



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 10:28 AM BST

PDB ID : 6XJF  
Title : X-ray crystal structure of Pyrococcus furiosus general transcription factor  
TFE-alpha (SeMet labeled protein)  
Authors : Murakami, K.S.; Jun, S.H.  
Deposited on : 2020-06-23  
Resolution : 3.20 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

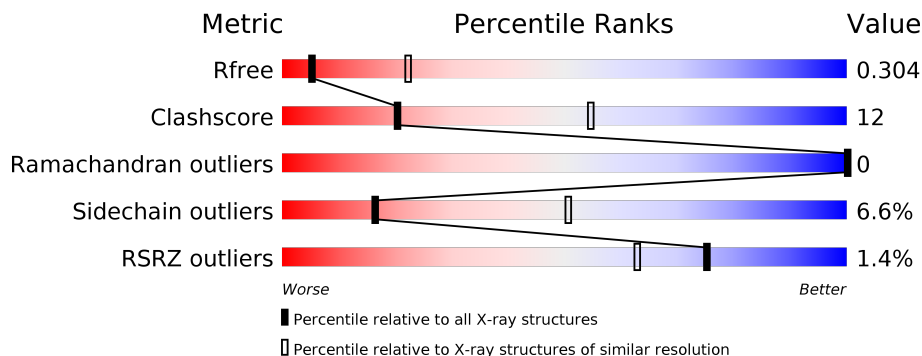
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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.



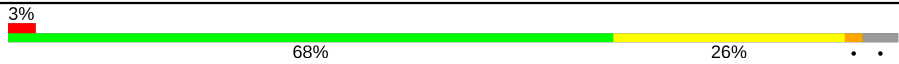

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 respectively. 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	110	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div>
1	B	110	<div style="display: flex; align-items: center;"> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div>
1	C	110	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div>
1	D	110	<div style="display: flex; align-items: center;"> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div>
1	E	110	<div style="display: flex; align-items: center;"> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div>
1	F	110	<div style="display: flex; align-items: center;"> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
1	G	110	
1	H	110	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 6810 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 Transcription factor E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	102	842	531	147	160	4	0	0	0
1	B	103	850	535	149	162	4	0	0	0
1	C	103	850	535	149	162	4	0	0	0
1	D	102	842	531	147	160	4	0	0	0
1	E	103	850	535	149	162	4	0	0	0
1	F	103	850	535	149	162	4	0	0	0
1	G	106	876	551	154	167	4	0	0	0
1	H	103	850	535	149	162	4	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MSE	ILE	conflict	UNP Q8U3H5
A	54	MSE	ILE	conflict	UNP Q8U3H5
A	66	MSE	PHE	conflict	UNP Q8U3H5
B	13	MSE	ILE	conflict	UNP Q8U3H5
B	54	MSE	ILE	conflict	UNP Q8U3H5
B	66	MSE	PHE	conflict	UNP Q8U3H5
C	13	MSE	ILE	conflict	UNP Q8U3H5
C	54	MSE	ILE	conflict	UNP Q8U3H5
C	66	MSE	PHE	conflict	UNP Q8U3H5
D	13	MSE	ILE	conflict	UNP Q8U3H5
D	54	MSE	ILE	conflict	UNP Q8U3H5
D	66	MSE	PHE	conflict	UNP Q8U3H5
E	13	MSE	ILE	conflict	UNP Q8U3H5

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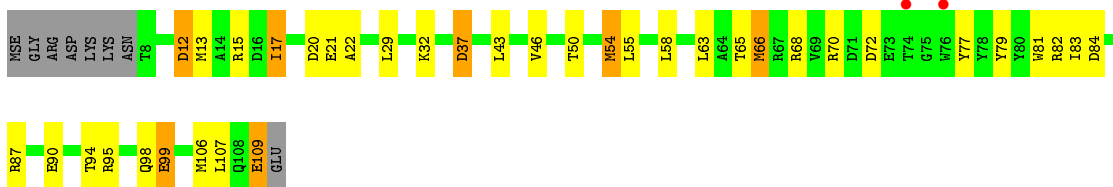
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<b>Chain</b>	<b>Residue</b>	<b>Modelled</b>	<b>Actual</b>	<b>Comment</b>	<b>Reference</b>
E	54	MSE	ILE	conflict	UNP Q8U3H5
E	66	MSE	PHE	conflict	UNP Q8U3H5
F	13	MSE	ILE	conflict	UNP Q8U3H5
F	54	MSE	ILE	conflict	UNP Q8U3H5
F	66	MSE	PHE	conflict	UNP Q8U3H5
G	13	MSE	ILE	conflict	UNP Q8U3H5
G	54	MSE	ILE	conflict	UNP Q8U3H5
G	66	MSE	PHE	conflict	UNP Q8U3H5
H	13	MSE	ILE	conflict	UNP Q8U3H5
H	54	MSE	ILE	conflict	UNP Q8U3H5
H	66	MSE	PHE	conflict	UNP Q8U3H5

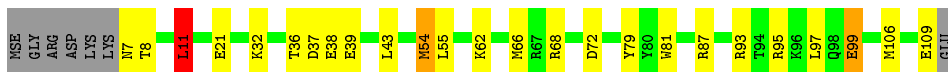
### 3 Residue-property plots [i](#)

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

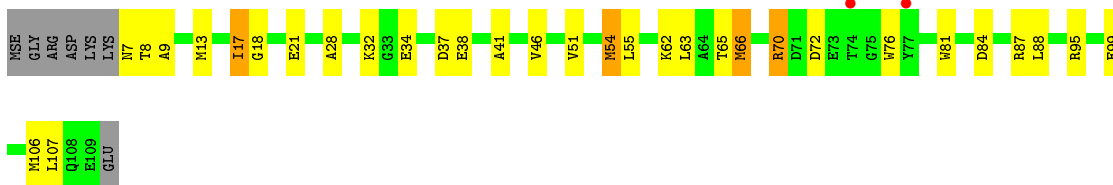
- Molecule 1: Transcription factor E



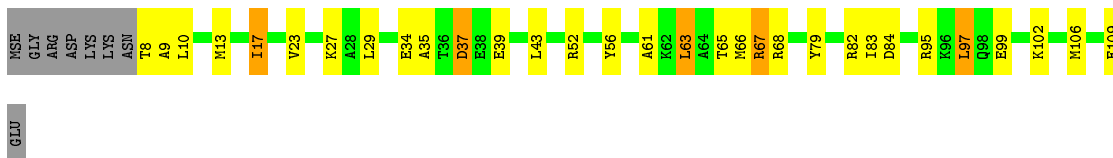
- Molecule 1: Transcription factor E



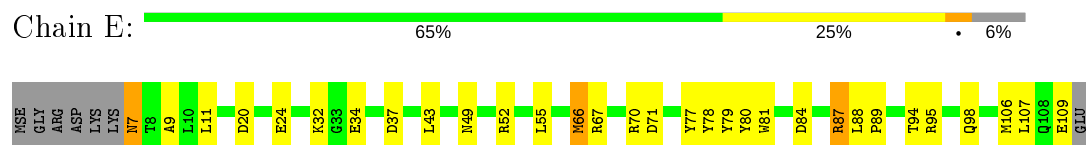
- Molecule 1: Transcription factor E



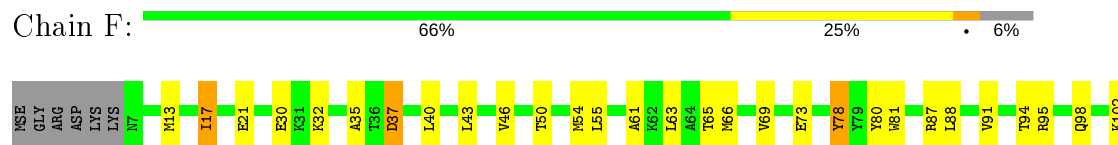
- Molecule 1: Transcription factor E



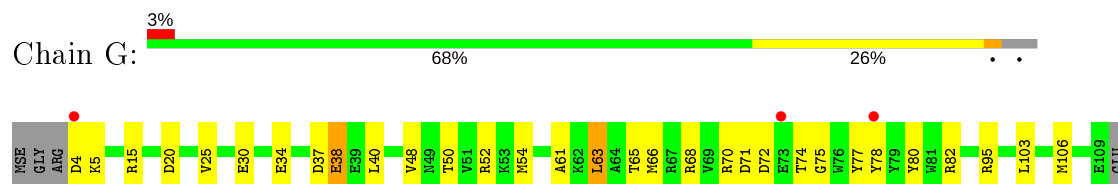
- Molecule 1: Transcription factor E



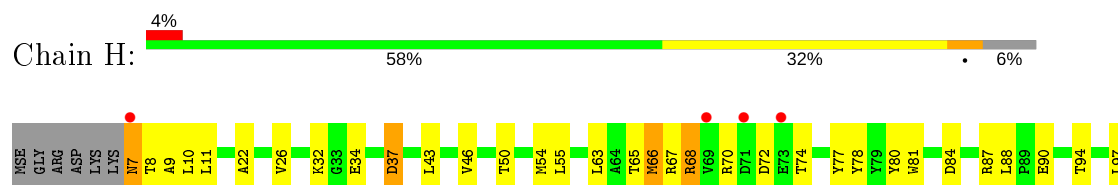
- Molecule 1: Transcription factor E



- Molecule 1: Transcription factor E



- Molecule 1: Transcription factor E



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.20Å 115.61Å 124.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.44 – 3.20 46.05 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.44-3.20) 97.7 (46.05-3.20)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.237 , 0.304 0.237 , 0.304	Depositor DCC
$R_{free}$ test set	1359 reflections (7.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.7	Xtrriage
Anisotropy	0.331	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 8.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6810	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.54	0/848	1.02	2/1133 (0.2%)
1	B	0.65	0/856	1.04	3/1144 (0.3%)
1	C	0.66	0/856	1.12	5/1144 (0.4%)
1	D	0.64	0/848	0.99	2/1133 (0.2%)
1	E	0.60	0/856	0.92	0/1144
1	F	0.68	0/856	0.97	1/1144 (0.1%)
1	G	0.75	1/882 (0.1%)	1.00	2/1177 (0.2%)
1	H	0.58	0/856	0.91	1/1144 (0.1%)
All	All	0.64	1/6858 (0.0%)	1.00	16/9163 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	38	GLU	CB-CG	-6.19	1.40	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	97	LEU	CB-CG-CD2	-7.07	98.99	111.00
1	C	38	GLU	N-CA-CB	-6.79	98.37	110.60
1	C	63	LEU	CA-CB-CG	6.32	129.83	115.30
1	D	63	LEU	CA-CB-CG	6.30	129.79	115.30
1	C	38	GLU	CA-CB-CG	6.06	126.72	113.40

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	842	0	861	32	0
1	B	850	0	867	23	0
1	C	850	0	867	18	0
1	D	842	0	861	25	0
1	E	850	0	867	21	0
1	F	850	0	867	23	0
1	G	876	0	897	15	1
1	H	850	0	867	33	1
All	All	6810	0	6954	171	1

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 12.

The worst 5 of 171 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:G:65:THR:OG1	1:G:82:ARG:NH2	2.09	0.85
1:D:29:LEU:HD21	1:D:82:ARG:HA	1.64	0.80
1:B:36:THR:HG22	1:B:39:GLU:HG3	1.62	0.78
1:F:13:MSE:HE2	1:F:63:LEU:HD11	1.66	0.75
1:C:18:GLY:HA3	1:C:54:MSE:HE1	1.69	0.75

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:68:ARG:NH2	1:H:74:THR:O[4_534]	2.03	0.17

## 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	100/110 (91%)	99 (99%)	1 (1%)	0	100	100
1	B	101/110 (92%)	100 (99%)	1 (1%)	0	100	100
1	C	101/110 (92%)	98 (97%)	3 (3%)	0	100	100
1	D	100/110 (91%)	100 (100%)	0	0	100	100
1	E	101/110 (92%)	99 (98%)	2 (2%)	0	100	100
1	F	101/110 (92%)	98 (97%)	3 (3%)	0	100	100
1	G	104/110 (94%)	102 (98%)	2 (2%)	0	100	100
1	H	101/110 (92%)	101 (100%)	0	0	100	100
All	All	809/880 (92%)	797 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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

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	88/90 (98%)	81 (92%)	7 (8%)	12	42
1	B	89/90 (99%)	83 (93%)	6 (7%)	16	50
1	C	89/90 (99%)	81 (91%)	8 (9%)	9	34
1	D	88/90 (98%)	83 (94%)	5 (6%)	20	56
1	E	89/90 (99%)	85 (96%)	4 (4%)	27	63
1	F	89/90 (99%)	84 (94%)	5 (6%)	21	57
1	G	92/90 (102%)	86 (94%)	6 (6%)	17	51
1	H	89/90 (99%)	83 (93%)	6 (7%)	16	50
All	All	713/720 (99%)	666 (93%)	47 (7%)	16	51

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	17	ILE
1	E	7	ASN

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Mol	Chain	Res	Type
1	H	37	ASP
1	D	66	MSE
1	E	37	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	7	ASN

### 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 monosaccharides 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	98/110 (89%)	0.14	2 (2%) 65 51	49, 107, 134, 146	0
1	B	99/110 (90%)	-0.22	0 100 100	49, 69, 90, 94	0
1	C	99/110 (90%)	-0.00	2 (2%) 65 51	50, 73, 148, 164	0
1	D	98/110 (89%)	-0.12	0 100 100	49, 75, 136, 150	0
1	E	99/110 (90%)	-0.14	0 100 100	56, 80, 105, 120	0
1	F	99/110 (90%)	-0.18	0 100 100	52, 70, 90, 107	0
1	G	102/110 (92%)	0.09	3 (2%) 51 36	46, 72, 105, 121	0
1	H	99/110 (90%)	0.00	4 (4%) 38 25	60, 96, 147, 167	0
All	All	793/880 (90%)	-0.05	11 (1%) 75 63	46, 76, 126, 167	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	77	TYR	3.8
1	G	78	TYR	3.4
1	H	71	ASP	3.1
1	G	73	GLU	3.0
1	H	69	VAL	2.9

### 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 monosaccharides 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.