

# Full wwPDB X-ray Structure Validation Report (i)

#### May 15, 2020 - 03:45 am BST

PDB ID : 2AQ2

Title : Crystal structure of T-cell receptor V beta domain variant complexed with

superantigen SEC3 mutant

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Deposited on : 2005-08-17

Resolution : 1.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.11

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)

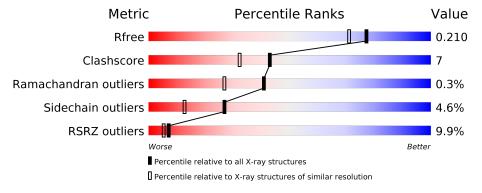
Validation Pipeline (wwPDB-VP) : 2.11

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 1.80 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 >=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 <=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	112	88%	8%	
2	В	237	83%	14%	



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3024 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 T-CELL RECEPTOR BETA CHAIN V.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	110	Total	С	N	О	S	0	0	0
1	A	110	841	520	148	170	3	U	0	0

• Molecule 2 is a protein called Enterotoxin type C-3.

Mol	Chain	Residues		$\mathbf{A}\mathbf{t}$	oms			ZeroOcc	AltConf	Trace
2	В	234	Total 1923	C 1224	N 314	O 375	S 10	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	?	-	GLY	SEE REMARK 999	UNP P0A0L5
В	?	-	LYS	SEE REMARK 999	UNP P0A0L5
В	102	TRP	VAL	SEE REMARK 999	UNP P0A0L5
В	103	TRP	THR	SEE REMARK 999	UNP P0A0L5
В	104	PRO	GLY	SEE REMARK 999	UNP P0A0L5

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

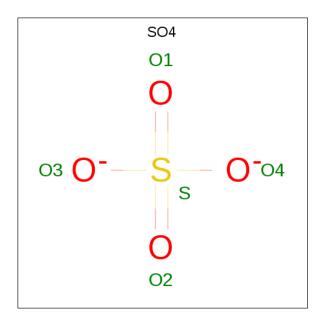
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Zn 1 1	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	3	Total Na 3 3	0	0

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total O S 5 4 1	0	0
5	В	1	Total O S 5 4 1	0	0
5	В	1	Total O S 5 4 1	0	0
5	В	1	Total O S 5 4 1	0	0
5	В	1	Total O S 5 4 1	0	0

#### • Molecule 6 is water.

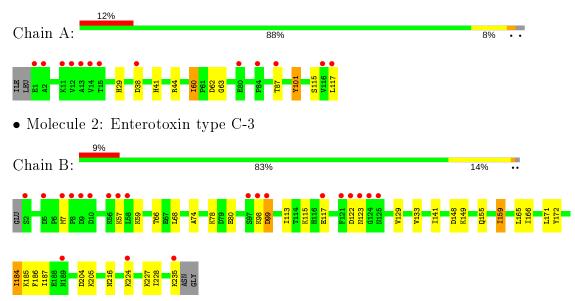
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	60	Total O 60 60	0	0
6	В	171	Total O 171 171	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: T-CELL RECEPTOR BETA CHAIN V





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants	96.54Å 96.54Å 92.18Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	40.00 - 1.80	Depositor
rtesolution (A)	38.07 - 1.80	EDS
% Data completeness	99.1 (40.00-1.80)	Depositor
(in resolution range)	99.1 (38.07-1.80)	EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.36 \; ({\rm at} \; 1.79 {\rm \AA})$	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
$R, R_{free}$	0.185 , $0.213$	Depositor
It, It free	0.184 , $0.210$	DCC
$R_{free}$ test set	2257  reflections  (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	$0.42\;,53.4$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.041 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3024	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ZN, SO4

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	Boı	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z >5	
1	A	0.77	$2/859 \ (0.2\%)$	0.73	2/1164 (0.2%)	
2	В	0.71	0/1969	0.70	0/2657	
All	All	0.73	$2/2828 \; (0.1\%)$	0.71	2/3821 (0.1%)	

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	Α	0	1

#### All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	A	101	TYR	C-N	9.29	1.55	1.34
1	A	62	ASP	C-N	-9.09	1.16	1.33

#### All (2) bond angle outliers are listed below:

ľ	Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
	1	A	63	GLY	O-C-N	-7.64	110.47	122.70
	1	Α	101	TYR	O-C-N	-5.62	113.71	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

$\mathbf{Mol}$	Chain	${f Res}$	$\mathbf{Type}$	$\mathbf{Group}$
1	A	101	TYR	Mainchain



### 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	841	0	794	8	0
2	В	1923	0	1854	29	0
3	В	1	0	0	0	0
4	В	3	0	0	0	0
5	В	25	0	0	1	0
6	A	60	0	0	5	0
6	В	171	0	0	2	0
All	All	3024	0	2648	37	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 7.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
2:B:155:GLN:O	2:B:159:ILE:HD13	1.68	0.93
2:B:166:ILE:HD11	2:B:172:TYR:CD1	2.09	0.87
2:B:80:GLU:HG3	2:B:115:LYS:NZ	1.99	0.77
2:B:80:GLU:HG3	2:B:115:LYS:CE	2.16	0.75
2:B:166:ILE:HD11	2:B:172:TYR:HD1	1.54	0.71
1:A:60:ILE:HG12	1:A:60:ILE:O	1.93	0.68
2:B:80:GLU:HG3	2:B:115:LYS:HZ3	1.59	0.67
1:A:41:HIS:HE1	6:A:147:HOH:O	1.79	0.65
1:A:29:HIS:ND1	6:A:161:HOH:O	2.31	0.61
2:B:184:ILE:HD12	2:B:186:PHE:CE1	2.36	0.61
2:B:227:LYS:C	2:B:228:ILE:HD12	2.22	0.60
2:B:185:LYS:HE2	2:B:187:ILE:CD1	2.32	0.59
2:B:129:VAL:HG12	2:B:228:ILE:HD13	1.85	0.58
2:B:80:GLU:HG3	2:B:115:LYS:HE2	1.86	0.57
2:B:184:ILE:HD11	2:B:228:ILE:HG23	1.88	0.56
2:B:66:THR:HG21	2:B:113:ILE:HD11	1.88	0.55
2:B:129:VAL:CG1	2:B:228:ILE:HD13	2.36	0.55
1:A:44:ARG:HB3	1:A:60:ILE:HD12	1.89	0.54
2:B:148:ASP:OD2	2:B:149:LYS:HG3	2.08	0.54
1:A:38:ASP:HB3	1:A:41:HIS:HB2	1.90	0.53

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Atom-1	Atom-2	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	Clash overlap (Å)
1:A:87:THR:HG23	1:A:115:SER:HA	1.92	0.52
2:B:99:ASP:OD2	2:B:99:ASP:N	2.43	0.51
1:A:41:HIS:CD2	6:A:169:HOH:O	2.63	0.50
2:B:228:ILE:N	2:B:228:ILE:HD12	2.27	0.49
2:B:235:LYS:HE2	6:B:1089:HOH:O	2.13	0.47
2:B:185:LYS:HE2	2:B:187:ILE:HD11	1.95	0.47
2:B:133:VAL:HB	2:B:141:ILE:HG23	1.97	0.47
2:B:166:ILE:HD13	2:B:171:LEU:HB3	1.99	0.44
2:B:117:GLU:HG2	6:B:1167:HOH:O	2.18	0.44
2:B:184:ILE:CD1	2:B:186:PHE:CE1	3.00	0.44
2:B:68:LEU:HD13	2:B:74:ALA:HA	1.99	0.43
2:B:78:LYS:HE2	5:B:503:SO4:O1	2.19	0.43
6:A:136:HOH:O	2:B:205:LYS:HE2	2.19	0.42
1:A:41:HIS:CE1	6:A:147:HOH:O	2.64	0.41
2:B:159:ILE:N	2:B:159:ILE:CD1	2.83	0.41
2:B:235:LYS:HB2	2:B:235:LYS:HE3	1.84	0.41
2:B:166:ILE:HD13	2:B:172:TYR:H	1.87	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		Allowed	$\mathbf{Outliers}$	Perce	$\mathbf{ntiles}$
1	A	$108/112 \; (96\%)$	106 (98%)	2 (2%)	0	100	100
2	В	232/237~(98%)	224 (97%)	7 (3%)	1 (0%)	34	21
All	All	340/349 (97%)	330 (97%)	9 (3%)	1 (0%)	41	27

#### All (1) Ramachandran outliers are listed below:

Mo	ol	Chain	Res	Type
2		В	122	ASP



#### 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	Analysed Rotameric		Percentiles
1	A	90/92 (98%)	88 (98%)	2 (2%)	52 39
2	В	217/219 (99%)	205 (94%)	12 (6%)	21 8
All	All	307/311 (99%)	293 (95%)	14 (5%)	27 13

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ILE
1	A	117	LEU
2	В	7	MET
2	В	57	LYS
2	В	59	LYS
2	В	98	LYS
2	В	99	ASP
2	В	123	ASN
2	В	159	ILE
2	В	165	LEU
2	В	184	ILE
2	В	204	ASP
2	В	216	ASN
2	В	224	LYS

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

Mol	Chain	Res	Type
1	A	29	HIS
2	В	216	ASN

#### 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 carbohydrates in this entry.

## 5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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 the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Type Chair		Chain	Chain Res Lin	T in le	Link Bond lengths			Bond angles		
10101	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	В	500	_	4,4,4	0.11	0	6,6,6	0.36	0
5	SO4	В	503	-	4,4,4	0.13	0	6,6,6	0.30	0
5	SO4	В	501	_	4,4,4	0.11	0	6,6,6	0.25	0
5	SO4	В	504	-	4,4,4	0.15	0	6,6,6	0.18	0
5	SO4	В	502	_	4,4,4	0.13	0	6,6,6	0.16	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type	Clashes	Symm-Clashes
5	В	503	SO4	1	0

## 5.7 Other polymers (i)

There are no such residues in this entry.



# 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	62:ASP	С	63:GLY	N	1.16



## 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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q < 0.9	
1	A	110/112 (98%)	0.57	13 (11%)	4	3	19, 33, 53, 54	0
2	В	$234/237 \ (98\%)$	0.35	21 (8%)	9	7	15, 24, 47, 57	0
All	All	344/349 (98%)	0.42	34 (9%)	7	5	15, 25, 50, 57	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	123	ASN	7.6
2	В	124	GLY	7.6
1	A	117	LEU	7.2
1	A	14	VAL	6.9
2	В	7	MET	5.6
2	В	99	ASP	5.1
2	В	122	ASP	4.8
2	В	121	PHE	4.8
2	В	58	LEU	4.4
2	В	56	LYS	4.3
1	A	12	VAL	4.3
2	В	97	SER	3.9
2	В	9	ASP	3.8
2	В	125	ASN	3.7
2	В	57	LYS	2.9
2	В	8	PRO	2.9
2	В	10	ASP	2.8
2	В	98	LYS	2.7
2	В	189	ASN	2.5
1	A	116	VAL	2.5
2	В	2	SER	2.4
1	A	11	LYS	2.3
2	В	235	LYS	2.3
2	В	117	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	В	5	ASP	2.3
1	A	2	ALA	2.3
1	A	84	PRO	2.2
1	A	87	THR	2.2
1	A	13	ALA	2.2
1	A	38	ASP	2.2
1	A	80	GLU	2.1
1	A	1	GLU	2.1
1	A	15	THR	2.1
2	В	224	LYS	2.0

### 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 carbohydrates 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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	NA	В	1004	1/1	0.88	0.24	40,40,40,40	0
4	NA	В	1003	1/1	0.89	0.27	48,48,48,48	0
5	SO4	В	504	5/5	0.93	0.30	74,74,75,75	0
5	SO4	В	500	5/5	0.94	0.12	41,44,46,48	0
5	SO4	В	503	5/5	0.95	0.10	64,65,66,66	0
4	NA	В	1002	1/1	0.96	0.13	39,39,39,39	0
3	ZN	В	1001	1/1	0.97	0.17	54,54,54,54	0
5	SO4	В	502	5/5	0.98	0.07	43,43,44,45	0
5	SO4	В	501	5/5	0.98	0.14	52,53,55,56	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

