



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:23 PM GMT

PDB ID : 1AIP
Title : EF-TU EF-TS COMPLEX FROM THERMUS THERMOPHILUS
Authors : Wang, Y.; Jiang, Y.; Meyering-Voss, M.; Sprinzl, M.; Sigler, P.B.
Deposited on : 1997-04-22
Resolution : 3.00 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
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 : 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

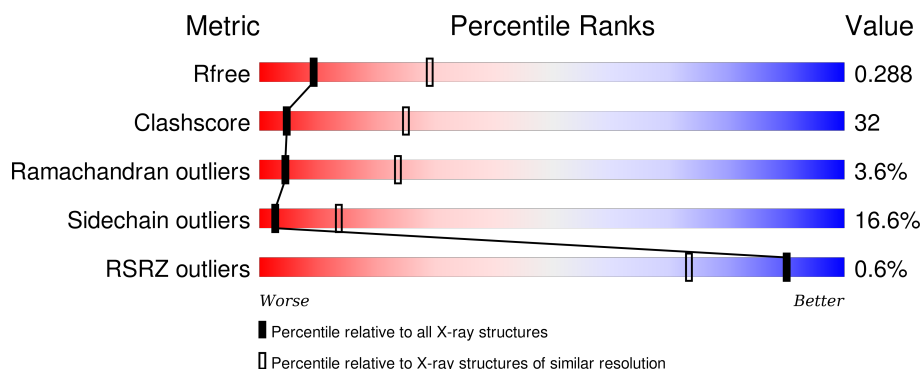
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 ≥ 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	405	
1	B	405	
1	E	405	
1	F	405	
2	C	196	

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Mol	Chain	Length	Quality of chain
2	D	196	<div><div></div><div>44%44%10%..</div></div>
2	G	196	<div><div></div><div>45%42%12%..</div></div>
2	H	196	<div><div></div><div>45%42%11%..</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17575 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 ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2865	1810	503	541	11			
1	B	373	Total	C	N	O	S	0	0	0
			2859	1807	495	545	12			
1	E	372	Total	C	N	O	S	0	0	0
			2869	1812	502	543	12			
1	F	372	Total	C	N	O	S	0	0	0
			2841	1792	495	542	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	THR	ALA	CONFLICT	UNP P60338
B	35	THR	ALA	CONFLICT	UNP P60338
E	35	THR	ALA	CONFLICT	UNP P60338
F	35	THR	ALA	CONFLICT	UNP P60338

- Molecule 2 is a protein called ELONGATION FACTOR TS.

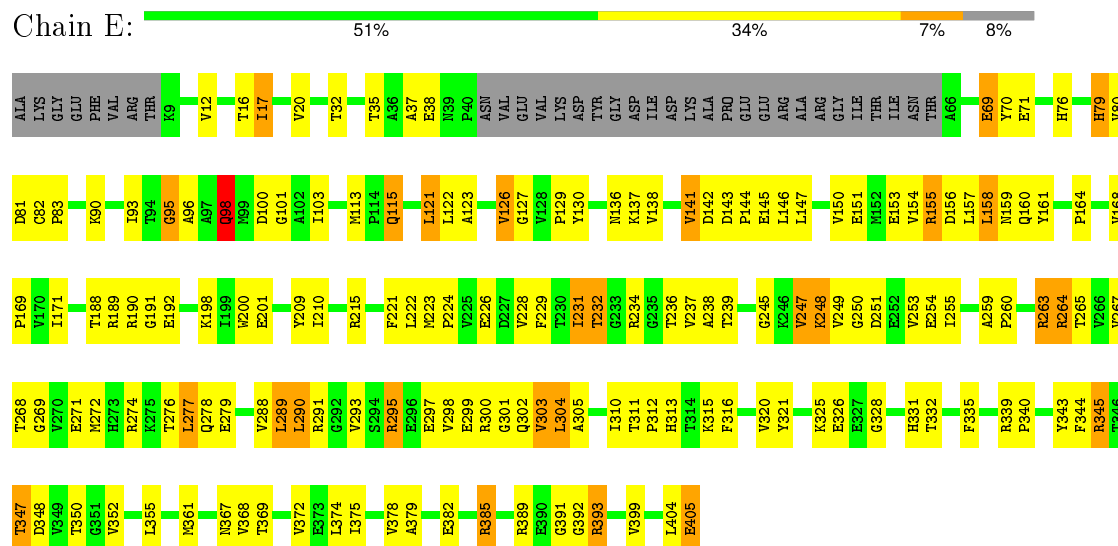
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	195	Total	C	N	O	S	0	0	0
			1544	969	276	290	9			
2	D	195	Total	C	N	O	S	0	0	0
			1513	952	268	284	9			
2	G	195	Total	C	N	O	S	0	0	0
			1546	970	279	288	9			
2	H	194	Total	C	N	O	S	0	0	0
			1523	957	274	283	9			

- Molecule 3 is water.

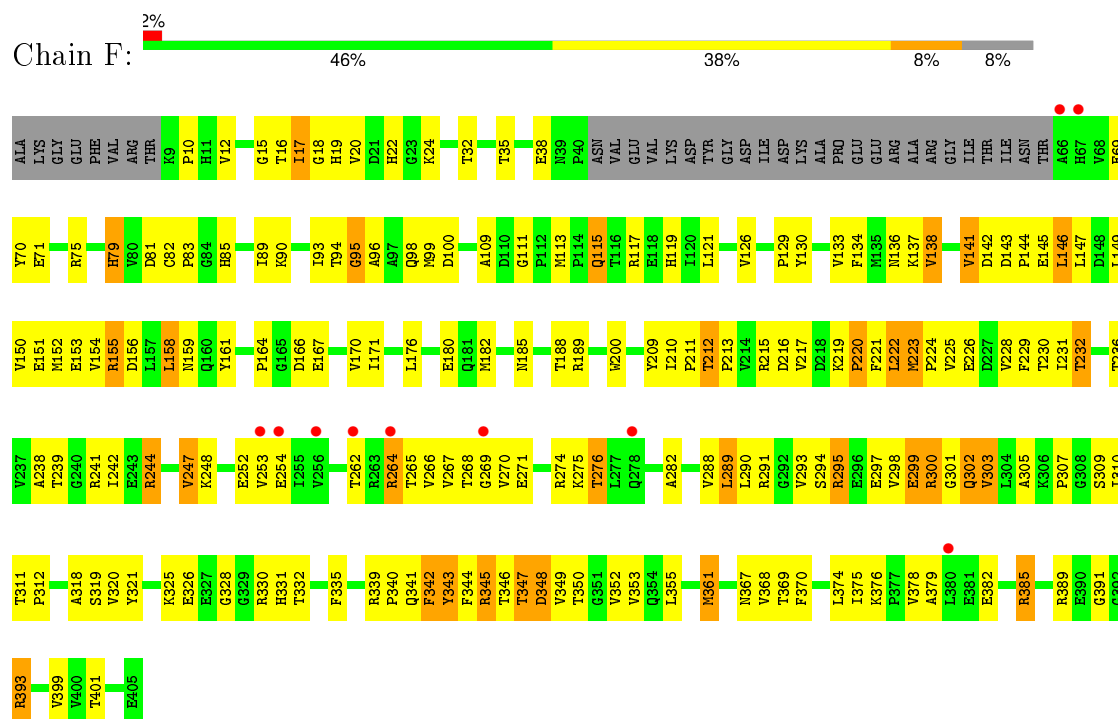
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	O 2	0	0
3	C	1	Total 1	O 1	0	0
3	D	4	Total 4	O 4	0	0
3	E	3	Total 3	O 3	0	0
3	G	4	Total 4	O 4	0	0
3	H	1	Total 1	O 1	0	0



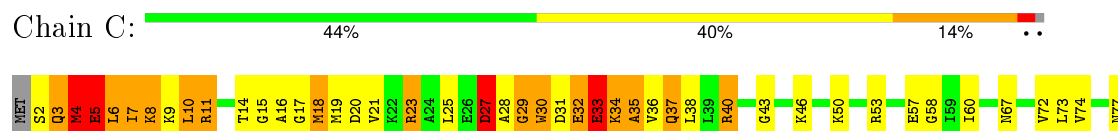
• Molecule 1: ELONGATION FACTOR TU

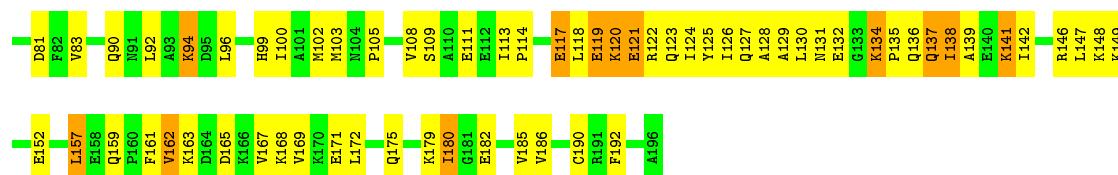


• Molecule 1: ELONGATION FACTOR TU



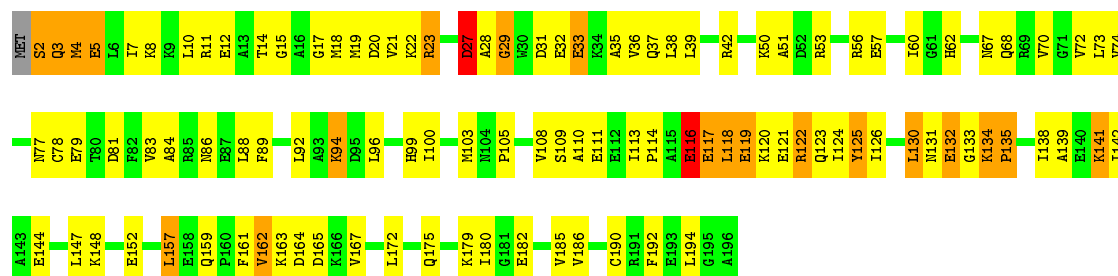
• Molecule 2: ELONGATION FACTOR TS





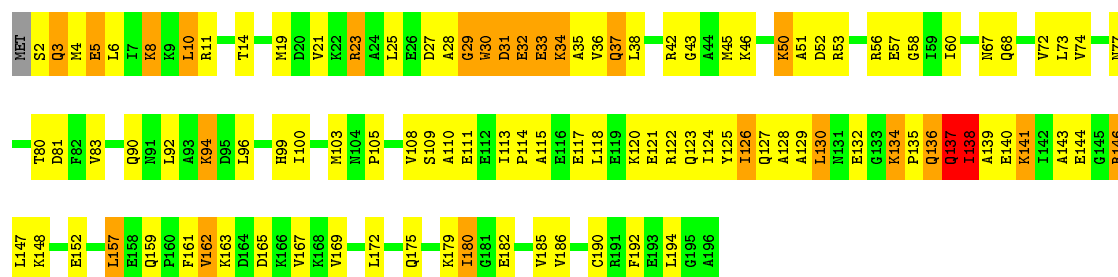
• Molecule 2: ELONGATION FACTOR TS

Chain D: 44% 44% 10% ..



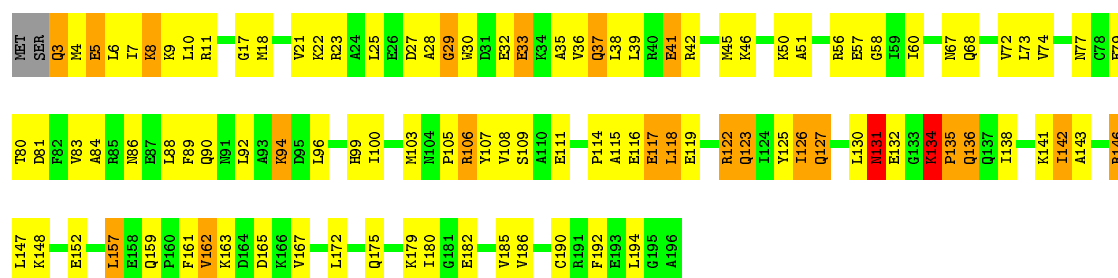
• Molecule 2: ELONGATION FACTOR TS

Chain G: 45% 42% 12% ..



• Molecule 2: ELONGATION FACTOR TS

Chain H: 45% 42% 11% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.30Å 127.50Å 123.70Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	100.00 – 3.00 44.39 – 2.78	Depositor EDS
% Data completeness (in resolution range)	92.0 (100.00-3.00) 90.2 (44.39-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.77Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.216 , 0.289 0.229 , 0.288	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.890	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.3	EDS
Estimated twinning fraction	0.011 for l,k,-h 0.100 for h,-k,-l 0.017 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 84816 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17575	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.49	1/2922 (0.0%)	0.68	0/3974
1	B	0.43	1/2915 (0.0%)	0.65	0/3965
1	E	0.49	1/2926 (0.0%)	0.69	0/3977
1	F	0.46	1/2897 (0.0%)	0.66	0/3941
2	C	0.43	0/1562	0.66	0/2094
2	D	0.41	0/1531	0.63	0/2056
2	G	0.44	0/1564	0.64	0/2096
2	H	0.43	0/1541	0.63	0/2067
All	All	0.45	4/17858 (0.0%)	0.66	0/24170

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	71	GLU	CD-OE2	7.53	1.33	1.25
1	B	71	GLU	CD-OE2	7.42	1.33	1.25
1	A	71	GLU	CD-OE2	6.74	1.33	1.25
1	E	71	GLU	CD-OE2	6.67	1.32	1.25

There are no bond angle outliers.

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	2865	0	2847	168	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2859	0	2835	218	0
1	E	2869	0	2855	153	0
1	F	2841	0	2802	172	0
2	C	1544	0	1558	127	0
2	D	1513	0	1507	119	0
2	G	1546	0	1565	110	0
2	H	1523	0	1530	103	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	D	4	0	0	0	0
3	E	3	0	0	0	0
3	G	4	0	0	0	0
3	H	1	0	0	0	0
All	All	17575	0	17499	1122	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 32.

The worst 5 of 1122 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:264:ARG:HG2	1:B:264:ARG:HH11	1.19	1.07
1:F:95:GLY:HA2	1:F:385:ARG:HH21	1.18	1.04
1:A:341:GLN:HB3	1:A:343:TYR:HE1	1.25	1.02
1:B:228:VAL:HG21	1:B:298:VAL:HG12	1.42	1.01
1:B:75:ARG:HH11	1:B:212:THR:HG23	1.26	1.00

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	369/405 (91%)	327 (89%)	34 (9%)	8 (2%)	8	38
1	B	369/405 (91%)	308 (84%)	46 (12%)	15 (4%)	3	20
1	E	368/405 (91%)	319 (87%)	39 (11%)	10 (3%)	6	32
1	F	368/405 (91%)	308 (84%)	46 (12%)	14 (4%)	4	22
2	C	193/196 (98%)	164 (85%)	20 (10%)	9 (5%)	3	17
2	D	193/196 (98%)	161 (83%)	25 (13%)	7 (4%)	4	24
2	G	193/196 (98%)	162 (84%)	20 (10%)	11 (6%)	2	12
2	H	192/196 (98%)	165 (86%)	20 (10%)	7 (4%)	4	24
All	All	2245/2404 (93%)	1914 (85%)	250 (11%)	81 (4%)	4	24

5 of 81 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	THR
1	B	67	HIS
1	B	232	THR
1	B	276	THR
2	C	29	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	306/339 (90%)	266 (87%)	40 (13%)	5	22
1	B	306/339 (90%)	256 (84%)	50 (16%)	3	14
1	E	308/339 (91%)	270 (88%)	38 (12%)	6	25
1	F	302/339 (89%)	254 (84%)	48 (16%)	3	15
2	C	157/162 (97%)	121 (77%)	36 (23%)	1	5
2	D	150/162 (93%)	119 (79%)	31 (21%)	1	7
2	G	157/162 (97%)	129 (82%)	28 (18%)	2	11
2	H	152/162 (94%)	118 (78%)	34 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1838/2004 (92%)	1533 (83%)	305 (17%)	3 13

5 of 305 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	56	ARG
1	E	158	LEU
2	H	56	ARG
2	D	118	LEU
2	D	175	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	90	GLN
1	E	79	HIS
2	G	99	HIS
2	D	99	HIS
2	D	183	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	373/405 (92%)	-0.73	1 (0%) 94 84	25, 50, 91, 109	0
1	B	373/405 (92%)	-0.44	2 (0%) 91 76	45, 94, 109, 110	0
1	E	372/405 (91%)	-0.74	0 100 100	20, 46, 84, 110	0
1	F	372/405 (91%)	-0.21	10 (2%) 58 28	34, 96, 110, 110	0
2	C	195/196 (99%)	-0.80	0 100 100	23, 60, 90, 100	0
2	D	195/196 (99%)	-0.68	0 100 100	31, 75, 109, 110	0
2	G	195/196 (99%)	-0.80	0 100 100	18, 49, 91, 104	0
2	H	194/196 (98%)	-0.66	0 100 100	23, 76, 109, 110	0
All	All	2269/2404 (94%)	-0.60	13 (0%) 90 73	18, 67, 109, 110	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	253	VAL	6.7
1	F	66	ALA	5.5
1	B	253	VAL	5.0
1	F	262	THR	3.5
1	B	65	THR	2.5

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.