



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:09 am BST

PDB ID : 6IN9
Title : Crystal structure of MucB in complex with MucA(peri)
Authors : Li, S.; Zhang, Q.; Bartlam, M.
Deposited on : 2018-10-24
Resolution : 1.80 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

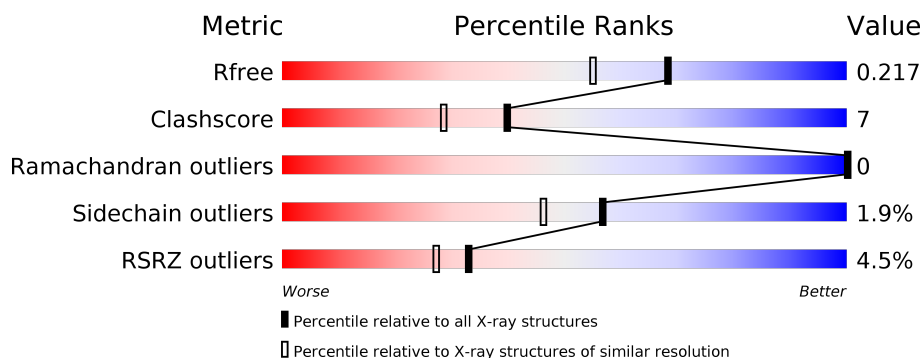
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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	295	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 85%, yellow 85%, yellow 88%, orange 88%, orange 91%, grey 91%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 85% 7% • 8% </div> </div>
1	B	295	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, green 4%, green 79%, yellow 79%, yellow 89%, orange 89%, orange 92%, grey 92%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 4% 79% 10% • 9% </div> </div>
2	C	89	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 6%, green 6%, green 42%, yellow 42%, yellow 50%, grey 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 6% 42% 8% 51% </div> </div>
2	D	89	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 9%, green 9%, green 43%, yellow 43%, yellow 50%, grey 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 9% 43% 7% 51% </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5317 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 Sigma factor AlgU regulatory protein MucB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	1	0
			2113	1316	388	402	7			
1	B	268	Total	C	N	O	S	0	1	0
			2083	1300	384	393	6			

- Molecule 2 is a protein called Sigma factor AlgU negative regulatory protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	44	Total	C	N	O	0	0	0
			349	214	66	69			
2	D	44	Total	C	N	O	0	0	0
			351	216	67	68			

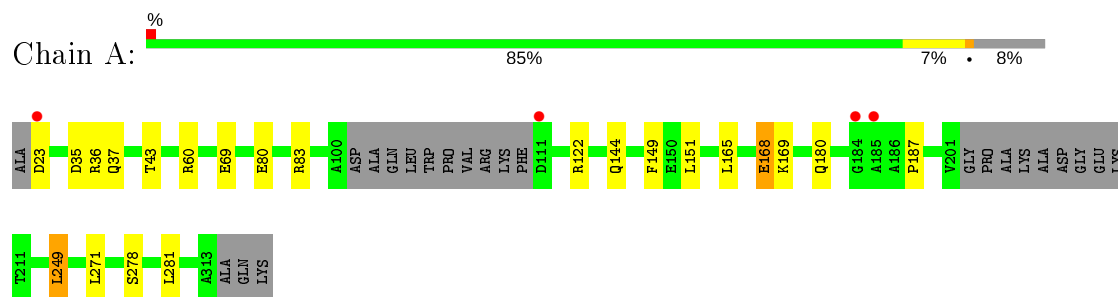
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	212	Total	O	0	0
			212	212		
3	B	171	Total	O	0	0
			171	171		
3	C	19	Total	O	0	0
			19	19		
3	D	19	Total	O	0	0
			19	19		

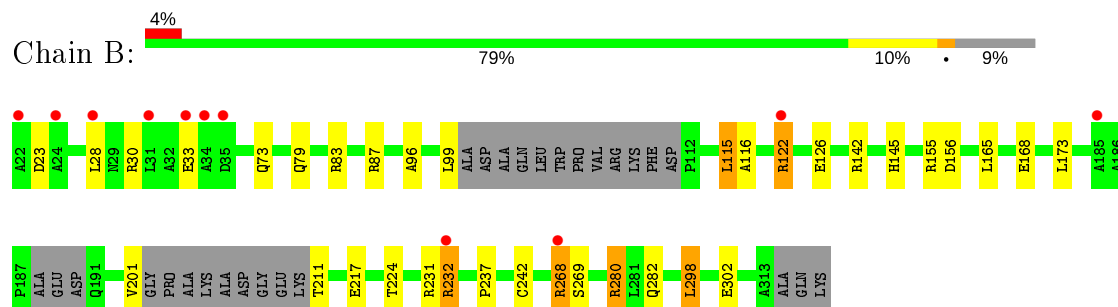
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

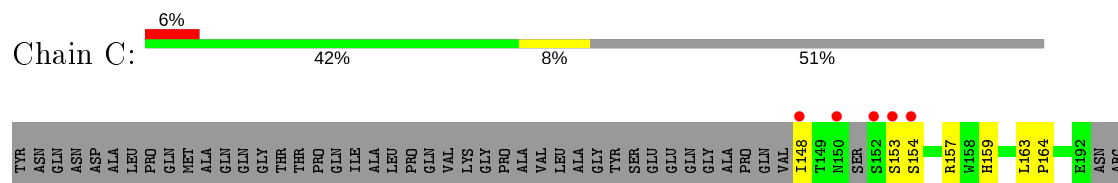
- Molecule 1: Sigma factor AlgU regulatory protein MucB



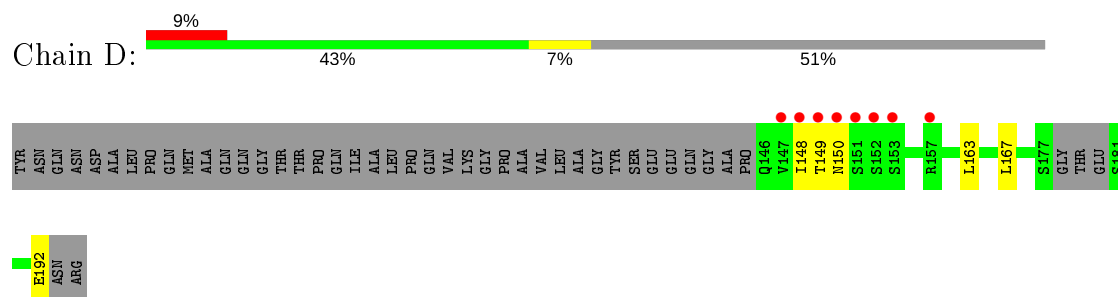
- Molecule 1: Sigma factor AlgU regulatory protein MucB



- Molecule 2: Sigma factor AlgU negative regulatory protein



- Molecule 2: Sigma factor AlgU negative regulatory protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.15Å 50.27Å 100.14Å 90.00° 109.05° 90.00°	Depositor
Resolution (Å)	44.40 – 1.80 44.40 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.40-1.80) 99.6 (44.40-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.188 , 0.216 0.189 , 0.217	Depositor DCC
R_{free} test set	3039 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5317	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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, 0.333 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	0.39	0/2153	0.62	0/2923
1	B	0.49	3/2122 (0.1%)	0.84	7/2878 (0.2%)
2	C	0.38	0/355	0.58	0/481
2	D	0.45	0/357	0.61	0/484
All	All	0.44	3/4987 (0.1%)	0.72	7/6766 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	298	LEU	CG-CD2	-6.31	1.28	1.51
1	B	268	ARG	CD-NE	-5.14	1.37	1.46
1	B	268	ARG	CG-CD	-5.07	1.39	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	ARG	NE-CZ-NH1	-17.83	111.39	120.30
1	B	298	LEU	CB-CG-CD1	-10.97	92.34	111.00
1	B	298	LEU	CA-CB-CG	-9.45	93.56	115.30
1	B	232	ARG	NE-CZ-NH2	8.81	124.70	120.30
1	B	232	ARG	CA-CB-CG	7.45	129.79	113.40
1	B	268	ARG	NE-CZ-NH1	-7.33	116.63	120.30
1	B	232	ARG	N-CA-CB	-5.09	101.43	110.60

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	2113	0	2067	21	0
1	B	2083	0	2048	36	0
2	C	349	0	334	6	0
2	D	351	0	340	10	0
3	A	212	0	0	6	0
3	B	171	0	0	15	0
3	C	19	0	0	0	0
3	D	19	0	0	3	0
All	All	5317	0	4789	71	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.

All (71) 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:87:ARG:NH1	3:B:401:HOH:O	1.90	1.04
2:D:149:THR:HB	2:D:150:ASN:HA	1.39	1.01
1:A:80:GLU:OE1	3:A:401:HOH:O	1.81	0.99
1:A:144:GLN:OE1	3:A:402:HOH:O	1.84	0.94
2:D:192:GLU:OE1	3:D:201:HOH:O	1.87	0.91
1:B:280:ARG:NH2	3:B:404:HOH:O	2.04	0.86
1:B:224:THR:HB	3:B:480:HOH:O	1.76	0.86
1:A:180:GLN:HG2	3:B:419:HOH:O	1.78	0.82
1:A:168:GLU:OE1	1:A:169:LYS:HE3	1.81	0.80
1:B:99:LEU:O	3:B:403:HOH:O	1.99	0.80
1:B:73:GLN:HE22	1:B:79:GLN:HE21	1.33	0.76
2:D:149:THR:H	2:D:150:ASN:HB2	1.51	0.74
1:B:201:VAL:O	3:B:405:HOH:O	2.07	0.72
1:B:268:ARG:HH22	1:B:298:LEU:HD21	1.54	0.72
1:A:37:GLN:NE2	3:A:406:HOH:O	2.22	0.72
1:B:282:GLN:OE1	3:B:406:HOH:O	2.08	0.70
1:A:69:GLU:OE1	1:A:83:ARG:NH1	2.25	0.69
2:C:154:SER:HA	2:C:157:ARG:HE	1.57	0.68
1:B:73:GLN:NE2	1:B:79:GLN:HE21	1.91	0.67
2:C:148:ILE:HD11	2:C:164:PRO:HD3	1.78	0.66
1:A:43:THR:HG23	1:A:180:GLN:HE21	1.62	0.65
1:B:268:ARG:NH2	1:B:298:LEU:HD21	2.12	0.63
1:B:268:ARG:NH2	1:B:298:LEU:HD11	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:192:GLU:OE1	3:D:202:HOH:O	2.15	0.63
1:A:35:ASP:HB3	1:A:36:ARG:NH1	2.15	0.62
1:B:268:ARG:NH2	1:B:302:GLU:OE1	2.33	0.62
2:D:149:THR:CB	2:D:150:ASN:HA	2.11	0.61
1:B:280:ARG:NE	3:B:402:HOH:O	1.99	0.58
1:A:23:ASP:OD1	3:A:405:HOH:O	2.17	0.58
1:B:28:LEU:HD11	1:B:115:LEU:HD23	1.87	0.57
1:A:60:ARG:NH2	1:A:187:PRO:O	2.39	0.55
1:B:122:ARG:HA	1:B:122:ARG:NE	2.22	0.55
2:C:157:ARG:HD3	2:C:157:ARG:H	1.71	0.55
1:B:122:ARG:NH2	3:B:412:HOH:O	2.34	0.54
1:A:271:LEU:HD22	2:D:167:LEU:HD21	1.90	0.54
1:A:168:GLU:CD	1:A:168:GLU:H	2.10	0.53
1:B:30:ARG:NH2	3:B:408:HOH:O	2.23	0.53
2:D:149:THR:H	2:D:150:ASN:CB	2.20	0.53
1:B:268:ARG:CZ	1:B:298:LEU:HD11	2.39	0.53
1:A:149:PHE:HB3	1:A:151:LEU:HD23	1.91	0.52
2:C:153:SER:O	2:C:157:ARG:HD3	2.10	0.52
1:B:122:ARG:HA	1:B:122:ARG:CZ	2.39	0.52
2:C:157:ARG:HD3	2:C:157:ARG:N	2.27	0.50
1:A:144:GLN:CD	3:A:402:HOH:O	2.36	0.49
2:D:192:GLU:HB3	3:D:202:HOH:O	2.12	0.49
1:B:155:ARG:NH1	3:B:411:HOH:O	2.32	0.48
1:B:231:ARG:HG2	1:B:242:CYS:SG	2.54	0.47
1:B:116:ALA:O	1:B:142:ARG:NH2	2.43	0.47
1:A:149:PHE:HB3	1:A:151:LEU:CD2	2.45	0.47
1:B:155:ARG:NH2	1:B:156:ASP:OD1	2.47	0.47
1:B:280:ARG:HD2	3:B:499:HOH:O	2.15	0.47
1:B:268:ARG:HG2	1:B:269:SER:N	2.31	0.46
1:B:126:GLU:OE1	3:B:407:HOH:O	2.20	0.46
1:A:122:ARG:NH2	1:A:122:ARG:HG3	2.31	0.46
1:A:168:GLU:CD	1:A:168:GLU:N	2.70	0.45
2:C:159:HIS:HB3	2:C:163:LEU:HD22	1.98	0.44
1:A:281:LEU:HD13	3:A:457:HOH:O	2.17	0.44
1:B:217:GLU:HG3	1:B:217:GLU:O	2.17	0.44
1:A:149:PHE:CZ	1:A:165:LEU:HD13	2.53	0.43
1:A:278:SER:OG	2:D:163:LEU:HD21	2.19	0.43
1:B:145:HIS:ND1	3:B:414:HOH:O	2.37	0.43
1:B:165:LEU:HD22	1:B:173:LEU:HD12	1.99	0.43
1:B:211:THR:O	1:B:211:THR:OG1	2.35	0.43
1:B:268:ARG:NH2	1:B:298:LEU:CD2	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:HA	1:A:249:LEU:HD12	1.83	0.42
1:B:168:GLU:H	1:B:168:GLU:CD	2.20	0.42
1:B:268:ARG:NH2	1:B:298:LEU:CD1	2.83	0.41
1:B:96:ALA:HA	1:B:99:LEU:HG	2.02	0.41
2:D:148:ILE:HA	2:D:149:THR:OG1	2.21	0.41
1:B:115:LEU:HA	1:B:115:LEU:HD12	1.86	0.41
1:B:155:ARG:NE	3:B:411:HOH:O	2.43	0.41

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	267/295 (90%)	261 (98%)	6 (2%)	0	100	100
1	B	261/295 (88%)	253 (97%)	8 (3%)	0	100	100
2	C	40/89 (45%)	39 (98%)	1 (2%)	0	100	100
2	D	40/89 (45%)	37 (92%)	3 (8%)	0	100	100
All	All	608/768 (79%)	590 (97%)	18 (3%)	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	224/239 (94%)	222 (99%)	2 (1%)	78	75
1	B	221/239 (92%)	213 (96%)	8 (4%)	35	20
2	C	38/73 (52%)	38 (100%)	0	100	100
2	D	39/73 (53%)	39 (100%)	0	100	100
All	All	522/624 (84%)	512 (98%)	10 (2%)	57	46

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	GLU
1	A	249	LEU
1	B	23	ASP
1	B	33	GLU
1	B	83	ARG
1	B	115	LEU
1	B	122	ARG
1	B	232	ARG
1	B	237	PRO
1	B	280	ARG

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

Mol	Chain	Res	Type
1	A	180	GLN
1	A	182	ASN
1	B	73	GLN

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

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, 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	272/295 (92%)	-0.32	4 (1%) 73 70	16, 26, 43, 64	0
1	B	268/295 (90%)	-0.06	11 (4%) 37 31	18, 29, 55, 68	0
2	C	44/89 (49%)	0.27	5 (11%) 5 3	20, 29, 60, 66	0
2	D	44/89 (49%)	0.62	8 (18%) 1 0	18, 28, 66, 79	0
All	All	628/768 (81%)	-0.10	28 (4%) 33 27	16, 28, 53, 79	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	151	SER	7.0
2	D	149	THR	7.0
2	D	150	ASN	4.9
1	B	34	ALA	4.8
1	B	185	ALA	4.7
1	B	31	LEU	4.5
2	D	148	ILE	4.4
2	C	150	ASN	4.4
2	D	157	ARG	4.1
1	B	232	ARG	4.0
2	C	153	SER	3.7
1	B	268	ARG	3.4
1	B	24	ALA	3.3
1	B	35	ASP	3.3
2	D	147	VAL	2.9
2	C	148	ILE	2.9
1	B	122	ARG	2.7
1	B	28	LEU	2.6
2	C	152	SER	2.6
2	C	154	SER	2.5
1	B	33	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	23	ASP	2.4
1	B	22	ALA	2.3
1	A	184	GLY	2.3
1	A	111	ASP	2.3
1	A	185	ALA	2.2
2	D	153	SER	2.1
2	D	152	SER	2.1

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.