



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:56 AM GMT

PDB ID : 3QDG
Title : The complex between TCR DMF5 and human Class I MHC HLA-A2 with the bound MART-1(26-35)(A27L) peptide
Authors : Borbulevych, O.Y.; Baker, B.M.
Deposited on : 2011-01-18
Resolution : 2.69 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 : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

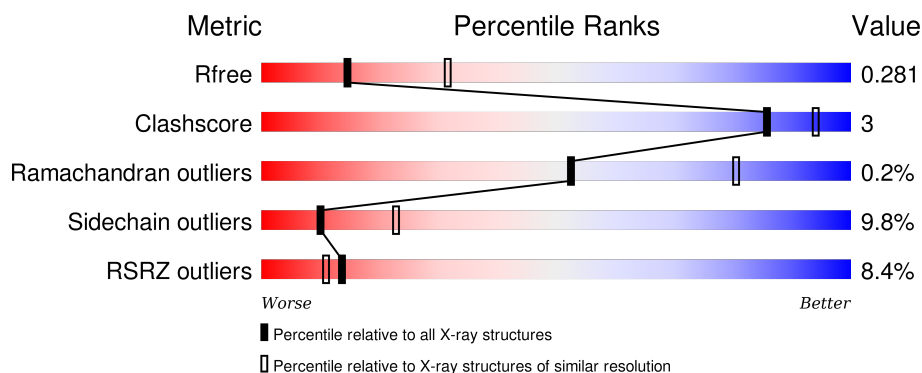
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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.

Mol	Chain	Length	Quality of chain
1	A	275	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>9%</div> </div> <div>•</div> </div>
2	B	100	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>7%</div> </div> <div>•</div> </div>
3	C	10	<div> <div>80%</div> <div>20%</div> </div>
4	D	199	<div> <div>19%</div> <div> <div></div> <div>80%</div> <div>18%</div> </div> <div>•</div> </div>
5	E	242	<div> <div>10%</div> <div> <div></div> <div>83%</div> <div>15%</div> </div> <div>•</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6633 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	1	0
			2255	1408	412	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	1	0
			842	537	141	159	5			

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 (26-35) peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			69	45	10	14			

- Molecule 4 is a protein called DMF5 alpha chain.

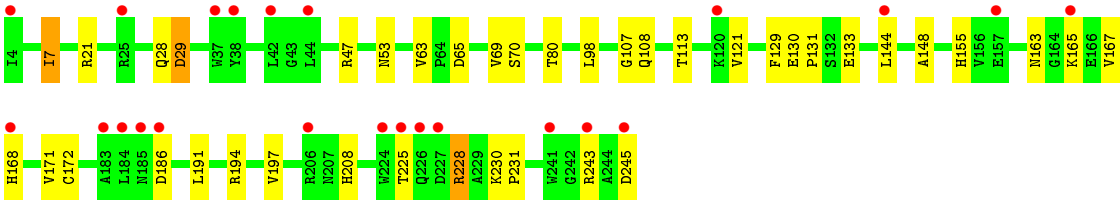
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	199	Total	C	N	O	S	0	0	0
			1546	965	255	318	8			

- Molecule 5 is a protein called DMF5 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	0	0
			1897	1191	333	365	8			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total 9	O 9	0	0
6	B	8	Total 8	O 8	0	0
6	C	3	Total 3	O 3	0	0
6	D	1	Total 1	O 1	0	0
6	E	3	Total 3	O 3	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	228.36Å 46.55Å 86.04Å 90.00° 106.73° 90.00°	Depositor
Resolution (Å)	20.00 – 2.69 19.79 – 2.69	Depositor EDS
% Data completeness (in resolution range)	90.2 (20.00-2.69) 90.2 (19.79-2.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.80 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.218 , 0.278 0.217 , 0.281	Depositor DCC
R_{free} test set	1123 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	66.4	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 22058 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6633	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.46	0/2323	0.68	1/3151 (0.0%)
2	B	0.50	0/868	0.67	0/1169
3	C	0.56	0/68	0.86	0/90
4	D	0.43	0/1579	0.63	0/2135
5	E	0.39	0/1946	0.63	0/2651
All	All	0.44	0/6784	0.66	1/9196 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	272	LEU	CA-CB-CG	5.13	127.10	115.30

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	2255	0	2109	11	0
2	B	842	0	812	2	0
3	C	69	0	79	1	0
4	D	1546	0	1460	13	1
5	E	1897	0	1808	14	0
6	A	9	0	0	0	0
6	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	3	0	0	0	0
6	D	1	0	0	0	0
6	E	3	0	0	0	0
All	All	6633	0	6268	36	1

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 3.

All (36) 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)
5:E:130:GLU:OE2	5:E:243:ARG:NH1	2.21	0.74
5:E:121:VAL:O	5:E:228:ARG:NH2	2.26	0.68
1:A:19:GLU:OE2	1:A:75:ARG:NH2	2.32	0.62
1:A:72:GLN:OE1	5:E:53:ASN:ND2	2.30	0.61
1:A:66:LYS:O	1:A:70:HIS:ND1	2.36	0.57
4:D:42:SER:OG	5:E:107:GLY:O	2.22	0.57
4:D:33:PHE:HB2	4:D:89:ALA:HB3	1.90	0.53
5:E:230:LYS:HA	5:E:231:PRO:HD3	1.68	0.47
1:A:65:ARG:HB3	4:D:94:GLY:H	1.78	0.47
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.96	0.47
1:A:258:THR:HG22	1:A:273:ARG:HB3	1.96	0.46
5:E:131:PRO:HD3	5:E:144:LEU:HG	1.97	0.46
4:D:142:ASN:OD1	4:D:142:ASN:N	2.48	0.46
4:D:179:ASP:N	4:D:179:ASP:OD1	2.44	0.46
2:B:48:LYS:H	2:B:48:LYS:HG3	1.30	0.46
5:E:113:THR:OG1	5:E:155:HIS:NE2	2.39	0.45
4:D:187:ASN:HD22	4:D:191:ILE:HG12	1.81	0.45
1:A:215:LEU:HD22	1:A:243:LYS:HD3	1.99	0.44
4:D:60:PHE:HD1	4:D:73:LEU:HD11	1.82	0.44
4:D:36:ARG:NH2	4:D:44:GLU:OE2	2.50	0.44
4:D:194:ASP:OD2	4:D:194:ASP:N	2.50	0.44
4:D:1:LYS:HE3	4:D:1:LYS:HB2	1.75	0.44
1:A:156:LEU:HD13	3:C:6:GLY:HA3	1.99	0.44
5:E:108:GLN:HG2	5:E:108:GLN:H	1.59	0.43
2:B:9:VAL:HG13	2:B:80:CYS:HB2	2.01	0.43
4:D:191:ILE:H	4:D:191:ILE:HG13	1.58	0.42
5:E:7:ILE:HD13	5:E:7:ILE:HG23	1.68	0.42
1:A:213:ILE:HG13	1:A:263:HIS:HB2	2.01	0.42
5:E:29:ASP:OD2	5:E:29:ASP:N	2.53	0.41
4:D:46:ILE:HG22	4:D:47:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:7:ILE:HD12	5:E:7:ILE:HG21	1.68	0.41
1:A:9:PHE:HB2	1:A:97:ARG:HB3	2.03	0.41
5:E:148:ALA:HB3	5:E:191:LEU:HB3	2.02	0.41
4:D:123:ASP:HA	5:E:129:PHE:HA	2.03	0.41
1:A:72:GLN:H	1:A:72:GLN:HG2	1.71	0.40
5:E:163:ASN:HA	5:E:208:HIS:HB3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:SER:OG	4:D:110:ASN:OD1[2_657]	2.17	0.03

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	274/275 (100%)	265 (97%)	7 (3%)	2 (1%)	26	55
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
4	D	197/199 (99%)	179 (91%)	18 (9%)	0	100	100
5	E	240/242 (99%)	227 (95%)	13 (5%)	0	100	100
All	All	817/826 (99%)	775 (95%)	40 (5%)	2 (0%)	52	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	PRO
1	A	226	GLN

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	232/231 (100%)	220 (95%)	12 (5%)	29	58
2	B	96/95 (101%)	88 (92%)	8 (8%)	14	31
3	C	7/7 (100%)	6 (86%)	1 (14%)	4	10
4	D	176/176 (100%)	150 (85%)	26 (15%)	4	9
5	E	204/204 (100%)	181 (89%)	23 (11%)	7	16
All	All	715/713 (100%)	645 (90%)	70 (10%)	10	23

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	72	GLN
1	A	75	ARG
1	A	106	ASP
1	A	113	TYR
1	A	121	LYS
1	A	156	LEU
1	A	196	ASP
1	A	197	HIS
1	A	207	SER
1	A	225	THR
1	A	248	VAL
2	B	4	THR
2	B	9	VAL
2	B	20	SER
2	B	48	LYS
2	B	58	LYS
2	B	70	PHE
2	B	74	GLU
2	B	89	GLN
3	C	1	GLU
4	D	1	LYS
4	D	20	LEU

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Mol	Chain	Res	Type
4	D	27	ARG
4	D	47	MET
4	D	56	GLU
4	D	68	SER
4	D	69	GLN
4	D	71	VAL
4	D	79	GLN
4	D	87	LEU
4	D	98	ILE
4	D	101	GLN
4	D	103	THR
4	D	105	LEU
4	D	112	GLN
4	D	127	SER
4	D	130	SER
4	D	131	VAL
4	D	143	VAL
4	D	148	ASP
4	D	152	TYR
4	D	168	SER
4	D	179	ASP
4	D	187	ASN
4	D	190	ILE
4	D	196	PHE
5	E	7	ILE
5	E	21	ARG
5	E	28	GLN
5	E	29	ASP
5	E	47	ARG
5	E	63	VAL
5	E	65	ASP
5	E	69	VAL
5	E	70	SER
5	E	80	THR
5	E	98	LEU
5	E	133	GLU
5	E	165	LYS
5	E	167	VAL
5	E	168	HIS
5	E	171	VAL
5	E	172	CYS
5	E	186	ASP

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Mol	Chain	Res	Type
5	E	194	ARG
5	E	197	VAL
5	E	225	THR
5	E	228	ARG
5	E	245	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	GLN
4	D	187	ASN
5	E	108	GLN
5	E	208	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 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%)	0.05	6 (2%) 65 66	53, 74, 122, 146	0
2	B	100/100 (100%)	-0.02	3 (3%) 54 54	52, 67, 88, 97	0
3	C	10/10 (100%)	-0.30	0 100 100	55, 62, 66, 75	0
4	D	199/199 (100%)	0.90	37 (18%) 2 1	66, 106, 159, 170	0
5	E	242/242 (100%)	0.55	23 (9%) 10 8	61, 102, 137, 151	0
All	All	826/826 (100%)	0.39	69 (8%) 14 11	52, 86, 145, 170	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	177	LYS	6.8
4	D	126	SER	6.5
5	E	42	LEU	5.5
4	D	189	SER	5.1
5	E	184	LEU	4.9
4	D	146	SER	4.8
4	D	147	LYS	4.6
4	D	176	ASN	4.5
4	D	196	PHE	4.4
4	D	190	ILE	4.3
5	E	44	LEU	4.2
4	D	132	CYS	4.1
1	A	16	GLY	4.0
5	E	185	ASN	3.9
4	D	199	SER	3.8
5	E	245	ASP	3.7
4	D	1	LYS	3.5
4	D	113	ASN	3.5
5	E	206	ARG	3.5
5	E	227	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
5	E	243	ARG	3.4
1	A	1	GLY	3.4
5	E	186	ASP	3.4
4	D	179	ASP	3.2
4	D	128	ASP	3.1
4	D	124	SER	3.0
4	D	193	GLU	2.9
4	D	149	SER	2.9
4	D	122	ARG	2.9
4	D	162	ARG	2.9
5	E	157	GLU	2.8
2	B	3	ARG	2.8
2	B	99[A]	MET	2.8
5	E	241	TRP	2.8
2	B	98	ASP	2.8
1	A	225	THR	2.8
5	E	25	ARG	2.7
1	A	223	ASP	2.7
4	D	188	ASN	2.7
4	D	173	ALA	2.7
4	D	172	VAL	2.6
5	E	226	GLN	2.6
4	D	148	ASP	2.6
4	D	112	GLN	2.6
4	D	180	PHE	2.6
5	E	168	HIS	2.5
5	E	183	ALA	2.4
5	E	38	TYR	2.4
5	E	165	LYS	2.4
4	D	110	ASN	2.4
4	D	127	SER	2.3
4	D	89	ALA	2.3
4	D	134	PHE	2.3
4	D	111	ILE	2.2
5	E	4	ILE	2.2
5	E	224	TRP	2.2
5	E	225	THR	2.2
4	D	198	PRO	2.2
1	A	217	TRP	2.2
5	E	37	TRP	2.2
4	D	185	ALA	2.2
4	D	108	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	120	LYS	2.1
5	E	144	LEU	2.1
4	D	195	THR	2.1
4	D	125	LYS	2.1
4	D	152	TYR	2.1
1	A	275	GLU	2.1
4	D	175	SER	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.