag	UNP Q6PJ56
B	215	ARG	-	expression tag	UNP Q6PJ56
B	216	GLY	-	expression tag	UNP Q6PJ56
B	217	GLY	-	expression tag	UNP Q6PJ56
B	218	LEU	-	expression tag	UNP Q6PJ56
B	219	GLU	-	expression tag	UNP Q6PJ56
B	220	VAL	-	expression tag	UNP Q6PJ56
B	221	LEU	-	expression tag	UNP Q6PJ56
B	222	PHE	-	expression tag	UNP Q6PJ56
B	223	GLN	-	expression tag	UNP Q6PJ56
D	-2	ALA	-	expression tag	UNP Q6PJ56
D	-1	ASP	-	expression tag	UNP Q6PJ56
D	0	PRO	-	expression tag	UNP Q6PJ56
D	96	PRO	SER	conflict	UNP Q6PJ56
D	97	SER	PHE	conflict	UNP Q6PJ56
D	98	TYR	LEU	conflict	UNP Q6PJ56
D	99	TRP	PRO	conflict	UNP Q6PJ56
D	100	GLY	PHE	conflict	UNP Q6PJ56
D	101	PHE	ARG	conflict	UNP Q6PJ56
D	102	PRO	GLY	conflict	UNP Q6PJ56
D	103	ARG	ASN	conflict	UNP Q6PJ56

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Chain	Residue	Modelled	Actual	Comment	Reference
D	104	THR	PHE	conflict	UNP Q6PJ56
D	105	THR	HIS	conflict	UNP Q6PJ56
D	106	ARG	TYR	conflict	UNP Q6PJ56
D	107	VAL	-	linker	UNP Q6PJ56
D	108	ILE	-	linker	UNP Q6PJ56
D	109	PHE	-	linker	UNP Q6PJ56
D	110	GLY	-	linker	UNP Q6PJ56
D	111	LYS	-	linker	UNP Q6PJ56
D	112	GLY	-	expression tag	UNP Q6PJ56
D	113	THR	-	expression tag	UNP Q6PJ56
D	114	ARG	-	expression tag	UNP Q6PJ56
D	115	VAL	-	expression tag	UNP Q6PJ56
D	116	THR	-	expression tag	UNP Q6PJ56
D	117	VAL	-	expression tag	UNP Q6PJ56
D	118	GLU	-	expression tag	UNP Q6PJ56
D	119	PRO	-	expression tag	UNP Q6PJ56
D	120	ASN	-	expression tag	UNP Q6PJ56
D	121	ILE	-	expression tag	UNP Q6PJ56
D	122	GLN	-	expression tag	UNP Q6PJ56
D	123	ASN	-	expression tag	UNP Q6PJ56
D	124	PRO	-	expression tag	UNP Q6PJ56
D	125	ASP	-	expression tag	UNP Q6PJ56
D	126	PRO	-	expression tag	UNP Q6PJ56
D	127	ALA	-	expression tag	UNP Q6PJ56
D	128	VAL	-	expression tag	UNP Q6PJ56
D	129	TYR	-	expression tag	UNP Q6PJ56
D	130	GLN	-	expression tag	UNP Q6PJ56
D	131	LEU	-	expression tag	UNP Q6PJ56
D	132	ARG	-	expression tag	UNP Q6PJ56
D	133	ASP	-	expression tag	UNP Q6PJ56
D	134	SER	-	expression tag	UNP Q6PJ56
D	135	LYS	-	expression tag	UNP Q6PJ56
D	136	SER	-	expression tag	UNP Q6PJ56
D	137	SER	-	expression tag	UNP Q6PJ56
D	138	ASP	-	expression tag	UNP Q6PJ56
D	139	LYS	-	expression tag	UNP Q6PJ56
D	140	SER	-	expression tag	UNP Q6PJ56
D	141	VAL	-	expression tag	UNP Q6PJ56
D	142	CYS	-	expression tag	UNP Q6PJ56
D	143	LEU	-	expression tag	UNP Q6PJ56
D	144	PHE	-	expression tag	UNP Q6PJ56
D	145	THR	-	expression tag	UNP Q6PJ56

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Chain	Residue	Modelled	Actual	Comment	Reference
D	146	ASP	-	expression tag	UNP Q6PJ56
D	147	PHE	-	expression tag	UNP Q6PJ56
D	148	ASP	-	expression tag	UNP Q6PJ56
D	149	SER	-	expression tag	UNP Q6PJ56
D	150	GLN	-	expression tag	UNP Q6PJ56
D	151	THR	-	expression tag	UNP Q6PJ56
D	152	ASN	-	expression tag	UNP Q6PJ56
D	153	VAL	-	expression tag	UNP Q6PJ56
D	154	SER	-	expression tag	UNP Q6PJ56
D	155	GLN	-	expression tag	UNP Q6PJ56
D	156	SER	-	expression tag	UNP Q6PJ56
D	157	LYS	-	expression tag	UNP Q6PJ56
D	158	ASP	-	expression tag	UNP Q6PJ56
D	159	SER	-	expression tag	UNP Q6PJ56
D	160	ASP	-	expression tag	UNP Q6PJ56
D	161	VAL	-	expression tag	UNP Q6PJ56
D	162	TYR	-	expression tag	UNP Q6PJ56
D	163	ILE	-	expression tag	UNP Q6PJ56
D	164	THR	-	expression tag	UNP Q6PJ56
D	165	ASP	-	expression tag	UNP Q6PJ56
D	166	LYS	-	expression tag	UNP Q6PJ56
D	167	CYS	-	expression tag	UNP Q6PJ56
D	168	VAL	-	expression tag	UNP Q6PJ56
D	169	LEU	-	expression tag	UNP Q6PJ56
D	170	ASP	-	expression tag	UNP Q6PJ56
D	171	MET	-	expression tag	UNP Q6PJ56
D	172	ARG	-	expression tag	UNP Q6PJ56
D	173	SER	-	expression tag	UNP Q6PJ56
D	174	MET	-	expression tag	UNP Q6PJ56
D	175	ASP	-	expression tag	UNP Q6PJ56
D	176	PHE	-	expression tag	UNP Q6PJ56
D	177	LYS	-	expression tag	UNP Q6PJ56
D	178	SER	-	expression tag	UNP Q6PJ56
D	179	ASN	-	expression tag	UNP Q6PJ56
D	180	SER	-	expression tag	UNP Q6PJ56
D	181	ALA	-	expression tag	UNP Q6PJ56
D	182	VAL	-	expression tag	UNP Q6PJ56
D	183	ALA	-	expression tag	UNP Q6PJ56
D	184	TRP	-	expression tag	UNP Q6PJ56
D	185	SER	-	expression tag	UNP Q6PJ56
D	186	ASN	-	expression tag	UNP Q6PJ56
D	187	LYS	-	expression tag	UNP Q6PJ56

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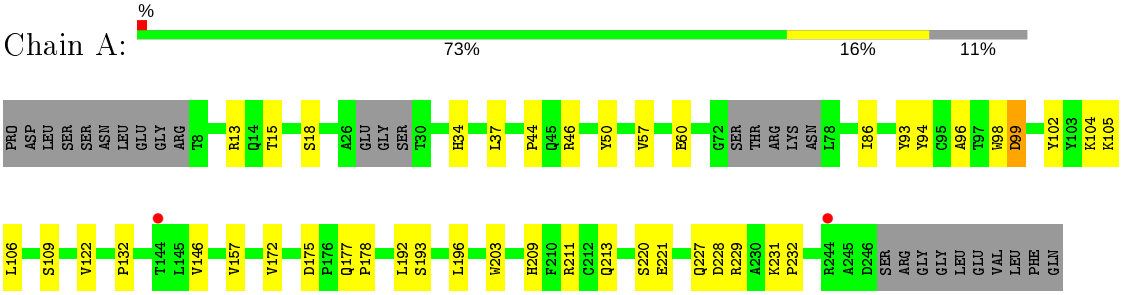
Chain	Residue	Modelled	Actual	Comment	Reference
D	188	SER	-	expression tag	UNP Q6PJ56
D	189	ASP	-	expression tag	UNP Q6PJ56
D	190	PHE	-	expression tag	UNP Q6PJ56
D	191	ALA	-	expression tag	UNP Q6PJ56
D	192	CYS	-	expression tag	UNP Q6PJ56
D	193	ALA	-	expression tag	UNP Q6PJ56
D	194	ASN	-	expression tag	UNP Q6PJ56
D	195	ALA	-	expression tag	UNP Q6PJ56
D	196	PHE	-	expression tag	UNP Q6PJ56
D	197	ASN	-	expression tag	UNP Q6PJ56
D	198	ASN	-	expression tag	UNP Q6PJ56
D	199	SER	-	expression tag	UNP Q6PJ56
D	200	ILE	-	expression tag	UNP Q6PJ56
D	201	ILE	-	expression tag	UNP Q6PJ56
D	202	PRO	-	expression tag	UNP Q6PJ56
D	203	GLU	-	expression tag	UNP Q6PJ56
D	204	ASP	-	expression tag	UNP Q6PJ56
D	205	THR	-	expression tag	UNP Q6PJ56
D	206	PHE	-	expression tag	UNP Q6PJ56
D	207	PHE	-	expression tag	UNP Q6PJ56
D	208	PRO	-	expression tag	UNP Q6PJ56
D	209	SER	-	expression tag	UNP Q6PJ56
D	210	PRO	-	expression tag	UNP Q6PJ56
D	211	GLU	-	expression tag	UNP Q6PJ56
D	212	SER	-	expression tag	UNP Q6PJ56
D	213	SER	-	expression tag	UNP Q6PJ56
D	214	SER	-	expression tag	UNP Q6PJ56
D	215	ARG	-	expression tag	UNP Q6PJ56
D	216	GLY	-	expression tag	UNP Q6PJ56
D	217	GLY	-	expression tag	UNP Q6PJ56
D	218	LEU	-	expression tag	UNP Q6PJ56
D	219	GLU	-	expression tag	UNP Q6PJ56
D	220	VAL	-	expression tag	UNP Q6PJ56
D	221	LEU	-	expression tag	UNP Q6PJ56
D	222	PHE	-	expression tag	UNP Q6PJ56
D	223	GLN	-	expression tag	UNP Q6PJ56

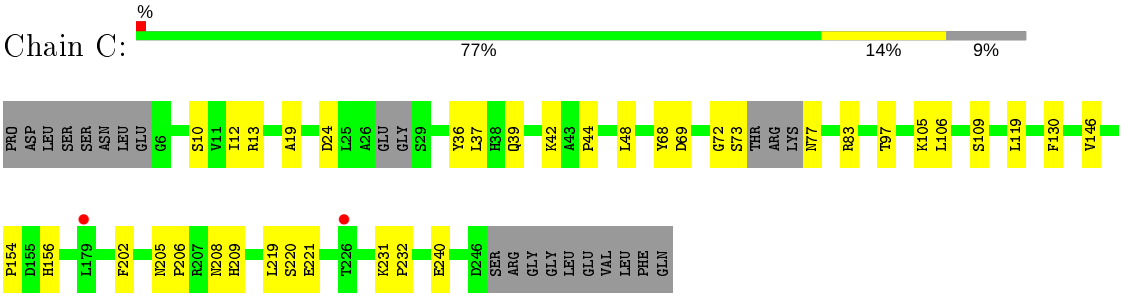
3 Residue-property plots (i)

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.

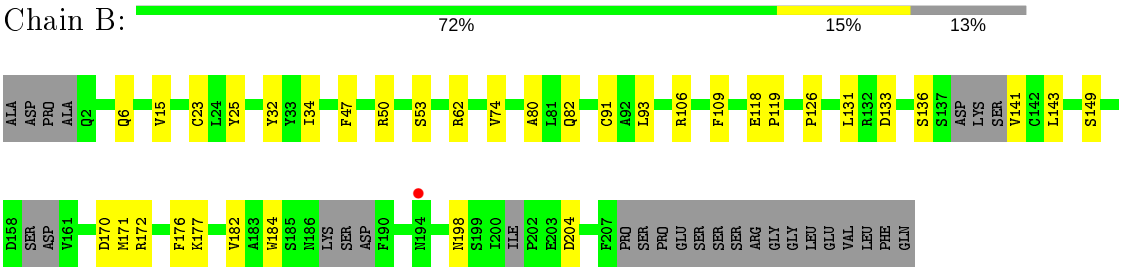
• Molecule 1: T-cell receptor gamma chain V region PT-gamma-1/2, Human nkt tcr beta chain



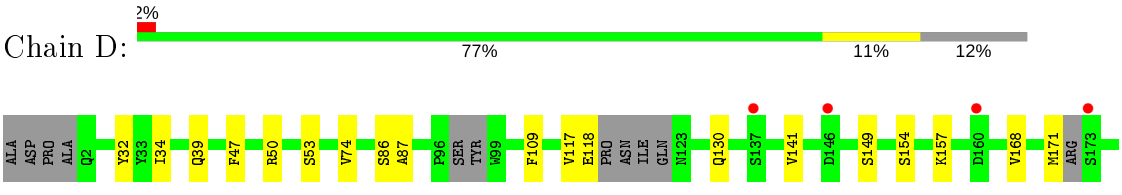
• Molecule 1: T-cell receptor gamma chain V region PT-gamma-1/2, Human nkt tcr beta chain

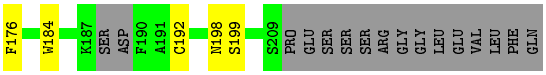


• Molecule 2: Human nkt tcr alpha chain



• Molecule 2: Human nkt tcr alpha chain




F176
W184
K187
SER
ASP
F190
A191
C192
N198
S199
S209
PRO
GLU
SER
SER
SER
ARG
GLY
GLY
LEU
GLU
VAL
LEU
PHE
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.26Å 60.84Å 99.09Å 90.00° 113.33° 90.00°	Depositor
Resolution (Å)	49.41 – 3.30 49.41 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.41-3.30) 99.1 (49.41-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.231 , 0.285 0.233 , 0.287	Depositor DCC
R_{free} test set	758 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	72.1	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6440	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0/1799	0.40	0/2462
1	C	0.21	0/1851	0.39	0/2531
2	B	0.22	0/1480	0.40	0/2012
2	D	0.22	0/1467	0.38	0/2000
All	All	0.21	0/6597	0.39	0/9005

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	1751	0	1585	25	0
1	C	1803	0	1629	20	0
2	B	1449	0	1317	22	0
2	D	1437	0	1241	12	0
All	All	6440	0	5772	75	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 6.

All (75) 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)
2:B:32:TYR:H	2:B:53:SER:HB3	1.56	0.71
2:B:170:ASP:OD1	2:B:177:LYS:NZ	2.24	0.70
1:A:104:LYS:HE3	1:A:106:LEU:HD21	1.73	0.69
2:D:32:TYR:H	2:D:53:SER:HB2	1.58	0.67
2:B:141:VAL:HG23	2:B:184:TRP:HB3	1.76	0.67
2:B:118:GLU:HB3	2:B:149:SER:HB3	1.76	0.67
1:A:211:ARG:NH1	1:A:213:GLN:OE1	2.29	0.65
2:D:34:ILE:HG21	2:D:74:VAL:HG21	1.84	0.59
1:A:122:VAL:O	1:A:229:ARG:NH2	2.34	0.59
2:B:34:ILE:HG21	2:B:74:VAL:HG11	1.85	0.58
1:C:36:TYR:OH	1:C:105:LYS:NZ	2.33	0.57
1:A:46:ARG:CZ	2:B:106:ARG:HG2	2.35	0.56
2:D:171:MET:HG3	2:D:176:PHE:HB3	1.88	0.56
1:A:13:ARG:NH1	1:A:18:SER:O	2.39	0.56
2:B:15:VAL:HG13	2:B:82:GLN:HA	1.89	0.55
1:A:94:TYR:HA	1:A:109:SER:HB2	1.89	0.55
1:C:12:ILE:HG12	1:C:154:PRO:HG3	1.89	0.55
2:D:130:GLN:NE2	2:D:192:CYS:SG	2.80	0.54
1:A:34:HIS:HB2	1:A:96:ALA:HB3	1.89	0.54
1:C:10:SER:OG	1:C:156:HIS:ND1	2.36	0.54
1:A:175:ASP:OD2	1:A:193:SER:OG	2.24	0.53
1:A:99:ASP:HB2	1:A:102:TYR:O	2.09	0.53
1:C:24:ASP:HB2	1:C:109:SER:HB3	1.91	0.53
2:B:143:LEU:HB3	2:B:182:VAL:HG12	1.91	0.52
1:C:69:ASP:HB2	1:C:83:ARG:HH12	1.74	0.52
1:A:227:GLN:HG2	1:A:228:ASP:H	1.73	0.52
1:A:50:TYR:HD1	1:A:57:VAL:HG22	1.75	0.50
2:D:47:PHE:HZ	2:D:50:ARG:HB2	1.75	0.50
1:C:209:HIS:NE2	1:C:240:GLU:OE1	2.45	0.49
1:A:172:VAL:HG12	1:A:196:LEU:HD12	1.95	0.49
1:C:13:ARG:HG3	1:C:19:ALA:HB2	1.95	0.49
2:B:47:PHE:HZ	2:B:50:ARG:HB2	1.78	0.48
2:D:141:VAL:HG12	2:D:184:TRP:HB3	1.95	0.48
2:D:154:SER:H	2:D:199:SER:HB2	1.79	0.47
2:B:198:ASN:OD1	2:B:198:ASN:N	2.48	0.47
1:C:73:SER:N	1:C:77:ASN:O	2.48	0.46
1:A:98:TRP:CE2	1:A:105:LYS:HD3	2.50	0.46
1:A:132:PRO:HD2	1:A:203:TRP:CZ2	2.51	0.46
2:B:133:ASP:HB3	2:B:136:SER:O	2.16	0.46
2:B:25:TYR:HB2	2:B:93:LEU:HD22	1.97	0.46
1:A:229:ARG:HH12	1:A:232:PRO:HG3	1.80	0.46
1:A:44:PRO:HD2	2:B:109:PHE:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:GLN:NE2	2:B:91:CYS:H	2.15	0.45
1:C:48:LEU:HD21	1:C:68:TYR:HB2	1.99	0.45
1:C:205:ASN:HA	1:C:206:PRO:HD3	1.82	0.45
1:C:219:LEU:HD12	1:C:219:LEU:H	1.82	0.45
1:C:37:LEU:HD21	1:C:39:GLN:HE21	1.79	0.45
1:A:15:THR:HG23	1:A:86:ILE:HA	1.99	0.45
1:C:130:PHE:HB2	1:C:146:VAL:HG23	1.98	0.45
2:B:119:PRO:O	2:B:149:SER:OG	2.30	0.45
1:C:231:LYS:HA	1:C:232:PRO:HD3	1.88	0.45
2:B:126:PRO:HG2	2:B:204:ASP:O	2.17	0.44
1:A:46:ARG:NH2	1:A:60:GLU:OE2	2.44	0.44
2:B:171:MET:HG3	2:B:176:PHE:HB3	2.00	0.44
1:A:231:LYS:HA	1:A:232:PRO:HD3	1.84	0.44
2:D:118:GLU:HG2	2:D:149:SER:HB3	2.00	0.43
1:A:146:VAL:HG12	2:B:131:LEU:HD12	2.01	0.43
1:C:39:GLN:HB2	1:C:42:LYS:HE3	2.00	0.43
1:C:44:PRO:HG2	2:D:109:PHE:CG	2.53	0.43
2:D:86:SER:OG	2:D:117:VAL:HG22	2.19	0.43
1:A:209:HIS:CE1	1:A:211:ARG:HB2	2.54	0.43
1:C:202:PHE:O	1:C:208:ASN:ND2	2.49	0.42
1:A:220:SER:OG	1:A:221:GLU:N	2.52	0.42
2:B:62:ARG:NH1	2:B:80:ALA:O	2.52	0.42
1:A:37:LEU:HD12	1:A:93:TYR:CE1	2.54	0.42
1:C:97:THR:O	1:C:106:LEU:N	2.48	0.42
1:A:177:GLN:HA	1:A:178:PRO:HD2	1.87	0.41
2:B:23:CYS:HB3	2:B:74:VAL:O	2.21	0.41
2:B:34:ILE:HG21	2:B:74:VAL:HG21	2.03	0.41
1:A:96:ALA:HB1	1:A:105:LYS:HE2	2.02	0.41
2:B:172:ARG:HA	2:B:172:ARG:HD3	1.84	0.40
1:C:220:SER:OG	1:C:221:GLU:N	2.53	0.40
2:D:157:LYS:H	2:D:198:ASN:ND2	2.19	0.40
2:D:39:GLN:O	2:D:87:ALA:HB1	2.22	0.40
1:C:72:GLY:HA2	1:C:73:SER:HA	1.91	0.40

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	225/259 (87%)	219 (97%)	6 (3%)	0	100	100
1	C	230/259 (89%)	226 (98%)	4 (2%)	0	100	100
2	B	187/226 (83%)	181 (97%)	6 (3%)	0	100	100
2	D	189/226 (84%)	187 (99%)	2 (1%)	0	100	100
All	All	831/970 (86%)	813 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	171/226 (76%)	168 (98%)	3 (2%)	59	78
1	C	178/226 (79%)	177 (99%)	1 (1%)	86	91
2	B	141/201 (70%)	141 (100%)	0	100	100
2	D	132/201 (66%)	131 (99%)	1 (1%)	81	89
All	All	622/854 (73%)	617 (99%)	5 (1%)	81	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ASP
1	A	157	VAL

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Mol	Chain	Res	Type
1	A	192	LEU
1	C	119	LEU
2	D	168	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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, 95^{th} 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	231/259 (89%)	-0.05	2 (0%)	84	84	50, 74, 118, 148	0
1	C	236/259 (91%)	0.06	2 (0%)	86	86	49, 71, 103, 124	0
2	B	197/226 (87%)	-0.01	1 (0%)	91	91	50, 80, 127, 147	0
2	D	199/226 (88%)	0.12	4 (2%)	65	64	53, 88, 128, 144	0
All	All	863/970 (88%)	0.03	9 (1%)	82	82	49, 78, 121, 148	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	137	SER	4.1
2	D	173	SER	3.8
1	A	144	THR	3.2
1	C	226	THR	2.6
2	D	160	ASP	2.3
2	B	194	ASN	2.3
2	D	146	ASP	2.1
1	A	244	ARG	2.1
1	C	179	LEU	2.1

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.