



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 06:16 AM UTC

PDB ID : 1MI5 / pdb_00001mi5
Title : The crystal structure of LC13 TcR in complex with HLAB8-EBV peptide complex
Authors : Kjer-Nielsen, L.; Clements, C.S.; Purcell, A.W.; Brooks, A.G.; Whisstock, J.C.; Burrows, S.R.; McCluskey, J.; Rossjohn, J.
Deposited on : 2002-08-21
Resolution : 2.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

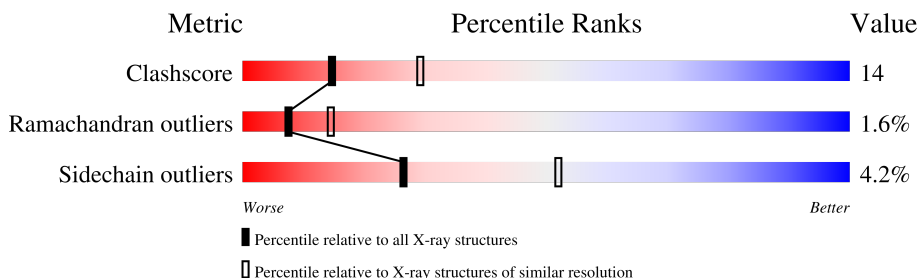
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 of 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	277	67% 28% 5%
2	B	99	64% 31% 5%
3	C	9	78% 22%
4	D	201	70% 27% .
5	E	241	74% 24% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6848 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 MHC heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2226	1377	406	436	7			

- Molecule 2 is a protein called beta 2 microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called Epstein Barr Virus peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			75	49	15	11			

- Molecule 4 is a protein called TcR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	201	Total	C	N	O	S	0	0	0
			1567	975	267	317	8			

- Molecule 5 is a protein called TcR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	241	Total	C	N	O	S	0	0	0
			1919	1209	335	371	4			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	71	Total	O	0	0
			71	71		

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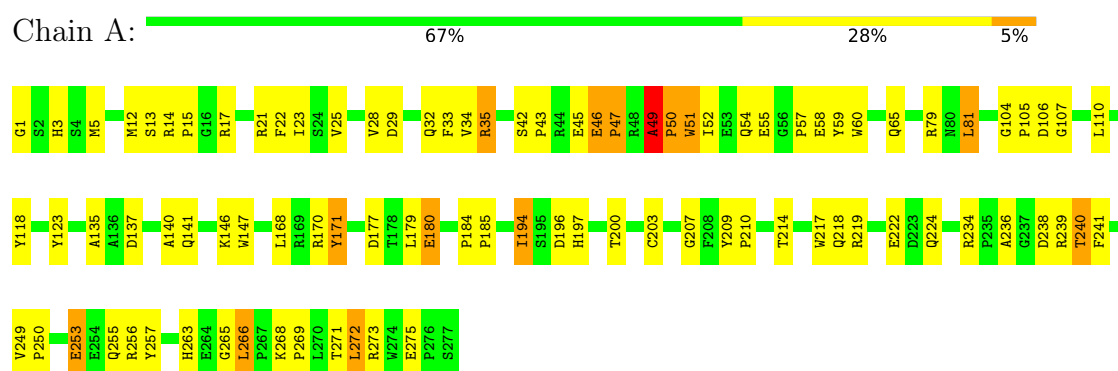
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	35	Total 35	O 35	0	0
6	C	4	Total 4	O 4	0	0
6	D	57	Total 57	O 57	0	0
6	E	65	Total 65	O 65	0	0

3 Residue-property plots [i](#)

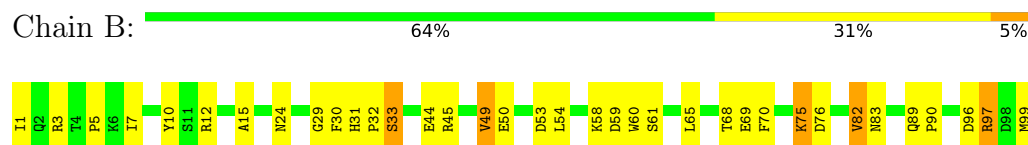
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

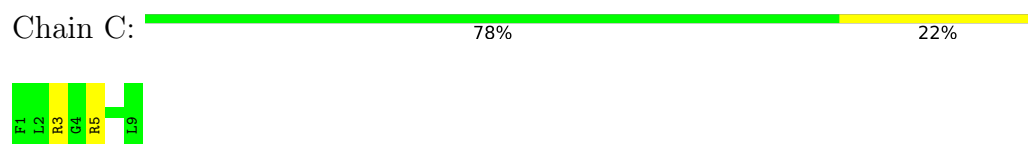
- Molecule 1: MHC heavy chain



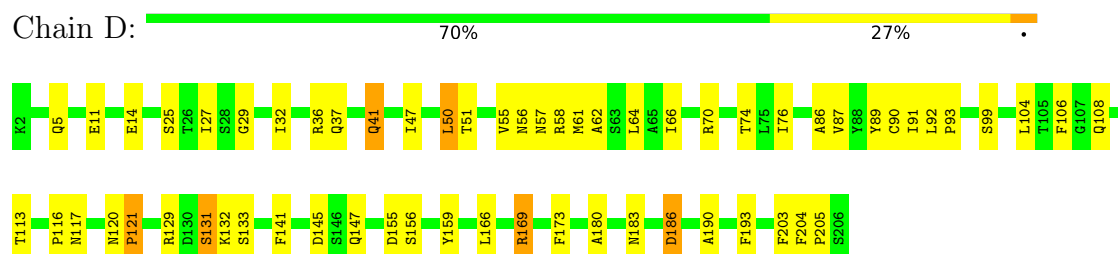
- Molecule 2: beta 2 microglobulin



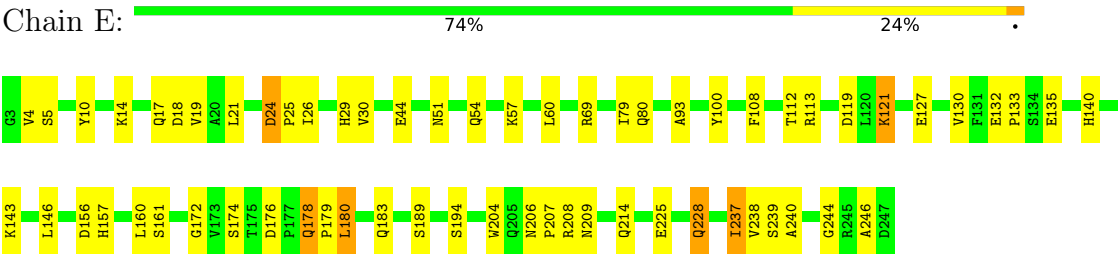
- Molecule 3: Epstein Barr Virus peptide



- Molecule 4: TcR alpha chain



● Molecule 5: TcR beta chain



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.49Å 105.90Å 144.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	92.9 (50.00-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.226 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6848	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/2286	0.97	12/3105 (0.4%)
2	B	0.42	0/852	0.89	3/1152 (0.3%)
3	C	0.39	0/76	0.90	0/98
4	D	0.42	0/1603	1.04	8/2181 (0.4%)
5	E	0.40	0/1971	0.94	11/2681 (0.4%)
All	All	0.42	0/6788	0.97	34/9217 (0.4%)

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	D	186	ASP	N-CA-C	-11.91	85.42	110.80
1	A	47	PRO	N-CA-C	-11.21	89.37	112.47
1	A	104	GLY	CA-C-N	9.01	129.19	119.28
1	A	104	GLY	C-N-CA	9.01	129.19	119.28
4	D	131	SER	N-CA-C	-7.40	104.49	113.97

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	2226	0	2046	85	0
2	B	829	0	794	24	0
3	C	75	0	79	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1567	0	1492	37	0
5	E	1919	0	1820	44	0
6	A	71	0	0	5	0
6	B	35	0	0	3	0
6	C	4	0	0	0	0
6	D	57	0	0	1	0
6	E	65	0	0	4	0
All	All	6848	0	6231	179	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 179 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:A:35:ARG:HH11	1:A:35:ARG:HB3	1.23	1.01
5:E:214:GLN:HG3	5:E:237:ILE:HD13	1.47	0.95
1:A:21:ARG:HE	1:A:23:ILE:HD11	1.33	0.94
2:B:75:LYS:HD3	2:B:75:LYS:H	1.43	0.83
5:E:30:VAL:HG22	5:E:51:ASN:HD21	1.44	0.83

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	275/277 (99%)	239 (87%)	29 (10%)	7 (2%)	4	7
2	B	97/99 (98%)	91 (94%)	5 (5%)	1 (1%)	12	24
3	C	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
4	D	199/201 (99%)	173 (87%)	22 (11%)	4 (2%)	6	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	239/241 (99%)	226 (95%)	12 (5%)	1 (0%)	30	49
All	All	817/827 (99%)	734 (90%)	70 (9%)	13 (2%)	7	14

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	SER
1	A	43	PRO
1	A	46	GLU
1	A	47	PRO
4	D	169	ARG

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	229/236 (97%)	214 (93%)	15 (7%)	15	32
2	B	94/94 (100%)	88 (94%)	6 (6%)	16	33
3	C	6/6 (100%)	5 (83%)	1 (17%)	2	4
4	D	180/180 (100%)	177 (98%)	3 (2%)	53	78
5	E	207/207 (100%)	202 (98%)	5 (2%)	43	70
All	All	716/723 (99%)	686 (96%)	30 (4%)	26	52

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	GLU
5	E	180	LEU
2	B	53	ASP
5	E	237	ILE
4	D	50	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	51	ASN
5	E	84	GLN
5	E	80	GLN
5	E	106	GLN
1	A	226	GLN

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 oligosaccharides 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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.