



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 08:24 PM EDT

PDB ID : 3MWT / pdb_00003mwt
Title : Crystal structure of Lassa fever virus nucleoprotein in complex with Mn²⁺
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Deposited on : 2010-05-06
Resolution : 1.98 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

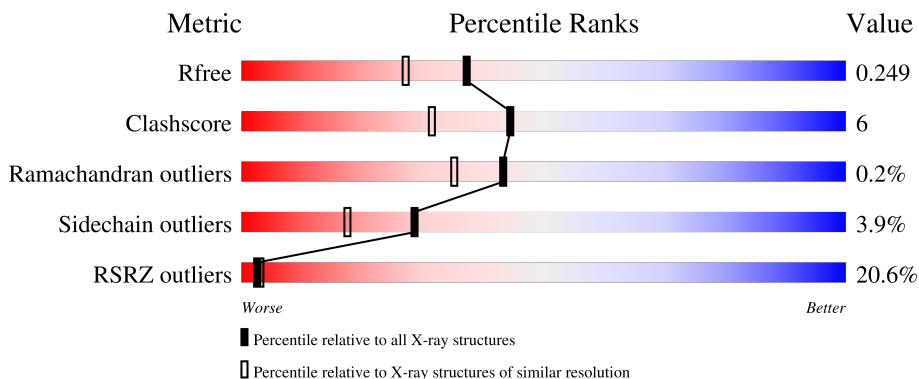
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	577	 20% 76% 11% • 11%
1	B	577	 15% 72% 15% • 11%
1	C	577	 19% 72% 13% • 13%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12279 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	513	4012	2521	697	767	27	0	0	0
1	B	512	4001	2510	696	768	27	0	0	0
1	C	500	3918	2463	681	747	27	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP P13699
A	-6	ALA	-	expression tag	UNP P13699
A	-5	MET	-	expression tag	UNP P13699
A	-4	ASP	-	expression tag	UNP P13699
A	-3	HIS	-	expression tag	UNP P13699
A	-2	VAL	-	expression tag	UNP P13699
A	-1	GLU	-	expression tag	UNP P13699
A	0	PHE	-	expression tag	UNP P13699
B	-7	GLY	-	expression tag	UNP P13699
B	-6	ALA	-	expression tag	UNP P13699
B	-5	MET	-	expression tag	UNP P13699
B	-4	ASP	-	expression tag	UNP P13699
B	-3	HIS	-	expression tag	UNP P13699
B	-2	VAL	-	expression tag	UNP P13699
B	-1	GLU	-	expression tag	UNP P13699
B	0	PHE	-	expression tag	UNP P13699
C	-7	GLY	-	expression tag	UNP P13699
C	-6	ALA	-	expression tag	UNP P13699
C	-5	MET	-	expression tag	UNP P13699
C	-4	ASP	-	expression tag	UNP P13699
C	-3	HIS	-	expression tag	UNP P13699
C	-2	VAL	-	expression tag	UNP P13699
C	-1	GLU	-	expression tag	UNP P13699

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	PHE	-	expression tag	UNP P13699

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0

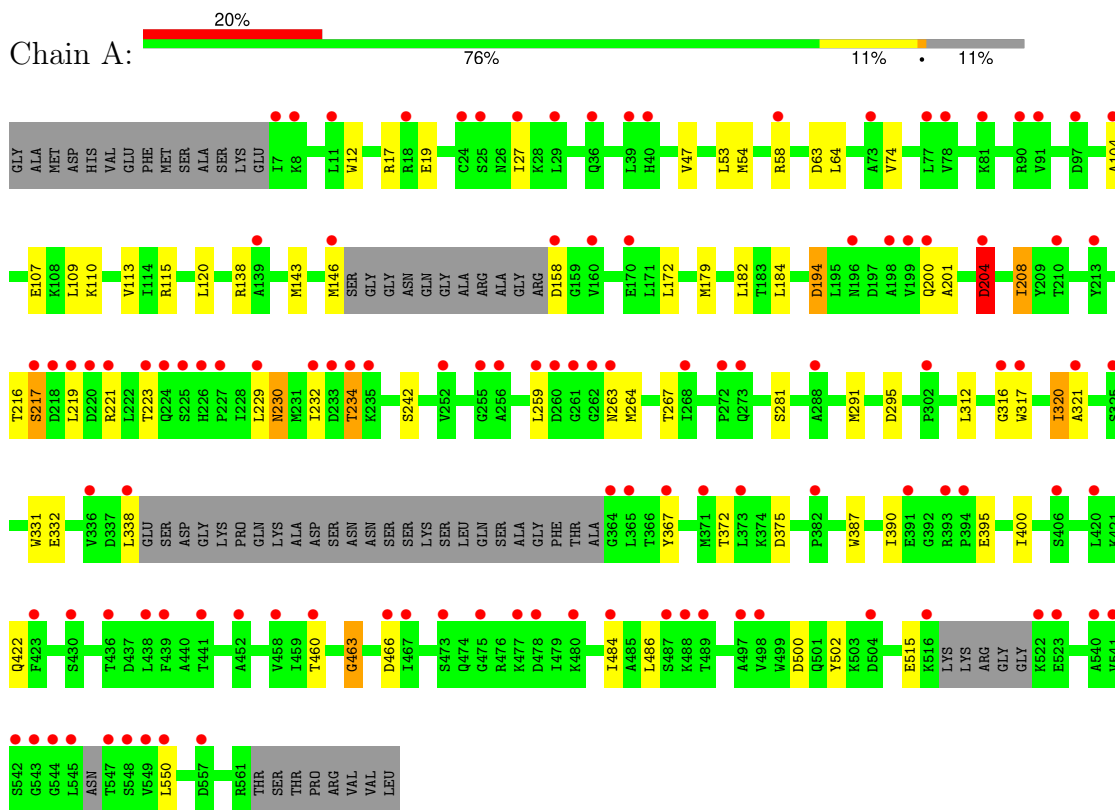
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total 135	O 135	0	0
4	B	158	Total 158	O 158	0	0
4	C	49	Total 49	O 49	0	0

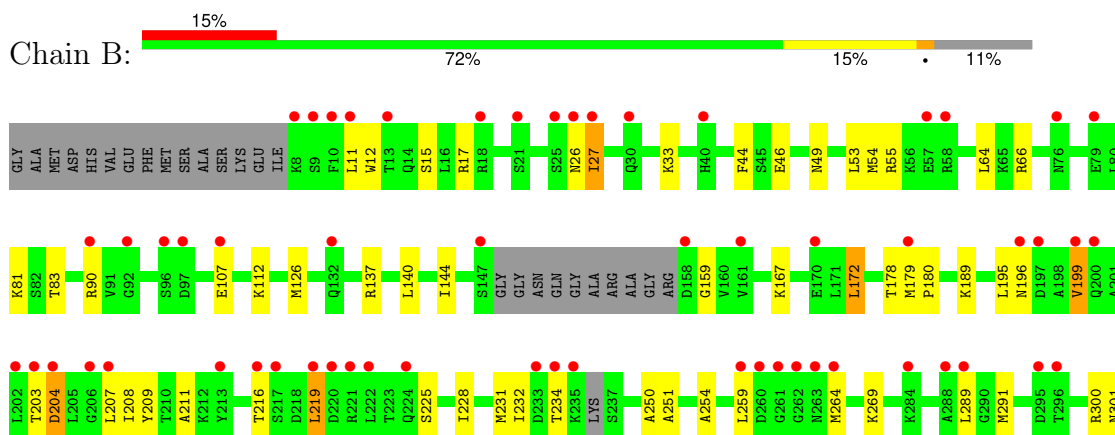
3 Residue-property plots [i](#)

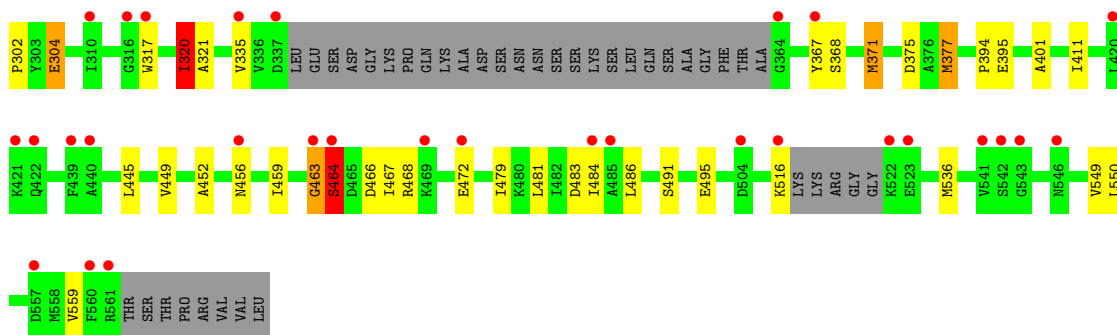
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nucleoprotein

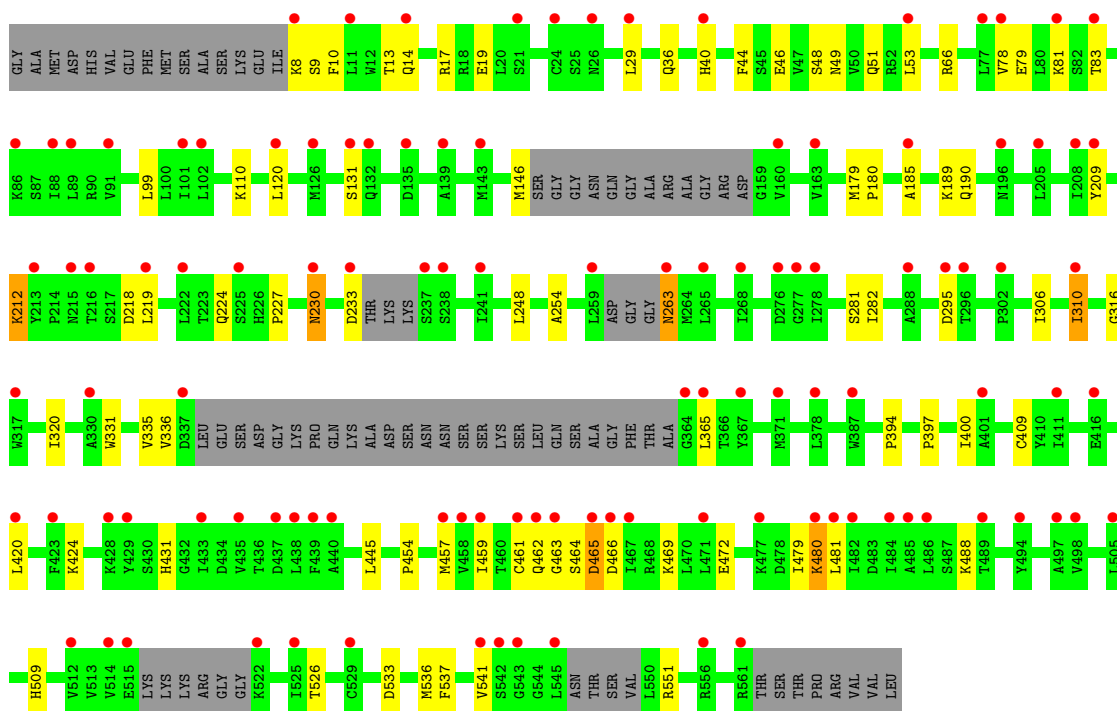


- Molecule 1: Nucleoprotein





● Molecule 1: Nucleoprotein



4 Data and refinement statistics i

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	176.88Å 176.88Å 56.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	153.18 – 1.98 153.18 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.5 (153.18-1.98) 99.8 (153.18-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.181 , 0.218 0.211 , 0.249	Depositor DCC
R_{free} test set	6843 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtrriage
Anisotropy	0.677	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l 0.069 for h,-h-k,-l 0.000 for -k,-h,-l	Xtrriage
Reported twinning fraction	0.553 for H, K, L 0.447 for K, H, -L	Depositor
Outliers	0 of 136770 reflections	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12279	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: ZN, MN

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	0.97	3/4068 (0.1%)	1.06	5/5491 (0.1%)
1	B	1.15	3/4057 (0.1%)	1.17	10/5477 (0.2%)
1	C	0.92	1/3972 (0.0%)	1.06	4/5360 (0.1%)
All	All	1.02	7/12097 (0.1%)	1.10	19/16328 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	449	VAL	CA-CB	6.72	1.62	1.54
1	A	204	ASP	CA-C	5.97	1.61	1.52
1	A	104	ALA	CA-CB	5.50	1.61	1.53
1	B	204	ASP	CA-CB	5.27	1.61	1.53
1	B	559	VAL	CA-CB	5.21	1.60	1.54

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	MET	CG-SD-CE	-7.99	83.32	100.90
1	C	316	GLY	N-CA-C	6.87	119.39	110.45
1	B	27	ILE	N-CA-C	6.46	118.37	112.43
1	A	316	GLY	N-CA-C	6.14	118.87	110.58
1	B	259	LEU	N-CA-C	6.12	119.21	109.24

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	4012	0	4084	51	0
1	B	4001	0	4060	56	0
1	C	3918	0	3980	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	135	0	0	4	0
4	B	158	0	0	3	2
4	C	49	0	0	2	0
All	All	12279	0	12124	144	2

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 6.

The worst 5 of 144 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:464:SER:HB3	1:B:483:ASP:OD2	1.85	0.77
1:A:502:TYR:CE1	1:A:550:LEU:HD13	2.21	0.75
1:B:459:ILE:HD12	1:B:479:ILE:HG21	1.69	0.75
1:A:74:VAL:CG1	1:A:179:MET:HE1	2.18	0.73
1:A:216:THR:OG1	1:A:234:THR:CG2	2.40	0.69

All (2) 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)
4:B:573:HOH:O	4:B:727:HOH:O[2_455]	1.78	0.42
4:B:623:HOH:O	4:B:679:HOH:O[3_445]	2.18	0.02

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	503/577 (87%)	494 (98%)	8 (2%)	1 (0%)	43	35
1	B	502/577 (87%)	490 (98%)	11 (2%)	1 (0%)	43	35
1	C	486/577 (84%)	478 (98%)	7 (1%)	1 (0%)	43	35
All	All	1491/1731 (86%)	1462 (98%)	26 (2%)	3 (0%)	43	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	463	GLY
1	C	463	GLY
1	A	463	GLY

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	450/498 (90%)	436 (97%)	14 (3%)	35	26
1	B	449/498 (90%)	428 (95%)	21 (5%)	23	12
1	C	439/498 (88%)	422 (96%)	17 (4%)	28	17
All	All	1338/1494 (90%)	1286 (96%)	52 (4%)	28	17

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	395	GLU
1	C	8	LYS
1	C	465	ASP
1	B	456	ASN
1	B	516	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	51	GLN
1	C	200	GLN
1	C	528	HIS
1	C	383	ASN
1	A	383	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are 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	A	513/577 (88%)	1.39	114 (22%) 2 2	25, 40, 58, 83	1 (0%)
1	B	512/577 (88%)	1.10	88 (17%) 4 5	24, 34, 51, 79	0
1	C	500/577 (86%)	1.41	112 (22%) 2 2	32, 44, 64, 76	0
All	All	1525/1731 (88%)	1.30	314 (20%) 2 3	24, 40, 59, 83	1 (0%)

The worst 5 of 314 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	463	GLY	7.5
1	A	7	ILE	7.5
1	A	439	PHE	6.2
1	B	207	LEU	6.1
1	A	234	THR	6.0

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 oligosaccharides 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	MN	A	680	1/1	0.83	0.20	76,76,76,76	0
2	MN	C	680	1/1	0.91	0.12	87,87,87,87	0
2	MN	B	680	1/1	0.94	0.10	54,54,54,54	0
3	ZN	A	690	1/1	0.94	0.12	57,57,57,57	0
3	ZN	C	690	1/1	0.94	0.09	61,61,61,61	0
3	ZN	B	690	1/1	0.97	0.10	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.