



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:02 AM UTC

PDB ID : 8T7R / pdb_00008t7r
Title : Crystal structure of human leukocyte antigen A*0101 in complex with the Fab of alloreactive antibody E07
Authors : Green, T.J.; Killian Jr, J.T.; Qiu, S.; Macon, K.J.; Yang, G.; King, R.G.; Lund, F.E.
Deposited on : 2023-06-21
Resolution : 3.84 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

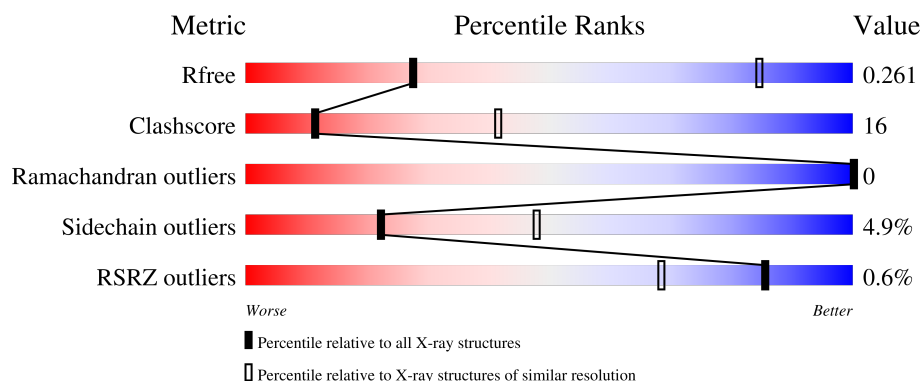
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 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	1169 (4.00-3.68)
Clashscore	190562	1211 (4.00-3.68)
Ramachandran outliers	187476	1156 (4.00-3.68)
Sidechain outliers	187428	1149 (4.00-3.68)
RSRZ outliers	180081	1168 (4.00-3.68)

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	214	
1	E	214	
1	I	214	
1	M	214	
1	Q	214	

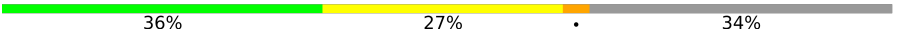
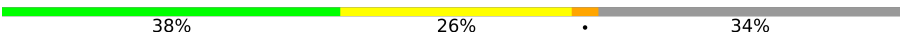
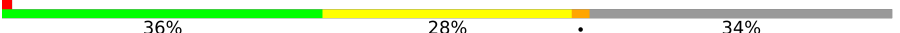
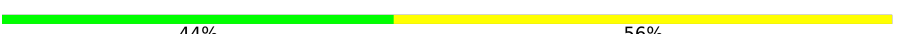
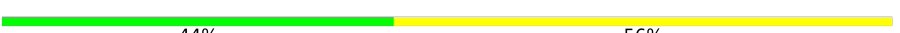
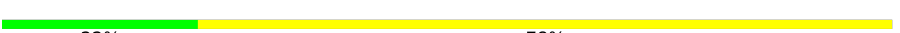
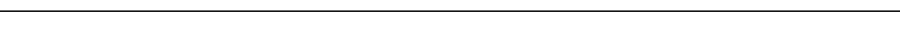
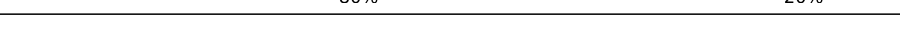
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Mol	Chain	Length	Quality of chain
1	U	214	
1	Y	214	
1	c	214	
1	g	214	
1	k	214	
1	o	214	
1	s	214	
2	B	240	
2	F	240	
2	J	240	
2	N	240	
2	R	240	
2	V	240	
2	Z	240	
2	d	240	
2	h	240	
2	l	240	
2	p	240	
2	t	240	
3	C	274	
3	G	274	
3	K	274	
3	O	274	
3	S	274	
3	W	274	

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Mol	Chain	Length	Quality of chain
3	a	274	
3	e	274	
3	i	274	
4	0	9	
4	1	9	
4	2	9	
4	3	9	
4	4	9	
4	5	9	
4	6	9	
4	7	9	
4	8	9	
5	D	99	
5	H	99	
5	L	99	
5	P	99	
5	T	99	
5	X	99	
5	b	99	
5	f	99	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 63611 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 Light chain from antibody JTK191b E07.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1535	957	266	308	4			
1	E	205	Total	C	N	O	S	0	0	0
			1535	957	266	308	4			
1	I	205	Total	C	N	O	S	0	0	0
			1535	957	266	308	4			
1	M	205	Total	C	N	O	S	0	0	0
			1535	957	266	308	4			
1	Q	205	Total	C	N	O	S	0	0	0
			1535	957	266	308	4			
1	U	205	Total	C	N	O	S	0	0	0
			1535	957	266	308	4			
1	Y	205	Total	C	N	O	S	0	0	0
			1535	957	266	308	4			
1	c	205	Total	C	N	O	S	0	0	0
			1535	957	266	308	4			
1	g	205	Total	C	N	O	S	0	0	0
			1535	957	266	308	4			
1	k	205	Total	C	N	O	S	0	0	0
			1535	957	266	308	4			
1	o	203	Total	C	N	O	S	0	0	0
			1517	946	263	304	4			
1	s	205	Total	C	N	O	S	0	0	0
			1535	957	266	308	4			

- Molecule 2 is a protein called Fab heavy chain from antibody JTK191b E07.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	0	0	0
			1680	1065	289	320	6			
2	F	221	Total	C	N	O	S	0	0	0
			1680	1065	289	320	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	220	Total	C	N	O	S	0	0	0
			1671	1059	287	319	6			
2	N	220	Total	C	N	O	S	0	0	0
			1671	1059	287	319	6			
2	R	221	Total	C	N	O	S	0	0	0
			1675	1061	288	320	6			
2	V	220	Total	C	N	O	S	0	0	0
			1671	1059	287	319	6			
2	Z	220	Total	C	N	O	S	0	0	0
			1676	1063	288	319	6			
2	d	220	Total	C	N	O	S	0	0	0
			1675	1062	288	319	6			
2	h	223	Total	C	N	O	S	0	0	0
			1690	1070	291	323	6			
2	l	219	Total	C	N	O	S	0	0	0
			1662	1054	285	317	6			
2	p	218	Total	C	N	O	S	0	0	0
			1656	1051	284	315	6			
2	t	221	Total	C	N	O	S	0	0	0
			1675	1061	288	320	6			

- Molecule 3 is a protein called MHC class I antigen (Fragment).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	274	Total	C	N	O	S	0	0	0
			2227	1383	408	426	10			
3	G	274	Total	C	N	O	S	0	0	0
			2227	1383	408	426	10			
3	K	274	Total	C	N	O	S	0	0	0
			2227	1383	408	426	10			
3	O	274	Total	C	N	O	S	0	0	0
			2227	1383	408	426	10			
3	S	274	Total	C	N	O	S	0	0	0
			2227	1383	408	426	10			
3	W	274	Total	C	N	O	S	0	0	0
			2227	1383	408	426	10			
3	a	182	Total	C	N	O	S	0	0	0
			1483	915	276	285	7			
3	e	182	Total	C	N	O	S	0	0	0
			1483	915	276	285	7			
3	i	182	Total	C	N	O	S	0	0	0
			1483	915	276	285	7			

- Molecule 4 is a protein called peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	0	9	Total	C	N	O	0	0	0
			76	49	11	16			
4	1	9	Total	C	N	O	0	0	0
			76	49	11	16			
4	2	9	Total	C	N	O	0	0	0
			76	49	11	16			
4	3	9	Total	C	N	O	0	0	0
			76	49	11	16			
4	4	9	Total	C	N	O	0	0	0
			76	49	11	16			
4	5	9	Total	C	N	O	0	0	0
			76	49	11	16			
4	6	9	Total	C	N	O	0	0	0
			76	49	11	16			
4	7	9	Total	C	N	O	0	0	0
			76	49	11	16			
4	8	9	Total	C	N	O	0	0	0
			76	49	11	16			

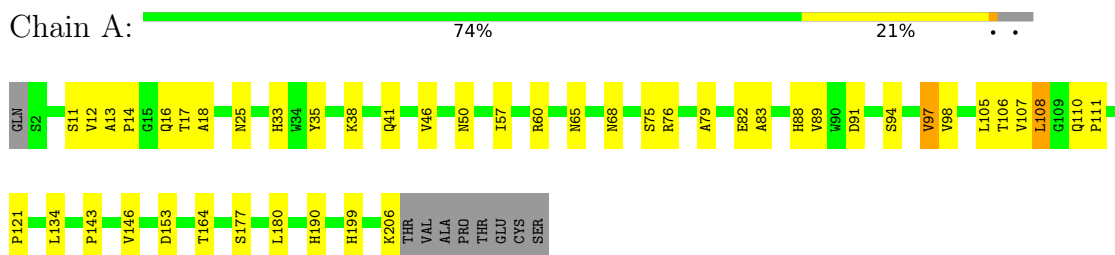
- Molecule 5 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
5	H	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
5	L	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
5	P	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
5	T	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
5	X	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
5	b	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
5	f	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

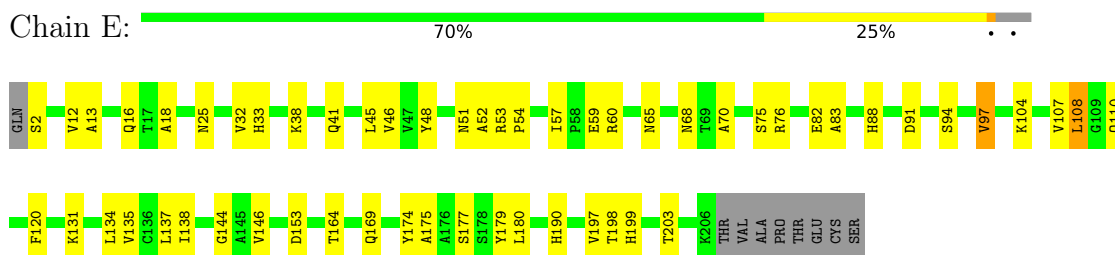
3 Residue-property plots

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.

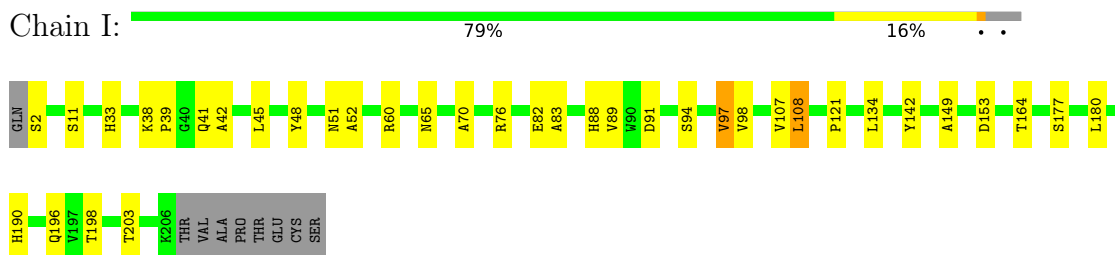
- Molecule 1: Light chain from antibody JTK191b E07



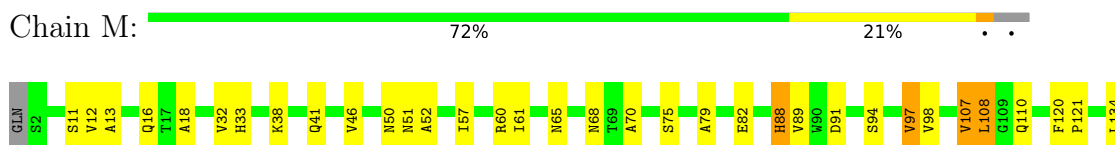
- Molecule 1: Light chain from antibody JTK191b E07



- Molecule 1: Light chain from antibody JTK191b E07



- Molecule 1: Light chain from antibody JTK191b E07





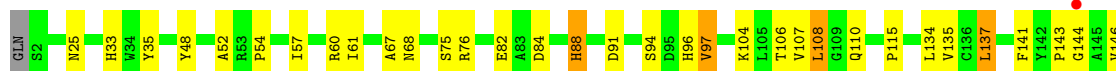
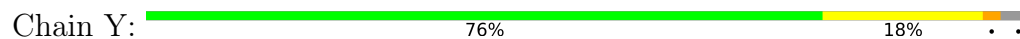
- Molecule 1: Light chain from antibody JTK191b E07



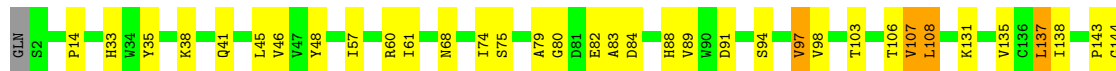
- Molecule 1: Light chain from antibody JTK191b E07



- Molecule 1: Light chain from antibody JTK191b E07

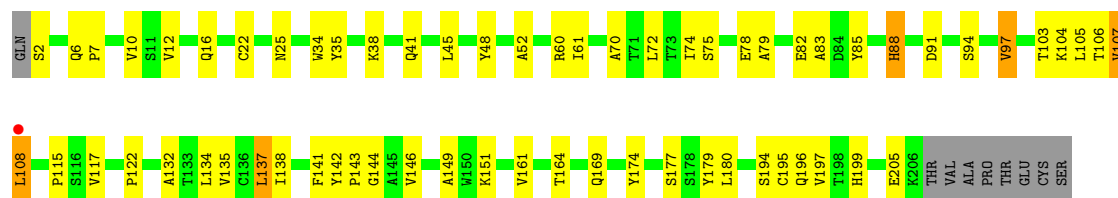


- Molecule 1: Light chain from antibody JTK191b E07



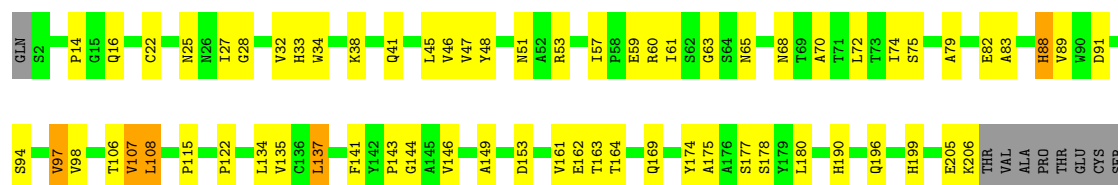
- Molecule 1: Light chain from antibody JTK191b E07





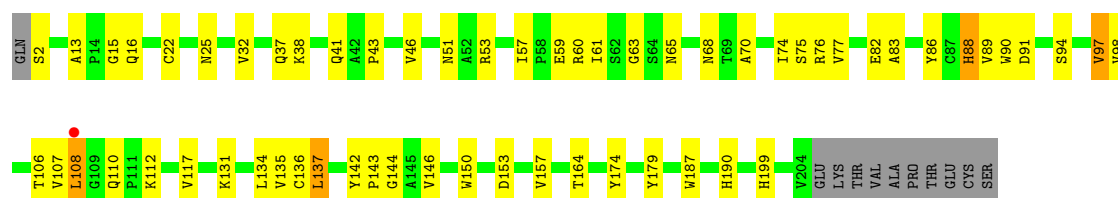
• Molecule 1: Light chain from antibody JTK191b E07

Chain k: 65% 29% 6%



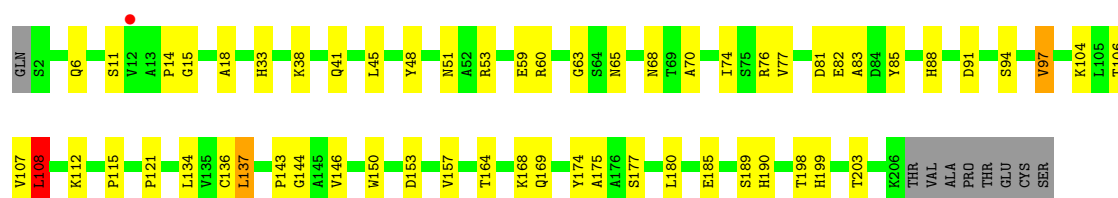
• Molecule 1: Light chain from antibody JTK191b E07

Chain o: 67% 26% 7%



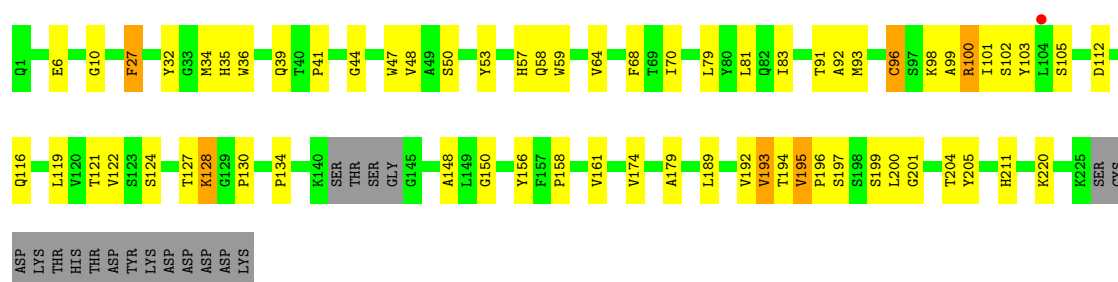
• Molecule 1: Light chain from antibody JTK191b E07

Chain s: 69% 26% 5%



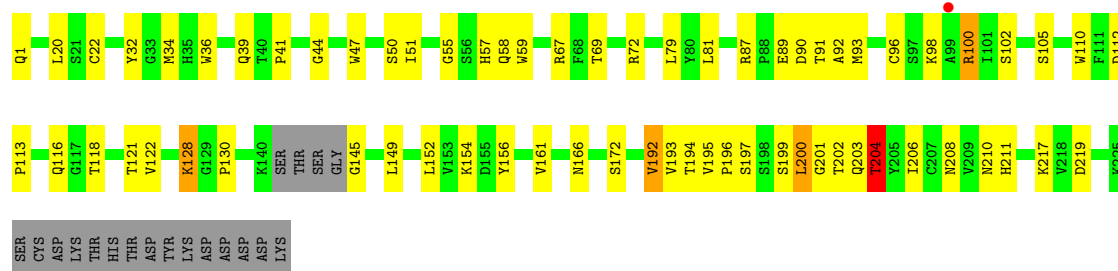
• Molecule 2: Fab heavy chain from antibody JTK191b E07

Chain B: 65% 25% 10%



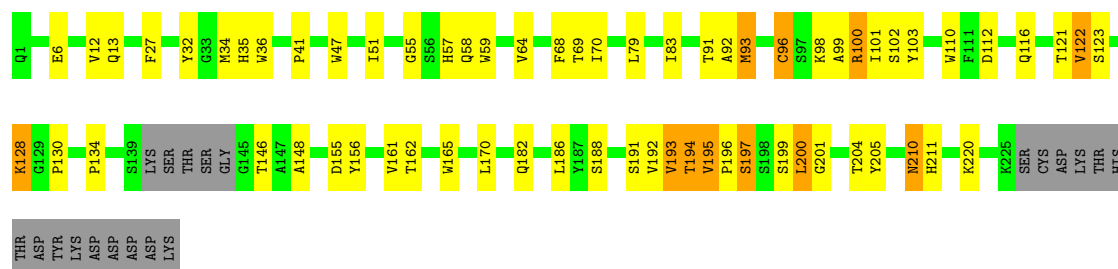
- Molecule 2: Fab heavy chain from antibody JTK191b E07

Chain F:  64% 26% 8%



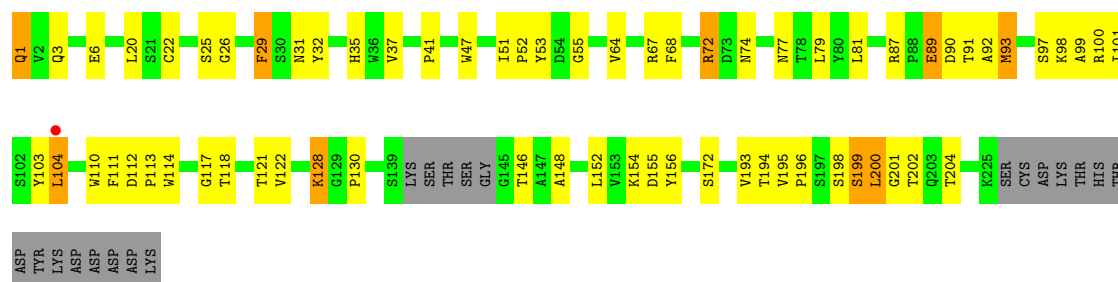
- Molecule 2: Fab heavy chain from antibody JTK191b E07

Chain J:  64% 23% 5% 8%



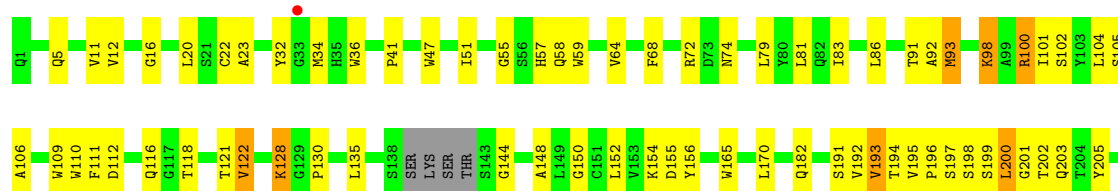
- Molecule 2: Fab heavy chain from antibody JTK191b E07

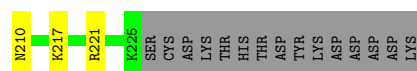
Chain N:  64% 24% 8%



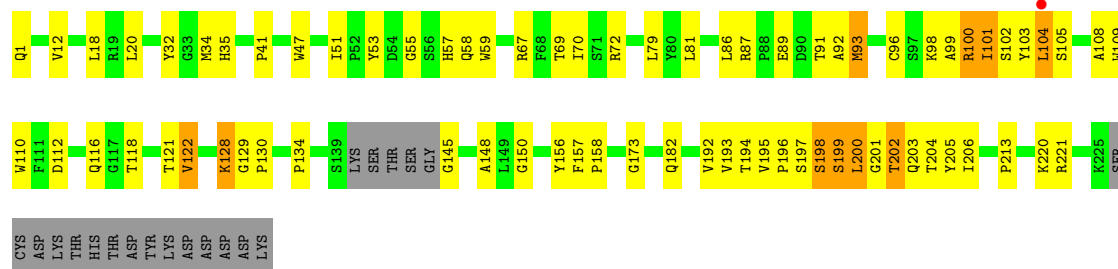
- Molecule 2: Fab heavy chain from antibody JTK191b E07

Chain R:  62% 28% 8%

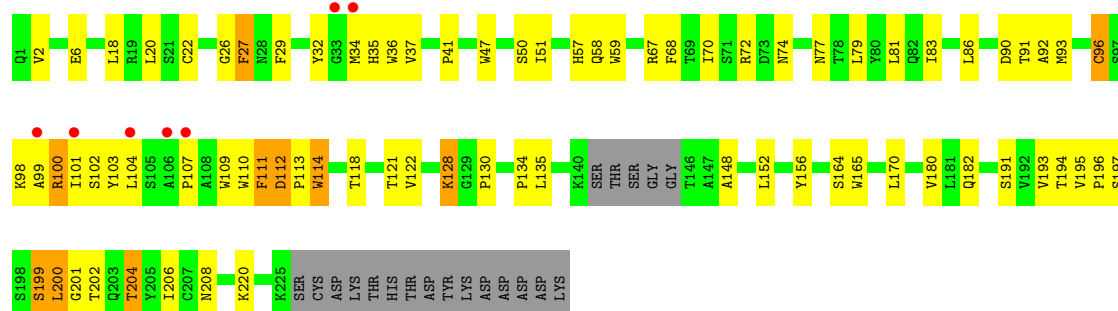




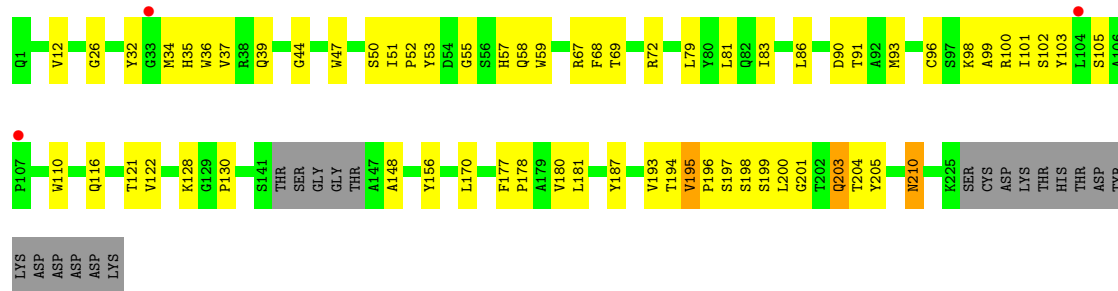
- Molecule 2: Fab heavy chain from antibody JTK191b E07



- Molecule 2: Fab heavy chain from antibody JTK191b E07

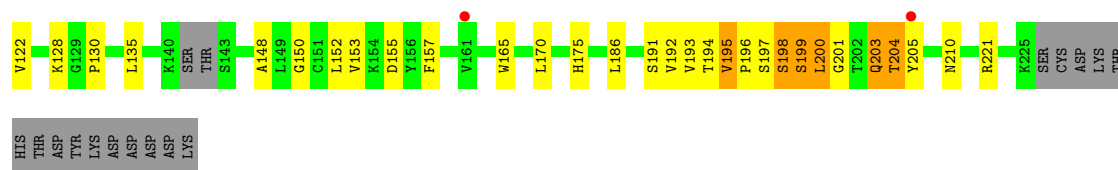


- Molecule 2: Fab heavy chain from antibody JTK191b E07

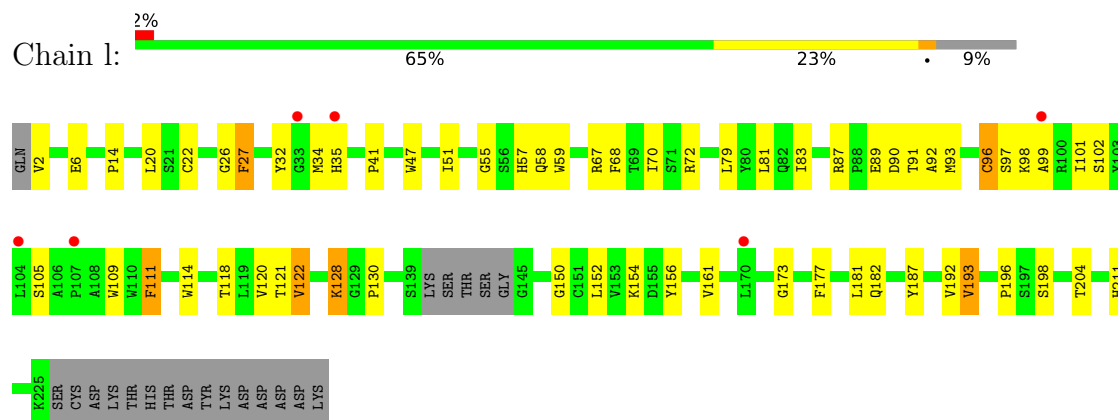


- Molecule 2: Fab heavy chain from antibody JTK191b E07

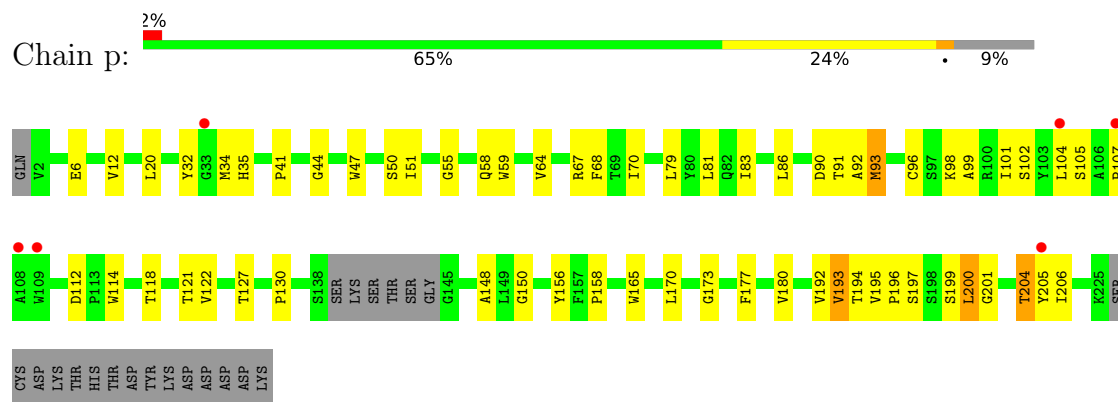




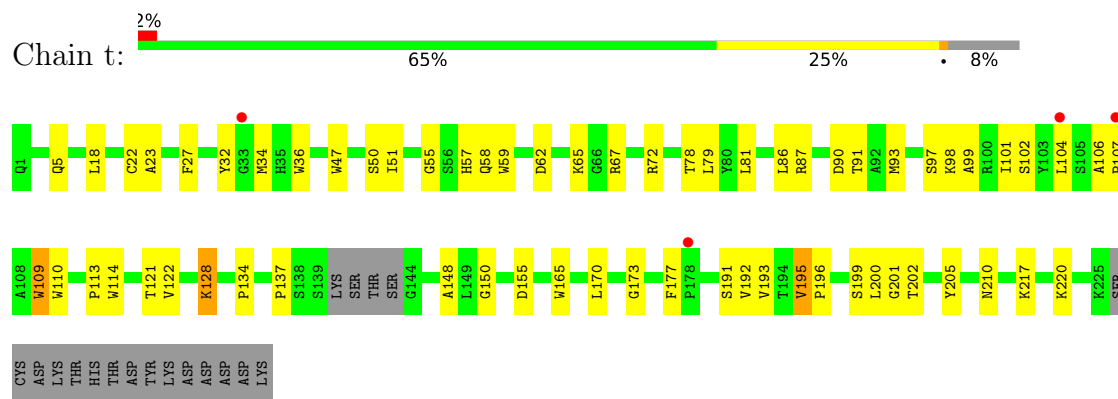
- Molecule 2: Fab heavy chain from antibody JTK191b E07



- Molecule 2: Fab heavy chain from antibody JTK191b E07

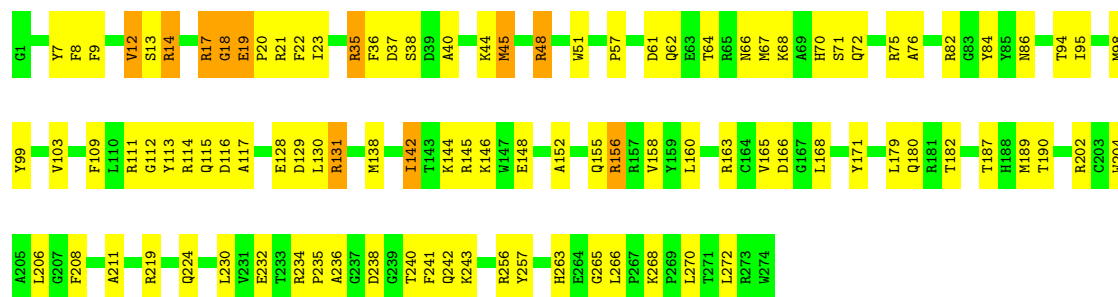


- Molecule 2: Fab heavy chain from antibody JTK191b E07



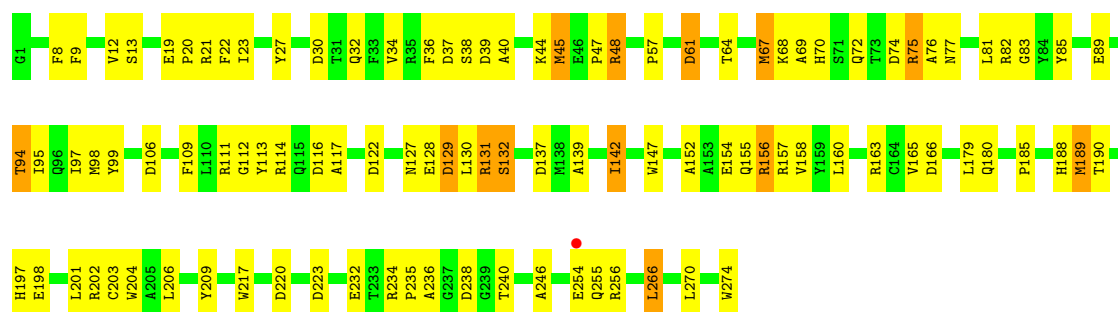
- Molecule 3: MHC class I antigen (Fragment)





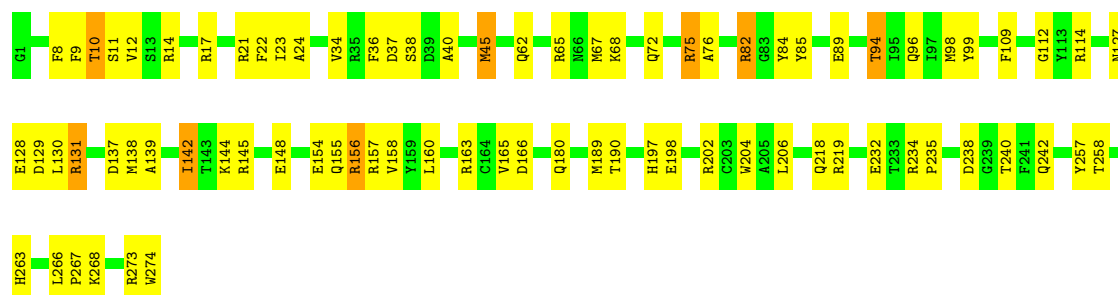
• Molecule 3: MHC class I antigen (Fragment)

Chain G: 62% 33% 5%



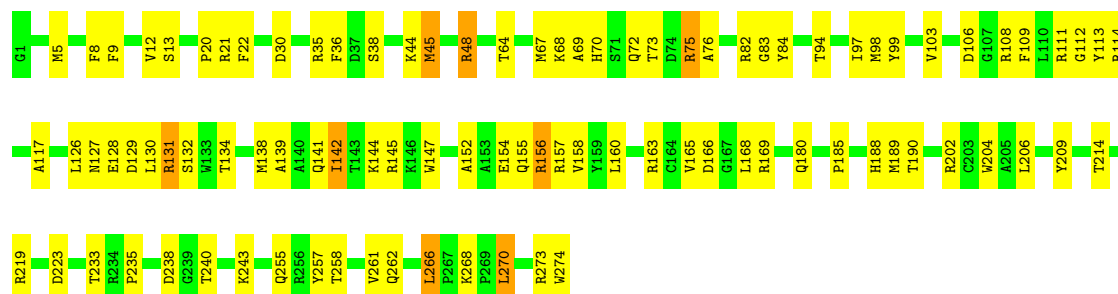
• Molecule 3: MHC class I antigen (Fragment)

Chain K: 71% 26% 3%

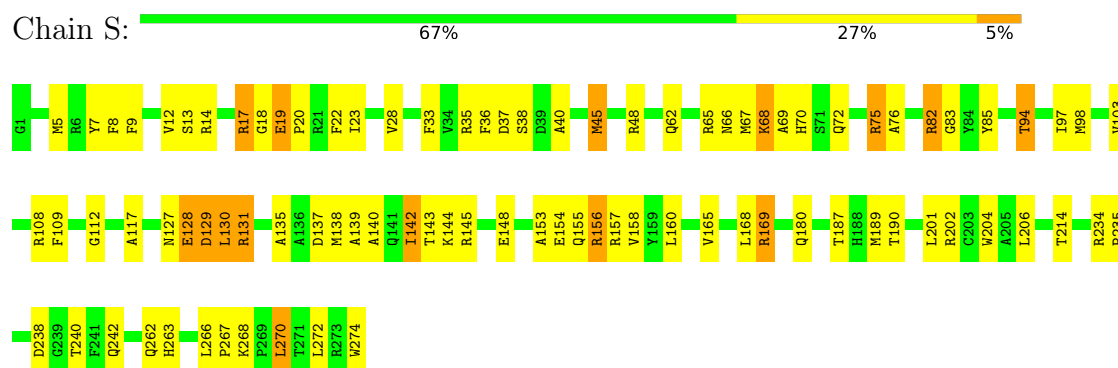


• Molecule 3: MHC class I antigen (Fragment)

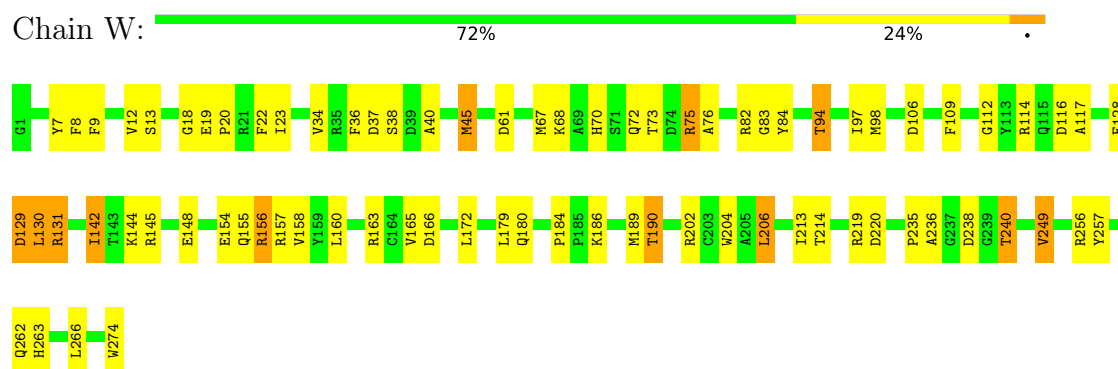
Chain O: 66% 31% 3%



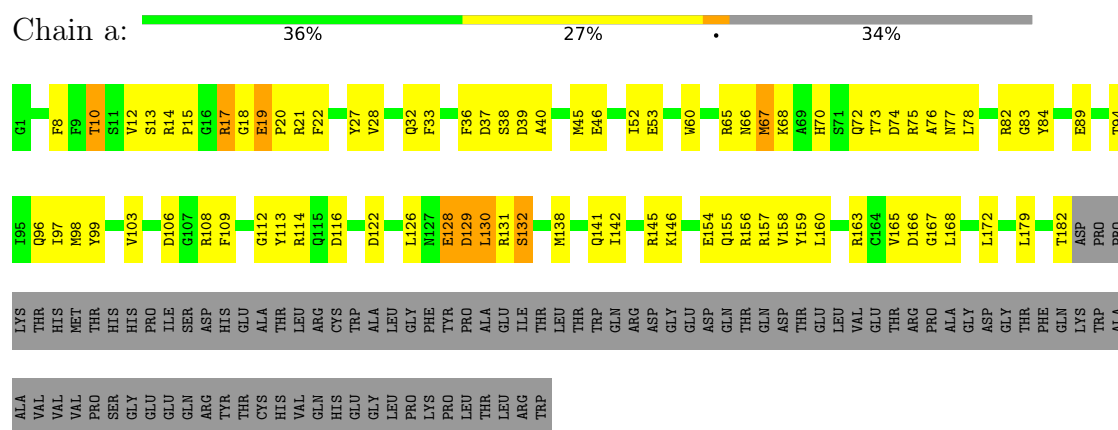
- Molecule 3: MHC class I antigen (Fragment)



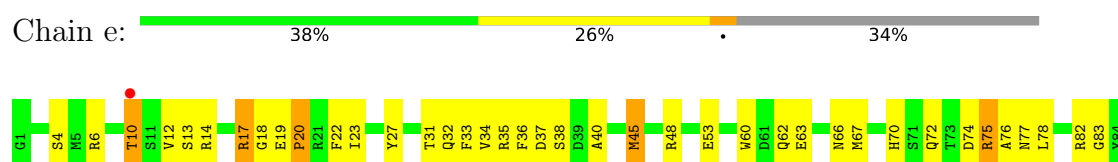
- Molecule 3: MHC class I antigen (Fragment)

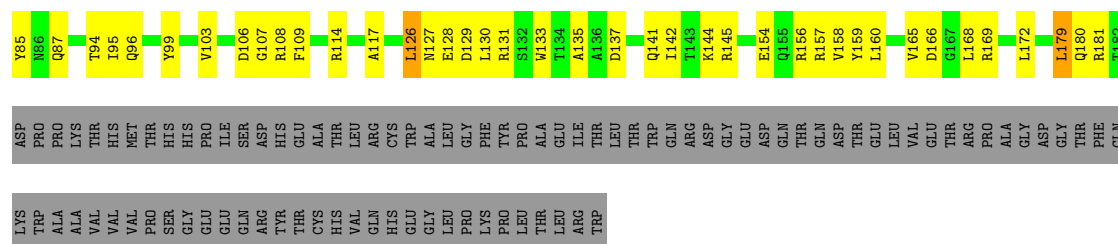


- Molecule 3: MHC class I antigen (Fragment)

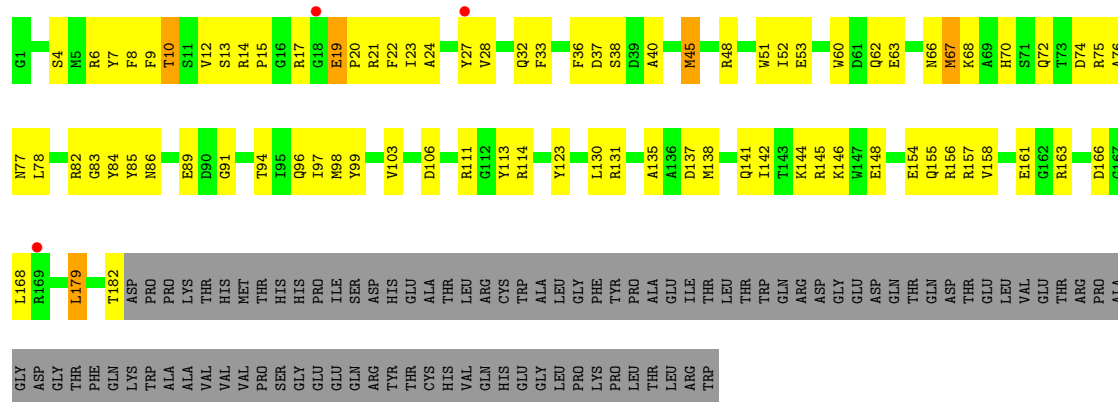


- Molecule 3: MHC class I antigen (Fragment)





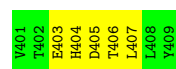
• Molecule 3: MHC class I antigen (Fragment)



• Molecule 4: peptide



• Molecule 4: peptide



• Molecule 4: peptide



• Molecule 4: peptide





- Molecule 4: peptide



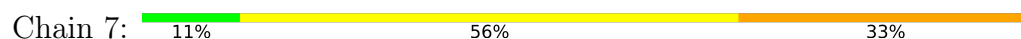
- Molecule 4: peptide



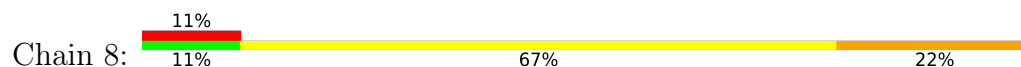
- Molecule 4: peptide



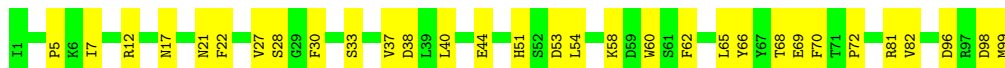
- Molecule 4: peptide



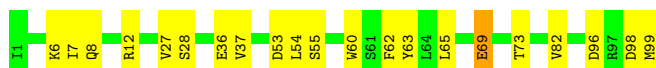
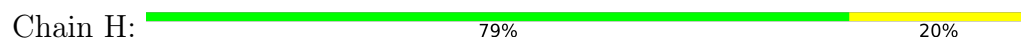
- Molecule 4: peptide



- Molecule 5: Beta-2-microglobulin



- Molecule 5: Beta-2-microglobulin



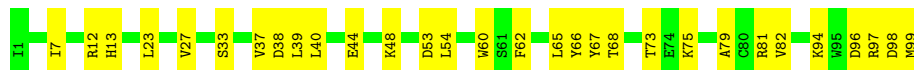
- Molecule 5: Beta-2-microglobulin

Chain L:  80% 20%



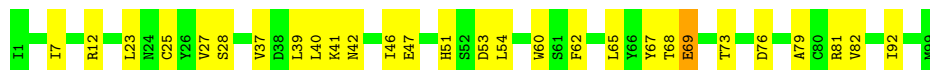
- Molecule 5: Beta-2-microglobulin

Chain P:  70% 30%



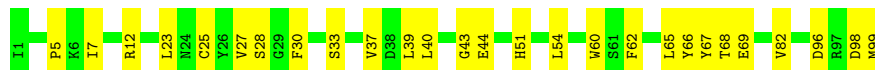
- Molecule 5: Beta-2-microglobulin

Chain T:  72% 27%



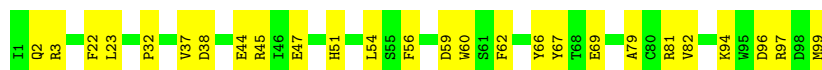
- Molecule 5: Beta-2-microglobulin

Chain X:  73% 27%



- Molecule 5: Beta-2-microglobulin

Chain b:  74% 26%



- Molecule 5: Beta-2-microglobulin

Chain f:  72% 28%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	357.08Å 259.58Å 255.36Å 90.00° 133.13° 90.00°	Depositor
Resolution (Å)	30.13 – 3.84 30.13 – 3.84	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.13-3.84) 90.6 (30.13-3.84)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.86Å)	Xtriage
Refinement program	PHENIX v1.20.1_4487	Depositor
R, R_{free}	0.216 , 0.263 0.217 , 0.261	Depositor DCC
R_{free} test set	2018 reflections (1.31%)	wwPDB-VP
Wilson B-factor (Å ²)	95.5	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 83.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.016 for h+2*k,-h-l 0.018 for k+l,h+l,-l 0.017 for -k+l,-h-l,-l 0.020 for -h+k-l,-l,-k 0.017 for -h-k-l,l,k 0.077 for h-k+l,l,-h-l 0.054 for -k-l,-h-l,k 0.045 for h+k+l,-l,-h-l 0.068 for k-l,h+l,-k 0.023 for h,-k,-h-l 0.044 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	63611	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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	0.19	0/1574	0.40	0/2152
1	E	0.19	0/1574	0.41	0/2152
1	I	0.21	0/1574	0.41	0/2152
1	M	0.21	0/1574	0.44	0/2152
1	Q	0.21	0/1574	0.41	0/2152
1	U	0.21	0/1574	0.43	0/2152
1	Y	0.17	0/1574	0.41	1/2152 (0.0%)
1	c	0.17	0/1574	0.38	0/2152
1	g	0.18	0/1574	0.44	1/2152 (0.0%)
1	k	0.16	0/1574	0.38	0/2152
1	o	0.17	0/1556	0.42	1/2129 (0.0%)
1	s	0.16	0/1574	0.41	1/2152 (0.0%)
2	B	0.23	0/1728	0.47	0/2357
2	F	0.26	0/1728	0.53	1/2357 (0.0%)
2	J	0.28	0/1719	0.48	0/2346
2	N	0.37	0/1719	0.60	1/2346 (0.0%)
2	R	0.26	0/1723	0.52	0/2351
2	V	0.25	0/1719	0.54	1/2346 (0.0%)
2	Z	0.25	0/1724	0.49	0/2352
2	d	0.21	0/1723	0.47	0/2350
2	h	0.21	0/1738	0.54	2/2370 (0.1%)
2	l	0.17	0/1710	0.38	0/2334
2	p	0.17	0/1704	0.42	0/2326
2	t	0.21	0/1723	0.48	1/2351 (0.0%)
3	C	0.25	0/2287	0.48	1/3101 (0.0%)
3	G	0.26	0/2287	0.45	0/3101
3	K	0.26	0/2287	0.48	0/3101
3	O	0.27	0/2287	0.47	0/3101
3	S	0.25	0/2287	0.47	1/3101 (0.0%)
3	W	0.27	0/2287	0.48	0/3101
3	a	0.27	0/1517	0.51	1/2045 (0.0%)
3	e	0.27	1/1517 (0.1%)	0.53	0/2045
3	i	0.20	0/1517	0.45	0/2045
4	0	0.28	0/77	0.66	0/105

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	1	0.31	0/77	0.65	0/105
4	2	0.30	0/77	0.63	0/105
4	3	0.27	0/77	0.60	0/105
4	4	0.41	0/77	0.69	0/105
4	5	0.30	0/77	0.62	0/105
4	6	0.23	0/77	0.37	0/105
4	7	0.22	0/77	0.36	0/105
4	8	0.28	0/77	0.43	0/105
5	D	0.20	0/852	0.40	0/1152
5	H	0.21	0/852	0.41	0/1152
5	L	0.20	0/852	0.39	0/1152
5	P	0.21	0/852	0.42	0/1152
5	T	0.21	0/852	0.43	0/1152
5	X	0.20	0/852	0.43	0/1152
5	b	0.18	0/852	0.42	0/1152
5	f	0.17	0/852	0.42	0/1152
All	All	0.23	1/65310 (0.0%)	0.46	13/88889 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	e	20	PRO	N-CD	5.06	1.54	1.47

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	202	THR	N-CA-C	8.36	120.39	111.28
3	C	18	GLY	N-CA-C	8.06	122.24	112.49
1	g	108	LEU	N-CA-C	7.94	121.79	109.96
1	o	108	LEU	N-CA-C	7.43	121.03	109.96
1	s	108	LEU	N-CA-C	7.27	120.28	109.59

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	1535	0	1482	40	0
1	E	1535	0	1482	39	0
1	I	1535	0	1482	27	0
1	M	1535	0	1482	34	0
1	Q	1535	0	1482	35	0
1	U	1535	0	1482	36	0
1	Y	1535	0	1482	45	0
1	c	1535	0	1482	39	0
1	g	1535	0	1482	52	0
1	k	1535	0	1482	43	0
1	o	1517	0	1463	62	0
1	s	1535	0	1482	49	0
2	B	1680	0	1632	49	0
2	F	1680	0	1632	60	0
2	J	1671	0	1619	59	0
2	N	1671	0	1619	64	0
2	R	1675	0	1622	68	0
2	V	1671	0	1619	74	0
2	Z	1676	0	1629	99	0
2	d	1675	0	1627	50	0
2	h	1690	0	1640	47	0
2	l	1662	0	1608	47	0
2	p	1656	0	1603	42	0
2	t	1675	0	1622	62	0
3	C	2227	0	2086	122	0
3	G	2227	0	2086	100	0
3	K	2227	0	2086	72	0
3	O	2227	0	2086	101	0
3	S	2227	0	2086	93	0
3	W	2227	0	2086	83	0
3	a	1483	0	1392	115	0
3	e	1483	0	1392	82	0
3	i	1483	0	1392	105	0
4	0	76	0	70	8	0
4	1	76	0	70	3	0
4	2	76	0	70	3	0
4	3	76	0	70	7	0
4	4	76	0	70	12	0
4	5	76	0	70	6	0
4	6	76	0	70	9	0
4	7	76	0	70	7	0
4	8	76	0	70	20	0
5	D	829	0	794	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	829	0	794	18	0
5	L	829	0	794	16	0
5	P	829	0	794	24	0
5	T	829	0	794	21	0
5	X	829	0	794	17	0
5	b	829	0	794	17	0
5	f	829	0	794	20	0
All	All	63611	0	60911	2005	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 16.

The worst 5 of 2005 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:101:ILE:CD1	3:a:158:VAL:HG23	1.57	1.33
3:O:129:ASP:HB3	3:O:131:ARG:CG	1.60	1.31
2:J:195:VAL:HG22	2:J:196:PRO:CD	1.64	1.27
3:O:129:ASP:CB	3:O:131:ARG:HG2	1.67	1.23
3:C:9:PHE:CG	3:C:70:HIS:HE1	1.56	1.22

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	203/214 (95%)	188 (93%)	15 (7%)	0	100	100
1	E	203/214 (95%)	187 (92%)	16 (8%)	0	100	100
1	I	203/214 (95%)	189 (93%)	14 (7%)	0	100	100
1	M	203/214 (95%)	188 (93%)	15 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	203/214 (95%)	190 (94%)	13 (6%)	0	100	100
1	U	203/214 (95%)	189 (93%)	14 (7%)	0	100	100
1	Y	203/214 (95%)	187 (92%)	16 (8%)	0	100	100
1	c	203/214 (95%)	188 (93%)	15 (7%)	0	100	100
1	g	203/214 (95%)	188 (93%)	15 (7%)	0	100	100
1	k	203/214 (95%)	187 (92%)	16 (8%)	0	100	100
1	o	201/214 (94%)	187 (93%)	14 (7%)	0	100	100
1	s	203/214 (95%)	186 (92%)	17 (8%)	0	100	100
2	B	217/240 (90%)	207 (95%)	10 (5%)	0	100	100
2	F	217/240 (90%)	205 (94%)	12 (6%)	0	100	100
2	J	216/240 (90%)	204 (94%)	12 (6%)	0	100	100
2	N	216/240 (90%)	207 (96%)	9 (4%)	0	100	100
2	R	217/240 (90%)	208 (96%)	9 (4%)	0	100	100
2	V	216/240 (90%)	206 (95%)	10 (5%)	0	100	100
2	Z	216/240 (90%)	206 (95%)	10 (5%)	0	100	100
2	d	216/240 (90%)	206 (95%)	10 (5%)	0	100	100
2	h	219/240 (91%)	209 (95%)	10 (5%)	0	100	100
2	l	215/240 (90%)	205 (95%)	10 (5%)	0	100	100
2	p	214/240 (89%)	205 (96%)	9 (4%)	0	100	100
2	t	217/240 (90%)	205 (94%)	12 (6%)	0	100	100
3	C	272/274 (99%)	256 (94%)	16 (6%)	0	100	100
3	G	272/274 (99%)	258 (95%)	14 (5%)	0	100	100
3	K	272/274 (99%)	257 (94%)	15 (6%)	0	100	100
3	O	272/274 (99%)	259 (95%)	13 (5%)	0	100	100
3	S	272/274 (99%)	258 (95%)	14 (5%)	0	100	100
3	W	272/274 (99%)	259 (95%)	13 (5%)	0	100	100
3	a	180/274 (66%)	170 (94%)	10 (6%)	0	100	100
3	e	180/274 (66%)	171 (95%)	9 (5%)	0	100	100
3	i	180/274 (66%)	167 (93%)	13 (7%)	0	100	100
4	0	7/9 (78%)	7 (100%)	0	0	100	100
4	1	7/9 (78%)	7 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	2	7/9 (78%)	7 (100%)	0	0	100	100
4	3	7/9 (78%)	7 (100%)	0	0	100	100
4	4	7/9 (78%)	7 (100%)	0	0	100	100
4	5	7/9 (78%)	7 (100%)	0	0	100	100
4	6	7/9 (78%)	7 (100%)	0	0	100	100
4	7	7/9 (78%)	7 (100%)	0	0	100	100
4	8	7/9 (78%)	7 (100%)	0	0	100	100
5	D	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
5	H	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
5	L	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
5	P	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
5	T	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
5	X	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
5	b	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
5	f	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
All	All	8041/8787 (92%)	7579 (94%)	462 (6%)	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	172/180 (96%)	170 (99%)	2 (1%)	63	72
1	E	172/180 (96%)	168 (98%)	4 (2%)	44	63
1	I	172/180 (96%)	169 (98%)	3 (2%)	53	68
1	M	172/180 (96%)	167 (97%)	5 (3%)	37	58
1	Q	172/180 (96%)	168 (98%)	4 (2%)	44	63
1	U	172/180 (96%)	168 (98%)	4 (2%)	44	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	172/180 (96%)	169 (98%)	3 (2%)	53	68
1	c	172/180 (96%)	168 (98%)	4 (2%)	44	63
1	g	172/180 (96%)	167 (97%)	5 (3%)	37	58
1	k	172/180 (96%)	166 (96%)	6 (4%)	32	55
1	o	170/180 (94%)	167 (98%)	3 (2%)	51	67
1	s	172/180 (96%)	168 (98%)	4 (2%)	44	63
2	B	187/205 (91%)	174 (93%)	13 (7%)	14	40
2	F	187/205 (91%)	172 (92%)	15 (8%)	11	36
2	J	186/205 (91%)	170 (91%)	16 (9%)	10	33
2	N	186/205 (91%)	172 (92%)	14 (8%)	12	38
2	R	186/205 (91%)	177 (95%)	9 (5%)	23	48
2	V	186/205 (91%)	173 (93%)	13 (7%)	14	40
2	Z	187/205 (91%)	174 (93%)	13 (7%)	14	40
2	d	187/205 (91%)	176 (94%)	11 (6%)	18	44
2	h	188/205 (92%)	175 (93%)	13 (7%)	14	41
2	l	185/205 (90%)	177 (96%)	8 (4%)	26	50
2	p	184/205 (90%)	175 (95%)	9 (5%)	22	48
2	t	186/205 (91%)	180 (97%)	6 (3%)	34	56
3	C	231/231 (100%)	216 (94%)	15 (6%)	15	42
3	G	231/231 (100%)	212 (92%)	19 (8%)	10	35
3	K	231/231 (100%)	220 (95%)	11 (5%)	23	48
3	O	231/231 (100%)	218 (94%)	13 (6%)	19	45
3	S	231/231 (100%)	213 (92%)	18 (8%)	11	37
3	W	231/231 (100%)	217 (94%)	14 (6%)	17	43
3	a	151/231 (65%)	141 (93%)	10 (7%)	15	42
3	e	151/231 (65%)	142 (94%)	9 (6%)	17	44
3	i	151/231 (65%)	143 (95%)	8 (5%)	20	46
4	0	9/9 (100%)	7 (78%)	2 (22%)	1	6
4	1	9/9 (100%)	7 (78%)	2 (22%)	1	6
4	2	9/9 (100%)	7 (78%)	2 (22%)	1	6
4	3	9/9 (100%)	7 (78%)	2 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	4	9/9 (100%)	8 (89%)	1 (11%)	6	24
4	5	9/9 (100%)	6 (67%)	3 (33%)	0	1
4	6	9/9 (100%)	5 (56%)	4 (44%)	0	0
4	7	9/9 (100%)	4 (44%)	5 (56%)	0	0
4	8	9/9 (100%)	3 (33%)	6 (67%)	0	0
5	D	94/94 (100%)	94 (100%)	0	100	100
5	H	94/94 (100%)	92 (98%)	2 (2%)	47	64
5	L	94/94 (100%)	92 (98%)	2 (2%)	47	64
5	P	94/94 (100%)	94 (100%)	0	100	100
5	T	94/94 (100%)	90 (96%)	4 (4%)	26	50
5	X	94/94 (100%)	93 (99%)	1 (1%)	65	73
5	b	94/94 (100%)	93 (99%)	1 (1%)	65	73
5	f	94/94 (100%)	93 (99%)	1 (1%)	65	73
All	All	6969/7532 (92%)	6627 (95%)	342 (5%)	22	48

5 of 342 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	a	19	GLU
2	h	193	VAL
3	a	182	THR
3	e	17	ARG
4	8	401	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
2	d	60	HIS
1	s	196	GLN
3	e	70	HIS
1	k	190	HIS
3	K	191	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	205/214 (95%)	-0.19	0 100 100	83, 110, 158, 171	0
1	E	205/214 (95%)	-0.23	0 100 100	80, 106, 145, 172	0
1	I	205/214 (95%)	-0.18	0 100 100	77, 102, 149, 163	0
1	M	205/214 (95%)	-0.21	0 100 100	74, 104, 138, 154	0
1	Q	205/214 (95%)	-0.24	0 100 100	72, 97, 133, 165	0
1	U	205/214 (95%)	-0.17	0 100 100	69, 103, 155, 171	0
1	Y	205/214 (95%)	-0.09	1 (0%) 87 71	97, 120, 142, 163	0
1	c	205/214 (95%)	0.11	1 (0%) 87 71	106, 143, 164, 183	0
1	g	205/214 (95%)	0.29	1 (0%) 87 71	111, 152, 169, 174	0
1	k	205/214 (95%)	0.09	0 100 100	135, 159, 176, 183	0
1	o	203/214 (94%)	0.07	1 (0%) 87 71	137, 160, 176, 181	0
1	s	205/214 (95%)	0.18	1 (0%) 87 71	140, 167, 181, 190	0
2	B	221/240 (92%)	-0.03	1 (0%) 87 71	82, 114, 163, 184	0
2	F	221/240 (92%)	-0.09	1 (0%) 87 71	77, 115, 163, 193	0
2	J	220/240 (91%)	-0.13	0 100 100	76, 114, 160, 187	0
2	N	220/240 (91%)	-0.08	1 (0%) 87 71	74, 110, 150, 179	0
2	R	221/240 (92%)	-0.12	1 (0%) 87 71	77, 107, 143, 174	0
2	V	220/240 (91%)	-0.09	1 (0%) 87 71	73, 110, 158, 175	0
2	Z	220/240 (91%)	0.08	7 (3%) 50 35	100, 126, 160, 179	0
2	d	220/240 (91%)	0.09	3 (1%) 73 52	112, 135, 164, 179	0
2	h	223/240 (92%)	0.37	6 (2%) 56 38	118, 146, 172, 190	0
2	l	219/240 (91%)	0.17	6 (2%) 56 38	138, 161, 177, 182	0
2	p	218/240 (90%)	0.18	6 (2%) 55 38	129, 160, 179, 190	0
2	t	221/240 (92%)	0.28	4 (1%) 67 47	132, 159, 180, 189	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	C	274/274 (100%)	-0.15	0 100 100	78, 102, 151, 170	0
3	G	274/274 (100%)	-0.17	1 (0%) 88 74	74, 97, 147, 175	0
3	K	274/274 (100%)	-0.24	0 100 100	70, 94, 137, 164	0
3	O	274/274 (100%)	-0.24	0 100 100	69, 93, 142, 166	0
3	S	274/274 (100%)	-0.25	0 100 100	70, 91, 146, 177	0
3	W	274/274 (100%)	-0.15	0 100 100	72, 92, 150, 187	0
3	a	182/274 (66%)	0.09	0 100 100	104, 125, 142, 162	0
3	e	182/274 (66%)	0.23	1 (0%) 87 71	118, 135, 152, 166	0
3	i	182/274 (66%)	0.38	3 (1%) 70 49	126, 147, 167, 180	0
4	0	9/9 (100%)	-0.15	0 100 100	84, 89, 104, 109	0
4	1	9/9 (100%)	-0.01	0 100 100	76, 92, 101, 106	0
4	2	9/9 (100%)	-0.05	0 100 100	78, 84, 105, 110	0
4	3	9/9 (100%)	-0.06	0 100 100	76, 83, 98, 100	0
4	4	9/9 (100%)	-0.33	0 100 100	70, 83, 97, 99	0
4	5	9/9 (100%)	0.16	0 100 100	77, 79, 96, 100	0
4	6	9/9 (100%)	0.29	0 100 100	118, 126, 137, 147	0
4	7	9/9 (100%)	0.57	0 100 100	118, 131, 136, 141	0
4	8	9/9 (100%)	0.88	1 (11%) 10 13	130, 142, 150, 151	0
5	D	99/99 (100%)	-0.17	0 100 100	89, 110, 138, 149	0
5	H	99/99 (100%)	-0.17	0 100 100	76, 105, 131, 141	0
5	L	99/99 (100%)	-0.17	0 100 100	73, 103, 131, 152	0
5	P	99/99 (100%)	-0.29	0 100 100	76, 99, 128, 143	0
5	T	99/99 (100%)	-0.25	0 100 100	74, 95, 125, 141	0
5	X	99/99 (100%)	-0.15	0 100 100	78, 106, 140, 153	0
5	b	99/99 (100%)	-0.09	0 100 100	106, 125, 146, 165	0
5	f	99/99 (100%)	0.19	1 (1%) 79 58	122, 140, 158, 173	0
All	All	8165/8787 (92%)	-0.03	49 (0%) 85 68	69, 122, 170, 193	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	33	GLY	5.1
2	h	101	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
2	Z	99	ALA	4.1
2	1	104	LEU	3.9
2	1	33	GLY	3.6

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 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.