wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 09:17 AM EDT

PDB ID	:	8DNT
Title	:	SARS-CoV-2 specific T cell receptor
Authors	:	Gallagher, D.T.; Wu, D.; Gowthaman, R.; Pierce, B.G.; Mariuzza, R.A.; Weng, N.P.
Deposited on	:	2022-07-11
Resolution	:	3.18 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 (i) 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 (1)) were used in the production of this report:

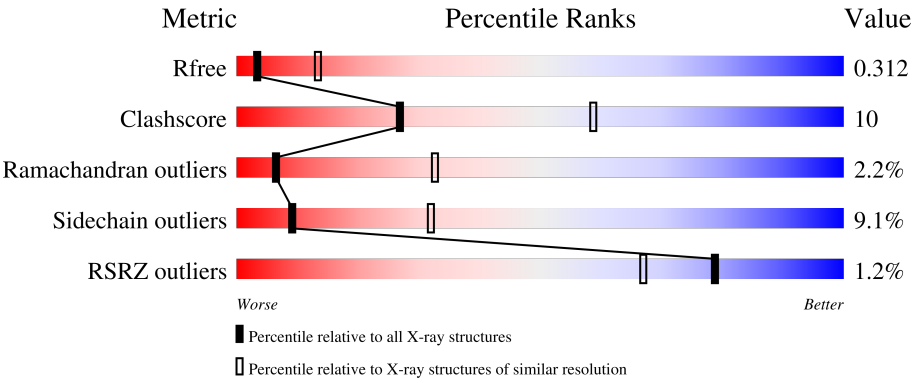
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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 <=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	203	4% 70% 27%
1	H	203	2% 65% 27% 5%
1	M	203	2% 71% 24%
1	V	203	3% 69% 28%
2	B	244	2% 61% 35%

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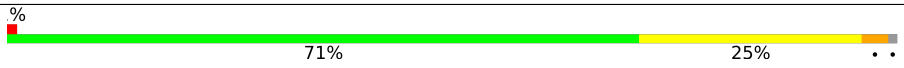
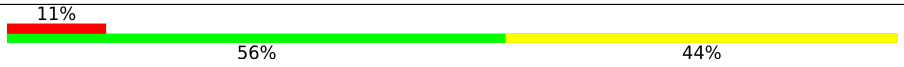
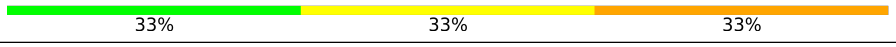
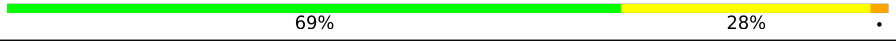
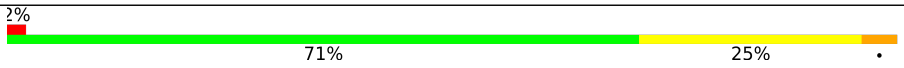
Mol	Chain	Length	Quality of chain
2	I	244	
2	P	244	
2	W	244	
3	D	9	
3	J	9	
3	Q	9	
3	X	9	
4	E	279	
4	K	279	
4	R	279	
4	Y	279	
5	F	100	
5	L	100	
5	T	100	
5	Z	100	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 26210 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 T-cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1548	964	260	316	8			
1	H	198	Total	C	N	O	S	0	0	0
			1543	961	259	315	8			
1	M	198	Total	C	N	O	S	0	0	0
			1543	961	259	315	8			
1	V	198	Total	C	N	O	S	0	0	0
			1539	958	258	315	8			

- Molecule 2 is a protein called T-cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1894	1189	328	372	5			
2	I	242	Total	C	N	O	S	0	0	0
			1881	1180	327	369	5			
2	P	242	Total	C	N	O	S	0	0	0
			1897	1190	330	372	5			
2	W	242	Total	C	N	O	S	0	0	0
			1894	1189	328	372	5			

- Molecule 3 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	9	Total	C	N	O	0	0	0
			77	49	14	14			
3	J	9	Total	C	N	O	0	0	0
			77	49	14	14			
3	Q	9	Total	C	N	O	0	0	0
			77	49	14	14			
3	X	9	Total	C	N	O	0	0	0
			77	49	14	14			

- Molecule 4 is a protein called MHC class I antigen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	275	Total	C	N	O	S	0	0	0
			2239	1399	408	423	9			
4	K	276	Total	C	N	O	S	0	0	0
			2236	1398	403	426	9			
4	R	278	Total	C	N	O	S	0	0	0
			2241	1400	408	424	9			
4	Y	274	Total	C	N	O	S	0	0	0
			2196	1380	395	413	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	initiating methionine	UNP U5YKE0
E	276	GLY	-	expression tag	UNP U5YKE0
E	277	GLY	-	expression tag	UNP U5YKE0
E	278	GLY	-	expression tag	UNP U5YKE0
K	0	MET	-	initiating methionine	UNP U5YKE0
K	276	GLY	-	expression tag	UNP U5YKE0
K	277	GLY	-	expression tag	UNP U5YKE0
K	278	GLY	-	expression tag	UNP U5YKE0
R	0	MET	-	initiating methionine	UNP U5YKE0
R	276	GLY	-	expression tag	UNP U5YKE0
R	277	GLY	-	expression tag	UNP U5YKE0
R	278	GLY	-	expression tag	UNP U5YKE0
Y	0	MET	-	initiating methionine	UNP U5YKE0
Y	276	GLY	-	expression tag	UNP U5YKE0
Y	277	GLY	-	expression tag	UNP U5YKE0
Y	278	GLY	-	expression tag	UNP U5YKE0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	100	Total	C	N	O	S	0	0	0
			813	518	137	154	4			
5	L	100	Total	C	N	O	S	0	0	0
			822	525	139	154	4			
5	T	100	Total	C	N	O	S	0	0	0
			804	516	135	150	3			
5	Z	100	Total	C	N	O	S	0	0	0
			812	519	138	152	3			

There are 4 discrepancies between the modelled and reference sequences:

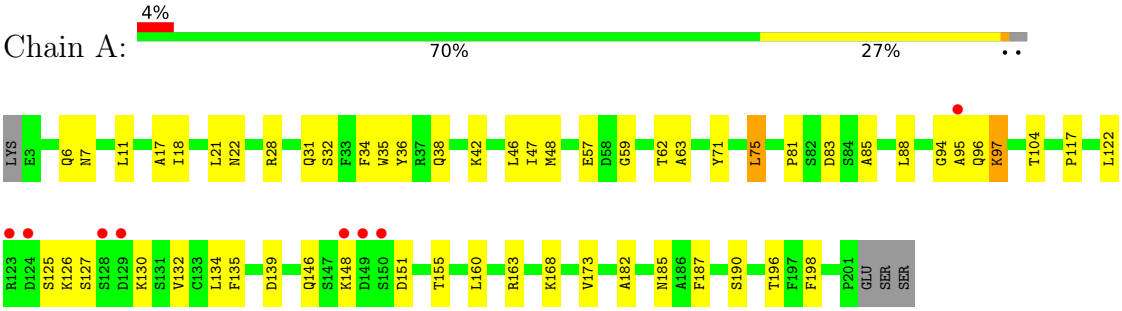
Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	initiating methionine	UNP P61769
L	1	MET	-	initiating methionine	UNP P61769
T	1	MET	-	initiating methionine	UNP P61769
Z	1	MET	-	initiating methionine	UNP P61769

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.

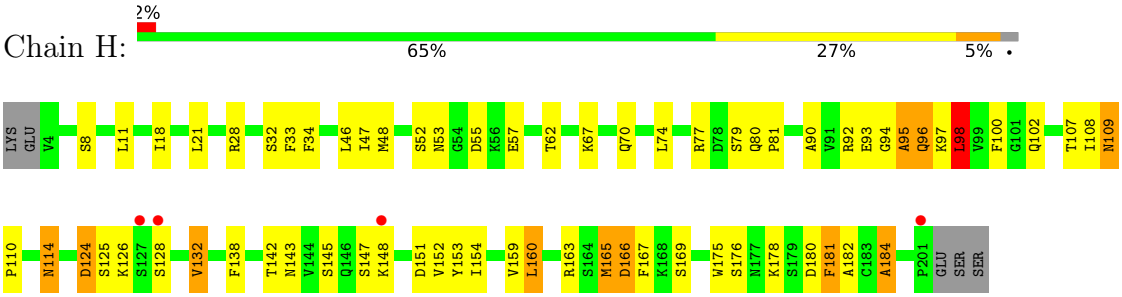
• Molecule 1: T-cell receptor alpha chain

Chain A:



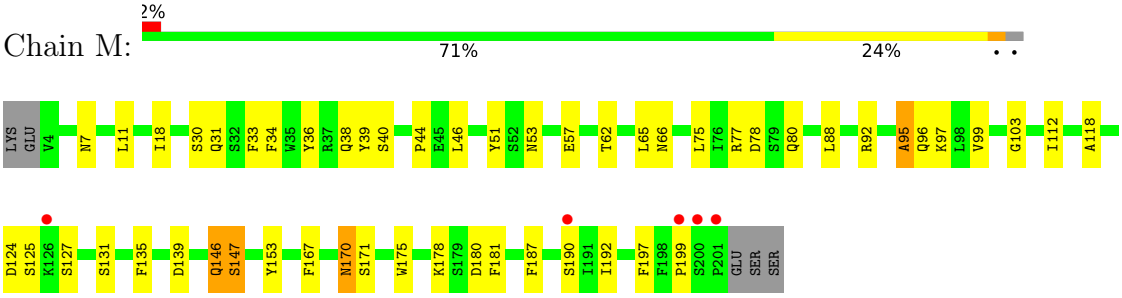
• Molecule 1: T-cell receptor alpha chain

Chain H:



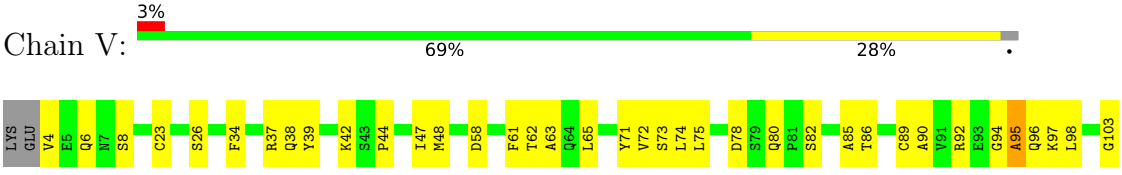
• Molecule 1: T-cell receptor alpha chain

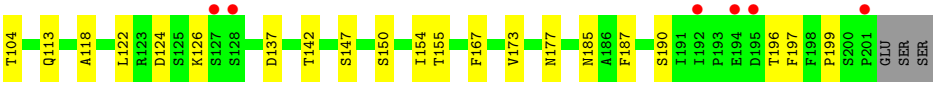
Chain M:



• Molecule 1: T-cell receptor alpha chain

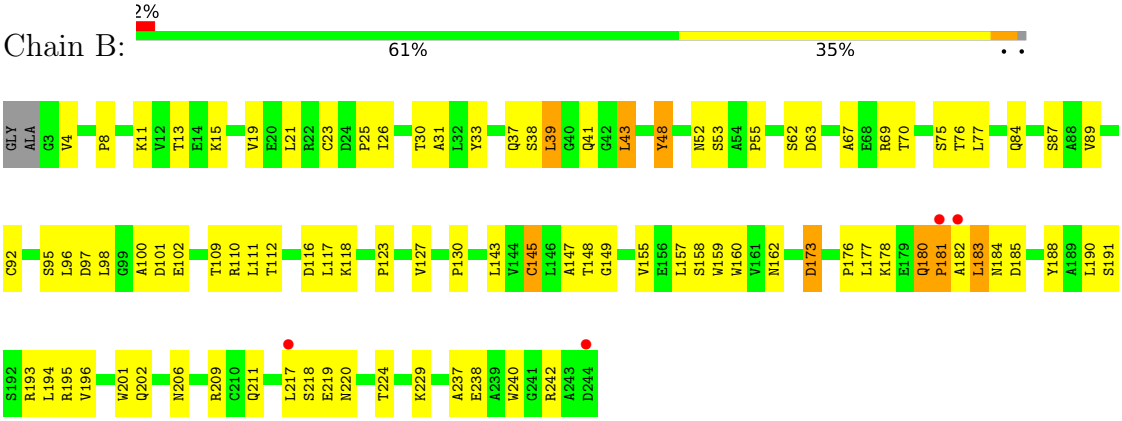
Chain V:





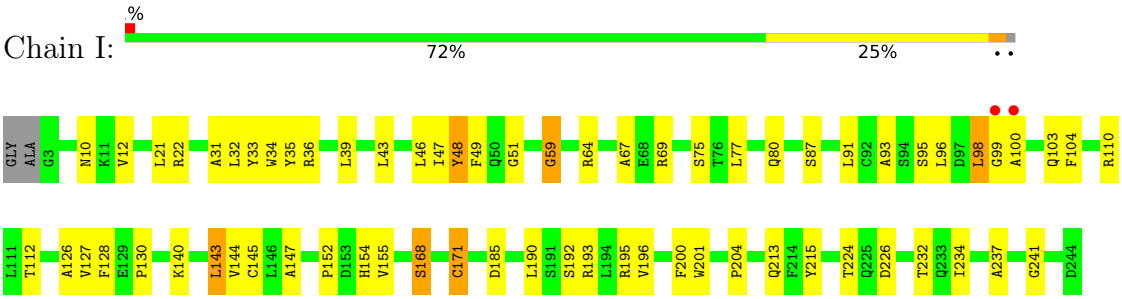
• Molecule 2: T-cell receptor beta chain

Chain B:



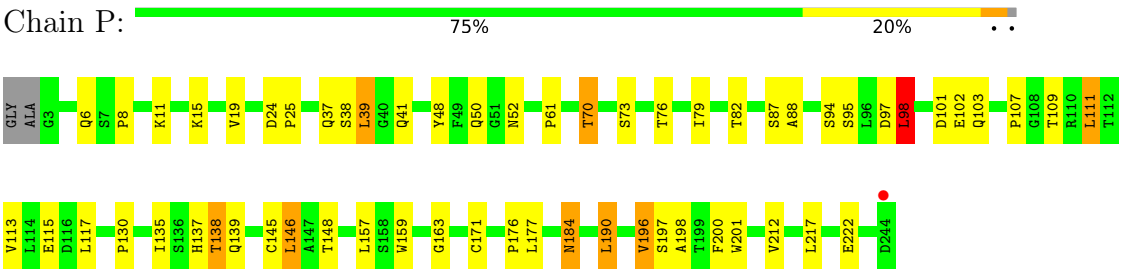
• Molecule 2: T-cell receptor beta chain

Chain I:



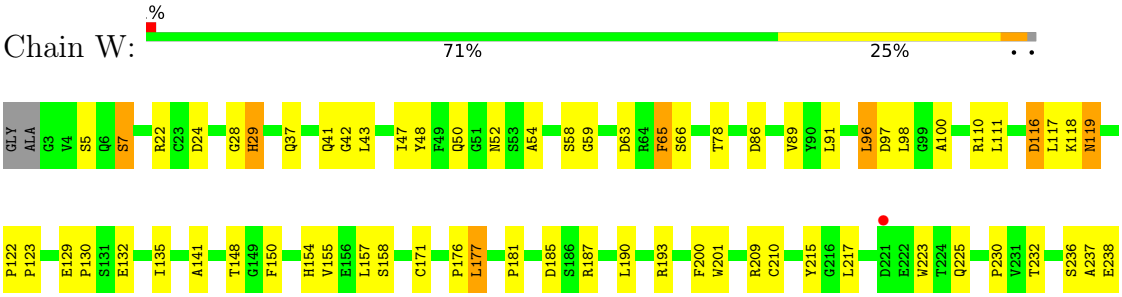
• Molecule 2: T-cell receptor beta chain

Chain P:



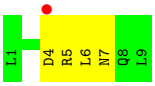
• Molecule 2: T-cell receptor beta chain

Chain W:



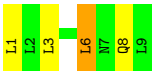
• Molecule 3: Nucleoprotein

Chain D:



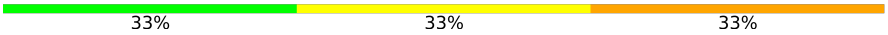
• Molecule 3: Nucleoprotein

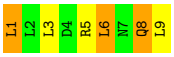
Chain J:



• Molecule 3: Nucleoprotein

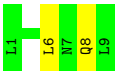
Chain Q:





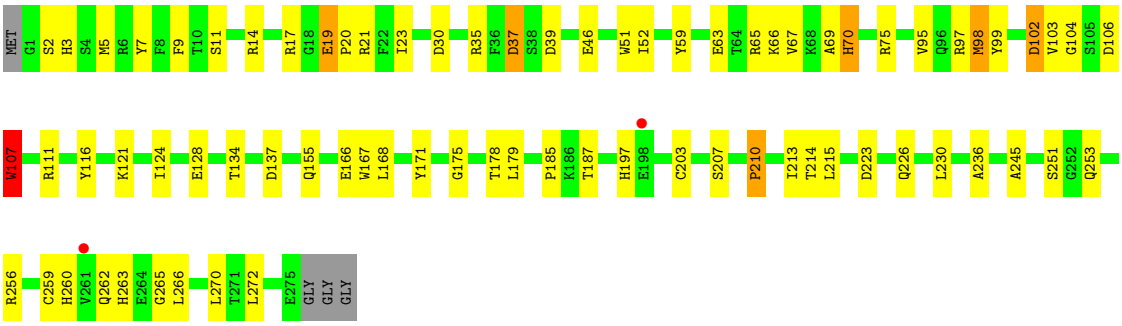
• Molecule 3: Nucleoprotein

Chain X:



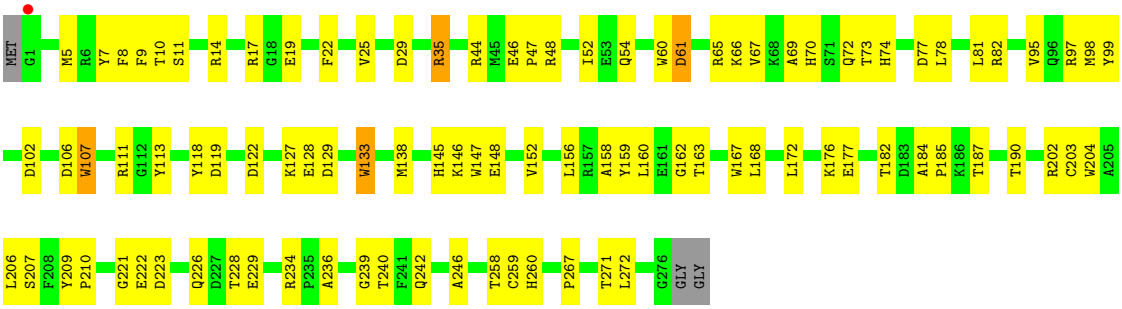
• Molecule 4: MHC class I antigen alpha chain

Chain E:



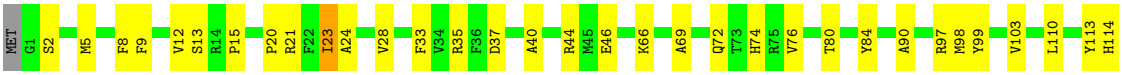
• Molecule 4: MHC class I antigen alpha chain

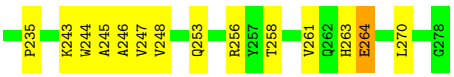
Chain K:



• Molecule 4: MHC class I antigen alpha chain

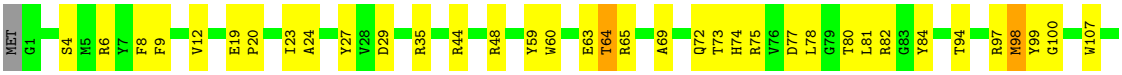
Chain R:

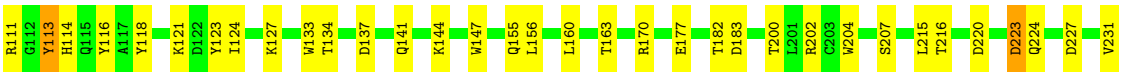


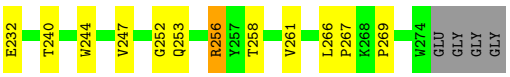


• Molecule 4: MHC class I antigen alpha chain

Chain Y:

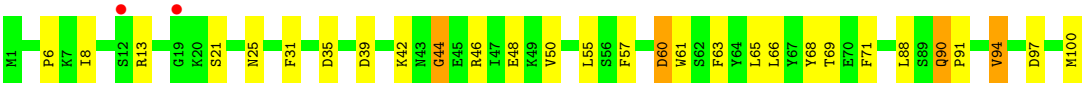






• Molecule 5: Beta-2-microglobulin

Chain F:

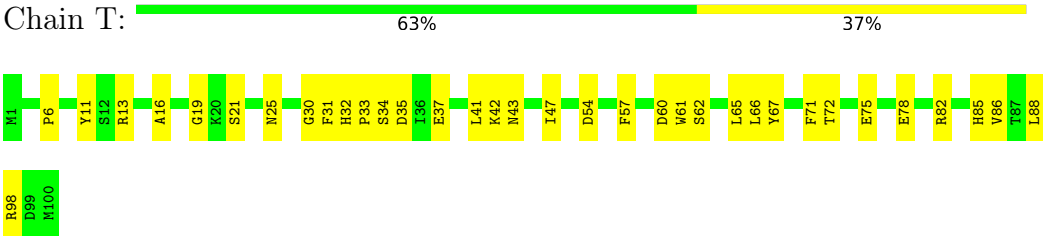


• Molecule 5: Beta-2-microglobulin

Chain L:

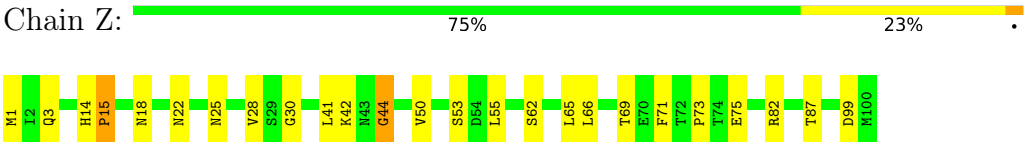
• Molecule 5: Beta-2-microglobulin

Chain T:



• Molecule 5: Beta-2-microglobulin

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	182.16Å 121.83Å 210.56Å 90.00° 100.02° 90.00°	Depositor
Resolution (Å)	30.00 – 3.18 29.90 – 3.18	Depositor EDS
% Data completeness (in resolution range)	74.7 (30.00-3.18) 74.8 (29.90-3.18)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.221 , 0.313 0.216 , 0.312	Depositor DCC
R_{free} test set	2857 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	107.6	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 74.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26210	wwPDB-VP
Average B, all atoms (Å^2)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.26	0/1581	0.57	0/2143
1	H	0.27	0/1576	0.57	0/2136
1	M	0.28	0/1576	0.58	0/2136
1	V	0.27	0/1572	0.59	0/2132
2	B	0.27	0/1942	0.55	0/2643
2	I	0.27	0/1929	0.58	0/2629
2	P	0.28	0/1945	0.57	0/2647
2	W	0.26	0/1942	0.55	0/2643
3	D	0.28	0/76	0.61	0/100
3	J	0.28	0/76	0.74	0/100
3	Q	0.28	0/76	0.69	0/100
3	X	0.26	0/76	0.54	0/100
4	E	0.25	0/2304	0.55	0/3129
4	K	0.26	0/2301	0.58	0/3126
4	R	0.26	0/2306	0.58	0/3132
4	Y	0.25	0/2258	0.56	0/3069
5	F	0.27	0/836	0.57	0/1137
5	L	0.27	0/845	0.64	0/1146
5	T	0.27	0/827	0.58	0/1125
5	Z	0.26	0/835	0.56	0/1135
All	All	0.27	0/26879	0.57	0/36508

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
3	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	5	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1548	0	1460	36	0
1	H	1543	0	1458	44	0
1	M	1543	0	1458	42	0
1	V	1539	0	1447	29	0
2	B	1894	0	1796	45	0
2	I	1881	0	1769	43	0
2	P	1897	0	1801	26	0
2	W	1894	0	1796	34	0
3	D	77	0	88	1	0
3	J	77	0	88	3	0
3	Q	77	0	88	8	0
3	X	77	0	88	2	0
4	E	2239	0	2083	45	0
4	K	2236	0	2070	63	0
4	R	2241	0	2077	54	0
4	Y	2196	0	2025	42	0
5	F	813	0	753	13	0
5	L	822	0	777	23	0
5	T	804	0	746	19	0
5	Z	812	0	757	11	0
All	All	26210	0	24625	518	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 10.

The worst 5 of 518 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:M:46:LEU:HB3	2:P:102:GLU:HG3	1.23	1.09
4:R:230:LEU:HD11	4:R:243:LYS:HE3	1.43	1.01
1:M:96:GLN:HE22	3:Q:6:LEU:HB3	1.23	0.98
2:W:41:GLN:HG2	2:W:42:GLY:H	1.29	0.98
4:K:127:LYS:HD3	4:K:128:GLU:H	1.29	0.96

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	197/203 (97%)	157 (80%)	33 (17%)	7 (4%)	3 21
1	H	196/203 (97%)	162 (83%)	28 (14%)	6 (3%)	4 24
1	M	196/203 (97%)	161 (82%)	30 (15%)	5 (3%)	5 29
1	V	196/203 (97%)	167 (85%)	26 (13%)	3 (2%)	10 43
2	B	240/244 (98%)	203 (85%)	31 (13%)	6 (2%)	5 30
2	I	240/244 (98%)	195 (81%)	42 (18%)	3 (1%)	12 46
2	P	240/244 (98%)	200 (83%)	33 (14%)	7 (3%)	4 26
2	W	240/244 (98%)	201 (84%)	34 (14%)	5 (2%)	7 34
3	D	7/9 (78%)	7 (100%)	0	0	100 100
3	J	7/9 (78%)	7 (100%)	0	0	100 100
3	Q	7/9 (78%)	7 (100%)	0	0	100 100
3	X	7/9 (78%)	7 (100%)	0	0	100 100
4	E	273/279 (98%)	240 (88%)	28 (10%)	5 (2%)	8 38
4	K	274/279 (98%)	233 (85%)	36 (13%)	5 (2%)	8 38
4	R	276/279 (99%)	243 (88%)	31 (11%)	2 (1%)	22 60
4	Y	272/279 (98%)	247 (91%)	19 (7%)	6 (2%)	6 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	F	98/100 (98%)	85 (87%)	10 (10%)	3 (3%)	4 24
5	L	98/100 (98%)	87 (89%)	9 (9%)	2 (2%)	7 35
5	T	98/100 (98%)	87 (89%)	8 (8%)	3 (3%)	4 24
5	Z	98/100 (98%)	84 (86%)	10 (10%)	4 (4%)	3 19
All	All	3260/3340 (98%)	2780 (85%)	408 (12%)	72 (2%)	6 33

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	LYS
1	A	126	LYS
2	B	39	LEU
2	B	181	PRO
4	E	107	TRP

5.3.2 Protein sidechains (i)

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	176/181 (97%)	164 (93%)	12 (7%)	16 47
1	H	176/181 (97%)	157 (89%)	19 (11%)	6 25
1	M	176/181 (97%)	168 (96%)	8 (4%)	27 61
1	V	175/181 (97%)	160 (91%)	15 (9%)	10 36
2	B	206/208 (99%)	186 (90%)	20 (10%)	8 29
2	I	203/208 (98%)	188 (93%)	15 (7%)	13 43
2	P	207/208 (100%)	187 (90%)	20 (10%)	8 29
2	W	206/208 (99%)	190 (92%)	16 (8%)	12 41
3	D	9/9 (100%)	7 (78%)	2 (22%)	1 4
3	J	9/9 (100%)	6 (67%)	3 (33%)	0 0
3	Q	9/9 (100%)	6 (67%)	3 (33%)	0 0
3	X	9/9 (100%)	9 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	E	229/232 (99%)	207 (90%)	22 (10%)	8 30
4	K	228/232 (98%)	202 (89%)	26 (11%)	5 23
4	R	227/232 (98%)	207 (91%)	20 (9%)	10 34
4	Y	218/232 (94%)	192 (88%)	26 (12%)	5 21
5	F	89/95 (94%)	81 (91%)	8 (9%)	9 33
5	L	91/95 (96%)	80 (88%)	11 (12%)	5 20
5	T	86/95 (90%)	81 (94%)	5 (6%)	20 53
5	Z	88/95 (93%)	83 (94%)	5 (6%)	20 54
All	All	2817/2900 (97%)	2561 (91%)	256 (9%)	9 32

5 of 256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Y	80	THR
4	Y	163	THR
2	I	234	ILE
2	I	200	PHE
4	Y	215	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
2	W	37	GLN
2	W	84	GLN
4	Y	191	HIS
2	I	84	GLN
2	I	50	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	199/203 (98%)	0.00	8 (4%) 38 24	116, 171, 247, 291	0
1	H	198/203 (97%)	-0.17	4 (2%) 65 50	99, 160, 250, 281	0
1	M	198/203 (97%)	-0.07	5 (2%) 57 43	89, 159, 236, 307	0
1	V	198/203 (97%)	-0.17	6 (3%) 50 34	94, 161, 253, 288	0
2	B	242/244 (99%)	-0.01	4 (1%) 70 57	116, 187, 247, 278	0
2	I	242/244 (99%)	-0.34	2 (0%) 86 77	111, 159, 215, 273	0
2	P	242/244 (99%)	-0.41	1 (0%) 92 89	87, 147, 207, 234	0
2	W	242/244 (99%)	-0.31	2 (0%) 86 77	116, 156, 193, 221	0
3	D	9/9 (100%)	0.93	1 (11%) 5 3	135, 141, 181, 188	0
3	J	9/9 (100%)	0.34	0 100 100	101, 111, 134, 151	0
3	Q	9/9 (100%)	0.21	0 100 100	88, 109, 141, 153	0
3	X	9/9 (100%)	0.51	0 100 100	116, 125, 171, 174	0
4	E	275/279 (98%)	-0.25	2 (0%) 87 81	104, 157, 200, 226	0
4	K	276/279 (98%)	-0.46	1 (0%) 92 89	77, 127, 161, 191	0
4	R	278/279 (99%)	-0.54	0 100 100	77, 128, 164, 187	0
4	Y	274/279 (98%)	-0.29	0 100 100	106, 147, 186, 220	0
5	F	100/100 (100%)	-0.05	2 (2%) 65 50	128, 177, 232, 255	0
5	L	100/100 (100%)	-0.39	0 100 100	86, 123, 157, 182	0
5	T	100/100 (100%)	-0.36	0 100 100	93, 127, 168, 177	0
5	Z	100/100 (100%)	-0.26	0 100 100	116, 154, 196, 238	0
All	All	3300/3340 (98%)	-0.26	38 (1%) 79 67	77, 151, 222, 307	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	201	PRO	11.5
1	M	200	SER	8.2
1	V	201	PRO	6.0
3	D	4	ASP	4.2
2	B	181	PRO	4.2

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 monosaccharides 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.