



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:34 PM GMT

PDB ID : 1G6R  
Title : A FUNCTIONAL HOT SPOT FOR ANTIGEN RECOGNITION IN A SUPERAGONIST TCR/MHC COMPLEX  
Authors : Degano, M.; Garcia, K.C.; Apostolopoulos, V.; Rudolph, M.G.; Teyton, L.; Wilson, I.A.  
Deposited on : 2000-11-07  
Resolution : 2.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

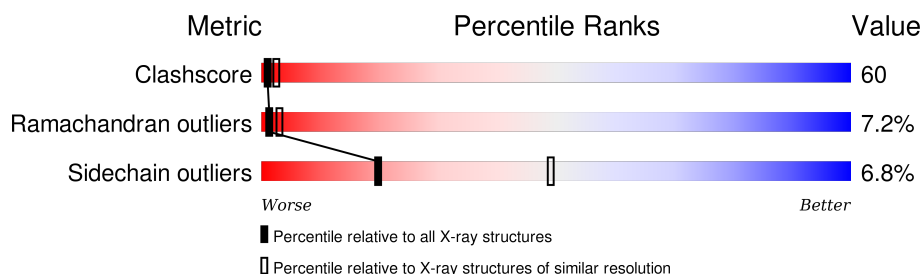
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)




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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	202	
1	C	202	
2	B	237	
2	D	237	
3	H	274	
3	I	274	
4	L	99	

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Mol	Chain	Length	Quality of chain
4	M	99	 23% 65% 12%
5	P	8	 13% 63% 13% 13%
5	Q	8	 75% 13% 13%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13100 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 ALPHA T CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1570	999	253	310	8			
1	C	202	Total	C	N	O	S	0	0	0
			1570	999	253	310	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	GLN	CONFLICT	UNP P01738
A	165	ALA	LYS	CONFLICT	UNP P01738
C	127	ALA	GLN	CONFLICT	UNP P01738
C	165	ALA	LYS	CONFLICT	UNP P01738

- Molecule 2 is a protein called BETA T CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	0	0
			1853	1160	331	355	7			
2	D	237	Total	C	N	O	S	0	0	0
			1853	1160	331	355	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	97	GLY	GLN	CONFLICT	UNP P01852
B	105	THR	ARG	CONFLICT	UNP P01852
B	11	LYS	ALA	CONFLICT	UNP P01852
B	107	TYR	GLU	CONFLICT	UNP P01852
B	108	PHE	GLN	CONFLICT	UNP P01852
B	109	GLY	PHE	CONFLICT	UNP P01852
B	110	ALA	PHE	CONFLICT	UNP P01852
B	?	-	PRO	DELETION	UNP P01852

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	DELETION	UNP P01852
B	115	SER	THR	CONFLICT	UNP P01852
D	97	GLY	GLN	CONFLICT	UNP P01852
D	105	THR	ARG	CONFLICT	UNP P01852
D	11	LYS	ALA	CONFLICT	UNP P01852
D	107	TYR	GLU	CONFLICT	UNP P01852
D	108	PHE	GLN	CONFLICT	UNP P01852
D	109	GLY	PHE	CONFLICT	UNP P01852
D	110	ALA	PHE	CONFLICT	UNP P01852
D	?	-	PRO	DELETION	UNP P01852
D	?	-	GLY	DELETION	UNP P01852
D	115	SER	THR	CONFLICT	UNP P01852

- Molecule 3 is a protein called MAJOR HISTOCOMPATIBILITY COMPLEX CLASS I MOLECULE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	274	Total	C	N	O	S	0	0	0
			2232	1408	393	422	9			
3	I	274	Total	C	N	O	S	0	0	0
			2232	1408	393	422	9			

- 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
			821	524	138	152	7			
4	M	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 5 is a protein called SIYR PEPTIDE.

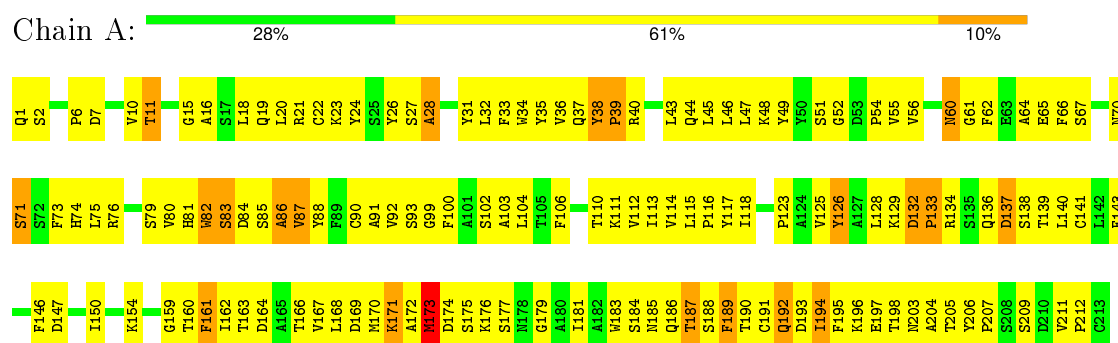
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	P	8	Total	C	N	O	0	0	0
			74	50	11	13			
5	Q	8	Total	C	N	O	0	0	0
			74	50	11	13			

### 3 Residue-property plots

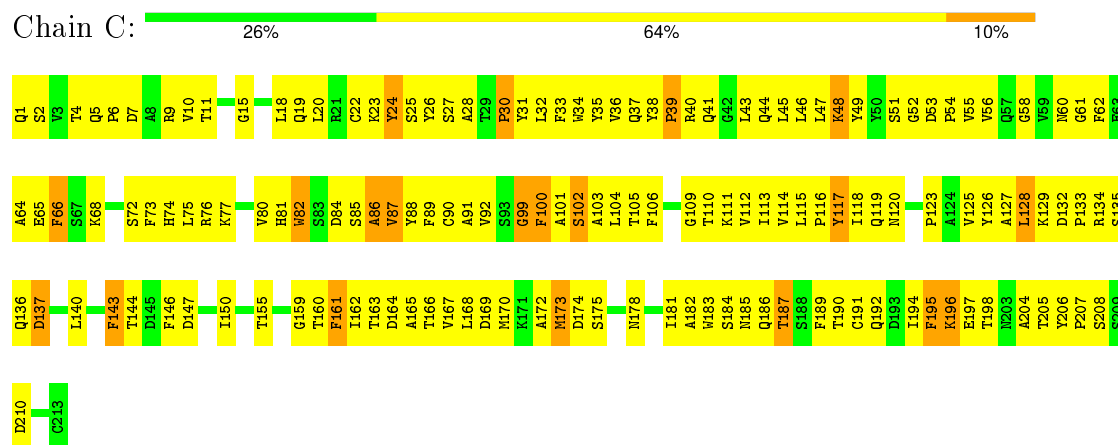
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

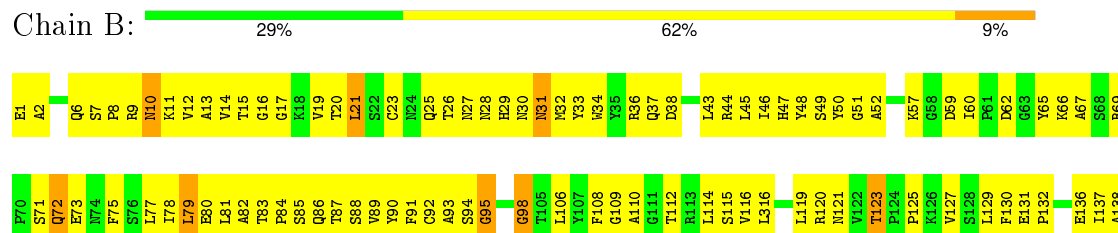
#### • Molecule 1: ALPHA T CELL RECEPTOR



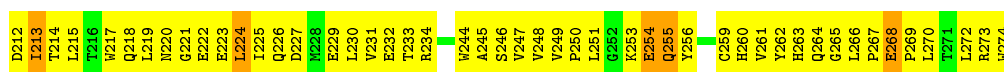
#### • Molecule 1: ALPHA T CELL RECEPTOR



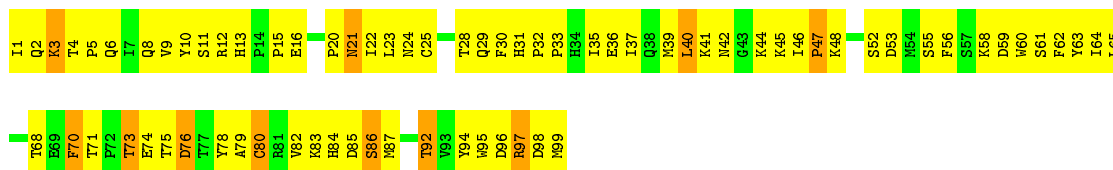
#### • Molecule 2: BETA T CELL RECEPTOR



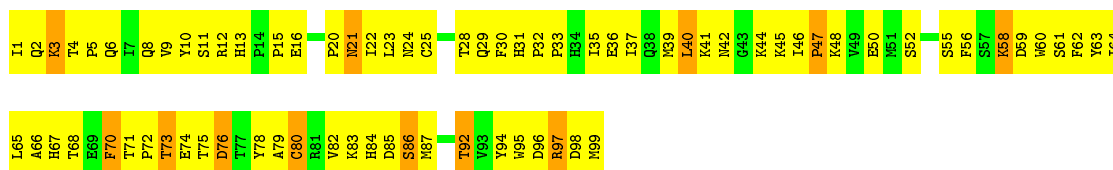




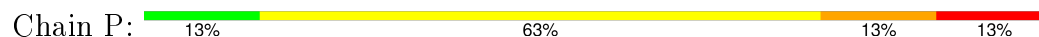
• Molecule 4: BETA-2 MICROGLOBULIN



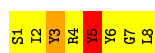
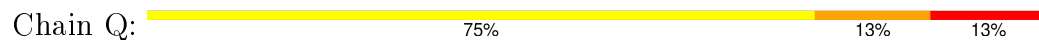
• Molecule 4: BETA-2 MICROGLOBULIN



• Molecule 5: SIYR PEPTIDE



• Molecule 5: SIYR PEPTIDE





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	297.71Å 94.57Å 84.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.80)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.298 , 0.327	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13100	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

## 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	0.56	0/1611	0.82	0/2193
1	C	0.43	0/1611	0.66	0/2193
2	B	0.56	0/1904	0.84	1/2586 (0.0%)
2	D	0.36	0/1904	0.62	0/2586
3	H	0.53	0/2293	0.76	1/3113 (0.0%)
3	I	0.48	0/2293	0.73	0/3113
4	L	0.50	0/847	0.74	0/1148
4	M	0.47	0/847	0.70	0/1148
5	P	0.69	0/76	0.84	0/100
5	Q	0.64	0/76	0.79	0/100
All	All	0.49	0/13462	0.74	2/18280 (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
2	B	0	1
5	P	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	201	LEU	N-CA-C	-5.49	96.18	111.00
2	B	221	GLU	N-CA-C	-5.48	96.20	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	50	TYR	Sidechain
5	P	3	TYR	Sidechain

## 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	1570	0	1508	205	0
1	C	1570	0	1508	206	0
2	B	1853	0	1767	242	0
2	D	1853	0	1767	242	0
3	H	2232	0	2127	249	0
3	I	2232	0	2127	235	0
4	L	821	0	798	107	0
4	M	821	0	798	108	0
5	P	74	0	72	19	0
5	Q	74	0	72	19	0
All	All	13100	0	12544	1521	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 60.

The worst 5 of 1521 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:C:85:SER:HB2	1:C:114:VAL:HG12	1.28	1.15
1:A:10:VAL:HB	1:A:112:VAL:HG12	1.27	1.14
1:A:85:SER:HB2	1:A:114:VAL:HG12	1.31	1.07
3:H:133:TRP:HB2	3:H:144:LYS:HE2	1.33	1.07
3:H:126:LEU:HD22	3:H:156:LEU:HD13	1.38	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	200/202 (99%)	155 (78%)	28 (14%)	17 (8%)	1	2
1	C	200/202 (99%)	148 (74%)	35 (18%)	17 (8%)	1	2
2	B	235/237 (99%)	186 (79%)	38 (16%)	11 (5%)	3	9
2	D	235/237 (99%)	178 (76%)	34 (14%)	23 (10%)	1	1
3	H	272/274 (99%)	202 (74%)	57 (21%)	13 (5%)	3	9
3	I	272/274 (99%)	205 (75%)	54 (20%)	13 (5%)	3	9
4	L	97/99 (98%)	78 (80%)	10 (10%)	9 (9%)	1	1
4	M	97/99 (98%)	79 (81%)	9 (9%)	9 (9%)	1	1
5	P	6/8 (75%)	1 (17%)	3 (50%)	2 (33%)	0	0
5	Q	6/8 (75%)	1 (17%)	3 (50%)	2 (33%)	0	0
All	All	1620/1640 (99%)	1233 (76%)	271 (17%)	116 (7%)	1	3

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ALA
1	A	38	TYR
1	A	61	GLY
1	A	82	TRP
1	A	173	MET

### 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	176/176 (100%)	165 (94%)	11 (6%)	22	53
1	C	176/176 (100%)	165 (94%)	11 (6%)	22	53
2	B	200/200 (100%)	182 (91%)	18 (9%)	12	34
2	D	200/200 (100%)	192 (96%)	8 (4%)	38	73
3	H	232/232 (100%)	215 (93%)	17 (7%)	17	44
3	I	232/232 (100%)	217 (94%)	15 (6%)	21	52
4	L	94/94 (100%)	86 (92%)	8 (8%)	13	36
4	M	94/94 (100%)	86 (92%)	8 (8%)	13	36
5	P	7/7 (100%)	7 (100%)	0	100	100
5	Q	7/7 (100%)	6 (86%)	1 (14%)	4	12
All	All	1418/1418 (100%)	1321 (93%)	97 (7%)	20	49

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	201	LEU
1	C	24	TYR
4	M	21	ASN
3	H	268	GLU
4	L	58	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
4	L	8	GLN
1	C	186	GLN
3	I	192	HIS
4	L	24	ASN
2	D	6	GLN

### 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 [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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.