



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:04 PM GMT

PDB ID : 4NQX  
Title : Crystal Structure of HLA A\*0101 in complex with NP44-S7N, an 9-mer influenza epitope  
Authors : Rossjohn, J.; Gras, S.  
Deposited on : 2013-11-26  
Resolution : 2.00 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

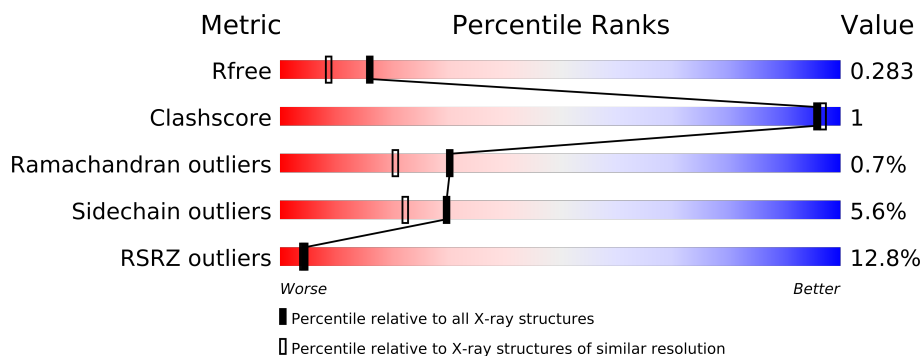
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	<b>FAILED</b>
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	284	
1	C	284	
1	E	284	
1	G	284	
1	I	284	
1	K	284	
2	B	100	
2	D	100	
2	F	100	
2	H	100	
2	J	100	
2	L	100	
3	M	9	
3	N	9	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	O	9	
3	P	9	
3	Q	9	
3	R	9	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19771 atoms, of which 0 are hydrogen and 0 are deuterium.

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-1 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	3	0
			2255	1399	416	430	10			
1	C	275	Total	C	N	O	S	0	1	0
			2245	1394	411	430	10			
1	E	275	Total	C	N	O	S	0	2	0
			2256	1399	415	432	10			
1	G	274	Total	C	N	O	S	0	2	0
			2248	1395	415	428	10			
1	I	274	Total	C	N	O	S	0	2	0
			2247	1394	413	430	10			
1	K	275	Total	C	N	O	S	0	1	0
			2243	1392	410	431	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	1	0
			845	539	142	160	4			
2	D	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	F	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	J	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	L	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	EXPRESSION TAG	UNP P61769

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	EXPRESSION TAG	UNP P61769
F	0	MET	-	EXPRESSION TAG	UNP P61769
H	0	MET	-	EXPRESSION TAG	UNP P61769
J	0	MET	-	EXPRESSION TAG	UNP P61769
L	0	MET	-	EXPRESSION TAG	UNP P61769

- Molecule 3 is a protein called NP44-S7N mutant peptide, CTELKLNDY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			
3	N	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			
3	O	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			
3	P	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			
3	Q	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			
3	R	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total	O	0	0
			116	116		
4	B	49	Total	O	0	0
			49	49		
4	C	110	Total	O	0	0
			110	110		
4	D	51	Total	O	0	0
			51	51		
4	E	90	Total	O	0	0
			90	90		
4	F	43	Total	O	0	0
			43	43		
4	G	70	Total	O	0	0
			70	70		
4	H	34	Total	O	0	0
			34	34		
4	I	55	Total	O	0	0
			55	55		

*Continued on next page...*

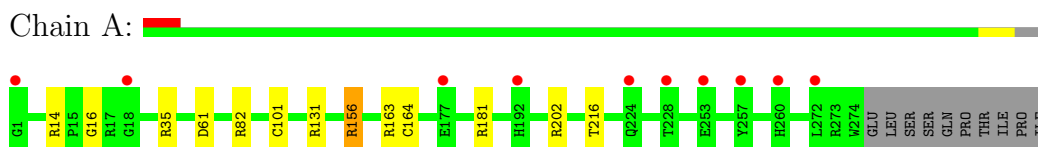
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	27	Total 27	O 27	0	0
4	K	97	Total 97	O 97	0	0
4	L	32	Total 32	O 32	0	0
4	M	7	Total 7	O 7	0	0
4	N	5	Total 5	O 5	0	0
4	O	2	Total 2	O 2	0	0
4	P	4	Total 4	O 4	0	0
4	Q	3	Total 3	O 3	0	0
4	R	4	Total 4	O 4	0	0

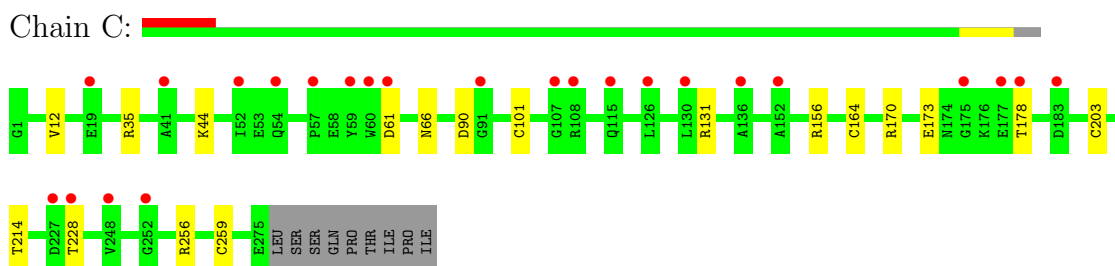
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

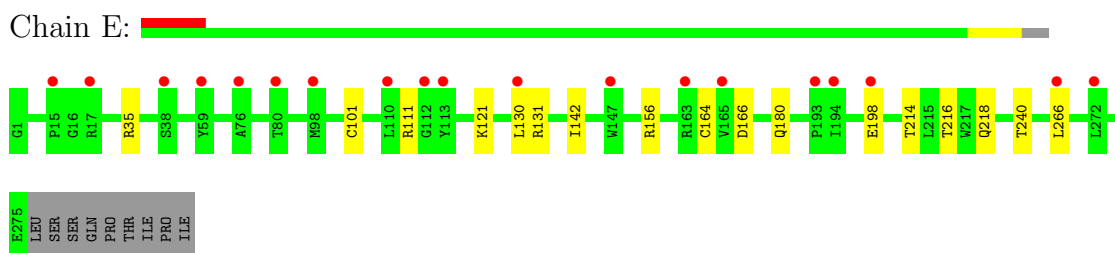
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



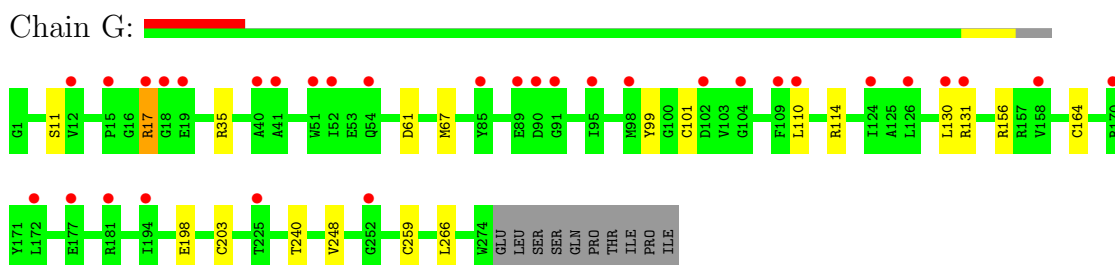
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



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

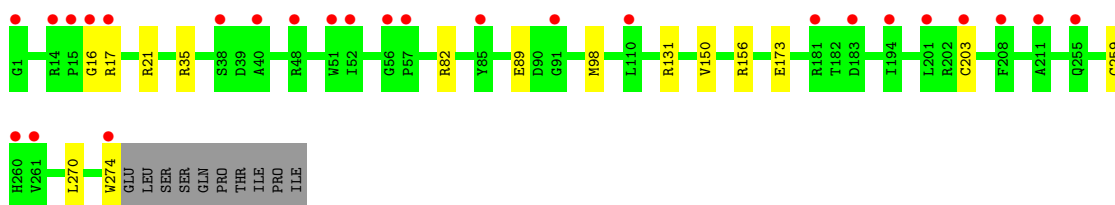


- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



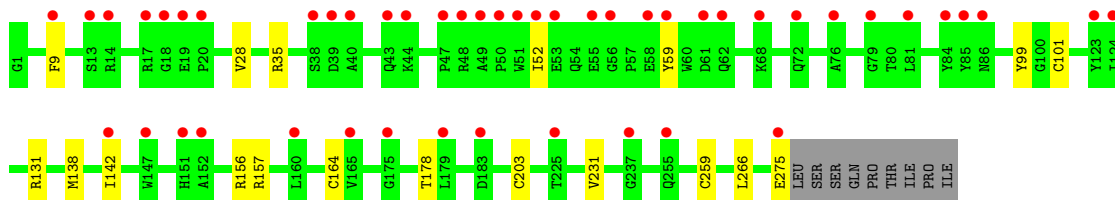
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain





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

Chain K:



- Molecule 2: Beta-2-microglobulin

Chain B:



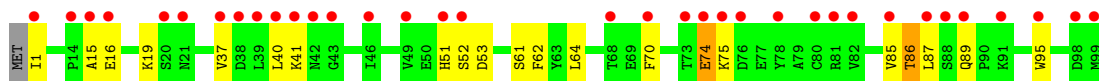
- Molecule 2: Beta-2-microglobulin

Chain D:



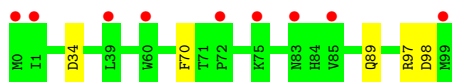
- Molecule 2: Beta-2-microglobulin

Chain F:



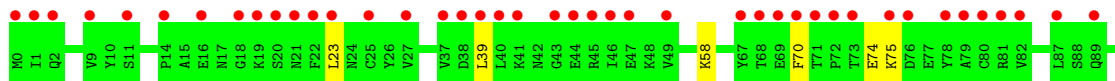
- Molecule 2: Beta-2-microglobulin

Chain H:

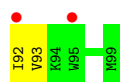


- Molecule 2: Beta-2-microglobulin

Chain J:

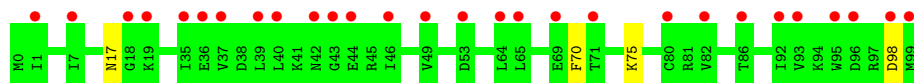






- Molecule 2: Beta-2-microglobulin

Chain L:



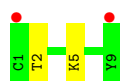
- Molecule 3: NP44-S7N mutant peptide, CTTELKLNDY

Chain M:

There are no outlier residues recorded for this chain.

- Molecule 3: NP44-S7N mutant peptide, CTTELKLNDY

Chain N:



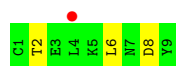
- Molecule 3: NP44-S7N mutant peptide, CTTELKLNDY

Chain O:



- Molecule 3: NP44-S7N mutant peptide, CTTELKLNDY

Chain P:



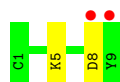
- Molecule 3: NP44-S7N mutant peptide, CTTELKLNDY

Chain Q:



- Molecule 3: NP44-S7N mutant peptide, CTTELKLNDY

Chain R:



## 4 Data and refinement statistics

Xtriage (Phenix) failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	264.61Å 81.41Å 140.29Å 90.00° 121.82° 90.00°	Depositor
Resolution (Å)	45.75 – 2.00 45.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (45.75-2.00) 96.2 (45.75-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.270 , 0.283 0.275 , 0.283	Depositor DCC
$R_{free}$ test set	8305 reflections (5.28%)	DCC
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 32.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	19771	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.37	0/2316	0.58	0/3140
1	C	0.38	0/2305	0.58	0/3125
1	E	0.39	0/2316	0.61	0/3139
1	G	0.37	0/2309	0.59	0/3131
1	I	0.35	0/2307	0.58	0/3127
1	K	0.38	0/2303	0.61	0/3123
2	B	0.38	0/868	0.64	0/1173
2	D	0.37	0/860	0.63	0/1162
2	F	0.45	0/852	0.83	2/1152 (0.2%)
2	H	0.39	0/860	0.63	0/1162
2	J	0.40	0/860	0.61	0/1162
2	L	0.37	0/860	0.63	0/1162
3	M	0.35	0/76	0.63	0/100
3	N	0.35	0/76	0.57	0/100
3	O	0.33	0/76	0.54	0/100
3	P	0.38	0/76	0.83	0/100
3	Q	0.31	0/76	0.61	0/100
3	R	0.36	0/76	0.51	0/100
All	All	0.38	0/19472	0.61	2/26358 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	85	VAL	C-N-CA	9.21	144.74	121.70
2	F	74	GLU	C-N-CA	5.33	135.03	121.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2255	0	0	4	0
1	C	2245	0	0	3	0
1	E	2256	0	0	1	0
1	G	2248	0	0	4	0
1	I	2247	0	0	1	0
1	K	2243	0	0	4	0
2	B	845	0	0	2	0
2	D	837	0	0	0	0
2	F	829	0	0	1	0
2	H	837	0	0	0	0
2	J	837	0	0	0	0
2	L	837	0	0	0	0
3	M	76	0	74	0	0
3	N	76	0	74	1	0
3	O	76	0	74	0	0
3	P	76	0	74	2	0
3	Q	76	0	74	0	0
3	R	76	0	74	0	0
4	A	116	0	0	2	0
4	B	49	0	0	0	0
4	C	110	0	0	0	0
4	D	51	0	0	0	0
4	E	90	0	0	0	0
4	F	43	0	0	0	0
4	G	70	0	0	0	0
4	H	34	0	0	0	0
4	I	55	0	0	0	0
4	J	27	0	0	0	0
4	K	97	0	0	1	0
4	L	32	0	0	0	0
4	M	7	0	0	0	0
4	N	5	0	0	0	0
4	O	2	0	0	0	0
4	P	4	0	0	0	0
4	Q	3	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	4	0	0	0	0
All	All	19771	0	444	19	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

The worst 5 of 19 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:67:MET:CE	3:P:2:THR:HG21	2.15	0.77
2:B:7:ILE:CD1	2:B:25:CYS:SG	2.92	0.57
1:K:157:ARG:NH1	4:K:333:HOH:O	2.38	0.57
1:C:203:CYS:SG	1:C:259:CYS:SG	3.03	0.56
1:I:203:CYS:SG	1:I:259:CYS:SG	3.03	0.56

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	275/284 (97%)	270 (98%)	4 (2%)	1 (0%)	43	36
1	C	274/284 (96%)	268 (98%)	6 (2%)	0	100	100
1	E	275/284 (97%)	269 (98%)	6 (2%)	0	100	100
1	G	274/284 (96%)	269 (98%)	4 (2%)	1 (0%)	43	36
1	I	274/284 (96%)	270 (98%)	3 (1%)	1 (0%)	43	36
1	K	274/284 (96%)	262 (96%)	11 (4%)	1 (0%)	43	36
2	B	99/100 (99%)	98 (99%)	0	1 (1%)	22	12
2	D	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	F	97/100 (97%)	79 (81%)	8 (8%)	10 (10%)	1	0
2	H	98/100 (98%)	94 (96%)	3 (3%)	1 (1%)	22	12
2	J	98/100 (98%)	94 (96%)	4 (4%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	98/100 (98%)	92 (94%)	6 (6%)	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
3	R	7/9 (78%)	7 (100%)	0	0	100	100
All	All	2276/2358 (96%)	2204 (97%)	56 (2%)	16 (1%)	30	20

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	15	ALA
2	F	61	SER
2	F	62	PHE
2	F	86	THR
1	G	17	ARG

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/241 (97%)	226 (97%)	8 (3%)	49	45
1	C	233/241 (97%)	220 (94%)	13 (6%)	30	22
1	E	234/241 (97%)	218 (93%)	16 (7%)	22	15
1	G	233/241 (97%)	220 (94%)	13 (6%)	30	22
1	I	233/241 (97%)	221 (95%)	12 (5%)	32	25
1	K	233/241 (97%)	222 (95%)	11 (5%)	36	29
2	B	96/95 (101%)	92 (96%)	4 (4%)	40	34
2	D	95/95 (100%)	91 (96%)	4 (4%)	40	34
2	F	94/95 (99%)	85 (90%)	9 (10%)	12	6
2	H	95/95 (100%)	91 (96%)	4 (4%)	40	34

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	95/95 (100%)	87 (92%)	8 (8%)	16	9
2	L	95/95 (100%)	91 (96%)	4 (4%)	40	34
3	M	9/9 (100%)	9 (100%)	0	100	100
3	N	9/9 (100%)	8 (89%)	1 (11%)	9	5
3	O	9/9 (100%)	8 (89%)	1 (11%)	9	5
3	P	9/9 (100%)	7 (78%)	2 (22%)	1	0
3	Q	9/9 (100%)	8 (89%)	1 (11%)	9	5
3	R	9/9 (100%)	7 (78%)	2 (22%)	1	0
All	All	2024/2070 (98%)	1911 (94%)	113 (6%)	30	22

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	86	THR
1	G	198	GLU
2	L	75	LYS
2	F	87	LEU
1	G	61	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

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 ⓘ

### 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<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	274/284 (96%)	0.58	10 (3%) 41 40	19, 38, 61, 79	0
1	C	275/284 (96%)	0.93	24 (8%) 10 10	26, 42, 70, 82	0
1	E	275/284 (96%)	0.90	19 (6%) 17 16	27, 41, 64, 93	0
1	G	274/284 (96%)	1.03	32 (11%) 5 5	26, 45, 73, 95	0
1	I	274/284 (96%)	0.96	26 (9%) 8 8	24, 49, 81, 109	0
1	K	275/284 (96%)	1.28	48 (17%) 2 2	28, 47, 90, 119	0
2	B	100/100 (100%)	0.78	8 (8%) 12 12	20, 36, 58, 64	0
2	D	100/100 (100%)	0.70	5 (5%) 28 27	25, 36, 62, 70	0
2	F	99/100 (99%)	1.93	35 (35%) 1 1	25, 53, 89, 99	0
2	H	100/100 (100%)	0.76	9 (9%) 10 9	27, 39, 61, 67	0
2	J	100/100 (100%)	2.10	44 (44%) 1 1	26, 57, 95, 104	0
2	L	100/100 (100%)	1.37	28 (28%) 1 1	32, 49, 77, 84	0
3	M	9/9 (100%)	0.18	0 100 100	21, 27, 30, 43	0
3	N	9/9 (100%)	1.22	2 (22%) 1 2	35, 42, 48, 61	0
3	O	9/9 (100%)	0.93	1 (11%) 6 6	31, 40, 44, 58	0
3	P	9/9 (100%)	1.28	1 (11%) 6 6	38, 43, 45, 60	0
3	Q	9/9 (100%)	0.26	0 100 100	31, 35, 39, 49	0
3	R	9/9 (100%)	1.62	2 (22%) 1 2	40, 47, 62, 63	0
All	All	2300/2358 (97%)	1.03	294 (12%) 4 4	19, 43, 76, 119	0

The worst 5 of 294 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	82	VAL	10.8
1	K	53	GLU	8.5
2	J	18	GLY	8.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	F	40	LEU	7.3
2	J	80	CYS	7.2

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.