wwPDB X-ray Structure Validation Summary Report (i)

May 25, 2020 – 06:28 am BST

PDB ID	:	3MV7
Title	:	Crystal Structure of the TK3 TCR in complex with HLA-B*3501/HPVG
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Deposited on	:	2010-05-03
Resolution	:	2.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

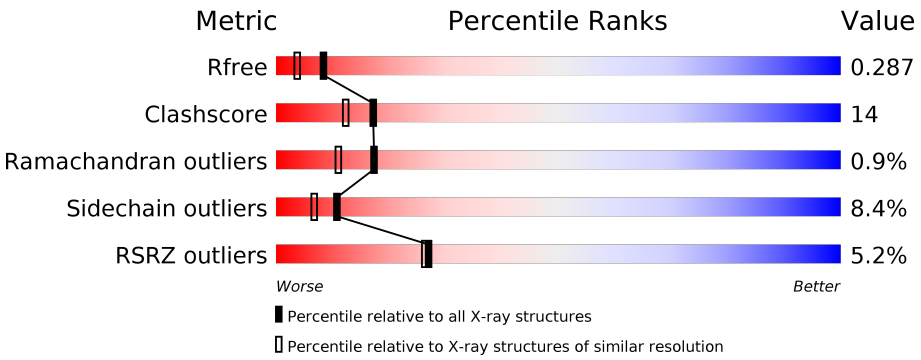
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	276	9%, 76%, 19%, 5%
2	B	99	4%, 72%, 24%, •
3	C	11	100%
4	D	200	4%, 73%, 21%, 7%
5	E	241	2%, 75%, 21%, •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7407 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, B-35 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2370	1471	436	455	8	0	13	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	870	551	146	170	3	0	5	0

- Molecule 3 is a protein called HPVG peptide from Epstein-Barr nuclear antigen 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	11	95	62	13	20	0	0	0

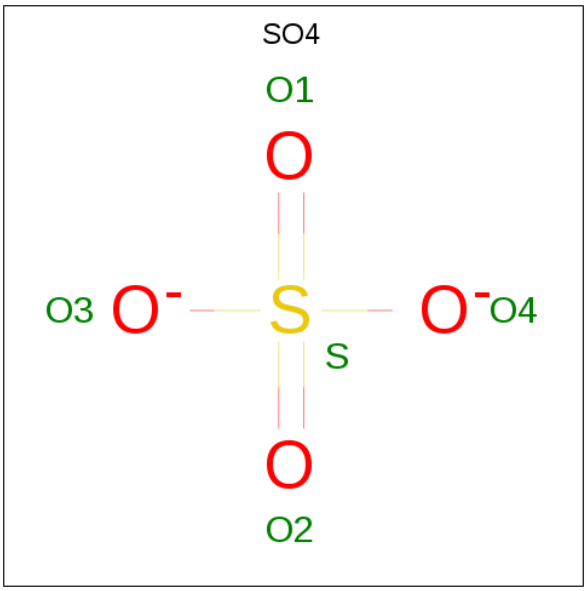
- Molecule 4 is a protein called alpha chain of the TK3 TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	200	1709	1063	281	357	8	0	19	0

- Molecule 5 is a protein called beta chain of the TK3 TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	241	2061	1291	362	403	5	0	17	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

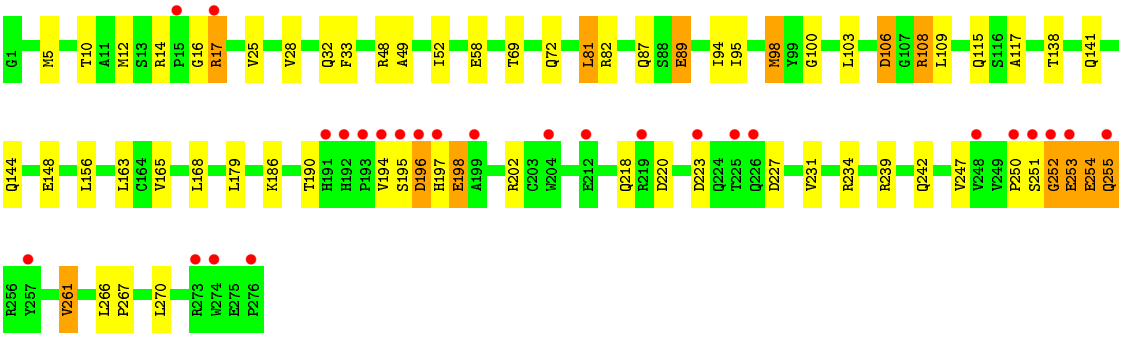
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	134	Total O 134 134	0	0
7	B	37	Total O 37 37	0	0
7	C	10	Total O 10 10	0	0
7	D	55	Total O 55 55	0	0
7	E	61	Total O 61 61	0	0

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.

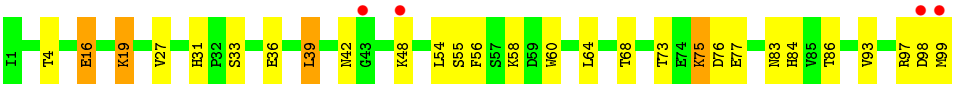
- Molecule 1: HLA class I histocompatibility antigen, B-35 alpha chain

Chain A:



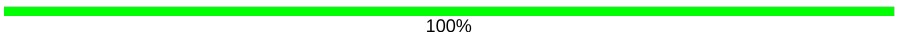
- Molecule 2: Beta-2-microglobulin

Chain B:



- Molecule 3: HPVG peptide from Epstein-Barr nuclear antigen 1

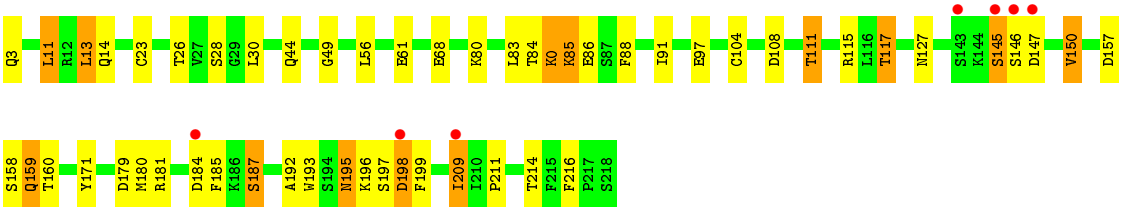
Chain C:



There are no outlier residues recorded for this chain.

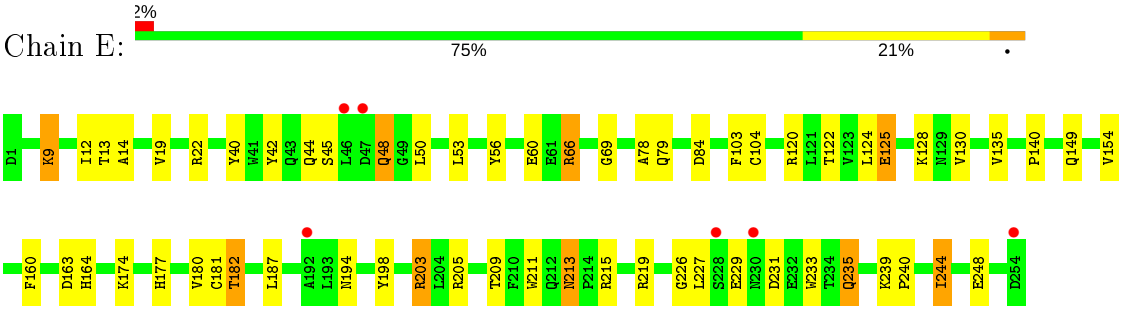
- Molecule 4: alpha chain of the TK3 TCR

Chain D:



• Molecule 5: beta chain of the TK3 TCR

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	44.86Å 62.24Å 92.56Å 94.64° 103.92° 109.31°	Depositor
Resolution (Å)	57.83 – 2.00 52.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (57.83-2.00) 97.1 (52.83-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.286 0.237 , 0.287	Depositor DCC
R_{free} test set	3014 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7407	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.47	0/2433	0.63	0/3304
2	B	0.42	0/893	0.55	0/1206
3	C	0.73	0/99	0.59	0/133
4	D	0.50	1/1743 (0.1%)	0.65	0/2360
5	E	0.49	0/2110	0.65	0/2865
All	All	0.48	1/7278 (0.0%)	0.63	0/9868

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	104	CYS	CB-SG	-5.17	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2370	0	2218	57	0
2	B	870	0	823	23	0
3	C	95	0	76	0	0
4	D	1709	0	1607	64	0
5	E	2061	0	1956	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	5	0	0	0	0
7	A	134	0	0	14	0
7	B	37	0	0	2	0
7	C	10	0	0	0	0
7	D	55	0	0	4	0
7	E	61	0	0	2	0
All	All	7407	0	6680	193	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 14.

The worst 5 of 193 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:D:0[B]:LYS:N	4:D:0[B]:LYS:HE2	1.52	1.24
4:D:84[A]:THR:CG2	4:D:0[A]:LYS:HD3	1.72	1.18
1:A:12[A]:MET:HG2	1:A:94[A]:ILE:HG22	1.17	1.16
5:E:163[A]:ASP:OD1	5:E:163[A]:ASP:O	1.64	1.15
1:A:25:VAL:HB	7:A:408:HOH:O	1.45	1.14

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	287/276 (104%)	269 (94%)	14 (5%)	4 (1%)	11 5
2	B	102/99 (103%)	98 (96%)	4 (4%)	0	100 100
3	C	9/11 (82%)	8 (89%)	1 (11%)	0	100 100
4	D	217/200 (108%)	208 (96%)	6 (3%)	3 (1%)	11 5
5	E	256/241 (106%)	246 (96%)	10 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	871/827 (105%)	829 (95%)	35 (4%)	7 (1%)	17 13

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	SER
1	A	196	ASP
1	A	220	ASP
4	D	184	ASP
4	D	198	ASP

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	247/234 (106%)	223 (90%)	24 (10%)	8 4
2	B	99/94 (105%)	91 (92%)	8 (8%)	11 7
3	C	9/9 (100%)	9 (100%)	0	100 100
4	D	197/178 (111%)	178 (90%)	19 (10%)	8 5
5	E	226/209 (108%)	203 (90%)	23 (10%)	7 4
All	All	778/724 (108%)	704 (90%)	74 (10%)	11 5

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	13	LEU
4	D	117	THR
5	E	213	ASN
4	D	30	LEU
4	D	0[B]	LYS

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

Mol	Chain	Res	Type
2	B	42	ASN
4	D	3	GLN
5	E	212	GLN
2	B	17	ASN
2	B	24	ASN

5.3.3 RNA (i)

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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SO4	E	255	-	4,4,4	0.16	0	6,6,6	0.06	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	276/276 (100%)	0.38	26 (9%) 8 8	12, 33, 108, 161	11 (3%)
2	B	99/99 (100%)	0.56	4 (4%) 38 37	24, 59, 86, 103	6 (6%)
3	C	11/11 (100%)	0.62	0 100 100	21, 33, 37, 38	0
4	D	200/200 (100%)	0.17	7 (3%) 44 43	16, 29, 76, 102	6 (3%)
5	E	241/241 (100%)	-0.08	6 (2%) 57 56	17, 31, 60, 97	8 (3%)
All	All	827/827 (100%)	0.22	43 (5%) 27 26	12, 33, 88, 161	31 (3%)

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	GLY	9.4
1	A	253	GLU	6.9
1	A	195	SER	5.7
1	A	197	HIS	5.6
1	A	225	THR	4.9

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	E	255	5/5	0.94	0.16	57,57,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.