



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2016 – 05:03 AM EDT

PDB ID : 5K4A  
Title : Structure of the amidase mutant E79A at 2.3 Angstrom resolution  
Authors : Chowdhury, S.R.; Sen, U.  
Deposited on : 2016-05-20  
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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
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) : rb-20027674

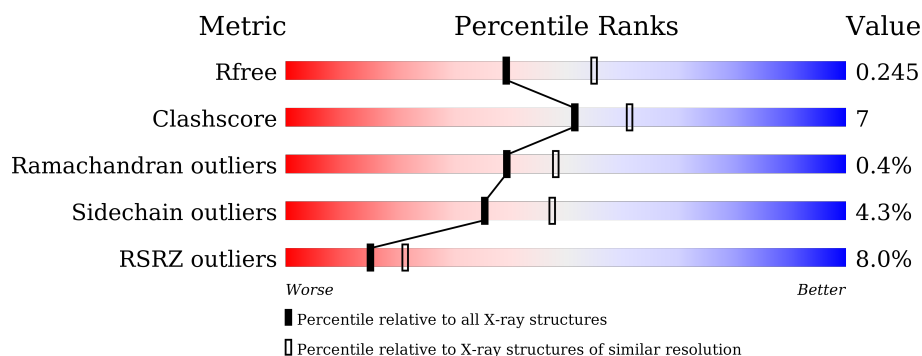
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 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	288	<div> <div>5%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	B	288	<div> <div>3%</div> <div>88%</div> <div>8%</div> <div>..</div> </div>
1	C	288	<div> <div>5%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	D	288	<div> <div>7%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	E	288	<div> <div>8%</div> <div>77%</div> <div>20%</div> <div>..</div> </div>
1	F	288	<div> <div>19%</div> <div>70%</div> <div>24%</div> <div>..</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13571 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 Intracellular protease/amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	281	Total	C	N	O	S	0	0	0
			2164	1391	353	410	10			
1	F	281	Total	C	N	O	S	0	0	0
			2167	1393	353	410	11			
1	A	281	Total	C	N	O	S	0	0	0
			2167	1393	353	410	11			
1	B	281	Total	C	N	O	S	0	0	0
			2167	1393	353	410	11			
1	D	281	Total	C	N	O	S	0	0	0
			2167	1393	353	410	11			
1	E	281	Total	C	N	O	S	0	0	0
			2164	1391	353	410	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP A0A0H3AFW5
C	0	SER	-	expression tag	UNP A0A0H3AFW5
C	79	ALA	GLU	engineered mutation	UNP A0A0H3AFW5
F	-1	GLY	-	expression tag	UNP A0A0H3AFW5
F	0	SER	-	expression tag	UNP A0A0H3AFW5
F	79	ALA	GLU	engineered mutation	UNP A0A0H3AFW5
A	-1	GLY	-	expression tag	UNP A0A0H3AFW5
A	0	SER	-	expression tag	UNP A0A0H3AFW5
A	79	ALA	GLU	engineered mutation	UNP A0A0H3AFW5
B	-1	GLY	-	expression tag	UNP A0A0H3AFW5
B	0	SER	-	expression tag	UNP A0A0H3AFW5
B	79	ALA	GLU	engineered mutation	UNP A0A0H3AFW5
D	-1	GLY	-	expression tag	UNP A0A0H3AFW5
D	0	SER	-	expression tag	UNP A0A0H3AFW5
D	79	ALA	GLU	engineered mutation	UNP A0A0H3AFW5
E	-1	GLY	-	expression tag	UNP A0A0H3AFW5
E	0	SER	-	expression tag	UNP A0A0H3AFW5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	79	ALA	GLU	engineered mutation	UNP A0A0H3AFW5

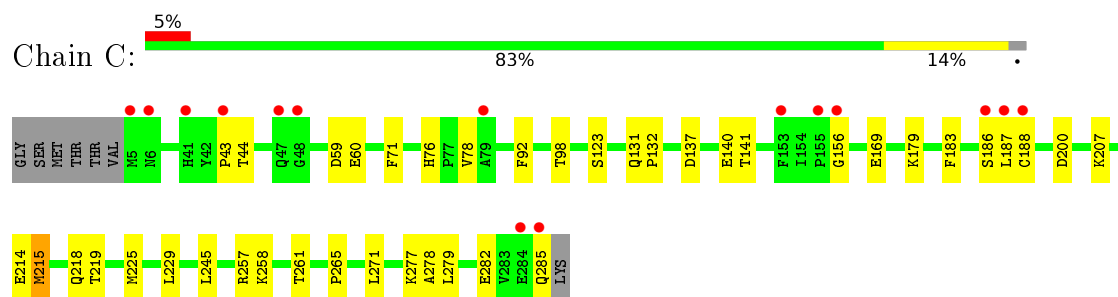
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	115	Total 115	O 115	0	0
2	F	41	Total 41	O 41	0	0
2	A	129	Total 129	O 129	0	0
2	B	142	Total 142	O 142	0	0
2	D	81	Total 81	O 81	0	0
2	E	67	Total 67	O 67	0	0

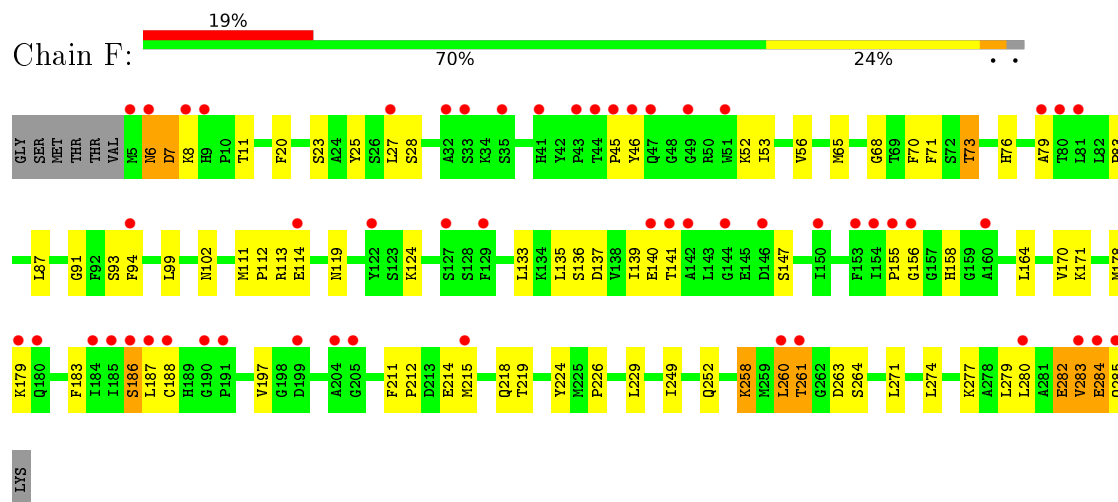
### 3 Residue-property plots

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.

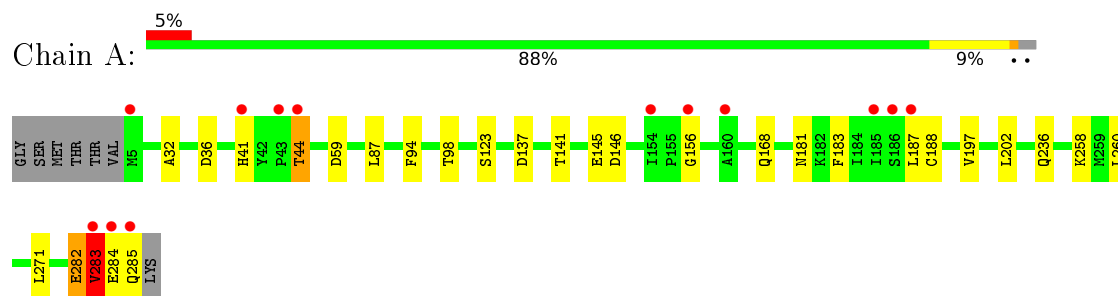
- Molecule 1: Intracellular protease/amidase



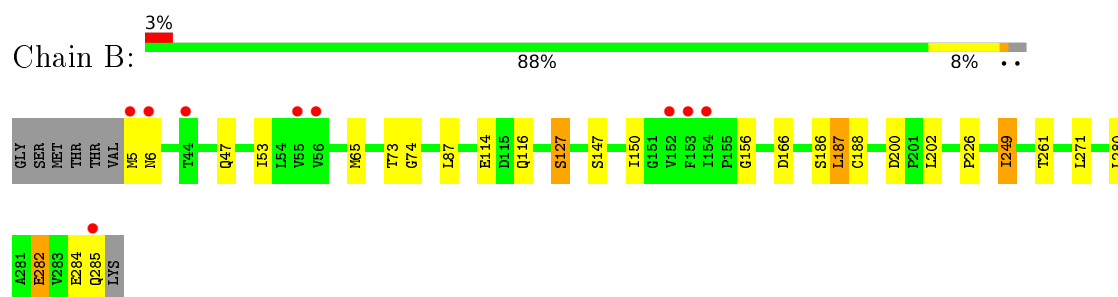
- Molecule 1: Intracellular protease/amidase



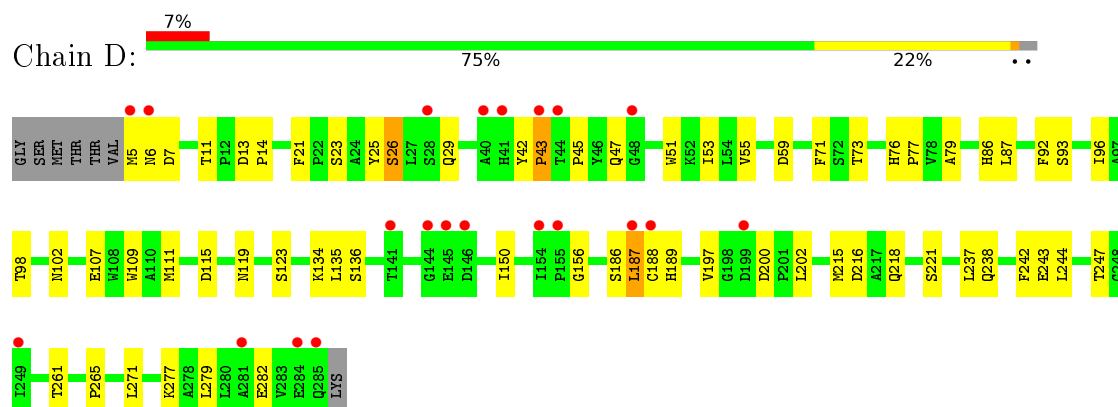
- Molecule 1: Intracellular protease/amidase



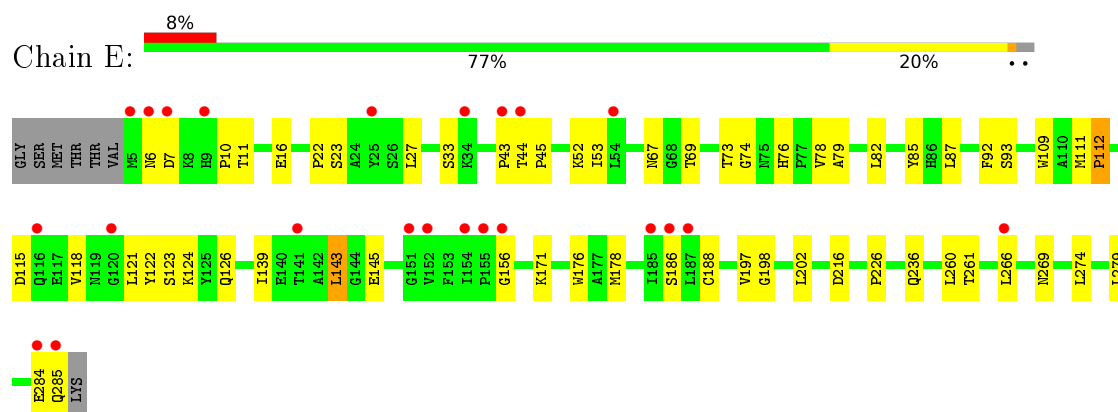
- Molecule 1: Intracellular protease/amidase



- Molecule 1: Intracellular protease/amidase



- Molecule 1: Intracellular protease/amidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.39 Å   79.63 Å   106.41 Å 90.00°   107.84°   90.00°	Depositor
Resolution (Å)	24.73 – 2.30 25.64 – 2.29	Depositor EDS
% Data completeness (in resolution range)	92.2 (24.73-2.30) 89.4 (25.64-2.29)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.180 , 0.246 0.177 , 0.245	Depositor DCC
$R_{free}$ test set	3338 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13571	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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 [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	0.44	0/2229	0.59	1/3028 (0.0%)
1	B	0.43	0/2229	0.56	0/3028
1	C	0.40	0/2226	0.55	0/3025
1	D	0.40	0/2229	0.57	0/3028
1	E	0.35	0/2226	0.52	0/3025
1	F	0.38	0/2229	0.53	0/3028
All	All	0.40	0/13368	0.55	1/18162 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	VAL	N-CA-C	5.22	125.10	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2167	0	2085	16	0
1	B	2167	0	2085	13	0
1	C	2164	0	2078	23	0
1	D	2167	0	2085	39	0
1	E	2164	0	2078	33	0
1	F	2167	0	2085	51	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	129	0	0	5	0
2	B	142	0	0	3	0
2	C	115	0	0	4	0
2	D	81	0	0	5	0
2	E	67	0	0	4	0
2	F	41	0	0	6	0
All	All	13571	0	12496	174	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 7.

The worst 5 of 174 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:F:178:MET:SD	2:F:341:HOH:O	2.20	0.98
1:F:73:THR:HG21	1:F:158:HIS:HB2	1.51	0.92
1:C:140:GLU:HG2	1:C:141:THR:HG23	1.57	0.85
1:F:68:GLY:O	2:F:301:HOH:O	1.94	0.85
1:D:47:GLN:HB2	2:D:308:HOH:O	1.76	0.84

There are no symmetry-related clashes.

## 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	279/288 (97%)	265 (95%)	12 (4%)	2 (1%)	26	31
1	B	279/288 (97%)	266 (95%)	13 (5%)	0	100	100
1	C	279/288 (97%)	267 (96%)	12 (4%)	0	100	100
1	D	279/288 (97%)	261 (94%)	17 (6%)	1 (0%)	39	48
1	E	279/288 (97%)	264 (95%)	12 (4%)	3 (1%)	17	18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	279/288 (97%)	250 (90%)	28 (10%)	1 (0%)	39	48
All	All	1674/1728 (97%)	1573 (94%)	94 (6%)	7 (0%)	39	48

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	283	VAL
1	A	282	GLU
1	A	283	VAL
1	D	43	PRO
1	E	198	GLY

### 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	227/233 (97%)	219 (96%)	8 (4%)	43	58
1	B	227/233 (97%)	216 (95%)	11 (5%)	31	42
1	C	226/233 (97%)	220 (97%)	6 (3%)	52	70
1	D	227/233 (97%)	220 (97%)	7 (3%)	47	64
1	E	226/233 (97%)	217 (96%)	9 (4%)	38	52
1	F	227/233 (97%)	209 (92%)	18 (8%)	15	19
All	All	1360/1398 (97%)	1301 (96%)	59 (4%)	35	47

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	THR
1	B	6	ASN
1	E	139	ILE
1	A	145	GLU
1	A	260	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	131	GLN
1	A	181	ASN
1	D	86	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 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	281/288 (97%)	-0.01	13 (4%)	36 45	18, 30, 49, 128	0
1	B	281/288 (97%)	0.00	9 (3%)	51 60	20, 32, 52, 93	0
1	C	281/288 (97%)	0.15	15 (5%)	30 39	21, 35, 57, 100	0
1	D	281/288 (97%)	0.30	21 (7%)	17 24	23, 46, 79, 124	0
1	E	281/288 (97%)	0.52	23 (8%)	14 20	27, 51, 78, 119	0
1	F	281/288 (97%)	1.06	54 (19%)	2 2	33, 62, 93, 134	0
All	All	1686/1728 (97%)	0.34	135 (8%)	15 21	18, 40, 82, 134	0

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	285	GLN	7.3
1	B	5	MET	7.1
1	E	5	MET	6.2
1	C	285	GLN	6.0
1	F	5	MET	5.9

### 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.