



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 07:59 PM EDT

PDB ID : 1THI  
Title : ESCHERICHIA COLI HEAT LABILE ENTEROTOXIN TYPE IIB  
Authors : Van Den Akker, F.; Hol, W.G.J.  
Deposited on : 1996-03-20  
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

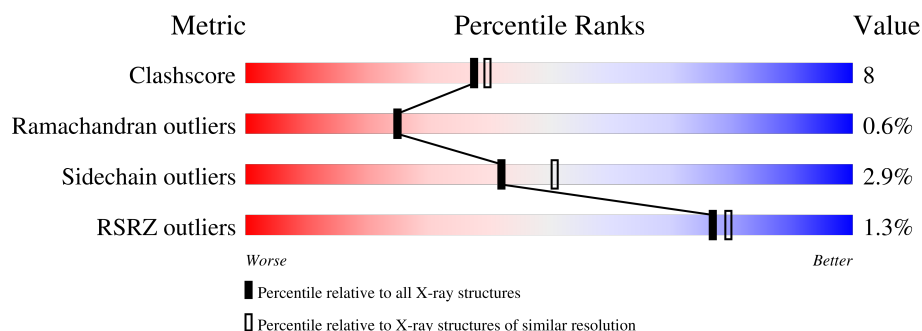
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 of 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	D	99	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	E	99	<div> <div>3%</div> <div>71%</div> <div>25%</div> <div>..</div> </div>
1	F	99	<div> <div>4%</div> <div>69%</div> <div>27%</div> <div>..</div> </div>
1	G	99	<div> <div>76%</div> <div>21%</div> <div>...</div> </div>
1	H	99	<div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	A	190	<div> <div>%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	53	 A horizontal bar chart showing the quality of chain C. The bar is divided into four segments: a small red segment at the beginning labeled '2%', followed by a green segment labeled '53%', a yellow segment labeled '15%', and a grey segment at the end labeled '32%'. The total length of the bar represents 100%.

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5684 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 HEAT LABILE ENTEROTOXIN TYPE IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	98	Total	C	N	O	S	0	0	0
			740	458	128	146	8			
1	E	98	Total	C	N	O	S	0	0	0
			740	458	128	146	8			
1	F	98	Total	C	N	O	S	0	0	0
			740	458	128	146	8			
1	G	98	Total	C	N	O	S	0	0	0
			740	458	128	146	8			
1	H	98	Total	C	N	O	S	0	0	0
			740	458	128	146	8			

- Molecule 2 is a protein called HEAT LABILE ENTEROTOXIN TYPE IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	186	Total	C	N	O	S	0	0	0
			1479	930	266	280	3			

- Molecule 3 is a protein called HEAT LABILE ENTEROTOXIN TYPE IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	36	Total	C	N	O	S	0	0	0
			290	185	50	53	2			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	34	Total	O	0	0
			34	34		
4	E	20	Total	O	0	0
			20	20		
4	F	14	Total	O	0	0
			14	14		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	17	Total 17	O 17	0	0
4	H	35	Total 35	O 35	0	0
4	A	80	Total 80	O 80	0	0
4	C	15	Total 15	O 15	0	0

### 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: HEAT LABILE ENTEROTOXIN TYPE IIB

Chain D: 



- Molecule 1: HEAT LABILE ENTEROTOXIN TYPE IIB

Chain E: 




- Molecule 1: HEAT LABILE ENTEROTOXIN TYPE IIB

Chain F: 




- Molecule 1: HEAT LABILE ENTEROTOXIN TYPE IIB

Chain G: 




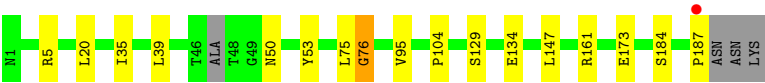
- Molecule 1: HEAT LABILE ENTEROTOXIN TYPE IIB

Chain H: 



- Molecule 2: HEAT LABILE ENTEROTOXIN TYPE IIB

Chain A: 



● Molecule 3: HEAT LABILE ENTEROTOXIN TYPE IIB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.70Å 105.70Å 171.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.25 50.51 – 2.25	Depositor EDS
% Data completeness (in resolution range)	82.4 (10.00-2.25) 83.1 (50.51-2.25)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.25Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.191 , 0.266 0.179 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 71.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5684	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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	D	0.54	0/751	0.75	0/1017
1	E	0.53	0/751	0.72	0/1017
1	F	0.51	0/751	0.71	0/1017
1	G	0.53	0/751	0.75	0/1017
1	H	0.56	0/751	0.73	0/1017
2	A	0.54	0/1521	0.75	1/2069 (0.0%)
3	C	0.56	0/293	0.69	0/392
All	All	0.54	0/5569	0.73	1/7546 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	76	GLY	N-CA-C	-5.10	100.35	113.10

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	D	740	0	729	13	0
1	E	740	0	729	25	0
1	F	740	0	729	23	0
1	G	740	0	729	15	0
1	H	740	0	729	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1479	0	1380	10	0
3	C	290	0	306	7	0
4	A	80	0	0	3	0
4	C	15	0	0	0	0
4	D	34	0	0	2	0
4	E	20	0	0	1	0
4	F	14	0	0	2	0
4	G	17	0	0	0	0
4	H	35	0	0	0	0
All	All	5684	0	5331	83	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 8.

All (83) 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:23:LEU:HD13	1:F:39:VAL:HG21	1.62	0.79
1:G:66:LYS:HE3	3:C:226:LEU:O	1.93	0.69
1:E:58:ASN:HD22	1:E:58:ASN:N	1.96	0.62
1:E:48:ARG:HD3	4:E:118:HOH:O	1.99	0.62
1:F:40:VAL:HG22	1:F:46:VAL:HG22	1.81	0.62
1:E:38:TYR:CD1	1:E:48:ARG:HB3	2.36	0.61
2:A:173:GLU:HG2	2:A:187:PRO:HG3	1.83	0.61
1:F:3:SER:HB2	4:F:113:HOH:O	2.01	0.60
1:G:67:ILE:HG23	1:G:96:LEU:HB2	1.84	0.60
1:E:40:VAL:HG22	1:E:46:VAL:HG22	1.84	0.59
1:G:48:ARG:HH21	1:G:51:ARG:NH1	2.01	0.59
1:E:58:ASN:HD22	1:E:58:ASN:H	1.52	0.58
1:E:55:TYR:HA	1:E:58:ASN:ND2	2.19	0.57
1:H:25:LYS:HB2	1:H:40:VAL:HB	1.85	0.57
2:A:50:ASN:HA	2:A:75:LEU:HD21	1.87	0.57
1:F:15:ALA:HB3	1:F:81:CYS:SG	2.45	0.56
1:D:67:ILE:HG23	1:D:96:LEU:HB2	1.88	0.55
1:E:12:ARG:CZ	1:F:33:ASN:HB3	2.37	0.55
1:D:85:ALA:HB3	4:D:130:HOH:O	2.06	0.54
1:E:22:GLU:HG2	1:E:42:SER:HB3	1.90	0.54
1:F:23:LEU:HD22	1:F:39:VAL:HG22	1.90	0.54
1:E:76:MET:SD	1:F:73:LEU:HD23	2.48	0.53
1:F:31:ASN:HB3	1:F:33:ASN:OD1	2.09	0.53
1:G:32:ASN:O	1:G:33:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:LYS:HB2	1:F:40:VAL:HB	1.91	0.52
1:D:9:ASN:CG	1:E:34:THR:HG21	2.31	0.51
2:A:104:PRO:HD2	4:A:202:HOH:O	2.11	0.51
1:E:12:ARG:HH11	1:E:13:THR:HG22	1.76	0.50
1:G:63:GLU:O	1:G:67:ILE:HG13	2.12	0.50
1:D:83:SER:HB2	1:D:92:TRP:CZ2	2.46	0.49
1:G:12:ARG:HH12	1:H:34:THR:HG21	1.77	0.49
1:F:50:SER:O	1:F:61:THR:HB	2.12	0.49
1:G:9:ASN:HA	1:G:12:ARG:NH1	2.28	0.49
1:E:84:PRO:HA	1:E:89:ASN:ND2	2.27	0.48
2:A:173:GLU:CG	2:A:187:PRO:HG3	2.43	0.48
1:F:55:TYR:CD1	1:F:56:PRO:HA	2.49	0.48
1:G:29:ASP:O	1:G:35:ASP:HA	2.14	0.48
1:E:12:ARG:C	1:E:12:ARG:HD3	2.34	0.47
1:G:70:ALA:HB2	3:C:226:LEU:HD21	1.96	0.47
1:D:25:LYS:HA	1:H:96:LEU:O	2.15	0.47
1:G:73:LEU:HD22	3:C:222:LEU:HD21	1.97	0.47
1:D:76:MET:CE	1:D:98:ALA:HA	2.45	0.47
1:E:38:TYR:CE1	1:E:48:ARG:HB3	2.50	0.46
1:F:12:ARG:HB3	1:F:12:ARG:NH1	2.31	0.46
1:G:13:THR:HG21	1:H:31:ASN:CG	2.35	0.46
1:F:76:MET:CE	1:F:98:ALA:HA	2.46	0.45
1:H:2:ALA:HB3	1:H:7:LYS:HG3	1.99	0.45
2:A:129:SER:HB3	2:A:134:GLU:CG	2.47	0.44
1:D:83:SER:HA	1:D:84:PRO:HD3	1.80	0.44
1:E:55:TYR:CG	1:F:53:LYS:HD3	2.53	0.44
1:E:55:TYR:CG	1:E:56:PRO:HA	2.53	0.44
1:D:9:ASN:OD1	1:E:34:THR:HG21	2.18	0.43
1:E:41:SER:HB3	1:E:47:TRP:HZ3	1.83	0.43
1:E:74:SER:O	3:C:217:LYS:HE3	2.18	0.43
3:C:200:LEU:O	3:C:204:LEU:HG	2.17	0.43
2:A:35:ILE:HG12	4:A:239:HOH:O	2.18	0.42
1:D:65:ARG:HD3	4:D:108:HOH:O	2.19	0.42
1:E:2:ALA:HB3	1:E:7:LYS:HG3	2.00	0.42
1:D:34:THR:HG21	1:H:9:ASN:CG	2.40	0.42
1:D:96:LEU:O	1:E:25:LYS:HA	2.20	0.42
1:D:92:TRP:O	1:E:30:ILE:HG12	2.19	0.42
1:F:21:VAL:HG12	1:F:22:GLU:N	2.34	0.42
1:F:38:TYR:CE1	1:F:48:ARG:HG3	2.55	0.42
2:A:5:ARG:HD3	2:A:20:LEU:HD13	2.02	0.42
1:F:56:PRO:O	1:F:59:VAL:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:GLU:HG3	1:G:37:MET:SD	2.60	0.42
2:A:76:GLY:HA2	4:A:197:HOH:O	2.19	0.41
1:E:27:ILE:O	1:E:37:MET:HE3	2.20	0.41
1:F:78:VAL:HA	1:F:95:GLU:O	2.20	0.41
3:C:216:ILE:HD13	3:C:216:ILE:HA	1.92	0.41
1:H:40:VAL:HG22	1:H:46:VAL:HG22	2.02	0.41
1:E:9:ASN:CG	1:F:34:THR:HG21	2.42	0.41
2:A:147:LEU:HD21	3:C:220:PHE:HA	2.02	0.41
1:D:76:MET:HE2	1:D:98:ALA:HA	2.03	0.40
1:F:12:ARG:HB3	1:F:12:ARG:HH11	1.85	0.40
1:G:81:CYS:HB3	1:G:93:ALA:HB3	2.03	0.40
2:A:39:LEU:HD11	2:A:95:VAL:HG22	2.03	0.40
1:F:76:MET:HE3	1:F:98:ALA:HA	2.02	0.40
1:G:25:LYS:HB2	1:G:40:VAL:HB	2.03	0.40
1:E:40:VAL:HA	1:E:45:GLY:O	2.21	0.40
1:F:4:GLN:N	4:F:113:HOH:O	2.55	0.40
1:G:87:SER:HA	1:G:88:PRO:HA	1.93	0.40
1:H:64:MET:HG2	1:H:94:ILE:CG2	2.51	0.40

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	D	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
1	E	96/99 (97%)	93 (97%)	1 (1%)	2 (2%)	7	3
1	F	96/99 (97%)	90 (94%)	6 (6%)	0	100	100
1	G	96/99 (97%)	94 (98%)	1 (1%)	1 (1%)	15	13
1	H	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
2	A	182/190 (96%)	175 (96%)	6 (3%)	1 (0%)	29	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	34/53 (64%)	34 (100%)	0	0	100	100
All	All	696/738 (94%)	674 (97%)	18 (3%)	4 (1%)	25	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	33	ASN
1	E	32	ASN
1	E	35	ASP
2	A	184	SER

### 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	D	81/82 (99%)	79 (98%)	2 (2%)	47	56
1	E	81/82 (99%)	78 (96%)	3 (4%)	34	40
1	F	81/82 (99%)	77 (95%)	4 (5%)	25	27
1	G	81/82 (99%)	78 (96%)	3 (4%)	34	40
1	H	81/82 (99%)	79 (98%)	2 (2%)	47	56
2	A	149/152 (98%)	147 (99%)	2 (1%)	69	79
3	C	34/47 (72%)	33 (97%)	1 (3%)	42	51
All	All	588/609 (97%)	571 (97%)	17 (3%)	42	51

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	14	THR
1	D	87	SER
1	E	12	ARG
1	E	22	GLU
1	E	58	ASN
1	F	12	ARG

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Mol	Chain	Res	Type
1	F	22	GLU
1	F	34	THR
1	F	69	MET
1	G	22	GLU
1	G	32	ASN
1	G	33	ASN
1	H	32	ASN
1	H	51	ARG
2	A	53	TYR
2	A	161	ARG
3	C	195	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	11	ASN
1	D	33	ASN
1	D	89	ASN
1	E	11	ASN
1	E	58	ASN
1	E	89	ASN
1	G	4	GLN
1	G	11	ASN
1	G	32	ASN
1	G	89	ASN
1	H	11	ASN
1	H	32	ASN
1	H	89	ASN
2	A	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 [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 ⓘ

### 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	D	98/99 (98%)	-0.78	0 100 100	7, 24, 50, 68	0
1	E	98/99 (98%)	-0.40	3 (3%) 49 52	13, 32, 67, 73	0
1	F	98/99 (98%)	-0.36	4 (4%) 37 40	19, 38, 66, 72	0
1	G	98/99 (98%)	-0.69	0 100 100	15, 29, 61, 75	0
1	H	98/99 (98%)	-0.90	0 100 100	8, 20, 47, 63	0
2	A	186/190 (97%)	-0.81	1 (0%) 91 91	10, 20, 49, 71	0
3	C	36/53 (67%)	-0.54	1 (2%) 53 55	13, 22, 40, 59	0
All	All	712/738 (96%)	-0.67	9 (1%) 77 79	7, 26, 60, 75	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	12	ARG	3.7
1	F	34	THR	3.5
1	F	15	ALA	2.8
1	F	84	PRO	2.6
1	F	33	ASN	2.4
3	C	195	THR	2.3
2	A	187	PRO	2.2
1	E	13	THR	2.2
1	E	15	ALA	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 [i](#)

There are no monosaccharides 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.