



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2024 – 05:32 AM EDT

PDB ID : 4MNQ
Title : TCR-peptide specificity overrides affinity enhancing TCR-MHC interactions
Authors : Rizkallah, P.J.; Cole, D.K.; Sewell, A.K.; Jakobsen, B.K.
Deposited on : 2013-09-11
Resolution : 2.74 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>.

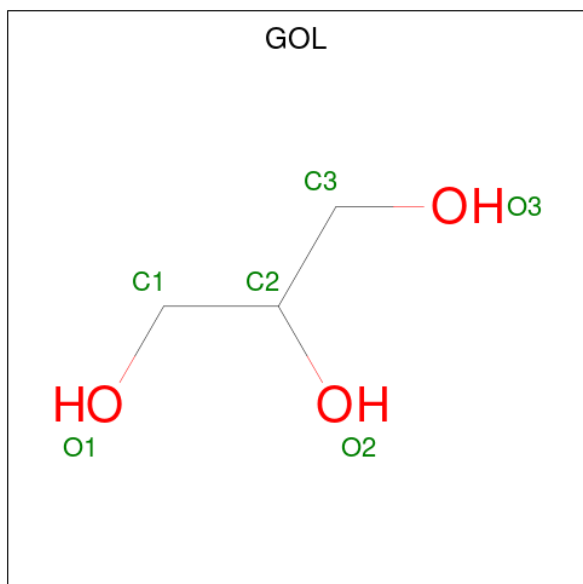
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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Chain	Residue	Modelled	Actual	Comment	Reference
E	99	GLU	-	linker	UNP A0A585
E	100	ALA	-	linker	UNP A0A585
E	101	PHE	-	linker	UNP A0A585
E	102	PHE	-	linker	UNP A0A585
E	103	GLY	-	linker	UNP A0A585
E	104	GLN	-	linker	UNP A0A585
E	105	GLY	-	linker	UNP A0A585
E	106	THR	-	linker	UNP A0A585
E	107	ARG	-	linker	UNP A0A585
E	108	LEU	-	linker	UNP A0A585
E	109	THR	-	linker	UNP A0A585
E	110	VAL	-	linker	UNP A0A585
E	111	VAL	-	linker	UNP A0A585
E	112	GLU	-	linker	UNP A0A585
E	148	TYR	PHE	conflict	UNP P01850
E	168	CYS	SER	conflict	UNP P01850
E	186	ALA	CYS	conflict	UNP P01850
E	200	ASP	ASN	conflict	UNP P01850

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		

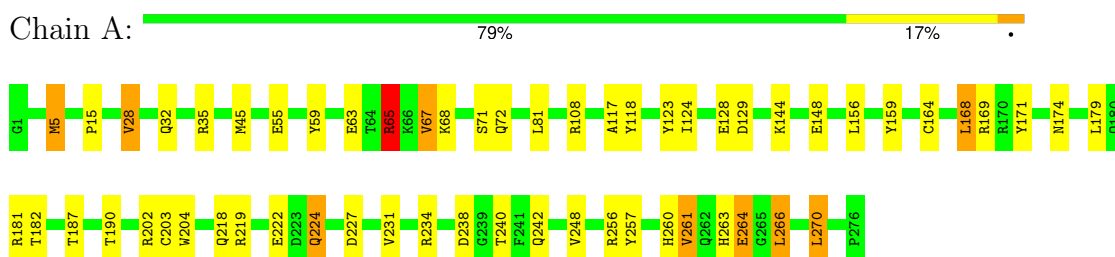
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	11	Total	O	0	0
			11	11		
8	B	5	Total	O	0	0
			5	5		
8	D	2	Total	O	0	0
			2	2		
8	E	3	Total	O	0	0
			3	3		

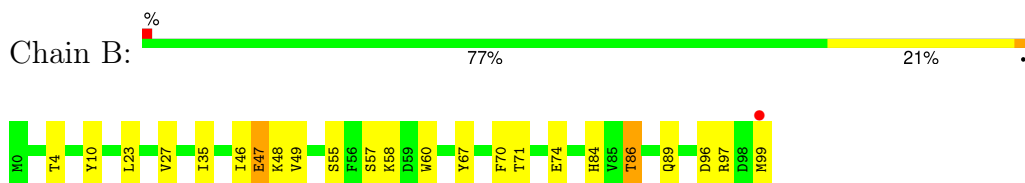
3 Residue-property plots

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



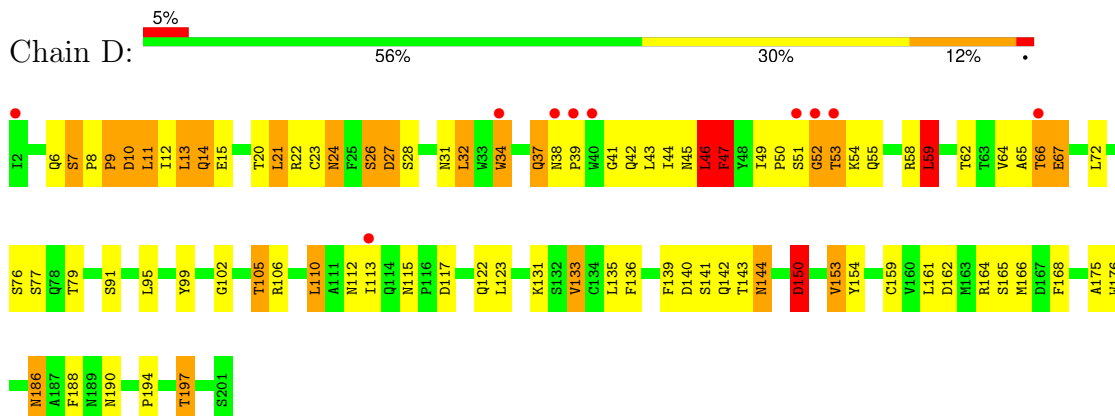
- Molecule 2: Beta-2-microglobulin



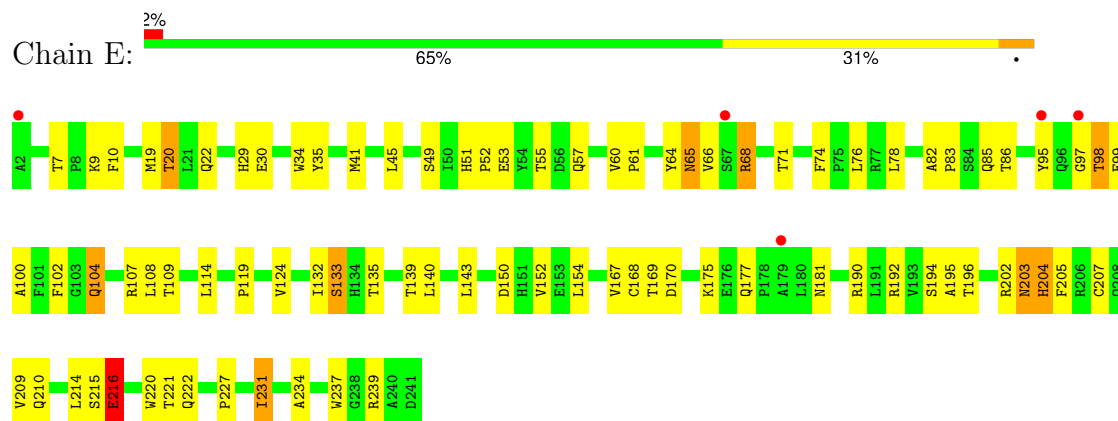
- Molecule 3: Telomerase reverse transcriptase



- Molecule 4: Uncharacterized protein, T-cell receptor, sp3.4 alpha chain



- Molecule 5: V_segment translation product, T-cell receptor beta-1 chain C region



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.22Å 48.49Å 118.07Å 90.00° 107.86° 90.00°	Depositor
Resolution (Å)	42.15 – 2.74 42.15 – 2.74	Depositor EDS
% Data completeness (in resolution range)	97.7 (42.15-2.74) 97.7 (42.15-2.74)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.214 , 0.284 0.217 , 0.286	Depositor DCC
R_{free} test set	1344 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6684	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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.

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Mol	Chain	Res	Type	Group
4	D	65	ALA	Peptide

5.2 Too-close contacts ⓘ

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	2254	0	2103	30	0
2	B	837	0	803	19	0
3	C	82	0	90	3	0
4	D	1565	0	1480	72	0
5	E	1911	0	1796	51	0
6	A	6	0	8	0	0
7	A	4	0	6	0	0
7	E	4	0	6	0	0
8	A	11	0	0	1	0
8	B	5	0	0	0	0
8	D	2	0	0	4	0
8	E	3	0	0	0	0
All	All	6684	0	6292	164	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 13.

The worst 5 of 164 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)
8:A:411:HOH:O	4:D:27:ASP:HB2	1.71	0.89
4:D:67:GLU:HA	8:D:402:HOH:O	1.74	0.86
4:D:49:ILE:O	4:D:64:VAL:HG21	1.79	0.81
4:D:67:GLU:CA	8:D:402:HOH:O	2.29	0.77
4:D:51:SER:O	4:D:53:THR:N	2.18	0.77

There are no symmetry-related clashes.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	209/209 (100%)	180 (86%)	29 (14%)	3	4
All	All	723/723 (100%)	628 (87%)	95 (13%)	3	5

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	131	LYS
5	E	65	ASN
4	D	144	ASN
4	D	197	THR
5	E	107	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	24	ASN
5	E	203	ASN
4	D	42	GLN
5	E	65	ASN
4	D	36	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

5.8 Polymer linkage issues ⓘ

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	276/276 (100%)	-0.10	0 100 100	27, 56, 101, 119	0
2	B	100/100 (100%)	-0.23	1 (1%) 79 81	26, 47, 75, 95	0
3	C	9/9 (100%)	-0.22	0 100 100	42, 46, 51, 54	0
4	D	200/200 (100%)	0.48	10 (5%) 35 36	42, 76, 110, 123	0
5	E	240/240 (100%)	0.06	5 (2%) 63 63	35, 68, 112, 129	0
All	All	825/825 (100%)	0.07	16 (1%) 66 66	26, 63, 107, 129	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	52	GLY	5.9
4	D	38	ASN	4.5
4	D	40	TRP	3.3
4	D	2	ILE	2.6
4	D	51	SER	2.6

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	A	302	4/4	0.68	0.15	59,65,67,68	0
7	EDO	E	301	4/4	0.78	0.16	61,61,65,70	0
6	GOL	A	301	6/6	0.86	0.10	70,73,75,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.