



# wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 12:49 PM GMT

PDB ID : 3E8K  
Title : Crystal structure of HK97 Prohead II  
Authors : Gertsman, I.; Speir, J.; Johnson, J.E.  
Deposited on : 2008-08-20  
Resolution : 3.65 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>

---

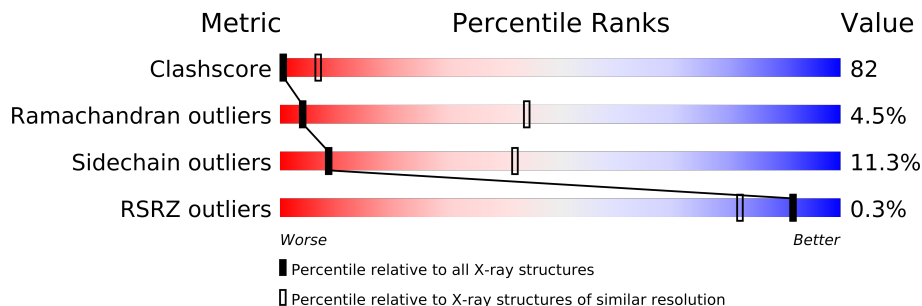
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
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 3.65 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	79885	1025 (3.90-3.42)
Ramachandran outliers	78287	1195 (3.92-3.40)
Sidechain outliers	78261	1193 (3.92-3.40)
RSRZ outliers	66119	1021 (3.94-3.38)

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	273	
1	B	273	
1	C	273	
1	D	273	
1	E	273	
1	F	273	
1	G	273	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13590 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 Major capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1978	1238	346	384	10			
1	B	250	Total	C	N	O	S	0	0	0
			1934	1209	339	377	9			
1	C	248	Total	C	N	O	S	0	0	0
			1918	1198	337	375	8			
1	D	254	Total	C	N	O	S	0	0	0
			1961	1228	343	381	9			
1	E	255	Total	C	N	O	S	0	0	0
			1970	1233	345	383	9			
1	F	248	Total	C	N	O	S	0	0	0
			1918	1198	337	375	8			
1	G	247	Total	C	N	O	S	0	0	0
			1911	1193	336	374	8			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	ALA	-	LINKER	UNP P49861
A	160	PRO	-	LINKER	UNP P49861
A	161	GLY	-	LINKER	UNP P49861
A	162	ASP	-	LINKER	UNP P49861
A	336	PHE	TRP	ENGINEERED	UNP P49861
B	159	ALA	-	LINKER	UNP P49861
B	160	PRO	-	LINKER	UNP P49861
B	161	GLY	-	LINKER	UNP P49861
B	162	ASP	-	LINKER	UNP P49861
B	336	PHE	TRP	ENGINEERED	UNP P49861
C	159	ALA	-	LINKER	UNP P49861
C	160	PRO	-	LINKER	UNP P49861
C	161	GLY	-	LINKER	UNP P49861
C	162	ASP	-	LINKER	UNP P49861
C	336	PHE	TRP	ENGINEERED	UNP P49861

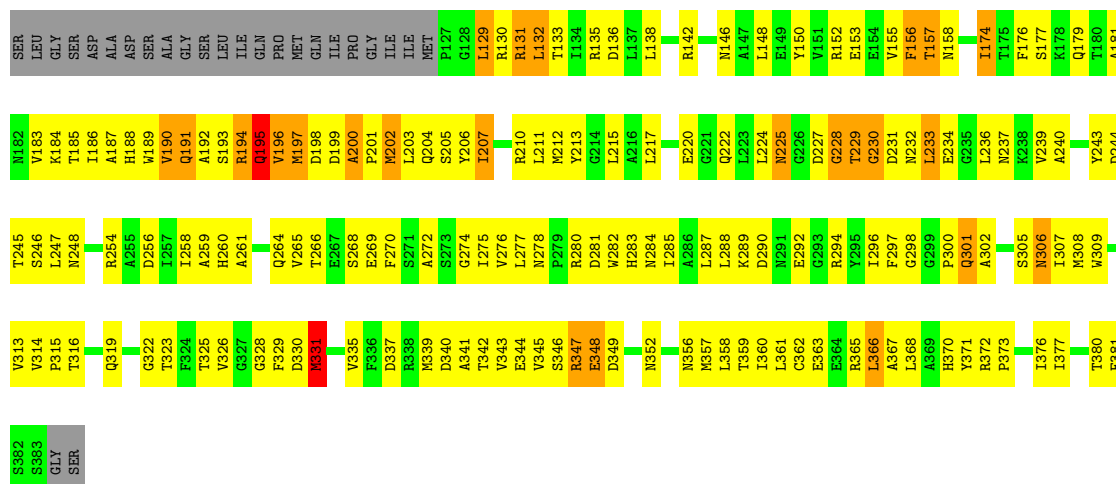
*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	159	ALA	-	LINKER	UNP P49861
D	160	PRO	-	LINKER	UNP P49861
D	161	GLY	-	LINKER	UNP P49861
D	162	ASP	-	LINKER	UNP P49861
D	336	PHE	TRP	ENGINEERED	UNP P49861
E	159	ALA	-	LINKER	UNP P49861
E	160	PRO	-	LINKER	UNP P49861
E	161	GLY	-	LINKER	UNP P49861
E	162	ASP	-	LINKER	UNP P49861
E	336	PHE	TRP	ENGINEERED	UNP P49861
F	159	ALA	-	LINKER	UNP P49861
F	160	PRO	-	LINKER	UNP P49861
F	161	GLY	-	LINKER	UNP P49861
F	162	ASP	-	LINKER	UNP P49861
F	336	PHE	TRP	ENGINEERED	UNP P49861
G	159	ALA	-	LINKER	UNP P49861
G	160	PRO	-	LINKER	UNP P49861
G	161	GLY	-	LINKER	UNP P49861
G	162	ASP	-	LINKER	UNP P49861
G	336	PHE	TRP	ENGINEERED	UNP P49861

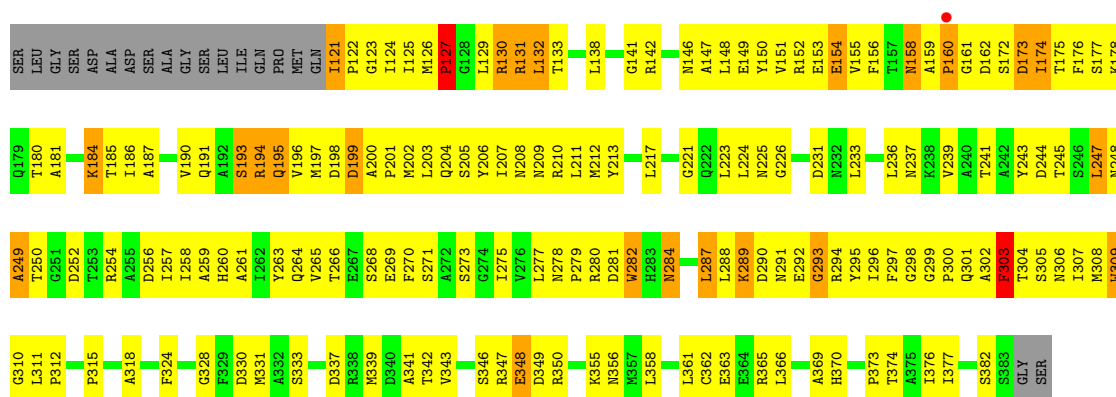


## Chain C:



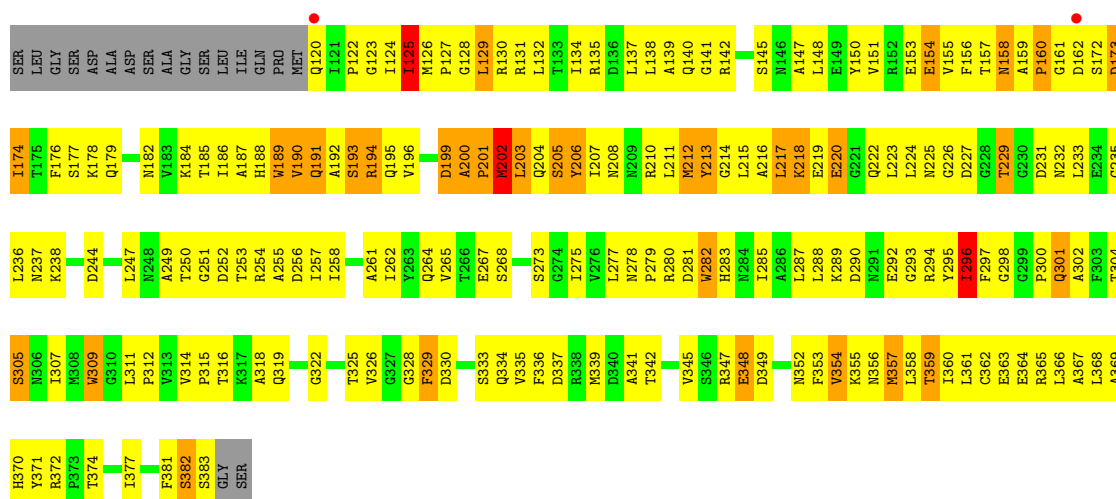
- Molecule 1: Major capsid protein

## Chain D:



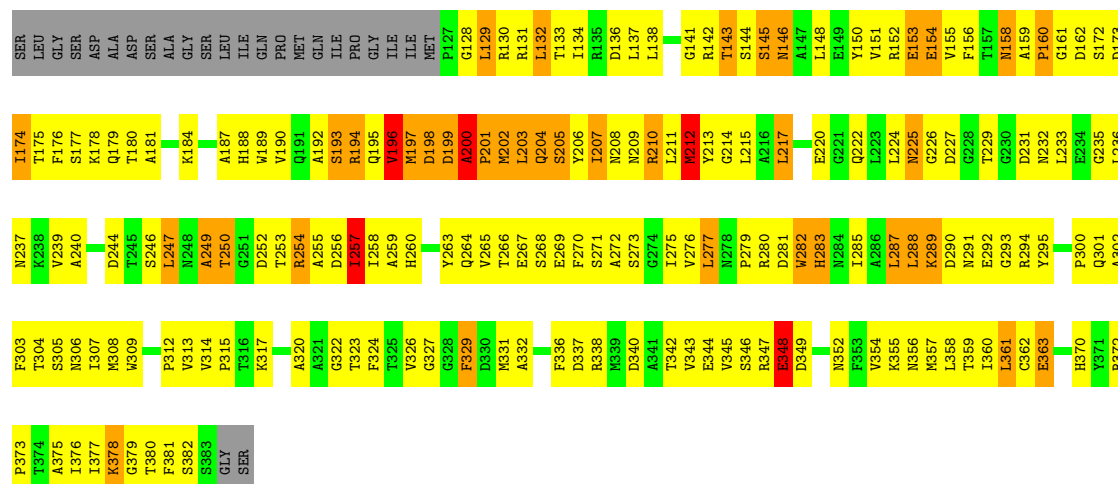
- Molecule 1: Major capsid protein

## Chain E:



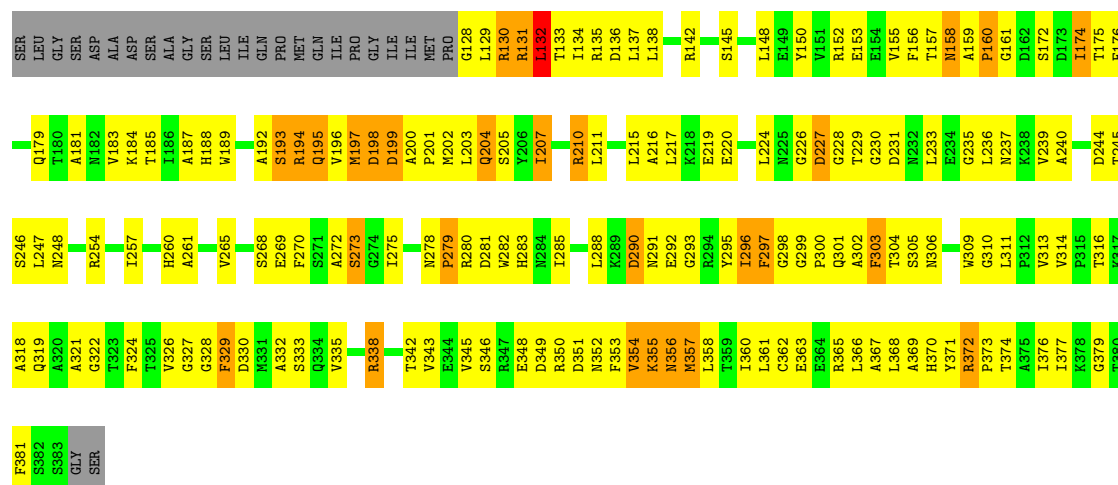
- Molecule 1: Major capsid protein

## Chain F:



## • Molecule 1: Major capsid protein

## Chain G:



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	553.03Å 574.39Å 587.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 3.65 34.99 – 3.65	Depositor EDS
% Data completeness (in resolution range)	64.8 (35.00-3.65) 54.3 (34.99-3.65)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 3.66Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.366 , (Not available) 0.332 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	72.5	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.96 , -20.0	EDS
Estimated twinning fraction	0.276 for -h,-l,-k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.23$ , $\langle L^2 \rangle = 0.09$	Xtriage
Outliers	0 of 656526 reflections	Xtriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	13590	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.41	1/2013 (0.0%)	0.68	2/2730 (0.1%)
1	B	0.42	0/1968	0.82	11/2669 (0.4%)
1	C	0.36	0/1952	0.68	2/2647 (0.1%)
1	D	0.37	1/1996 (0.1%)	0.68	5/2708 (0.2%)
1	E	0.40	1/2005 (0.0%)	0.70	5/2720 (0.2%)
1	F	0.42	0/1952	0.83	11/2647 (0.4%)
1	G	0.40	0/1944	0.77	9/2636 (0.3%)
All	All	0.40	3/13830 (0.0%)	0.74	45/18757 (0.2%)

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	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	329	PHE	C-N	-5.66	1.21	1.34
1	A	212	MET	C-N	-5.28	1.21	1.34
1	D	288	LEU	C-N	-5.03	1.22	1.34

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	200	ALA	C-N-CD	-9.66	99.35	120.60
1	G	272	ALA	CB-CA-C	-8.25	97.73	110.10
1	G	228	GLY	N-CA-C	8.21	133.63	113.10
1	D	193	SER	N-CA-CB	-7.66	99.01	110.50
1	G	195	GLN	N-CA-C	-7.24	91.46	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	369	ALA	Mainchain

## 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	1978	0	1946	311	0
1	B	1934	0	1896	343	0
1	C	1918	0	1878	343	0
1	D	1961	0	1929	330	0
1	E	1970	0	1937	365	0
1	F	1918	0	1878	347	0
1	G	1911	0	1870	285	0
All	All	13590	0	13334	2213	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 82.

The worst 5 of 2213 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:127:PRO:HB2	1:E:213:TYR:CD1	1.32	1.62
1:D:125:ILE:HD11	1:D:208:ASN:CG	1.32	1.49
1:D:125:ILE:HD11	1:D:208:ASN:ND2	1.26	1.45
1:C:196:VAL:HG12	1:C:203:LEU:CD1	1.44	1.45
1:B:201:PRO:O	1:B:204:GLN:CB	1.67	1.41

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	254/273 (93%)	195 (77%)	49 (19%)	10 (4%)	5	49
1	B	248/273 (91%)	189 (76%)	48 (19%)	11 (4%)	4	45
1	C	246/273 (90%)	188 (76%)	47 (19%)	11 (4%)	4	44
1	D	252/273 (92%)	209 (83%)	34 (14%)	9 (4%)	5	52
1	E	253/273 (93%)	190 (75%)	49 (19%)	14 (6%)	3	38
1	F	246/273 (90%)	192 (78%)	40 (16%)	14 (6%)	3	37
1	G	245/273 (90%)	199 (81%)	36 (15%)	10 (4%)	4	47
All	All	1744/1911 (91%)	1362 (78%)	303 (17%)	79 (4%)	4	44

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ILE
1	A	208	ASN
1	B	200	ALA
1	B	297	PHE
1	C	131	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	211/223 (95%)	184 (87%)	27 (13%)	6	35
1	B	206/223 (92%)	181 (88%)	25 (12%)	7	38
1	C	204/223 (92%)	184 (90%)	20 (10%)	12	51
1	D	209/223 (94%)	191 (91%)	18 (9%)	15	59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	210/223 (94%)	185 (88%)	25 (12%)	8	39
1	F	204/223 (92%)	173 (85%)	31 (15%)	4	26
1	G	203/223 (91%)	185 (91%)	18 (9%)	14	57
All	All	1447/1561 (93%)	1283 (89%)	164 (11%)	9	42

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	130	ARG
1	E	129	LEU
1	G	193	SER
1	D	132	LEU
1	D	282	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	232	ASN
1	C	284	ASN
1	G	158	ASN
1	C	237	ASN
1	C	264	GLN

### 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	256/273 (93%)	0.01	1 (0%) 90 77	1, 28, 53, 72	0
1	B	250/273 (91%)	0.05	2 (0%) 83 62	1, 31, 59, 78	0
1	C	248/273 (90%)	0.05	0 100 100	7, 33, 59, 69	0
1	D	254/273 (93%)	-0.00	1 (0%) 90 77	1, 32, 54, 79	0
1	E	255/273 (93%)	0.01	2 (0%) 83 62	5, 34, 57, 90	0
1	F	248/273 (90%)	0.01	0 100 100	1, 31, 54, 75	0
1	G	247/273 (90%)	0.04	0 100 100	3, 31, 57, 87	0
All	All	1758/1911 (91%)	0.02	6 (0%) 91 82	1, 31, 57, 90	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	162	ASP	2.9
1	A	160	PRO	2.8
1	E	120	GLN	2.5
1	B	125	ILE	2.4
1	B	383	SER	2.1

### 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.