



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2022 – 12:07 AM JST

PDB ID : 8GVB
Title : The complex between public TCR TD08 and HLA-A24 bound to HIV-1 Nef138-8 peptide
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Deposited on : 2022-09-14
Resolution : 3.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

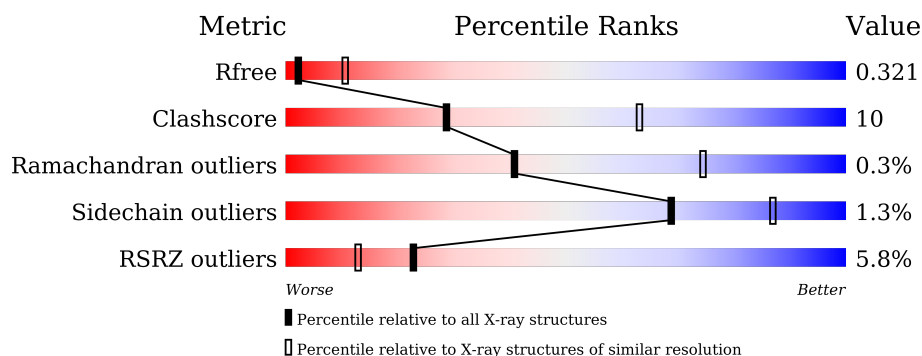
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	209	<div> <div>9%</div> <div>71% 15% 12%</div> </div>
2	B	246	<div> <div>8%</div> <div>78% 18% .</div> </div>
3	H	275	<div> <div>2%</div> <div>78% 21% ..</div> </div>
4	L	100	<div> <div>2%</div> <div>85% 14% .</div> </div>
5	P	8	<div> <div></div> <div>50% 50%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6462 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 TD08 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1427	901	235	285	6			

- Molecule 2 is a protein called TD08 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	0
			1914	1202	344	362	6			

- Molecule 3 is a protein called MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	273	Total	C	N	O	S	0	0	0
			2218	1380	402	426	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	0	MET	-	initiating methionine	UNP F6IQZ4

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	expression tag	UNP P61769

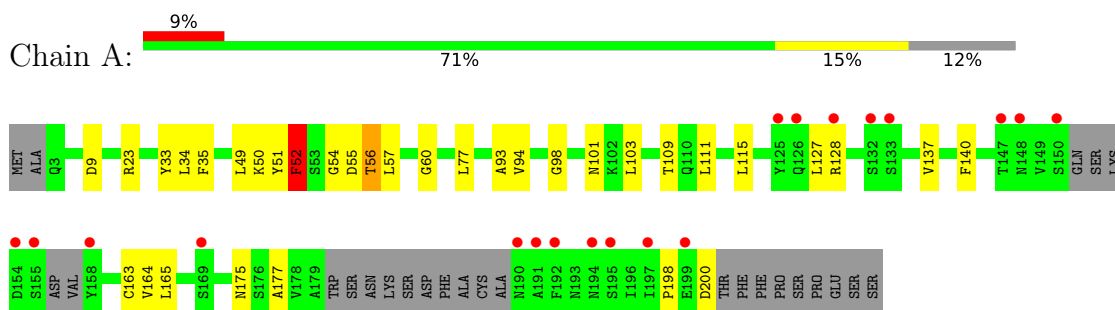
- Molecule 5 is a protein called 8-mer peptide from Protein Nef.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	P	8	Total	C	N	O	0	0	0
			75	52	12	11			

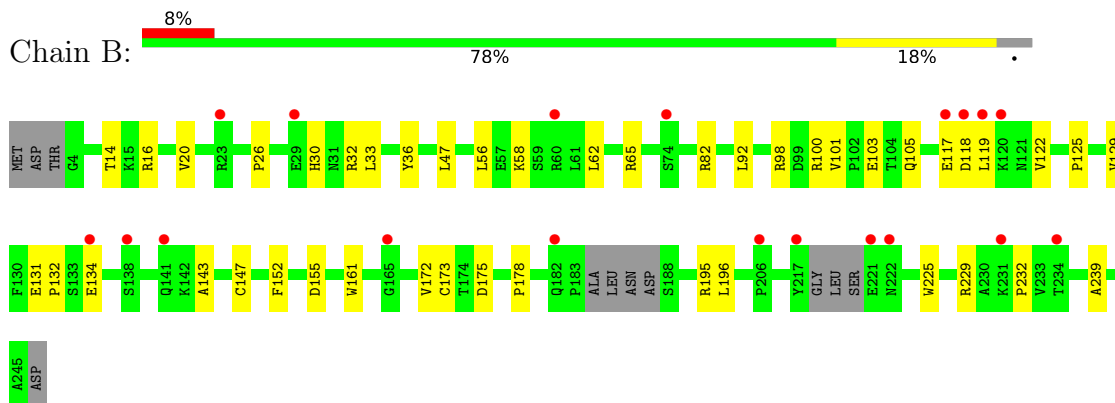
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

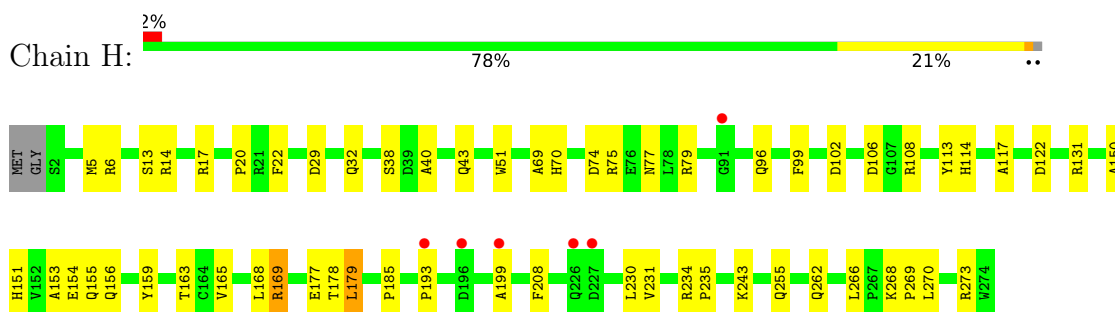
- Molecule 1: TD08 TCR alpha chain



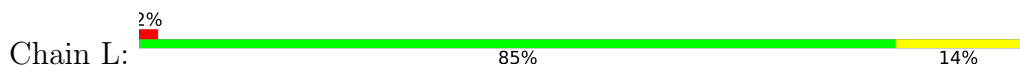
- Molecule 2: TD08 TCR beta chain

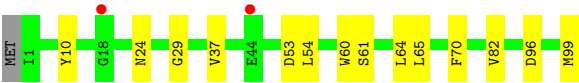


- Molecule 3: MHC class I antigen

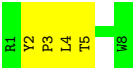


- Molecule 4: Beta-2-microglobulin





● Molecule 5: 8-mer peptide from Protein Nef



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.66Å 71.66Å 381.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.01 – 3.20 35.01 – 3.20	Depositor EDS
% Data completeness (in resolution range)	82.7 (35.01-3.20) 82.7 (35.01-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.81 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, REFMAC 5	Depositor
R, R_{free}	0.280 , 0.321 0.280 , 0.321	Depositor DCC
R_{free} test set	759 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 22.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	6462	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

5.1 Standard geometry

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	0.61	5/1456 (0.3%)	0.56	1/1968 (0.1%)
2	B	0.24	0/1964	0.44	0/2664
3	H	0.23	0/2278	0.43	0/3087
4	L	0.23	0/851	0.40	0/1152
5	P	0.29	0/79	0.51	0/106
All	All	0.35	5/6628 (0.1%)	0.46	1/8977 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	TYR	CE2-CZ	-6.58	1.29	1.38
1	A	51	TYR	CG-CD2	-6.13	1.31	1.39
1	A	51	TYR	CE1-CZ	-6.08	1.30	1.38
1	A	52	PHE	CG-CD2	-6.04	1.29	1.38
1	A	51	TYR	CG-CD1	-5.06	1.32	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	THR	N-CA-C	5.24	125.14	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	PHE	Peptide

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	1427	0	1358	45	0
2	B	1914	0	1823	39	0
3	H	2218	0	2076	42	0
4	L	828	0	794	9	0
5	P	75	0	71	9	0
All	All	6462	0	6122	122	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 10.

The worst 5 of 122 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:115:LEU:HD11	1:A:164:VAL:CG1	1.50	1.39
1:A:49:LEU:HD21	1:A:60:GLY:CA	1.71	1.21
1:A:49:LEU:CD2	1:A:60:GLY:HA3	1.74	1.17
1:A:101:ASN:HD21	5:P:4:LEU:HD22	1.15	1.08
1:A:49:LEU:CD2	1:A:60:GLY:CA	2.32	1.06

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	175/209 (84%)	160 (91%)	13 (7%)	2 (1%)	14	51
2	B	229/246 (93%)	220 (96%)	9 (4%)	0	100	100
3	H	271/275 (98%)	266 (98%)	5 (2%)	0	100	100
4	L	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
5	P	6/8 (75%)	6 (100%)	0	0	100	100
All	All	778/838 (93%)	747 (96%)	29 (4%)	2 (0%)	41	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	THR
1	A	54	GLY

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	160/183 (87%)	156 (98%)	4 (2%)	47	77
2	B	209/218 (96%)	207 (99%)	2 (1%)	76	90
3	H	230/231 (100%)	228 (99%)	2 (1%)	78	91
4	L	94/95 (99%)	93 (99%)	1 (1%)	73	88
5	P	7/7 (100%)	7 (100%)	0	100	100
All	All	700/734 (95%)	691 (99%)	9 (1%)	69	87

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	179	LEU
4	L	70	PHE
1	A	111	LEU
2	B	30	HIS
2	B	103	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
3	H	70	HIS

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 monosaccharides 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](#)

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	183/209 (87%)	0.47	19 (10%) 6 4	27, 59, 153, 196	0
2	B	235/246 (95%)	0.63	19 (8%) 12 6	38, 100, 149, 172	0
3	H	273/275 (99%)	0.30	6 (2%) 62 48	33, 69, 125, 168	0
4	L	99/100 (99%)	0.31	2 (2%) 65 51	48, 87, 114, 171	0
5	P	8/8 (100%)	0.37	0 100 100	31, 44, 52, 68	0
All	All	798/838 (95%)	0.44	46 (5%) 23 13	27, 80, 140, 196	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	60	ARG	5.8
2	B	134	GLU	5.1
1	A	190	ASN	4.5
2	B	118	ASP	4.4
1	A	148	ASN	4.0

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 monosaccharides 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.