



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 21, 2024 – 04:27 pm GMT

PDB ID : 8RJI  
Title : HLA A\*2402-NF9\_5R pMHC complex  
Authors : Wall, A.; Motozono, C.; Sewell, A.K.; Rizkallah, P.J.; Fuller, A.  
Deposited on : 2023-12-21  
Resolution : 2.30 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

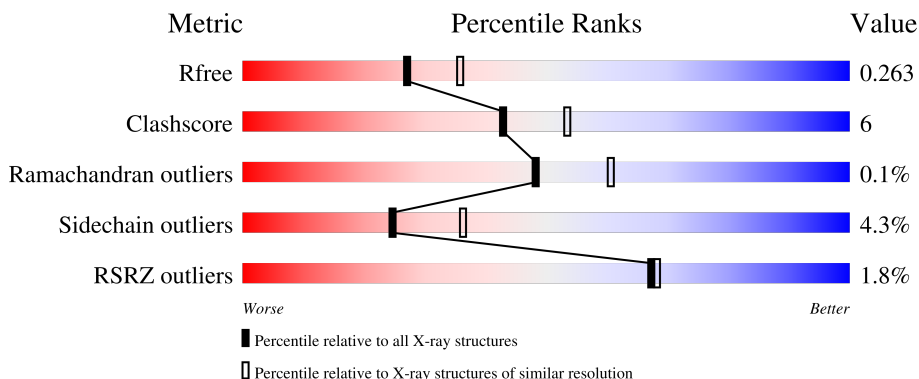
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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  $\geq 3$ , 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	 3% 85% 14% .
1	D	276	 3% 86% 13% .
1	G	276	 2% 84% 16%
1	J	276	 86% 13% .
2	B	100	 3% 84% 16%

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Mol	Chain	Length	Quality of chain
2	E	100	 <p>% 83% 17%</p>
2	H	100	 <p>% 79% 21%</p>
2	K	100	 <p>% 81% 19%</p>
3	C	9	 <p>56% 44%</p>
3	F	9	 <p>67% 33%</p>
3	I	9	 <p>44% 56%</p>
3	L	9	 <p>33% 56% 11%</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13033 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2238	1392	405	431	10	0	0	0
1	D	276	2238	1392	405	431	10	0	0	0
1	G	276	2238	1392	405	431	10	0	0	0
1	J	276	2238	1392	405	431	10	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	E	100	837	533	141	159	4	0	0	0
2	H	100	837	533	141	159	4	0	0	0
2	K	100	837	533	141	159	4	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769
K	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			94	62	17	15			
3	F	9	Total	C	N	O	0	0	0
			94	62	17	15			
3	L	9	Total	C	N	O	0	0	0
			94	62	17	15			
3	I	9	Total	C	N	O	0	0	0
			94	62	17	15			

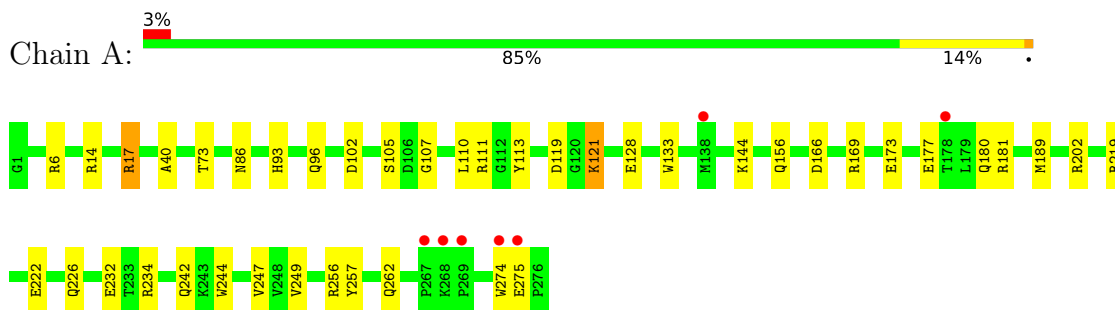
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		
4	B	25	Total	O	0	0
			25	25		
4	C	4	Total	O	0	0
			4	4		
4	D	46	Total	O	0	0
			46	46		
4	E	23	Total	O	0	0
			23	23		
4	G	53	Total	O	0	0
			53	53		
4	H	24	Total	O	0	0
			24	24		
4	J	85	Total	O	0	0
			85	85		
4	K	22	Total	O	0	0
			22	22		
4	L	1	Total	O	0	0
			1	1		
4	I	1	Total	O	0	0
			1	1		

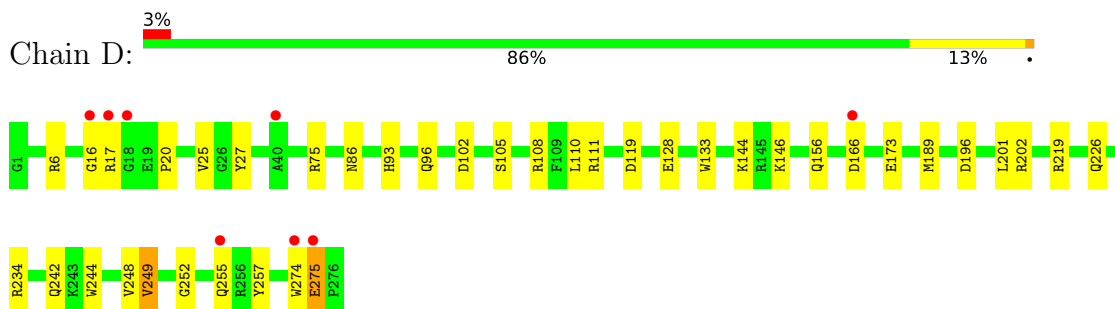
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

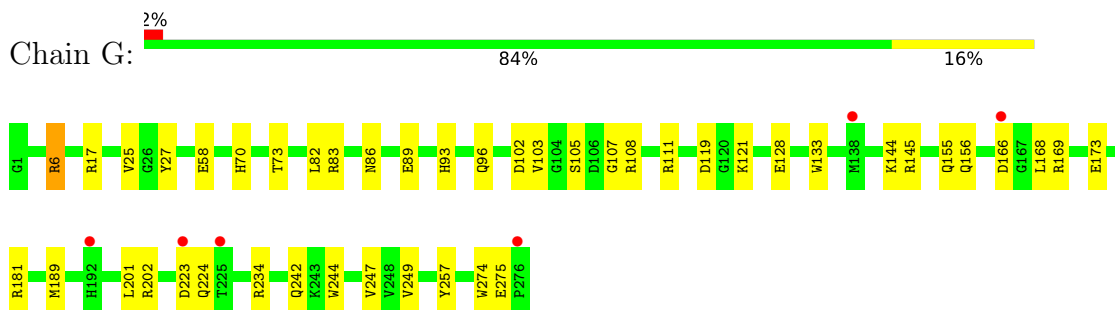
- Molecule 1: MHC class I antigen



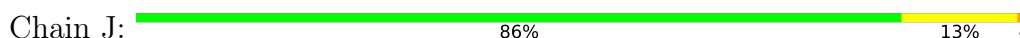
- Molecule 1: MHC class I antigen

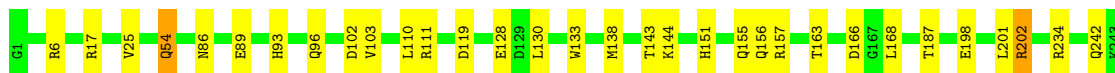


- Molecule 1: MHC class I antigen

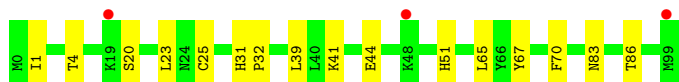
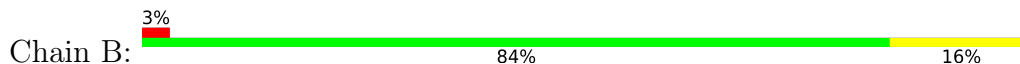


- Molecule 1: MHC class I antigen

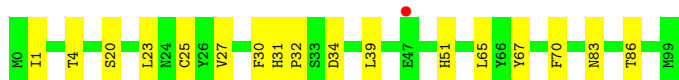
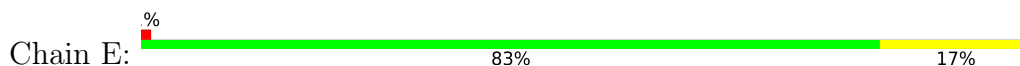




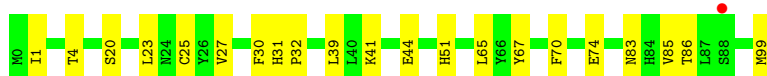
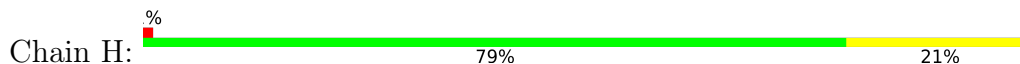
- Molecule 2: Beta-2-microglobulin



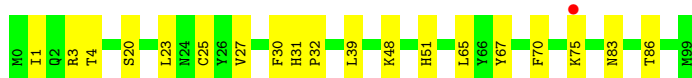
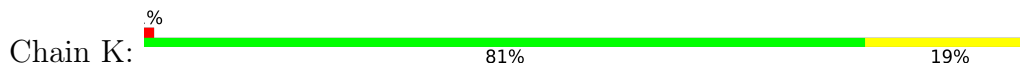
- Molecule 2: Beta-2-microglobulin



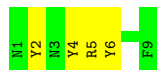
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



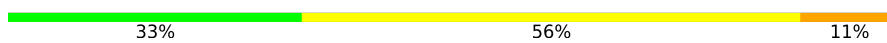
- Molecule 3: Spike glycoprotein

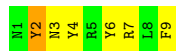


- Molecule 3: Spike glycoprotein



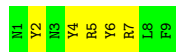
- Molecule 3: Spike glycoprotein

Chain L:  33% 56% 11%



- Molecule 3: Spike glycoprotein

Chain I:  44% 56%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.28Å 77.02Å 111.82Å 90.00° 110.58° 90.00°	Depositor
Resolution (Å)	54.80 – 2.30 54.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (54.80-2.30) 99.7 (54.80-2.30)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.217 , 0.265 0.221 , 0.263	Depositor DCC
$R_{free}$ test set	3602 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtrriage
Anisotropy	0.585	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 29.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.45 % 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 1.1421e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

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	0.80	2/2299 (0.1%)	0.85	2/3116 (0.1%)
1	D	0.75	0/2299	0.84	2/3116 (0.1%)
1	G	0.75	0/2299	0.84	2/3116 (0.1%)
1	J	0.81	1/2299 (0.0%)	0.86	2/3116 (0.1%)
2	B	0.73	0/860	0.76	0/1162
2	E	0.78	0/860	0.78	0/1162
2	H	0.75	0/860	0.76	0/1162
2	K	0.74	0/860	0.78	0/1162
3	C	0.76	0/97	0.95	0/128
3	F	0.66	0/97	0.90	0/128
3	I	0.70	0/97	0.91	0/128
3	L	0.79	0/97	0.89	0/128
All	All	0.77	3/13024 (0.0%)	0.83	8/17624 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	GLU	CD-OE1	-5.42	1.19	1.25
1	A	232	GLU	CD-OE2	-5.27	1.19	1.25
1	J	198	GLU	CD-OE2	5.07	1.31	1.25

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	166	ASP	CB-CG-OD1	8.56	126.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	D	166	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	J	202	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	J	166	ASP	CB-CG-OD2	-6.17	112.75	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	2	TYR	Peptide,Mainchain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2238	0	2095	27	1
1	D	2238	0	2095	33	1
1	G	2238	0	2095	32	1
1	J	2238	0	2095	27	0
2	B	837	0	803	10	0
2	E	837	0	803	9	0
2	H	837	0	803	13	1
2	K	837	0	803	10	0
3	C	94	0	87	3	0
3	F	94	0	87	1	0
3	I	94	0	87	3	0
3	L	94	0	87	3	0
4	A	73	0	0	2	0
4	B	25	0	0	2	0
4	C	4	0	0	1	0
4	D	46	0	0	2	0
4	E	23	0	0	2	0
4	G	53	0	0	0	0
4	H	24	0	0	1	0
4	I	1	0	0	0	0
4	J	85	0	0	5	0
4	K	22	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1	0	0	0	0
All	All	13033	0	11940	151	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 151 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:G:155:GLN:OE1	3:I:7:ARG:NH1	2.02	0.92
1:D:255:GLN:CD	1:D:255:GLN:H	1.83	0.82
1:D:255:GLN:HG2	1:G:83:ARG:O	1.80	0.80
2:K:4:THR:HG22	2:K:86:THR:HB	1.68	0.75
1:D:173:GLU:OE1	1:D:173:GLU:HA	1.87	0.74

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:GLN:NE2	1:D:16:GLY:O[2_646]	2.11	0.09
1:G:108:ARG:NH1	2:H:85:VAL:O[2_546]	2.17	0.03

## 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%)	11 (4%)	0	100 100
1	D	274/276 (99%)	267 (97%)	7 (3%)	0	100 100
1	G	274/276 (99%)	263 (96%)	11 (4%)	0	100 100
1	J	274/276 (99%)	265 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	E	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	H	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	K	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
3	I	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
3	L	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
All	All	1516/1540 (98%)	1463 (96%)	51 (3%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	3	ASN
3	I	5	ARG

### 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%)	224 (97%)	8 (3%)	32	47
1	D	232/232 (100%)	226 (97%)	6 (3%)	41	58
1	G	232/232 (100%)	222 (96%)	10 (4%)	25	36
1	J	232/232 (100%)	224 (97%)	8 (3%)	32	47
2	B	95/95 (100%)	92 (97%)	3 (3%)	34	50
2	E	95/95 (100%)	90 (95%)	5 (5%)	19	28
2	H	95/95 (100%)	91 (96%)	4 (4%)	25	37
2	K	95/95 (100%)	89 (94%)	6 (6%)	15	21
3	C	9/9 (100%)	7 (78%)	2 (22%)	1	0
3	F	9/9 (100%)	7 (78%)	2 (22%)	1	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	9/9 (100%)	7 (78%)	2 (22%)	1	0
3	L	9/9 (100%)	7 (78%)	2 (22%)	1	0
All	All	1344/1344 (100%)	1286 (96%)	58 (4%)	25	36

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	86	ASN
3	L	6	TYR
1	G	275	GLU
3	L	2	TYR
2	K	20	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	155	GLN
1	J	174	ASN
2	K	31	HIS
1	D	218	GLN
1	D	197	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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%)	0.14	7 (2%) 58 59	20, 37, 61, 82	0
1	D	276/276 (100%)	0.30	8 (2%) 54 55	22, 43, 72, 90	0
1	G	276/276 (100%)	0.28	6 (2%) 62 63	24, 43, 67, 80	0
1	J	276/276 (100%)	0.02	1 (0%) 89 89	20, 35, 58, 81	0
2	B	100/100 (100%)	0.21	3 (3%) 52 54	20, 41, 73, 81	0
2	E	100/100 (100%)	0.01	1 (1%) 79 79	20, 33, 54, 64	0
2	H	100/100 (100%)	0.30	1 (1%) 79 79	25, 44, 70, 80	0
2	K	100/100 (100%)	0.26	1 (1%) 79 79	20, 41, 80, 102	0
3	C	9/9 (100%)	-0.20	0 100 100	23, 29, 38, 40	0
3	F	9/9 (100%)	0.34	0 100 100	34, 43, 54, 58	0
3	I	9/9 (100%)	0.53	0 100 100	34, 40, 56, 65	0
3	L	9/9 (100%)	0.00	0 100 100	27, 34, 46, 50	0
All	All	1540/1540 (100%)	0.19	28 (1%) 67 68	20, 39, 68, 102	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	18	GLY	3.7
1	D	16	GLY	3.5
1	D	40	ALA	3.3
2	K	75	LYS	3.1
1	D	275	GLU	2.8

### 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.