# wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:53 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 1MI5 |
| 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

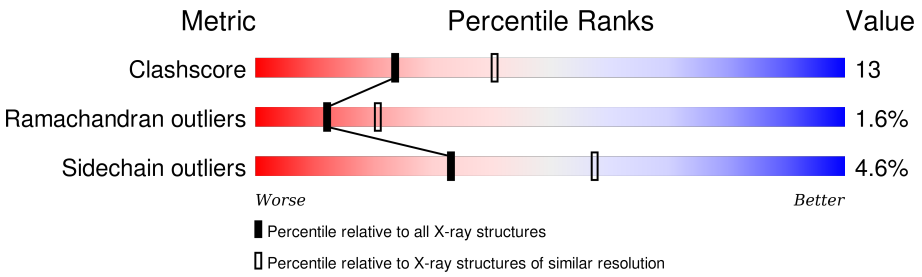
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | NOT EXECUTED |
| EDS | : | NOT EXECUTED |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 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 2.50 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 | 102246 | 4242 (2.50-2.50) |
| Ramachandran outliers | 100387 | 4156 (2.50-2.50) |
| Sidechain outliers | 100360 | 4158 (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 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 <=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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 277 | 69% 28% • |
| 2 | B | 99 | 67% 31% • |
| 3 | C | 9 | 89% 11% |
| 4 | D | 201 | 73% 25% • |
| 5 | E | 241 | 75% 23% • |

# 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 |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 277 | 2226 | 1377 | 406 | 436 | 7 | 0 | 0 | 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 | 829 | 528 | 140 | 158 | 3 | 0 | 0 | 0 |

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

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

- Molecule 4 is a protein called TcR alpha chain.

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

- Molecule 5 is a protein called TcR beta chain.

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

- Molecule 6 is water.

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

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

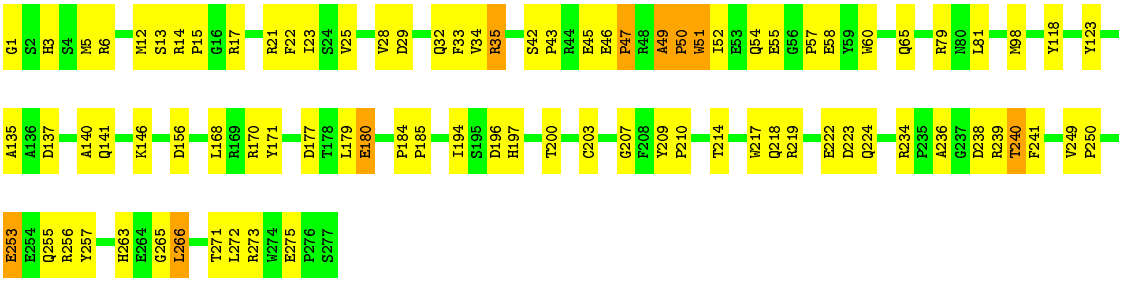
# 3 Residue-property plots (i)

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

Note EDS was not executed.

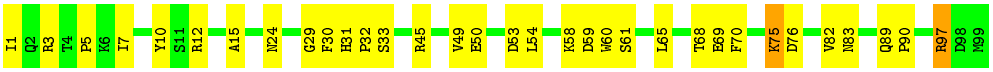
- Molecule 1: MHC heavy chain

Chain A:




- Molecule 2: beta 2 microglobulin

Chain B:

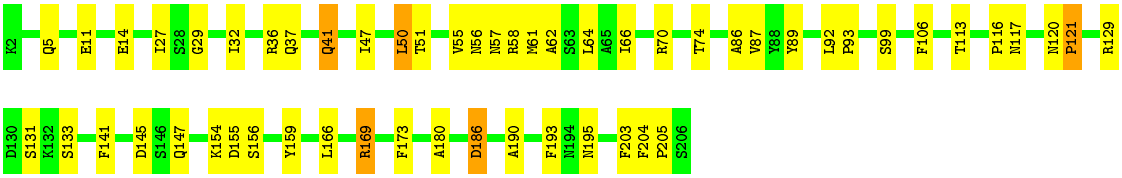



- Molecule 3: Epstein Barr Virus peptide

Chain C:

- Molecule 4: TcR alpha chain

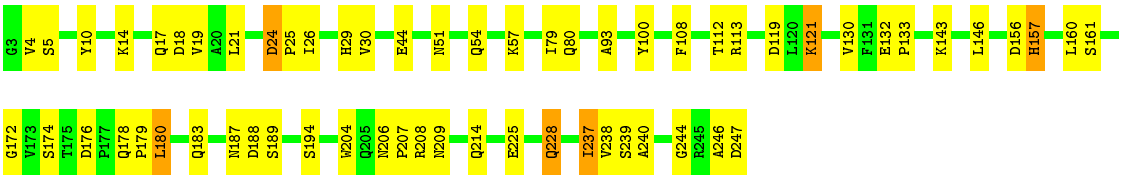
Chain D:




- Molecule 5: TcR beta chain

Chain E:

75%
23%


G3 V4 S5 Y10 K14 Q17 D18 V19 A20 L21 D24 P25 I26 H29 V30 E44 N51 Q54 K57 I79 Q80 A93 Y100 F108 T112 R113 D119 L120 K121 V130 F131 E132 P133 K143 L146 D156 H157 L160 S161
G172 V173 S174 T175 D176 P177 Q178 P179 L180 Q183 N187 D188 S189 S194 W204 Q205 N206 P207 R208 N209 Q214 E225 Q228 I237 V238 S239 A240 G244 R245 A246 D247

# 4 Data and refinement statistics (i)

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

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 56.49Å 105.90Å 144.50Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 2.50 | Depositor |
| % Data completeness<br>(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 | 0.36 | 0/2286 | 0.64 | 1/3105 (0.0%) |
| 2 | B | 0.36 | 0/852 | 0.61 | 0/1152 |
| 3 | C | 0.39 | 0/76 | 0.61 | 0/98 |
| 4 | D | 0.35 | 0/1603 | 0.70 | 2/2181 (0.1%) |
| 5 | E | 0.36 | 0/1971 | 0.60 | 0/2681 |
| All | All | 0.36 | 0/6788 | 0.64 | 3/9217 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | D | 186 | ASP | N-CA-C | -9.47 | 85.42 | 111.00 |
| 1 | A | 47 | PRO | N-CA-C | -8.74 | 89.37 | 112.10 |
| 4 | D | 169 | ARG | N-CA-C | 5.34 | 125.43 | 111.00 |

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 | 81 | 0 |
| 2 | B | 829 | 0 | 794 | 24 | 0 |
| 3 | C | 75 | 0 | 79 | 1 | 0 |
| 4 | D | 1567 | 0 | 1492 | 35 | 0 |
| 5 | E | 1919 | 0 | 1820 | 42 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 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 | 170 | 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 13.

The worst 5 of 170 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:H | 2:B:75:LYS:HD3 | 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%) | 7 10 |
| 2 | B | 97/99 (98%) | 91 (94%) | 5 (5%) | 1 (1%) | 19 34 |
| 3 | C | 7/9 (78%) | 5 (71%) | 2 (29%) | 0 | 100 100 |
| 4 | D | 199/201 (99%) | 173 (87%) | 22 (11%) | 4 (2%) | 9 15 |
| 5 | E | 239/241 (99%) | 226 (95%) | 12 (5%) | 1 (0%) | 39 61 |
| All | All | 817/827 (99%) | 734 (90%) | 70 (9%) | 13 (2%) | 12 21 |

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 (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 | 229/236 (97%) | 214 (93%) | 15 (7%) | 21 | 38 |
| 2 | B | 94/94 (100%) | 89 (95%) | 5 (5%) | 28 | 50 |
| 3 | C | 6/6 (100%) | 6 (100%) | 0 | 100 | 100 |
| 4 | D | 180/180 (100%) | 177 (98%) | 3 (2%) | 68 | 89 |
| 5 | E | 207/207 (100%) | 197 (95%) | 10 (5%) | 31 | 55 |
| All | All | 716/723 (99%) | 683 (95%) | 33 (5%) | 33 | 57 |

5 of 33 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 275 | GLU |
| 2 | B | 70 | PHE |
| 5 | E | 228 | GLN |
| 2 | B | 50 | GLU |
| 2 | B | 53 | ASP |

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

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | D | 41 | GLN |
| 5 | E | 29 | HIS |
| 5 | E | 122 | ASN |
| 2 | B | 2 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 83 | 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)

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 (i)

## 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section will therefore be empty.

## 6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

## 6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

## 6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.