



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:32 PM UTC

PDB ID : 3MWP / pdb_00003mwp
Title : Nucleoprotein structure of lassa fever virus
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Deposited on : 2010-05-06
Resolution : 1.79 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	:	4-5-2 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

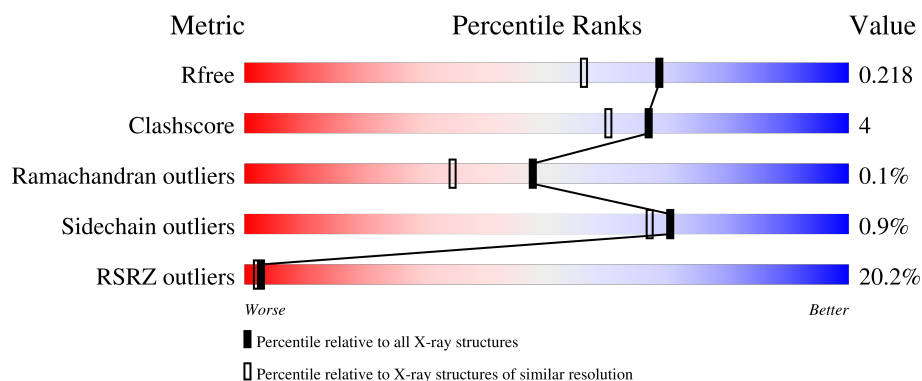
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 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	14% 83% 5% 11%
1	B	577	18% 82% 7% 11%
1	C	577	22% 77% 11% 12%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12477 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
1	A	512	Total	C	N	O	S	0	1	0
			4011	2521	697	766	27			
1	B	515	Total	C	N	O	S	0	0	0
			4027	2528	701	771	27			
1	C	506	Total	C	N	O	S	0	0	0
			3961	2488	688	758	27			

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 ZINC ION (CCD ID: ZN) (formula: Zn).

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

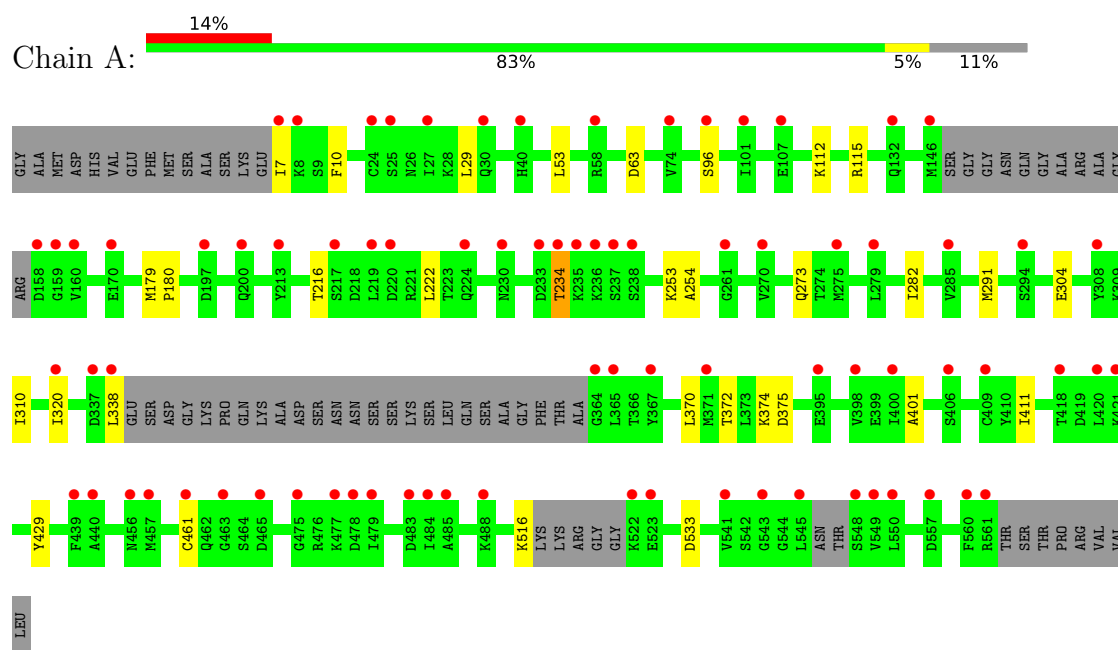
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	175	Total	O	0	0
			175	175		
3	B	192	Total	O	0	0
			192	192		
3	C	108	Total	O	0	0
			108	108		

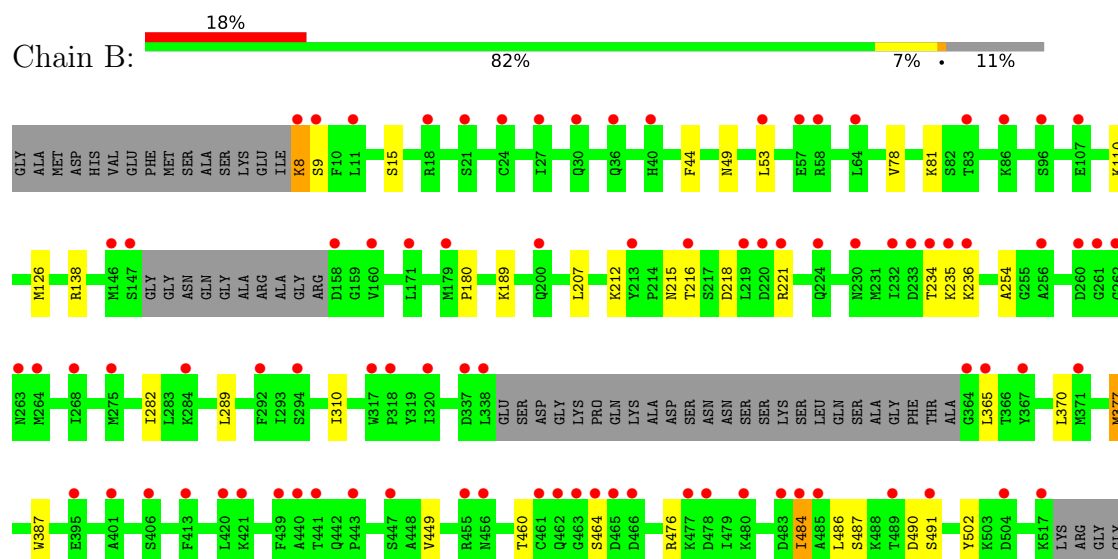
3 Residue-property plots [i](#)

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

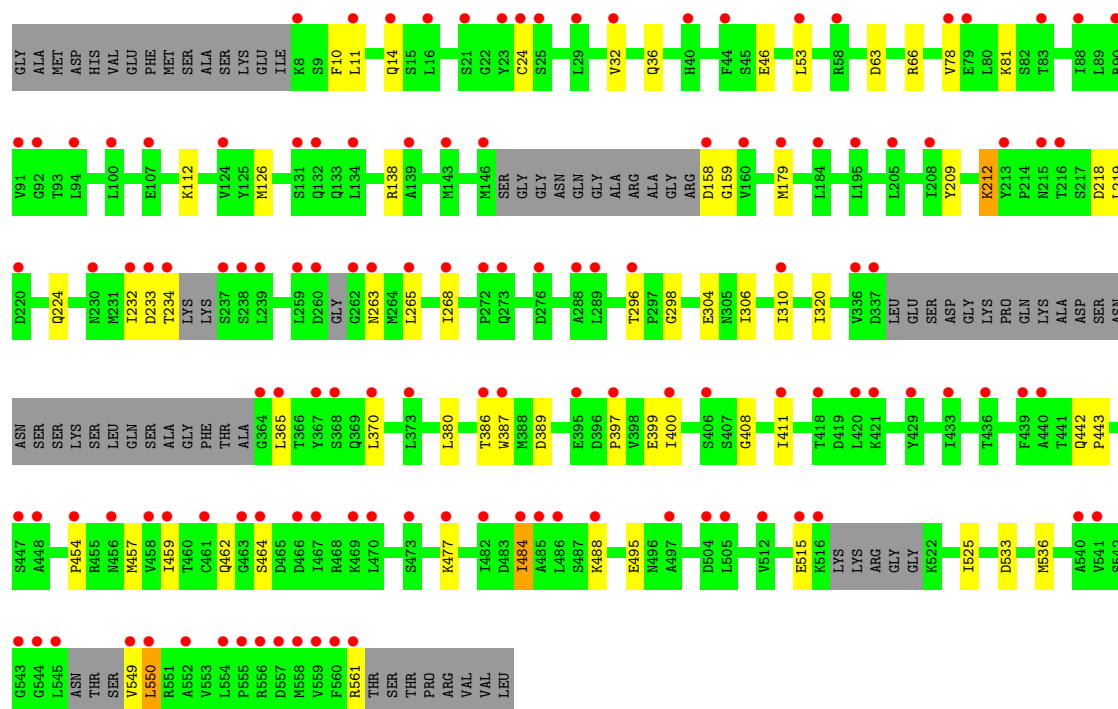
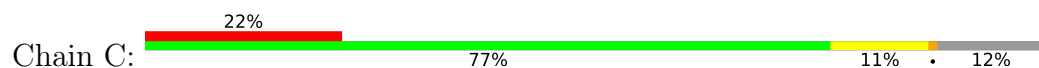


• Molecule 1: Nucleoprotein





● Molecule 1: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	176.82Å 176.82Å 56.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	153.18 – 1.79 153.13 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.7 (153.18-1.79) 99.9 (153.13-1.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.178 , 0.196 0.200 , 0.218	Depositor DCC
R_{free} test set	9260 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l 0.021 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.348 for H, K, L 0.652 for K, H, -L	Depositor
Outliers	0 of 184177 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12477	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.73	0/4070	0.90	1/5493 (0.0%)
1	B	0.78	0/4084	0.92	4/5513 (0.1%)
1	C	0.70	0/4015	0.90	0/5418
All	All	0.74	0/12169	0.91	5/16424 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	MET	CG-SD-CE	-10.16	78.55	100.90
1	A	461	CYS	CB-CA-C	-6.38	98.95	109.80
1	B	490	ASP	CA-C-N	5.59	128.04	120.38
1	B	490	ASP	C-N-CA	5.59	128.04	120.38
1	B	476	ARG	N-CA-C	5.33	116.06	108.54

There are no chirality outliers.

There are no planarity outliers.

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	4011	0	4085	22	0
1	B	4027	0	4098	30	0
1	C	3961	0	4019	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	175	0	0	3	0
3	B	192	0	0	2	0
3	C	108	0	0	2	0
All	All	12477	0	12202	90	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 4.

All (90) 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:C:219:LEU:HD23	1:C:234:THR:HG22	1.37	1.01
1:C:24:CYS:SG	1:C:268:ILE:HG12	2.17	0.85
1:B:502:TYR:CE1	1:B:550:LEU:HD13	2.16	0.80
1:C:265:LEU:O	1:C:268:ILE:HG13	1.82	0.78
1:C:408:GLY:O	1:C:550:LEU:HA	1.83	0.78
1:C:533:ASP:OD2	3:C:655:HOH:O	2.01	0.78
1:C:397:PRO:HB2	1:C:400:ILE:HD11	1.75	0.69
1:C:219:LEU:HD23	1:C:234:THR:CG2	2.19	0.66
1:B:502:TYR:CE1	1:B:550:LEU:CD1	2.79	0.66
1:A:533:ASP:OD2	3:A:728:HOH:O	2.13	0.65
1:C:219:LEU:CD2	1:C:234:THR:HG22	2.22	0.63
1:A:7:ILE:HG23	1:A:10:PHE:H	1.65	0.62
1:C:112:LYS:HE3	1:C:304:GLU:OE1	2.00	0.61
1:C:515:GLU:HG3	1:C:525:ILE:HD13	1.82	0.61
1:A:216:THR:HG23	1:A:234:THR:HG21	1.86	0.57
1:C:365:LEU:HD22	1:C:370:LEU:HD23	1.86	0.57
1:C:387:TRP:CH2	1:C:484:ILE:HG12	2.41	0.56
1:C:389:ASP:OD1	3:C:655:HOH:O	2.18	0.56
1:B:212:LYS:HE3	1:B:218:ASP:OD2	2.07	0.54
1:A:115:ARG:HD2	1:A:375:ASP:OD2	2.08	0.54
1:B:49:ASN:O	1:B:53:LEU:HG	2.08	0.53
1:B:365:LEU:HD22	1:B:370:LEU:HD23	1.88	0.53
1:B:78:VAL:O	1:B:81:LYS:HE2	2.09	0.52
1:A:179:MET:HG3	1:A:320:ILE:O	2.10	0.52
1:B:215:ASN:HB2	3:B:681:HOH:O	2.11	0.51
1:C:112:LYS:NZ	1:C:298:GLY:O	2.44	0.50
1:C:442:GLN:NE2	1:C:443:PRO:HD2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ILE:HG12	1:C:310:ILE:HD12	1.94	0.50
1:C:179:MET:HG3	1:C:320:ILE:O	2.10	0.50
1:C:386:THR:HB	1:C:459:ILE:HD13	1.93	0.50
1:A:216:THR:HA	1:A:234:THR:HG21	1.94	0.50
1:C:265:LEU:HD22	1:C:268:ILE:HD11	1.92	0.50
1:A:370:LEU:HG	1:A:374:LYS:HE3	1.92	0.49
1:B:484:ILE:CG2	1:B:486:LEU:HG	2.42	0.49
1:A:273:GLN:HG2	3:A:646:HOH:O	2.12	0.49
1:B:502:TYR:HE1	1:B:550:LEU:HD13	1.71	0.49
1:C:219:LEU:HD21	1:C:232:ILE:HB	1.96	0.48
1:B:216:THR:HG22	1:B:234:THR:CB	2.43	0.48
1:B:126:MET:CE	1:B:138:ARG:HG3	2.44	0.47
1:C:126:MET:HE1	1:C:138:ARG:HG3	1.96	0.47
1:C:10:PHE:CE2	1:C:14:GLN:HG3	2.49	0.47
1:B:216:THR:HG22	1:B:234:THR:HB	1.95	0.47
1:B:126:MET:HE1	1:B:138:ARG:HG3	1.98	0.46
1:C:399:GLU:O	1:C:400:ILE:HD13	2.15	0.46
1:C:454:PRO:HD2	1:C:457:MET:SD	2.55	0.46
1:A:29:LEU:C	1:A:29:LEU:HD23	2.41	0.46
1:C:212:LYS:HE2	1:C:218:ASP:OD2	2.16	0.46
1:C:112:LYS:HE2	1:C:296:THR:O	2.16	0.46
1:A:222:LEU:HD23	1:B:207:LEU:HD13	1.98	0.46
1:A:96:SER:OG	1:A:338:LEU:HD21	2.16	0.45
1:C:380:LEU:HD11	1:C:411:ILE:HD11	1.98	0.45
1:A:429:TYR:CZ	1:A:516:LYS:HE2	2.52	0.45
1:C:462:GLN:HB2	1:C:484:ILE:HD11	1.98	0.45
1:C:484:ILE:H	1:C:484:ILE:HG13	1.71	0.44
1:C:209:TYR:HA	1:C:212:LYS:O	2.18	0.44
1:B:180:PRO:HB3	1:B:254:ALA:HA	1.99	0.44
1:A:53:LEU:HD22	1:A:63:ASP:OD1	2.18	0.44
1:A:115:ARG:HD3	1:A:372:THR:HA	2.00	0.44
1:A:338:LEU:HD11	3:A:654:HOH:O	2.18	0.44
1:B:484:ILE:HG22	1:B:486:LEU:HG	2.00	0.44
1:B:282:ILE:HD11	1:B:310:ILE:CD1	2.48	0.43
1:B:110:LYS:NZ	3:B:695:HOH:O	2.51	0.43
1:C:443:PRO:HG3	1:C:561:ARG:HH21	1.83	0.43
1:C:387:TRP:HH2	1:C:484:ILE:HG12	1.84	0.42
1:B:387:TRP:CH2	1:B:484:ILE:HG13	2.54	0.42
1:A:180:PRO:HG3	1:A:253:LYS:HG2	2.01	0.42
1:B:502:TYR:CZ	1:B:550:LEU:HD11	2.54	0.42
1:A:216:THR:CB	1:A:234:THR:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:GLU:HG3	1:C:536:MET:HE1	2.02	0.42
1:A:180:PRO:HB3	1:A:254:ALA:HA	2.01	0.42
1:B:460:THR:CG2	1:B:484:ILE:HG12	2.50	0.42
1:A:112:LYS:HD2	1:A:304:GLU:OE2	2.19	0.42
1:B:484:ILE:HD13	1:B:484:ILE:HA	1.80	0.42
1:A:401:ALA:HA	1:A:411:ILE:O	2.20	0.41
1:B:487:SER:O	1:B:491:SER:HB2	2.20	0.41
1:C:32:VAL:O	1:C:36:GLN:HG3	2.21	0.41
1:A:282:ILE:HD11	1:A:310:ILE:CD1	2.51	0.41
1:A:291:MET:O	1:C:477:LYS:NZ	2.53	0.41
1:C:53:LEU:HD22	1:C:63:ASP:OD1	2.20	0.41
1:C:488:LYS:HD3	1:C:488:LYS:HA	1.80	0.41
1:B:377:MET:HE1	1:B:449:VAL:HG13	2.01	0.41
1:B:8:LYS:HB2	1:B:9:SER:H	1.68	0.41
1:B:44:PHE:CG	1:B:189:LYS:HG2	2.56	0.41
1:B:221:ARG:HA	1:B:221:ARG:HD3	1.91	0.41
1:C:46:GLU:OE2	1:C:66:ARG:HD2	2.21	0.41
1:B:235:LYS:HG3	1:B:236:LYS:N	2.36	0.41
1:B:15:SER:CB	1:B:289:LEU:HD11	2.51	0.40
1:B:550:LEU:N	1:B:550:LEU:HD12	2.35	0.40
1:C:78:VAL:O	1:C:81:LYS:HE3	2.21	0.40
1:C:158:ASP:HB3	1:C:159:GLY:H	1.67	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	A	503/577 (87%)	496 (99%)	7 (1%)	0	100	100
1	B	507/577 (88%)	502 (99%)	5 (1%)	0	100	100
1	C	492/577 (85%)	483 (98%)	8 (2%)	1 (0%)	43	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1502/1731 (87%)	1481 (99%)	20 (1%)	1 (0%)	48 34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	550	LEU

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%)	449 (100%)	1 (0%)	87 87
1	B	452/498 (91%)	449 (99%)	3 (1%)	76 73
1	C	444/498 (89%)	436 (98%)	8 (2%)	51 43
All	All	1346/1494 (90%)	1334 (99%)	12 (1%)	70 67

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	THR
1	B	8	LYS
1	B	464	SER
1	B	484	ILE
1	C	11	LEU
1	C	212	LYS
1	C	224	GLN
1	C	233	ASP
1	C	263	ASN
1	C	464	SER
1	C	484	ILE
1	C	549	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	383	ASN
1	A	501	GLN
1	B	14	GLN
1	B	132	GLN
1	B	196	ASN
1	B	200	GLN
1	B	224	GLN
1	B	379	GLN
1	B	383	ASN
1	B	422	GLN
1	C	26	ASN
1	C	72	GLN
1	C	133	GLN
1	C	230	ASN
1	C	474	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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

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	512/577 (88%)	1.23	80 (15%) 5 4	20, 33, 45, 66	1 (0%)
1	B	515/577 (89%)	1.33	103 (20%) 3 2	31, 33, 45, 58	0
1	C	506/577 (87%)	1.55	127 (25%) 1 1	32, 36, 49, 65	0
All	All	1533/1731 (88%)	1.37	310 (20%) 3 2	20, 34, 47, 66	1 (0%)

All (310) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	549	VAL	9.9
1	B	338	LEU	9.0
1	A	7	ILE	7.7
1	A	338	LEU	6.5
1	B	260	ASP	5.9
1	B	147	SER	5.8
1	A	234	THR	5.6
1	B	262	GLY	5.5
1	C	439	PHE	5.2
1	C	545	LEU	4.9
1	C	262	GLY	4.8
1	A	439	PHE	4.8
1	A	549	VAL	4.8
1	C	516	LYS	4.7
1	B	263	ASN	4.5
1	A	235	LYS	4.5
1	C	158	ASP	4.5
1	B	549	VAL	4.3
1	B	235	LYS	4.3
1	C	24	CYS	4.3
1	B	546	ASN	4.3
1	A	337	ASP	4.2
1	C	234	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	236	LYS	4.2
1	B	463	GLY	4.1
1	A	545	LEU	4.1
1	A	364	GLY	4.0
1	C	337	ASP	4.0
1	A	238	SER	4.0
1	B	440	ALA	4.0
1	A	484	ILE	3.9
1	B	456	ASN	3.9
1	A	236	LYS	3.9
1	B	158	ASP	3.9
1	B	517	LYS	3.9
1	C	132	GLN	3.8
1	C	467	ILE	3.8
1	A	213	TYR	3.8
1	B	477	LYS	3.8
1	C	260	ASP	3.8
1	C	263	ASN	3.8
1	B	367	TYR	3.7
1	C	420	LEU	3.7
1	A	58	ARG	3.7
1	B	439	PHE	3.7
1	A	548	SER	3.7
1	A	8	LYS	3.6
1	C	458	VAL	3.6
1	C	40	HIS	3.6
1	B	179	MET	3.6
1	B	464	SER	3.6
1	A	365	LEU	3.6
1	B	234	THR	3.5
1	A	320	ILE	3.5
1	C	505	LEU	3.5
1	C	448	ALA	3.5
1	A	158	ASP	3.5
1	B	337	ASP	3.5
1	C	268	ILE	3.5
1	A	220	ASP	3.4
1	A	367	TYR	3.4
1	B	545	LEU	3.4
1	C	23	TYR	3.4
1	A	237	SER	3.4
1	C	484	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	421	LYS	3.4
1	C	550	LEU	3.4
1	B	522	LYS	3.3
1	A	456	ASN	3.3
1	B	484	ILE	3.3
1	B	365	LEU	3.3
1	C	131	SER	3.3
1	B	541	VAL	3.3
1	B	548	SER	3.2
1	C	237	SER	3.2
1	C	556	ARG	3.2
1	C	364	GLY	3.2
1	C	160	VAL	3.2
1	B	466	ASP	3.2
1	B	557	ASP	3.2
1	C	233	ASP	3.2
1	C	418	THR	3.2
1	B	561	ARG	3.1
1	C	463	GLY	3.1
1	B	317	TRP	3.1
1	B	221	ARG	3.1
1	C	367	TYR	3.1
1	C	107	GLU	3.1
1	A	270	VAL	3.1
1	A	261	GLY	3.1
1	C	365	LEU	3.1
1	B	230	ASN	3.1
1	A	406	SER	3.1
1	B	30	GLN	3.0
1	C	213	TYR	3.0
1	B	27	ILE	3.0
1	B	547	THR	3.0
1	A	371	MET	3.0
1	B	219	LEU	3.0
1	C	88	ILE	3.0
1	C	208	ILE	3.0
1	A	557	ASP	3.0
1	B	233	ASP	3.0
1	B	8	LYS	3.0
1	B	232	ILE	3.0
1	C	11	LEU	2.9
1	A	457	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	406	SER	2.9
1	C	485	ALA	2.9
1	C	230	ASN	2.9
1	B	443	PRO	2.9
1	A	107	GLU	2.9
1	C	216	THR	2.9
1	A	200	GLN	2.9
1	B	543	GLY	2.9
1	B	542	SER	2.9
1	C	473	SER	2.9
1	A	170	GLU	2.8
1	C	541	VAL	2.8
1	A	275	MET	2.8
1	A	25	SER	2.8
1	B	11	LEU	2.8
1	C	454	PRO	2.8
1	C	433	ILE	2.8
1	A	440	ALA	2.8
1	A	541	VAL	2.8
1	C	238	SER	2.8
1	C	512	VAL	2.8
1	C	195	LEU	2.8
1	B	371	MET	2.8
1	A	160	VAL	2.8
1	C	482	ILE	2.8
1	C	466	ASP	2.8
1	A	475	GLY	2.8
1	C	543	GLY	2.8
1	C	205	LEU	2.7
1	A	27	ILE	2.7
1	C	406	SER	2.7
1	C	78	VAL	2.7
1	A	40	HIS	2.7
1	B	9	SER	2.7
1	B	40	HIS	2.7
1	B	96	SER	2.7
1	C	447	SER	2.7
1	A	132	GLN	2.7
1	A	279	LEU	2.7
1	A	420	LEU	2.7
1	B	420	LEU	2.7
1	A	522	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	523	GLU	2.6
1	B	264	MET	2.6
1	C	146	MET	2.6
1	A	461	CYS	2.6
1	B	58	ARG	2.6
1	B	461	CYS	2.6
1	B	556	ARG	2.6
1	C	53	LEU	2.6
1	C	265	LEU	2.6
1	C	289	LEU	2.6
1	C	540	ALA	2.6
1	C	79	GLU	2.6
1	A	478	ASP	2.6
1	A	285	VAL	2.6
1	C	90	ARG	2.6
1	A	233	ASP	2.5
1	B	441	THR	2.5
1	B	550	LEU	2.5
1	C	259	LEU	2.5
1	C	470	LEU	2.5
1	C	310	ILE	2.5
1	B	216	THR	2.5
1	B	57	GLU	2.5
1	B	560	PHE	2.5
1	A	550	LEU	2.5
1	C	94	LEU	2.5
1	C	91	VAL	2.5
1	A	400	ILE	2.5
1	C	497	ALA	2.5
1	C	8	LYS	2.5
1	C	179	MET	2.5
1	A	395	GLU	2.5
1	B	320	ILE	2.5
1	C	459	ILE	2.5
1	C	25	SER	2.5
1	A	230	ASN	2.4
1	C	373	LEU	2.4
1	A	146	MET	2.4
1	C	288	ALA	2.4
1	C	296	THR	2.4
1	C	411	ILE	2.4
1	C	464	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	14	GLN	2.4
1	A	477	LYS	2.4
1	C	558	MET	2.4
1	C	16	LEU	2.4
1	C	134	LEU	2.4
1	B	256	ALA	2.4
1	A	308	TYR	2.4
1	B	491	SER	2.4
1	C	555	PRO	2.4
1	B	86	LYS	2.4
1	C	477	LYS	2.4
1	A	217	SER	2.3
1	A	543	GLY	2.3
1	B	294	SER	2.3
1	B	447	SER	2.3
1	B	318	PRO	2.3
1	A	561	ARG	2.3
1	B	465	ASP	2.3
1	C	400	ILE	2.3
1	A	398	VAL	2.3
1	B	364	GLY	2.3
1	B	504	ASP	2.3
1	A	24	CYS	2.3
1	C	386	THR	2.3
1	A	485	ALA	2.3
1	B	401	ALA	2.3
1	B	540	ALA	2.3
1	C	370	LEU	2.3
1	B	36	GLN	2.3
1	C	32	VAL	2.3
1	C	336	VAL	2.3
1	C	488	LYS	2.3
1	C	440	ALA	2.3
1	C	461	CYS	2.3
1	B	462	GLN	2.3
1	C	552	ALA	2.3
1	C	554	LEU	2.3
1	B	523	GLU	2.3
1	B	213	TYR	2.3
1	A	479	ILE	2.3
1	B	268	ILE	2.3
1	C	557	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	219	LEU	2.2
1	C	44	PHE	2.2
1	B	160	VAL	2.2
1	C	397	PRO	2.2
1	B	489	THR	2.2
1	C	436	THR	2.2
1	C	215	ASN	2.2
1	B	421	LYS	2.2
1	C	276	ASP	2.2
1	C	504	ASP	2.2
1	C	29	LEU	2.2
1	B	224	GLN	2.2
1	B	455	ARG	2.2
1	C	429	TYR	2.2
1	A	74	VAL	2.2
1	A	96	SER	2.2
1	C	220	ASP	2.2
1	B	24	CYS	2.2
1	C	387	TRP	2.2
1	C	273	GLN	2.2
1	A	463	GLY	2.2
1	B	18	ARG	2.2
1	A	560	PHE	2.2
1	B	292	PHE	2.2
1	A	421	LYS	2.2
1	A	488	LYS	2.2
1	C	469	LYS	2.2
1	C	232	ILE	2.2
1	C	21	SER	2.2
1	B	146	MET	2.1
1	B	220	ASP	2.1
1	B	261	GLY	2.1
1	C	92	GLY	2.1
1	C	544	GLY	2.1
1	B	53	LEU	2.1
1	C	239	LEU	2.1
1	C	486	LEU	2.1
1	B	21	SER	2.1
1	C	143	MET	2.1
1	C	368	SER	2.1
1	B	83	THR	2.1
1	C	83	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	30	GLN	2.1
1	B	395	GLU	2.1
1	B	485	ALA	2.1
1	C	456	ASN	2.1
1	B	64	LEU	2.1
1	A	465	ASP	2.1
1	B	478	ASP	2.1
1	C	58	ARG	2.1
1	C	561	ARG	2.1
1	C	560	PHE	2.1
1	A	101	ILE	2.1
1	A	159	GLY	2.1
1	C	124	VAL	2.1
1	B	558	MET	2.1
1	C	395	GLU	2.1
1	C	100	LEU	2.1
1	C	184	LEU	2.1
1	C	272	PRO	2.1
1	B	480	LYS	2.1
1	C	515	GLU	2.0
1	B	275	MET	2.0
1	A	224	GLN	2.0
1	A	483	ASP	2.0
1	C	559	VAL	2.0
1	A	409	CYS	2.0
1	B	171	LEU	2.0
1	A	418	THR	2.0
1	B	284	LYS	2.0
1	B	107	GLU	2.0
1	B	200	GLN	2.0
1	B	413	PHE	2.0
1	A	197	ASP	2.0
1	B	483	ASP	2.0
1	C	139	ALA	2.0
1	A	294	SER	2.0

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 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($\text{\AA}^2$)	Q<0.9
2	ZN	B	570	1/1	0.84	0.41	103,103,103,103	0
2	ZN	C	570	1/1	0.99	0.06	44,44,44,44	0
2	ZN	A	570	1/1	1.00	0.02	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.