



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 4, 2024 – 02:54 AM EST

PDB ID : 1ZNP
Title : X-Ray Crystal Structure of Protein Q8U9W0 from *Agrobacterium tumefaciens*. Northeast Structural Genomics Consortium Target AtR55.
Authors : Kuzin, A.P.; Chen, Y.; Forouhar, F.; Vorobiev, S.M.; Xiao, R.; Ma, L.-C.; Acton, T.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2005-05-11
Resolution : 2.50 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

<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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

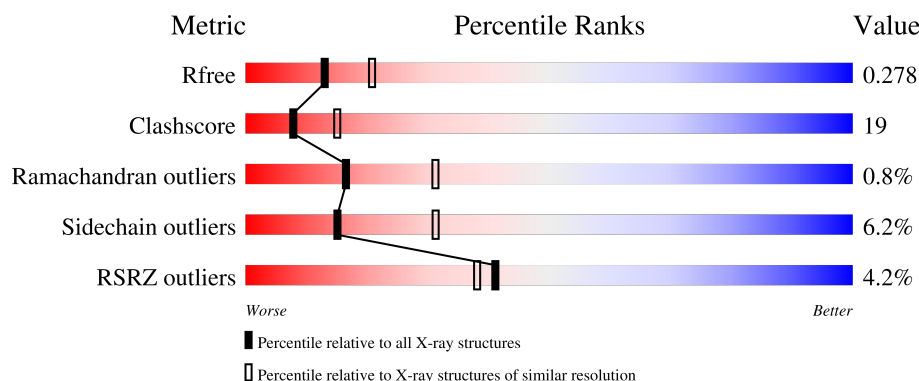
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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 ≥ 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	154	<div> <div>3%</div> <div>67%</div> <div>23%</div> <div>9%</div> </div>
1	B	154	<div> <div>3%</div> <div>58%</div> <div>28%</div> <div>9%</div> </div>
1	C	154	<div> <div>%</div> <div>56%</div> <div>31%</div> <div>10%</div> </div>
1	D	154	<div> <div>3%</div> <div>60%</div> <div>25%</div> <div>10%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	154	<div><div></div><div>5%</div><div>60%</div><div>27%</div><div>• •</div><div>10%</div></div>
1	F	154	<div><div></div><div>7%</div><div>53%</div><div>34%</div><div>5%</div><div>9%</div></div>
1	G	154	<div><div></div><div>4%</div><div>66%</div><div>21%</div><div>•</div><div>9%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7750 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 hypothetical protein Atu3615.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	Se	0	0	0
			1086	693	188	201	2	2			
1	B	140	Total	C	N	O	S	Se	0	0	0
			1086	693	188	201	2	2			
1	C	138	Total	C	N	O	S	Se	0	0	0
			1074	687	186	197	2	2			
1	D	138	Total	C	N	O	S	Se	0	0	0
			1074	687	186	197	2	2			
1	E	139	Total	C	N	O	S	Se	0	0	0
			1078	689	187	198	2	2			
1	F	140	Total	C	N	O	S	Se	0	0	0
			1086	693	188	201	2	2			
1	G	140	Total	C	N	O	S	Se	0	0	0
			1086	693	188	201	2	2			

There are 77 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q8U9W0
A	5	MSE	MET	modified residue	UNP Q8U9W0
A	135	MSE	MET	modified residue	UNP Q8U9W0
A	147	LEU	-	cloning artifact	UNP Q8U9W0
A	148	GLU	-	cloning artifact	UNP Q8U9W0
A	149	HIS	-	cloning artifact	UNP Q8U9W0
A	150	HIS	-	cloning artifact	UNP Q8U9W0
A	151	HIS	-	cloning artifact	UNP Q8U9W0
A	152	HIS	-	cloning artifact	UNP Q8U9W0
A	153	HIS	-	cloning artifact	UNP Q8U9W0
A	154	HIS	-	cloning artifact	UNP Q8U9W0
B	1	MSE	MET	modified residue	UNP Q8U9W0
B	5	MSE	MET	modified residue	UNP Q8U9W0
B	135	MSE	MET	modified residue	UNP Q8U9W0
B	147	LEU	-	cloning artifact	UNP Q8U9W0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	148	GLU	-	cloning artifact	UNP Q8U9W0
B	149	HIS	-	cloning artifact	UNP Q8U9W0
B	150	HIS	-	cloning artifact	UNP Q8U9W0
B	151	HIS	-	cloning artifact	UNP Q8U9W0
B	152	HIS	-	cloning artifact	UNP Q8U9W0
B	153	HIS	-	cloning artifact	UNP Q8U9W0
B	154	HIS	-	cloning artifact	UNP Q8U9W0
C	1	MSE	MET	modified residue	UNP Q8U9W0
C	5	MSE	MET	modified residue	UNP Q8U9W0
C	135	MSE	MET	modified residue	UNP Q8U9W0
C	147	LEU	-	cloning artifact	UNP Q8U9W0
C	148	GLU	-	cloning artifact	UNP Q8U9W0
C	149	HIS	-	cloning artifact	UNP Q8U9W0
C	150	HIS	-	cloning artifact	UNP Q8U9W0
C	151	HIS	-	cloning artifact	UNP Q8U9W0
C	152	HIS	-	cloning artifact	UNP Q8U9W0
C	153	HIS	-	cloning artifact	UNP Q8U9W0
C	154	HIS	-	cloning artifact	UNP Q8U9W0
D	1	MSE	MET	modified residue	UNP Q8U9W0
D	5	MSE	MET	modified residue	UNP Q8U9W0
D	135	MSE	MET	modified residue	UNP Q8U9W0
D	147	LEU	-	cloning artifact	UNP Q8U9W0
D	148	GLU	-	cloning artifact	UNP Q8U9W0
D	149	HIS	-	cloning artifact	UNP Q8U9W0
D	150	HIS	-	cloning artifact	UNP Q8U9W0
D	151	HIS	-	cloning artifact	UNP Q8U9W0
D	152	HIS	-	cloning artifact	UNP Q8U9W0
D	153	HIS	-	cloning artifact	UNP Q8U9W0
D	154	HIS	-	cloning artifact	UNP Q8U9W0
E	1	MSE	MET	modified residue	UNP Q8U9W0
E	5	MSE	MET	modified residue	UNP Q8U9W0
E	135	MSE	MET	modified residue	UNP Q8U9W0
E	147	LEU	-	cloning artifact	UNP Q8U9W0
E	148	GLU	-	cloning artifact	UNP Q8U9W0
E	149	HIS	-	cloning artifact	UNP Q8U9W0
E	150	HIS	-	cloning artifact	UNP Q8U9W0
E	151	HIS	-	cloning artifact	UNP Q8U9W0
E	152	HIS	-	cloning artifact	UNP Q8U9W0
E	153	HIS	-	cloning artifact	UNP Q8U9W0
E	154	HIS	-	cloning artifact	UNP Q8U9W0
F	1	MSE	MET	modified residue	UNP Q8U9W0
F	5	MSE	MET	modified residue	UNP Q8U9W0

Continued on next page...

Continued from previous page...

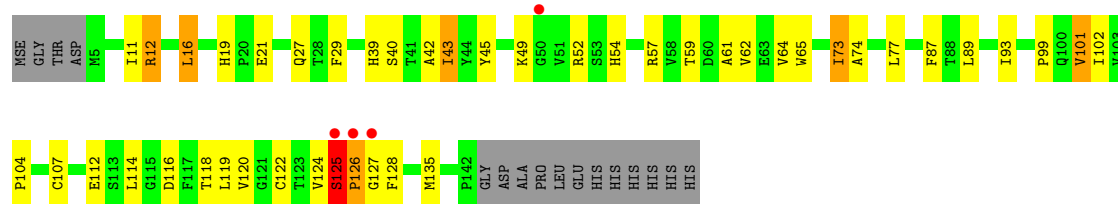
Chain	Residue	Modelled	Actual	Comment	Reference
F	135	MSE	MET	modified residue	UNP Q8U9W0
F	147	LEU	-	cloning artifact	UNP Q8U9W0
F	148	GLU	-	cloning artifact	UNP Q8U9W0
F	149	HIS	-	cloning artifact	UNP Q8U9W0
F	150	HIS	-	cloning artifact	UNP Q8U9W0
F	151	HIS	-	cloning artifact	UNP Q8U9W0
F	152	HIS	-	cloning artifact	UNP Q8U9W0
F	153	HIS	-	cloning artifact	UNP Q8U9W0
F	154	HIS	-	cloning artifact	UNP Q8U9W0
G	1	MSE	MET	modified residue	UNP Q8U9W0
G	5	MSE	MET	modified residue	UNP Q8U9W0
G	135	MSE	MET	modified residue	UNP Q8U9W0
G	147	LEU	-	cloning artifact	UNP Q8U9W0
G	148	GLU	-	cloning artifact	UNP Q8U9W0
G	149	HIS	-	cloning artifact	UNP Q8U9W0
G	150	HIS	-	cloning artifact	UNP Q8U9W0
G	151	HIS	-	cloning artifact	UNP Q8U9W0
G	152	HIS	-	cloning artifact	UNP Q8U9W0
G	153	HIS	-	cloning artifact	UNP Q8U9W0
G	154	HIS	-	cloning artifact	UNP Q8U9W0

- Molecule 2 is water.

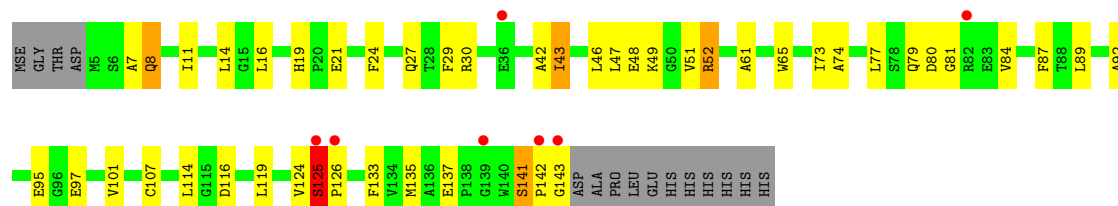
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	40	Total O 40 40	0	0
2	B	33	Total O 33 33	0	0
2	C	26	Total O 26 26	0	0
2	D	23	Total O 23 23	0	0
2	E	28	Total O 28 28	0	0
2	F	14	Total O 14 14	0	0
2	G	16	Total O 16 16	0	0

- Molecule 1: hypothetical protein Atu3615

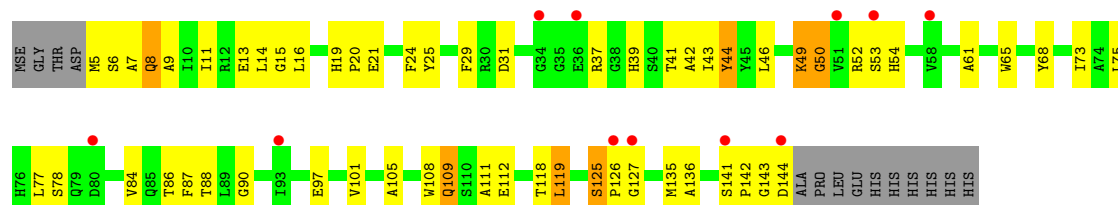




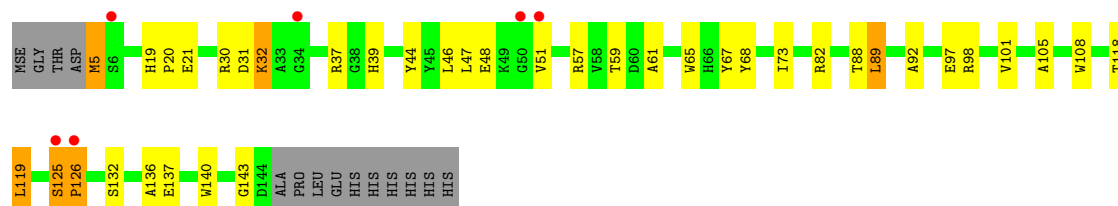
• Molecule 1: hypothetical protein Atu3615



• Molecule 1: hypothetical protein Atu3615



• Molecule 1: hypothetical protein Atu3615



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	75.97Å 91.32Å 291.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.11 – 2.50 27.11 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.0 (27.11-2.50) 95.3 (27.11-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.70 (at 2.47Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.267 0.216 , 0.278	Depositor DCC
R_{free} test set	1780 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7750	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% 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

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	0.42	0/1119	0.66	0/1521
1	B	0.49	0/1120	0.76	5/1524 (0.3%)
1	C	0.40	0/1108	0.65	1/1508 (0.1%)
1	D	0.35	0/1108	0.59	0/1508
1	E	0.52	0/1112	0.74	2/1513 (0.1%)
1	F	0.41	0/1120	0.70	2/1524 (0.1%)
1	G	0.49	1/1120 (0.1%)	0.91	6/1524 (0.4%)
All	All	0.44	1/7807 (0.0%)	0.72	16/10622 (0.2%)

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	E	0	1
1	G	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	5	MSE	CA-C	-5.14	1.39	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	5	MSE	N-CA-C	-11.28	80.55	111.00
1	G	5	MSE	C-N-CA	-11.28	93.51	121.70
1	G	125	SER	C-N-CD	9.08	147.47	128.40
1	B	5	MSE	C-N-CA	7.74	141.06	121.70
1	E	143	GLY	CA-C-O	7.74	134.53	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	125	SER	Mainchain
1	G	5	MSE	Mainchain

5.2 Too-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 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	1086	0	1022	38	0
1	B	1086	0	1022	61	0
1	C	1074	0	1015	60	0
1	D	1074	0	1015	35	0
1	E	1078	0	1018	36	0
1	F	1086	0	1022	48	0
1	G	1086	0	1022	31	0
2	A	40	0	0	1	0
2	B	33	0	0	1	0
2	C	26	0	0	0	0
2	D	23	0	0	0	0
2	E	28	0	0	2	0
2	F	14	0	0	1	0
2	G	16	0	0	0	0
All	All	7750	0	7136	286	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 19.

The worst 5 of 286 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:5:MSE:HE1	1:C:93:ILE:N	1.32	1.39
1:B:5:MSE:CE	1:C:93:ILE:H	1.60	1.12
1:B:5:MSE:CE	1:C:93:ILE:N	2.14	1.08
1:A:61:ALA:HA	1:A:126:PRO:HG2	1.46	0.96
1:E:8:GLN:H	1:E:8:GLN:NE2	1.67	0.91

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	138/154 (90%)	131 (95%)	6 (4%)	1 (1%)	19	35
1	B	138/154 (90%)	128 (93%)	7 (5%)	3 (2%)	5	9
1	C	136/154 (88%)	132 (97%)	4 (3%)	0	100	100
1	D	136/154 (88%)	125 (92%)	9 (7%)	2 (2%)	8	16
1	E	137/154 (89%)	130 (95%)	7 (5%)	0	100	100
1	F	138/154 (90%)	124 (90%)	12 (9%)	2 (1%)	9	17
1	G	138/154 (90%)	126 (91%)	12 (9%)	0	100	100
All	All	961/1078 (89%)	896 (93%)	57 (6%)	8 (1%)	16	31

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	127	GLY
1	F	125	SER
1	B	125	SER
1	A	126	PRO
1	B	51	VAL

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	111/120 (92%)	107 (96%)	4 (4%)	30	56
1	B	111/120 (92%)	101 (91%)	10 (9%)	8	16
1	C	110/120 (92%)	104 (94%)	6 (6%)	18	37
1	D	110/120 (92%)	103 (94%)	7 (6%)	14	30
1	E	110/120 (92%)	101 (92%)	9 (8%)	9	19
1	F	111/120 (92%)	104 (94%)	7 (6%)	15	30
1	G	111/120 (92%)	106 (96%)	5 (4%)	23	46
All	All	774/840 (92%)	726 (94%)	48 (6%)	15	31

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	43	ILE
1	E	141	SER
1	E	52	ARG
1	E	95	GLU
1	F	13	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	76	HIS
1	F	39	HIS
1	F	8	GLN
1	F	66	HIS
1	C	26	HIS

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 oligosaccharides 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, 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	138/154 (89%)	-0.16	5 (3%) 46 43	15, 24, 46, 65	0
1	B	138/154 (89%)	-0.08	5 (3%) 46 43	13, 26, 45, 54	0
1	C	136/154 (88%)	-0.14	2 (1%) 71 68	17, 28, 58, 65	0
1	D	136/154 (88%)	0.24	4 (2%) 54 50	24, 39, 56, 68	0
1	E	137/154 (88%)	0.16	7 (5%) 34 32	21, 32, 54, 64	0
1	F	138/154 (89%)	0.83	11 (7%) 20 19	29, 50, 67, 80	0
1	G	138/154 (89%)	0.42	6 (4%) 40 37	24, 43, 61, 69	0
All	All	961/1078 (89%)	0.18	40 (4%) 41 38	13, 35, 60, 80	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	125	SER	5.0
1	A	125	SER	4.7
1	B	6	SER	4.5
1	D	125	SER	4.2
1	E	143	GLY	4.0

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.