



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 01:18 AM UTC

PDB ID : 8I5C / pdb_00008i5c
Title : Crystal structure of a TCR in complex with HLA-A*11:01 bound to KRAS peptide (VVGAVGVGK)
Authors : Lu, D.; Chen, Y.; Jiang, M.; Tan, S.G.; Chai, Y.; Gao, G.F.
Deposited on : 2023-01-24
Resolution : 3.34 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
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

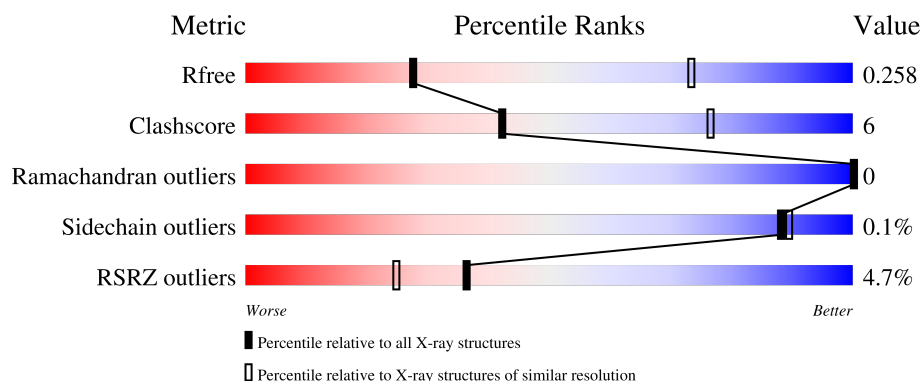
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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.



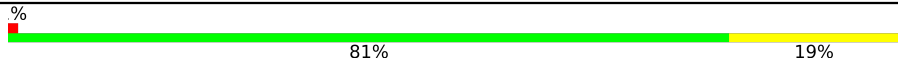
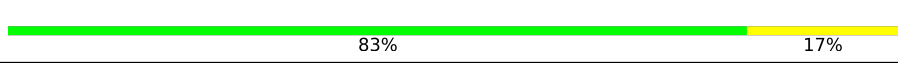
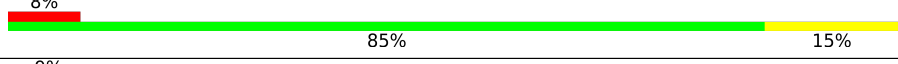
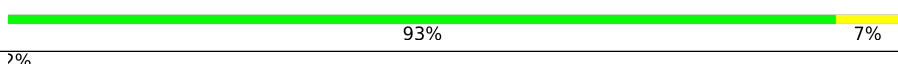
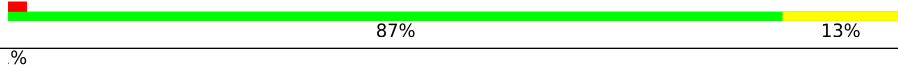
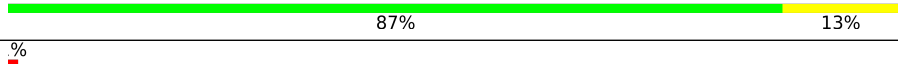
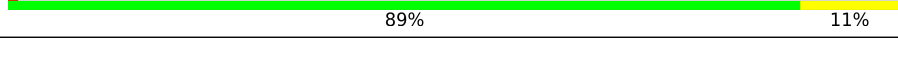
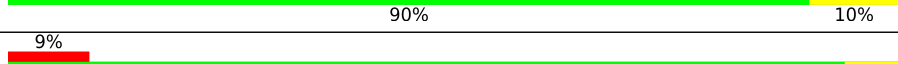
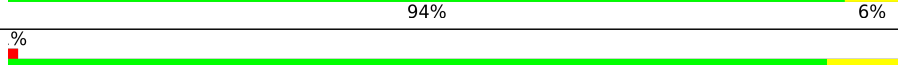
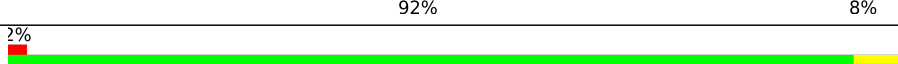
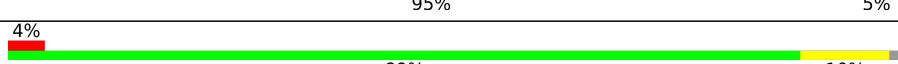
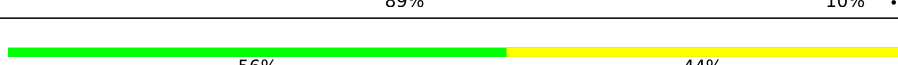
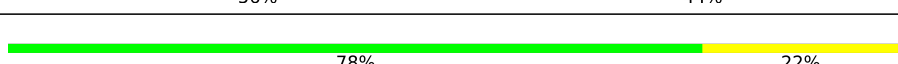
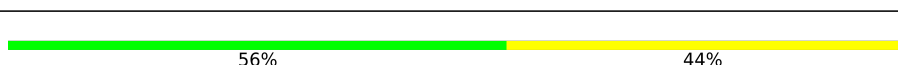
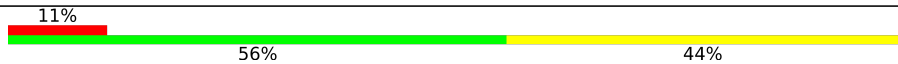
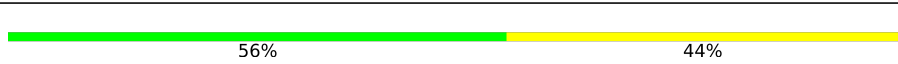
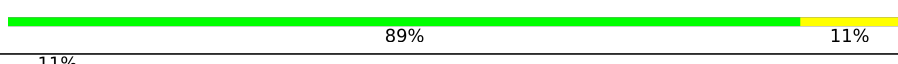
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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 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	274	79% 21%
1	F	274	84% 16%
1	K	274	82% 18%
1	P	274	81% 19%
1	U	274	82% 18%

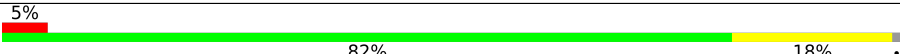
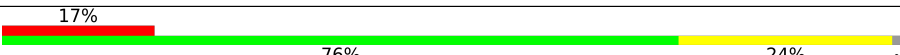
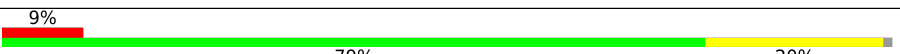
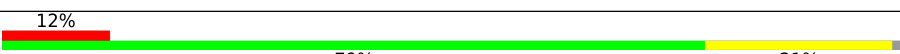
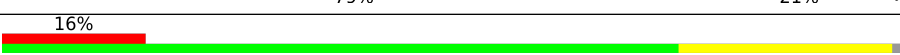
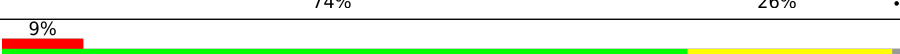
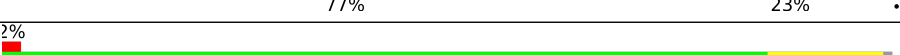
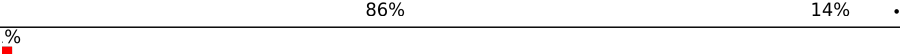
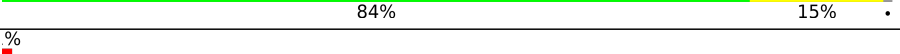
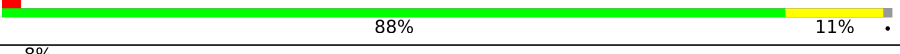
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Mol	Chain	Length	Quality of chain
1	Z	274	
1	e	274	
1	j	274	
1	o	274	
1	t	274	
2	B	99	
2	G	99	
2	L	99	
2	Q	99	
2	V	99	
2	a	99	
2	f	99	
2	k	99	
2	p	99	
2	u	99	
3	C	9	
3	H	9	
3	M	9	
3	R	9	
3	W	9	
3	b	9	
3	g	9	
3	l	9	
3	q	9	
3	v	9	

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Mol	Chain	Length	Quality of chain
4	D	199	
4	I	199	
4	N	199	
4	S	199	
4	X	199	
4	c	199	
4	h	199	
4	m	199	
4	r	199	
4	w	199	
5	E	242	
5	J	242	
5	O	242	
5	T	242	
5	Y	242	
5	d	242	
5	i	242	
5	n	242	
5	s	242	
5	x	242	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 65732 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 MHC class I antigen (Fragment).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	F	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	K	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	P	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	U	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	Z	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	e	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	j	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	o	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	t	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	245	VAL	ALA	engineered mutation	UNP U5YJJ6
A	253	GLN	GLU	engineered mutation	UNP U5YJJ6
F	245	VAL	ALA	engineered mutation	UNP U5YJJ6
F	253	GLN	GLU	engineered mutation	UNP U5YJJ6
K	245	VAL	ALA	engineered mutation	UNP U5YJJ6
K	253	GLN	GLU	engineered mutation	UNP U5YJJ6
P	245	VAL	ALA	engineered mutation	UNP U5YJJ6
P	253	GLN	GLU	engineered mutation	UNP U5YJJ6
U	245	VAL	ALA	engineered mutation	UNP U5YJJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
U	253	GLN	GLU	engineered mutation	UNP U5YJJ6
Z	245	VAL	ALA	engineered mutation	UNP U5YJJ6
Z	253	GLN	GLU	engineered mutation	UNP U5YJJ6
e	245	VAL	ALA	engineered mutation	UNP U5YJJ6
e	253	GLN	GLU	engineered mutation	UNP U5YJJ6
j	245	VAL	ALA	engineered mutation	UNP U5YJJ6
j	253	GLN	GLU	engineered mutation	UNP U5YJJ6
o	245	VAL	ALA	engineered mutation	UNP U5YJJ6
o	253	GLN	GLU	engineered mutation	UNP U5YJJ6
t	245	VAL	ALA	engineered mutation	UNP U5YJJ6
t	253	GLN	GLU	engineered mutation	UNP U5YJJ6

- 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
			828	528	140	157	3			
2	G	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	L	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	Q	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	V	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	a	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	f	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	k	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	p	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	u	98	Total	C	N	O	S	0	0	0
			820	523	139	156	2			

- Molecule 3 is a protein called peptide KRAS-G12V-9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	H	9	Total	C	N	O	0	0	0
			55	35	10	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	R	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	W	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	b	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	g	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	l	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	q	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	v	9	Total	C	N	O	0	0	0
			55	35	10	10			

- Molecule 4 is a protein called TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	I	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	N	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	S	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	X	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	c	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	h	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	m	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	r	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	w	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			

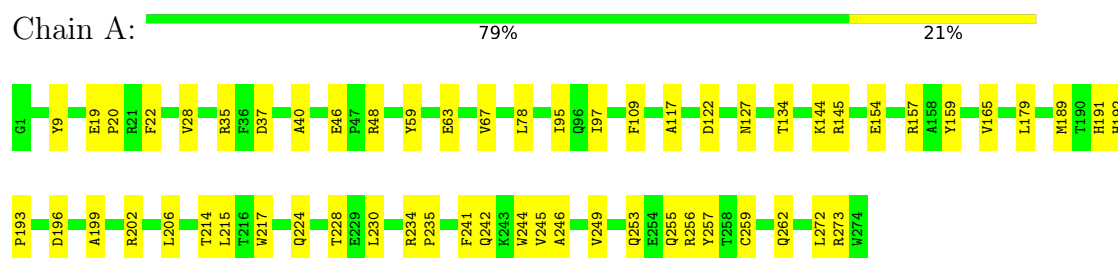
- Molecule 5 is a protein called TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	240	Total 1892	C 1186	N 331	O 369	S 6	0	0	0
5	J	240	Total 1892	C 1186	N 331	O 369	S 6	0	0	0
5	O	240	Total 1892	C 1186	N 331	O 369	S 6	0	0	0
5	T	240	Total 1892	C 1186	N 331	O 369	S 6	0	0	0
5	Y	240	Total 1892	C 1186	N 331	O 369	S 6	0	0	0
5	d	240	Total 1892	C 1186	N 331	O 369	S 6	0	0	0
5	i	240	Total 1892	C 1186	N 331	O 369	S 6	0	0	0
5	n	240	Total 1892	C 1186	N 331	O 369	S 6	0	0	0
5	s	240	Total 1892	C 1186	N 331	O 369	S 6	0	0	0
5	x	240	Total 1892	C 1186	N 331	O 369	S 6	0	0	0

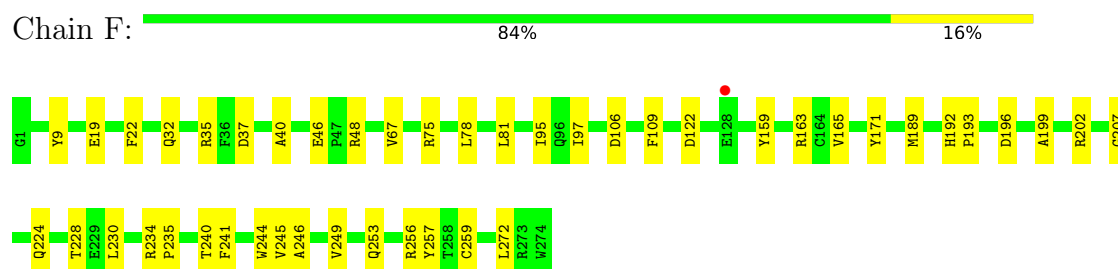
3 Residue-property plots

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.

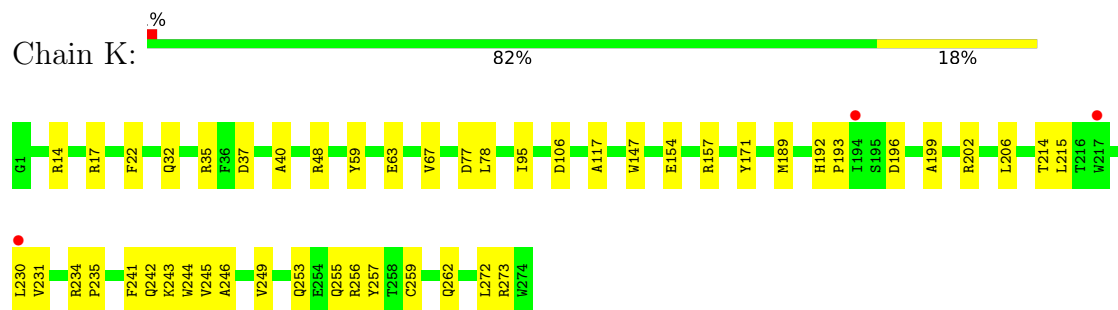
• Molecule 1: MHC class I antigen (Fragment)



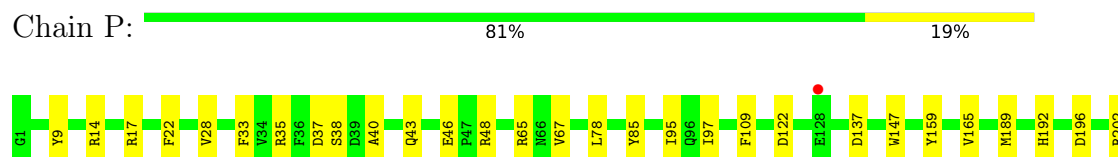
• Molecule 1: MHC class I antigen (Fragment)

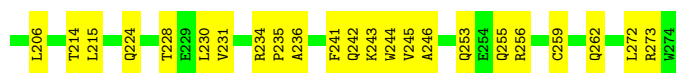


• Molecule 1: MHC class I antigen (Fragment)

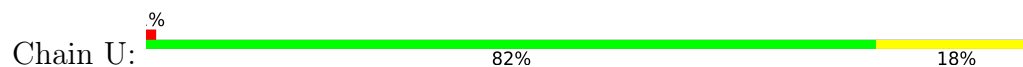


• Molecule 1: MHC class I antigen (Fragment)

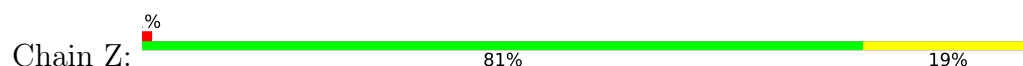




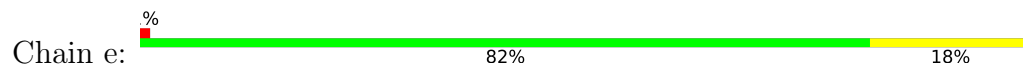
- Molecule 1: MHC class I antigen (Fragment)



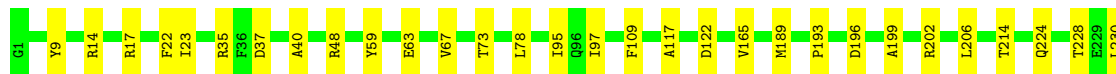
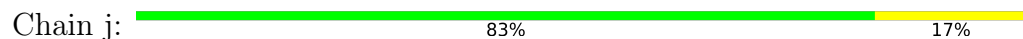
- Molecule 1: MHC class I antigen (Fragment)



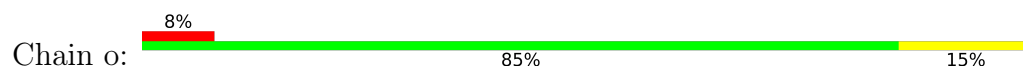
- Molecule 1: MHC class I antigen (Fragment)

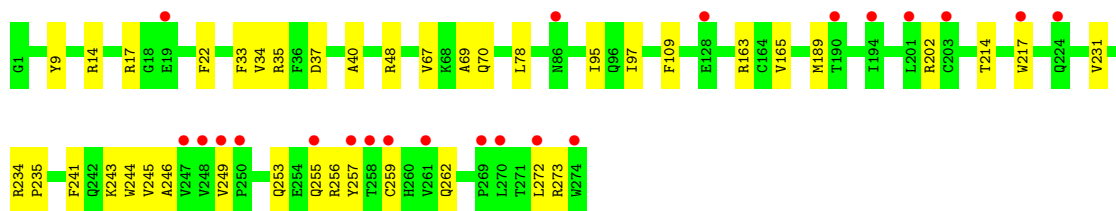


- Molecule 1: MHC class I antigen (Fragment)

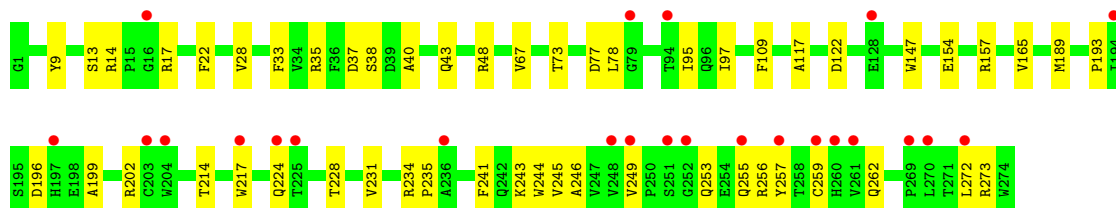
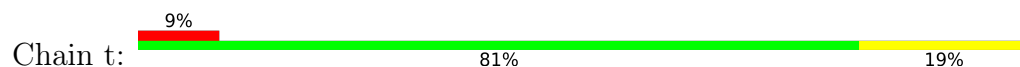


- Molecule 1: MHC class I antigen (Fragment)





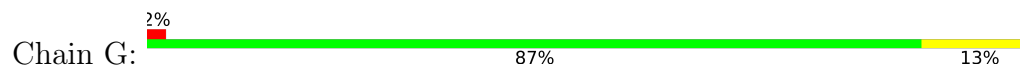
• Molecule 1: MHC class I antigen (Fragment)



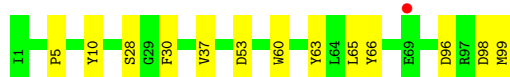
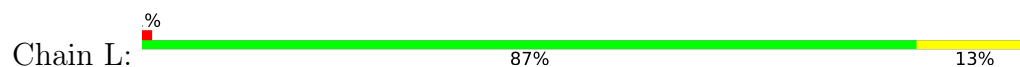
• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin



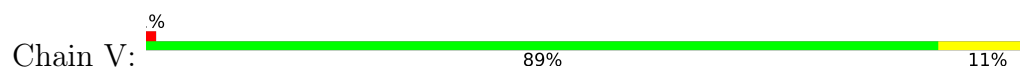
• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin





- Molecule 2: Beta-2-microglobulin

Chain a: 90% 10%



- Molecule 2: Beta-2-microglobulin

Chain f: 9% 94% 6%



- Molecule 2: Beta-2-microglobulin

Chain k: 0% 92% 8%



- Molecule 2: Beta-2-microglobulin

Chain p: 2% 95% 5%



- Molecule 2: Beta-2-microglobulin

Chain u: 4% 89% 10%



- Molecule 3: peptide KRAS-G12V-9

Chain C: 56% 44%

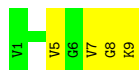


- Molecule 3: peptide KRAS-G12V-9

Chain H: 78% 22%



- Molecule 3: peptide KRAS-G12V-9



- Molecule 3: peptide KRAS-G12V-9



- Molecule 3: peptide KRAS-G12V-9



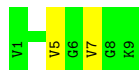
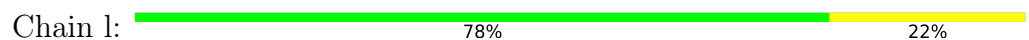
- Molecule 3: peptide KRAS-G12V-9



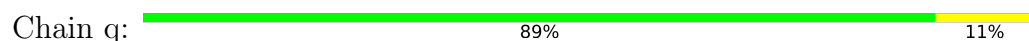
- Molecule 3: peptide KRAS-G12V-9



- Molecule 3: peptide KRAS-G12V-9

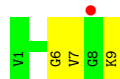


- Molecule 3: peptide KRAS-G12V-9

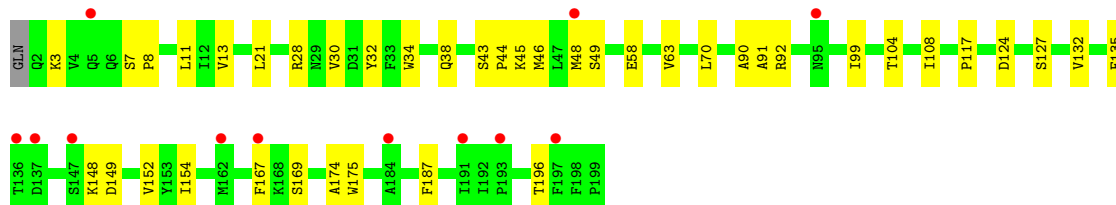




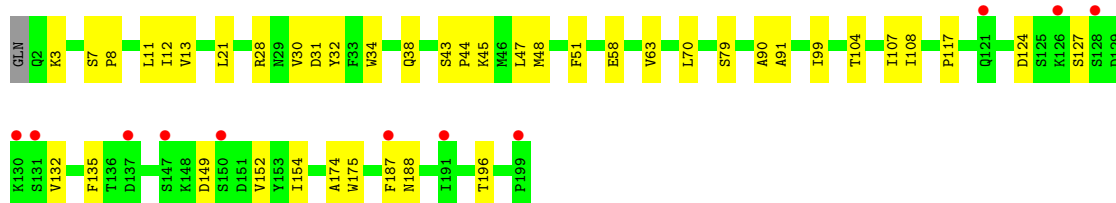
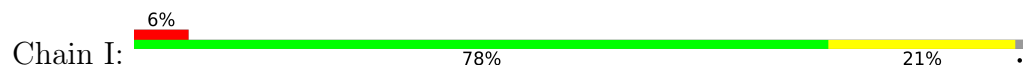
- Molecule 3: peptide KRAS-G12V-9



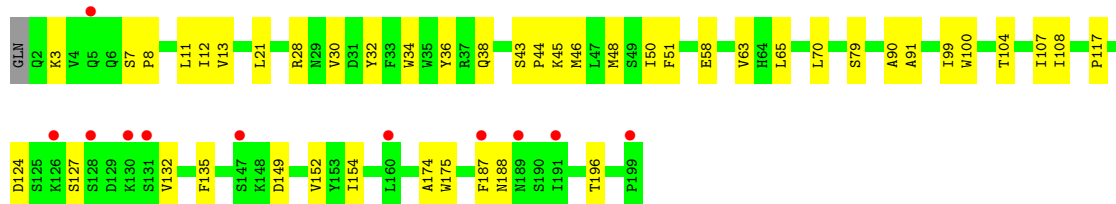
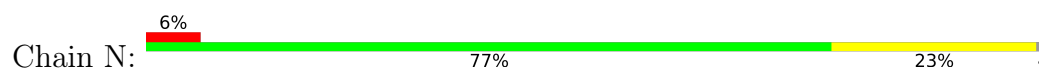
- Molecule 4: TCR alpha chain



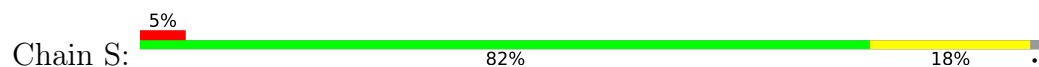
- Molecule 4: TCR alpha chain

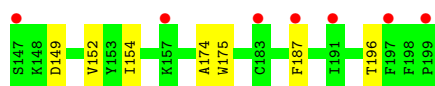


- Molecule 4: TCR alpha chain

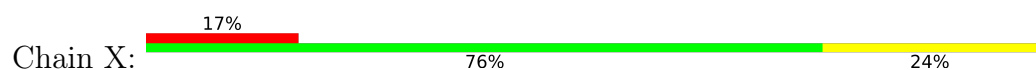


- Molecule 4: TCR alpha chain

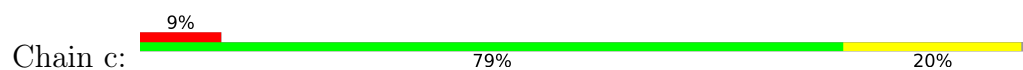




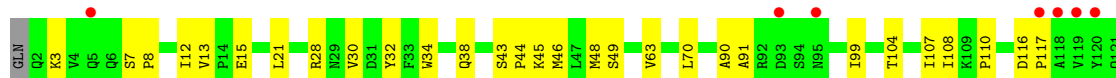
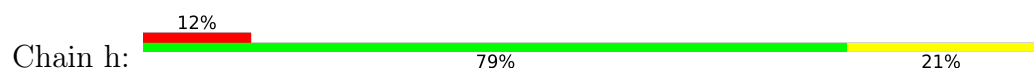
• Molecule 4: TCR alpha chain



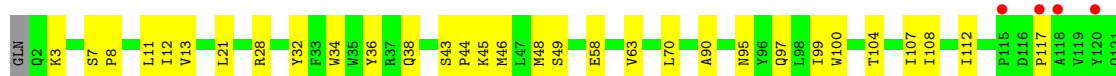
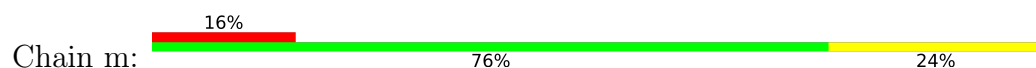
• Molecule 4: TCR alpha chain



• Molecule 4: TCR alpha chain

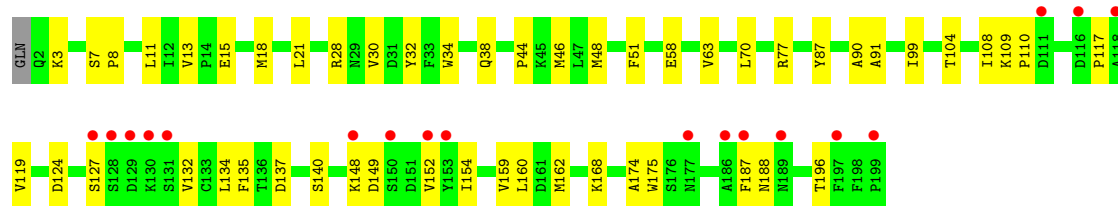


• Molecule 4: TCR alpha chain

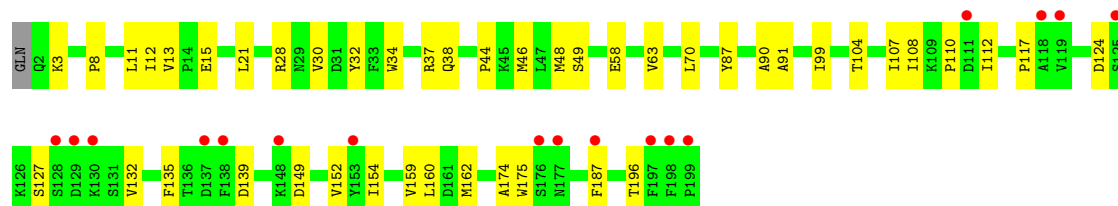
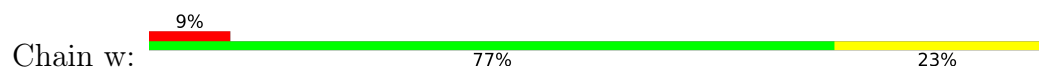


• Molecule 4: TCR alpha chain

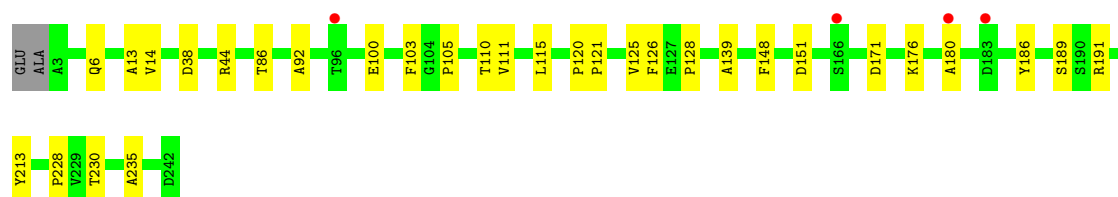
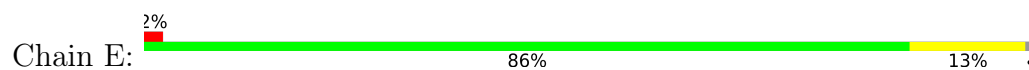




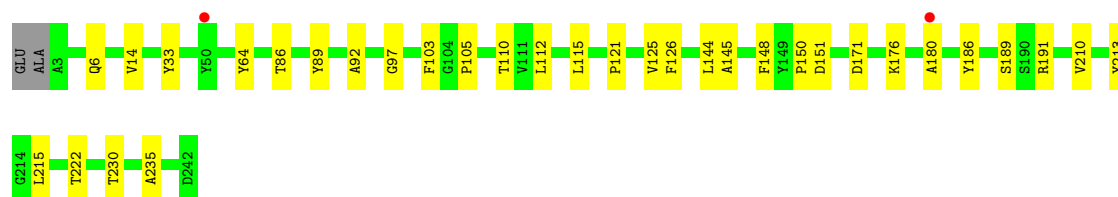
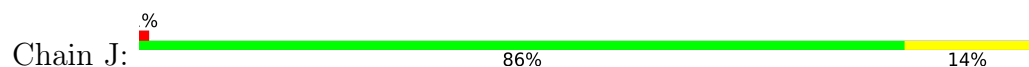
• Molecule 4: TCR alpha chain



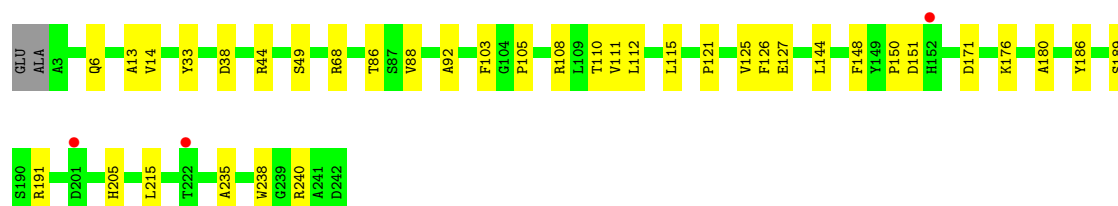
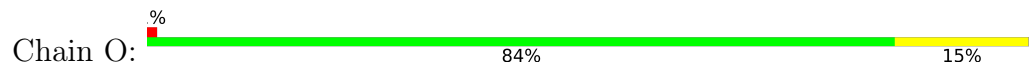
• Molecule 5: TCR beta chain



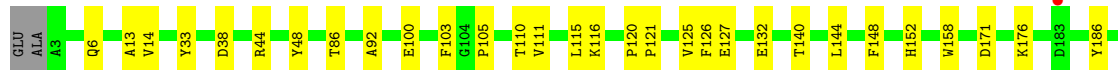
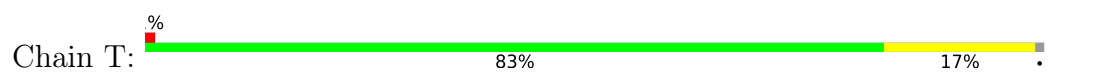
• Molecule 5: TCR beta chain



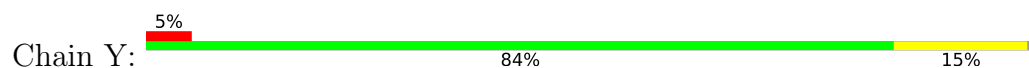
• Molecule 5: TCR beta chain



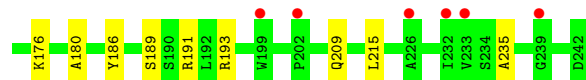
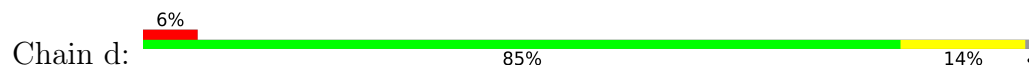
• Molecule 5: TCR beta chain



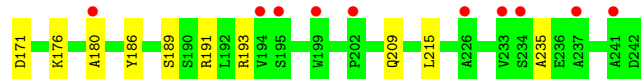
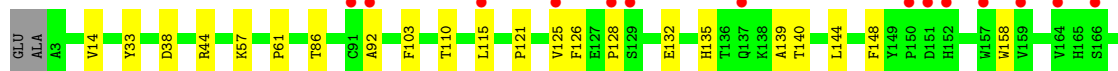
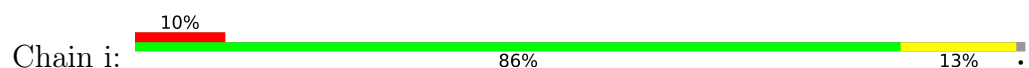
- Molecule 5: TCR beta chain



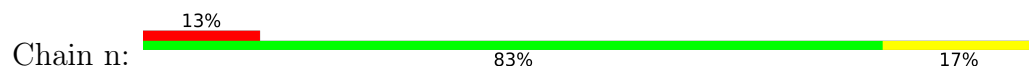
- Molecule 5: TCR beta chain

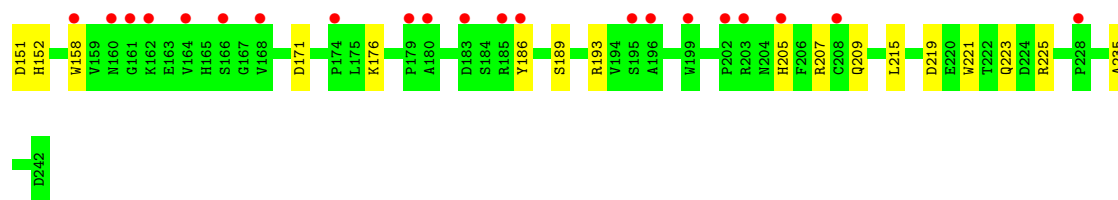


- Molecule 5: TCR beta chain

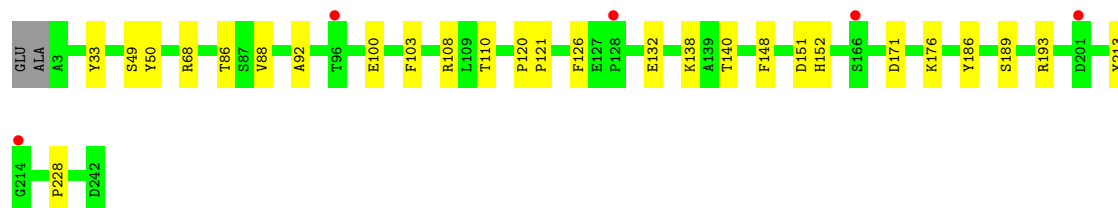
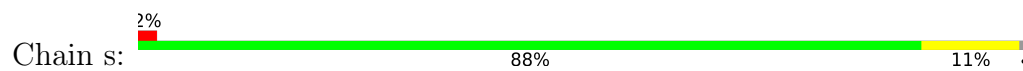


- Molecule 5: TCR beta chain

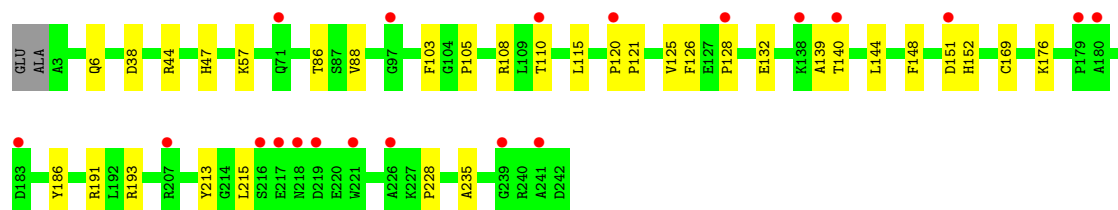
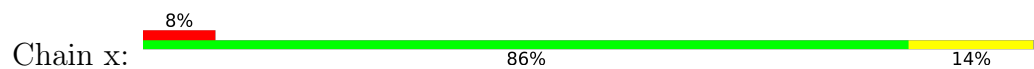




• Molecule 5: TCR beta chain



• Molecule 5: TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	156.86Å 156.89Å 191.97Å 77.37° 78.13° 82.27°	Depositor
Resolution (Å)	49.82 – 3.34 49.82 – 3.34	Depositor EDS
% Data completeness (in resolution range)	92.3 (49.82-3.34) 92.4 (49.82-3.34)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.224 , 0.258 0.224 , 0.258	Depositor DCC
R_{free} test set	11643 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	79.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	65732	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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

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	0.07	0/2298	0.23	0/3120
1	F	0.07	0/2298	0.23	0/3120
1	K	0.07	0/2298	0.23	0/3120
1	P	0.07	0/2298	0.23	0/3120
1	U	0.07	0/2298	0.22	0/3120
1	Z	0.07	0/2298	0.22	0/3120
1	e	0.07	0/2298	0.23	0/3120
1	j	0.08	0/2298	0.22	0/3120
1	o	0.08	0/2298	0.24	0/3120
1	t	0.07	0/2298	0.22	0/3120
2	B	0.09	0/851	0.27	0/1152
2	G	0.09	0/851	0.27	0/1152
2	L	0.09	0/851	0.27	0/1152
2	Q	0.09	0/851	0.28	0/1152
2	V	0.09	0/851	0.27	0/1152
2	a	0.12	0/851	0.27	0/1152
2	f	0.09	0/851	0.26	0/1152
2	k	0.11	0/851	0.25	0/1152
2	p	0.10	0/851	0.24	0/1152
2	u	0.08	0/843	0.24	0/1142
3	C	0.11	0/54	0.28	0/70
3	H	0.13	0/54	0.26	0/70
3	M	0.11	0/54	0.33	0/70
3	R	0.12	0/54	0.36	0/70
3	W	0.13	0/54	0.40	0/70
3	b	0.08	0/54	0.24	0/70
3	g	0.07	0/54	0.26	0/70
3	l	0.09	0/54	0.29	0/70
3	q	0.07	0/54	0.20	0/70
3	v	0.11	0/54	0.28	0/70
4	D	0.08	0/1598	0.22	0/2163
4	I	0.08	0/1598	0.24	0/2163
4	N	0.08	0/1598	0.24	0/2163
4	S	0.07	0/1598	0.22	0/2163

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	X	0.08	0/1598	0.24	0/2163
4	c	0.07	0/1598	0.22	0/2163
4	h	0.07	0/1598	0.21	0/2163
4	m	0.07	0/1598	0.21	0/2163
4	r	0.08	0/1598	0.24	0/2163
4	w	0.08	0/1598	0.24	0/2163
5	E	0.07	0/1944	0.24	0/2650
5	J	0.07	0/1944	0.24	0/2650
5	O	0.08	0/1944	0.24	0/2650
5	T	0.08	0/1944	0.24	0/2650
5	Y	0.10	0/1944	0.25	0/2650
5	d	0.07	0/1944	0.23	0/2650
5	i	0.07	0/1944	0.23	0/2650
5	n	0.08	0/1944	0.25	0/2650
5	s	0.07	0/1944	0.24	0/2650
5	x	0.08	0/1944	0.26	0/2650
All	All	0.08	0/67442	0.24	0/91540

There are no bond length outliers.

There are no bond angle outliers.

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	2237	0	2091	38	0
1	F	2237	0	2091	31	0
1	K	2237	0	2091	33	0
1	P	2237	0	2091	36	0
1	U	2237	0	2091	32	0
1	Z	2237	0	2091	32	0
1	e	2237	0	2091	31	0
1	j	2237	0	2091	28	0
1	o	2237	0	2091	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	t	2237	0	2091	34	0
2	B	828	0	794	8	0
2	G	828	0	794	11	0
2	L	828	0	794	11	0
2	Q	828	0	794	11	0
2	V	828	0	794	9	0
2	a	828	0	794	9	0
2	f	828	0	794	5	0
2	k	828	0	794	7	0
2	p	828	0	794	4	0
2	u	820	0	785	8	0
3	C	55	0	65	3	0
3	H	55	0	65	3	0
3	M	55	0	65	3	0
3	R	55	0	65	3	0
3	W	55	0	65	5	0
3	b	55	0	65	2	0
3	g	55	0	65	5	0
3	l	55	0	65	1	0
3	q	55	0	65	1	0
3	v	55	0	65	5	0
4	D	1562	0	1484	30	0
4	I	1562	0	1484	29	0
4	N	1562	0	1484	31	0
4	S	1562	0	1484	23	0
4	X	1562	0	1484	32	0
4	c	1562	0	1484	29	0
4	h	1562	0	1484	26	0
4	m	1562	0	1484	31	0
4	r	1562	0	1484	37	0
4	w	1562	0	1484	27	0
5	E	1892	0	1779	20	0
5	J	1892	0	1779	23	0
5	O	1892	0	1779	23	0
5	T	1892	0	1779	25	0
5	Y	1892	0	1779	23	0
5	d	1892	0	1779	24	0
5	i	1892	0	1779	20	0
5	n	1892	0	1779	24	0
5	s	1892	0	1779	20	0
5	x	1892	0	1779	20	0
All	All	65732	0	62121	810	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 6.

The worst 5 of 810 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)
1:t:255:GLN:O	1:t:273:ARG:NH1	2.21	0.73
1:o:255:GLN:O	1:o:273:ARG:NH1	2.23	0.72
1:P:14:ARG:HB3	1:P:17:ARG:HB2	1.73	0.70
5:n:221:TRP:HH2	5:n:225:ARG:HB2	1.56	0.70
1:A:35:ARG:HD3	1:A:48:ARG:HE	1.57	0.69

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	272/274 (99%)	270 (99%)	2 (1%)	0	100	100
1	F	272/274 (99%)	271 (100%)	1 (0%)	0	100	100
1	K	272/274 (99%)	271 (100%)	1 (0%)	0	100	100
1	P	272/274 (99%)	270 (99%)	2 (1%)	0	100	100
1	U	272/274 (99%)	269 (99%)	3 (1%)	0	100	100
1	Z	272/274 (99%)	271 (100%)	1 (0%)	0	100	100
1	e	272/274 (99%)	269 (99%)	3 (1%)	0	100	100
1	j	272/274 (99%)	269 (99%)	3 (1%)	0	100	100
1	o	272/274 (99%)	269 (99%)	3 (1%)	0	100	100
1	t	272/274 (99%)	269 (99%)	3 (1%)	0	100	100
2	B	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	G	97/99 (98%)	96 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	97/99 (98%)	97 (100%)	0	0	100	100
2	Q	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	V	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	a	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	f	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	k	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
2	p	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	u	96/99 (97%)	92 (96%)	4 (4%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	7 (100%)	0	0	100	100
3	M	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	R	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	W	7/9 (78%)	7 (100%)	0	0	100	100
3	b	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	g	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	l	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	q	7/9 (78%)	7 (100%)	0	0	100	100
3	v	7/9 (78%)	7 (100%)	0	0	100	100
4	D	196/199 (98%)	193 (98%)	3 (2%)	0	100	100
4	I	196/199 (98%)	193 (98%)	3 (2%)	0	100	100
4	N	196/199 (98%)	192 (98%)	4 (2%)	0	100	100
4	S	196/199 (98%)	190 (97%)	6 (3%)	0	100	100
4	X	196/199 (98%)	194 (99%)	2 (1%)	0	100	100
4	c	196/199 (98%)	194 (99%)	2 (1%)	0	100	100
4	h	196/199 (98%)	193 (98%)	3 (2%)	0	100	100
4	m	196/199 (98%)	193 (98%)	3 (2%)	0	100	100
4	r	196/199 (98%)	192 (98%)	4 (2%)	0	100	100
4	w	196/199 (98%)	192 (98%)	4 (2%)	0	100	100
5	E	238/242 (98%)	237 (100%)	1 (0%)	0	100	100
5	J	238/242 (98%)	234 (98%)	4 (2%)	0	100	100
5	O	238/242 (98%)	236 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	T	238/242 (98%)	233 (98%)	5 (2%)	0	100	100
5	Y	238/242 (98%)	236 (99%)	2 (1%)	0	100	100
5	d	238/242 (98%)	236 (99%)	2 (1%)	0	100	100
5	i	238/242 (98%)	237 (100%)	1 (0%)	0	100	100
5	n	238/242 (98%)	233 (98%)	5 (2%)	0	100	100
5	s	238/242 (98%)	235 (99%)	3 (1%)	0	100	100
5	x	238/242 (98%)	233 (98%)	5 (2%)	0	100	100
All	All	8099/8230 (98%)	7985 (99%)	114 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	F	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	K	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	P	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	U	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	Z	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	e	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	j	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	o	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	t	232/232 (100%)	231 (100%)	1 (0%)	84	83
2	B	94/94 (100%)	94 (100%)	0	100	100
2	G	94/94 (100%)	94 (100%)	0	100	100
2	L	94/94 (100%)	94 (100%)	0	100	100
2	Q	94/94 (100%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V	94/94 (100%)	94 (100%)	0	100	100
2	a	94/94 (100%)	94 (100%)	0	100	100
2	f	94/94 (100%)	94 (100%)	0	100	100
2	k	94/94 (100%)	94 (100%)	0	100	100
2	p	94/94 (100%)	94 (100%)	0	100	100
2	u	93/94 (99%)	93 (100%)	0	100	100
3	C	5/5 (100%)	5 (100%)	0	100	100
3	H	5/5 (100%)	5 (100%)	0	100	100
3	M	5/5 (100%)	5 (100%)	0	100	100
3	R	5/5 (100%)	5 (100%)	0	100	100
3	W	5/5 (100%)	5 (100%)	0	100	100
3	b	5/5 (100%)	5 (100%)	0	100	100
3	g	5/5 (100%)	5 (100%)	0	100	100
3	l	5/5 (100%)	5 (100%)	0	100	100
3	q	5/5 (100%)	5 (100%)	0	100	100
3	v	5/5 (100%)	5 (100%)	0	100	100
4	D	180/181 (99%)	180 (100%)	0	100	100
4	I	180/181 (99%)	180 (100%)	0	100	100
4	N	180/181 (99%)	180 (100%)	0	100	100
4	S	180/181 (99%)	180 (100%)	0	100	100
4	X	180/181 (99%)	180 (100%)	0	100	100
4	c	180/181 (99%)	180 (100%)	0	100	100
4	h	180/181 (99%)	180 (100%)	0	100	100
4	m	180/181 (99%)	180 (100%)	0	100	100
4	r	180/181 (99%)	180 (100%)	0	100	100
4	w	180/181 (99%)	180 (100%)	0	100	100
5	E	205/206 (100%)	205 (100%)	0	100	100
5	J	205/206 (100%)	205 (100%)	0	100	100
5	O	205/206 (100%)	205 (100%)	0	100	100
5	T	205/206 (100%)	205 (100%)	0	100	100
5	Y	205/206 (100%)	205 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	d	205/206 (100%)	205 (100%)	0	100	100
5	i	205/206 (100%)	205 (100%)	0	100	100
5	n	205/206 (100%)	205 (100%)	0	100	100
5	s	205/206 (100%)	205 (100%)	0	100	100
5	x	205/206 (100%)	205 (100%)	0	100	100
All	All	7159/7180 (100%)	7149 (100%)	10 (0%)	88	89

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	j	259	CYS
1	o	259	CYS
1	t	259	CYS
1	P	259	CYS
1	U	259	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
5	d	73	ASN
4	m	71	HIS
5	d	173	GLN
4	h	22	ASN
4	m	146	GLN

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 oligosaccharides 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	274/274 (100%)	-0.08	0 100 100	38, 61, 98, 129	0
1	F	274/274 (100%)	0.03	1 (0%) 88 80	46, 66, 101, 127	0
1	K	274/274 (100%)	0.10	3 (1%) 78 62	41, 68, 105, 130	0
1	P	274/274 (100%)	-0.05	1 (0%) 88 80	39, 61, 100, 136	0
1	U	274/274 (100%)	0.12	4 (1%) 72 53	42, 71, 113, 151	0
1	Z	274/274 (100%)	0.24	3 (1%) 78 62	50, 73, 108, 155	0
1	e	274/274 (100%)	0.26	3 (1%) 78 62	49, 80, 110, 128	0
1	j	274/274 (100%)	0.18	0 100 100	50, 75, 111, 142	0
1	o	274/274 (100%)	0.54	22 (8%) 18 14	48, 83, 175, 197	0
1	t	274/274 (100%)	0.60	24 (8%) 15 13	52, 91, 175, 192	0
2	B	99/99 (100%)	-0.06	0 100 100	45, 66, 97, 122	0
2	G	99/99 (100%)	0.12	2 (2%) 65 47	54, 76, 111, 126	0
2	L	99/99 (100%)	0.17	1 (1%) 79 64	50, 77, 109, 120	0
2	Q	99/99 (100%)	0.01	0 100 100	44, 65, 97, 120	0
2	V	99/99 (100%)	0.19	1 (1%) 79 64	59, 87, 116, 131	0
2	a	99/99 (100%)	0.20	0 100 100	59, 82, 111, 120	0
2	f	99/99 (100%)	0.83	9 (9%) 15 12	63, 102, 142, 148	0
2	k	99/99 (100%)	0.22	1 (1%) 79 64	62, 86, 111, 138	0
2	p	99/99 (100%)	0.47	2 (2%) 65 47	64, 96, 136, 143	0
2	u	98/99 (98%)	0.56	4 (4%) 41 27	67, 108, 133, 153	0
3	C	9/9 (100%)	0.34	0 100 100	47, 52, 58, 66	0
3	H	9/9 (100%)	0.42	0 100 100	54, 60, 64, 64	0
3	M	9/9 (100%)	0.65	0 100 100	47, 58, 66, 69	0
3	R	9/9 (100%)	0.61	1 (11%) 10 10	41, 55, 58, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
3	W	9/9 (100%)	0.67	0	100	100	52, 60, 65, 69	0
3	b	9/9 (100%)	0.66	0	100	100	52, 67, 70, 74	0
3	g	9/9 (100%)	0.71	0	100	100	59, 69, 80, 81	0
3	l	9/9 (100%)	0.77	0	100	100	58, 67, 73, 80	0
3	q	9/9 (100%)	0.07	0	100	100	58, 60, 62, 63	0
3	v	9/9 (100%)	1.21	1 (11%)	10	10	62, 74, 78, 95	0
4	D	198/199 (99%)	0.48	12 (6%)	27	19	42, 81, 160, 177	0
4	I	198/199 (99%)	0.52	11 (5%)	30	21	41, 78, 144, 176	0
4	N	198/199 (99%)	0.53	11 (5%)	30	21	36, 77, 143, 187	0
4	S	198/199 (99%)	0.53	9 (4%)	38	25	43, 79, 154, 174	0
4	X	198/199 (99%)	0.86	33 (16%)	4	4	46, 86, 169, 190	0
4	c	198/199 (99%)	0.73	18 (9%)	15	12	48, 92, 177, 198	0
4	h	198/199 (99%)	0.88	23 (11%)	9	9	56, 92, 176, 196	0
4	m	198/199 (99%)	0.86	32 (16%)	4	5	49, 93, 164, 196	0
4	r	198/199 (99%)	0.72	18 (9%)	15	12	44, 86, 151, 197	0
4	w	198/199 (99%)	0.70	17 (8%)	16	13	45, 85, 161, 195	0
5	E	240/242 (99%)	0.12	4 (1%)	69	51	47, 74, 117, 143	0
5	J	240/242 (99%)	0.09	2 (0%)	82	69	41, 65, 114, 136	0
5	O	240/242 (99%)	0.12	3 (1%)	75	57	41, 66, 113, 135	0
5	T	240/242 (99%)	0.11	2 (0%)	82	69	43, 73, 118, 155	0
5	Y	240/242 (99%)	0.57	11 (4%)	37	25	47, 93, 145, 182	0
5	d	240/242 (99%)	0.85	14 (5%)	29	19	56, 131, 176, 190	0
5	i	240/242 (99%)	0.94	24 (10%)	12	11	66, 136, 181, 198	0
5	n	240/242 (99%)	0.94	32 (13%)	7	7	46, 94, 151, 186	0
5	s	240/242 (99%)	0.35	5 (2%)	63	45	48, 78, 125, 151	0
5	x	240/242 (99%)	0.91	20 (8%)	17	13	54, 98, 147, 180	0
All	All	8199/8230 (99%)	0.42	384 (4%)	36	25	36, 79, 156, 198	0

The worst 5 of 384 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	o	257	TYR	5.0
4	D	147	SER	4.9

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Mol	Chain	Res	Type	RSRZ
4	N	147	SER	4.5
4	r	131	SER	4.5
4	m	191	ILE	4.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.