



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 06:25 PM EDT

PDB ID : 3QEQ
Title : The complex between TCR DMF4 and human Class I MHC HLA-A2 with the bound MART-1(27-35) nonameric peptide
Authors : Borbulevych, O.Y.; Baker, B.M.
Deposited on : unknown
Resolution : 2.59 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

<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	:	FAILED
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

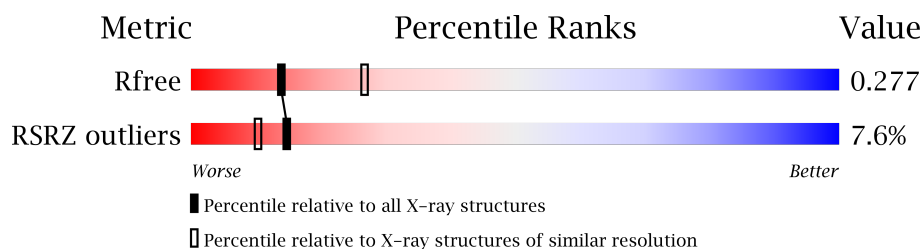
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	100719	2542 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6679 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, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	INITIATING METHIONINE	UNP P61769

- Molecule 3 is a protein called MART-1(27-35) peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			57	37	9	11			

- Molecule 4 is a protein called DMF4 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	194	Total	C	N	O	S	0	0	0
			1497	938	243	307	9			

- Molecule 5 is a protein called DMF4 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total	C	N	O	S	0	0	0
			1938	1213	340	379	6			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	39	Total 39	O 39	0	0
6	B	9	Total 9	O 9	0	0
6	C	1	Total 1	O 1	0	0
6	D	16	Total 16	O 16	0	0
6	E	38	Total 38	O 38	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.65Å 73.66Å 225.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.59 19.81 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.59) 99.1 (19.81-2.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.34 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.215 , 0.269 0.223 , 0.277	Depositor DCC
R_{free} test set	1591 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6679	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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, 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	275/275 (100%)	0.32	16 (5%) 24 18	27, 50, 99, 129	0
2	B	100/100 (100%)	0.48	7 (7%) 17 12	30, 56, 98, 111	0
3	C	9/9 (100%)	1.21	1 (11%) 6 3	34, 38, 44, 47	0
4	D	194/194 (100%)	0.88	26 (13%) 4 2	30, 73, 115, 139	0
5	E	243/243 (100%)	0.24	12 (4%) 30 24	27, 47, 78, 99	0
All	All	821/821 (100%)	0.46	62 (7%) 15 10	27, 52, 102, 139	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	56	SER	7.6
2	B	99	MET	6.7
4	D	2	GLN	6.3
5	E	243	ASP	6.2
4	D	127	ASP	4.9
4	D	126	SER	4.8
1	A	221	GLY	4.5
4	D	176	LYS	4.5
2	B	0	MET	4.4
5	E	1	ASP	4.0
3	C	4	ILE	4.0
1	A	220	ASP	4.0
4	D	57	ASN	3.8
1	A	1	GLY	3.8
1	A	226	GLN	3.8
1	A	224	GLN	3.7
4	D	177	SER	3.7
1	A	223	ASP	3.6
4	D	18	VAL	3.2
4	D	66	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	16	GLU	3.2
1	A	222	GLU	3.1
1	A	275	GLU	3.1
5	E	183	ASN	3.0
5	E	225	ASP	3.0
5	E	223	THR	3.0
5	E	117	ASN	2.9
1	A	225	THR	2.9
5	E	184	ASP	2.8
4	D	74	ASN	2.8
4	D	54	LEU	2.7
4	D	125	SER	2.7
4	D	77	ALA	2.7
2	B	75	LYS	2.7
4	D	145	SER	2.6
4	D	64	PHE	2.6
4	D	52	GLY	2.6
4	D	73	LEU	2.6
5	E	181	ALA	2.5
4	D	178	ASP	2.5
4	D	147	ASP	2.4
4	D	22	CYS	2.4
2	B	48	LYS	2.3
4	D	4	ASN	2.2
1	A	255	GLN	2.2
5	E	174	GLN	2.2
2	B	98	ASP	2.2
1	A	192	HIS	2.2
4	D	124	LYS	2.2
1	A	17	ARG	2.1
5	E	219	ASN	2.1
1	A	264	GLU	2.1
4	D	190	ILE	2.1
1	A	194	VAL	2.1
5	E	218	GLU	2.1
5	E	131	GLU	2.1
1	A	135	ALA	2.1
4	D	55	THR	2.1
4	D	183	ASN	2.1
2	B	74	GLU	2.1
1	A	261	VAL	2.0
4	D	144	GLN	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.