



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 11, 2016 – 06:41 PM EDT

PDB ID : 5E9D
Title : RD-1 Mart-1 High bound to Mart-1 decameric peptide (ELA) in complex with HLA-A2
Authors : Singh, N.K.; Baker, B.M.
Deposited on : 2015-10-15
Resolution : 2.51 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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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) : rb-20027790

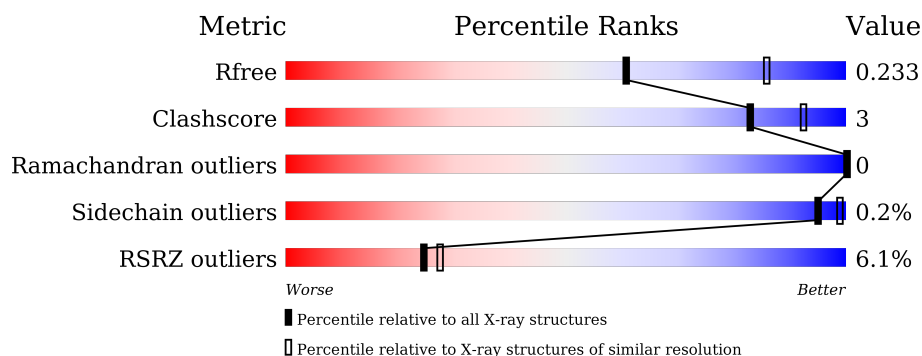
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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.

Mol	Chain	Length	Quality of chain
1	A	275	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div></div> </div> <div></div> </div>
1	F	275	<div> <div>8%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div></div> </div> <div></div> </div>
2	B	100	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div></div> </div> <div></div> </div>
2	G	100	<div> <div>6%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div></div> </div> <div></div> </div>
3	C	10	<div> <div></div> <div> <div></div> <div>80%</div> <div>20%</div> <div></div> </div> <div></div> </div>
3	H	10	<div> <div></div> <div> <div></div> <div>90%</div> <div>10%</div> <div></div> </div> <div></div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	129	 4% 77% 9% 15%
4	I	129	 3% 79% 5% 16%
5	E	156	 5% 71% 1% 26%
5	J	156	 7% 65% 8% 27%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9683 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	266	Total	C	N	O	S	0	0	0
			2174	1364	395	406	9			
1	F	272	Total	C	N	O	S	0	0	0
			2219	1388	404	418	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			816	518	138	157	3			
2	G	98	Total	C	N	O	S	0	0	0
			821	522	139	157	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Melanoma derived Mart-1 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			68	45	10	13			
3	H	10	Total	C	N	O	0	0	0
			68	45	10	13			

- Molecule 4 is a protein called A6-TCR Valpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	110	Total	C	N	O	S	0	0	0
			849	533	140	173	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	108	Total	C	N	O	S	0	0	0
			834	524	138	169	3			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	30	THR	GLN	engineered mutation	UNP A0A075B6T6
D	48	SER	PHE	engineered mutation	UNP A0A075B6T6
D	91	THR	-	linker	UNP A0A075B6T6
D	92	LYS	-	linker	UNP A0A075B6T6
D	93	TYR	-	linker	UNP A0A075B6T6
D	94	SER	-	linker	UNP A0A075B6T6
D	95	TRP	-	linker	UNP A0A075B6T6
D	96	GLY	-	linker	UNP A0A075B6T6
D	97	LYS	-	linker	UNP A0A075B6T6
D	98	LEU	-	linker	UNP A0A075B6T6
D	99	GLN	-	linker	UNP A0A075B6T6
D	100	PHE	-	linker	UNP A0A075B6T6
D	101	GLY	-	linker	UNP A0A075B6T6
D	102	ALA	-	linker	UNP A0A075B6T6
D	103	GLY	-	linker	UNP A0A075B6T6
D	104	THR	-	linker	UNP A0A075B6T6
D	105	GLN	-	linker	UNP A0A075B6T6
D	106	VAL	-	linker	UNP A0A075B6T6
D	107	VAL	-	linker	UNP A0A075B6T6
D	108	VAL	-	linker	UNP A0A075B6T6
D	109	THR	-	linker	UNP A0A075B6T6
D	110	PRO	-	linker	UNP A0A075B6T6
D	111	ASP	-	linker	UNP A0A075B6T6
D	112	GLY	-	expression tag	UNP A0A075B6T6
D	113	GLY	-	expression tag	UNP A0A075B6T6
D	114	GLY	-	expression tag	UNP A0A075B6T6
D	115	LEU	-	expression tag	UNP A0A075B6T6
D	116	ASN	-	expression tag	UNP A0A075B6T6
D	117	ASP	-	expression tag	UNP A0A075B6T6
D	118	ILE	-	expression tag	UNP A0A075B6T6
D	119	PHE	-	expression tag	UNP A0A075B6T6
D	120	GLU	-	expression tag	UNP A0A075B6T6
D	121	ALA	-	expression tag	UNP A0A075B6T6
D	122	GLN	-	expression tag	UNP A0A075B6T6
D	123	LYS	-	expression tag	UNP A0A075B6T6
D	124	ILE	-	expression tag	UNP A0A075B6T6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	125	GLU	-	expression tag	UNP A0A075B6T6
D	126	TRP	-	expression tag	UNP A0A075B6T6
D	127	HIS	-	expression tag	UNP A0A075B6T6
D	128	GLU	-	expression tag	UNP A0A075B6T6
I	30	THR	GLN	engineered mutation	UNP A0A075B6T6
I	48	SER	PHE	engineered mutation	UNP A0A075B6T6
I	91	THR	-	linker	UNP A0A075B6T6
I	92	LYS	-	linker	UNP A0A075B6T6
I	93	TYR	-	linker	UNP A0A075B6T6
I	94	SER	-	linker	UNP A0A075B6T6
I	95	TRP	-	linker	UNP A0A075B6T6
I	96	GLY	-	linker	UNP A0A075B6T6
I	97	LYS	-	linker	UNP A0A075B6T6
I	98	LEU	-	linker	UNP A0A075B6T6
I	99	GLN	-	linker	UNP A0A075B6T6
I	100	PHE	-	linker	UNP A0A075B6T6
I	101	GLY	-	linker	UNP A0A075B6T6
I	102	ALA	-	linker	UNP A0A075B6T6
I	103	GLY	-	linker	UNP A0A075B6T6
I	104	THR	-	linker	UNP A0A075B6T6
I	105	GLN	-	linker	UNP A0A075B6T6
I	106	VAL	-	linker	UNP A0A075B6T6
I	107	VAL	-	linker	UNP A0A075B6T6
I	108	VAL	-	linker	UNP A0A075B6T6
I	109	THR	-	linker	UNP A0A075B6T6
I	110	PRO	-	linker	UNP A0A075B6T6
I	111	ASP	-	linker	UNP A0A075B6T6
I	112	GLY	-	expression tag	UNP A0A075B6T6
I	113	GLY	-	expression tag	UNP A0A075B6T6
I	114	GLY	-	expression tag	UNP A0A075B6T6
I	115	LEU	-	expression tag	UNP A0A075B6T6
I	116	ASN	-	expression tag	UNP A0A075B6T6
I	117	ASP	-	expression tag	UNP A0A075B6T6
I	118	ILE	-	expression tag	UNP A0A075B6T6
I	119	PHE	-	expression tag	UNP A0A075B6T6
I	120	GLU	-	expression tag	UNP A0A075B6T6
I	121	ALA	-	expression tag	UNP A0A075B6T6
I	122	GLN	-	expression tag	UNP A0A075B6T6
I	123	LYS	-	expression tag	UNP A0A075B6T6
I	124	ILE	-	expression tag	UNP A0A075B6T6
I	125	GLU	-	expression tag	UNP A0A075B6T6
I	126	TRP	-	expression tag	UNP A0A075B6T6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	127	HIS	-	expression tag	UNP A0A075B6T6
I	128	GLU	-	expression tag	UNP A0A075B6T6

- Molecule 5 is a protein called A6-TCR Vbeta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	115	Total	C	N	O	S	0	0	0
			885	558	151	169	7			
5	J	114	Total	C	N	O	S	0	0	0
			876	553	150	166	7			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-18	MET	-	initiating methionine	UNP A0A0K0K1A5
E	-17	GLY	-	expression tag	UNP A0A0K0K1A5
E	-16	SER	-	expression tag	UNP A0A0K0K1A5
E	-15	SER	-	expression tag	UNP A0A0K0K1A5
E	-14	HIS	-	expression tag	UNP A0A0K0K1A5
E	-13	HIS	-	expression tag	UNP A0A0K0K1A5
E	-12	HIS	-	expression tag	UNP A0A0K0K1A5
E	-11	HIS	-	expression tag	UNP A0A0K0K1A5
E	-10	HIS	-	expression tag	UNP A0A0K0K1A5
E	-9	HIS	-	expression tag	UNP A0A0K0K1A5
E	-8	SER	-	expression tag	UNP A0A0K0K1A5
E	-7	SER	-	expression tag	UNP A0A0K0K1A5
E	-6	GLY	-	expression tag	UNP A0A0K0K1A5
E	-5	LEU	-	expression tag	UNP A0A0K0K1A5
E	-4	VAL	-	expression tag	UNP A0A0K0K1A5
E	-3	PRO	-	expression tag	UNP A0A0K0K1A5
E	-2	ARG	-	expression tag	UNP A0A0K0K1A5
E	-1	GLY	-	expression tag	UNP A0A0K0K1A5
E	0	SER	-	expression tag	UNP A0A0K0K1A5
E	33	ALA	SER	engineered mutation	UNP A0A0K0K1A5
E	52	VAL	ALA	engineered mutation	UNP A0A0K0K1A5
E	59	ASP	GLU	engineered mutation	UNP A0A0K0K1A5
E	62	ASP	ASN	engineered mutation	UNP A0A0K0K1A5
E	65	LYS	ASN	engineered mutation	UNP A0A0K0K1A5
E	94	ARG	-	expression tag	UNP A0A0K0K1A5
E	95	PRO	-	expression tag	UNP A0A0K0K1A5
E	96	GLY	-	expression tag	UNP A0A0K0K1A5
E	97	TRP	-	expression tag	UNP A0A0K0K1A5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	98	MET	-	expression tag	UNP A0A0K0K1A5
E	99	ALA	-	expression tag	UNP A0A0K0K1A5
E	100	GLY	-	expression tag	UNP A0A0K0K1A5
E	101	GLY	-	expression tag	UNP A0A0K0K1A5
E	102	VAL	-	expression tag	UNP A0A0K0K1A5
E	103	GLU	-	expression tag	UNP A0A0K0K1A5
E	104	LEU	-	expression tag	UNP A0A0K0K1A5
E	105	TYR	-	expression tag	UNP A0A0K0K1A5
E	106	PHE	-	expression tag	UNP A0A0K0K1A5
E	107	GLY	-	expression tag	UNP A0A0K0K1A5
E	108	PRO	-	expression tag	UNP A0A0K0K1A5
E	109	GLY	-	expression tag	UNP A0A0K0K1A5
E	110	THR	-	expression tag	UNP A0A0K0K1A5
E	111	ARG	-	expression tag	UNP A0A0K0K1A5
E	112	LEU	-	expression tag	UNP A0A0K0K1A5
E	113	THR	-	expression tag	UNP A0A0K0K1A5
E	114	VAL	-	expression tag	UNP A0A0K0K1A5
E	115	THR	-	expression tag	UNP A0A0K0K1A5
E	116	GLU	-	expression tag	UNP A0A0K0K1A5
E	117	ASP	-	expression tag	UNP A0A0K0K1A5
E	118	LEU	-	expression tag	UNP A0A0K0K1A5
E	119	ILE	-	linker	UNP A0A0K0K1A5
E	120	ASN	-	linker	UNP A0A0K0K1A5
E	121	GLY	-	linker	UNP A0A0K0K1A5
E	122	SER	-	linker	UNP A0A0K0K1A5
E	123	ALA	-	linker	UNP A0A0K0K1A5
E	124	ASP	-	linker	UNP A0A0K0K1A5
E	125	ASP	-	linker	UNP A0A0K0K1A5
E	126	ALA	-	linker	UNP A0A0K0K1A5
E	127	LYS	-	linker	UNP A0A0K0K1A5
E	128	LYS	-	linker	UNP A0A0K0K1A5
E	129	ASP	-	linker	UNP A0A0K0K1A5
E	130	ALA	-	linker	UNP A0A0K0K1A5
E	131	ALA	-	linker	UNP A0A0K0K1A5
E	132	LYS	-	linker	UNP A0A0K0K1A5
E	133	LYS	-	linker	UNP A0A0K0K1A5
E	134	ASP	-	linker	UNP A0A0K0K1A5
E	135	GLY	-	linker	UNP A0A0K0K1A5
E	136	LYS	-	linker	UNP A0A0K0K1A5
E	137	SER	-	linker	UNP A0A0K0K1A5
J	-18	MET	-	initiating methionine	UNP A0A0K0K1A5
J	-17	GLY	-	expression tag	UNP A0A0K0K1A5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	-16	SER	-	expression tag	UNP A0A0K0K1A5
J	-15	SER	-	expression tag	UNP A0A0K0K1A5
J	-14	HIS	-	expression tag	UNP A0A0K0K1A5
J	-13	HIS	-	expression tag	UNP A0A0K0K1A5
J	-12	HIS	-	expression tag	UNP A0A0K0K1A5
J	-11	HIS	-	expression tag	UNP A0A0K0K1A5
J	-10	HIS	-	expression tag	UNP A0A0K0K1A5
J	-9	HIS	-	expression tag	UNP A0A0K0K1A5
J	-8	SER	-	expression tag	UNP A0A0K0K1A5
J	-7	SER	-	expression tag	UNP A0A0K0K1A5
J	-6	GLY	-	expression tag	UNP A0A0K0K1A5
J	-5	LEU	-	expression tag	UNP A0A0K0K1A5
J	-4	VAL	-	expression tag	UNP A0A0K0K1A5
J	-3	PRO	-	expression tag	UNP A0A0K0K1A5
J	-2	ARG	-	expression tag	UNP A0A0K0K1A5
J	-1	GLY	-	expression tag	UNP A0A0K0K1A5
J	0	SER	-	expression tag	UNP A0A0K0K1A5
J	33	ALA	SER	engineered mutation	UNP A0A0K0K1A5
J	52	VAL	ALA	engineered mutation	UNP A0A0K0K1A5
J	59	ASP	GLU	engineered mutation	UNP A0A0K0K1A5
J	62	ASP	ASN	engineered mutation	UNP A0A0K0K1A5
J	65	LYS	ASN	engineered mutation	UNP A0A0K0K1A5
J	94	ARG	-	expression tag	UNP A0A0K0K1A5
J	95	PRO	-	expression tag	UNP A0A0K0K1A5
J	96	GLY	-	expression tag	UNP A0A0K0K1A5
J	97	TRP	-	expression tag	UNP A0A0K0K1A5
J	98	MET	-	expression tag	UNP A0A0K0K1A5
J	99	ALA	-	expression tag	UNP A0A0K0K1A5
J	100	GLY	-	expression tag	UNP A0A0K0K1A5
J	101	GLY	-	expression tag	UNP A0A0K0K1A5
J	102	VAL	-	expression tag	UNP A0A0K0K1A5
J	103	GLU	-	expression tag	UNP A0A0K0K1A5
J	104	LEU	-	expression tag	UNP A0A0K0K1A5
J	105	TYR	-	expression tag	UNP A0A0K0K1A5
J	106	PHE	-	expression tag	UNP A0A0K0K1A5
J	107	GLY	-	expression tag	UNP A0A0K0K1A5
J	108	PRO	-	expression tag	UNP A0A0K0K1A5
J	109	GLY	-	expression tag	UNP A0A0K0K1A5
J	110	THR	-	expression tag	UNP A0A0K0K1A5
J	111	ARG	-	expression tag	UNP A0A0K0K1A5
J	112	LEU	-	expression tag	UNP A0A0K0K1A5
J	113	THR	-	expression tag	UNP A0A0K0K1A5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	114	VAL	-	expression tag	UNP A0A0K0K1A5
J	115	THR	-	expression tag	UNP A0A0K0K1A5
J	116	GLU	-	expression tag	UNP A0A0K0K1A5
J	117	ASP	-	expression tag	UNP A0A0K0K1A5
J	118	LEU	-	expression tag	UNP A0A0K0K1A5
J	119	ILE	-	linker	UNP A0A0K0K1A5
J	120	ASN	-	linker	UNP A0A0K0K1A5
J	121	GLY	-	linker	UNP A0A0K0K1A5
J	122	SER	-	linker	UNP A0A0K0K1A5
J	123	ALA	-	linker	UNP A0A0K0K1A5
J	124	ASP	-	linker	UNP A0A0K0K1A5
J	125	ASP	-	linker	UNP A0A0K0K1A5
J	126	ALA	-	linker	UNP A0A0K0K1A5
J	127	LYS	-	linker	UNP A0A0K0K1A5
J	128	LYS	-	linker	UNP A0A0K0K1A5
J	129	ASP	-	linker	UNP A0A0K0K1A5
J	130	ALA	-	linker	UNP A0A0K0K1A5
J	131	ALA	-	linker	UNP A0A0K0K1A5
J	132	LYS	-	linker	UNP A0A0K0K1A5
J	133	LYS	-	linker	UNP A0A0K0K1A5
J	134	ASP	-	linker	UNP A0A0K0K1A5
J	135	GLY	-	linker	UNP A0A0K0K1A5
J	136	LYS	-	linker	UNP A0A0K0K1A5
J	137	SER	-	linker	UNP A0A0K0K1A5

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	11	Total O 11 11	0	0
6	B	13	Total O 13 13	0	0
6	C	2	Total O 2 2	0	0
6	D	7	Total O 7 7	0	0
6	E	12	Total O 12 12	0	0
6	F	9	Total O 9 9	0	0
6	G	2	Total O 2 2	0	0

Continued on next page...

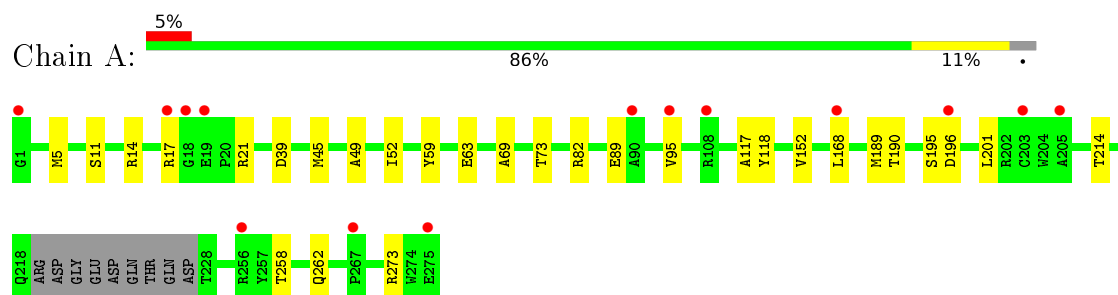
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	O	0	0
			1	1		
6	I	7	Total	O	0	0
			7	7		
6	J	9	Total	O	0	0
			9	9		

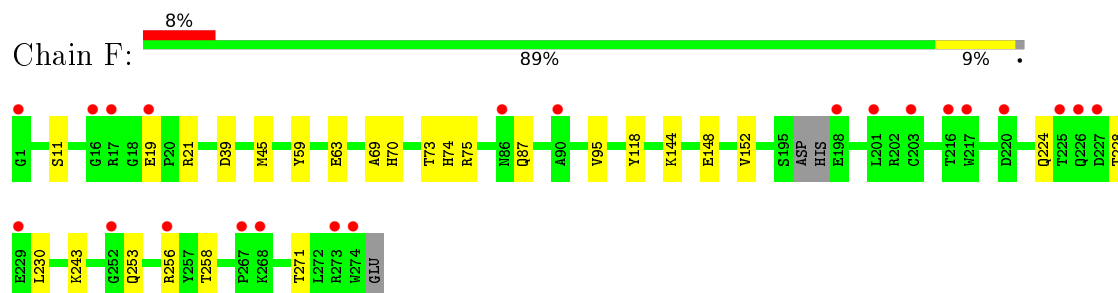
3 Residue-property plots [i](#)

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.

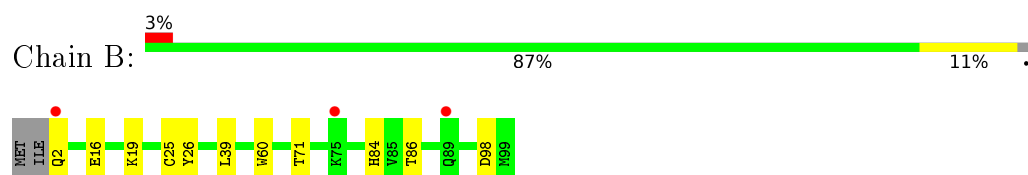
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



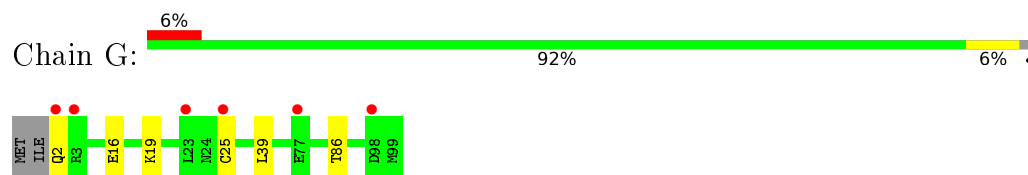
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



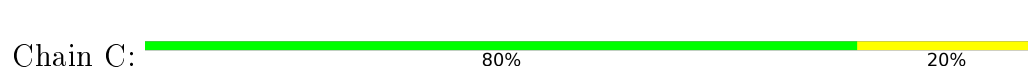
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



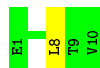
- Molecule 3: Melanoma derived Mart-1 peptide





- Molecule 3: Melanoma derived Mart-1 peptide

Chain H:



- Molecule 4: A6-TCR Valpha

Chain D:



- Molecule 4: A6-TCR Valpha

Chain I:



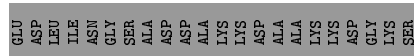
- Molecule 5: A6-TCR Vbeta

Chain E:



- Molecule 5: A6-TCR Vbeta

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.44 Å 164.48 Å 95.20 Å 90.00° 100.56° 90.00°	Depositor
Resolution (Å)	20.04 – 2.51 20.04 – 2.51	Depositor EDS
% Data completeness (in resolution range)	84.9 (20.04-2.51) 84.9 (20.04-2.51)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.50 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.180 , 0.232 0.180 , 0.233	Depositor DCC
R_{free} test set	1836 reflections (4.16%)	DCC
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9683	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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.

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	0.23	0/2238	0.40	0/3036
1	F	0.23	0/2282	0.40	0/3096
2	B	0.24	0/839	0.43	0/1135
2	G	0.24	0/844	0.41	0/1141
3	C	0.20	0/67	0.64	0/90
3	H	0.20	0/67	0.66	0/90
4	D	0.24	0/868	0.41	0/1178
4	I	0.25	0/852	0.43	0/1155
5	E	0.24	0/907	0.43	0/1232
5	J	0.32	0/898	0.46	0/1220
All	All	0.24	0/9862	0.42	0/13373

There are no bond length outliers.

There are no bond angle outliers.

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	2174	0	2038	17	0
1	F	2219	0	2078	14	0
2	B	816	0	768	9	0
2	G	821	0	780	3	0
3	C	68	0	79	2	0
3	H	68	0	79	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	849	0	807	6	0
4	I	834	0	796	4	0
5	E	885	0	853	2	0
5	J	876	0	847	8	0
6	A	11	0	0	0	0
6	B	13	0	0	4	0
6	C	2	0	0	0	0
6	D	7	0	0	0	0
6	E	12	0	0	0	0
6	F	9	0	0	0	0
6	G	2	0	0	0	0
6	H	1	0	0	0	0
6	I	7	0	0	0	0
6	J	9	0	0	2	0
All	All	9683	0	9125	58	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 3.

The worst 5 of 58 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:J:2:ALA:HB3	5:J:26:ASP:OD2	1.76	0.85
2:B:84:HIS:O	6:B:102:HOH:O	2.10	0.70
1:F:19:GLU:OE1	1:F:75:ARG:NE	2.25	0.66
2:B:26:TYR:OH	6:B:103:HOH:O	2.15	0.61
1:F:70:HIS:O	1:F:74:HIS:ND1	2.28	0.59

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	262/275 (95%)	254 (97%)	8 (3%)	0	100	100
1	F	268/275 (98%)	261 (97%)	7 (3%)	0	100	100
2	B	96/100 (96%)	95 (99%)	1 (1%)	0	100	100
2	G	96/100 (96%)	95 (99%)	1 (1%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
3	H	8/10 (80%)	8 (100%)	0	0	100	100
4	D	108/129 (84%)	103 (95%)	5 (5%)	0	100	100
4	I	106/129 (82%)	102 (96%)	4 (4%)	0	100	100
5	E	113/156 (72%)	108 (96%)	5 (4%)	0	100	100
5	J	112/156 (72%)	107 (96%)	5 (4%)	0	100	100
All	All	1177/1340 (88%)	1141 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	223/231 (96%)	223 (100%)	0	100	100
1	F	228/231 (99%)	228 (100%)	0	100	100
2	B	92/95 (97%)	92 (100%)	0	100	100
2	G	93/95 (98%)	93 (100%)	0	100	100
3	C	7/7 (100%)	7 (100%)	0	100	100
3	H	7/7 (100%)	7 (100%)	0	100	100
4	D	94/109 (86%)	94 (100%)	0	100	100
4	I	92/109 (84%)	92 (100%)	0	100	100
5	E	95/127 (75%)	94 (99%)	1 (1%)	80	94
5	J	94/127 (74%)	93 (99%)	1 (1%)	80	94
All	All	1025/1138 (90%)	1023 (100%)	2 (0%)	95	99

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	25	GLN
5	J	25	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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	266/275 (96%)	0.39	14 (5%) 30 34	38, 64, 104, 135	0
1	F	272/275 (98%)	0.46	22 (8%) 15 16	36, 65, 116, 140	0
2	B	98/100 (98%)	0.22	3 (3%) 52 57	42, 59, 93, 106	0
2	G	98/100 (98%)	0.42	6 (6%) 25 27	48, 66, 97, 118	0
3	C	10/10 (100%)	0.24	0 100 100	39, 43, 47, 62	0
3	H	10/10 (100%)	0.50	0 100 100	35, 44, 55, 61	0
4	D	110/129 (85%)	0.12	5 (4%) 37 42	29, 47, 71, 94	0
4	I	108/129 (83%)	0.26	4 (3%) 45 50	33, 54, 87, 108	0
5	E	115/156 (73%)	0.33	8 (6%) 19 22	30, 49, 76, 102	0
5	J	114/156 (73%)	0.34	11 (9%) 10 11	32, 52, 81, 102	0
All	All	1201/1340 (89%)	0.35	73 (6%) 25 27	29, 58, 101, 140	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	2	ALA	6.1
5	J	2	ALA	5.2
1	F	217	TRP	4.8
1	A	108	ARG	4.4
5	E	59	ASP	4.3

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

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.