



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 04:04 am 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

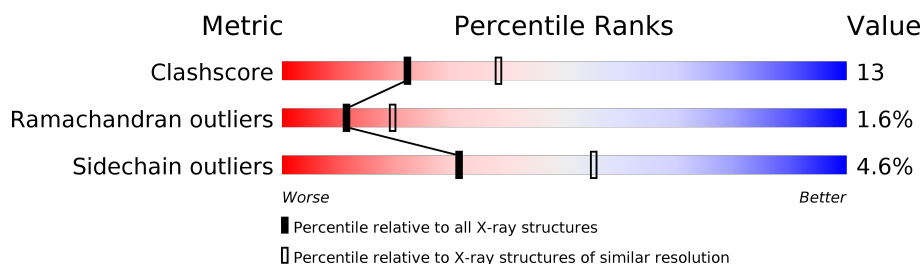
1 Overall quality at a glance

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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	277	
2	B	99	
3	C	9	
4	D	201	
5	E	241	

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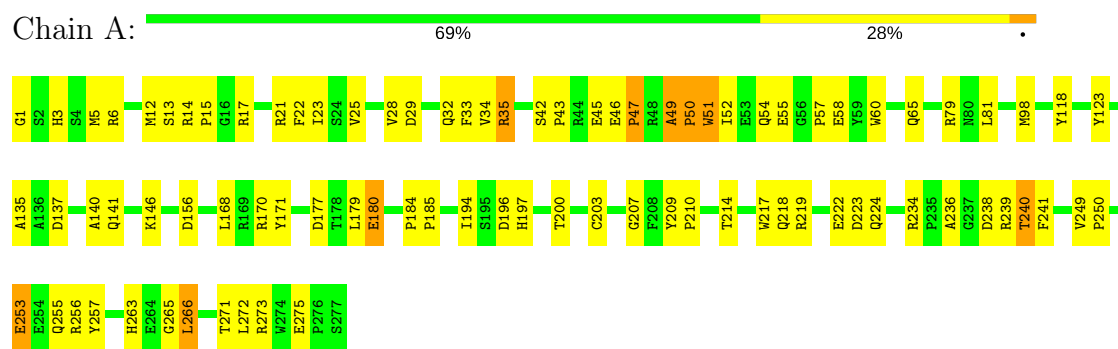
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	35	Total 35	O 35	0	0
6	C	4	Total 4	O 4	0	0
6	D	57	Total 57	O 57	0	0
6	E	65	Total 65	O 65	0	0

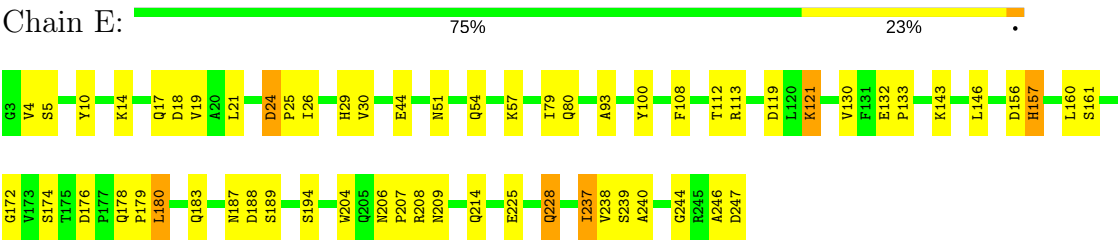
3 Residue-property plots

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.

Note EDS was not executed.

- Molecule 1: MHC heavy 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	0.36	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(°)	Ideal(°)
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%)	6	10
2	B	97/99 (98%)	91 (94%)	5 (5%)	1 (1%)	18	32
3	C	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
4	D	199/201 (99%)	173 (87%)	22 (11%)	4 (2%)	9	14
5	E	239/241 (99%)	226 (95%)	12 (5%)	1 (0%)	38	59
All	All	817/827 (99%)	734 (90%)	70 (9%)	13 (2%)	11	19

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%)	19	36
2	B	94/94 (100%)	89 (95%)	5 (5%)	26	48
3	C	6/6 (100%)	6 (100%)	0	100	100
4	D	180/180 (100%)	177 (98%)	3 (2%)	66	87
5	E	207/207 (100%)	197 (95%)	10 (5%)	30	53
All	All	716/723 (99%)	683 (95%)	33 (5%)	31	55

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

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.