



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 01:06 am BST

PDB ID : 5D2L
Title : Crystal structure of TCR C7 in complex with HCMV NLV epitope presented by HLA-A2
Authors : Gao, M.; Mariuzza, R.A.
Deposited on : 2015-08-05
Resolution : 3.51 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
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

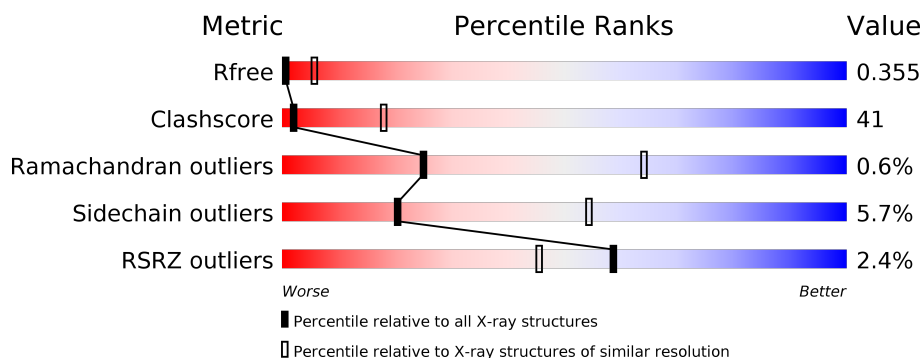
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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 $\leq 5\%$. 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	276	<div> <div>58%</div> <div>40%</div> <div>..</div> </div>
1	C	276	<div> <div>61%</div> <div>35%</div> <div>..</div> </div>
1	G	276	<div> <div>2%</div> <div>46%</div> <div>47%</div> <div>..</div> </div>
1	M	276	<div> <div>%</div> <div>48%</div> <div>48%</div> <div>..</div> </div>
2	B	100	<div> <div>3%</div> <div>48%</div> <div>50%</div> <div>..</div> </div>
2	D	100	<div> <div>55%</div> <div>41%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	100	
2	N	100	
3	E	205	
3	I	205	
3	K	205	
3	O	205	
4	F	245	
4	J	245	
4	L	245	
4	P	245	
5	Q	9	
5	R	9	
5	T	9	
5	U	9	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 25272 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2242	1401	408	424	9			
1	G	270	Total	C	N	O	S	0	0	0
			2199	1379	395	416	9			
1	M	273	Total	C	N	O	S	0	0	0
			2210	1379	401	421	9			
1	C	274	Total	C	N	O	S	0	0	0
			2242	1401	408	424	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01892
G	0	MET	-	initiating methionine	UNP P01892
M	0	MET	-	initiating methionine	UNP P01892
C	0	MET	-	initiating methionine	UNP P01892

- 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
			823	522	140	158	3			
2	H	96	Total	C	N	O	S	0	0	0
			777	494	128	152	3			
2	N	100	Total	C	N	O	S	0	0	0
			825	524	138	159	4			
2	D	100	Total	C	N	O	S	0	0	0
			827	527	137	159	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769
N	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called C7 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	185	Total	C	N	O	S	0	0	0
			1404	878	227	293	6			
3	K	192	Total	C	N	O	S	0	0	0
			1452	912	237	296	7			
3	O	187	Total	C	N	O	S	0	0	0
			1435	900	234	294	7			
3	E	187	Total	C	N	O	S	0	0	0
			1432	897	234	294	7			

- Molecule 4 is a protein called C7 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	226	Total	C	N	O	S	0	0	0
			1759	1108	303	343	5			
4	L	226	Total	C	N	O	S	0	0	0
			1699	1064	299	331	5			
4	P	235	Total	C	N	O	S	0	0	0
			1784	1122	306	351	5			
4	F	238	Total	C	N	O	S	0	0	0
			1852	1163	323	361	5			

- Molecule 5 is a protein called ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Q	9	Total	C	N	O	S	0	0	0
			64	42	10	11	1			
5	U	9	Total	C	N	O	S	0	0	0
			64	42	10	11	1			
5	T	9	Total	C	N	O	S	0	0	0
			64	42	10	11	1			
5	R	9	Total	C	N	O	S	0	0	0
			64	42	10	11	1			

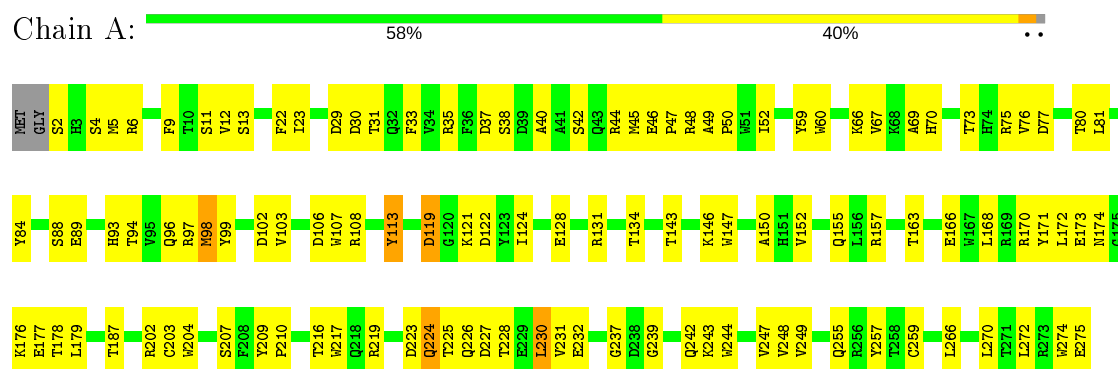
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	9	Total O 9 9	0	0
6	B	1	Total O 1 1	0	0
6	I	3	Total O 3 3	0	0
6	J	2	Total O 2 2	0	0
6	G	7	Total O 7 7	0	0
6	K	2	Total O 2 2	0	0
6	M	3	Total O 3 3	0	0
6	N	5	Total O 5 5	0	0
6	O	5	Total O 5 5	0	0
6	P	5	Total O 5 5	0	0
6	C	8	Total O 8 8	0	0
6	D	2	Total O 2 2	0	0
6	E	2	Total O 2 2	0	0

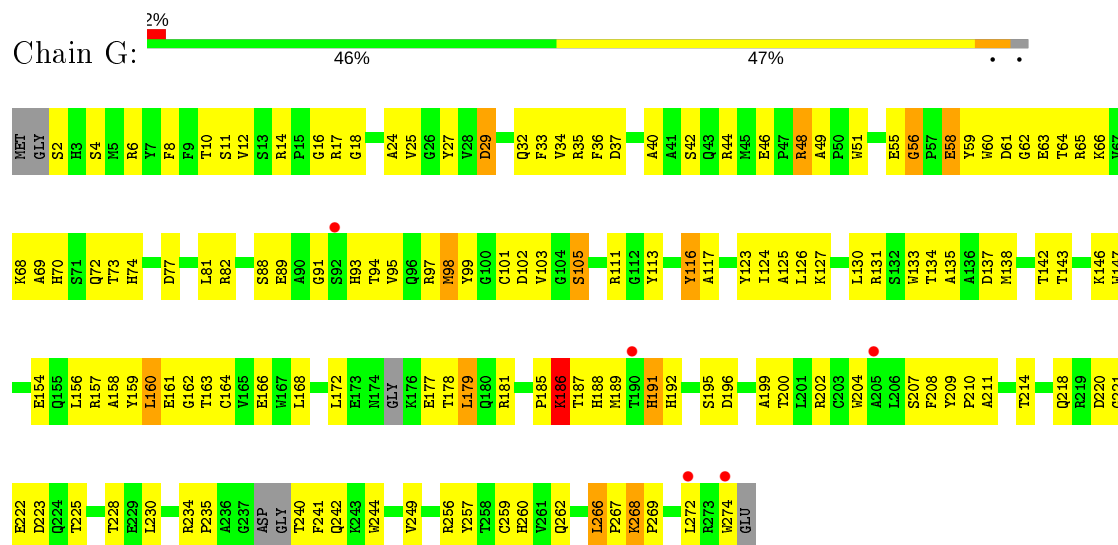
3 Residue-property plots [i](#)

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.

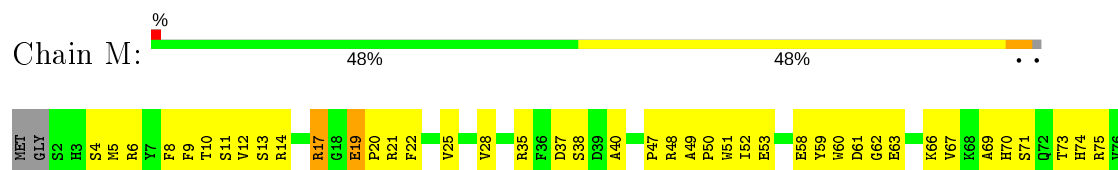
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

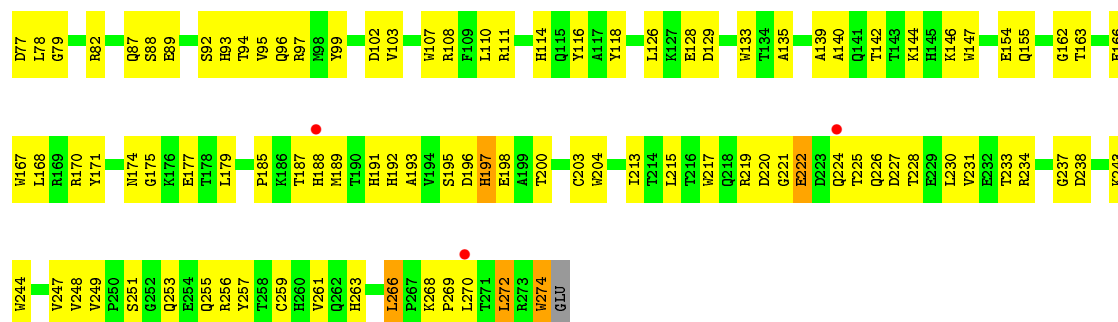


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



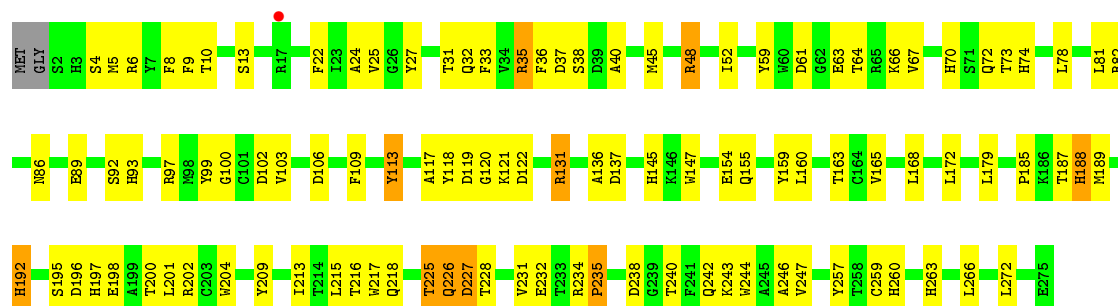
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain





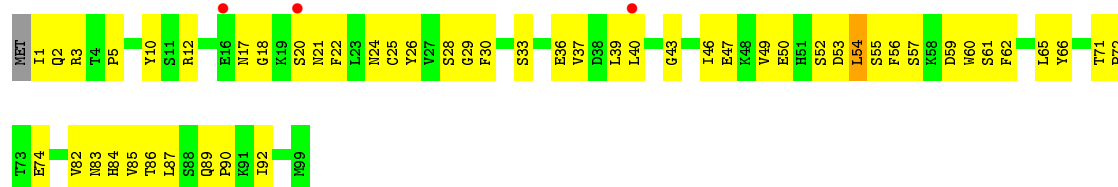
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain C: 61% 35%



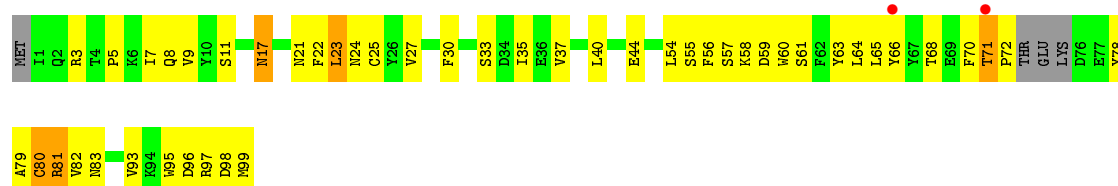
- Molecule 2: Beta-2-microglobulin

Chain B: 3% 48% 50%



- Molecule 2: Beta-2-microglobulin

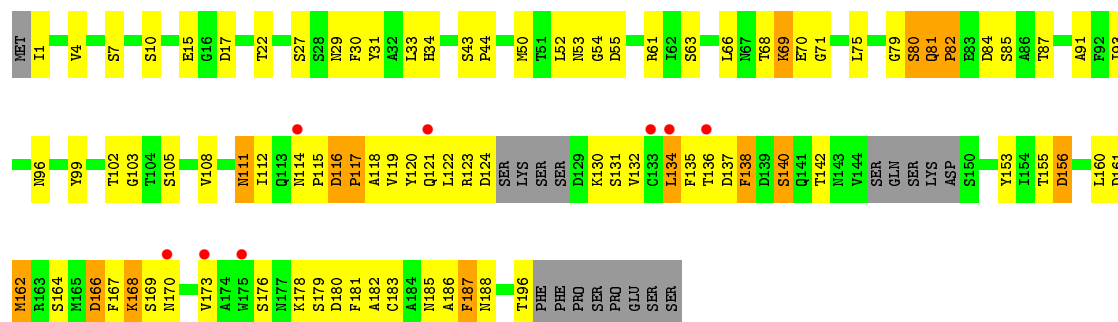
Chain H: 2% 49% 42% 5%



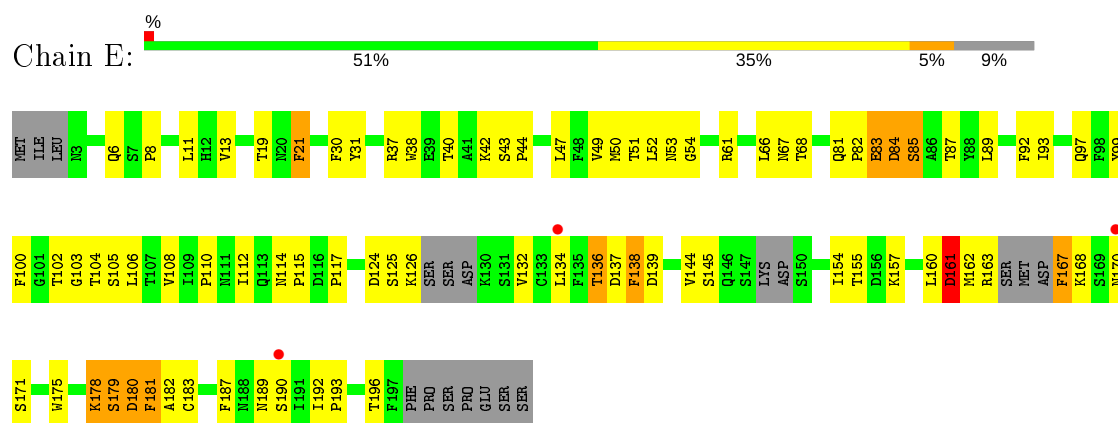
- Molecule 2: Beta-2-microglobulin

Chain N: 2% 44% 54%

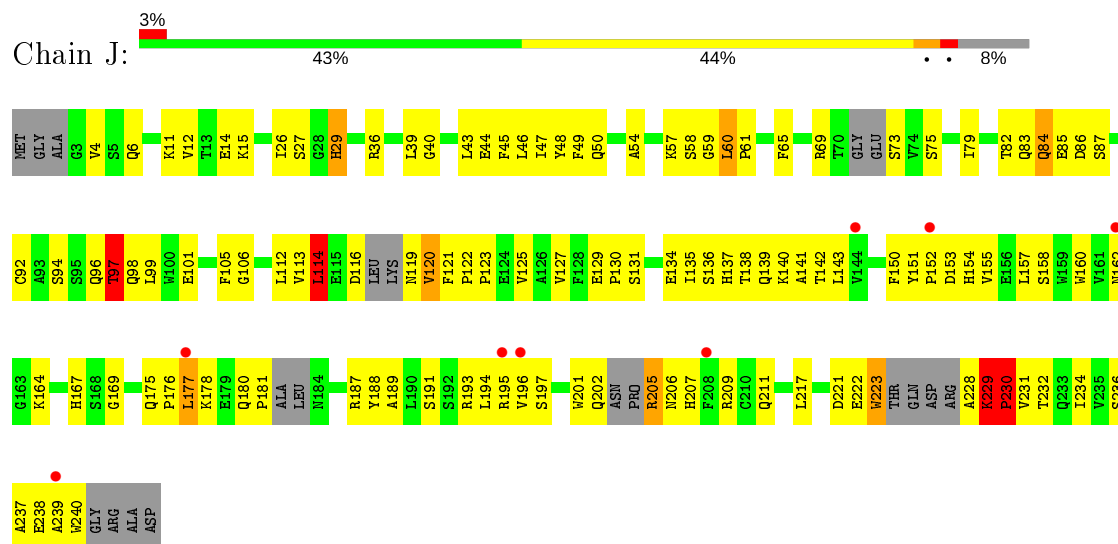




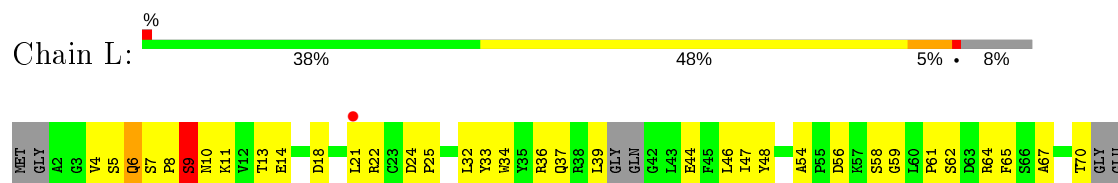
• Molecule 3: C7 TCR alpha chain

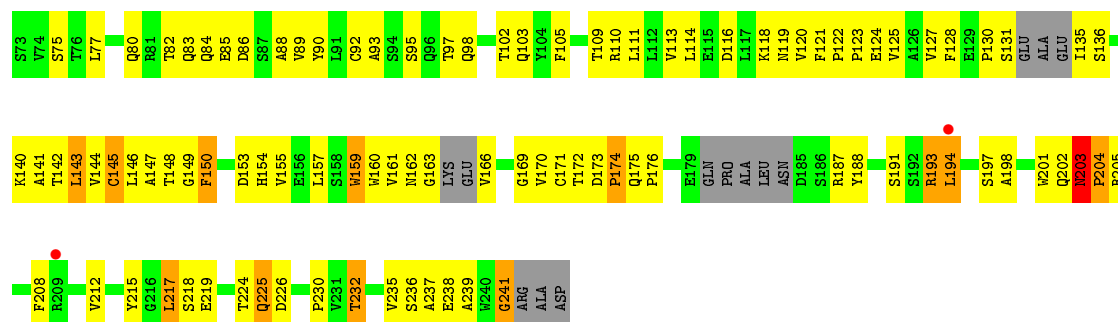


• Molecule 4: C7 TCR beta chain

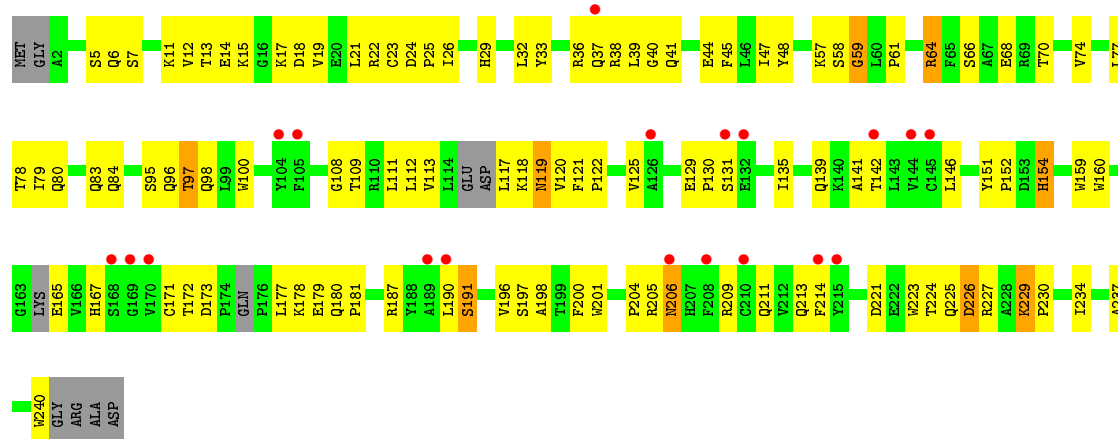


• Molecule 4: C7 TCR beta chain

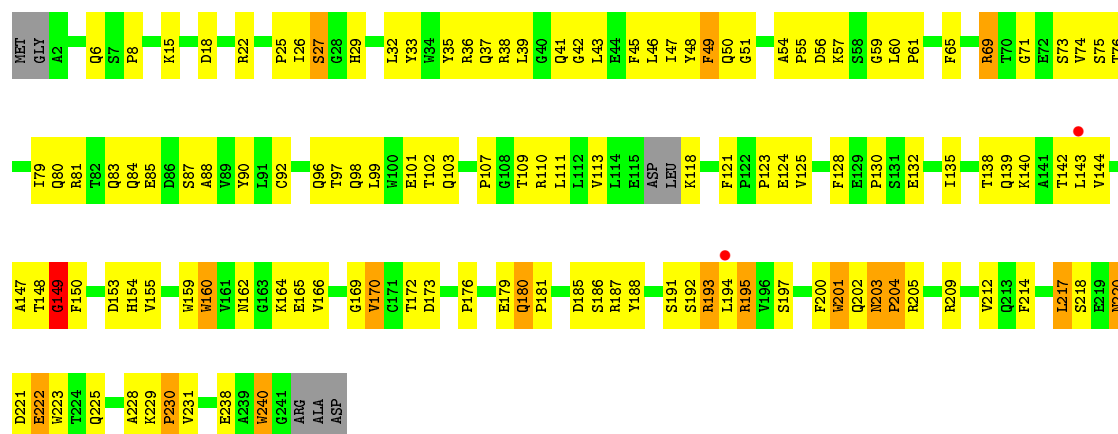
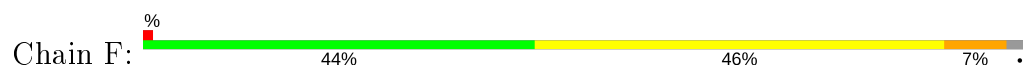




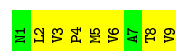
• Molecule 4: C7 TCR beta chain



• Molecule 4: C7 TCR beta chain

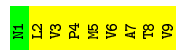


• Molecule 5: ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL




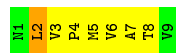
- Molecule 5: ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL

Chain U:  11% 89%



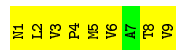
- Molecule 5: ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL

Chain T:  22% 67% 11%



- Molecule 5: ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL

Chain R:  11% 89%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	151.76Å 366.64Å 151.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 3.51 49.84 – 3.51	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.51-3.51) 91.4 (49.84-3.51)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.48Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.270 , 0.355 0.274 , 0.355	Depositor DCC
R_{free} test set	2702 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	79.4	Xtrriage
Anisotropy	0.599	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	25272	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6340e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

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	0.47	0/2307	0.61	1/3132 (0.0%)
1	C	0.46	0/2307	0.59	1/3132 (0.0%)
1	G	0.53	1/2262 (0.0%)	0.72	2/3072 (0.1%)
1	M	0.42	0/2272	0.69	2/3085 (0.1%)
2	B	0.43	0/845	0.66	0/1143
2	D	0.53	0/850	0.68	2/1151 (0.2%)
2	H	0.44	0/798	0.64	0/1083
2	N	0.52	0/848	0.80	0/1150
3	E	0.46	0/1463	0.70	0/1987
3	I	0.54	0/1433	0.80	4/1946 (0.2%)
3	K	0.56	1/1486 (0.1%)	0.85	4/2018 (0.2%)
3	O	0.54	2/1466 (0.1%)	0.82	4/1992 (0.2%)
4	F	0.54	1/1900 (0.1%)	0.77	3/2586 (0.1%)
4	J	0.50	2/1801 (0.1%)	0.76	2/2448 (0.1%)
4	L	0.52	0/1737	0.95	11/2362 (0.5%)
4	P	0.43	0/1829	0.73	2/2494 (0.1%)
5	Q	0.45	0/64	0.72	0/88
5	R	0.42	0/64	0.67	0/88
5	T	0.55	0/64	0.78	0/88
5	U	0.30	0/64	0.50	0/88
All	All	0.49	7/25860 (0.0%)	0.74	38/35133 (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	A	0	1
1	C	0	1
1	G	0	4
2	H	0	1
2	N	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	3
3	K	0	5
3	O	0	3
4	F	0	3
4	J	0	2
4	L	0	5
4	P	0	3
All	All	0	32

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	230	PRO	N-CD	5.28	1.55	1.47
1	G	267	PRO	N-CD	5.25	1.55	1.47
3	K	172	ALA	CA-CB	-5.25	1.41	1.52
3	O	82	PRO	N-CD	5.13	1.55	1.47
3	O	117	PRO	N-CD	5.13	1.55	1.47

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	241	GLY	N-CA-C	12.45	144.23	113.10
3	I	7	SER	C-N-CD	-11.91	94.40	120.60
4	L	149	GLY	N-CA-C	10.65	139.73	113.10
1	G	179	LEU	N-CA-C	8.08	132.81	111.00
3	I	192	ILE	C-N-CD	6.94	142.98	128.40

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	GLN	Mainchain
1	G	105	SER	Peptide
1	G	56	GLY	Peptide
4	J	229	LYS	Peptide
4	J	97	THR	Peptide

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	2242	0	2090	131	0
1	C	2242	0	2090	122	0
1	G	2199	0	2039	220	0
1	M	2210	0	2042	163	0
2	B	823	0	787	47	0
2	D	827	0	781	51	0
2	H	777	0	715	63	0
2	N	825	0	770	78	0
3	E	1432	0	1307	102	0
3	I	1404	0	1269	125	1
3	K	1452	0	1320	213	4
3	O	1435	0	1323	107	2
4	F	1852	0	1726	181	0
4	J	1759	0	1634	156	0
4	L	1699	0	1542	201	0
4	P	1784	0	1638	134	2
5	Q	64	0	74	12	0
5	R	64	0	74	12	0
5	T	64	0	74	13	0
5	U	64	0	74	27	0
6	A	9	0	0	4	0
6	B	1	0	0	0	0
6	C	8	0	0	1	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	G	7	0	0	3	0
6	I	3	0	0	1	0
6	J	2	0	0	1	0
6	K	2	0	0	0	0
6	M	3	0	0	3	0
6	N	5	0	0	2	0
6	O	5	0	0	0	0
6	P	5	0	0	1	0
All	All	25272	0	23369	1971	5

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 41.

The worst 5 of 1971 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)
3:I:192:ILE:HG23	3:I:193:PRO:CD	1.42	1.46
1:A:230:LEU:HD21	1:A:243:LYS:NZ	1.27	1.43
3:K:175:TRP:CZ2	4:L:146:LEU:HD22	1.53	1.42
4:L:88:ALA:CB	4:L:110:ARG:HG3	1.46	1.41
3:K:112:ILE:CG2	3:K:139:ASP:HB3	1.48	1.41

All (5) 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	Interatomic distance (Å)	Clash overlap (Å)
3:K:12:HIS:ND1	3:O:10:SER:OG[1_556]	1.92	0.28
3:K:12:HIS:CG	3:O:10:SER:OG[1_556]	2.00	0.20
3:K:189:ASN:OD1	4:P:181:PRO:CG[1_556]	2.09	0.11
3:I:10:SER:OG	3:I:12:HIS:ND1[3_655]	2.14	0.06
3:K:189:ASN:OD1	4:P:181:PRO:CD[1_556]	2.17	0.03

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	272/276 (99%)	255 (94%)	17 (6%)	0	100	100
1	C	272/276 (99%)	248 (91%)	23 (8%)	1 (0%)	34	71
1	G	264/276 (96%)	239 (90%)	25 (10%)	0	100	100
1	M	271/276 (98%)	242 (89%)	29 (11%)	0	100	100
2	B	97/100 (97%)	84 (87%)	13 (13%)	0	100	100
2	D	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
2	H	92/100 (92%)	82 (89%)	9 (10%)	1 (1%)	14	53
2	N	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
3	E	179/205 (87%)	152 (85%)	26 (14%)	1 (1%)	25	64
3	I	175/205 (85%)	137 (78%)	37 (21%)	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	188/205 (92%)	158 (84%)	26 (14%)	4 (2%)	7	39
3	O	181/205 (88%)	160 (88%)	20 (11%)	1 (1%)	25	64
4	F	234/245 (96%)	197 (84%)	34 (14%)	3 (1%)	12	49
4	J	214/245 (87%)	185 (86%)	28 (13%)	1 (0%)	29	67
4	L	214/245 (87%)	183 (86%)	29 (14%)	2 (1%)	17	57
4	P	227/245 (93%)	192 (85%)	32 (14%)	3 (1%)	12	49
5	Q	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
5	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
5	T	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
5	U	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	3104/3340 (93%)	2707 (87%)	379 (12%)	18 (1%)	25	64

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	122	LEU
4	J	114	LEU
3	K	147	SER
3	K	150	SER
4	L	174	PRO

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	231/232 (100%)	226 (98%)	5 (2%)	52	77
1	C	231/232 (100%)	221 (96%)	10 (4%)	29	62
1	G	226/232 (97%)	216 (96%)	10 (4%)	28	62
1	M	225/232 (97%)	216 (96%)	9 (4%)	31	64
2	B	93/95 (98%)	92 (99%)	1 (1%)	73	87
2	D	93/95 (98%)	88 (95%)	5 (5%)	22	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	86/95 (90%)	83 (96%)	3 (4%)	36	67
2	N	92/95 (97%)	90 (98%)	2 (2%)	52	77
3	E	158/185 (85%)	145 (92%)	13 (8%)	11	41
3	I	155/185 (84%)	145 (94%)	10 (6%)	17	50
3	K	158/185 (85%)	140 (89%)	18 (11%)	5	28
3	O	159/185 (86%)	145 (91%)	14 (9%)	10	39
4	F	198/212 (93%)	184 (93%)	14 (7%)	14	47
4	J	189/212 (89%)	176 (93%)	13 (7%)	15	48
4	L	174/212 (82%)	162 (93%)	12 (7%)	15	48
4	P	189/212 (89%)	178 (94%)	11 (6%)	20	54
5	Q	8/8 (100%)	7 (88%)	1 (12%)	4	24
5	R	8/8 (100%)	8 (100%)	0	100	100
5	T	8/8 (100%)	7 (88%)	1 (12%)	4	24
5	U	8/8 (100%)	8 (100%)	0	100	100
All	All	2689/2928 (92%)	2537 (94%)	152 (6%)	20	54

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	150	PHE
3	O	80	SER
4	F	160	TRP
4	L	193	ARG
1	M	197	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	93	HIS
2	N	13	HIS
4	F	98	GLN
1	M	96	GLN
2	N	2	GLN

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](#)

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

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	274/276 (99%)	-0.18	0 100 100	33, 56, 82, 107	0
1	C	274/276 (99%)	-0.20	1 (0%) 92 87	35, 51, 83, 100	0
1	G	270/276 (97%)	0.06	5 (1%) 66 53	57, 80, 102, 122	0
1	M	273/276 (98%)	0.06	3 (1%) 80 69	51, 77, 111, 119	0
2	B	99/100 (99%)	0.05	3 (3%) 50 37	45, 72, 108, 123	0
2	D	100/100 (100%)	-0.06	0 100 100	40, 66, 90, 113	0
2	H	96/100 (96%)	0.19	2 (2%) 63 50	59, 88, 110, 115	0
2	N	100/100 (100%)	0.18	2 (2%) 65 52	57, 87, 107, 116	0
3	E	187/205 (91%)	-0.05	3 (1%) 72 59	36, 63, 114, 131	0
3	I	185/205 (90%)	-0.04	3 (1%) 72 59	41, 72, 115, 126	0
3	K	192/205 (93%)	0.37	15 (7%) 13 10	55, 89, 129, 140	0
3	O	187/205 (91%)	0.15	8 (4%) 35 26	58, 91, 134, 151	0
4	F	238/245 (97%)	0.06	2 (0%) 86 75	38, 80, 125, 132	0
4	J	226/245 (92%)	0.17	8 (3%) 44 33	25, 88, 129, 141	0
4	L	226/245 (92%)	0.31	3 (1%) 77 65	74, 106, 127, 136	0
4	P	235/245 (95%)	0.33	19 (8%) 12 10	50, 95, 133, 154	0
5	Q	9/9 (100%)	0.07	0 100 100	43, 48, 51, 53	0
5	R	9/9 (100%)	-0.17	0 100 100	40, 41, 44, 46	0
5	T	9/9 (100%)	0.04	0 100 100	59, 63, 71, 72	0
5	U	9/9 (100%)	0.17	0 100 100	63, 67, 72, 73	0
All	All	3198/3340 (95%)	0.08	77 (2%) 59 45	25, 79, 122, 154	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	134	LEU	6.5
3	K	127	SER	6.3
3	K	128	SER	5.2
3	K	172	ALA	5.0
4	P	190	LEU	4.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.