



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 02:23 PM GMT

PDB ID : 2AQ3
Title : Crystal structure of T-cell receptor V beta domain variant complexed with superantigen SEC3
Authors : Cho, S.; Swaminathan, C.P.; Yang, J.; Kerzic, M.C.; Guan, R.; Kieke, M.C.; Kranz, D.M.; Mariuzza, R.A.; Sundberg, E.J.
Deposited on : 2005-08-17
Resolution : 2.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

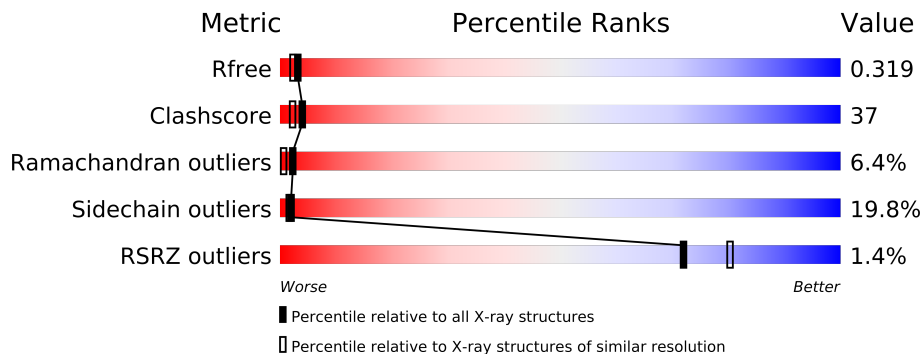
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	112	
1	C	112	
1	E	112	
1	G	112	
2	B	237	
2	D	237	
2	F	237	
2	H	237	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11155 atoms, of which 0 are hydrogen and 0 are deuterium.

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	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			828	513	147	165	3			
1	C	109	Total	C	N	O	S	0	0	0
			828	513	147	165	3			
1	E	109	Total	C	N	O	S	0	0	0
			828	513	147	165	3			
1	G	109	Total	C	N	O	S	0	0	0
			828	513	147	165	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1904	1207	312	375	10			
2	D	235	Total	C	N	O	S	0	0	0
			1913	1211	314	378	10			
2	F	234	Total	C	N	O	S	0	0	0
			1906	1205	312	379	10			
2	H	237	Total	C	N	O	S	0	0	0
			1922	1215	315	382	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	DELETION	UNP P0A0L5
B	?	-	VAL	DELETION	UNP P0A0L5
D	?	-	ASN	DELETION	UNP P0A0L5
D	?	-	VAL	DELETION	UNP P0A0L5
F	?	-	ASN	DELETION	UNP P0A0L5
F	?	-	VAL	DELETION	UNP P0A0L5
H	?	-	ASN	DELETION	UNP P0A0L5
H	?	-	VAL	DELETION	UNP P0A0L5

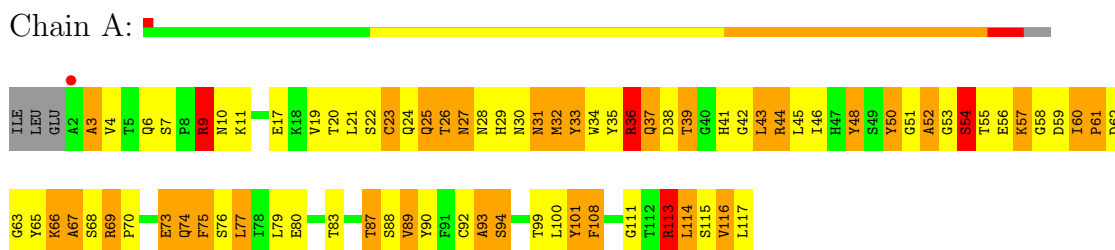
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total 21	O 21	0	0
3	B	48	Total 48	O 48	0	0
3	C	15	Total 15	O 15	0	0
3	D	31	Total 31	O 31	0	0
3	E	11	Total 11	O 11	0	0
3	F	31	Total 31	O 31	0	0
3	G	15	Total 15	O 15	0	0
3	H	26	Total 26	O 26	0	0

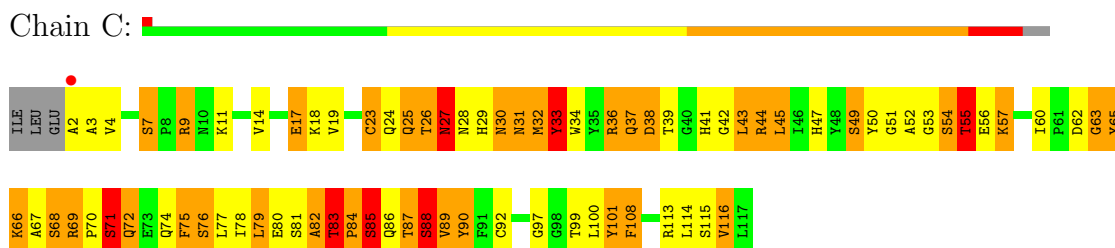
3 Residue-property plots

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.

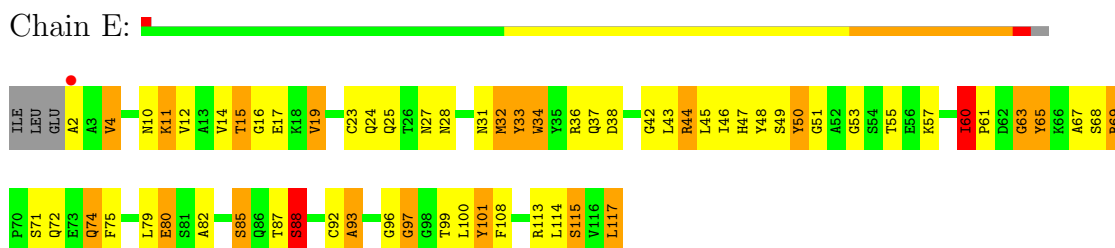
- Molecule 1: T-cell receptor beta chain V



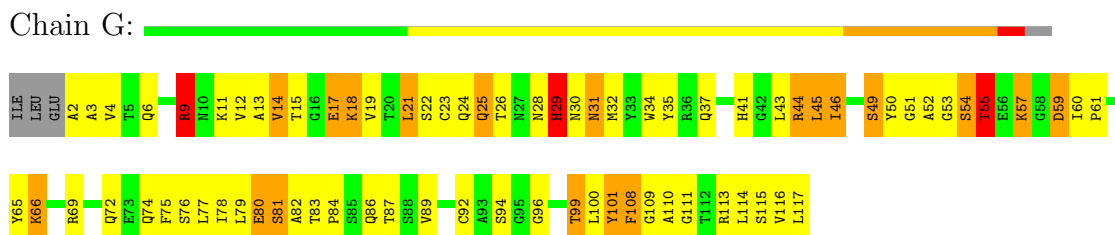
- Molecule 1: T-cell receptor beta chain V



- Molecule 1: T-cell receptor beta chain V



- Molecule 1: T-cell receptor beta chain V

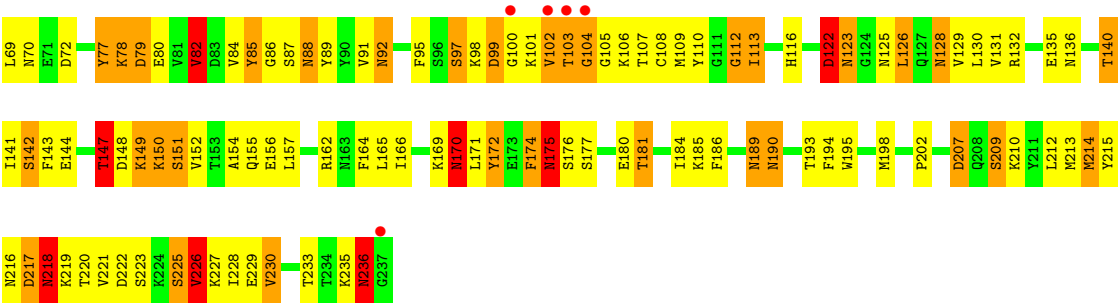


- Molecule 2: Enterotoxin type C-3



Response Category	Percentage
Strongly agree	25%
Agree	45%
Disagree	15%
Strongly disagree	15%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.16Å 70.46Å 98.37Å 74.18° 75.76° 88.40°	Depositor
Resolution (Å)	40.00 – 2.30 63.42 – 2.28	Depositor EDS
% Data completeness (in resolution range)	94.2 (40.00-2.30) 92.4 (63.42-2.28)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.206 , 0.271 0.213 , 0.319	Depositor DCC
R_{free} test set	3402 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 67372 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11155	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	2.51	38/845 (4.5%)	2.06	26/1142 (2.3%)
1	C	2.25	31/845 (3.7%)	1.88	19/1142 (1.7%)
1	E	2.20	24/846 (2.8%)	1.74	15/1145 (1.3%)
1	G	2.13	15/846 (1.8%)	1.98	22/1145 (1.9%)
2	B	2.05	63/1945 (3.2%)	1.72	37/2619 (1.4%)
2	D	1.83	26/1953 (1.3%)	1.67	32/2627 (1.2%)
2	F	1.83	31/1946 (1.6%)	1.60	22/2618 (0.8%)
2	H	1.77	30/1962 (1.5%)	1.56	22/2640 (0.8%)
All	All	2.00	258/11188 (2.3%)	1.73	195/15078 (1.3%)

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	6
1	E	0	1
1	G	0	1
2	B	0	5
2	D	0	1
2	F	0	4
2	H	0	1
All	All	0	19

The worst 5 of 258 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	TYR	C-N	23.04	1.87	1.34
1	E	101	TYR	C-N	21.36	1.83	1.34
1	C	63	GLY	C-N	20.06	1.80	1.34
1	E	63	GLY	C-N	18.65	1.76	1.34
1	G	101	TYR	C-N	17.43	1.74	1.34

The worst 5 of 195 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	101	TYR	O-C-N	-23.91	84.44	122.70
1	A	101	TYR	O-C-N	-22.11	87.32	122.70
1	E	101	TYR	O-C-N	-18.64	92.88	122.70
2	D	162	ARG	NE-CZ-NH1	-16.09	112.25	120.30
2	D	29	ASP	CB-CG-OD1	-13.04	106.57	118.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	ALA	Peptide
1	A	35	TYR	Peptide
1	A	54	SER	Mainchain
1	A	6	GLN	Peptide
1	A	61	PRO	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	828	0	786	79	1
1	C	828	0	786	79	1
1	E	828	0	786	60	0
1	G	828	0	787	66	0
2	B	1904	0	1847	125	0
2	D	1913	0	1852	121	0
2	F	1906	0	1839	135	0
2	H	1922	0	1853	155	0
3	A	21	0	0	1	0
3	B	48	0	0	12	0
3	C	15	0	0	1	0
3	D	31	0	0	3	0
3	E	11	0	0	0	0
3	F	31	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	15	0	0	1	0
3	H	26	0	0	2	0
All	All	11155	0	10536	803	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 37.

The worst 5 of 803 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:26:THR:CB	1:A:26:THR:CG2	1.76	1.60
2:B:27:LEU:CG	2:B:27:LEU:CD1	1.86	1.53
1:E:80:GLU:CG	1:E:80:GLU:CD	1.75	1.51
1:G:101:TYR:C	1:G:108:PHE:N	1.74	1.41
1:A:32:MET:SD	1:A:32:MET:CE	2.08	1.40

All (1) 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	Distance(Å)	Clash(Å)
1:A:26:THR:OG1	1:C:26:THR:CG2[1.455]	2.00	0.20

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	105/112 (94%)	91 (87%)	10 (10%)	4 (4%)	5	2
1	C	105/112 (94%)	92 (88%)	9 (9%)	4 (4%)	5	2
1	E	107/112 (96%)	83 (78%)	16 (15%)	8 (8%)	2	0
1	G	107/112 (96%)	88 (82%)	16 (15%)	3 (3%)	8	4
2	B	232/237 (98%)	188 (81%)	26 (11%)	18 (8%)	1	0
2	D	231/237 (98%)	175 (76%)	34 (15%)	22 (10%)	1	0
2	F	230/237 (97%)	185 (80%)	31 (14%)	14 (6%)	2	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	233/237 (98%)	167 (72%)	52 (22%)	14 (6%)	2	1
All	All	1350/1396 (97%)	1069 (79%)	194 (14%)	87 (6%)	2	0

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	28	ASN
1	A	39	THR
2	B	80	GLU
2	B	101	LYS

5.3.2 Protein sidechains ⓘ

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	88/91 (97%)	78 (89%)	10 (11%)	8	9
1	C	88/91 (97%)	60 (68%)	28 (32%)	0	0
1	E	88/91 (97%)	71 (81%)	17 (19%)	2	2
1	G	88/91 (97%)	67 (76%)	21 (24%)	1	0
2	B	215/217 (99%)	183 (85%)	32 (15%)	4	4
2	D	216/217 (100%)	177 (82%)	39 (18%)	2	2
2	F	215/217 (99%)	159 (74%)	56 (26%)	1	0
2	H	216/217 (100%)	179 (83%)	37 (17%)	3	3
All	All	1214/1232 (98%)	974 (80%)	240 (20%)	2	1

5 of 240 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	224	LYS
2	F	39	LYS
2	H	140	THR
1	E	37	GLN
1	E	85	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	88	ASN
2	D	163	ASN
2	H	189	ASN
2	D	92	ASN
2	D	128	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	109/112 (97%)	-0.24	1 (0%) 81 88	8, 35, 52, 59	0
1	C	109/112 (97%)	-0.23	1 (0%) 81 88	21, 39, 58, 66	0
1	E	109/112 (97%)	-0.14	1 (0%) 81 88	27, 47, 64, 70	0
1	G	109/112 (97%)	-0.17	0 100 100	24, 40, 59, 63	0
2	B	234/237 (98%)	-0.25	2 (0%) 81 88	10, 41, 65, 86	0
2	D	235/237 (99%)	-0.11	7 (2%) 48 58	23, 47, 71, 87	0
2	F	234/237 (98%)	-0.20	1 (0%) 90 95	29, 45, 75, 91	0
2	H	237/237 (100%)	-0.00	6 (2%) 54 65	27, 50, 76, 103	0
All	All	1376/1396 (98%)	-0.16	19 (1%) 72 80	8, 44, 69, 103	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	237	GLY	4.9
2	H	102	VAL	4.3
1	A	2	ALA	4.2
2	H	103	THR	3.8
1	E	2	ALA	3.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.