wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2023 – 04:32 PM EDT

PDB ID	:	3E3Q
Title	:	Structure of the 3alpham13 high-affinity mutant of the 2C TCR in complex with Ld/QL9
Authors	:	Colf, L.A.; Garcia, K.C.
Deposited on	:	2008-08-07
Resolution	:	2.95 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:

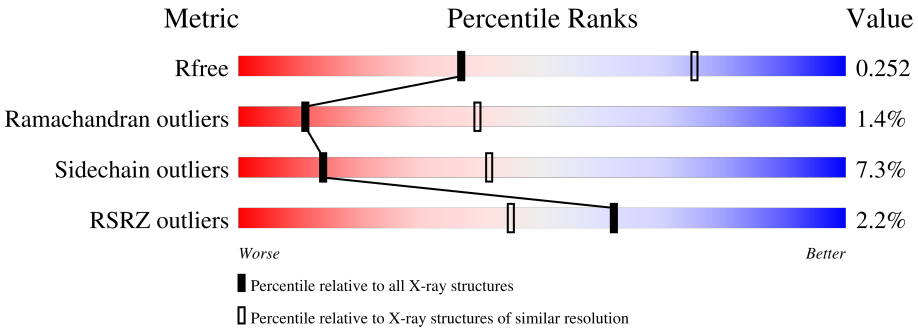
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.95 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	3104 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	175	3% 91% 6% ·
1	B	175	3% 92% 6% ·
1	H	175	5% 93% 6% ·
1	L	175	3% 93% 6% ·
1	P	175	3% 92% 7% ·
1	U	175	4% 92% 7% ·

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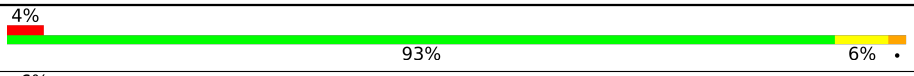
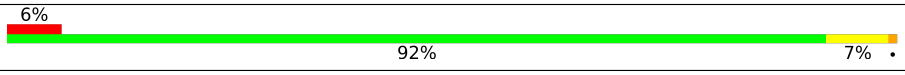
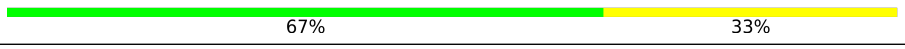
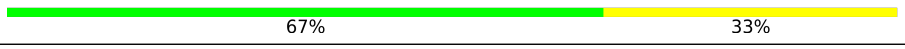
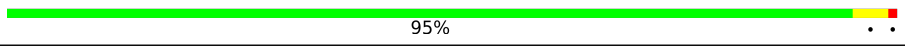
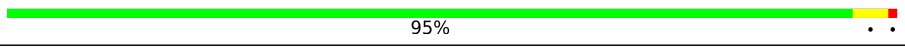
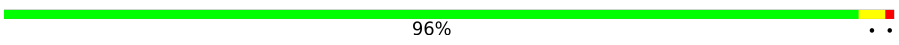
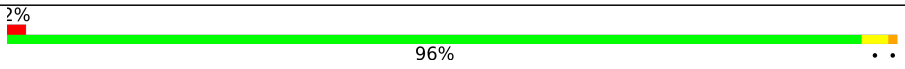
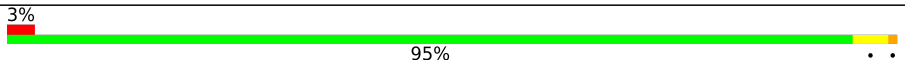
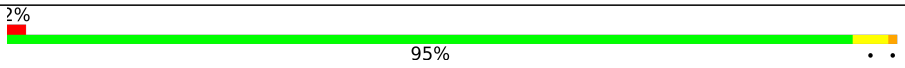
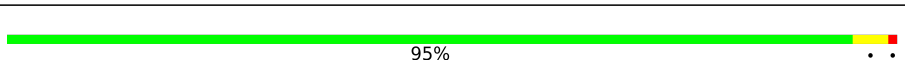
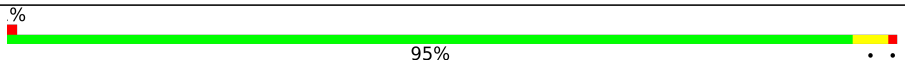
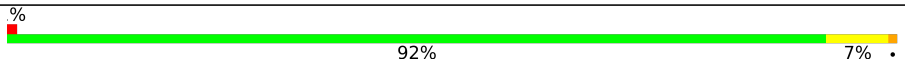
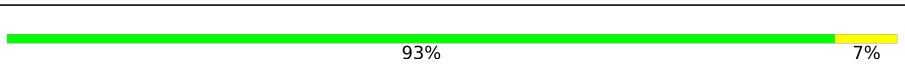
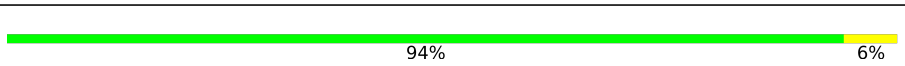
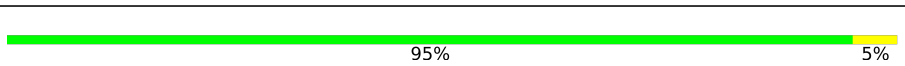
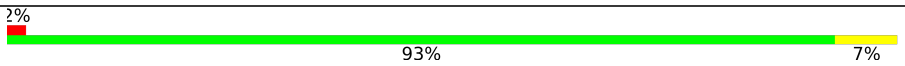
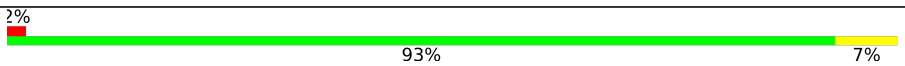
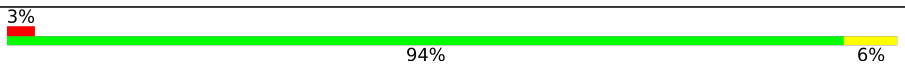
Mol	Chain	Length	Quality of chain
1	Y	175	
1	c	175	
2	G	9	
2	K	9	
2	O	9	
2	Q	9	
2	T	9	
2	X	9	
2	b	9	
2	f	9	
3	C	109	
3	D	109	
3	I	109	
3	M	109	
3	R	109	
3	V	109	
3	Z	109	
3	d	109	
4	E	111	
4	F	111	
4	J	111	
4	N	111	
4	S	111	
4	W	111	
4	a	111	

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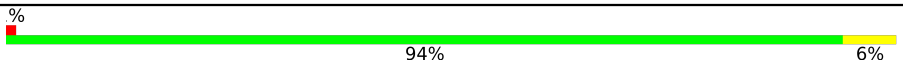
Mol	Chain	Length	Quality of chain
4	e	111	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 25808 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 H-2 class I histocompatibility antigen, L-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			
1	B	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			
1	c	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			
1	H	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			
1	L	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			
1	P	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			
1	U	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			
1	Y	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	TYR	PHE	engineered mutation	UNP P01897
A	12	THR	VAL	engineered mutation	UNP P01897
A	15	ARG	PRO	engineered mutation	UNP P01897
A	23	THR	ILE	engineered mutation	UNP P01897
A	30	ASP	ASN	engineered mutation	UNP P01897
A	49	VAL	ALA	engineered mutation	UNP P01897
A	66	VAL	ILE	engineered mutation	UNP P01897
A	97	ARG	TRP	engineered mutation	UNP P01897
A	131	ARG	LYS	engineered mutation	UNP P01897
B	8	TYR	PHE	engineered mutation	UNP P01897
B	12	THR	VAL	engineered mutation	UNP P01897
B	15	ARG	PRO	engineered mutation	UNP P01897
B	23	THR	ILE	engineered mutation	UNP P01897

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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	ASP	ASN	engineered mutation	UNP P01897
B	49	VAL	ALA	engineered mutation	UNP P01897
B	66	VAL	ILE	engineered mutation	UNP P01897
B	97	ARG	TRP	engineered mutation	UNP P01897
B	131	ARG	LYS	engineered mutation	UNP P01897
c	8	TYR	PHE	engineered mutation	UNP P01897
c	12	THR	VAL	engineered mutation	UNP P01897
c	15	ARG	PRO	engineered mutation	UNP P01897
c	23	THR	ILE	engineered mutation	UNP P01897
c	30	ASP	ASN	engineered mutation	UNP P01897
c	49	VAL	ALA	engineered mutation	UNP P01897
c	66	VAL	ILE	engineered mutation	UNP P01897
c	97	ARG	TRP	engineered mutation	UNP P01897
c	131	ARG	LYS	engineered mutation	UNP P01897
H	8	TYR	PHE	engineered mutation	UNP P01897
H	12	THR	VAL	engineered mutation	UNP P01897
H	15	ARG	PRO	engineered mutation	UNP P01897
H	23	THR	ILE	engineered mutation	UNP P01897
H	30	ASP	ASN	engineered mutation	UNP P01897
H	49	VAL	ALA	engineered mutation	UNP P01897
H	66	VAL	ILE	engineered mutation	UNP P01897
H	97	ARG	TRP	engineered mutation	UNP P01897
H	131	ARG	LYS	engineered mutation	UNP P01897
L	8	TYR	PHE	engineered mutation	UNP P01897
L	12	THR	VAL	engineered mutation	UNP P01897
L	15	ARG	PRO	engineered mutation	UNP P01897
L	23	THR	ILE	engineered mutation	UNP P01897
L	30	ASP	ASN	engineered mutation	UNP P01897
L	49	VAL	ALA	engineered mutation	UNP P01897
L	66	VAL	ILE	engineered mutation	UNP P01897
L	97	ARG	TRP	engineered mutation	UNP P01897
L	131	ARG	LYS	engineered mutation	UNP P01897
P	8	TYR	PHE	engineered mutation	UNP P01897
P	12	THR	VAL	engineered mutation	UNP P01897
P	15	ARG	PRO	engineered mutation	UNP P01897
P	23	THR	ILE	engineered mutation	UNP P01897
P	30	ASP	ASN	engineered mutation	UNP P01897
P	49	VAL	ALA	engineered mutation	UNP P01897
P	66	VAL	ILE	engineered mutation	UNP P01897
P	97	ARG	TRP	engineered mutation	UNP P01897
P	131	ARG	LYS	engineered mutation	UNP P01897
U	8	TYR	PHE	engineered mutation	UNP P01897

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Chain	Residue	Modelled	Actual	Comment	Reference
U	12	THR	VAL	engineered mutation	UNP P01897
U	15	ARG	PRO	engineered mutation	UNP P01897
U	23	THR	ILE	engineered mutation	UNP P01897
U	30	ASP	ASN	engineered mutation	UNP P01897
U	49	VAL	ALA	engineered mutation	UNP P01897
U	66	VAL	ILE	engineered mutation	UNP P01897
U	97	ARG	TRP	engineered mutation	UNP P01897
U	131	ARG	LYS	engineered mutation	UNP P01897
Y	8	TYR	PHE	engineered mutation	UNP P01897
Y	12	THR	VAL	engineered mutation	UNP P01897
Y	15	ARG	PRO	engineered mutation	UNP P01897
Y	23	THR	ILE	engineered mutation	UNP P01897
Y	30	ASP	ASN	engineered mutation	UNP P01897
Y	49	VAL	ALA	engineered mutation	UNP P01897
Y	66	VAL	ILE	engineered mutation	UNP P01897
Y	97	ARG	TRP	engineered mutation	UNP P01897
Y	131	ARG	LYS	engineered mutation	UNP P01897

- Molecule 2 is a protein called QL9 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	9	Total	C	N	O	0	0	0
			76	52	10	14			
2	G	9	Total	C	N	O	0	0	0
			76	52	10	14			
2	f	9	Total	C	N	O	0	0	0
			76	52	10	14			
2	K	9	Total	C	N	O	0	0	0
			76	52	10	14			
2	O	9	Total	C	N	O	0	0	0
			76	52	10	14			
2	T	9	Total	C	N	O	0	0	0
			76	52	10	14			
2	X	9	Total	C	N	O	0	0	0
			76	52	10	14			
2	b	9	Total	C	N	O	0	0	0
			76	52	10	14			

- Molecule 3 is a protein called T-cell receptor alpha chain V region PHDS58.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			
3	C	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			
3	d	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			
3	I	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			
3	M	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			
3	R	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			
3	V	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			
3	Z	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	43	PRO	LEU	engineered mutation	UNP P01738
D	82	ARG	TRP	engineered mutation	UNP P01738
D	99	ASP	GLY	engineered mutation	UNP P01738
D	100	PRO	PHE	engineered mutation	UNP P01738
D	101	PRO	ALA	engineered mutation	UNP P01738
D	102	PRO	SER	engineered mutation	UNP P01738
D	103	LEU	ALA	engineered mutation	UNP P01738
C	43	PRO	LEU	engineered mutation	UNP P01738
C	82	ARG	TRP	engineered mutation	UNP P01738
C	99	ASP	GLY	engineered mutation	UNP P01738
C	100	PRO	PHE	engineered mutation	UNP P01738
C	101	PRO	ALA	engineered mutation	UNP P01738
C	102	PRO	SER	engineered mutation	UNP P01738
C	103	LEU	ALA	engineered mutation	UNP P01738
d	43	PRO	LEU	engineered mutation	UNP P01738
d	82	ARG	TRP	engineered mutation	UNP P01738
d	99	ASP	GLY	engineered mutation	UNP P01738
d	100	PRO	PHE	engineered mutation	UNP P01738
d	101	PRO	ALA	engineered mutation	UNP P01738
d	102	PRO	SER	engineered mutation	UNP P01738
d	103	LEU	ALA	engineered mutation	UNP P01738
I	43	PRO	LEU	engineered mutation	UNP P01738
I	82	ARG	TRP	engineered mutation	UNP P01738
I	99	ASP	GLY	engineered mutation	UNP P01738

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Chain	Residue	Modelled	Actual	Comment	Reference
I	100	PRO	PHE	engineered mutation	UNP P01738
I	101	PRO	ALA	engineered mutation	UNP P01738
I	102	PRO	SER	engineered mutation	UNP P01738
I	103	LEU	ALA	engineered mutation	UNP P01738
M	43	PRO	LEU	engineered mutation	UNP P01738
M	82	ARG	TRP	engineered mutation	UNP P01738
M	99	ASP	GLY	engineered mutation	UNP P01738
M	100	PRO	PHE	engineered mutation	UNP P01738
M	101	PRO	ALA	engineered mutation	UNP P01738
M	102	PRO	SER	engineered mutation	UNP P01738
M	103	LEU	ALA	engineered mutation	UNP P01738
R	43	PRO	LEU	engineered mutation	UNP P01738
R	82	ARG	TRP	engineered mutation	UNP P01738
R	99	ASP	GLY	engineered mutation	UNP P01738
R	100	PRO	PHE	engineered mutation	UNP P01738
R	101	PRO	ALA	engineered mutation	UNP P01738
R	102	PRO	SER	engineered mutation	UNP P01738
R	103	LEU	ALA	engineered mutation	UNP P01738
V	43	PRO	LEU	engineered mutation	UNP P01738
V	82	ARG	TRP	engineered mutation	UNP P01738
V	99	ASP	GLY	engineered mutation	UNP P01738
V	100	PRO	PHE	engineered mutation	UNP P01738
V	101	PRO	ALA	engineered mutation	UNP P01738
V	102	PRO	SER	engineered mutation	UNP P01738
V	103	LEU	ALA	engineered mutation	UNP P01738
Z	43	PRO	LEU	engineered mutation	UNP P01738
Z	82	ARG	TRP	engineered mutation	UNP P01738
Z	99	ASP	GLY	engineered mutation	UNP P01738
Z	100	PRO	PHE	engineered mutation	UNP P01738
Z	101	PRO	ALA	engineered mutation	UNP P01738
Z	102	PRO	SER	engineered mutation	UNP P01738
Z	103	LEU	ALA	engineered mutation	UNP P01738

- Molecule 4 is a protein called TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	111	Total	C	N	O	S	0	0	0
			847	523	147	174	3			
4	F	111	Total	C	N	O	S	0	0	0
			847	523	147	174	3			
4	e	111	Total	C	N	O	S	0	0	0
			847	523	147	174	3			

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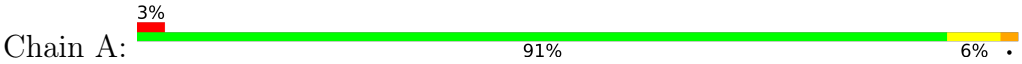
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	111	Total	C	N	O	S	0	0	0
			847	523	147	174	3			
4	N	111	Total	C	N	O	S	0	0	0
			847	523	147	174	3			
4	S	111	Total	C	N	O	S	0	0	0
			847	523	147	174	3			
4	W	111	Total	C	N	O	S	0	0	0
			847	523	147	174	3			
4	a	111	Total	C	N	O	S	0	0	0
			847	523	147	174	3			

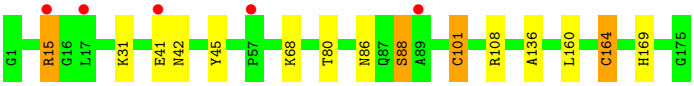
3 Residue-property plots (i)

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: H-2 class I histocompatibility antigen, L-D alpha chain

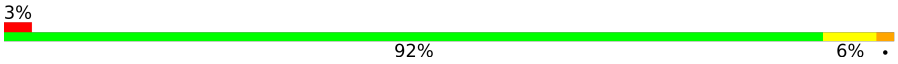
Chain A:

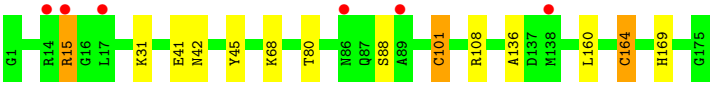




• Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain

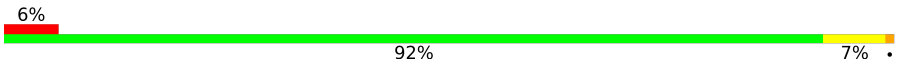
Chain B:

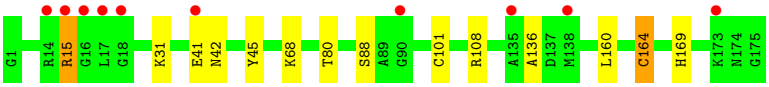




• Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain

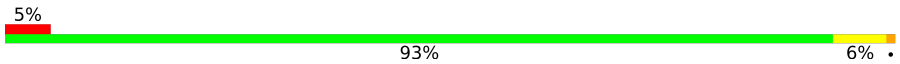
Chain c:

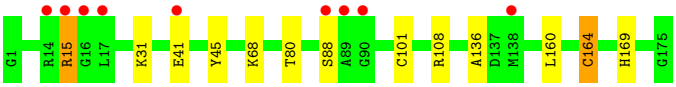




• Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain

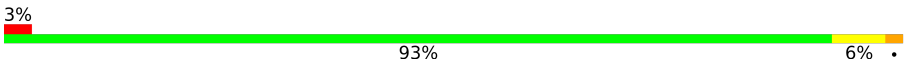
Chain H:





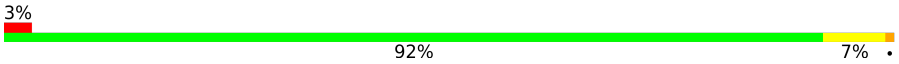
• Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain

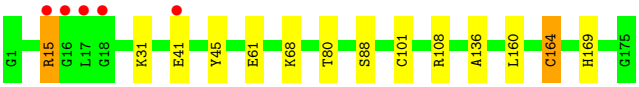
Chain L:



• Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain

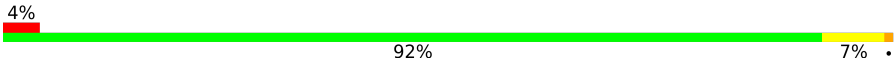
Chain P:

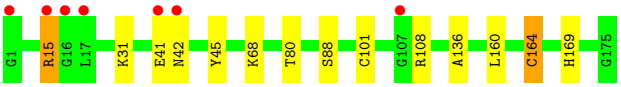




• Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain

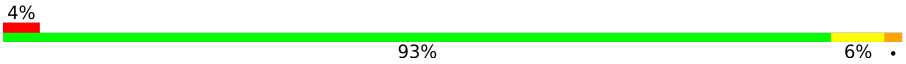
Chain U:

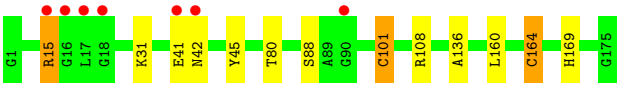




• Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain

Chain Y:





• Molecule 2: QL9 peptide

Chain Q:

• Molecule 2: QL9 peptide

Chain G:

• Molecule 2: QL9 peptide

Chain f:

• Molecule 2: QL9 peptide

Chain K:

• Molecule 2: QL9 peptide

Chain O:

• Molecule 2: QL9 peptide

Chain T:

• Molecule 2: QL9 peptide

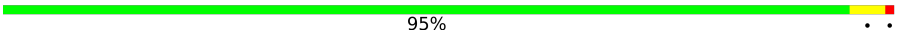
Chain X:

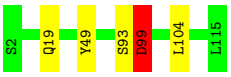
• Molecule 2: QL9 peptide

Chain b:

• Molecule 3: T-cell receptor alpha chain V region PHDS58

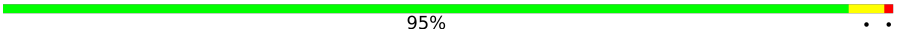
Chain D:





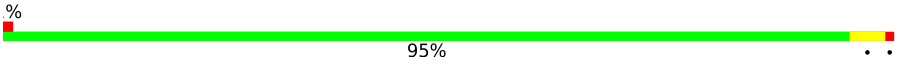
• Molecule 3: T-cell receptor alpha chain V region PHDS58

Chain C:



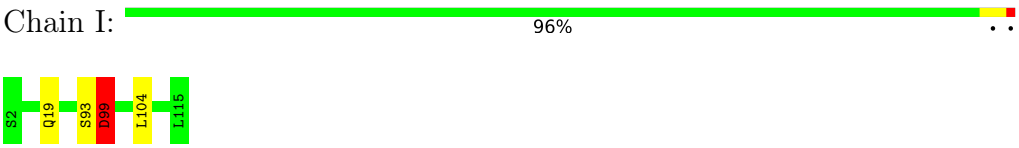
• Molecule 3: T-cell receptor alpha chain V region PHDS58

Chain d:



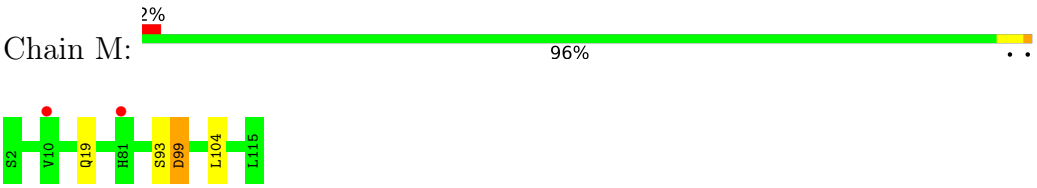
• Molecule 3: T-cell receptor alpha chain V region PHDS58

Chain I:



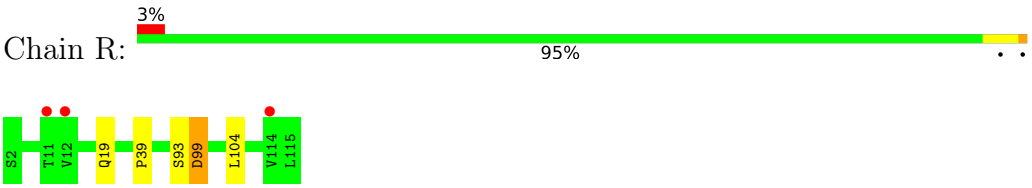
• Molecule 3: T-cell receptor alpha chain V region PHDS58

Chain M:



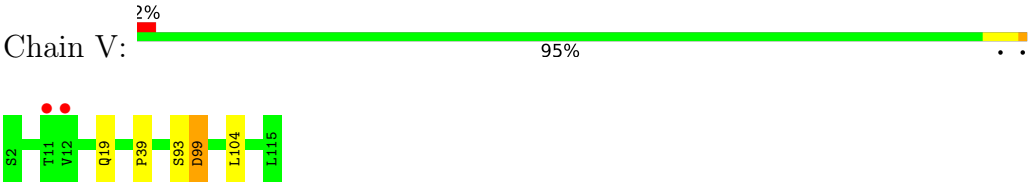
• Molecule 3: T-cell receptor alpha chain V region PHDS58

Chain R:



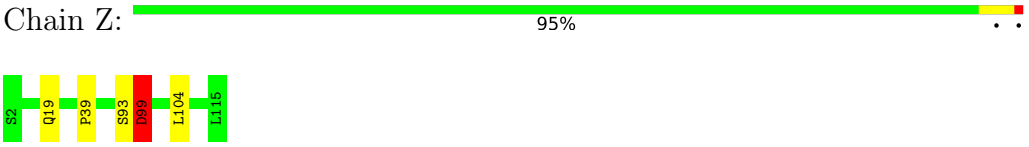
• Molecule 3: T-cell receptor alpha chain V region PHDS58

Chain V:



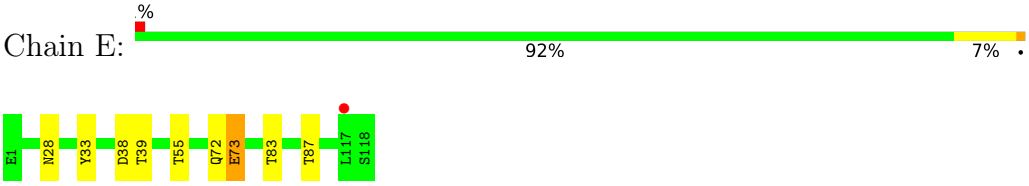
• Molecule 3: T-cell receptor alpha chain V region PHDS58

Chain Z:



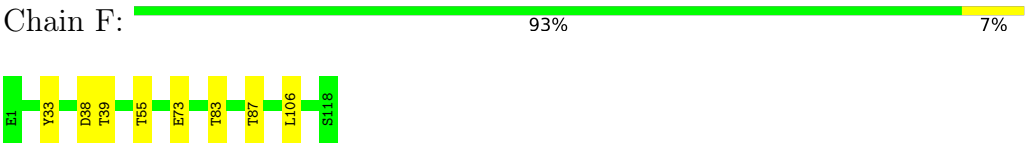
• Molecule 4: TCR beta chain

Chain E:



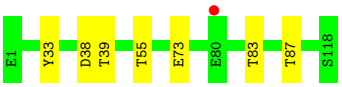
• Molecule 4: TCR beta chain

Chain F:



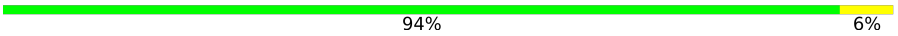
• Molecule 4: TCR beta chain

Chain e:



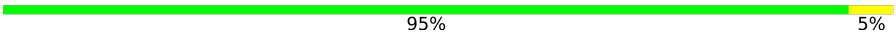
• Molecule 4: TCR beta chain

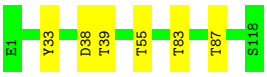
Chain J:



• Molecule 4: TCR beta chain

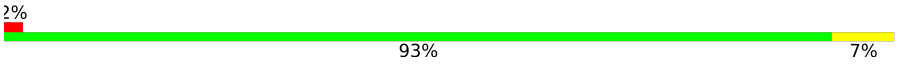
Chain N:

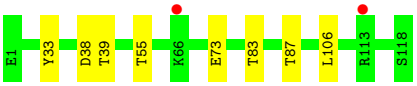




• Molecule 4: TCR beta chain

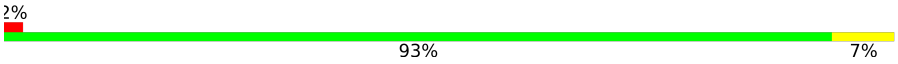
Chain S:

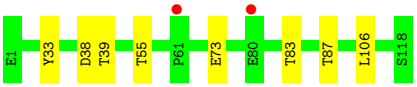




• Molecule 4: TCR beta chain

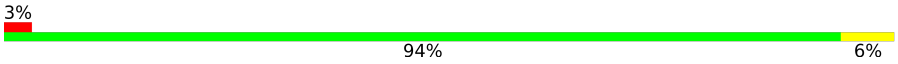
Chain W:

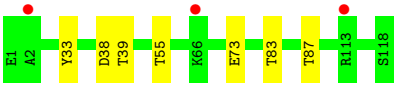




• Molecule 4: TCR beta chain

Chain a:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	158.47Å 160.46Å 357.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.52 – 2.95 41.51 – 2.93	Depositor EDS
% Data completeness (in resolution range)	97.4 (41.52-2.95) 96.8 (41.51-2.93)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.95Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.275 0.251 , 0.252	Depositor DCC
R_{free} test set	4707 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.2	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 35.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.054 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	25808	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2603e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

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	0.48	0/1489	0.67	2/2015 (0.1%)
1	B	0.44	0/1489	0.65	2/2015 (0.1%)
1	H	0.44	0/1489	0.64	1/2015 (0.0%)
1	L	0.45	0/1489	0.65	2/2015 (0.1%)
1	P	0.43	0/1489	0.64	1/2015 (0.0%)
1	U	0.43	0/1489	0.65	1/2015 (0.0%)
1	Y	0.44	0/1489	0.65	2/2015 (0.1%)
1	c	0.42	0/1489	0.63	1/2015 (0.0%)
2	G	0.58	0/79	0.74	0/106
2	K	0.54	0/79	0.68	0/106
2	O	0.58	0/79	0.74	0/106
2	Q	0.58	0/79	0.77	0/106
2	T	0.50	0/79	0.73	0/106
2	X	0.50	0/79	0.71	0/106
2	b	0.55	0/79	0.70	0/106
2	f	0.53	0/79	0.68	0/106
3	C	0.47	0/879	0.73	1/1196 (0.1%)
3	D	0.47	0/879	0.73	1/1196 (0.1%)
3	I	0.48	0/879	0.73	1/1196 (0.1%)
3	M	0.47	0/879	0.73	0/1196
3	R	0.46	0/879	0.73	1/1196 (0.1%)
3	V	0.44	0/879	0.70	0/1196
3	Z	0.46	0/879	0.72	1/1196 (0.1%)
3	d	0.44	0/879	0.71	1/1196 (0.1%)
4	E	0.50	0/865	0.72	0/1172
4	F	0.47	0/865	0.69	0/1172
4	J	0.46	0/865	0.69	0/1172
4	N	0.45	0/865	0.69	0/1172
4	S	0.46	0/865	0.68	0/1172
4	W	0.44	0/865	0.68	0/1172
4	a	0.46	0/865	0.67	0/1172
4	e	0.43	0/865	0.66	0/1172
All	All	0.45	0/26496	0.68	18/35912 (0.1%)

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.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	164	CYS	CA-CB-SG	-7.21	101.02	114.00
1	Y	164	CYS	CA-CB-SG	-7.14	101.15	114.00
1	U	164	CYS	CA-CB-SG	-7.02	101.37	114.00
1	L	164	CYS	CA-CB-SG	-6.94	101.50	114.00
1	H	164	CYS	CA-CB-SG	-6.62	102.08	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	49	TYR	Sidechain

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	173/175 (99%)	158 (91%)	12 (7%)	3 (2%)	9 34
1	B	173/175 (99%)	155 (90%)	15 (9%)	3 (2%)	9 34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	173/175 (99%)	155 (90%)	15 (9%)	3 (2%)	9	34
1	L	173/175 (99%)	157 (91%)	13 (8%)	3 (2%)	9	34
1	P	173/175 (99%)	156 (90%)	14 (8%)	3 (2%)	9	34
1	U	173/175 (99%)	158 (91%)	12 (7%)	3 (2%)	9	34
1	Y	173/175 (99%)	157 (91%)	13 (8%)	3 (2%)	9	34
1	c	173/175 (99%)	156 (90%)	14 (8%)	3 (2%)	9	34
2	G	7/9 (78%)	7 (100%)	0	0	100	100
2	K	7/9 (78%)	7 (100%)	0	0	100	100
2	O	7/9 (78%)	7 (100%)	0	0	100	100
2	Q	7/9 (78%)	7 (100%)	0	0	100	100
2	T	7/9 (78%)	7 (100%)	0	0	100	100
2	X	7/9 (78%)	7 (100%)	0	0	100	100
2	b	7/9 (78%)	7 (100%)	0	0	100	100
2	f	7/9 (78%)	7 (100%)	0	0	100	100
3	C	107/109 (98%)	98 (92%)	7 (6%)	2 (2%)	8	32
3	D	107/109 (98%)	101 (94%)	5 (5%)	1 (1%)	17	51
3	I	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	17	51
3	M	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	17	51
3	R	107/109 (98%)	100 (94%)	5 (5%)	2 (2%)	8	32
3	V	107/109 (98%)	100 (94%)	5 (5%)	2 (2%)	8	32
3	Z	107/109 (98%)	101 (94%)	4 (4%)	2 (2%)	8	32
3	d	107/109 (98%)	100 (94%)	5 (5%)	2 (2%)	8	32
4	E	109/111 (98%)	105 (96%)	3 (3%)	1 (1%)	17	51
4	F	109/111 (98%)	105 (96%)	3 (3%)	1 (1%)	17	51
4	J	109/111 (98%)	106 (97%)	2 (2%)	1 (1%)	17	51
4	N	109/111 (98%)	105 (96%)	3 (3%)	1 (1%)	17	51
4	S	109/111 (98%)	106 (97%)	2 (2%)	1 (1%)	17	51
4	W	109/111 (98%)	106 (97%)	2 (2%)	1 (1%)	17	51
4	a	109/111 (98%)	106 (97%)	2 (2%)	1 (1%)	17	51
4	e	109/111 (98%)	106 (97%)	2 (2%)	1 (1%)	17	51
All	All	3168/3232 (98%)	2953 (93%)	170 (5%)	45 (1%)	11	39

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	99	ASP
3	C	99	ASP
3	d	99	ASP
3	I	99	ASP
3	M	99	ASP

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	144/144 (100%)	132 (92%)	12 (8%)	11	35
1	B	144/144 (100%)	132 (92%)	12 (8%)	11	35
1	H	144/144 (100%)	133 (92%)	11 (8%)	13	39
1	L	144/144 (100%)	133 (92%)	11 (8%)	13	39
1	P	144/144 (100%)	132 (92%)	12 (8%)	11	35
1	U	144/144 (100%)	132 (92%)	12 (8%)	11	35
1	Y	144/144 (100%)	133 (92%)	11 (8%)	13	39
1	c	144/144 (100%)	132 (92%)	12 (8%)	11	35
2	G	9/9 (100%)	6 (67%)	3 (33%)	0	1
2	K	9/9 (100%)	6 (67%)	3 (33%)	0	1
2	O	9/9 (100%)	7 (78%)	2 (22%)	1	3
2	Q	9/9 (100%)	6 (67%)	3 (33%)	0	1
2	T	9/9 (100%)	6 (67%)	3 (33%)	0	1
2	X	9/9 (100%)	6 (67%)	3 (33%)	0	1
2	b	9/9 (100%)	6 (67%)	3 (33%)	0	1
2	f	9/9 (100%)	6 (67%)	3 (33%)	0	1
3	C	95/95 (100%)	91 (96%)	4 (4%)	30	63
3	D	95/95 (100%)	91 (96%)	4 (4%)	30	63
3	I	95/95 (100%)	91 (96%)	4 (4%)	30	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	95/95 (100%)	91 (96%)	4 (4%)	30	63
3	R	95/95 (100%)	92 (97%)	3 (3%)	39	71
3	V	95/95 (100%)	91 (96%)	4 (4%)	30	63
3	Z	95/95 (100%)	91 (96%)	4 (4%)	30	63
3	d	95/95 (100%)	91 (96%)	4 (4%)	30	63
4	E	91/91 (100%)	84 (92%)	7 (8%)	13	39
4	F	91/91 (100%)	84 (92%)	7 (8%)	13	39
4	J	91/91 (100%)	85 (93%)	6 (7%)	16	46
4	N	91/91 (100%)	86 (94%)	5 (6%)	21	53
4	S	91/91 (100%)	84 (92%)	7 (8%)	13	39
4	W	91/91 (100%)	84 (92%)	7 (8%)	13	39
4	a	91/91 (100%)	85 (93%)	6 (7%)	16	46
4	e	91/91 (100%)	85 (93%)	6 (7%)	16	46
All	All	2712/2712 (100%)	2514 (93%)	198 (7%)	14	41

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	93	SER
4	S	55	THR
4	N	38	ASP
1	P	101	CYS
1	U	41	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	87	GLN
3	R	5	GLN
4	a	10	ASN
3	M	5	GLN
4	N	72	GLN

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 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	175/175 (100%)	0.00	5 (2%) 51 35	24, 40, 68, 92	0
1	B	175/175 (100%)	0.16	6 (3%) 45 29	33, 49, 74, 92	0
1	H	175/175 (100%)	0.20	9 (5%) 28 17	31, 50, 76, 97	0
1	L	175/175 (100%)	0.10	5 (2%) 51 35	32, 46, 69, 89	0
1	P	175/175 (100%)	0.18	5 (2%) 51 35	30, 49, 70, 92	0
1	U	175/175 (100%)	0.20	7 (4%) 38 25	28, 49, 74, 93	0
1	Y	175/175 (100%)	0.11	7 (4%) 38 25	30, 46, 69, 89	0
1	c	175/175 (100%)	0.25	10 (5%) 23 14	38, 53, 76, 94	0
2	G	9/9 (100%)	-0.10	0 100 100	37, 42, 44, 51	0
2	K	9/9 (100%)	-0.17	0 100 100	39, 41, 48, 54	0
2	O	9/9 (100%)	-0.07	0 100 100	36, 38, 46, 48	0
2	Q	9/9 (100%)	-0.01	0 100 100	35, 37, 42, 49	0
2	T	9/9 (100%)	0.45	0 100 100	35, 43, 46, 55	0
2	X	9/9 (100%)	0.07	0 100 100	39, 43, 47, 52	0
2	b	9/9 (100%)	-0.02	0 100 100	32, 36, 43, 45	0
2	f	9/9 (100%)	0.32	0 100 100	45, 47, 53, 56	0
3	C	109/109 (100%)	-0.01	0 100 100	30, 44, 59, 69	0
3	D	109/109 (100%)	-0.06	0 100 100	25, 39, 56, 65	0
3	I	109/109 (100%)	-0.00	0 100 100	32, 44, 58, 68	0
3	M	109/109 (100%)	0.02	2 (1%) 68 51	32, 46, 62, 75	0
3	R	109/109 (100%)	0.02	3 (2%) 53 36	31, 44, 58, 71	0
3	V	109/109 (100%)	0.10	2 (1%) 68 51	34, 46, 60, 74	0
3	Z	109/109 (100%)	-0.02	0 100 100	32, 41, 55, 66	0
3	d	109/109 (100%)	0.15	1 (0%) 84 71	35, 49, 61, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
4	E	111/111 (100%)	-0.15	1 (0%) 84 71	26, 38, 58, 74	0
4	F	111/111 (100%)	-0.01	0 100 100	29, 45, 63, 77	0
4	J	111/111 (100%)	-0.10	0 100 100	32, 45, 65, 80	0
4	N	111/111 (100%)	-0.15	0 100 100	30, 42, 58, 80	0
4	S	111/111 (100%)	0.10	2 (1%) 68 51	33, 45, 62, 75	0
4	W	111/111 (100%)	0.22	2 (1%) 68 51	32, 48, 63, 78	0
4	a	111/111 (100%)	0.08	3 (2%) 54 38	31, 44, 59, 72	0
4	e	111/111 (100%)	-0.02	1 (0%) 84 71	35, 49, 64, 78	0
All	All	3232/3232 (100%)	0.07	71 (2%) 62 45	24, 46, 68, 97	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	16	GLY	6.0
1	H	89	ALA	4.6
1	A	17	LEU	4.1
1	c	16	GLY	3.8
1	Y	17	LEU	3.8

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.