



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 02:01 am GMT

PDB ID : 6TWP
Title : Binding domain of BoNT/A5
Authors : Davies, J.R.; Acharya, K.R.
Deposited on : 2020-01-13
Resolution : 1.15 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 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

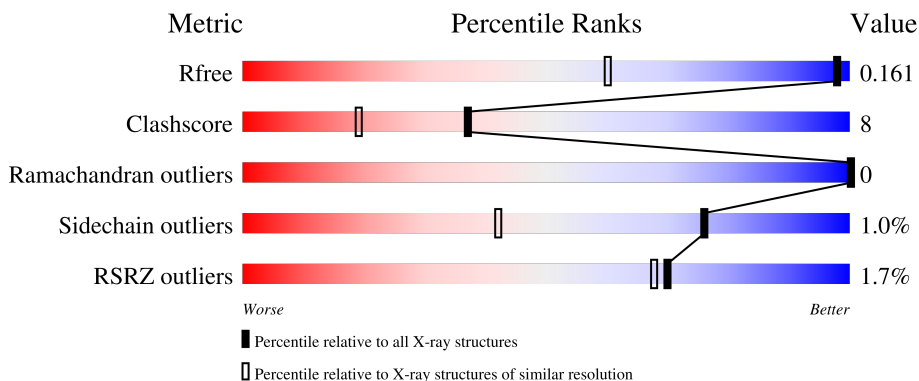
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.15 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	1492 (1.18-1.10)
Clashscore	141614	1537 (1.18-1.10)
Ramachandran outliers	138981	1483 (1.18-1.10)
Sidechain outliers	138945	1480 (1.18-1.10)
RSRZ outliers	127900	1464 (1.18-1.10)

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	AAA	433	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4350 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 Botulinum neurotoxin A5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	415	3827	2443	646	723	15	0	52	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	864	MET	-	initiating methionine	UNP C7BEA8
AAA	865	HIS	-	expression tag	UNP C7BEA8
AAA	866	HIS	-	expression tag	UNP C7BEA8
AAA	867	HIS	-	expression tag	UNP C7BEA8
AAA	868	HIS	-	expression tag	UNP C7BEA8
AAA	869	HIS	-	expression tag	UNP C7BEA8
AAA	870	HIS	-	expression tag	UNP C7BEA8

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	Cl	0	0
			1	1		

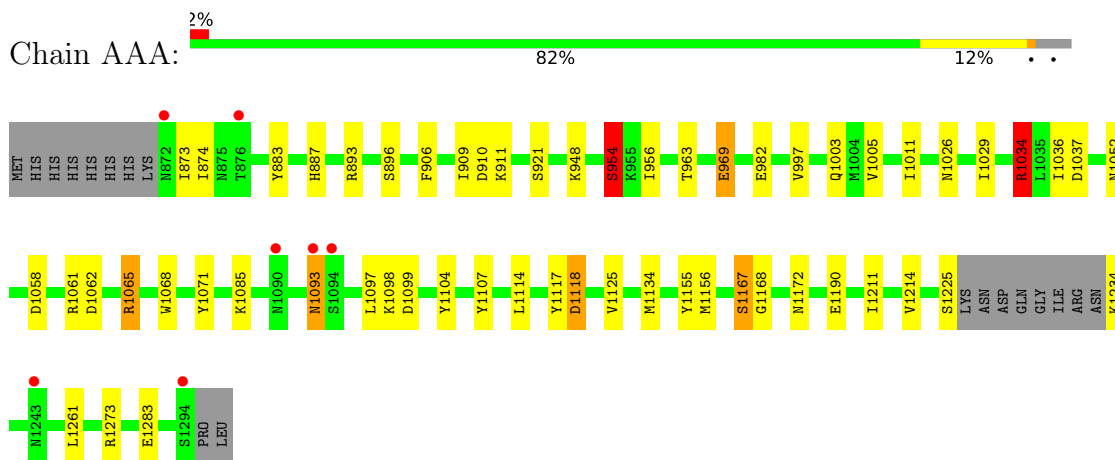
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	509	Total	O	0	25
			522	522		

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: Botulinum neurotoxin A5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.55Å 60.27Å 185.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.57 – 1.15 50.51 – 1.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (92.57-1.15) 99.9 (50.51-1.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.15Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.135 , 0.161 0.136 , 0.161	Depositor DCC
R_{free} test set	3494 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	12.5	Xtrriage
Anisotropy	0.207	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4350	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MLZ, CL

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	AAA	0.95	10/3917 (0.3%)	1.12	20/5290 (0.4%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	982	GLU	CD-OE1	-11.81	1.12	1.25
1	AAA	1093	ASN	CG-ND2	8.56	1.54	1.32
1	AAA	969	GLU	CD-OE1	7.97	1.34	1.25
1	AAA	954	SER	CA-CB	6.17	1.62	1.52
1	AAA	896	SER	CB-OG	6.08	1.50	1.42
1	AAA	1167[A]	SER	CB-OG	6.07	1.50	1.42
1	AAA	1167[B]	SER	CB-OG	6.07	1.50	1.42
1	AAA	1190	GLU	CD-OE1	-6.03	1.19	1.25
1	AAA	969	GLU	CD-OE2	-5.44	1.19	1.25
1	AAA	921	SER	CA-CB	-5.28	1.45	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	1273	ARG	NE-CZ-NH1	-9.47	115.56	120.30
1	AAA	1117[A]	TYR	CA-C-O	9.06	139.13	120.10
1	AAA	1117[B]	TYR	CA-C-O	9.06	139.13	120.10
1	AAA	1273	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	AAA	1261	LEU	CB-CG-CD2	7.61	123.94	111.00
1	AAA	1155	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	AAA	893	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	AAA	1118	ASP	CB-CA-C	-6.80	96.80	110.40
1	AAA	1061	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	AAA	1071	TYR	CB-CG-CD1	5.84	124.51	121.00
1	AAA	1061	ARG	NE-CZ-NH1	5.81	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	893	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	AAA	1118	ASP	CA-CB-CG	-5.75	100.74	113.40
1	AAA	1107	TYR	CB-CG-CD2	5.51	124.31	121.00
1	AAA	954	SER	N-CA-CB	5.22	118.33	110.50
1	AAA	1034	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	AAA	1099	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	AAA	1117[A]	TYR	CA-C-N	-5.06	106.07	117.20
1	AAA	1117[B]	TYR	CA-C-N	-5.06	106.07	117.20
1	AAA	1273	ARG	CB-CA-C	5.00	120.40	110.40

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	AAA	3827	0	3765	60	1
2	AAA	1	0	0	0	0
3	AAA	522	0	0	18	0
All	All	4350	0	3765	60	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 8.

All (60) 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:AAA:1034:ARG:NH2	1:AAA:1036:ILE:HD11	1.36	1.41
1:AAA:1034:ARG:HH22	1:AAA:1036:ILE:CD1	1.41	1.31
1:AAA:1034:ARG:NH2	1:AAA:1036:ILE:CD1	1.93	1.27
1:AAA:1062[B]:ASP:OD2	1:AAA:1065[B]:ARG:CD	1.97	1.11
1:AAA:948[A]:LYS:HE2	3:AAA:1421:HOH:O	1.50	1.09
1:AAA:1062[B]:ASP:OD2	1:AAA:1065[B]:ARG:HD3	1.52	1.06
1:AAA:1034:ARG:HH22	1:AAA:1036:ILE:HD11	0.93	0.94
1:AAA:1026[A]:ASN:ND2	3:AAA:1404:HOH:O	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:1052[A]:ASN:OD1	3:AAA:1401:HOH:O	1.90	0.88
1:AAA:1062[B]:ASP:CG	1:AAA:1065[B]:ARG:HG2	1.95	0.87
1:AAA:911[B]:LYS:NZ	3:AAA:1405:HOH:O	2.10	0.85
1:AAA:1118:ASP:OD1	3:AAA:1402:HOH:O	1.97	0.83
1:AAA:1058[A]:ASP:OD2	3:AAA:1403:HOH:O	1.98	0.80
1:AAA:1034:ARG:NH2	1:AAA:1036:ILE:HD13	1.96	0.80
1:AAA:1034:ARG:HH21	1:AAA:1036:ILE:CD1	1.95	0.76
1:AAA:1062[B]:ASP:CB	1:AAA:1065[B]:ARG:HG2	2.15	0.76
1:AAA:1172[A]:ASN:ND2	3:AAA:1406:HOH:O	2.18	0.76
1:AAA:1062[B]:ASP:HB3	1:AAA:1065[B]:ARG:HG2	1.68	0.75
1:AAA:1005[B]:VAL:CG2	3:AAA:1443:HOH:O	2.34	0.74
1:AAA:1062[B]:ASP:OD2	1:AAA:1065[B]:ARG:CG	2.40	0.70
1:AAA:1005[B]:VAL:HG22	3:AAA:1443:HOH:O	1.90	0.69
1:AAA:1234:LYS:HD2	1:AAA:1283[B]:GLU:OE2	1.93	0.68
1:AAA:1034:ARG:HH22	1:AAA:1036:ILE:HD12	1.55	0.68
1:AAA:873:ILE:HG21	3:AAA:1716:HOH:O	1.95	0.66
1:AAA:1062[B]:ASP:OD2	1:AAA:1065[B]:ARG:HG2	2.00	0.62
1:AAA:1118:ASP:HB2	3:AAA:1402:HOH:O	2.02	0.60
1:AAA:1034:ARG:HH21	1:AAA:1034:ARG:CG	2.15	0.59
1:AAA:1062[B]:ASP:OD2	1:AAA:1065[B]:ARG:HD2	2.00	0.58
1:AAA:1062[B]:ASP:HB3	1:AAA:1065[B]:ARG:CG	2.33	0.58
1:AAA:1168:GLY:HA2	3:AAA:1447:HOH:O	2.07	0.55
1:AAA:954:SER:HB2	1:AAA:956:ILE:HG22	1.89	0.54
1:AAA:1036:ILE:O	1:AAA:1037[B]:ASP:HB2	2.06	0.54
1:AAA:1085:LYS:HE2	3:AAA:1433:HOH:O	2.08	0.54
1:AAA:1211:ILE:O	1:AAA:1214[A]:VAL:HG23	2.07	0.54
1:AAA:948[B]:LYS:NZ	3:AAA:1646[B]:HOH:O	2.42	0.53
1:AAA:1118:ASP:CB	3:AAA:1402:HOH:O	2.56	0.53
1:AAA:1156[B]:MET:SD	3:AAA:1559:HOH:O	2.59	0.52
1:AAA:963:THR:HB	1:AAA:1058[A]:ASP:HB3	1.92	0.50
1:AAA:1034:ARG:NH2	1:AAA:1034:ARG:HG2	2.28	0.49
1:AAA:997[B]:VAL:HG12	1:AAA:1029:ILE:HG22	1.94	0.48
1:AAA:1034:ARG:HH21	1:AAA:1036:ILE:HD13	1.65	0.48
1:AAA:873:ILE:HG23	1:AAA:874:ILE:N	2.29	0.48
1:AAA:1034:ARG:HH21	1:AAA:1034:ARG:HG2	1.77	0.48
1:AAA:948[A]:LYS:HB3	1:AAA:1068:TRP:HB2	1.96	0.47
1:AAA:948[A]:LYS:HE3	1:AAA:1068:TRP:CD1	2.50	0.46
1:AAA:1114[A]:LEU:HB3	1:AAA:1283[A]:GLU:HB2	1.98	0.46
1:AAA:1234:LYS:CD	1:AAA:1283[B]:GLU:OE2	2.60	0.46
1:AAA:1125:VAL:HG22	1:AAA:1134[B]:MET:HG2	2.00	0.43
1:AAA:910[B]:ASP:OD2	1:AAA:1104[B]:TYR:OH	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:1098[B]:LYS:HE2	3:AAA:1629:HOH:O	2.18	0.43
1:AAA:1234:LYS:NZ	1:AAA:1283[B]:GLU:OE2	2.51	0.43
1:AAA:1167[B]:SER:OG	1:AAA:1168:GLY:N	2.52	0.42
1:AAA:909:ILE:HG22	1:AAA:1104[B]:TYR:CD2	2.54	0.42
1:AAA:873:ILE:HG23	1:AAA:874:ILE:H	1.83	0.42
1:AAA:1097:LEU:HG	1:AAA:1225[A]:SER:HB3	2.02	0.41
1:AAA:1062[A]:ASP:C	1:AAA:1062[A]:ASP:OD1	2.58	0.41
1:AAA:1005[B]:VAL:HG23	3:AAA:1443:HOH:O	2.11	0.41
1:AAA:883[A]:TYR:CE2	1:AAA:906:PHE:CD2	3.08	0.41
1:AAA:1003:GLN:HA	1:AAA:1011:ILE:HD11	2.03	0.40
1:AAA:1093:ASN:HB2	1:AAA:1098[A]:LYS:NZ	2.36	0.40

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:AAA:883[B]:TYR:OH	1:AAA:969:GLU:OE2[3_644]	2.00	0.20

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	AAA	461/433 (106%)	444 (96%)	17 (4%)	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	AAA	434/400 (108%)	429 (99%)	5 (1%)	71 35

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	887	HIS
1	AAA	954	SER
1	AAA	1034	ARG
1	AAA	1065[A]	ARG
1	AAA	1065[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MLZ	AAA	1236	1	8,9,10	0.72	0	4,9,11	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLZ	AAA	1236	1	-	0/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	AAA	414/433 (95%)	0.12	7 (1%) 70 68	8, 15, 33, 50	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	872	ASN	3.7
1	AAA	876	THR	3.6
1	AAA	1243	ASN	3.4
1	AAA	1094	SER	3.3
1	AAA	1294	SER	3.2
1	AAA	1093	ASN	2.5
1	AAA	1090	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	MLZ	AAA	1236	10/11	0.97	0.07	11,13,16,16	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CL	AAA	1301	1/1	1.00	0.11	17,17,17,17	1

6.5 Other polymers [i](#)

There are no such residues in this entry.