



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 20, 2016 – 05:57 PM EDT

PDB ID : 5SWZ  
Title : Crystal Structure of NP1-B17 TCR-H2Db-NP complex  
Authors : Gras, S.; Del Campo, C.M.; Farenc, C.; Josephs, T.M.; Rossjohn, J.  
Deposited on : 2016-08-09  
Resolution : 2.65 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

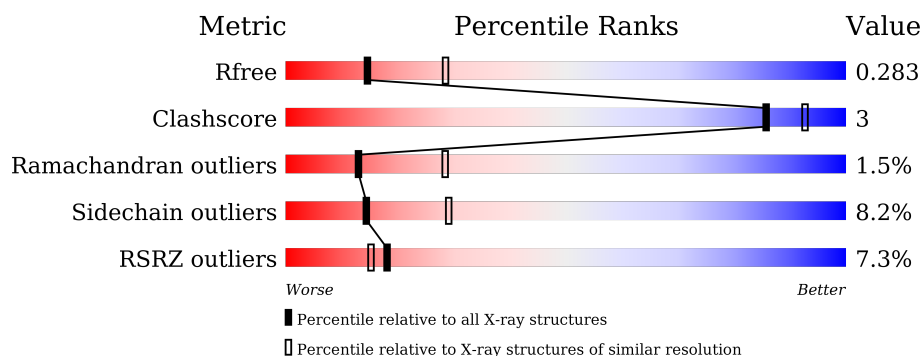
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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.

Mol	Chain	Length	Quality of chain
1	A	280	<div> <div>3%</div> <div>86% 12% ..</div> </div>
1	F	280	<div> <div>8%</div> <div>82% 16% ..</div> </div>
1	K	280	<div> <div>8%</div> <div>84% 14% ..</div> </div>
1	P	280	<div> <div>13%</div> <div>72% 13% 15%</div> </div>
2	B	99	<div> <div>%</div> <div>86% 12% .</div> </div>
2	G	99	<div> <div>8%</div> <div>81% 16% .</div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	L	99	
2	Q	99	
3	C	9	
3	H	9	
3	M	9	
3	R	9	
4	D	207	
4	I	207	
4	N	207	
4	S	207	
5	E	243	
5	J	243	
5	O	243	
5	T	243	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	D	301	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27034 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	5	0
			2317	1460	415	433	9			
1	F	277	Total	C	N	O	S	0	5	0
			2317	1460	415	433	9			
1	K	277	Total	C	N	O	S	0	5	0
			2317	1460	415	433	9			
1	P	238	Total	C	N	O	S	0	4	0
			1983	1250	353	371	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			818	523	138	150	7			
2	G	99	Total	C	N	O	S	0	1	0
			826	528	139	151	8			
2	L	99	Total	C	N	O	S	0	1	0
			826	528	139	151	8			
2	Q	98	Total	C	N	O	S	0	1	0
			818	522	138	150	8			

- Molecule 3 is a protein called influenza NP366 epitope.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			68	38	10	18	2			
3	H	9	Total	C	N	O	S	0	0	0
			68	38	10	18	2			
3	M	9	Total	C	N	O	S	0	0	0
			68	38	10	18	2			
3	R	9	Total	C	N	O	S	0	0	0
			68	38	10	18	2			

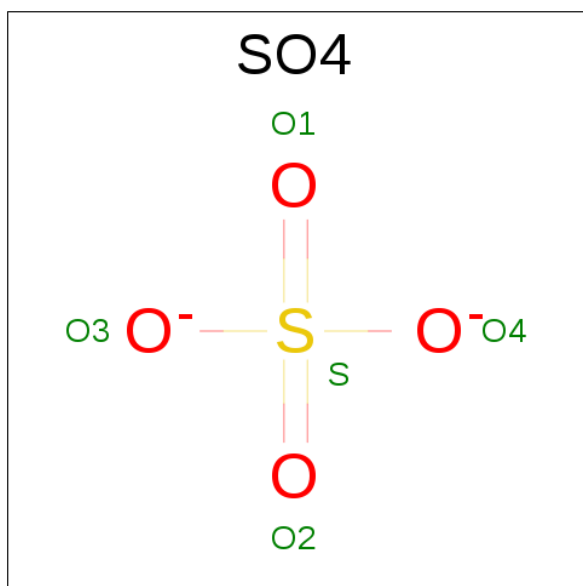
- Molecule 4 is a protein called NP1-B17 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	198	Total	C	N	O	S	0	0	0
			1557	977	256	318	6			
4	I	186	Total	C	N	O	S	0	0	0
			1461	916	241	299	5			
4	N	201	Total	C	N	O	S	0	0	0
			1586	996	260	323	7			
4	S	203	Total	C	N	O	S	0	0	0
			1598	1002	262	327	7			

- Molecule 5 is a protein called NP1-B17 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	240	Total	C	N	O	S	0	0	0
			1940	1231	338	362	9			
5	J	240	Total	C	N	O	S	0	0	0
			1940	1231	338	362	9			
5	O	241	Total	C	N	O	S	0	1	0
			1960	1241	343	367	9			
5	T	239	Total	C	N	O	S	0	0	0
			1935	1228	337	361	9			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	O	1	Total	O	S	0	0
			5	4	1		
6	T	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	Na	0	0
			1	1		
7	I	1	Total	Na	0	0
			1	1		
7	T	2	Total	Na	0	0
			2	2		
7	K	1	Total	Na	0	0
			1	1		
7	E	1	Total	Na	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	55	Total	O	0	0
			55	55		
8	B	15	Total	O	0	0
			15	15		
8	C	4	Total	O	0	0
			4	4		
8	D	30	Total	O	0	0
			30	30		
8	E	50	Total	O	0	0
			50	50		
8	F	31	Total	O	0	0
			31	31		
8	G	18	Total	O	0	0
			18	18		
8	H	2	Total	O	0	0
			2	2		

*Continued on next page...*

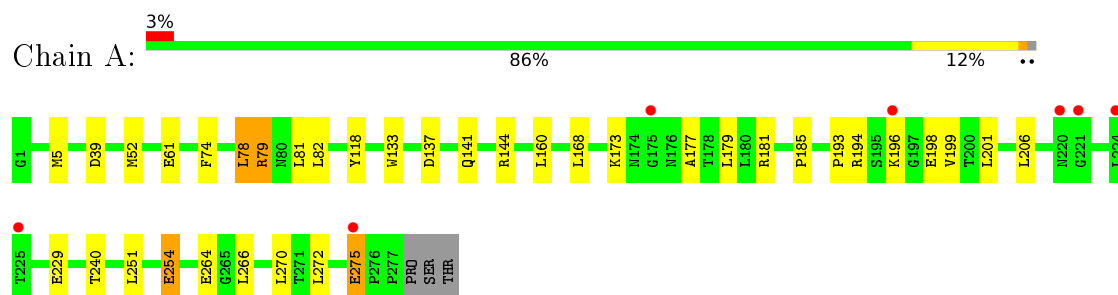
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	23	Total 23	O 23	0	0
8	J	33	Total 33	O 33	0	0
8	K	40	Total 40	O 40	0	0
8	L	19	Total 19	O 19	0	0
8	M	1	Total 1	O 1	0	0
8	N	32	Total 32	O 32	0	0
8	O	57	Total 57	O 57	0	0
8	P	40	Total 40	O 40	0	0
8	Q	14	Total 14	O 14	0	0
8	R	2	Total 2	O 2	0	0
8	S	22	Total 22	O 22	0	0
8	T	44	Total 44	O 44	0	0

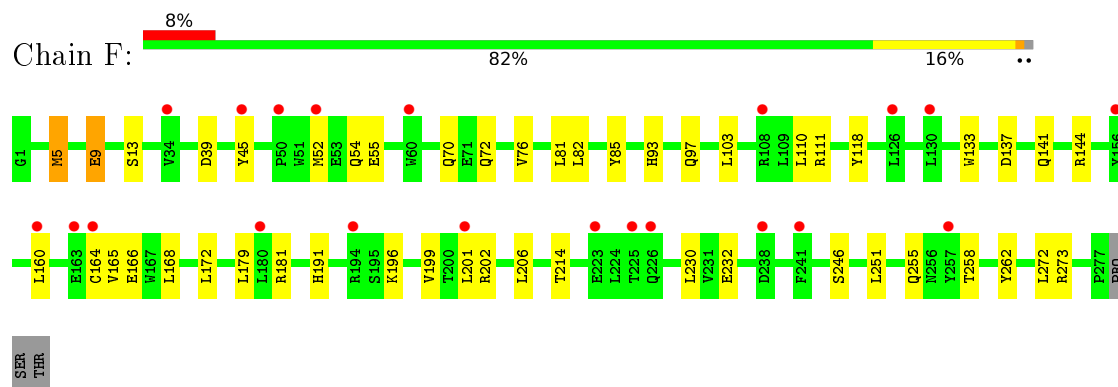
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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.

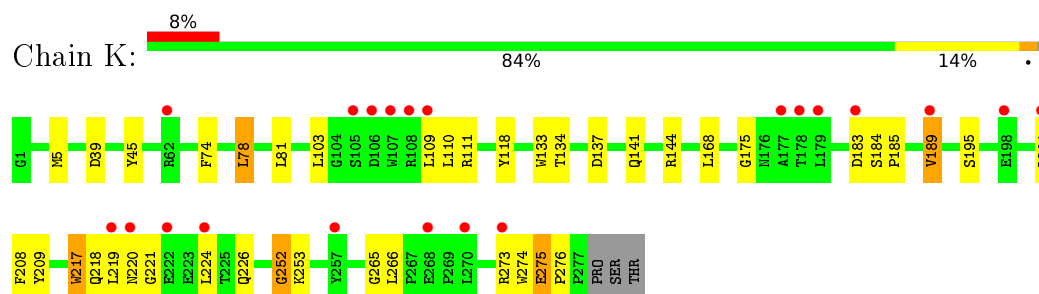
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



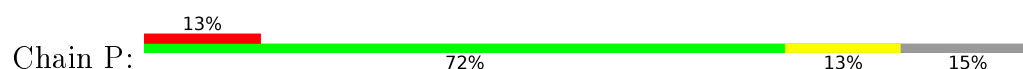
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



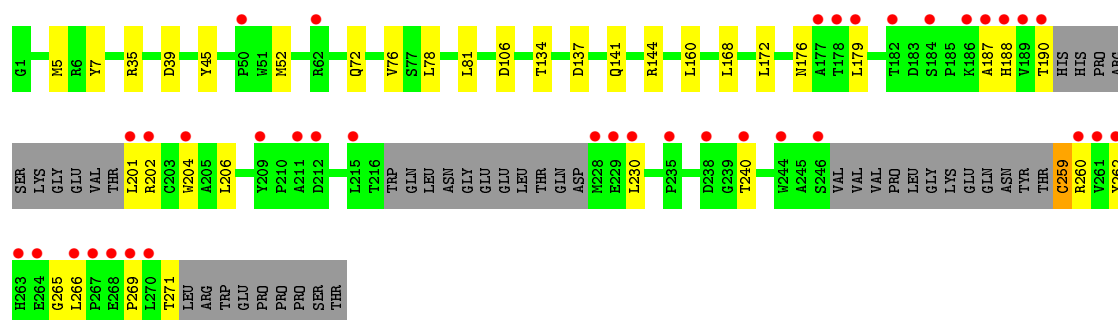
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



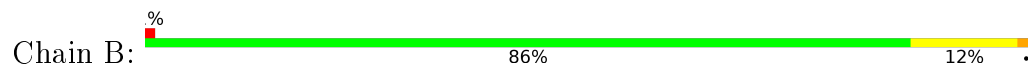
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



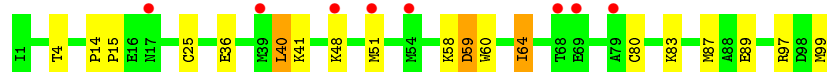
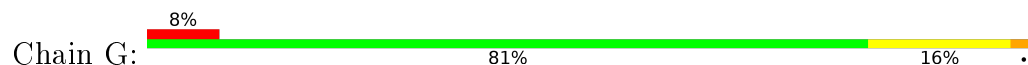




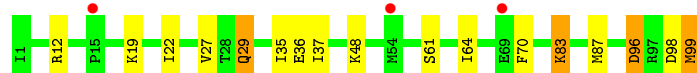
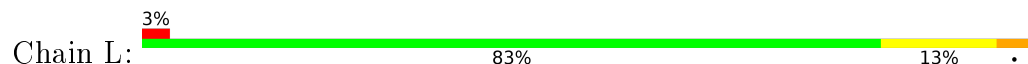
- Molecule 2: Beta-2-microglobulin



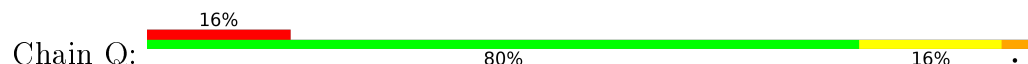
- Molecule 2: Beta-2-microglobulin



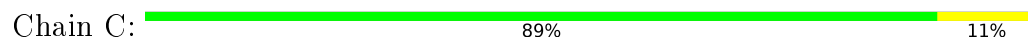
- Molecule 2: Beta-2-microglobulin



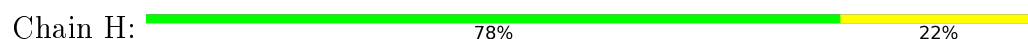
- Molecule 2: Beta-2-microglobulin



- Molecule 3: influenza NP366 epitope



- Molecule 3: influenza NP366 epitope





- Molecule 3: influenza NP366 epitope

Chain M: 78% 22%



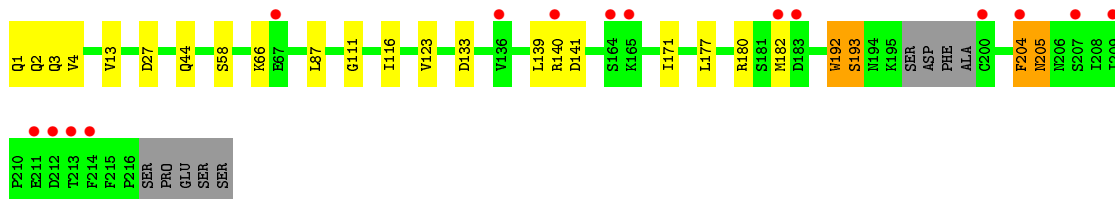
- Molecule 3: influenza NP366 epitope

Chain R: 78% 22%



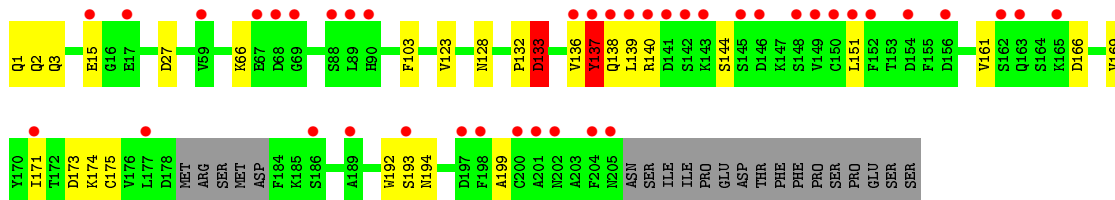
- Molecule 4: NP1-B17 TCR alpha chain

Chain D: 7% 84% 10% . .



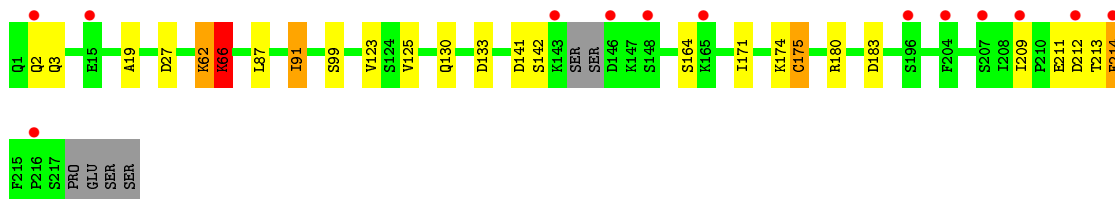
- Molecule 4: NP1-B17 TCR alpha chain

Chain I: 20% 76% 13% . 10%



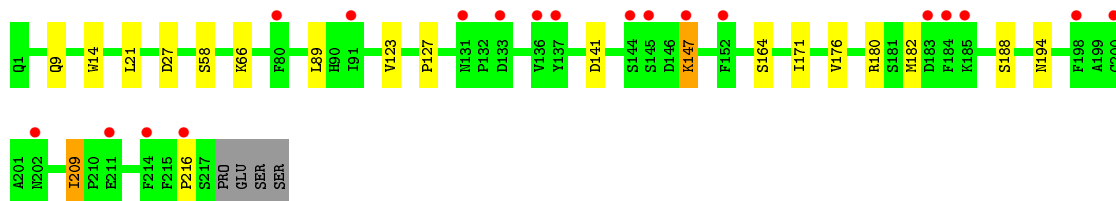
- Molecule 4: NP1-B17 TCR alpha chain

Chain N: 6% 85% 10% . .



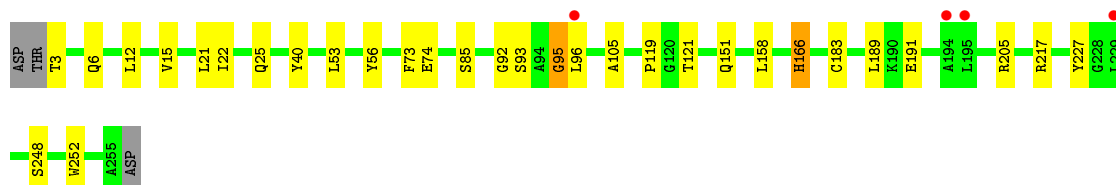
- Molecule 4: NP1-B17 TCR alpha chain

Chain S: 9% 88% 9% ..



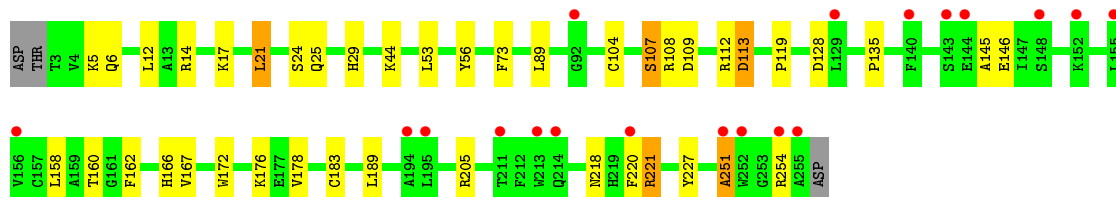
• Molecule 5: NP1-B17 TCR beta chain

Chain E: 2% 86% 12% ..



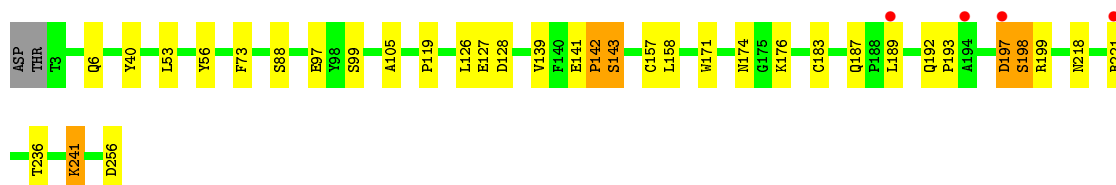
• Molecule 5: NP1-B17 TCR beta chain

Chain J: 8% 81% 15% ..



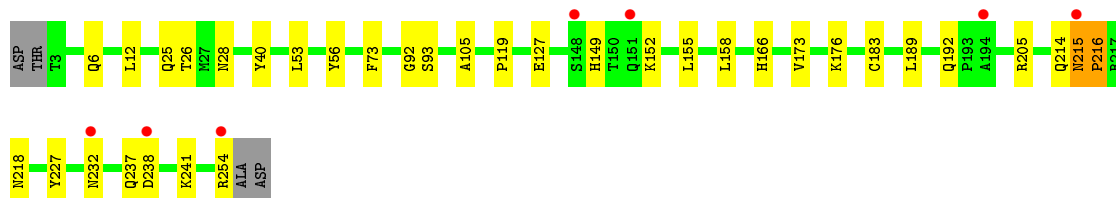
• Molecule 5: NP1-B17 TCR beta chain

Chain O: 2% 85% 12% ..



• Molecule 5: NP1-B17 TCR beta chain

Chain T: 3% 84% 14% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.23Å 100.19Å 469.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.80 – 2.65 47.71 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.80-2.65) 100.0 (47.71-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, $R_{free}$	0.226 , 0.249 0.258 , 0.283	Depositor DCC
$R_{free}$ test set	6526 reflections (5.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.7	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	27034	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.35	0/2385	0.56	0/3240
1	F	0.37	0/2385	0.59	2/3240 (0.1%)
1	K	0.38	0/2385	0.60	2/3240 (0.1%)
1	P	0.36	0/2037	0.56	0/2759
2	B	0.39	0/844	0.61	1/1144 (0.1%)
2	G	0.39	0/852	0.64	2/1154 (0.2%)
2	L	0.38	0/852	0.61	0/1154
2	Q	0.39	0/844	0.60	0/1143
3	C	0.29	0/67	0.48	0/86
3	H	0.30	0/67	0.48	0/86
3	M	0.30	0/67	0.47	0/86
3	R	0.30	0/67	0.50	0/86
4	D	0.38	0/1594	0.61	1/2164 (0.0%)
4	I	0.42	0/1495	0.66	2/2028 (0.1%)
4	N	0.36	0/1624	0.56	0/2203
4	S	0.37	0/1637	0.56	0/2222
5	E	0.34	0/1994	0.58	0/2711
5	J	0.37	0/1994	0.63	1/2711 (0.0%)
5	O	0.35	0/2014	0.65	4/2736 (0.1%)
5	T	0.35	0/1989	0.62	0/2704
All	All	0.37	0/27193	0.60	15/36897 (0.0%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	142	PRO	C-N-CA	6.40	137.70	121.70
5	O	197	ASP	C-N-CA	6.00	136.69	121.70
1	F	164	CYS	C-N-CA	5.93	136.51	121.70
5	J	104	CYS	CA-CB-SG	5.74	124.33	114.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	40	LEU	C-N-CA	5.65	135.83	121.70

There are no chirality outliers.

There are no planarity outliers.

## 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	2317	0	2193	11	0
1	F	2317	0	2193	11	0
1	K	2317	0	2193	17	0
1	P	1983	0	1872	10	0
2	B	818	0	797	5	0
2	G	826	0	807	9	0
2	L	826	0	805	6	0
2	Q	818	0	793	6	0
3	C	68	0	54	0	0
3	H	68	0	54	1	0
3	M	68	0	54	0	0
3	R	68	0	54	2	0
4	D	1557	0	1458	7	0
4	I	1461	0	1373	11	0
4	N	1586	0	1491	8	0
4	S	1598	0	1502	5	0
5	E	1940	0	1867	7	0
5	J	1940	0	1869	14	0
5	O	1960	0	1885	10	0
5	T	1935	0	1863	9	0
6	D	5	0	0	0	0
6	E	5	0	0	0	0
6	K	5	0	0	0	0
6	O	5	0	0	0	0
6	T	5	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	K	1	0	0	0	0
7	T	2	0	0	0	0
8	A	55	0	0	0	0
8	B	15	0	0	0	0
8	C	4	0	0	0	0
8	D	30	0	0	0	0
8	E	50	0	0	0	0
8	F	31	0	0	0	0
8	G	18	0	0	0	0
8	H	2	0	0	0	0
8	I	23	0	0	0	0
8	J	33	0	0	0	0
8	K	40	0	0	0	0
8	L	19	0	0	0	0
8	M	1	0	0	0	0
8	N	32	0	0	0	0
8	O	57	0	0	0	0
8	P	40	0	0	0	0
8	Q	14	0	0	0	0
8	R	2	0	0	0	0
8	S	22	0	0	0	0
8	T	44	0	0	0	0
All	All	27034	0	25177	142	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 3.

The worst 5 of 142 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)
2:G:25:CYS:HG	2:G:80:CYS:HG	1.03	0.96
5:J:109:ASP:OD2	5:J:113:ASP:HB2	1.67	0.94
5:J:108:ARG:NH2	5:J:113:ASP:OD1	2.06	0.85
5:J:145:ALA:HB1	5:J:146:GLU:HA	1.57	0.84
4:D:3:GLN:H	4:D:4:VAL:HA	1.44	0.83

There are no symmetry-related clashes.

## 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	280/280 (100%)	262 (94%)	14 (5%)	4 (1%)	14	31
1	F	280/280 (100%)	264 (94%)	15 (5%)	1 (0%)	39	65
1	K	280/280 (100%)	250 (89%)	25 (9%)	5 (2%)	11	23
1	P	234/280 (84%)	221 (94%)	11 (5%)	2 (1%)	21	44
2	B	97/99 (98%)	94 (97%)	2 (2%)	1 (1%)	19	41
2	G	98/99 (99%)	93 (95%)	5 (5%)	0	100	100
2	L	98/99 (99%)	94 (96%)	4 (4%)	0	100	100
2	Q	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
3	H	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
3	M	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
3	R	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
4	D	194/207 (94%)	175 (90%)	15 (8%)	4 (2%)	9	20
4	I	182/207 (88%)	160 (88%)	18 (10%)	4 (2%)	8	19
4	N	197/207 (95%)	185 (94%)	8 (4%)	4 (2%)	9	21
4	S	201/207 (97%)	178 (89%)	19 (10%)	4 (2%)	9	21
5	E	238/243 (98%)	224 (94%)	11 (5%)	3 (1%)	15	33
5	J	238/243 (98%)	221 (93%)	15 (6%)	2 (1%)	24	47
5	O	240/243 (99%)	221 (92%)	14 (6%)	5 (2%)	9	20
5	T	237/243 (98%)	212 (90%)	20 (8%)	5 (2%)	9	20
All	All	3219/3352 (96%)	2972 (92%)	199 (6%)	48 (2%)	13	28

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	196	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
4	I	137	TYR
4	I	140	ARG
1	K	195	SER
1	K	275	GLU

### 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	240/238 (101%)	223 (93%)	17 (7%)	18	38
1	F	240/238 (101%)	211 (88%)	29 (12%)	6	12
1	K	240/238 (101%)	225 (94%)	15 (6%)	22	44
1	P	203/238 (85%)	182 (90%)	21 (10%)	9	18
2	B	93/93 (100%)	87 (94%)	6 (6%)	21	43
2	G	94/93 (101%)	88 (94%)	6 (6%)	22	43
2	L	94/93 (101%)	84 (89%)	10 (11%)	8	17
2	Q	93/93 (100%)	83 (89%)	10 (11%)	8	16
3	C	8/8 (100%)	8 (100%)	0	100	100
3	H	8/8 (100%)	8 (100%)	0	100	100
3	M	8/8 (100%)	7 (88%)	1 (12%)	6	11
3	R	8/8 (100%)	8 (100%)	0	100	100
4	D	178/188 (95%)	164 (92%)	14 (8%)	15	32
4	I	167/188 (89%)	157 (94%)	10 (6%)	24	47
4	N	182/188 (97%)	166 (91%)	16 (9%)	12	25
4	S	184/188 (98%)	175 (95%)	9 (5%)	31	58
5	E	212/215 (99%)	196 (92%)	16 (8%)	17	35
5	J	212/215 (99%)	192 (91%)	20 (9%)	11	22
5	O	214/215 (100%)	197 (92%)	17 (8%)	15	32
5	T	212/215 (99%)	194 (92%)	18 (8%)	13	27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2890/2968 (97%)	2655 (92%)	235 (8%)	14	30

5 of 235 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	J	128	ASP
1	K	224	LEU
5	T	12	LEU
5	J	167	VAL
1	K	45	TYR

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

Mol	Chain	Res	Type
5	J	82	ASN
5	J	83	ASN
4	S	202	ASN
5	J	7	ASN
5	O	174	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 6 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	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	SO4	D	301	-	4,4,4	0.19	0	6,6,6	0.08	0
6	SO4	E	301	-	4,4,4	0.17	0	6,6,6	0.07	0
6	SO4	K	301	-	4,4,4	0.18	0	6,6,6	0.06	0
6	SO4	O	301	-	4,4,4	0.17	0	6,6,6	0.08	0
6	SO4	T	301	-	4,4,4	0.19	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	D	301	-	-	0/0/0/0	0/0/0/0
6	SO4	E	301	-	-	0/0/0/0	0/0/0/0
6	SO4	K	301	-	-	0/0/0/0	0/0/0/0
6	SO4	O	301	-	-	0/0/0/0	0/0/0/0
6	SO4	T	301	-	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

## 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	277/280 (98%)	0.30	7 (2%) 61 59	33, 61, 99, 120	7 (2%)
1	F	277/280 (98%)	0.66	21 (7%) 17 14	40, 84, 117, 143	7 (2%)
1	K	277/280 (98%)	0.49	21 (7%) 17 14	34, 67, 109, 123	7 (2%)
1	P	238/280 (85%)	0.81	37 (15%) 3 2	37, 66, 159, 198	5 (2%)
2	B	99/99 (100%)	0.32	1 (1%) 84 84	41, 59, 79, 88	2 (2%)
2	G	99/99 (100%)	0.78	8 (8%) 15 12	54, 75, 103, 111	0
2	L	99/99 (100%)	0.33	3 (3%) 54 52	43, 63, 91, 102	0
2	Q	98/99 (98%)	0.88	16 (16%) 2 1	48, 85, 108, 115	0
3	C	9/9 (100%)	-0.05	0 100 100	40, 42, 48, 51	0
3	H	9/9 (100%)	0.06	0 100 100	50, 60, 68, 72	0
3	M	9/9 (100%)	-0.17	0 100 100	42, 49, 59, 60	0
3	R	9/9 (100%)	0.19	0 100 100	41, 49, 56, 59	0
4	D	198/207 (95%)	0.43	15 (7%) 17 14	39, 64, 115, 129	1 (0%)
4	I	186/207 (89%)	1.14	41 (22%) 1 1	52, 84, 162, 187	1 (0%)
4	N	201/207 (97%)	0.61	13 (6%) 22 20	46, 72, 109, 144	1 (0%)
4	S	203/207 (98%)	0.69	19 (9%) 11 8	43, 79, 122, 140	1 (0%)
5	E	240/243 (98%)	0.18	4 (1%) 73 72	32, 56, 92, 106	1 (0%)
5	J	240/243 (98%)	0.58	19 (7%) 15 13	40, 74, 138, 163	0
5	O	241/243 (99%)	0.23	4 (1%) 73 72	34, 57, 87, 108	2 (0%)
5	T	239/243 (98%)	0.39	7 (2%) 55 53	34, 64, 100, 124	1 (0%)
All	All	3248/3352 (96%)	0.53	236 (7%) 18 15	32, 68, 117, 198	36 (1%)

The worst 5 of 236 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	187	ALA	11.2
4	I	138	GLN	10.0
4	I	139	LEU	9.1
4	I	140	ARG	8.9
1	P	268	GLU	8.4

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	D	301	5/5	0.71	0.25	3.58	118,118,119,119	0
6	SO4	T	301	5/5	0.73	0.35	1.37	115,115,115,115	0
7	NA	E	302	1/1	0.85	0.17	0.43	50,50,50,50	0
7	NA	I	301	1/1	0.92	0.23	0.23	48,48,48,48	0
6	SO4	E	301	5/5	0.80	0.17	-0.15	115,116,116,116	0
7	NA	J	301	1/1	0.85	0.16	-0.55	38,38,38,38	0
7	NA	T	302	1/1	0.91	0.11	-1.63	42,42,42,42	0
6	SO4	O	301	5/5	0.92	0.13	-1.76	102,102,102,102	0
7	NA	T	303	1/1	0.88	0.10	-1.94	49,49,49,49	0
6	SO4	K	301	5/5	0.88	0.12	-	114,114,114,115	0
7	NA	K	302	1/1	0.95	0.06	-	79,79,79,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.