



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 02:50 PM BST

PDB ID : 4L29  
Title : Structure of wtMHC class I with NY-ESO1 double mutant  
Authors : Halabelian, L.; Giorgetti, S.; Bellotti, V.; Bolognesi, M.; Ricagno, S.  
Deposited on : 2013-06-04  
Resolution : 3.09 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
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) : 2.13

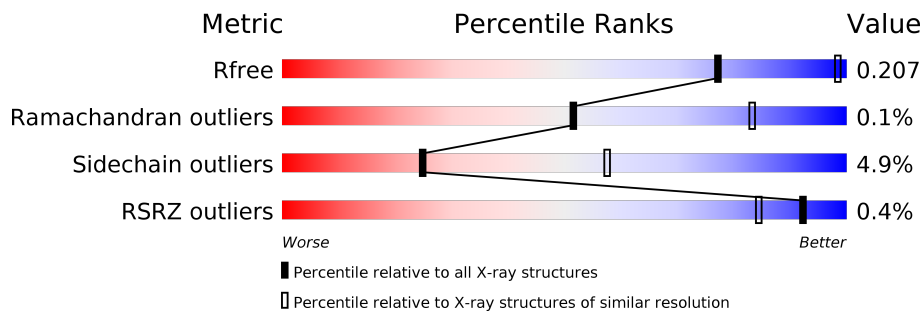
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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.




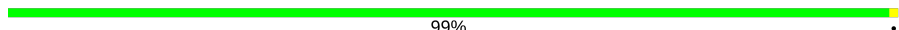

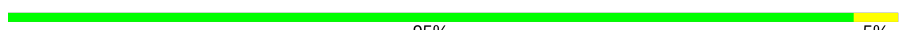











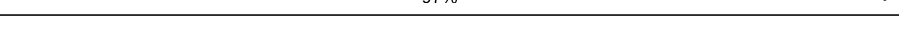
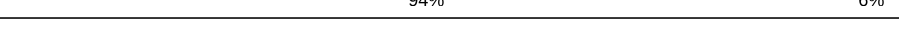
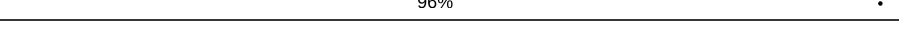
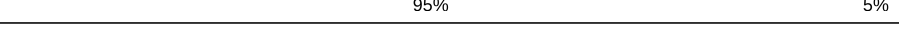
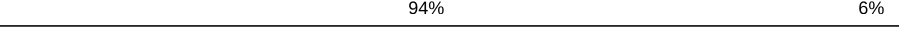
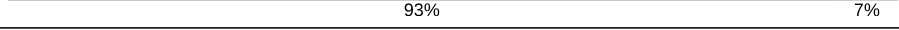
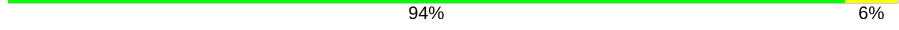

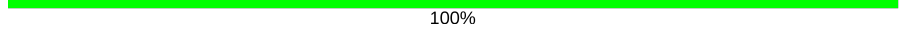

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	 99%
1	C	276	 95% 5%
1	E	276	 95% 5%
1	G	276	 96% .
1	I	276	 96% .
1	K	276	 94% 6%
1	M	276	 97% .


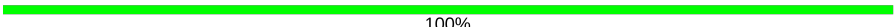

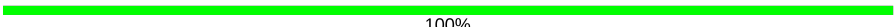
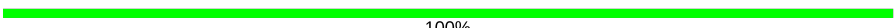


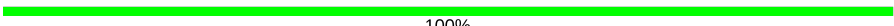
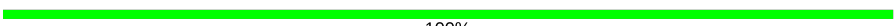

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Mol	Chain	Length	Quality of chain
1	O	276	 96%
1	Q	276	 99%
1	S	276	 95% 5%
1	U	276	 95% 5%
1	W	276	 96%
1	Y	276	 95% 5%
1	a	276	 96%
2	B	100	 94% 6%
2	D	100	 95% 5%
2	F	100	 95% 5%
2	H	100	 94% 6%
2	J	100	 97%
2	L	100	 96%
2	N	100	 94% 6%
2	P	100	 97%
2	R	100	 94% 6%
2	T	100	 96%
2	V	100	 95% 5%
2	X	100	 94% 6%
2	Z	100	 93% 7%
2	b	100	 94% 6%
3	c	9	 89% 11%
3	e	9	 100%
3	f	9	 89% 11%
3	g	9	 100%

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Mol	Chain	Length	Quality of chain
3	h	9	 89% 11%
3	i	9	 100%
3	j	9	 89% 11%
3	k	9	 100%
3	l	9	 100%
3	m	9	 89% 11%
3	n	9	 89% 11%
3	o	9	 100%
3	p	9	 100%
3	q	9	 100%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 44627 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2254	1408	410	427	9	0	0	0
1	C	276	2254	1408	410	427	9	0	0	0
1	E	276	2254	1408	410	427	9	0	0	0
1	G	276	2254	1408	410	427	9	0	0	0
1	I	276	2254	1408	410	427	9	0	0	0
1	K	276	2254	1408	410	427	9	0	0	0
1	M	276	2254	1408	410	427	9	0	0	0
1	O	276	2254	1408	410	427	9	0	0	0
1	Q	276	2254	1408	410	427	9	0	0	0
1	S	276	2254	1408	410	427	9	0	0	0
1	U	276	2254	1408	410	427	9	0	0	0
1	W	276	2254	1408	410	427	9	0	0	0
1	Y	276	2254	1408	410	427	9	0	0	0
1	a	276	2254	1408	410	427	9	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	837	533	141	159	4	0	0	0
2	D	100	837	533	141	159	4	0	0	0
2	F	100	837	533	141	159	4	0	0	0
2	H	100	837	533	141	159	4	0	0	0
2	J	100	837	533	141	159	4	0	0	0
2	L	100	837	533	141	159	4	0	0	0
2	N	100	837	533	141	159	4	0	0	0
2	P	100	837	533	141	159	4	0	0	0
2	R	100	837	533	141	159	4	0	0	0
2	T	100	837	533	141	159	4	0	0	0
2	V	100	837	533	141	159	4	0	0	0
2	X	100	837	533	141	159	4	0	0	0
2	Z	100	837	533	141	159	4	0	0	0
2	b	100	837	533	141	159	4	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	INITIATING METHIONINE	UNP P61769
D	0	MET	-	INITIATING METHIONINE	UNP P61769
F	0	MET	-	INITIATING METHIONINE	UNP P61769
H	0	MET	-	INITIATING METHIONINE	UNP P61769
J	0	MET	-	INITIATING METHIONINE	UNP P61769
L	0	MET	-	INITIATING METHIONINE	UNP P61769
N	0	MET	-	INITIATING METHIONINE	UNP P61769
P	0	MET	-	INITIATING METHIONINE	UNP P61769
R	0	MET	-	INITIATING METHIONINE	UNP P61769
T	0	MET	-	INITIATING METHIONINE	UNP P61769
V	0	MET	-	INITIATING METHIONINE	UNP P61769
X	0	MET	-	INITIATING METHIONINE	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	0	MET	-	INITIATING METHIONINE	UNP P61769
b	0	MET	-	INITIATING METHIONINE	UNP P61769

- Molecule 3 is a protein called NY-ESO1 DOUBLE MUTANT (1Y, 9V).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	m	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	i	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	k	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	f	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	l	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	h	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	e	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	n	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	p	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	o	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	c	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	g	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	q	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			
3	j	9	Total	C	N	O	S	0	0	0
			82	57	11	13	1			

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total	Cl	0	0
			1	1		
4	K	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	W	1	Total Cl 1 1	0	0
4	N	2	Total Cl 2 2	0	0
4	S	1	Total Cl 1 1	0	0
4	J	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0
4	b	1	Total Cl 1 1	0	0
4	V	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0
4	R	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	I	3	Total Cl 3 3	0	0
4	Z	1	Total Cl 1 1	0	0
4	a	1	Total Cl 1 1	0	0
4	U	1	Total Cl 1 1	0	0
4	L	1	Total Cl 1 1	0	0
4	G	1	Total Cl 1 1	0	0
4	Q	2	Total Cl 2 2	0	0
4	H	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	T	1	Total Cl 1 1	0	0

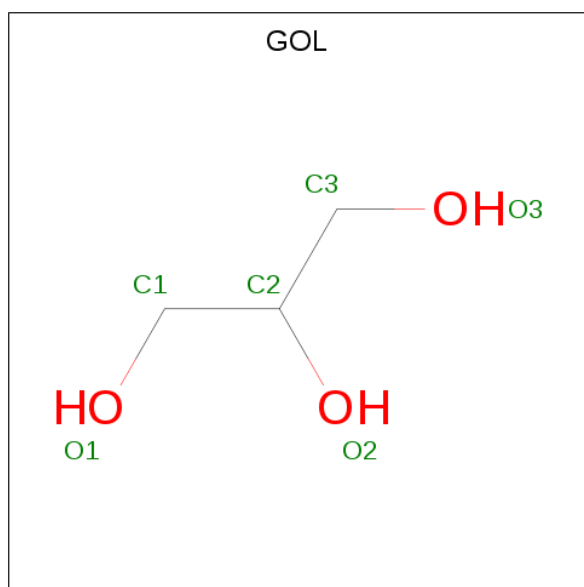
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	1	Total Cl 1 1	0	0
4	Y	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	i	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	f	1	Total C O 6 3 3	0	0
5	l	1	Total C O 6 3 3	0	0
5	K	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	h	1	Total C O 6 3 3	0	0
5	e	1	Total C O 6 3 3	0	0
5	O	1	Total C O 6 3 3	0	0
5	O	1	Total C O 6 3 3	0	0
5	Q	1	Total C O 6 3 3	0	0
5	S	1	Total C O 6 3 3	0	0
5	o	1	Total C O 6 3 3	0	0
5	c	1	Total C O 6 3 3	0	0
5	g	1	Total C O 6 3 3	0	0
5	Y	1	Total C O 6 3 3	0	0
5	q	1	Total C O 6 3 3	0	0
5	a	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total O 2 2	0	0
6	C	4	Total O 4 4	0	0
6	D	2	Total O 2 2	0	0
6	E	3	Total O 3 3	0	0
6	F	2	Total O 2 2	0	0
6	G	7	Total O 7 7	0	0
6	H	1	Total O 1 1	0	0

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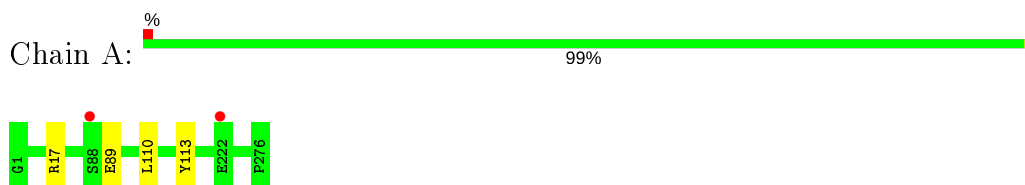
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
6	I	3	Total O 3 3	0	0
6	J	2	Total O 2 2	0	0
6	K	3	Total O 3 3	0	0
6	L	3	Total O 3 3	0	0
6	M	1	Total O 1 1	0	0
6	P	3	Total O 3 3	0	0
6	Q	2	Total O 2 2	0	0
6	R	3	Total O 3 3	0	0
6	S	1	Total O 1 1	0	0
6	T	1	Total O 1 1	0	0
6	U	3	Total O 3 3	0	0
6	V	2	Total O 2 2	0	0
6	X	3	Total O 3 3	0	0
6	Y	2	Total O 2 2	0	0
6	Z	2	Total O 2 2	0	0

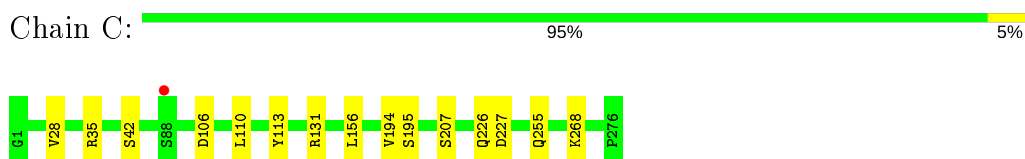
### 3 Residue-property plots [i](#)

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.

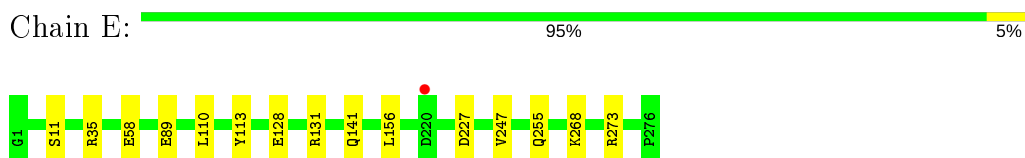
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



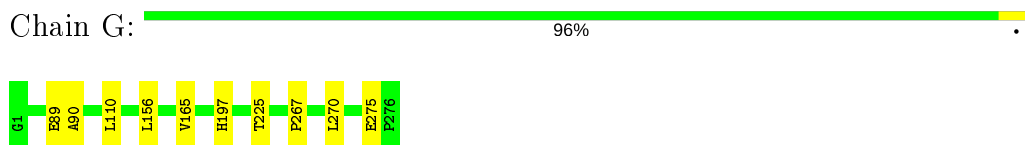
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



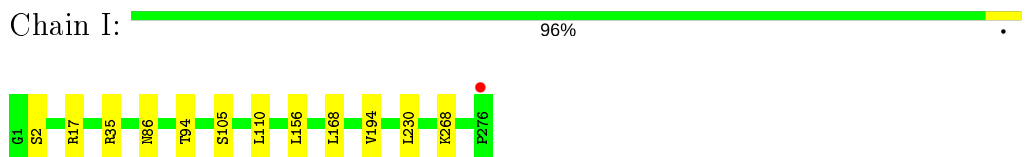
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



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



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



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

Chain K:  94% 6%



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

Chain M:  97%



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

Chain O:  96%



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

Chain Q:  99%



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

Chain S:  95% 5%



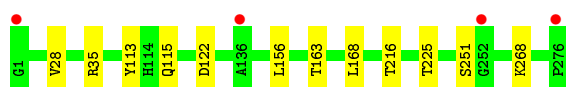
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain U:  95% 5%

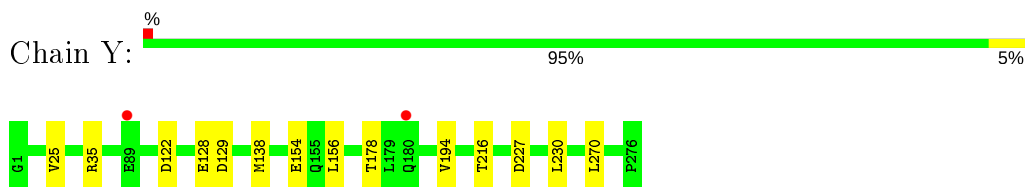


- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

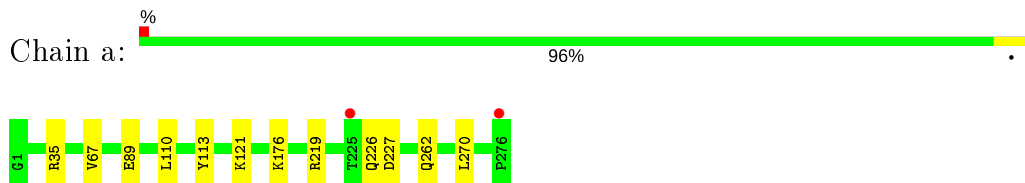
Chain W:  96%



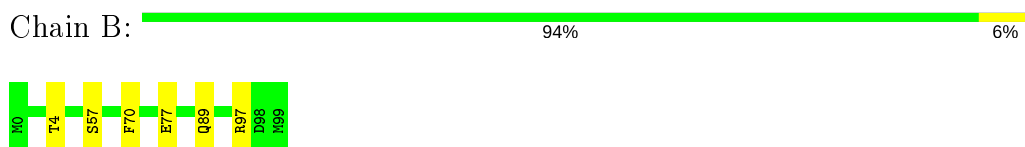
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



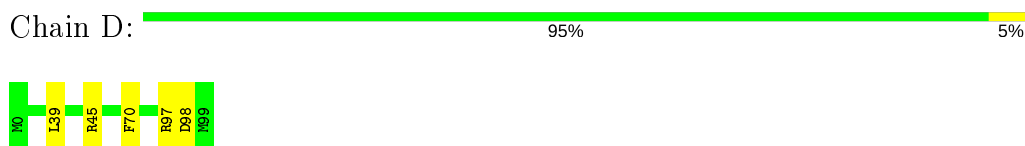
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



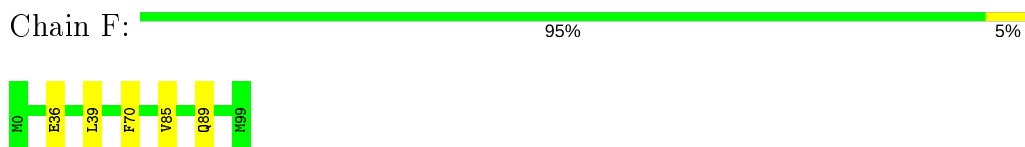
- Molecule 2: Beta-2-microglobulin



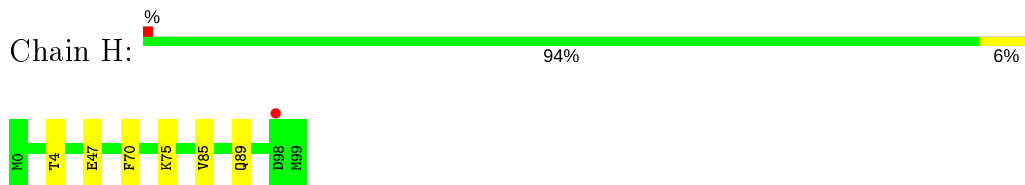
- Molecule 2: Beta-2-microglobulin



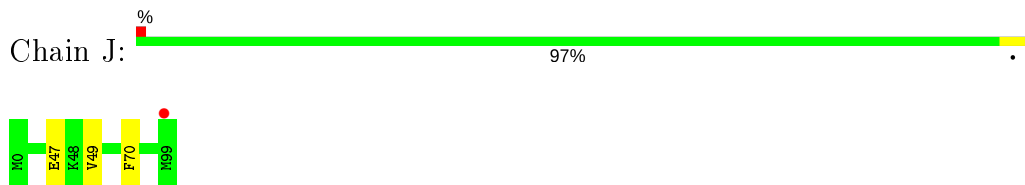
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

Chain L:  96%



- Molecule 2: Beta-2-microglobulin

Chain N:  94%



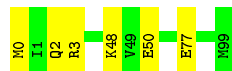
- Molecule 2: Beta-2-microglobulin

Chain P:  97%



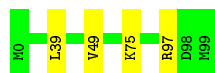
- Molecule 2: Beta-2-microglobulin

Chain R:  94%



- Molecule 2: Beta-2-microglobulin

Chain T:  96%



- Molecule 2: Beta-2-microglobulin

Chain V:  95%



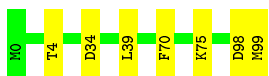
- Molecule 2: Beta-2-microglobulin

Chain X:  94%



- Molecule 2: Beta-2-microglobulin

Chain Z:  93% 7%




- Molecule 2: Beta-2-microglobulin

Chain b:  94% 6%



- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain m:  89% 11%



- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain i:  100%


There are no outlier residues recorded for this chain.

- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain f:  89% 11%




- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain h:  89% 11%





- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain e: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain n: 89% 11%



- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain p: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain o: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain c: 89% 11%



- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain g: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain q: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: NY-ESO1 DOUBLE MUTANT (1Y, 9V)

Chain j: 89% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.57Å 313.36Å 314.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.80 – 3.09 53.88 – 3.09	Depositor EDS
% Data completeness (in resolution range)	98.8 (53.80-3.09) 99.1 (53.88-3.09)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.171 , 0.201 0.185 , 0.207	Depositor DCC
$R_{free}$ test set	9171 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.6	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
Reported twinning fraction	0.671 for H, K, L 0.329 for -H, L, K	Depositor
Outliers	1 of 182843 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	44627	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL

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	0.49	0/2320	0.64	0/3149
1	C	0.58	1/2320 (0.0%)	0.65	0/3149
1	E	0.49	0/2320	0.64	0/3149
1	G	0.52	1/2320 (0.0%)	0.61	0/3149
1	I	0.51	0/2320	0.61	0/3149
1	K	0.49	0/2320	0.63	0/3149
1	M	0.48	0/2320	0.62	0/3149
1	O	0.46	0/2320	0.60	0/3149
1	Q	0.52	0/2320	0.64	0/3149
1	S	0.47	0/2320	0.61	0/3149
1	U	0.47	0/2320	0.58	0/3149
1	W	0.52	1/2320 (0.0%)	0.61	0/3149
1	Y	0.47	0/2320	0.60	0/3149
1	a	0.44	0/2320	0.59	0/3149
2	B	0.47	0/860	0.59	0/1162
2	D	0.53	0/860	0.63	0/1162
2	F	0.50	0/860	0.59	0/1162
2	H	0.48	0/860	0.60	0/1162
2	J	0.50	0/860	0.57	0/1162
2	L	0.50	0/860	0.60	0/1162
2	N	0.50	0/860	0.61	0/1162
2	P	0.46	0/860	0.58	0/1162
2	R	0.47	0/860	0.56	0/1162
2	T	0.56	1/860 (0.1%)	0.63	0/1162
2	V	0.49	0/860	0.58	0/1162
2	X	0.48	0/860	0.59	0/1162
2	Z	0.45	0/860	0.58	0/1162
2	b	0.46	0/860	0.56	0/1162
3	c	0.51	0/84	0.55	0/113
3	e	0.43	0/84	0.58	0/113
3	f	0.45	0/84	0.50	0/113
3	g	0.46	0/84	0.51	0/113

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	h	0.48	0/84	0.58	0/113
3	i	0.46	0/84	0.62	0/113
3	j	0.46	0/84	0.53	0/113
3	k	0.51	0/84	0.59	0/113
3	l	0.42	0/84	0.59	0/113
3	m	0.46	0/84	0.69	0/113
3	n	0.45	0/84	0.68	0/113
3	o	0.45	0/84	0.48	0/113
3	p	0.48	0/84	0.57	0/113
3	q	0.43	0/84	0.54	0/113
All	All	0.49	4/45696 (0.0%)	0.61	0/61936

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	49	VAL	CB-CG1	-5.63	1.41	1.52
1	C	28	VAL	CB-CG1	-5.37	1.41	1.52
1	G	90	ALA	CA-CB	-5.34	1.41	1.52
1	W	28	VAL	CA-CB	-5.01	1.44	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	274/276 (99%)	263 (96%)	10 (4%)	1 (0%)	34	69
1	C	274/276 (99%)	262 (96%)	12 (4%)	0	100	100
1	E	274/276 (99%)	262 (96%)	12 (4%)	0	100	100
1	G	274/276 (99%)	264 (96%)	9 (3%)	1 (0%)	34	69
1	I	274/276 (99%)	268 (98%)	6 (2%)	0	100	100
1	K	274/276 (99%)	264 (96%)	10 (4%)	0	100	100
1	M	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
1	O	274/276 (99%)	265 (97%)	9 (3%)	0	100	100
1	Q	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
1	S	274/276 (99%)	264 (96%)	10 (4%)	0	100	100
1	U	274/276 (99%)	265 (97%)	9 (3%)	0	100	100
1	W	274/276 (99%)	266 (97%)	8 (3%)	0	100	100
1	Y	274/276 (99%)	258 (94%)	16 (6%)	0	100	100
1	a	274/276 (99%)	260 (95%)	14 (5%)	0	100	100
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	D	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	F	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	H	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	J	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	L	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	N	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	P	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	R	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
2	T	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	V	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	X	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	Z	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	b	98/100 (98%)	94 (96%)	3 (3%)	1 (1%)	15	49
3	c	7/9 (78%)	7 (100%)	0	0	100	100
3	e	7/9 (78%)	7 (100%)	0	0	100	100
3	f	7/9 (78%)	7 (100%)	0	0	100	100
3	g	7/9 (78%)	7 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	h	7/9 (78%)	7 (100%)	0	0	100	100
3	i	7/9 (78%)	7 (100%)	0	0	100	100
3	j	7/9 (78%)	7 (100%)	0	0	100	100
3	k	7/9 (78%)	7 (100%)	0	0	100	100
3	l	7/9 (78%)	7 (100%)	0	0	100	100
3	m	7/9 (78%)	7 (100%)	0	0	100	100
3	n	7/9 (78%)	7 (100%)	0	0	100	100
3	o	7/9 (78%)	7 (100%)	0	0	100	100
3	p	7/9 (78%)	7 (100%)	0	0	100	100
3	q	7/9 (78%)	7 (100%)	0	0	100	100
All	All	5306/5390 (98%)	5121 (96%)	182 (3%)	3 (0%)	51	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	G	267	PRO
2	b	35	ILE

### 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	232/232 (100%)	229 (99%)	3 (1%)	69	87
1	C	232/232 (100%)	218 (94%)	14 (6%)	19	49
1	E	232/232 (100%)	217 (94%)	15 (6%)	17	47
1	G	232/232 (100%)	224 (97%)	8 (3%)	37	69
1	I	232/232 (100%)	220 (95%)	12 (5%)	23	55
1	K	232/232 (100%)	215 (93%)	17 (7%)	14	43
1	M	232/232 (100%)	223 (96%)	9 (4%)	32	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	232/232 (100%)	221 (95%)	11 (5%)	26	59
1	Q	232/232 (100%)	228 (98%)	4 (2%)	60	83
1	S	232/232 (100%)	219 (94%)	13 (6%)	21	52
1	U	232/232 (100%)	219 (94%)	13 (6%)	21	52
1	W	232/232 (100%)	221 (95%)	11 (5%)	26	59
1	Y	232/232 (100%)	218 (94%)	14 (6%)	19	49
1	a	232/232 (100%)	220 (95%)	12 (5%)	23	55
2	B	95/95 (100%)	89 (94%)	6 (6%)	18	48
2	D	95/95 (100%)	90 (95%)	5 (5%)	22	54
2	F	95/95 (100%)	90 (95%)	5 (5%)	22	54
2	H	95/95 (100%)	89 (94%)	6 (6%)	18	48
2	J	95/95 (100%)	92 (97%)	3 (3%)	39	69
2	L	95/95 (100%)	91 (96%)	4 (4%)	30	62
2	N	95/95 (100%)	89 (94%)	6 (6%)	18	48
2	P	95/95 (100%)	92 (97%)	3 (3%)	39	69
2	R	95/95 (100%)	89 (94%)	6 (6%)	18	48
2	T	95/95 (100%)	92 (97%)	3 (3%)	39	69
2	V	95/95 (100%)	90 (95%)	5 (5%)	22	54
2	X	95/95 (100%)	89 (94%)	6 (6%)	18	48
2	Z	95/95 (100%)	88 (93%)	7 (7%)	13	42
2	b	95/95 (100%)	90 (95%)	5 (5%)	22	54
3	c	9/9 (100%)	8 (89%)	1 (11%)	6	24
3	e	9/9 (100%)	9 (100%)	0	100	100
3	f	9/9 (100%)	8 (89%)	1 (11%)	6	24
3	g	9/9 (100%)	9 (100%)	0	100	100
3	h	9/9 (100%)	8 (89%)	1 (11%)	6	24
3	i	9/9 (100%)	9 (100%)	0	100	100
3	j	9/9 (100%)	8 (89%)	1 (11%)	6	24
3	k	9/9 (100%)	9 (100%)	0	100	100
3	l	9/9 (100%)	9 (100%)	0	100	100
3	m	9/9 (100%)	8 (89%)	1 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	n	9/9 (100%)	8 (89%)	1 (11%)	6	24
3	o	9/9 (100%)	9 (100%)	0	100	100
3	p	9/9 (100%)	9 (100%)	0	100	100
3	q	9/9 (100%)	9 (100%)	0	100	100
All	All	4704/4704 (100%)	4472 (95%)	232 (5%)	25	57

5 of 232 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	113	TYR
2	P	70	PHE
1	a	35	ARG
1	M	268	LYS
1	O	35	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	155	GLN
1	S	32	GLN
1	Y	32	GLN
1	I	155	GLN
1	a	32	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

Of 50 ligands modelled in this entry, 30 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	O	302	-	5,5,5	0.41	0	5,5,5	0.29	0
5	GOL	K	302	-	5,5,5	0.38	0	5,5,5	0.63	0
5	GOL	l	101	-	5,5,5	0.25	0	5,5,5	0.38	0
5	GOL	C	303	-	5,5,5	0.37	0	5,5,5	0.23	0
5	GOL	a	302	-	5,5,5	0.49	0	5,5,5	0.50	0
5	GOL	O	303	-	5,5,5	0.40	0	5,5,5	0.28	0
5	GOL	S	302	-	5,5,5	0.41	0	5,5,5	0.55	0
5	GOL	i	101	-	5,5,5	0.51	0	5,5,5	0.48	0
5	GOL	f	101	-	5,5,5	0.56	0	5,5,5	0.88	0
5	GOL	e	101	-	5,5,5	0.51	0	5,5,5	0.38	0
5	GOL	Y	302	-	5,5,5	0.50	0	5,5,5	0.27	0
5	GOL	g	101	-	5,5,5	0.51	0	5,5,5	0.27	0
5	GOL	Q	303	-	5,5,5	0.60	0	5,5,5	0.47	0
5	GOL	E	302	-	5,5,5	0.54	0	5,5,5	0.80	0
5	GOL	c	101	-	5,5,5	0.41	0	5,5,5	0.44	0
5	GOL	h	101	-	5,5,5	0.51	0	5,5,5	0.53	0
5	GOL	o	101	-	5,5,5	0.47	0	5,5,5	0.29	0
5	GOL	C	302	-	5,5,5	0.53	0	5,5,5	0.37	0
5	GOL	A	302	-	5,5,5	0.61	0	5,5,5	0.76	0
5	GOL	q	101	-	5,5,5	0.43	0	5,5,5	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	O	302	-	-	2/4/4/4	-
5	GOL	K	302	-	-	0/4/4/4	-
5	GOL	l	101	-	-	4/4/4/4	-
5	GOL	C	303	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	a	302	-	-	2/4/4/4	-
5	GOL	O	303	-	-	2/4/4/4	-
5	GOL	S	302	-	-	0/4/4/4	-
5	GOL	i	101	-	-	2/4/4/4	-
5	GOL	f	101	-	-	2/4/4/4	-
5	GOL	e	101	-	-	2/4/4/4	-
5	GOL	Y	302	-	-	2/4/4/4	-
5	GOL	g	101	-	-	2/4/4/4	-
5	GOL	Q	303	-	-	2/4/4/4	-
5	GOL	E	302	-	-	2/4/4/4	-
5	GOL	c	101	-	-	2/4/4/4	-
5	GOL	h	101	-	-	3/4/4/4	-
5	GOL	o	101	-	-	0/4/4/4	-
5	GOL	C	302	-	-	2/4/4/4	-
5	GOL	A	302	-	-	2/4/4/4	-
5	GOL	q	101	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	303	GOL	O1-C1-C2-C3
5	f	101	GOL	O1-C1-C2-C3
5	e	101	GOL	C1-C2-C3-O3
5	Y	302	GOL	O1-C1-C2-C3
5	A	302	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	276/276 (100%)	0.09	2 (0%) 87 75	38, 51, 71, 87	2 (0%)
1	C	276/276 (100%)	0.02	1 (0%) 92 84	34, 47, 68, 82	2 (0%)
1	E	276/276 (100%)	0.05	1 (0%) 92 84	34, 49, 66, 81	1 (0%)
1	G	276/276 (100%)	-0.06	0 100 100	36, 50, 69, 80	1 (0%)
1	I	276/276 (100%)	-0.00	1 (0%) 92 84	33, 49, 71, 83	1 (0%)
1	K	276/276 (100%)	0.04	1 (0%) 92 84	33, 51, 65, 72	2 (0%)
1	M	276/276 (100%)	0.01	0 100 100	40, 53, 70, 83	1 (0%)
1	O	276/276 (100%)	0.10	1 (0%) 92 84	39, 54, 69, 78	2 (0%)
1	Q	276/276 (100%)	0.03	1 (0%) 92 84	35, 48, 63, 80	1 (0%)
1	S	276/276 (100%)	0.13	1 (0%) 92 84	41, 58, 74, 82	2 (0%)
1	U	276/276 (100%)	0.02	0 100 100	41, 56, 72, 102	2 (0%)
1	W	276/276 (100%)	0.27	4 (1%) 75 56	41, 60, 74, 87	2 (0%)
1	Y	276/276 (100%)	0.17	2 (0%) 87 75	39, 58, 73, 78	2 (0%)
1	a	276/276 (100%)	0.33	2 (0%) 87 75	45, 63, 78, 98	2 (0%)
2	B	100/100 (100%)	0.04	0 100 100	38, 53, 71, 93	0
2	D	100/100 (100%)	0.06	0 100 100	34, 50, 72, 89	0
2	F	100/100 (100%)	0.07	0 100 100	34, 52, 69, 83	0
2	H	100/100 (100%)	0.09	1 (1%) 82 67	39, 57, 73, 113	0
2	J	100/100 (100%)	0.07	1 (1%) 82 67	38, 53, 70, 85	0
2	L	100/100 (100%)	0.07	0 100 100	38, 53, 70, 86	0
2	N	100/100 (100%)	-0.02	1 (1%) 82 67	42, 55, 73, 155	0
2	P	100/100 (100%)	-0.02	0 100 100	41, 56, 79, 116	0
2	R	100/100 (100%)	-0.03	0 100 100	37, 52, 69, 80	0
2	T	100/100 (100%)	0.07	0 100 100	43, 60, 79, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	V	100/100 (100%)	0.05	0 100 100	42, 57, 71, 84	0
2	X	100/100 (100%)	0.00	0 100 100	45, 57, 73, 84	0
2	Z	100/100 (100%)	0.06	0 100 100	44, 58, 75, 83	0
2	b	100/100 (100%)	0.08	0 100 100	48, 61, 75, 85	0
3	c	9/9 (100%)	-0.09	0 100 100	58, 58, 60, 62	0
3	e	9/9 (100%)	-0.03	0 100 100	52, 55, 56, 57	0
3	f	9/9 (100%)	0.13	0 100 100	42, 44, 50, 50	0
3	g	9/9 (100%)	0.18	0 100 100	50, 52, 56, 56	0
3	h	9/9 (100%)	-0.00	0 100 100	47, 49, 53, 54	0
3	i	9/9 (100%)	-0.08	0 100 100	40, 41, 43, 45	0
3	j	9/9 (100%)	0.21	0 100 100	56, 61, 66, 66	0
3	k	9/9 (100%)	-0.15	0 100 100	39, 43, 48, 49	0
3	l	9/9 (100%)	0.17	0 100 100	39, 42, 48, 48	0
3	m	9/9 (100%)	-0.06	0 100 100	42, 47, 49, 51	0
3	n	9/9 (100%)	0.11	0 100 100	53, 55, 58, 58	0
3	o	9/9 (100%)	0.32	0 100 100	55, 61, 64, 64	0
3	p	9/9 (100%)	0.01	0 100 100	38, 42, 45, 46	0
3	q	9/9 (100%)	0.34	0 100 100	67, 71, 73, 73	0
All	All	5390/5390 (100%)	0.07	20 (0%) 92 84	33, 54, 73, 155	23 (0%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	88	SER	3.4
1	Q	225	THR	3.3
1	W	1	GLY	3.2
1	O	88	SER	3.2
1	I	276	PRO	3.0

## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CL	J	101	1/1	0.72	0.32	67,67,67,67	0
4	CL	Z	101	1/1	0.74	0.14	59,59,59,59	0
5	GOL	S	302	6/6	0.79	0.23	53,55,55,55	0
5	GOL	O	303	6/6	0.80	0.34	79,80,81,82	0
4	CL	T	101	1/1	0.80	0.15	63,63,63,63	0
4	CL	a	301	1/1	0.81	0.13	67,67,67,67	0
5	GOL	C	303	6/6	0.81	0.29	55,57,58,58	0
4	CL	V	101	1/1	0.83	0.15	69,69,69,69	0
4	CL	H	101	1/1	0.84	0.12	83,83,83,83	0
4	CL	D	101	1/1	0.84	0.13	76,76,76,76	0
5	GOL	a	302	6/6	0.84	0.22	57,58,59,59	0
5	GOL	Y	302	6/6	0.86	0.20	58,59,59,60	0
4	CL	L	101	1/1	0.87	0.12	74,74,74,74	0
4	CL	Y	301	1/1	0.87	0.23	60,60,60,60	0
5	GOL	K	302	6/6	0.87	0.19	50,52,54,54	0
4	CL	K	301	1/1	0.87	0.27	69,69,69,69	0
4	CL	I	301	1/1	0.88	0.23	57,57,57,57	0
4	CL	Q	301	1/1	0.88	0.32	46,46,46,46	0
4	CL	O	301	1/1	0.89	0.21	59,59,59,59	0
4	CL	B	101	1/1	0.89	0.26	64,64,64,64	0
4	CL	b	101	1/1	0.90	0.09	73,73,73,73	0
5	GOL	h	101	6/6	0.90	0.28	50,51,52,52	0
4	CL	C	301	1/1	0.90	0.22	60,60,60,60	0
4	CL	N	102	1/1	0.91	0.19	50,50,50,50	0
5	GOL	c	101	6/6	0.91	0.30	60,61,62,63	0
5	GOL	l	101	6/6	0.91	0.28	35,38,39,41	0
5	GOL	i	101	6/6	0.91	0.30	68,68,69,69	0
4	CL	P	101	1/1	0.93	0.11	70,70,70,70	0
5	GOL	g	101	6/6	0.93	0.34	56,56,57,57	0
5	GOL	o	101	6/6	0.93	0.34	58,58,58,58	0
4	CL	S	301	1/1	0.94	0.13	52,52,52,52	0
5	GOL	q	101	6/6	0.94	0.29	61,61,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	e	101	6/6	0.94	0.26	51,53,54,55	0
5	GOL	O	302	6/6	0.94	0.38	53,54,55,56	0
4	CL	G	301	1/1	0.95	0.20	54,54,54,54	0
4	CL	R	101	1/1	0.95	0.15	72,72,72,72	0
5	GOL	f	101	6/6	0.95	0.22	35,37,37,38	0
4	CL	F	101	1/1	0.95	0.10	68,68,68,68	0
5	GOL	E	302	6/6	0.95	0.27	38,39,43,45	0
4	CL	E	301	1/1	0.96	0.13	44,44,44,44	0
5	GOL	A	302	6/6	0.96	0.30	25,28,28,29	0
4	CL	N	101	1/1	0.96	0.09	65,65,65,65	0
4	CL	A	301	1/1	0.96	0.21	66,66,66,66	0
4	CL	U	301	1/1	0.97	0.23	64,64,64,64	0
5	GOL	C	302	6/6	0.97	0.24	37,39,40,41	0
4	CL	I	303	1/1	0.97	0.23	50,50,50,50	0
4	CL	Q	302	1/1	0.97	0.14	57,57,57,57	0
4	CL	I	302	1/1	0.98	0.25	52,52,52,52	0
4	CL	W	301	1/1	0.98	0.25	59,59,59,59	0
5	GOL	Q	303	6/6	0.98	0.21	36,37,38,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.