



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 03:00 PM UTC

PDB ID : 5SWZ / pdb_00005swz
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

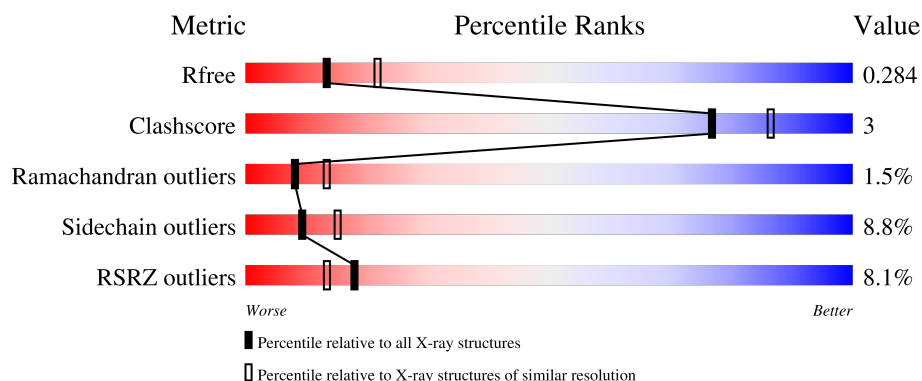
1 Overall quality at a glance

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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 of 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 $\leq 5\%$. 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	4% 85% 12% ..
1	F	280	11% 81% 17% ..
1	K	280	8% 81% 14% ..
1	P	280	8% 71% 13% 15%
2	B	99	5% 89% 8% .

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Mol	Chain	Length	Quality of chain
2	G	99	
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	

2 Entry composition [i](#)

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			

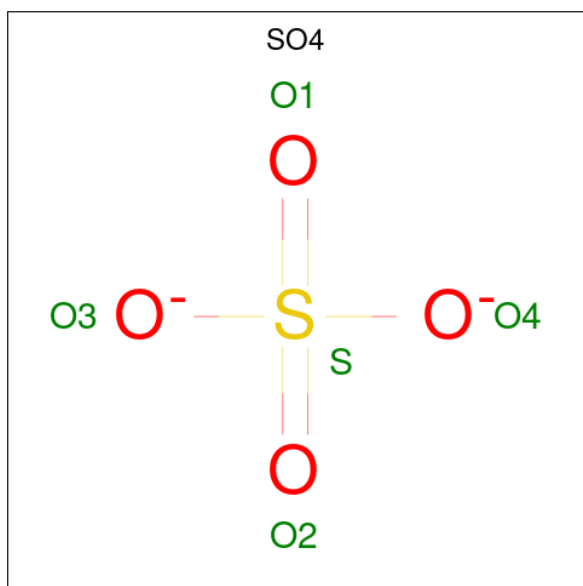
- Molecule 4 is a protein called NP1-B17 TCR alpha chain.

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 (CCD ID: SO4) (formula: O₄S).



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

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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 (CCD ID: NA) (formula: Na).

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

- 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		

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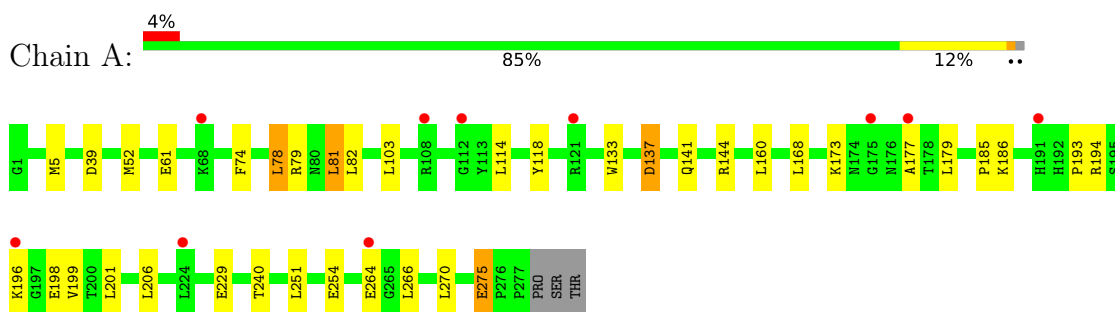
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	23	Total 23	O 23	0	0
8	J	33	Total 33	O 33	0	0
8	K	40	Total 40	O 40	0	0
8	L	19	Total 19	O 19	0	0
8	M	1	Total 1	O 1	0	0
8	N	32	Total 32	O 32	0	0
8	O	57	Total 57	O 57	0	0
8	P	40	Total 40	O 40	0	0
8	Q	14	Total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

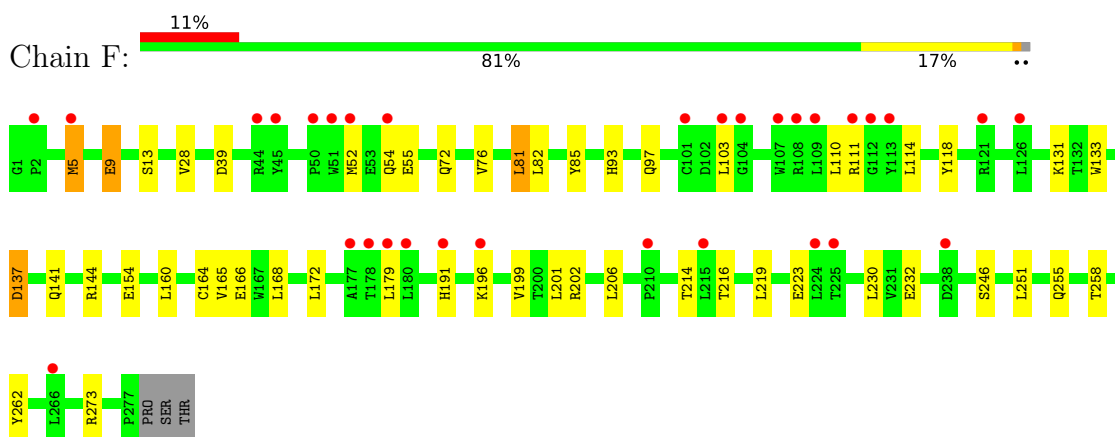
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

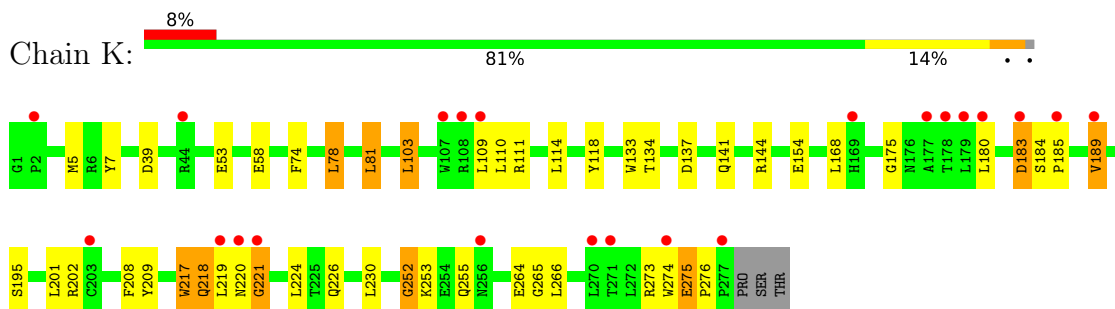
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



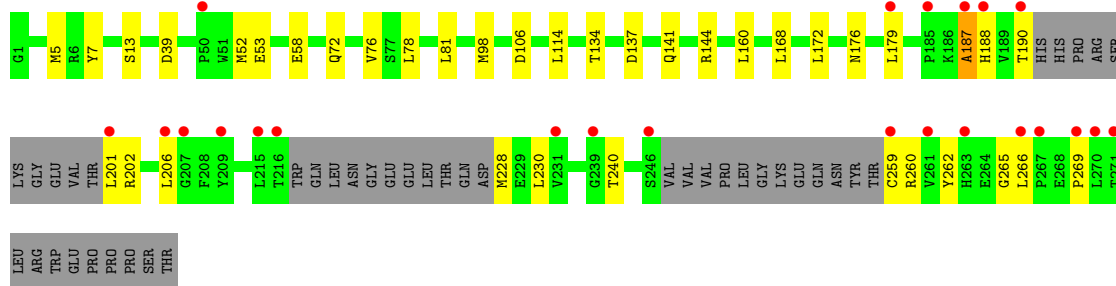
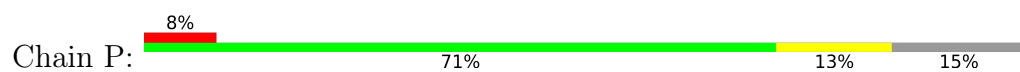
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



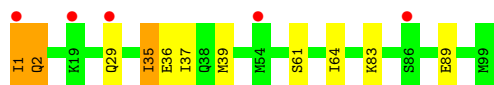
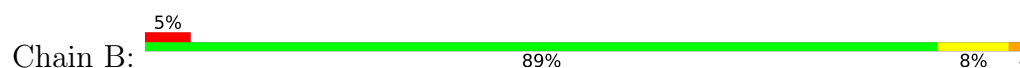
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



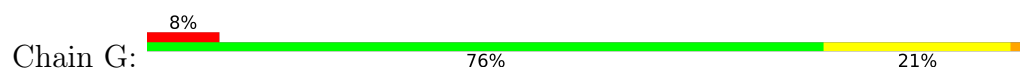
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



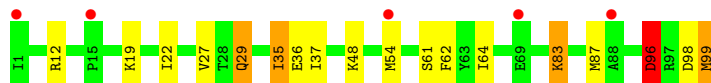
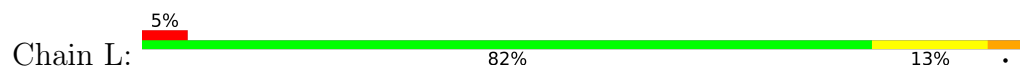
- Molecule 2: Beta-2-microglobulin



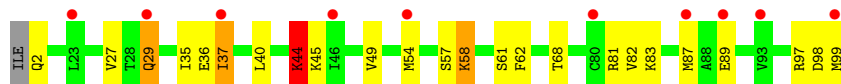
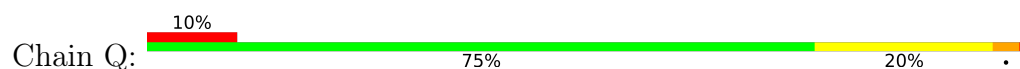
- Molecule 2: Beta-2-microglobulin



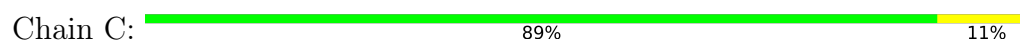
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: influenza NP366 epitope



- Molecule 3: influenza NP366 epitope

Chain H:  78% 22%



- Molecule 3: influenza NP366 epitope

Chain M:  78% 22%



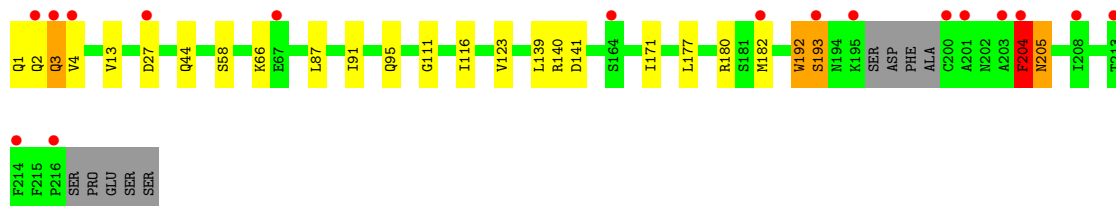
- Molecule 3: influenza NP366 epitope

Chain R:  78% 22%



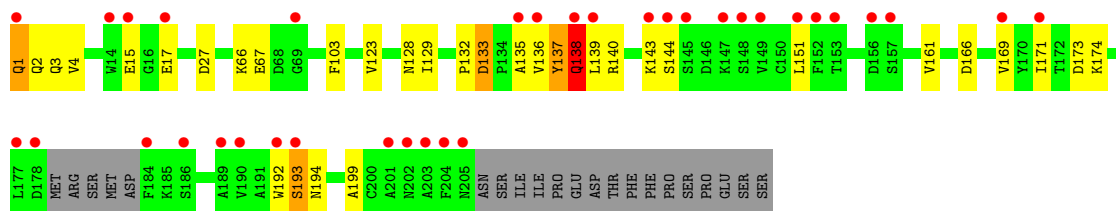
- Molecule 4: NP1-B17 TCR alpha chain

Chain D:  8% 83% 10% . .



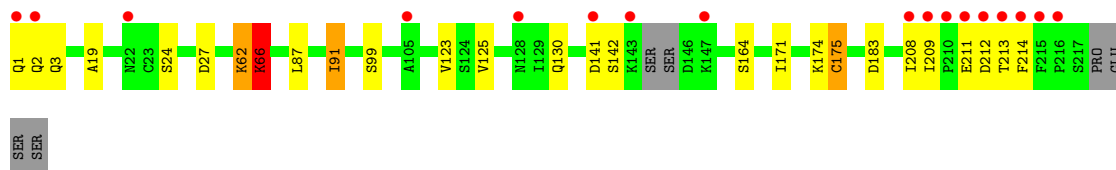
- Molecule 4: NP1-B17 TCR alpha chain

Chain I:  17% 73% 14% . 10%

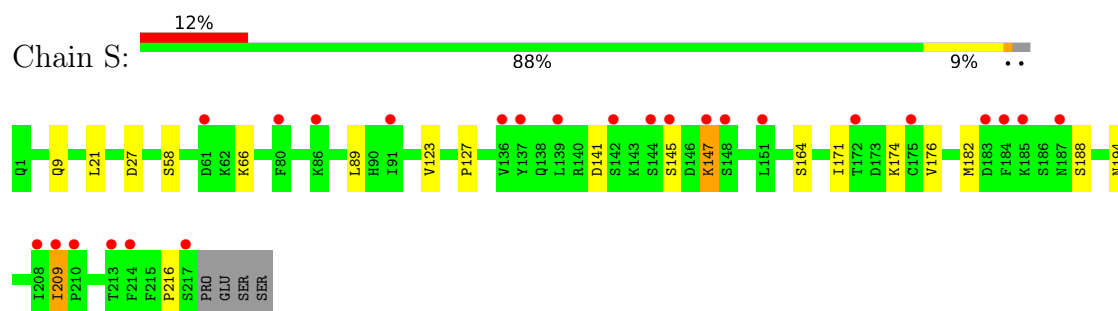


- Molecule 4: NP1-B17 TCR alpha chain

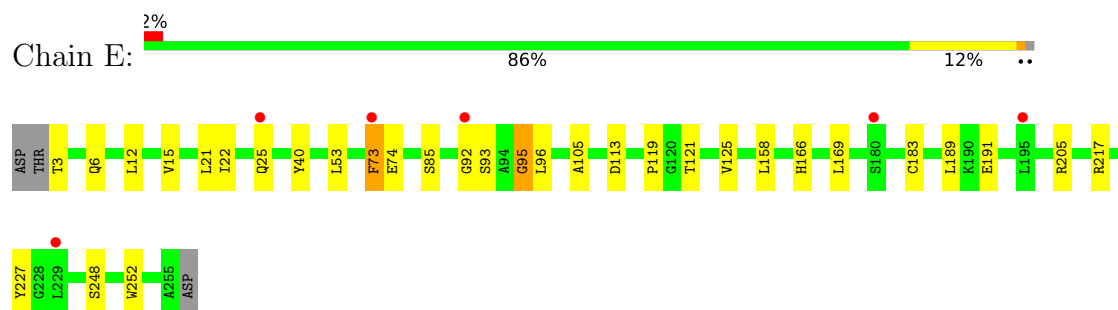
Chain N:  8% 84% 11% . .



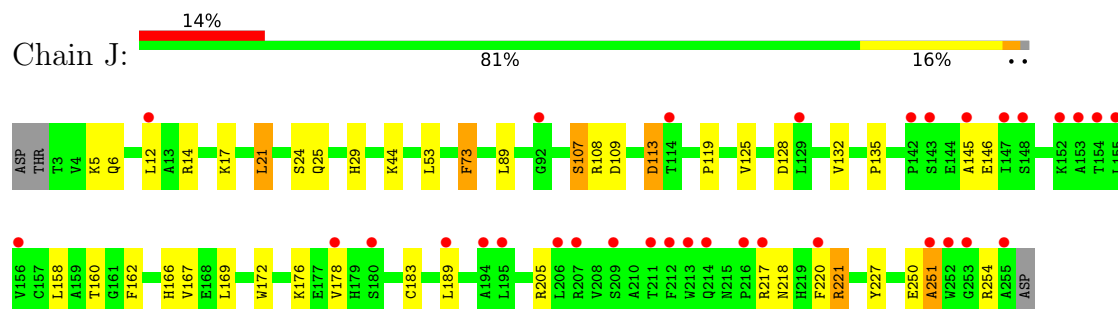
- Molecule 4: NP1-B17 TCR alpha chain



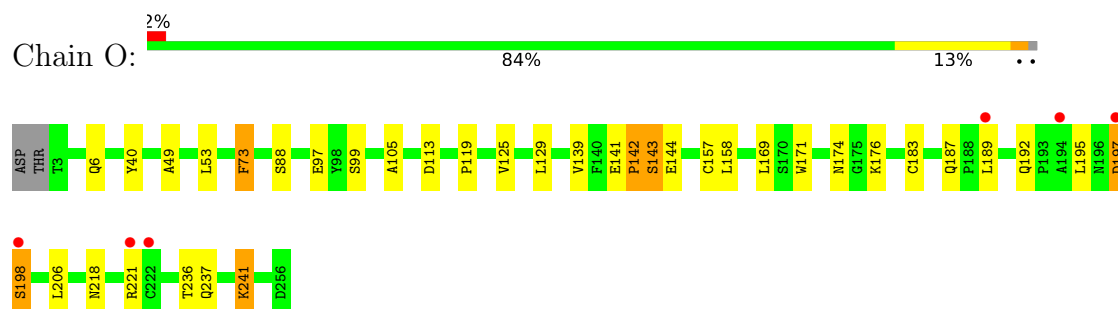
- Molecule 5: NP1-B17 TCR beta chain



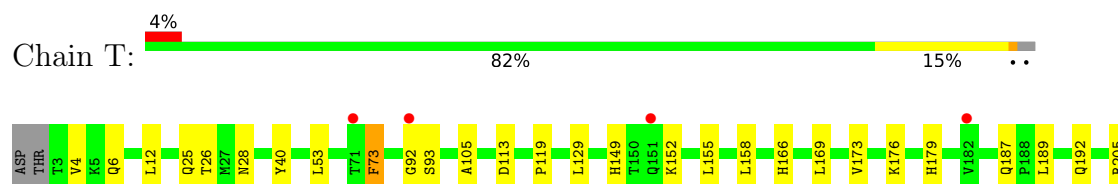
- Molecule 5: NP1-B17 TCR beta chain

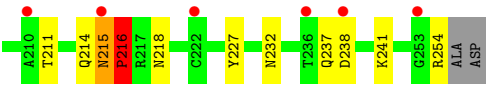


- Molecule 5: NP1-B17 TCR beta chain



- Molecule 5: NP1-B17 TCR beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.23Å 100.19Å 469.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.80 – 2.65 38.80 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.80-2.65) 99.9 (38.80-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.226 , 0.249 0.260 , 0.284	Depositor DCC
R_{free} test set	6523 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	27034	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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.

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: SO4, NA

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	0.65	0/2385	1.16	1/3240 (0.0%)
1	F	0.69	0/2385	1.19	5/3240 (0.2%)
1	K	0.69	0/2385	1.23	12/3240 (0.4%)
1	P	0.65	0/2037	1.16	4/2759 (0.1%)
2	B	0.73	0/844	1.12	2/1144 (0.2%)
2	G	0.74	0/852	1.20	5/1154 (0.4%)
2	L	0.74	0/852	1.15	2/1154 (0.2%)
2	Q	0.75	0/844	1.20	4/1143 (0.3%)
3	C	0.57	0/67	1.00	0/86
3	H	0.59	0/67	0.98	0/86
3	M	0.58	0/67	0.97	0/86
3	R	0.57	0/67	1.00	0/86
4	D	0.72	0/1594	1.13	8/2164 (0.4%)
4	I	0.76	0/1495	1.16	9/2028 (0.4%)
4	N	0.70	0/1624	1.09	2/2203 (0.1%)
4	S	0.70	0/1637	1.10	2/2222 (0.1%)
5	E	0.66	0/1994	1.12	4/2711 (0.1%)
5	J	0.68	0/1994	1.13	4/2711 (0.1%)
5	O	0.67	0/2014	1.19	11/2736 (0.4%)
5	T	0.65	0/1989	1.14	8/2704 (0.3%)
All	All	0.69	0/27193	1.16	83/36897 (0.2%)

There are no bond length outliers.

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	217	ARG	N-CA-C	-9.10	102.69	113.88
5	O	142	PRO	CA-C-N	8.89	137.70	121.70
5	O	142	PRO	C-N-CA	8.89	137.70	121.70
5	O	197	ASP	CA-C-N	8.33	136.69	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	197	ASP	C-N-CA	8.33	136.69	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	18	0
1	P	1983	0	1872	10	0
2	B	818	0	797	5	0
2	G	826	0	807	11	0
2	L	826	0	805	7	0
2	Q	818	0	793	8	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	11	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

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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	147	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 147 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	1.05	0.99
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%)	9	14
1	F	280/280 (100%)	264 (94%)	15 (5%)	1 (0%)	30	45
1	K	280/280 (100%)	250 (89%)	25 (9%)	5 (2%)	6	11
1	P	234/280 (84%)	221 (94%)	11 (5%)	2 (1%)	14	24
2	B	97/99 (98%)	94 (97%)	2 (2%)	1 (1%)	12	20
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%)	5	9
4	I	182/207 (88%)	160 (88%)	18 (10%)	4 (2%)	5	9
4	N	197/207 (95%)	185 (94%)	8 (4%)	4 (2%)	6	10
4	S	201/207 (97%)	178 (89%)	19 (10%)	4 (2%)	6	10
5	E	238/243 (98%)	224 (94%)	11 (5%)	3 (1%)	9	16
5	J	238/243 (98%)	221 (93%)	15 (6%)	2 (1%)	16	27
5	O	240/243 (99%)	221 (92%)	14 (6%)	5 (2%)	5	9
5	T	237/243 (98%)	212 (90%)	20 (8%)	5 (2%)	5	9
All	All	3219/3352 (96%)	2972 (92%)	199 (6%)	48 (2%)	8	13

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	196	LYS

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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%)	13	23
1	F	240/238 (101%)	207 (86%)	33 (14%)	3	5
1	K	240/238 (101%)	218 (91%)	22 (9%)	8	14
1	P	203/238 (85%)	181 (89%)	22 (11%)	6	9
2	B	93/93 (100%)	89 (96%)	4 (4%)	26	44
2	G	94/93 (101%)	86 (92%)	8 (8%)	10	17
2	L	94/93 (101%)	84 (89%)	10 (11%)	6	10
2	Q	93/93 (100%)	81 (87%)	12 (13%)	4	6
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%)	4	6
3	R	8/8 (100%)	8 (100%)	0	100	100
4	D	178/188 (95%)	164 (92%)	14 (8%)	11	19
4	I	167/188 (89%)	154 (92%)	13 (8%)	11	20
4	N	182/188 (97%)	167 (92%)	15 (8%)	10	18
4	S	184/188 (98%)	176 (96%)	8 (4%)	26	44
5	E	212/215 (99%)	197 (93%)	15 (7%)	13	23
5	J	212/215 (99%)	191 (90%)	21 (10%)	7	11
5	O	214/215 (100%)	197 (92%)	17 (8%)	11	19
5	T	212/215 (99%)	193 (91%)	19 (9%)	9	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2890/2968 (97%)	2639 (91%)	251 (9%)	9 16

5 of 251 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	J	167	VAL
2	Q	97	ARG
1	K	230	LEU
2	Q	87	MET
5	T	28	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
5	O	131	ASN
2	Q	29	GLN
5	O	232	ASN
1	P	176	ASN
4	S	131	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	K	301	-	4,4,4	0.26	0	6,6,6	0.07	0
6	SO4	E	301	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	T	301	-	4,4,4	0.25	0	6,6,6	0.09	0
6	SO4	O	301	-	4,4,4	0.25	0	6,6,6	0.09	0
6	SO4	D	301	-	4,4,4	0.24	0	6,6,6	0.08	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, 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	277/280 (98%)	0.45	10 (3%) 46 38	19, 61, 98, 120	12 (4%)
1	F	277/280 (98%)	0.99	31 (11%) 10 8	24, 83, 117, 143	12 (4%)
1	K	277/280 (98%)	0.63	22 (7%) 18 14	21, 66, 109, 123	12 (4%)
1	P	238/280 (85%)	0.67	23 (9%) 13 10	19, 65, 159, 198	9 (3%)
2	B	99/99 (100%)	0.40	5 (5%) 33 26	37, 58, 79, 88	2 (2%)
2	G	99/99 (100%)	0.92	8 (8%) 18 13	35, 75, 103, 111	1 (1%)
2	L	99/99 (100%)	0.65	5 (5%) 33 26	27, 62, 91, 102	1 (1%)
2	Q	98/99 (98%)	0.97	10 (10%) 12 9	31, 85, 108, 115	1 (1%)
3	C	9/9 (100%)	-0.15	0 100 100	40, 42, 48, 51	0
3	H	9/9 (100%)	0.58	0 100 100	50, 60, 68, 72	0
3	M	9/9 (100%)	0.16	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%)	0.65	17 (8%) 16 12	39, 64, 115, 129	1 (0%)
4	I	186/207 (89%)	1.22	35 (18%) 3 2	52, 84, 162, 187	1 (0%)
4	N	201/207 (97%)	0.89	17 (8%) 16 12	46, 72, 109, 144	1 (0%)
4	S	203/207 (98%)	0.92	25 (12%) 8 7	43, 79, 122, 140	1 (0%)
5	E	240/243 (98%)	0.35	6 (2%) 58 52	32, 56, 92, 106	1 (0%)
5	J	240/243 (98%)	0.91	33 (13%) 6 5	40, 74, 138, 163	0
5	O	241/243 (99%)	0.40	6 (2%) 58 52	31, 56, 87, 108	3 (1%)
5	T	239/243 (98%)	0.63	10 (4%) 40 32	34, 64, 100, 124	1 (0%)
All	All	3248/3352 (96%)	0.71	263 (8%) 18 13	19, 67, 117, 198	59 (1%)

The worst 5 of 263 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	139	LEU	4.9
5	T	215	ASN	4.9
1	A	108[A]	ARG	4.8
4	D	200	CYS	4.7
4	S	184	PHE	4.4

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
6	SO4	K	301	5/5	0.68	0.12	114,114,114,115	0
6	SO4	T	301	5/5	0.69	0.16	115,115,115,115	0
6	SO4	E	301	5/5	0.75	0.17	115,116,116,116	0
6	SO4	D	301	5/5	0.76	0.17	118,118,119,119	0
7	NA	J	301	1/1	0.79	0.09	38,38,38,38	0
7	NA	E	302	1/1	0.86	0.17	50,50,50,50	0
6	SO4	O	301	5/5	0.89	0.12	102,102,102,102	0
7	NA	K	302	1/1	0.90	0.13	79,79,79,79	0
7	NA	T	302	1/1	0.90	0.11	42,42,42,42	0
7	NA	T	303	1/1	0.91	0.22	49,49,49,49	0
7	NA	I	301	1/1	0.94	0.17	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.