



# wwPDB X-ray Structure Validation Summary Report i

Mar 1, 2014 – 01:57 AM GMT

PDB ID : 3E20  
Title : Crystal structure of S.pombe eRF1/eRF3 complex  
Authors : Cheng, Z.; Lim, M.; Kong, C.; Song, H.  
Deposited on : 2008-08-05  
Resolution : 3.50 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>

---

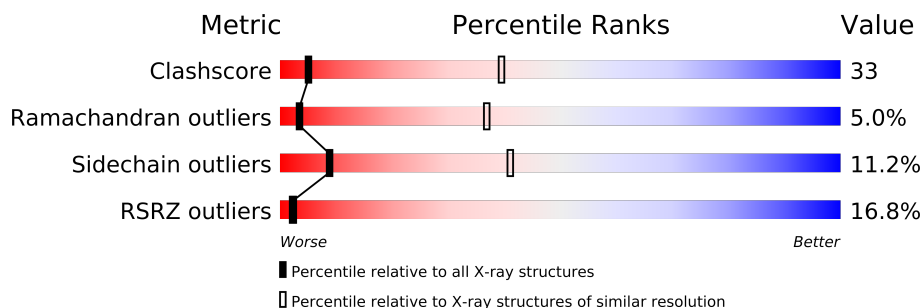
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.50 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	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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. 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	201	
1	D	201	
1	E	201	
1	J	201	
2	B	441	
2	C	441	
2	H	441	
2	K	441	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13096 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 Eukaryotic peptide chain release factor GTP-binding subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1524	965	256	293	10			
1	D	196	Total	C	N	O	S	0	0	0
			1524	965	256	293	10			
1	E	196	Total	C	N	O	S	0	0	0
			1524	965	256	293	10			
1	J	196	Total	C	N	O	S	0	0	0
			1524	965	256	293	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	462	GLY	-	EXPRESSION TAG	UNP O74718
A	463	PRO	-	EXPRESSION TAG	UNP O74718
A	464	LEU	-	EXPRESSION TAG	UNP O74718
A	465	GLY	-	EXPRESSION TAG	UNP O74718
A	466	SER	-	EXPRESSION TAG	UNP O74718
D	462	GLY	-	EXPRESSION TAG	UNP O74718
D	463	PRO	-	EXPRESSION TAG	UNP O74718
D	464	LEU	-	EXPRESSION TAG	UNP O74718
D	465	GLY	-	EXPRESSION TAG	UNP O74718
D	466	SER	-	EXPRESSION TAG	UNP O74718
E	462	GLY	-	EXPRESSION TAG	UNP O74718
E	463	PRO	-	EXPRESSION TAG	UNP O74718
E	464	LEU	-	EXPRESSION TAG	UNP O74718
E	465	GLY	-	EXPRESSION TAG	UNP O74718
E	466	SER	-	EXPRESSION TAG	UNP O74718
J	462	GLY	-	EXPRESSION TAG	UNP O74718
J	463	PRO	-	EXPRESSION TAG	UNP O74718
J	464	LEU	-	EXPRESSION TAG	UNP O74718
J	465	GLY	-	EXPRESSION TAG	UNP O74718
J	466	SER	-	EXPRESSION TAG	UNP O74718

- Molecule 2 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	261	Total 2088	C 1321	N 347	O 405	S 15	0	0	0
2	B	261	Total 2088	C 1321	N 347	O 405	S 15	0	0	0
2	H	175	Total 1412	C 900	N 225	O 277	S 10	0	0	0
2	K	175	Total 1412	C 900	N 225	O 277	S 10	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	MET	-	EXPRESSION TAG	UNP P79063
C	-6	HIS	-	EXPRESSION TAG	UNP P79063
C	-5	HIS	-	EXPRESSION TAG	UNP P79063
C	-4	HIS	-	EXPRESSION TAG	UNP P79063
C	-3	HIS	-	EXPRESSION TAG	UNP P79063
C	-2	HIS	-	EXPRESSION TAG	UNP P79063
C	-1	HIS	-	EXPRESSION TAG	UNP P79063
C	0	MET	-	EXPRESSION TAG	UNP P79063
B	-7	MET	-	EXPRESSION TAG	UNP P79063
B	-6	HIS	-	EXPRESSION TAG	UNP P79063
B	-5	HIS	-	EXPRESSION TAG	UNP P79063
B	-4	HIS	-	EXPRESSION TAG	UNP P79063
B	-3	HIS	-	EXPRESSION TAG	UNP P79063
B	-2	HIS	-	EXPRESSION TAG	UNP P79063
B	-1	HIS	-	EXPRESSION TAG	UNP P79063
B	0	MET	-	EXPRESSION TAG	UNP P79063
H	-7	MET	-	EXPRESSION TAG	UNP P79063
H	-6	HIS	-	EXPRESSION TAG	UNP P79063
H	-5	HIS	-	EXPRESSION TAG	UNP P79063
H	-4	HIS	-	EXPRESSION TAG	UNP P79063
H	-3	HIS	-	EXPRESSION TAG	UNP P79063
H	-2	HIS	-	EXPRESSION TAG	UNP P79063
H	-1	HIS	-	EXPRESSION TAG	UNP P79063
H	0	MET	-	EXPRESSION TAG	UNP P79063
K	-7	MET	-	EXPRESSION TAG	UNP P79063
K	-6	HIS	-	EXPRESSION TAG	UNP P79063
K	-5	HIS	-	EXPRESSION TAG	UNP P79063
K	-4	HIS	-	EXPRESSION TAG	UNP P79063
K	-3	HIS	-	EXPRESSION TAG	UNP P79063
K	-2	HIS	-	EXPRESSION TAG	UNP P79063

*Continued on next page...*

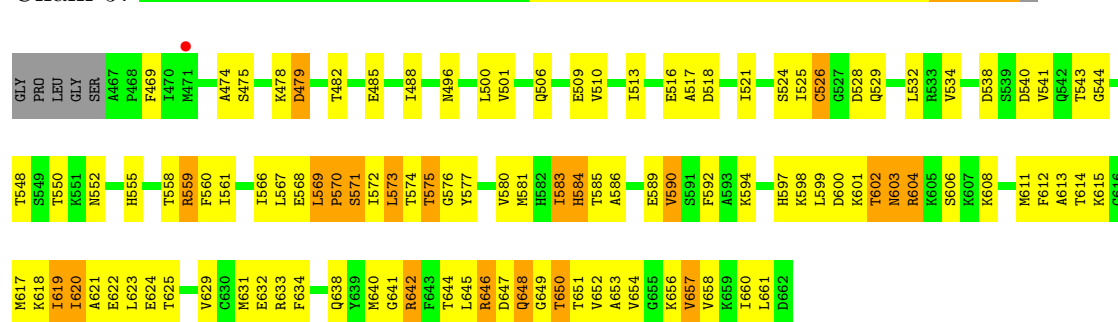
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	EXPRESSION TAG	UNP P79063
K	0	MET	-	EXPRESSION TAG	UNP P79063



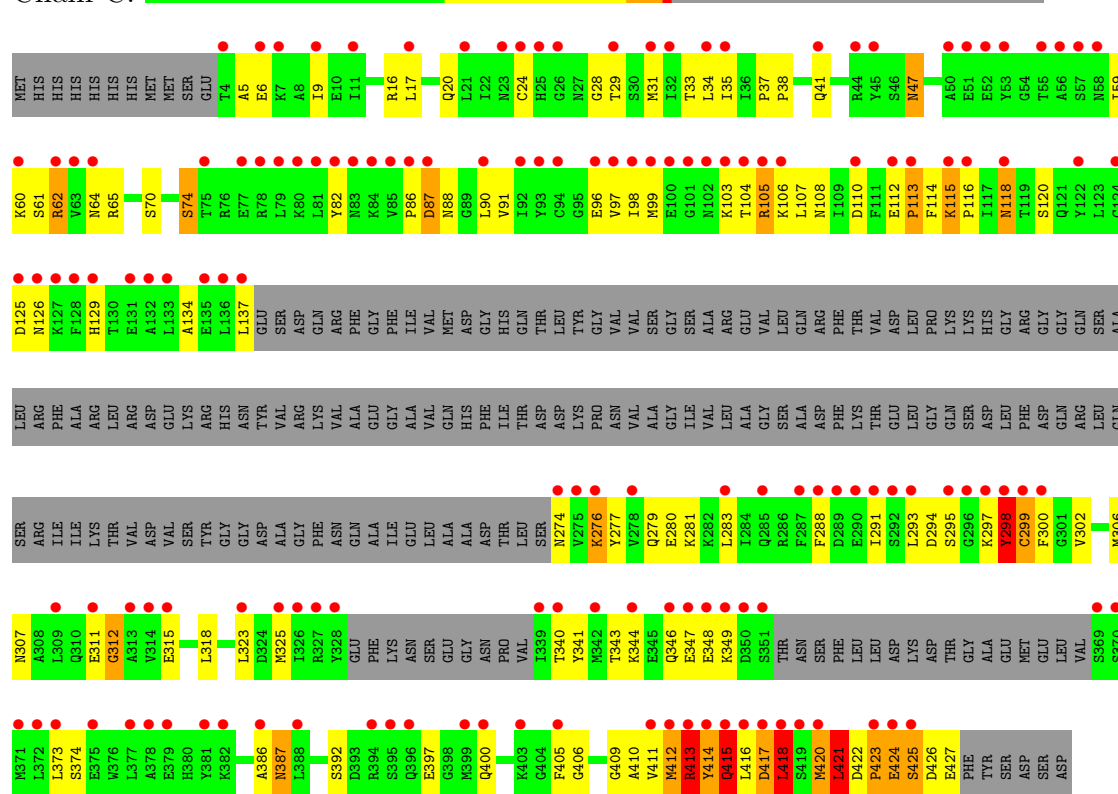
- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit

Chain J:



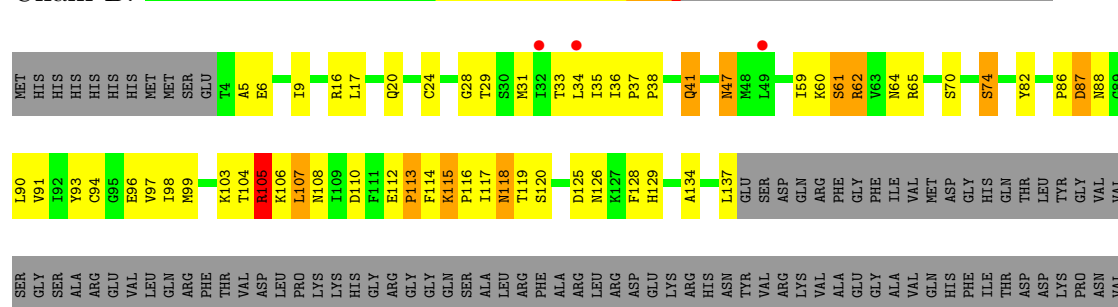
- Molecule 2: Eukaryotic peptide chain release factor subunit 1

Chain C:



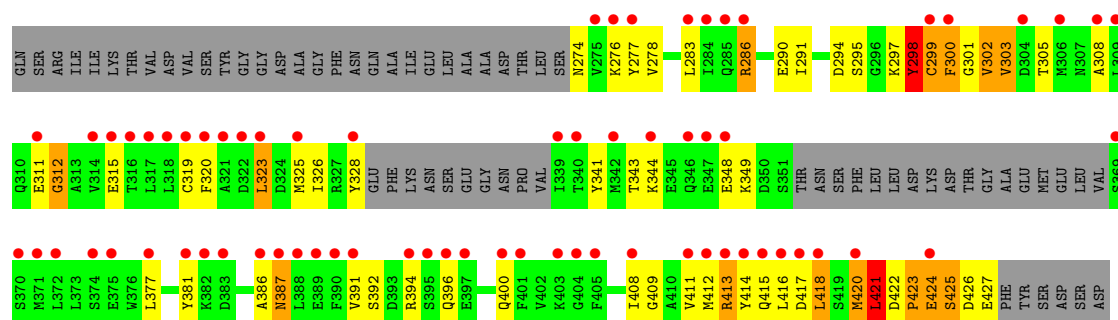
- Molecule 2: Eukaryotic peptide chain release factor subunit 1

Chain B:









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.85Å 129.85Å 332.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50 88.51 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-3.50) 99.7 (88.51-3.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, $R_{free}$	0.258 , 0.280 0.273 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	123.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 156.5	EDS
Estimated twinning fraction	0.439 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 68782 reflections	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	13096	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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	0.36	0/1547	0.57	1/2089 (0.0%)
1	D	0.36	0/1547	0.55	0/2089
1	E	0.49	0/1547	0.63	1/2089 (0.0%)
1	J	0.48	1/1547 (0.1%)	0.65	1/2089 (0.0%)
2	B	0.34	0/2119	0.61	6/2848 (0.2%)
2	C	0.34	0/2119	0.63	7/2848 (0.2%)
2	H	0.34	0/1425	0.55	1/1901 (0.1%)
2	K	0.34	0/1425	0.56	1/1901 (0.1%)
All	All	0.38	1/13276 (0.0%)	0.60	18/17854 (0.1%)

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	2
1	D	0	2
1	E	0	3
1	J	0	1
2	B	0	1
2	C	0	1
2	H	0	1
2	K	0	1
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	646	ARG	CB-CG	-5.26	1.38	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	413	ARG	NE-CZ-NH2	9.76	125.18	120.30
2	B	105	ARG	CG-CD-NE	8.50	129.65	111.80
2	C	413	ARG	NE-CZ-NH2	-8.02	116.29	120.30
2	C	413	ARG	NE-CZ-NH1	7.61	124.11	120.30
2	B	413	ARG	NE-CZ-NH1	-7.29	116.66	120.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	569	LEU	Peptide
1	A	647	ASP	Peptide
2	C	413	ARG	Peptide
1	D	569	LEU	Peptide
1	D	647	ASP	Peptide

## 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	1524	0	1569	89	0
1	D	1524	0	1569	92	0
1	E	1524	0	1569	117	0
1	J	1524	0	1569	104	0
2	B	2088	0	2077	144	0
2	C	2088	0	2077	133	0
2	H	1412	0	1388	117	0
2	K	1412	0	1388	86	0
All	All	13096	0	13206	878	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 33.

The worst 5 of 878 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:425:SER:CB	2:B:426:ASP:HA	1.52	1.38

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:414:TYR:CE2	2:H:416:LEU:HD11	1.60	1.36
2:C:425:SER:CB	2:C:426:ASP:HA	1.52	1.34
2:H:425:SER:CB	2:H:426:ASP:HA	1.51	1.29
2:K:425:SER:CB	2:K:426:ASP:HA	1.52	1.23

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	194/201 (96%)	170 (88%)	20 (10%)	4 (2%)	11	62
1	D	194/201 (96%)	170 (88%)	20 (10%)	4 (2%)	11	62
1	E	194/201 (96%)	164 (84%)	23 (12%)	7 (4%)	5	49
1	J	194/201 (96%)	166 (86%)	23 (12%)	5 (3%)	8	57
2	B	253/441 (57%)	201 (79%)	33 (13%)	19 (8%)	2	24
2	C	253/441 (57%)	203 (80%)	31 (12%)	19 (8%)	2	24
2	H	155/441 (35%)	113 (73%)	30 (19%)	12 (8%)	1	22
2	K	155/441 (35%)	114 (74%)	31 (20%)	10 (6%)	2	29
All	All	1592/2568 (62%)	1301 (82%)	211 (13%)	80 (5%)	3	37

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	479	ASP
1	A	575	THR
1	A	648	GLN
2	C	87	ASP
2	C	299	CYS

### 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	172/175 (98%)	153 (89%)	19 (11%)	9	43
1	D	172/175 (98%)	151 (88%)	21 (12%)	7	36
1	E	172/175 (98%)	144 (84%)	28 (16%)	3	21
1	J	172/175 (98%)	145 (84%)	27 (16%)	4	23
2	B	232/383 (61%)	208 (90%)	24 (10%)	10	47
2	C	232/383 (61%)	210 (90%)	22 (10%)	12	51
2	H	154/383 (40%)	144 (94%)	10 (6%)	24	71
2	K	154/383 (40%)	141 (92%)	13 (8%)	16	59
All	All	1460/2232 (65%)	1296 (89%)	164 (11%)	9	41

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

Mol	Chain	Res	Type
2	B	298	TYR
1	E	543	THR
2	K	78	ARG
2	B	323	LEU
2	B	418	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	555	HIS
2	B	88	ASN
1	J	555	HIS
1	D	563	GLN
1	D	584	HIS

### 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	196/201 (97%)	0.99	20 (10%) 7 5	69, 77, 80, 82	0
1	D	196/201 (97%)	0.68	5 (2%) 53 24	69, 77, 80, 82	0
1	E	196/201 (97%)	0.88	17 (8%) 10 6	49, 58, 67, 72	0
1	J	196/201 (97%)	0.57	1 (0%) 88 64	49, 58, 67, 72	0
2	B	261/441 (59%)	0.44	4 (1%) 70 36	66, 79, 83, 83	0
2	C	261/441 (59%)	3.13	149 (57%) 0 1	66, 79, 83, 83	0
2	H	175/441 (39%)	0.46	9 (5%) 27 11	66, 83, 116, 122	0
2	K	175/441 (39%)	1.96	74 (42%) 1 1	66, 83, 118, 138	0
All	All	1656/2568 (64%)	1.19	279 (16%) 2 2	49, 77, 98, 138	0

The worst 5 of 279 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	99	MET	25.0
2	C	326	ILE	12.4
2	C	371	MET	11.6
2	C	328	TYR	11.0
2	C	104	THR	10.6

### 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.