



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:02 PM GMT

PDB ID : 3QPR  
Title : HK97 Prohead I encapsidating inactive virally encoded protease  
Authors : Huang, R.K.; Khayat, R.; Lee, K.K.; Gertsman, I.; Duda, R.L.; Hendrix, R.W.; Johnson, J.E.  
Deposited on : 2011-02-14  
Resolution : 5.20 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

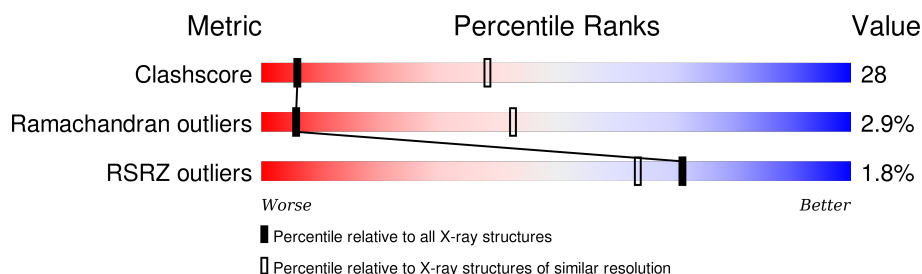
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 5.20 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))
Clashscore	102246	1042 (6.74-3.66)
Ramachandran outliers	100387	1011 (6.76-3.62)
RSRZ outliers	91569	1146 (6.80-3.60)

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. 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	385	
1	B	385	
1	C	385	
1	D	385	
1	E	385	
1	F	385	
1	G	385	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8654 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.

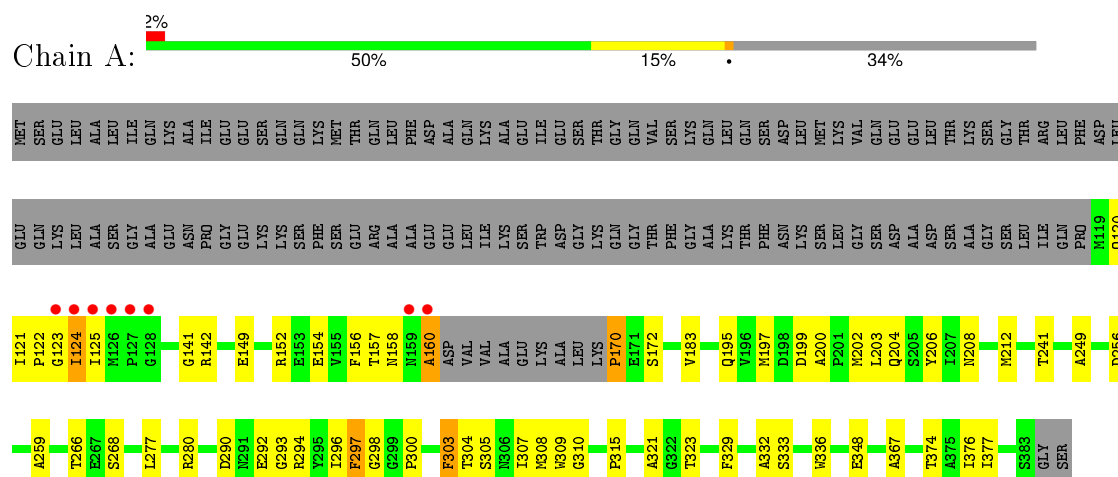
- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	0	0	0
			1260	748	256	256			
1	B	250	Total	C	N	O	0	0	0
			1231	731	250	250			
1	C	248	Total	C	N	O	0	0	0
			1221	725	248	248			
1	D	254	Total	C	N	O	0	0	0
			1250	742	254	254			
1	E	255	Total	C	N	O	0	0	0
			1255	745	255	255			
1	F	248	Total	C	N	O	0	0	0
			1221	725	248	248			
1	G	247	Total	C	N	O	0	0	0
			1216	722	247	247			

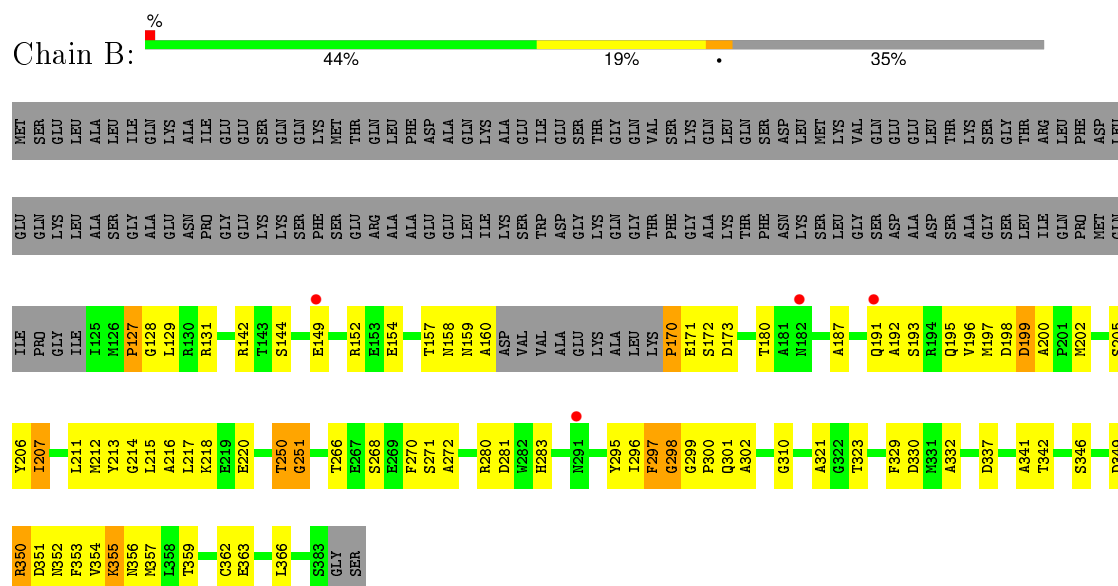
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: Major capsid protein



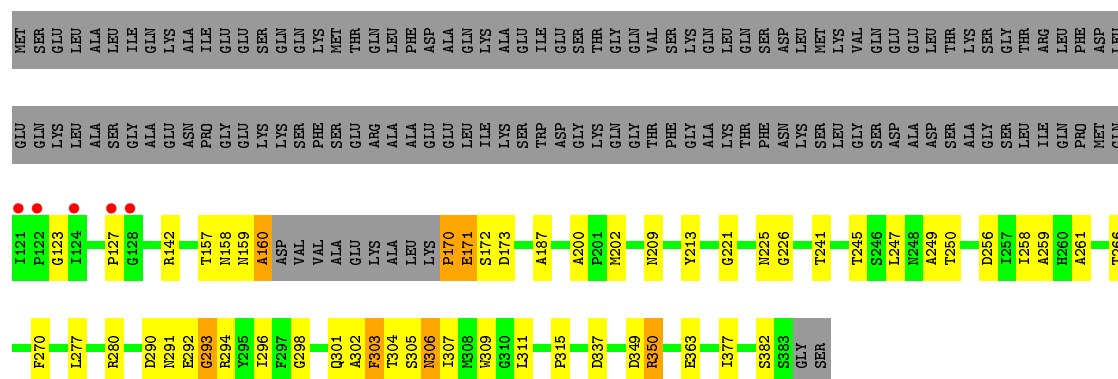
#### • Molecule 1: Major capsid protein



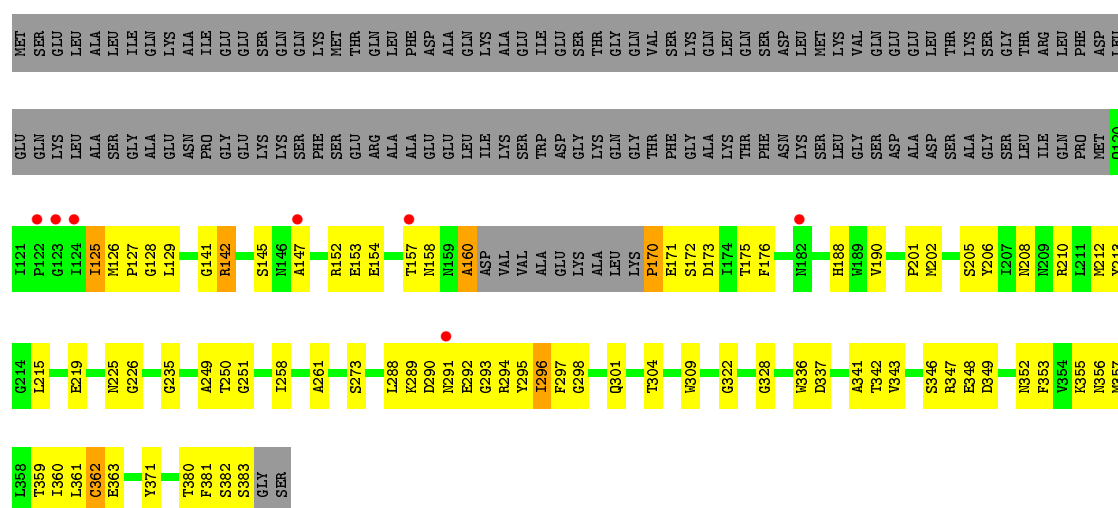
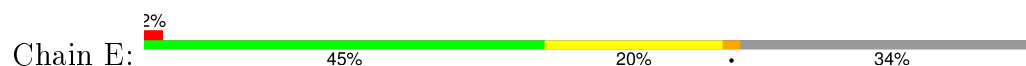
#### • Molecule 1: Major capsid protein



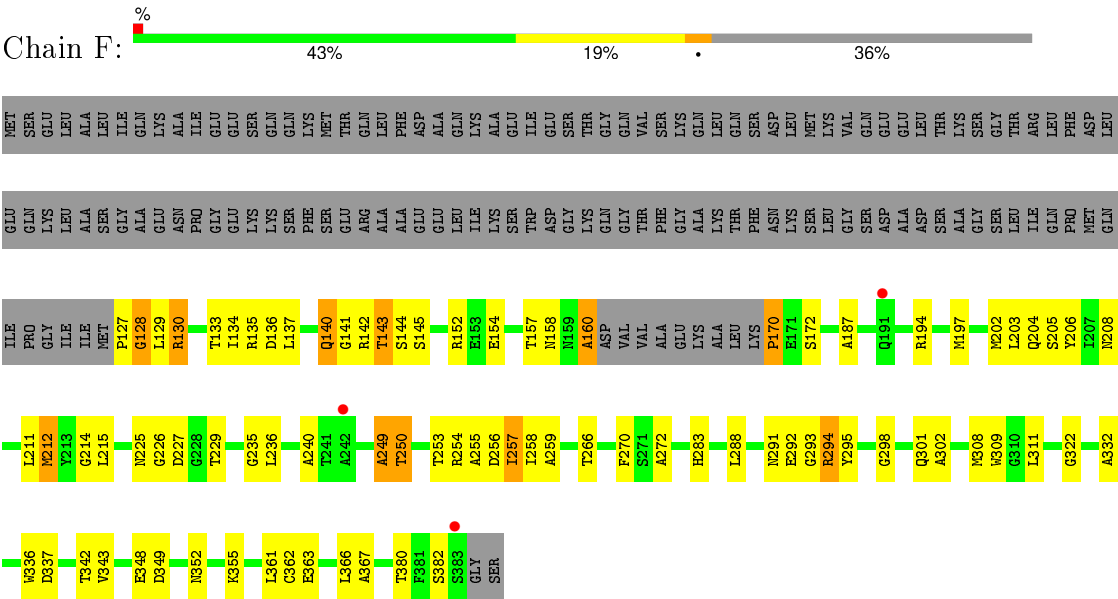
- Molecule 1: Major capsid protein



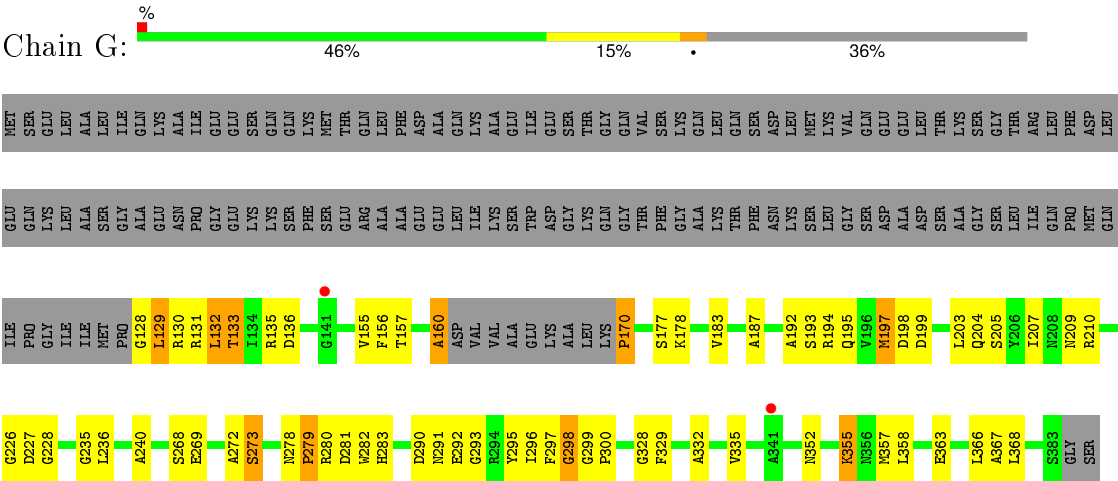
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	560.12Å 560.12Å 560.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 5.20 44.56 – 5.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (45.00-5.20) 77.2 (44.56-5.19)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 5.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.461 , 0.467 0.396 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	175.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.08 , 16.6	EDS
Estimated twinning fraction	0.125 for -l,-k,-h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.32$ , $\langle L^2 \rangle = 0.16$	Xtriage
Outliers	0 of 86454 reflections	Xtriage
$F_o, F_c$ correlation	0.73	EDS
Total number of atoms	8654	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.39	1/1259 (0.1%)	0.94	15/1749 (0.9%)
1	B	0.42	0/1230	0.90	11/1709 (0.6%)
1	C	0.34	0/1220	0.80	9/1695 (0.5%)
1	D	0.35	0/1249	0.85	8/1735 (0.5%)
1	E	0.32	0/1254	0.81	9/1742 (0.5%)
1	F	0.43	0/1220	1.07	19/1695 (1.1%)
1	G	0.38	0/1215	1.10	22/1688 (1.3%)
All	All	0.38	1/8647 (0.0%)	0.93	93/12013 (0.8%)

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
1	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	MET	C-N	-5.26	1.22	1.34

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	297	PHE	N-CA-C	-9.22	86.10	111.00
1	A	298	GLY	N-CA-C	8.91	135.37	113.10
1	B	128	GLY	N-CA-C	-8.58	91.65	113.10
1	D	123	GLY	N-CA-C	-8.24	92.50	113.10
1	G	272	ALA	CB-CA-C	-8.23	97.76	110.10

There are no chirality outliers.



All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	362	CYS	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	1260	0	595	42	0
1	B	1231	0	583	78	0
1	C	1221	0	580	49	0
1	D	1250	0	591	44	0
1	E	1255	0	593	71	0
1	F	1221	0	580	63	0
1	G	1216	0	578	50	0
All	All	8654	0	4100	361	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

The worst 5 of 361 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:B:158:ASN:CB	1:B:172:SER:HA	1.21	1.57
1:B:158:ASN:CB	1:B:172:SER:CA	2.08	1.31
1:E:202:MET:HA	1:F:142:ARG:O	1.26	1.26
1:B:193:SER:CB	1:C:149:GLU:CB	2.14	1.26
1:A:293:GLY:O	1:C:298:GLY:CA	1.84	1.24

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	254/385 (66%)	194 (76%)	54 (21%)	6 (2%)	7	47
1	B	248/385 (64%)	194 (78%)	47 (19%)	7 (3%)	6	44
1	C	246/385 (64%)	200 (81%)	36 (15%)	10 (4%)	3	34
1	D	252/385 (66%)	205 (81%)	39 (16%)	8 (3%)	5	41
1	E	253/385 (66%)	215 (85%)	33 (13%)	5 (2%)	9	51
1	F	246/385 (64%)	201 (82%)	36 (15%)	9 (4%)	4	37
1	G	245/385 (64%)	201 (82%)	38 (16%)	6 (2%)	7	47
All	All	1744/2695 (65%)	1410 (81%)	283 (16%)	51 (3%)	6	43

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ILE
1	A	170	PRO
1	A	208	ASN
1	B	170	PRO
1	B	350	ARG

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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 carbohydrates 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	256/385 (66%)	-0.36	8 (3%)	52 44	118, 145, 169, 195	0
1	B	250/385 (64%)	-0.37	4 (1%)	74 67	118, 149, 175, 187	0
1	C	248/385 (64%)	-0.38	3 (1%)	81 74	121, 150, 174, 189	0
1	D	254/385 (65%)	-0.39	5 (1%)	68 60	118, 149, 170, 188	0
1	E	255/385 (66%)	-0.33	7 (2%)	58 50	120, 152, 173, 203	0
1	F	248/385 (64%)	-0.41	3 (1%)	81 74	123, 147, 170, 191	0
1	G	247/385 (64%)	-0.46	2 (0%)	87 83	122, 149, 172, 193	0
All	All	1758/2695 (65%)	-0.39	32 (1%)	71 64	118, 149, 173, 203	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	141	GLY	4.3
1	A	126	MET	4.1
1	A	160	ALA	3.9
1	E	122	PRO	3.6
1	A	127	PRO	3.6

### 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 carbohydrates 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.