



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 11:40 PM JST

PDB ID : 7DZM
Title : Crystal Structure of the cross-restricted T18A TCR and HLAB8101 bound to HIV-1 Gag TL9 peptide
Authors : Liu, Y.; Yin, L.
Deposited on : 2021-01-25
Resolution : 2.25 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

<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 : 2.36
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) : 2.36

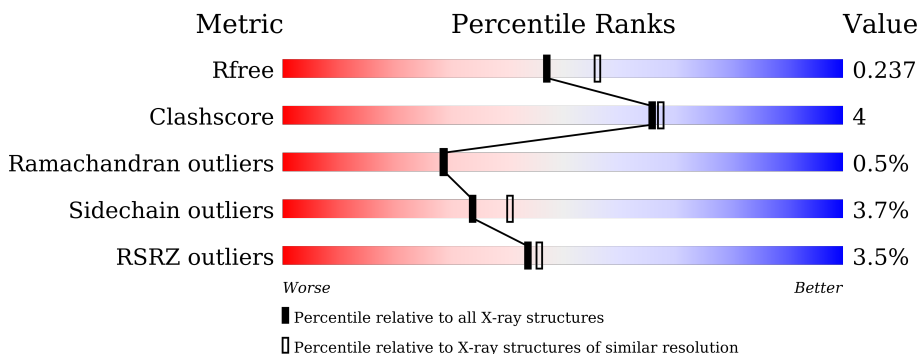
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	278	 7% 86% 12%
2	B	100	 % 90% 8%
3	C	9	 100%
4	D	241	 % 90% 10%
5	E	207	 2% 83% 14%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7079 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 class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	278	2263	1404	413	440	6	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP I3ZN85

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	9	71	43	11	16	1	0	0	0

- Molecule 4 is a protein called beta chain T18A TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	1919	1214	330	365	10	0	0	0

- Molecule 5 is a protein called alpha chain T18A TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	201	1566	971	269	314	12	0	0	0

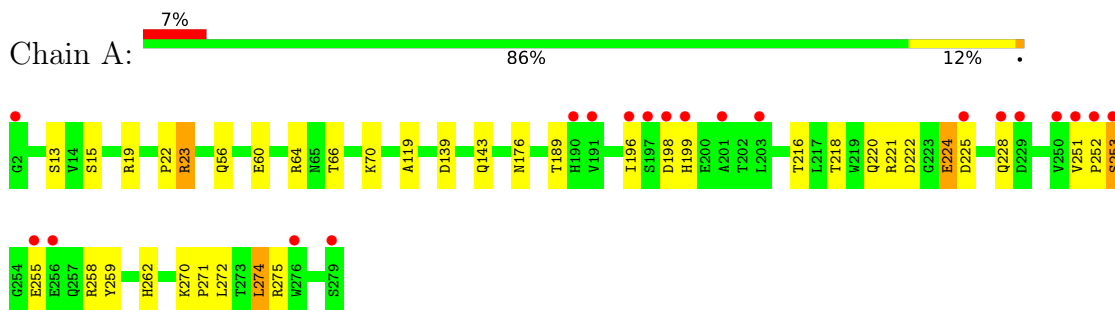
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	107	Total 107	O 107	0	0
6	B	54	Total 54	O 54	0	0
6	C	8	Total 8	O 8	0	0
6	D	156	Total 156	O 156	0	0
6	E	98	Total 98	O 98	0	0

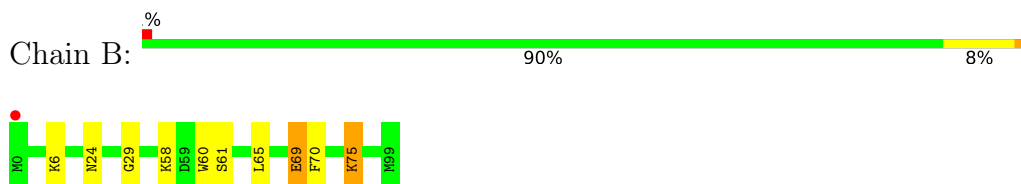
3 Residue-property plots [i](#)

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: MHC class I antigen



- Molecule 2: Beta-2-microglobulin

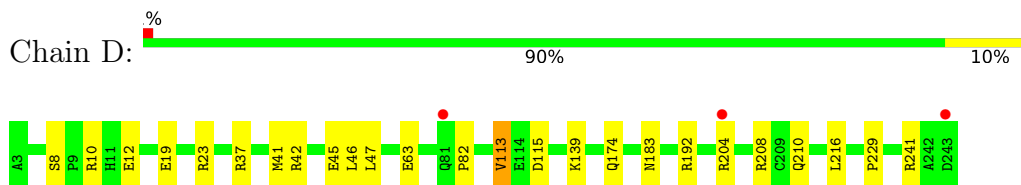


- Molecule 3: Gag-Pol polyprotein

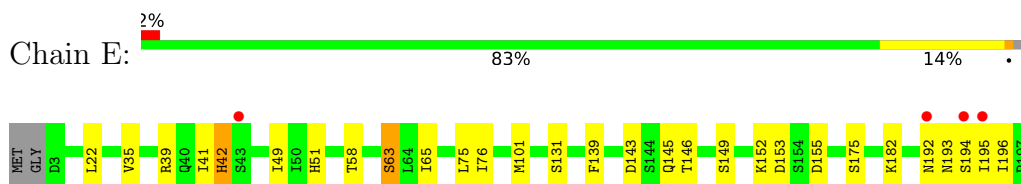


There are no outlier residues recorded for this chain.

- Molecule 4: beta chain T18A TCR



- Molecule 5: alpha chain T18A TCR



PRO
GLU
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.10Å 93.10Å 263.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.55 – 2.25 46.55 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.55-2.25) 99.9 (46.55-2.24)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.24Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.196 , 0.240 0.194 , 0.237	Depositor DCC
R_{free} test set	1999 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtrriage
Anisotropy	0.567	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7079	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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	0.34	0/2324	0.62	0/3156
2	B	0.35	0/860	0.56	0/1162
3	C	0.38	0/71	0.57	0/95
4	D	0.40	0/1973	0.59	0/2687
5	E	0.36	0/1599	0.60	0/2171
All	All	0.37	0/6827	0.60	0/9271

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	2263	0	2114	21	0
2	B	837	0	803	5	0
3	C	71	0	72	0	0
4	D	1919	0	1825	12	0
5	E	1566	0	1492	17	0
6	A	107	0	0	3	0
6	B	54	0	0	1	0
6	C	8	0	0	0	0
6	D	156	0	0	3	0
6	E	98	0	0	2	0
All	All	7079	0	6306	52	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 4.

All (52) 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:199:HIS:O	1:A:253:SER:N	2.23	0.71
5:E:58:THR:HG22	5:E:63:SER:HB2	1.74	0.69
5:E:39:ARG:HB3	5:E:49:ILE:HD11	1.77	0.67
5:E:143:ASP:OD2	5:E:145:GLN:NE2	2.31	0.63
2:B:69:GLU:CD	2:B:69:GLU:H	2.02	0.63
4:D:41:MET:HG2	4:D:42:ARG:HG2	1.81	0.62
2:B:75:LYS:NZ	6:B:101:HOH:O	2.35	0.59
4:D:183:ASN:O	6:D:301:HOH:O	2.17	0.58
5:E:192:ASN:O	5:E:194:SER:N	2.36	0.57
5:E:192:ASN:ND2	6:E:304:HOH:O	2.38	0.57
4:D:113:VAL:HG13	4:D:115:ASP:H	1.70	0.57
1:A:189:THR:HG21	1:A:272:LEU:HD13	1.86	0.56
1:A:119:ALA:HB2	2:B:60:TRP:CE2	2.42	0.55
1:A:60:GLU:H	1:A:60:GLU:CD	2.12	0.53
1:A:270:LYS:HG2	1:A:271:PRO:HD2	1.89	0.53
5:E:146:THR:OG1	6:E:301:HOH:O	2.18	0.53
1:A:64:ARG:NH1	6:A:301:HOH:O	2.24	0.53
4:D:208:ARG:NH1	4:D:210:GLN:HB2	2.25	0.52
5:E:139:PHE:CZ	5:E:196:ILE:HG22	2.45	0.52
1:A:19:ARG:HG3	6:A:320:HOH:O	2.09	0.51
5:E:153:ASP:OD2	5:E:182:LYS:HE3	2.11	0.51
4:D:139:LYS:NZ	6:D:303:HOH:O	2.35	0.50
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.94	0.50
1:A:15:SER:HA	1:A:22:PRO:HB3	1.94	0.49
1:A:251:VAL:HG12	1:A:259:TYR:CE1	2.47	0.49
1:A:139:ASP:O	1:A:143:GLN:HG3	2.13	0.48
4:D:216:LEU:HD22	4:D:229:PRO:HD2	1.95	0.48
5:E:65:ILE:HD13	5:E:76:ILE:HD12	1.94	0.48
5:E:131:SER:O	5:E:131:SER:OG	2.31	0.48
1:A:255:GLU:O	1:A:258:ARG:HB2	2.15	0.47
4:D:42:ARG:HD2	4:D:45:GLU:OE2	2.15	0.46
1:A:252:PRO:HG2	1:A:255:GLU:OE1	2.15	0.46
5:E:196:ILE:HD13	5:E:202:PHE:HZ	1.80	0.46
1:A:220:GLN:OE1	1:A:262:HIS:NE2	2.48	0.46
1:A:220:GLN:HG2	1:A:224:GLU:N	2.31	0.46
4:D:8:SER:OG	4:D:23:ARG:NH2	2.48	0.46
5:E:35:VAL:O	5:E:51:HIS:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASP:OD1	1:A:258:ARG:HG2	2.16	0.45
4:D:174:GLN:HG3	5:E:42:HIS:NE2	2.32	0.45
1:A:189:THR:OG1	1:A:274:LEU:HD21	2.17	0.44
1:A:13:SER:HA	1:A:23:ARG:O	2.17	0.44
1:A:255:GLU:HB2	1:A:258:ARG:HD3	2.01	0.42
4:D:37:ARG:HB2	4:D:47:LEU:HD11	2.01	0.42
5:E:153:ASP:OD1	5:E:155:ASP:HB2	2.19	0.42
1:A:66:THR:HG22	1:A:70:LYS:HE3	2.02	0.42
5:E:22:LEU:HD22	5:E:75:LEU:HD23	2.02	0.41
4:D:46:LEU:HD22	5:E:101:MET:HG3	2.01	0.41
2:B:29:GLY:HA2	2:B:61:SER:OG	2.21	0.41
4:D:19:GLU:HG2	6:D:304:HOH:O	2.21	0.41
1:A:56:GLN:N	6:A:310:HOH:O	2.39	0.40
1:A:221:ARG:HH21	1:A:258:ARG:HH22	1.70	0.40
5:E:149:SER:H	5:E:195:ILE:HG12	1.86	0.40

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	276/278 (99%)	259 (94%)	16 (6%)	1 (0%)	34	37
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	239/241 (99%)	232 (97%)	6 (2%)	1 (0%)	34	37
5	E	199/207 (96%)	189 (95%)	8 (4%)	2 (1%)	15	13
All	All	819/835 (98%)	782 (96%)	33 (4%)	4 (0%)	29	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	41	ILE
5	E	193	ASN
1	A	253	SER
4	D	82	PRO

5.3.2 Protein sidechains [i](#)

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	236/236 (100%)	225 (95%)	11 (5%)	26	29
2	B	95/95 (100%)	90 (95%)	5 (5%)	22	23
3	C	9/9 (100%)	9 (100%)	0	100	100
4	D	211/211 (100%)	204 (97%)	7 (3%)	38	46
5	E	178/183 (97%)	174 (98%)	4 (2%)	52	61
All	All	729/734 (99%)	702 (96%)	27 (4%)	34	40

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	176	ASN
1	A	196	ILE
1	A	198	ASP
1	A	216	THR
1	A	218	THR
1	A	224	GLU
1	A	225	ASP
1	A	228	GLN
1	A	274	LEU
1	A	275	ARG
2	B	6	LYS
2	B	58	LYS
2	B	69	GLU
2	B	70	PHE
2	B	75	LYS

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Mol	Chain	Res	Type
4	D	10	ARG
4	D	12	GLU
4	D	63	GLU
4	D	113	VAL
4	D	192	ARG
4	D	204	ARG
4	D	241	ARG
5	E	42	HIS
5	E	63	SER
5	E	152	LYS
5	E	175	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	176	ASN
1	A	190	HIS
1	A	193	HIS
4	D	81	GLN

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

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	278/278 (100%)	0.21	20 (7%) 15 16	28, 47, 99, 114	0
2	B	100/100 (100%)	-0.21	1 (1%) 82 84	32, 41, 57, 74	0
3	C	9/9 (100%)	-0.55	0 100 100	31, 34, 36, 37	0
4	D	241/241 (100%)	-0.36	3 (1%) 79 81	27, 37, 59, 87	0
5	E	201/207 (97%)	0.03	5 (2%) 57 60	31, 42, 69, 98	0
All	All	829/835 (99%)	-0.06	29 (3%) 44 46	27, 42, 86, 114	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	194	SER	7.0
1	A	201	ALA	6.9
1	A	253	SER	5.2
1	A	196	ILE	4.9
5	E	43	SER	4.6
1	A	2	GLY	4.3
1	A	255	GLU	4.3
4	D	81	GLN	4.3
1	A	250	VAL	4.0
1	A	279	SER	3.9
1	A	276	TRP	3.8
1	A	198	ASP	3.7
5	E	192	ASN	3.6
5	E	198	GLU	3.6
1	A	190	HIS	3.6
1	A	199	HIS	3.6
1	A	203	LEU	3.6
1	A	252	PRO	3.3
2	B	0	MET	3.1
5	E	195	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	228	GLN	2.8
1	A	229	ASP	2.8
1	A	256	GLU	2.7
1	A	225	ASP	2.6
1	A	197	SER	2.3
1	A	191	VAL	2.3
1	A	251	VAL	2.3
4	D	243	ASP	2.3
4	D	204	ARG	2.1

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.