



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 02:30 AM EDT

PDB ID : 8RRO / pdb_00008rro
Title : G12V-TCR complex with HLA-A3
Authors : Sim, M.J.W.; Sun, P.D.
Deposited on : 2024-01-23
Resolution : 3.50 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

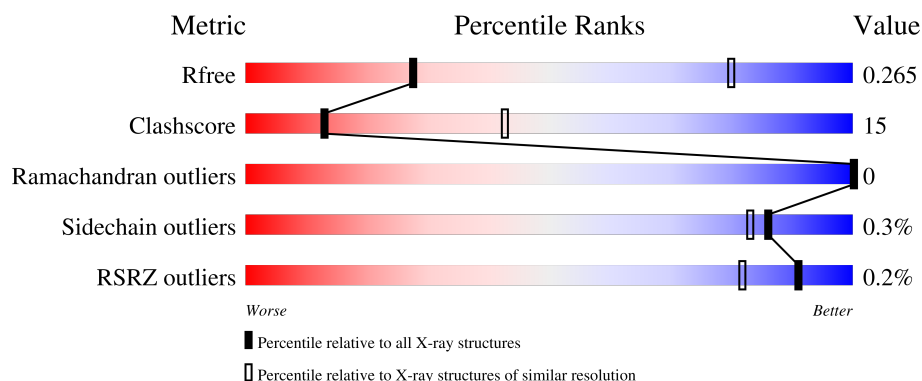
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	206	
1	F	206	
1	K	206	
1	P	206	
1	U	206	

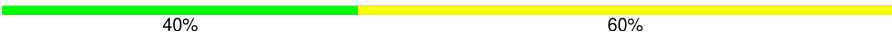
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Mol	Chain	Length	Quality of chain
1	Z	206	
1	e	206	
1	j	206	
2	B	246	
2	G	246	
2	L	246	
2	Q	246	
2	V	246	
2	a	246	
2	f	246	
2	k	246	
3	C	279	
3	H	279	
3	M	279	
3	R	279	
3	W	279	
3	b	279	
3	g	279	
3	l	279	
4	D	100	
4	I	100	
4	N	100	
4	S	100	
4	X	100	
4	c	100	

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Mol	Chain	Length	Quality of chain
4	h	100	
4	m	100	
5	E	10	
5	J	10	
5	O	10	
5	T	10	
5	Y	10	
5	d	10	
5	i	10	
5	n	10	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 53193 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 G12V-TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1593	1003	265	317	8			
1	F	202	Total	C	N	O	S	0	0	0
			1591	1002	265	316	8			
1	K	203	Total	C	N	O	S	0	0	0
			1597	1005	266	318	8			
1	P	201	Total	C	N	O	S	0	0	0
			1587	1000	264	315	8			
1	U	201	Total	C	N	O	S	0	0	0
			1587	1000	264	315	8			
1	Z	201	Total	C	N	O	S	0	0	0
			1587	1000	264	315	8			
1	e	202	Total	C	N	O	S	0	0	0
			1593	1003	265	317	8			
1	j	200	Total	C	N	O	S	0	0	0
			1580	995	263	314	8			

- Molecule 2 is a protein called G12V-TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1958	1235	351	364	8			
2	G	240	Total	C	N	O	S	0	0	0
			1942	1226	349	359	8			
2	L	240	Total	C	N	O	S	0	0	0
			1942	1226	349	359	8			
2	Q	240	Total	C	N	O	S	0	0	0
			1942	1226	349	359	8			
2	V	240	Total	C	N	O	S	0	0	0
			1942	1226	349	359	8			
2	a	240	Total	C	N	O	S	0	0	0
			1942	1226	349	359	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	f	240	Total	C	N	O	S	0	0	0
			1942	1226	349	359	8			
2	k	240	Total	C	N	O	S	0	0	0
			1942	1226	349	359	8			

- Molecule 3 is a protein called HLA class I histocompatibility antigen, A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	274	Total	C	N	O	S	0	0	0
			2228	1386	403	430	9			
3	H	275	Total	C	N	O	S	0	0	0
			2237	1391	404	433	9			
3	M	276	Total	C	N	O	S	0	0	0
			2245	1397	405	434	9			
3	R	277	Total	C	N	O	S	0	0	0
			2251	1400	406	436	9			
3	W	276	Total	C	N	O	S	0	0	0
			2245	1397	405	434	9			
3	b	276	Total	C	N	O	S	0	0	0
			2245	1397	405	434	9			
3	g	274	Total	C	N	O	S	0	0	0
			2228	1386	403	430	9			
3	l	273	Total	C	N	O	S	0	0	0
			2214	1375	401	429	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP P04439
H	0	MET	-	initiating methionine	UNP P04439
M	0	MET	-	initiating methionine	UNP P04439
R	0	MET	-	initiating methionine	UNP P04439
W	0	MET	-	initiating methionine	UNP P04439
b	0	MET	-	initiating methionine	UNP P04439
g	0	MET	-	initiating methionine	UNP P04439
l	0	MET	-	initiating methionine	UNP P04439

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	98	Total	C	N	O	S	0	0	0
			820	523	139	156	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	97	Total	C	N	O	S	0	0	0
			812	519	138	153	2			
4	N	98	Total	C	N	O	S	0	0	0
			820	523	139	156	2			
4	S	98	Total	C	N	O	S	0	0	0
			820	523	139	156	2			
4	X	98	Total	C	N	O	S	0	0	0
			820	523	139	156	2			
4	c	98	Total	C	N	O	S	0	0	0
			820	523	139	156	2			
4	h	97	Total	C	N	O	S	0	0	0
			812	519	138	153	2			
4	m	97	Total	C	N	O	S	0	0	0
			812	519	138	153	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P61769
I	0	MET	-	initiating methionine	UNP P61769
N	0	MET	-	initiating methionine	UNP P61769
S	0	MET	-	initiating methionine	UNP P61769
X	0	MET	-	initiating methionine	UNP P61769
c	0	MET	-	initiating methionine	UNP P61769
h	0	MET	-	initiating methionine	UNP P61769
m	0	MET	-	initiating methionine	UNP P61769

- Molecule 5 is a protein called GTPase KRas, N-terminally processed.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	10	Total	C	N	O	0	0	0
			62	40	11	11			
5	J	10	Total	C	N	O	0	0	0
			62	40	11	11			
5	O	10	Total	C	N	O	0	0	0
			62	40	11	11			
5	T	10	Total	C	N	O	0	0	0
			62	40	11	11			
5	Y	10	Total	C	N	O	0	0	0
			62	40	11	11			
5	d	10	Total	C	N	O	0	0	0
			62	40	11	11			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	i	10	Total	C	N	O	0	0	0
			62	40	11	11			
5	n	10	Total	C	N	O	0	0	0
			62	40	11	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	6	VAL	GLY	variant	UNP P01116
J	6	VAL	GLY	variant	UNP P01116
O	6	VAL	GLY	variant	UNP P01116
T	6	VAL	GLY	variant	UNP P01116
Y	6	VAL	GLY	variant	UNP P01116
d	6	VAL	GLY	variant	UNP P01116
i	6	VAL	GLY	variant	UNP P01116
n	6	VAL	GLY	variant	UNP P01116

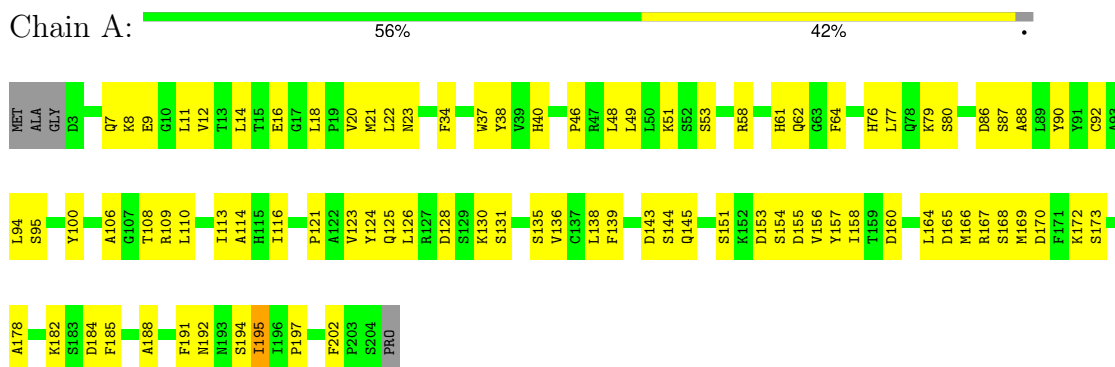
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	O	0	0
			1	1		

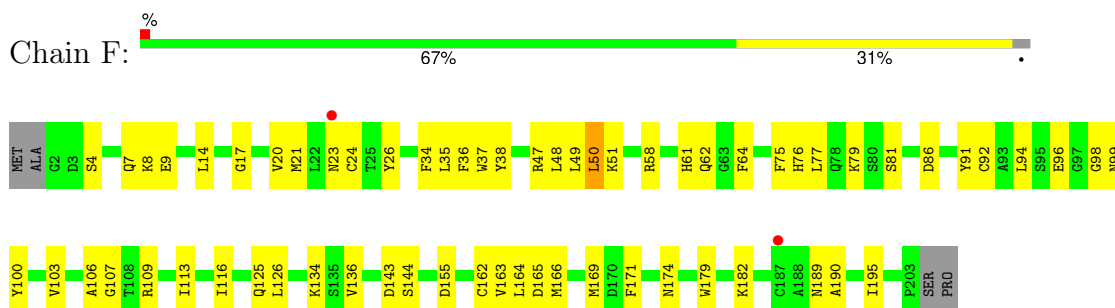
3 Residue-property plots [i](#)

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.

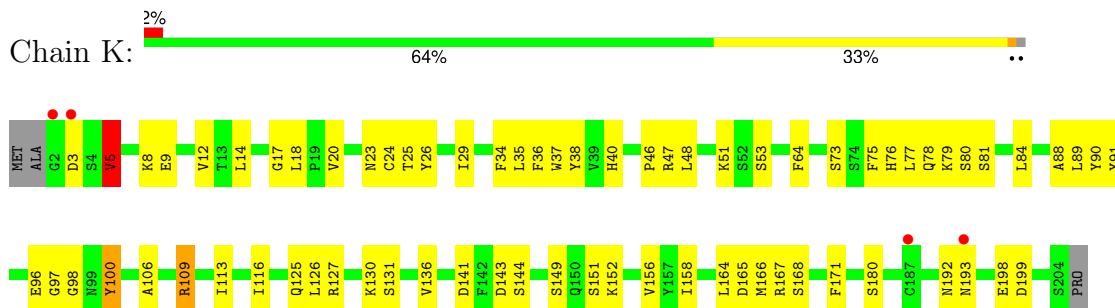
- Molecule 1: G12V-TCR alpha chain



- Molecule 1: G12V-TCR alpha chain

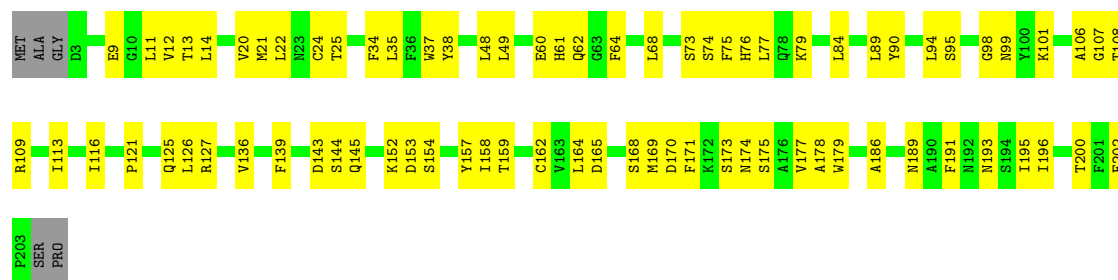


- Molecule 1: G12V-TCR alpha chain

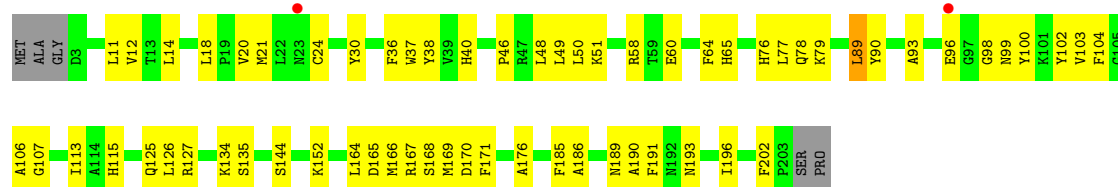


- Molecule 1: G12V-TCR alpha chain

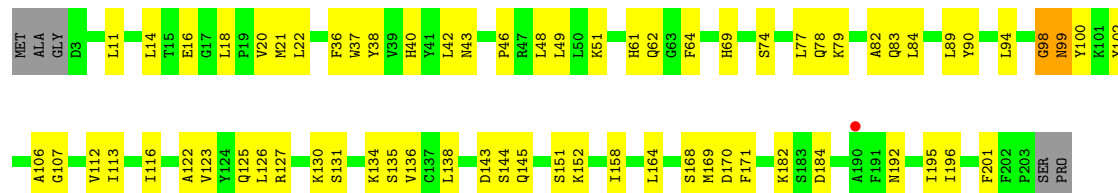




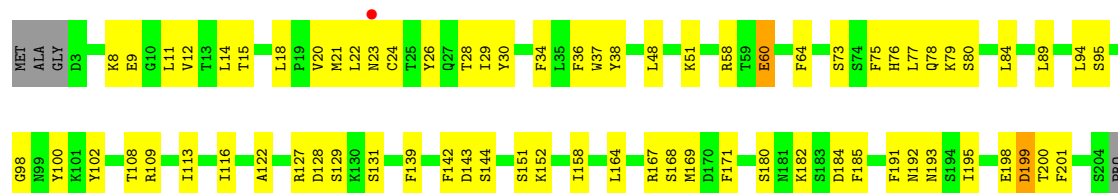
- Molecule 1: G12V-TCR alpha chain



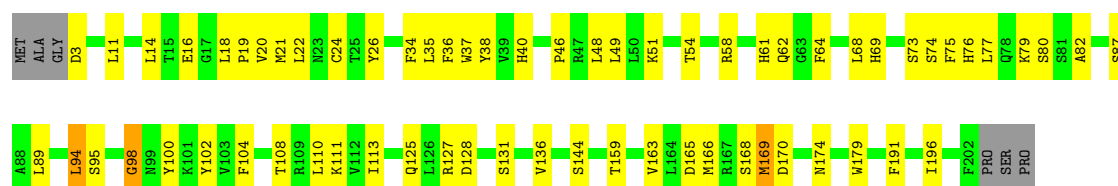
- Molecule 1: G12V-TCR alpha chain



- Molecule 1: G12V-TCR alpha chain

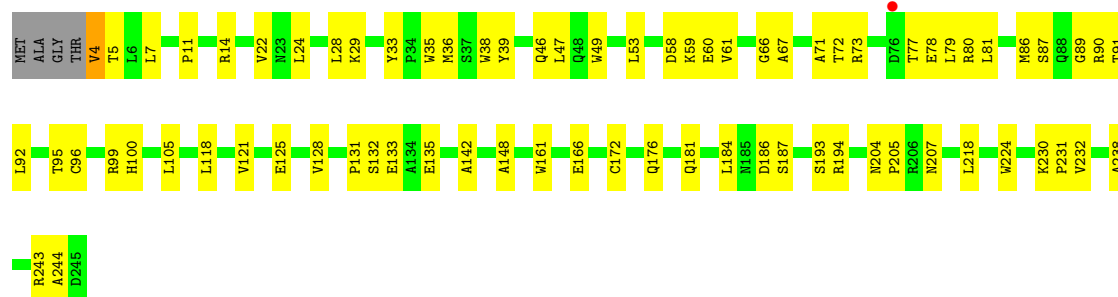


- Molecule 1: G12V-TCR alpha chain



- Molecule 2: G12V-TCR beta chain

Chain B:  68% 30%



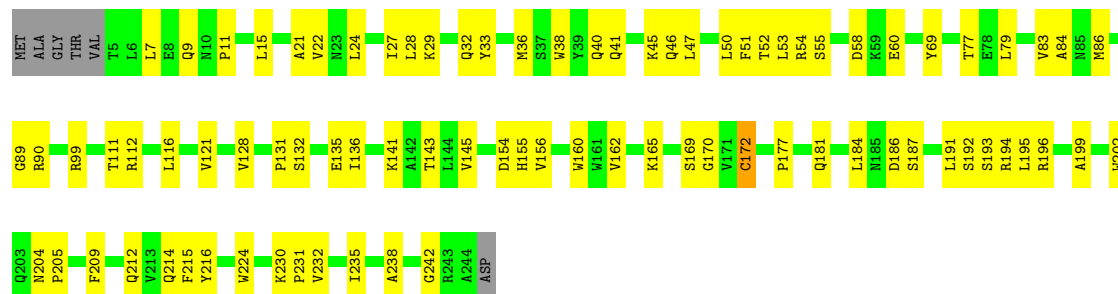
- Molecule 2: G12V-TCR beta chain

Chain G:  70% 28%



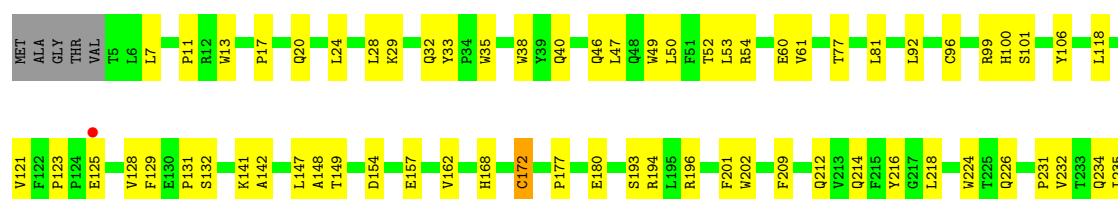
- Molecule 2: G12V-TCR beta chain

Chain L:  63% 34%



- Molecule 2: G12V-TCR beta chain

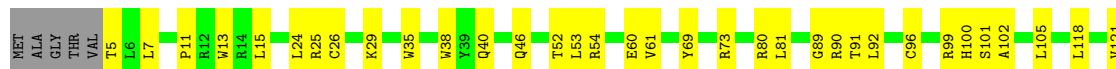
Chain Q:  70% 27%





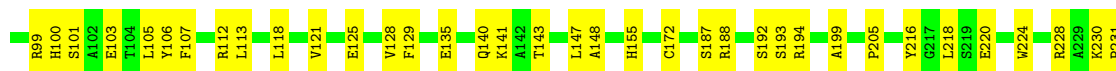
- Molecule 2: G12V-TCR beta chain

Chain V: 71% 26%



- Molecule 2: G12V-TCR beta chain

Chain a: 67% 30%



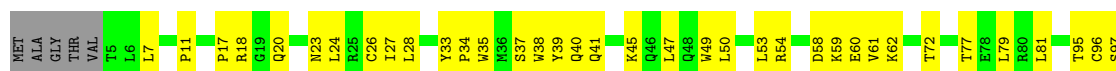
- Molecule 2: G12V-TCR beta chain

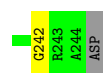
Chain f: 70% 27%



- Molecule 2: G12V-TCR beta chain

Chain k: 67% 30%



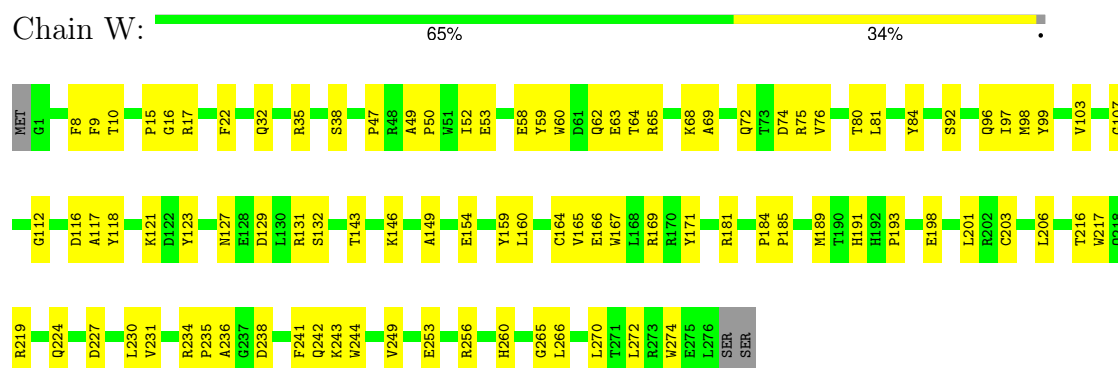


- Molecule 3: HLA class I histocompatibility antigen, A alpha chain

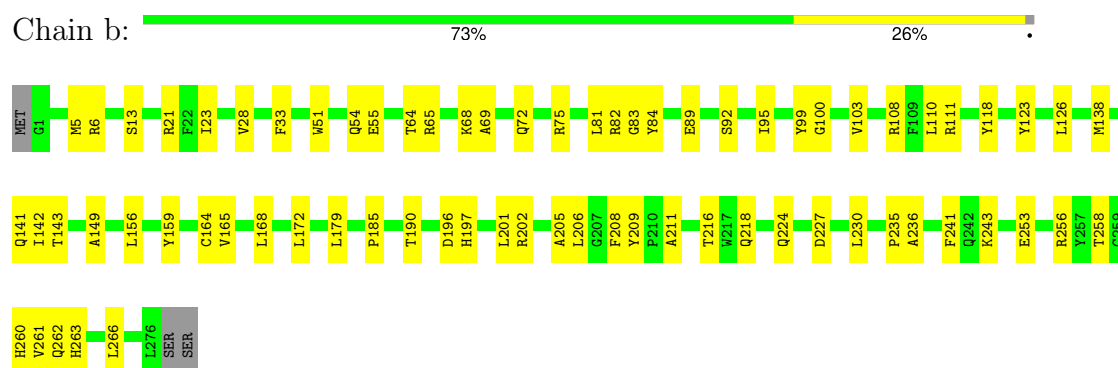
Chain C: 65% 33% ..



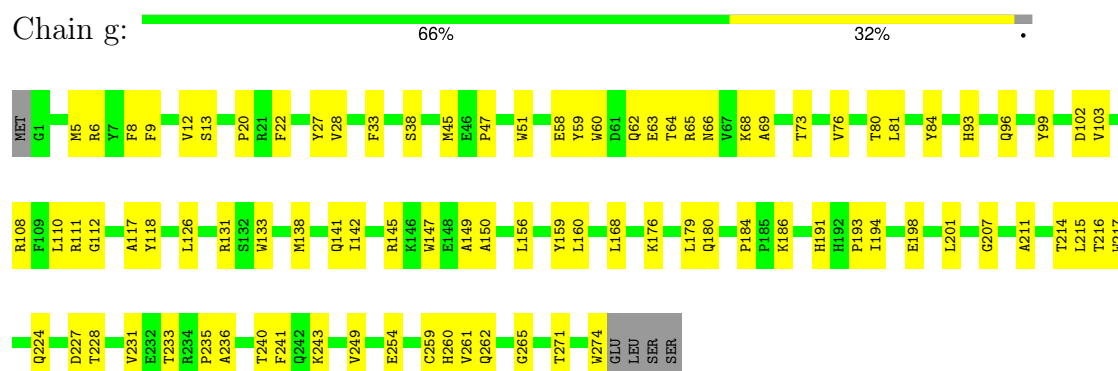
- Molecule 3: HLA class I histocompatibility antigen, A alpha chain



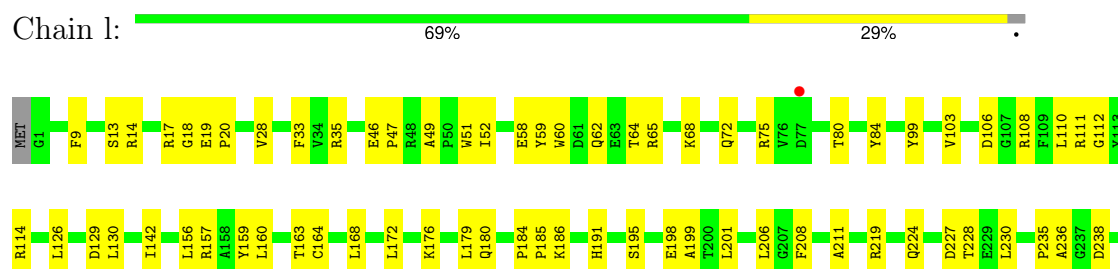
- Molecule 3: HLA class I histocompatibility antigen, A alpha chain

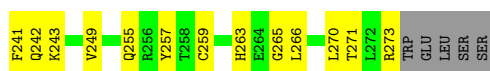


- Molecule 3: HLA class I histocompatibility antigen, A alpha chain



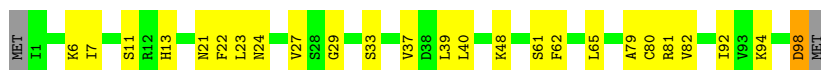
- Molecule 3: HLA class I histocompatibility antigen, A alpha chain





• Molecule 4: Beta-2-microglobulin

Chain D: 73% 24%



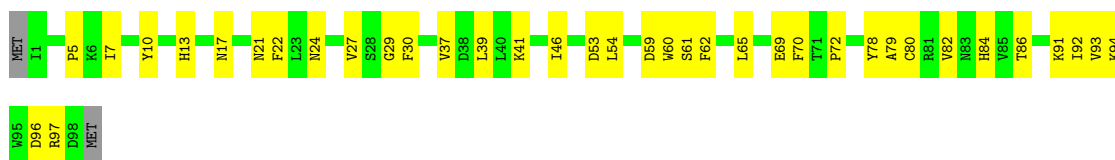
• Molecule 4: Beta-2-microglobulin

Chain I: 73% 24%



• Molecule 4: Beta-2-microglobulin

Chain N: 61% 37%



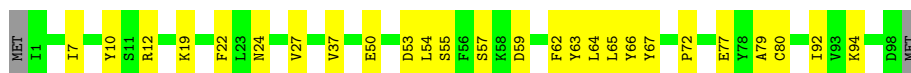
• Molecule 4: Beta-2-microglobulin

Chain S: 79% 19%



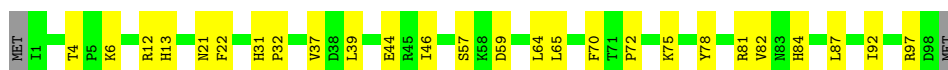
• Molecule 4: Beta-2-microglobulin

Chain X: 72% 26%



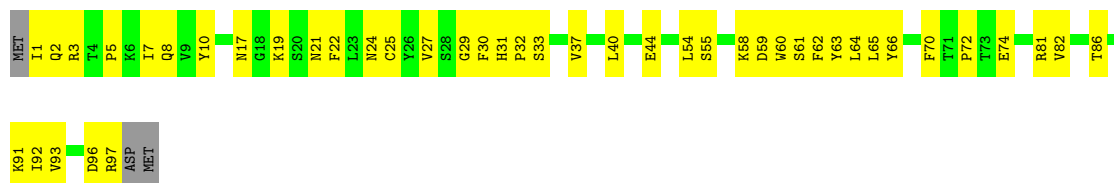
• Molecule 4: Beta-2-microglobulin

Chain c: 72% 26%



• Molecule 4: Beta-2-microglobulin

Chain h:  53% 44%



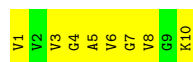
- Molecule 4: Beta-2-microglobulin

Chain m:  69% 28%



- Molecule 5: GTPase KRas, N-terminally processed

Chain E:  20% 80%



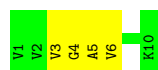
- Molecule 5: GTPase KRas, N-terminally processed

Chain J:  40% 60%



- Molecule 5: GTPase KRas, N-terminally processed

Chain O:  60% 40%



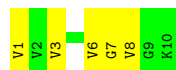
- Molecule 5: GTPase KRas, N-terminally processed

Chain T:  50% 50%



- Molecule 5: GTPase KRas, N-terminally processed

Chain Y:  50% 50%



- Molecule 5: GTPase KRas, N-terminally processed

Chain d:  50% 50%



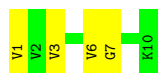
- Molecule 5: GTPase KRas, N-terminally processed

Chain i:  50% 50%



- Molecule 5: GTPase KRas, N-terminally processed

Chain n:  60% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.48Å 195.79Å 442.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.46 – 3.50 46.46 – 3.50	Depositor EDS
% Data completeness (in resolution range)	84.4 (46.46-3.50) 95.4 (46.46-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.238 , 0.286 0.268 , 0.265	Depositor DCC
R_{free} test set	6903 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 97.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	53193	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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	0.64	0/1630	0.94	1/2209 (0.0%)
1	F	0.66	0/1628	0.95	1/2206 (0.0%)
1	K	0.70	1/1634 (0.1%)	1.01	2/2214 (0.1%)
1	P	0.63	1/1624 (0.1%)	0.96	0/2201
1	U	0.61	0/1624	0.93	2/2201 (0.1%)
1	Z	0.66	1/1624 (0.1%)	1.11	7/2201 (0.3%)
1	e	0.62	0/1630	0.98	2/2209 (0.1%)
1	j	0.70	1/1616 (0.1%)	0.96	1/2189 (0.0%)
2	B	0.56	2/2010 (0.1%)	0.81	0/2739
2	G	0.54	0/1994	0.80	0/2718
2	L	0.54	0/1994	0.84	0/2718
2	Q	0.52	0/1994	0.80	0/2718
2	V	0.52	0/1994	0.80	0/2718
2	a	0.50	0/1994	0.78	0/2718
2	f	0.51	0/1994	0.82	2/2718 (0.1%)
2	k	0.47	0/1994	0.77	1/2718 (0.0%)
3	C	0.63	2/2288 (0.1%)	0.91	3/3106 (0.1%)
3	H	0.58	0/2297	0.86	0/3118
3	M	0.68	6/2305 (0.3%)	0.90	2/3129 (0.1%)
3	R	0.62	0/2311	0.93	3/3137 (0.1%)
3	W	0.55	0/2305	0.85	0/3129
3	b	0.60	0/2305	0.84	0/3129
3	g	0.53	0/2288	0.81	0/3106
3	l	0.52	0/2272	0.81	0/3083
4	D	0.65	2/843 (0.2%)	0.77	0/1142
4	I	0.50	0/835	0.75	0/1131
4	N	0.50	0/843	0.81	0/1142
4	S	0.49	0/843	0.80	0/1142
4	X	0.44	0/843	0.74	0/1142
4	c	0.50	0/843	0.76	0/1142
4	h	0.43	0/835	0.77	0/1131
4	m	0.41	0/835	0.67	0/1131
5	E	0.70	0/61	1.18	0/80
5	J	0.70	0/61	1.10	0/80

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	O	0.68	0/61	0.87	0/80
5	T	0.84	0/61	0.98	0/80
5	Y	0.64	0/61	1.17	0/80
5	d	0.57	0/61	0.91	0/80
5	i	0.65	0/61	0.91	0/80
5	n	0.65	0/61	0.80	0/80
All	All	0.58	16/54557 (0.0%)	0.87	27/74075 (0.0%)

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	F	0	1
1	K	0	2
1	e	0	2
2	V	0	1
3	C	0	2
3	H	0	2
3	M	0	2
All	All	0	13

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	275	GLU	CG-CD	10.09	1.77	1.52
3	M	275	GLU	CD-OE1	8.22	1.41	1.25
4	D	98	ASP	CB-CG	7.53	1.70	1.52
3	M	276	LEU	C-O	6.93	1.37	1.23
1	Z	99	ASN	CB-CG	6.59	1.68	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	99	ASN	N-CA-CB	-13.39	91.51	111.19
3	C	108	ARG	CG-CD-NE	-11.50	86.70	112.00
1	Z	99	ASN	CA-C-N	-10.49	105.86	122.65
1	Z	99	ASN	C-N-CA	-10.49	105.86	122.65
1	Z	98	GLY	CA-C-N	-9.83	107.29	121.83

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
3	C	108	ARG	Sidechain
3	C	21	ARG	Sidechain
1	F	109	ARG	Sidechain
3	H	14	ARG	Sidechain

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	1593	0	1516	74	0
1	F	1591	0	1514	56	0
1	K	1597	0	1519	75	0
1	P	1587	0	1511	81	0
1	U	1587	0	1511	64	0
1	Z	1587	0	1511	75	1
1	e	1593	0	1516	60	0
1	j	1580	0	1503	62	1
2	B	1958	0	1896	55	0
2	G	1942	0	1883	62	0
2	L	1942	0	1883	75	0
2	Q	1942	0	1883	51	0
2	V	1942	0	1883	62	0
2	a	1942	0	1883	75	0
2	f	1942	0	1883	57	0
2	k	1942	0	1883	52	0
3	C	2228	0	2080	81	0
3	H	2237	0	2086	64	0
3	M	2245	0	2097	65	1
3	R	2251	0	2102	57	0
3	W	2245	0	2097	78	0
3	b	2245	0	2097	60	1
3	g	2228	0	2080	72	0
3	l	2214	0	2070	65	0
4	D	820	0	785	18	0
4	I	812	0	781	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	820	0	785	27	0
4	S	820	0	785	12	0
4	X	820	0	785	19	0
4	c	820	0	785	21	0
4	h	812	0	781	33	0
4	m	812	0	781	19	0
5	E	62	0	74	15	0
5	J	62	0	74	12	0
5	O	62	0	74	4	0
5	T	62	0	74	9	0
5	Y	62	0	74	10	0
5	d	62	0	74	13	0
5	i	62	0	74	7	0
5	n	62	0	74	4	0
6	C	1	0	0	0	0
All	All	53193	0	50747	1557	2

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 15.

The worst 5 of 1557 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:M:275:GLU:CD	3:M:275:GLU:CG	1.77	1.53
1:Z:99:ASN:ND2	2:a:100:HIS:CE1	1.92	1.35
1:P:34:PHE:O	1:P:94:LEU:HD12	1.37	1.25
1:Z:99:ASN:HD21	2:a:100:HIS:CE1	1.55	1.20
1:K:5:VAL:CG2	1:K:26:TYR:CB	2.33	1.06

All (2) 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:b:108:ARG:NH2	1:j:170:ASP:OD1[4_545]	1.40	0.80
3:M:108:ARG:NH2	1:Z:170:ASP:OD1[3_555]	2.18	0.02

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	200/206 (97%)	186 (93%)	14 (7%)	0	100	100
1	F	200/206 (97%)	195 (98%)	5 (2%)	0	100	100
1	K	201/206 (98%)	185 (92%)	16 (8%)	0	100	100
1	P	199/206 (97%)	187 (94%)	12 (6%)	0	100	100
1	U	199/206 (97%)	192 (96%)	7 (4%)	0	100	100
1	Z	199/206 (97%)	192 (96%)	7 (4%)	0	100	100
1	e	200/206 (97%)	192 (96%)	8 (4%)	0	100	100
1	j	198/206 (96%)	187 (94%)	11 (6%)	0	100	100
2	B	240/246 (98%)	230 (96%)	10 (4%)	0	100	100
2	G	238/246 (97%)	232 (98%)	6 (2%)	0	100	100
2	L	238/246 (97%)	233 (98%)	5 (2%)	0	100	100
2	Q	238/246 (97%)	230 (97%)	8 (3%)	0	100	100
2	V	238/246 (97%)	228 (96%)	10 (4%)	0	100	100
2	a	238/246 (97%)	232 (98%)	6 (2%)	0	100	100
2	f	238/246 (97%)	229 (96%)	9 (4%)	0	100	100
2	k	238/246 (97%)	227 (95%)	11 (5%)	0	100	100
3	C	272/279 (98%)	258 (95%)	14 (5%)	0	100	100
3	H	273/279 (98%)	262 (96%)	11 (4%)	0	100	100
3	M	274/279 (98%)	264 (96%)	10 (4%)	0	100	100
3	R	275/279 (99%)	262 (95%)	13 (5%)	0	100	100
3	W	274/279 (98%)	263 (96%)	11 (4%)	0	100	100
3	b	274/279 (98%)	262 (96%)	12 (4%)	0	100	100
3	g	272/279 (98%)	262 (96%)	10 (4%)	0	100	100
3	l	271/279 (97%)	259 (96%)	12 (4%)	0	100	100
4	D	96/100 (96%)	95 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	I	95/100 (95%)	94 (99%)	1 (1%)	0	100	100
4	N	96/100 (96%)	95 (99%)	1 (1%)	0	100	100
4	S	96/100 (96%)	95 (99%)	1 (1%)	0	100	100
4	X	96/100 (96%)	96 (100%)	0	0	100	100
4	c	96/100 (96%)	96 (100%)	0	0	100	100
4	h	95/100 (95%)	94 (99%)	1 (1%)	0	100	100
4	m	95/100 (95%)	93 (98%)	2 (2%)	0	100	100
5	E	8/10 (80%)	8 (100%)	0	0	100	100
5	J	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
5	O	8/10 (80%)	8 (100%)	0	0	100	100
5	T	8/10 (80%)	8 (100%)	0	0	100	100
5	Y	8/10 (80%)	8 (100%)	0	0	100	100
5	d	8/10 (80%)	8 (100%)	0	0	100	100
5	i	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
5	n	8/10 (80%)	8 (100%)	0	0	100	100
All	All	6516/6728 (97%)	6269 (96%)	247 (4%)	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	182/184 (99%)	181 (100%)	1 (0%)	81	80
1	F	181/184 (98%)	180 (99%)	1 (1%)	78	79
1	K	182/184 (99%)	179 (98%)	3 (2%)	55	70
1	P	181/184 (98%)	181 (100%)	0	100	100
1	U	181/184 (98%)	181 (100%)	0	100	100
1	Z	181/184 (98%)	180 (99%)	1 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	182/184 (99%)	179 (98%)	3 (2%)	55	70
1	j	180/184 (98%)	178 (99%)	2 (1%)	65	74
2	B	214/216 (99%)	214 (100%)	0	100	100
2	G	212/216 (98%)	211 (100%)	1 (0%)	81	80
2	L	212/216 (98%)	211 (100%)	1 (0%)	81	80
2	Q	212/216 (98%)	211 (100%)	1 (0%)	81	80
2	V	212/216 (98%)	212 (100%)	0	100	100
2	a	212/216 (98%)	212 (100%)	0	100	100
2	f	212/216 (98%)	212 (100%)	0	100	100
2	k	212/216 (98%)	212 (100%)	0	100	100
3	C	231/236 (98%)	230 (100%)	1 (0%)	84	81
3	H	232/236 (98%)	232 (100%)	0	100	100
3	M	233/236 (99%)	233 (100%)	0	100	100
3	R	234/236 (99%)	232 (99%)	2 (1%)	70	76
3	W	233/236 (99%)	233 (100%)	0	100	100
3	b	233/236 (99%)	233 (100%)	0	100	100
3	g	231/236 (98%)	231 (100%)	0	100	100
3	l	230/236 (98%)	230 (100%)	0	100	100
4	D	93/95 (98%)	93 (100%)	0	100	100
4	I	92/95 (97%)	92 (100%)	0	100	100
4	N	93/95 (98%)	93 (100%)	0	100	100
4	S	93/95 (98%)	93 (100%)	0	100	100
4	X	93/95 (98%)	93 (100%)	0	100	100
4	c	93/95 (98%)	93 (100%)	0	100	100
4	h	92/95 (97%)	92 (100%)	0	100	100
4	m	92/95 (97%)	92 (100%)	0	100	100
5	E	6/6 (100%)	6 (100%)	0	100	100
5	J	6/6 (100%)	6 (100%)	0	100	100
5	O	6/6 (100%)	6 (100%)	0	100	100
5	T	6/6 (100%)	6 (100%)	0	100	100
5	Y	6/6 (100%)	5 (83%)	1 (17%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	d	6/6 (100%)	6 (100%)	0	100	100
5	i	6/6 (100%)	6 (100%)	0	100	100
5	n	6/6 (100%)	6 (100%)	0	100	100
All	All	5794/5896 (98%)	5776 (100%)	18 (0%)	86	83

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	e	198	GLU
1	j	169	MET
1	j	94	LEU
2	Q	172	CYS
1	e	169	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
3	g	188	HIS
4	h	13	HIS
2	k	41	GLN
3	M	87	GLN
3	M	66	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	U	1
1	j	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	17:GLY	C	18:LEU	N	1.19
1	j	17:GLY	C	18:LEU	N	1.14

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	202/206 (98%)	-0.34	0 100 100	75, 107, 163, 181	0
1	F	202/206 (98%)	-0.26	2 (0%) 79 56	81, 106, 169, 182	0
1	K	203/206 (98%)	-0.17	4 (1%) 65 39	30, 107, 157, 194	0
1	P	201/206 (97%)	-0.27	0 100 100	79, 108, 183, 228	0
1	U	201/206 (97%)	-0.32	2 (0%) 79 56	74, 109, 197, 223	0
1	Z	201/206 (97%)	-0.23	1 (0%) 87 68	86, 114, 182, 213	0
1	e	202/206 (98%)	-0.24	1 (0%) 87 68	84, 114, 178, 208	0
1	j	200/206 (97%)	-0.28	0 100 100	68, 112, 198, 238	0
2	B	242/246 (98%)	-0.38	1 (0%) 88 72	61, 116, 164, 184	0
2	G	240/246 (97%)	-0.38	1 (0%) 88 72	81, 120, 163, 185	0
2	L	240/246 (97%)	-0.42	0 100 100	79, 115, 151, 174	0
2	Q	240/246 (97%)	-0.32	1 (0%) 88 72	82, 129, 164, 184	0
2	V	240/246 (97%)	-0.31	0 100 100	84, 138, 166, 174	0
2	a	240/246 (97%)	-0.33	0 100 100	85, 136, 177, 211	0
2	f	240/246 (97%)	-0.32	1 (0%) 88 72	83, 128, 171, 193	0
2	k	240/246 (97%)	-0.35	0 100 100	87, 135, 176, 198	0
3	C	274/279 (98%)	-0.35	0 100 100	30, 113, 189, 205	0
3	H	275/279 (98%)	-0.51	0 100 100	74, 104, 174, 206	0
3	M	276/279 (98%)	-0.44	0 100 100	55, 113, 155, 180	0
3	R	277/279 (99%)	-0.40	0 100 100	77, 105, 148, 179	0
3	W	276/279 (98%)	-0.46	0 100 100	78, 108, 160, 176	0
3	b	276/279 (98%)	-0.45	0 100 100	80, 104, 142, 183	0
3	g	274/279 (98%)	-0.42	0 100 100	85, 118, 209, 227	0
3	l	273/279 (97%)	-0.32	1 (0%) 88 72	92, 128, 230, 253	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
4	D	98/100 (98%)	-0.51	0	100	100	76, 140, 165, 170	0
4	I	97/100 (97%)	-0.49	0	100	100	91, 115, 138, 179	0
4	N	98/100 (98%)	-0.41	0	100	100	95, 131, 161, 169	0
4	S	98/100 (98%)	-0.43	0	100	100	92, 125, 158, 166	0
4	X	98/100 (98%)	-0.52	0	100	100	99, 129, 152, 157	0
4	c	98/100 (98%)	-0.60	0	100	100	86, 112, 143, 157	0
4	h	97/100 (97%)	-0.44	0	100	100	104, 148, 170, 183	0
4	m	97/100 (97%)	-0.44	0	100	100	117, 159, 184, 193	0
5	E	10/10 (100%)	-0.28	0	100	100	95, 98, 109, 113	0
5	J	10/10 (100%)	-0.27	0	100	100	85, 92, 98, 103	0
5	O	10/10 (100%)	-0.08	0	100	100	96, 100, 104, 114	0
5	T	10/10 (100%)	-0.34	0	100	100	88, 90, 96, 103	0
5	Y	10/10 (100%)	-0.14	0	100	100	84, 96, 105, 108	0
5	d	10/10 (100%)	-0.22	0	100	100	89, 96, 102, 103	0
5	i	10/10 (100%)	0.00	0	100	100	97, 101, 109, 113	0
5	n	10/10 (100%)	0.01	0	100	100	102, 109, 117, 119	0
All	All	6596/6728 (98%)	-0.37	15 (0%)	91	82	30, 118, 177, 253	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	193	ASN	4.2
1	K	3	ASP	4.1
2	B	76	ASP	3.4
2	G	76	ASP	3.0
1	F	23	ASN	2.9

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.