



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 15, 2026 – 06:09 PM JST

PDB ID : 9LLU / pdb_00009llu
Title : p53 epitope specific TCR 4414A binding to p53Y220D-HLA-A2
Authors : Duan, Z.H.; Wu, D.C.
Deposited on : 2025-01-17
Resolution : 2.87 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

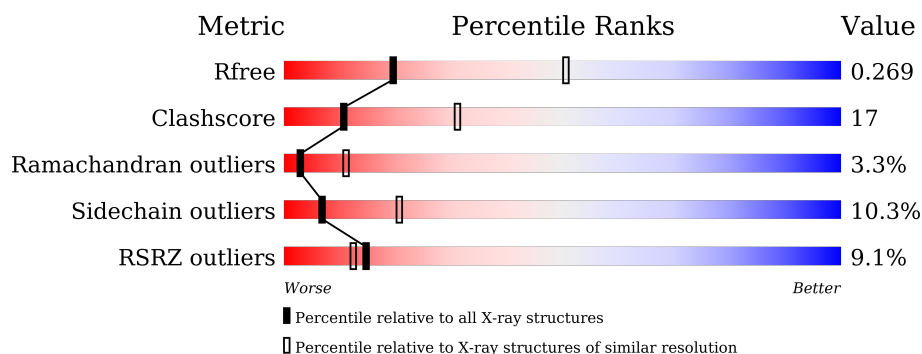
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	276	3% 71% 22% 6%
2	B	100	4% 72% 28%
3	C	9	56% 44%
4	E	247	17% 48% 41% 8% . .
5	D	207	10% 55% 26% 11% . 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12873 atoms, of which 6263 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
1	A	275	Total	C	H	N	O	S	0	0	0
			4340	1403	2094	409	425	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q8WLS4

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	100	Total	C	H	N	O	S	0	3	0
			1671	541	823	142	161	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 VAL-VAL-PRO-ASP-GLU-PRO-PRO-GLU-VAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	9	Total	C	H	N	O		0	0	0
			134	44	66	9	15				

- Molecule 4 is a protein called T cell receptor 4414A chain beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	E	243	Total	C	H	N	O	S	0	0	0
			3745	1215	1817	338	370	5			

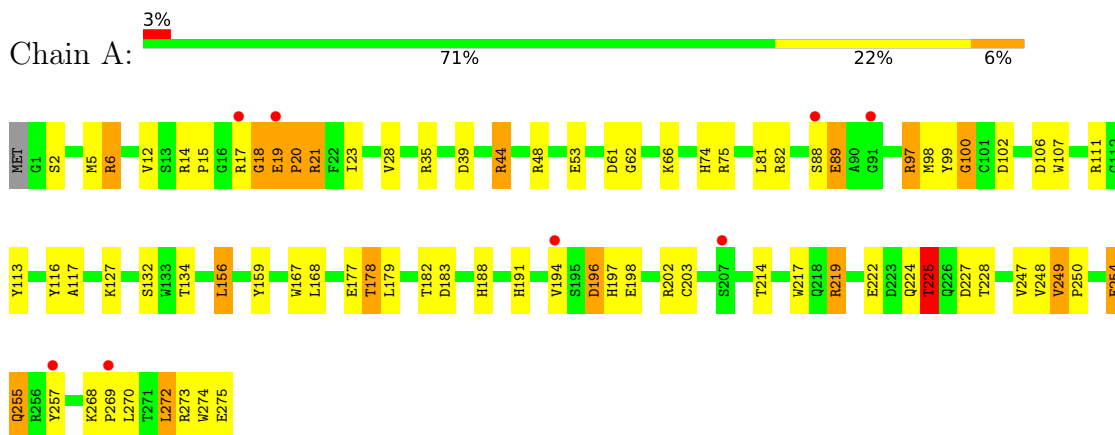
- Molecule 5 is a protein called T cell receptor 4414A chain alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	D	193	Total	C	H	N	O	S	0	0	0
			2983	953	1463	248	310	9			

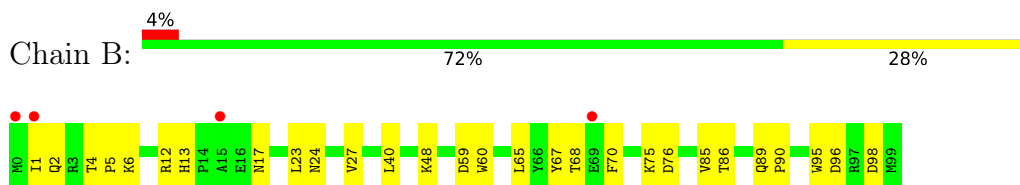
3 Residue-property plots [i](#)

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



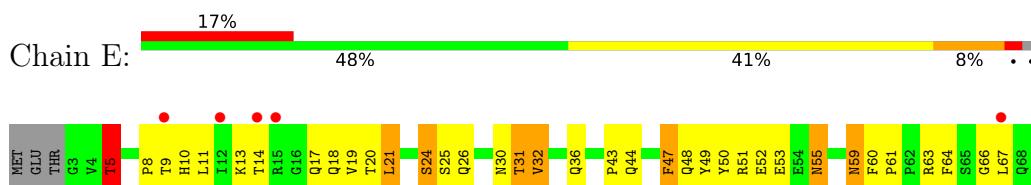
- Molecule 2: Beta-2-microglobulin

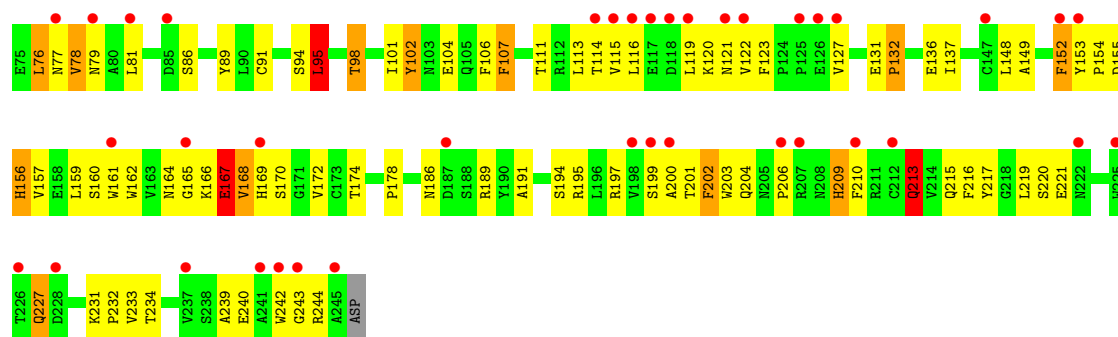


- Molecule 3: VAL-VAL-PRO-ASP-GLU-PRO-PRO-GLU-VAL

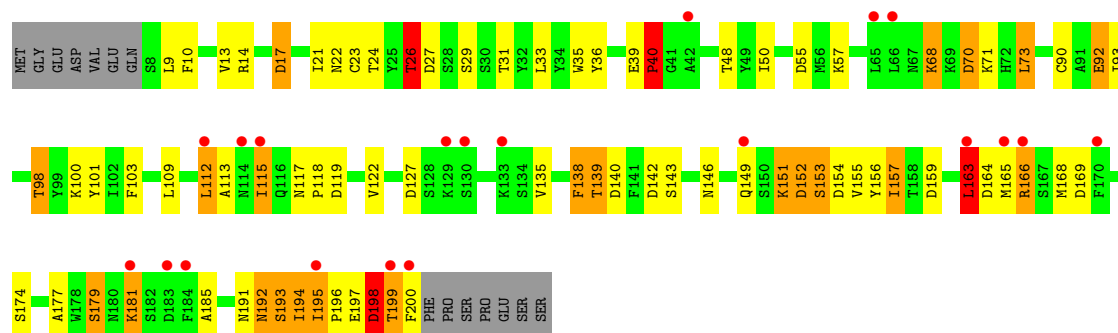


- Molecule 4: T cell receptor 4414A chain beta





• Molecule 5: T cell receptor 4414A chain alpha



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.64Å 44.05Å 207.88Å 90.00° 104.59° 90.00°	Depositor
Resolution (Å)	34.77 – 2.87 34.77 – 2.87	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.77-2.87) 99.8 (34.77-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.47 (at 2.85Å)	Xtriage
Refinement program	PHENIX (???)	Depositor
R, R_{free}	0.266 , 0.270 0.266 , 0.269	Depositor DCC
R_{free} test set	2000 reflections (8.94%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.862	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.7	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	0.89	EDS
Total number of atoms	12873	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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	0.63	1/2311 (0.0%)	1.25	13/3137 (0.4%)
2	B	0.60	0/884	1.17	2/1194 (0.2%)
3	C	0.72	0/70	1.18	0/98
4	E	0.59	0/1982	1.19	10/2700 (0.4%)
5	D	0.59	0/1548	1.31	12/2095 (0.6%)
All	All	0.61	1/6795 (0.0%)	1.24	37/9224 (0.4%)

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	3
4	E	0	1
5	D	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	ARG	NE-CZ	5.67	1.39	1.33

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	55	ASP	CA-CB-CG	9.07	121.67	112.60
2	B	70	PHE	CA-CB-CG	7.91	121.71	113.80
4	E	234	THR	CA-CB-OG1	-7.84	97.84	109.60
1	A	188	HIS	CA-CB-CG	7.54	121.34	113.80
4	E	5	THR	CA-CB-OG1	-7.39	98.51	109.60

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	VAL	Peptide
1	A	48	ARG	Sidechain
1	A	82	ARG	Sidechain
5	D	98	THR	Peptide
4	E	195	ARG	Sidechain

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	2246	2094	2096	50	0
2	B	848	823	817	15	0
3	C	68	66	66	2	1
4	E	1928	1817	1817	101	2
5	D	1520	1463	1463	51	1
All	All	6610	6263	6259	215	2

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 17.

The worst 5 of 215 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)
4:E:153:TYR:CD1	4:E:154:PRO:HA	2.07	0.89
1:A:97:ARG:HH11	1:A:97:ARG:CG	1.84	0.89
4:E:101:ILE:O	4:E:102:TYR:O	1.95	0.85
1:A:97:ARG:NH1	1:A:97:ARG:HB2	1.96	0.80
1:A:97:ARG:HH11	1:A:97:ARG:HG3	1.48	0.78

All (2) 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)
3:C:5:GLU:OE1	4:E:98:THR:O[4_444]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:197:ARG:HH12	5:D:140:ASP:OD1[3_454]	1.57	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	273/276 (99%)	248 (91%)	19 (7%)	6 (2%)	5	18
2	B	101/100 (101%)	89 (88%)	11 (11%)	1 (1%)	12	35
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	E	241/247 (98%)	202 (84%)	33 (14%)	6 (2%)	4	15
5	D	191/207 (92%)	148 (78%)	29 (15%)	14 (7%)	1	2
All	All	813/839 (97%)	693 (85%)	93 (11%)	27 (3%)	3	11

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
4	E	102	TYR
5	D	40	PRO
5	D	115	ILE
5	D	153	SER

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	231/232 (100%)	208 (90%)	23 (10%)	7	22
2	B	98/95 (103%)	96 (98%)	2 (2%)	48	76
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	17
4	E	209/213 (98%)	186 (89%)	23 (11%)	6	18
5	D	175/188 (93%)	150 (86%)	25 (14%)	3	9
All	All	722/737 (98%)	648 (90%)	74 (10%)	7	21

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	68	LYS
5	D	179	SER
5	D	92	GLU
5	D	149	GLN
2	B	85	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	215	GLN
5	D	22	ASN
5	D	191	ASN
2	B	13	HIS
2	B	42	ASN

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 oligosaccharides 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	275/276 (99%)	0.36	8 (2%) 53 45	42, 56, 86, 116	0
2	B	100/100 (100%)	0.33	4 (4%) 42 34	30, 55, 81, 114	3 (3%)
3	C	9/9 (100%)	0.18	0 100 100	43, 44, 50, 55	0
4	E	243/247 (98%)	1.09	43 (17%) 4 3	41, 66, 95, 121	0
5	D	193/207 (93%)	0.93	20 (10%) 11 10	44, 62, 101, 141	0
All	All	820/839 (97%)	0.71	75 (9%) 15 12	30, 60, 92, 141	3 (0%)

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	115	ILE	4.8
4	E	122	VAL	4.4
4	E	165	GLY	4.3
5	D	200	PHE	3.8
5	D	66	LEU	3.7

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 oligosaccharides 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.