



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:41 PM BST

PDB ID : 3IYK
EMDB ID: : EMD-5147
Title : Bluetongue virus structure reveals a sialic acid binding domain, amphipathic helices and a central coiled coil in the outer capsid proteins
Authors : Zhang, X.; Boyce, M.; Bhattacharya, B.; Zhang, X.; Schein, S.; Roy, P.; Zhou, Z.H.
Deposited on : 2010-01-25
Resolution : 7.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

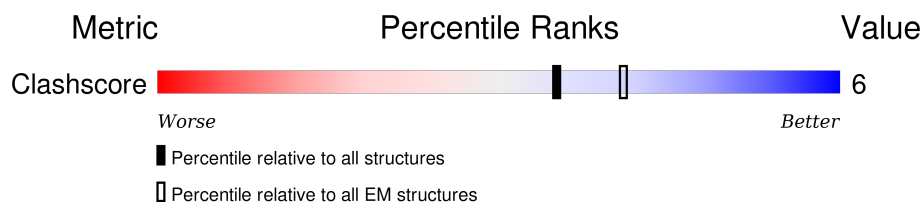
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY










The reported resolution of this entry is 7.00 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)	EM structures (#Entries)
Clashscore	114402	924

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	526	 58% 42%
1	B	526	 58% 42%
1	C	526	 58% 42%
1	D	526	 58% 42%
1	E	526	 58% 42%
1	F	526	 58% 42%
2	G	600	 23% 77% •
2	I	600	 23% 77% •
2	K	600	 23% 77% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2331 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

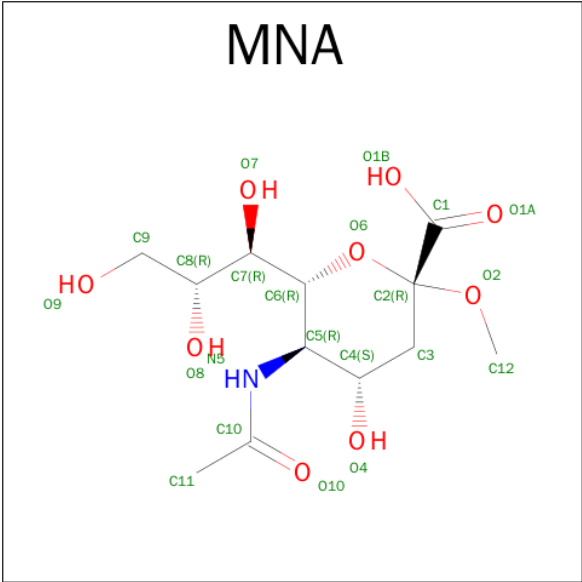
- Molecule 1 is a protein called VP5.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	307	Total C 307 307	0	307
1	B	307	Total C 307 307	0	307
1	C	307	Total C 307 307	0	307
1	D	307	Total C 307 307	0	307
1	E	307	Total C 307 307	0	307
1	F	307	Total C 307 307	0	307

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	G	141	Total C 141 141	0	141
2	I	141	Total C 141 141	0	141
2	K	141	Total C 141 141	0	141

- Molecule 3 is 2-O-METHYL-5-N-ACETYL-ALPHA-D- NEURAMINIC ACID (three-letter code: MNA) (formula: C₁₂H₂₁NO₉).

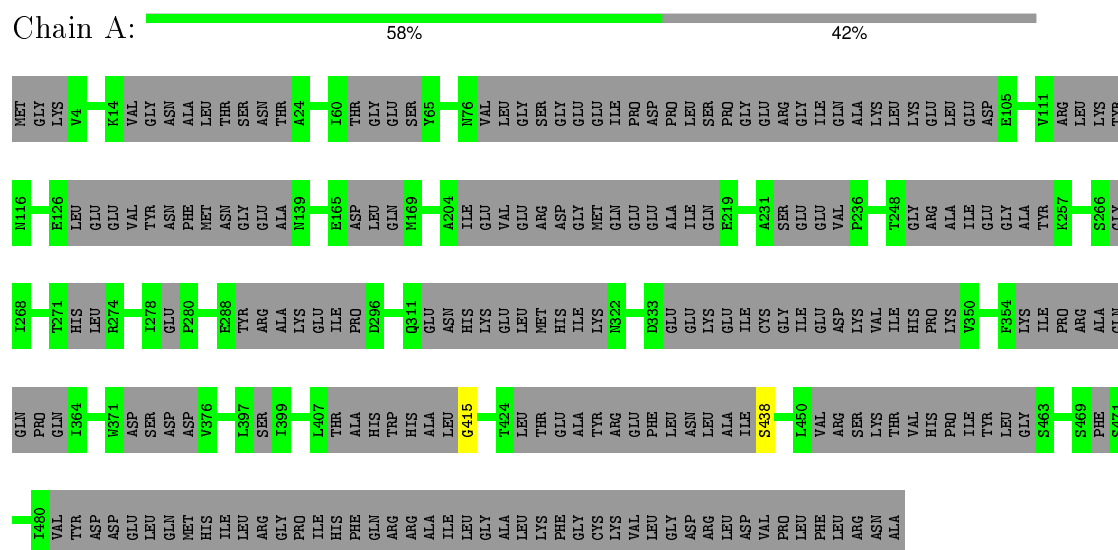


Mol	Chain	Residues	Atoms				AltConf
3	G	1	Total	C	N	O	1
			22	12	1	9	
3	I	1	Total	C	N	O	1
			22	12	1	9	
3	K	1	Total	C	N	O	1
			22	12	1	9	

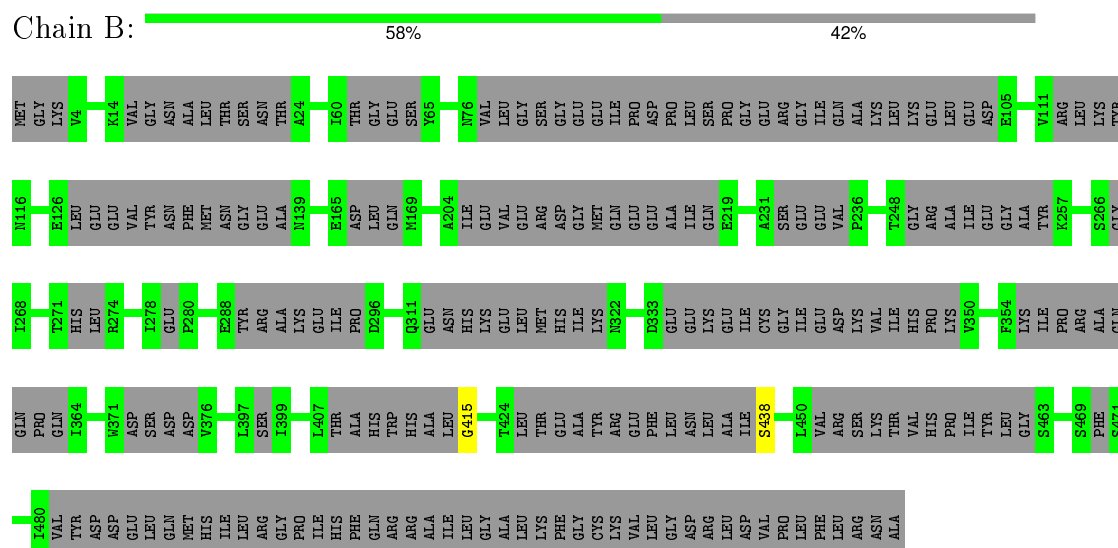
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: VP5

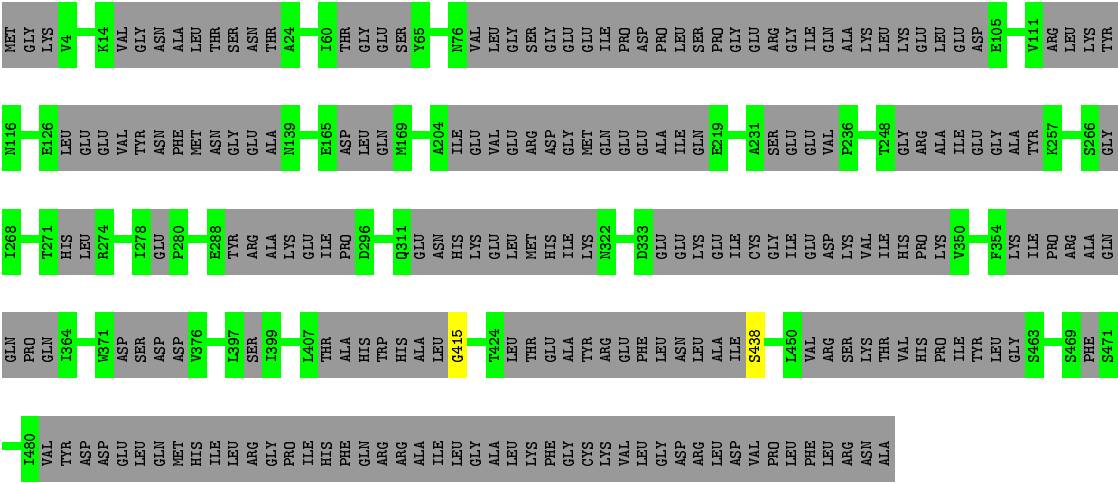


• Molecule 1: VP5

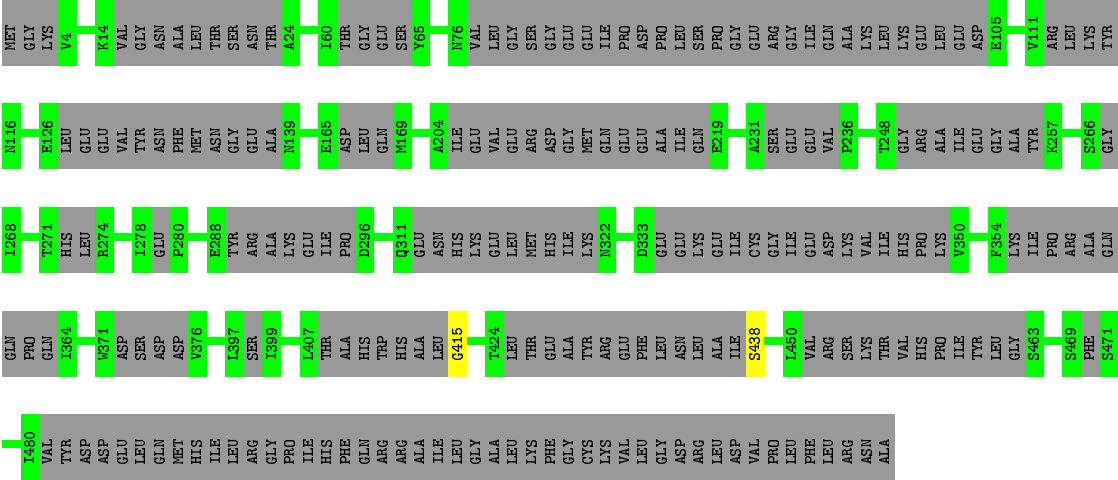


• Molecule 1: VP5

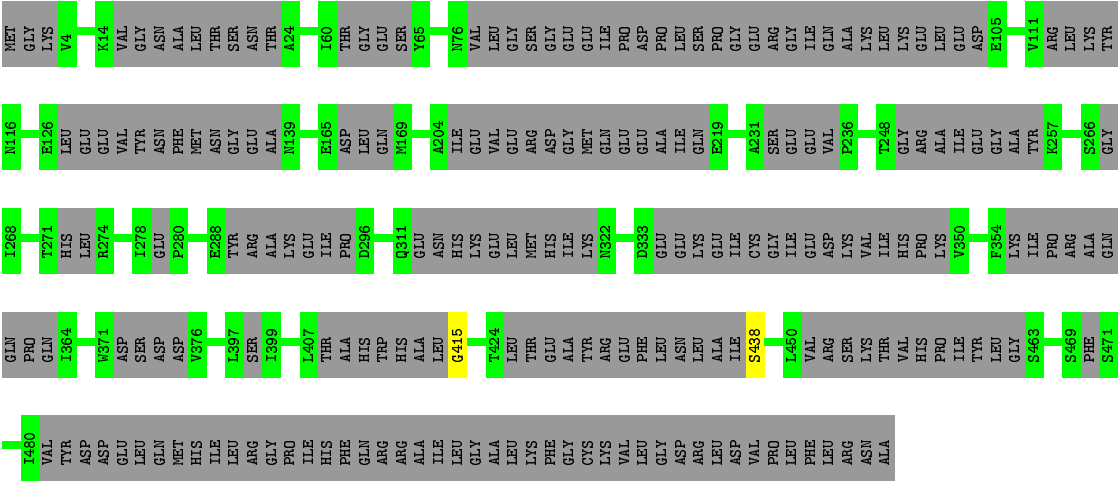




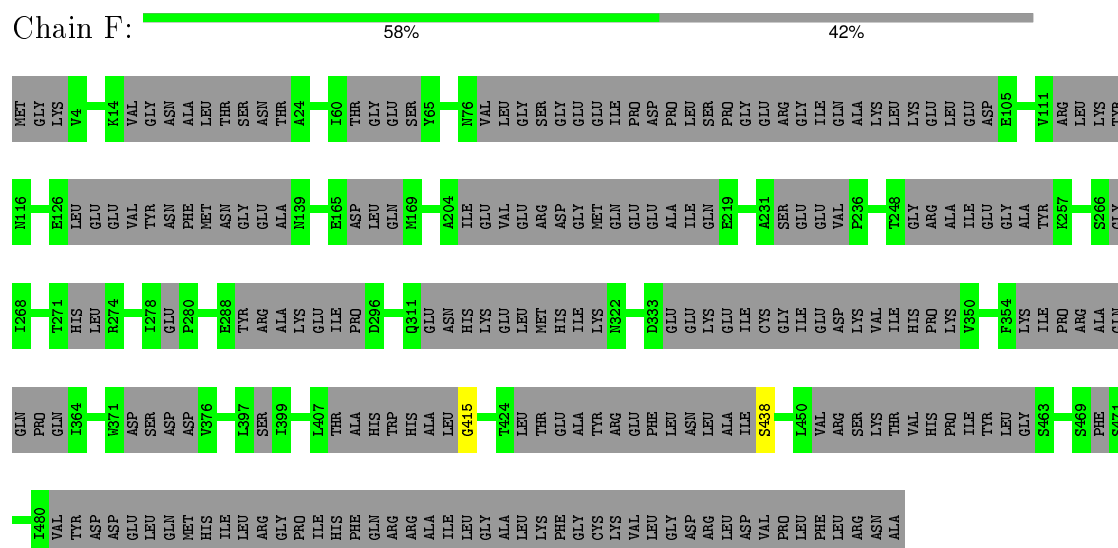
• Molecule 1: VP5



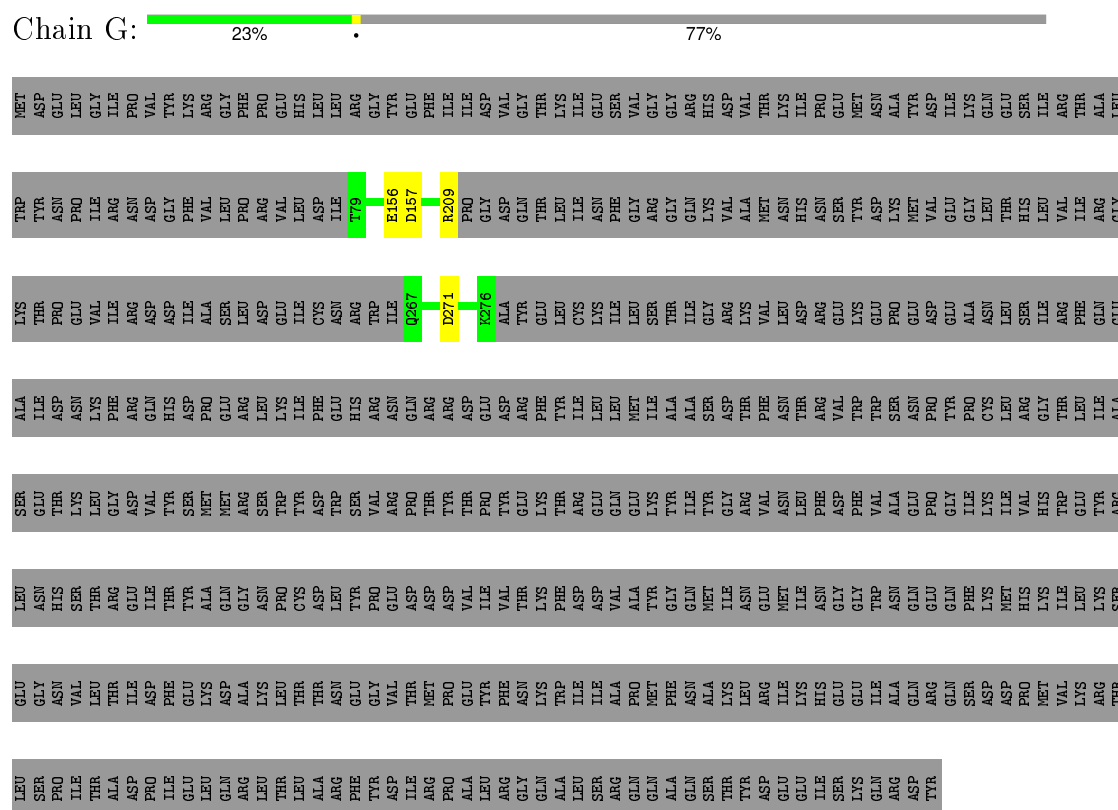
• Molecule 1: VP5



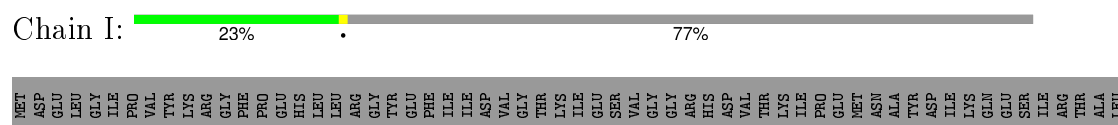
- Molecule 1: VP5



- Molecule 2: VP2



- Molecule 2: VP2



TRP	TRR	ASN	PRO	PRO	ARG	ASN	ASP	GLY	PHE	VAL	LEU	PRO	ARG	VAL	LEU	ASP	ILE	Tyr	D156	R209	PRO	GLY	ASP	GLN	THR	LEU	ILE	ASN	PHE	GLY	ARG	GLY	GLN	LVS	VAL	ALA	ASN	ASN	SER	TYR	ASP	LVS	MET	MET	HIS	THR	GLY	LEU	THR	HIS	LEU	VAL	ILE	ARG	TYR
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LNS	THR	PRO	GLU	VAL	ILE	ARG	ASP	ASP	ASP	ALA	LEU	SER	ASN	ARG	TRP	CYS	Q267	D271	E276	ALA	TYR	GLU	LEU	CYS	LNS	ILE	LEU	SER	THR	ILE	GLY	ARG	LNS	VAL	LEU	ASP	ARG	GLU	LNS	GLU	PRO	GLU	ASP	GLU	ALA	ASN	LEU	SER	ILE	ARG	PHE	GLN	GLU
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ALA ILE ASP ASN LYS PHE ARG GLN HIS ASP PRO LEU ARG GLY THR TYR TRP SER CYS VAL MET THR

SER	GLU	THR	LYS	LEU	GLY	ASP	VAL	TYR	SER	SER	MET	NET	ARG	ARG	SER	TRP	TRP	ASP	ASP	TRP	SER	SER	VAL	VAL	ARG	PRO	PRO	THR	THR	THR	THR	PRO	TYR	GLU	GLU	LYS	LYS	THR	THR	ANG	GLU	GLU	GLN	GLU	GLU	LYS	TYR	Tyr	ILE	ILE	TYR	TYR	GLY	ARG	ARG	VAL	ASN	LEU	PHE	PHE	ASP	ASP	ALA	ALA	VAL	GLU	GLY	GLY	ILE	ILE	LYS	LYS	ILE	ILE	VAL	HIS	TRP	TRP	GLU	THR	THR	TYR	ARG
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LEU ASN HIS SER THR ARG GLU ILE THR TYR GLN GLY ASN ASP CYS ASP LEU TYR PRO GLU ASP ASP VAL ILE VAL THR LYS PHE ASP ASP VAL TYR GLN MET ILE MET GLU MET ILE ASN GLN GLU GLN PHE PHE MET HIS LYS ILE LEU LYS

GLU GLY ASN VAL LEU THR ILE ASP PHE GLU LYS ASP ALA LYS LEU THR THR ASN GLU GLY VAL THR MET PRO GLU TYR PHE ASN LYS TRP ILE ILE ILE LYS HIS GLU GLU ILE ILE GLN ARG GLN SER ASP ASP PRO MET LYS VAL ARG THR

LEU SER PRO ILE THR ALA ASP PRO GLU LEU GLN ARG LEU THR LEU ALA ARG PHE TYR ASP ILE ARG PRO ALA LEU GLY GLN ALA LEU SER ARG GLN GLN ALA GLN SER THR TYR ASP GLU GLU ILE SER LYS GLN ARG ASP

- Molecule 2: VP2

Chain K: 23% . 77%

[illegible]

TRP	TYR	ASN	PRO	PRO	ARG	ASN	ASP	GLY	PHE	VAL	VAL	LEU	PRO	ARG	VAL	LEU	ASP	ILE	Tyr	D156	D157	R209	PRO	GLY	ASP	ASN	GLN	THR	LEU	ILE	ASN	PHE	GLY	ARG	GLY	GLN	LYS	VAL	ALA	ALA	ASN	ASN	SER	TYR	ASP	LYS	MET	VAL	GLU	GLY	LEU	THR	HIS	LEU	ILE	VAL	ARG	TYR
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LYS	THR	PRO	GLU	VAL	ILE	ARG	ASP	ASP	ALA	ALA	SER	LEU	ASP	GLU	CYS	ILE	ASN	ARG	TRP	Q267	D271	E276	ALA	TYR	GLU	LEU	CYS	LYS	ILE	LEU	SER	THR	ILE	ARG	GLU	LYS	GLU	VAL	LEU	ASP	ARG	GLU	GLU	PRO	GLU	ASP	GLU	ALA	ASN	LEU	SER	ILE	ARG	PHE	GLN
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ALA ILE ASP ASN LYS PHE ARG GLN GLU LEU LYS ILE PHE GLU HIS ARG ASN GLN ARG ARG ASP GLU ASP ARG PHE TYR ILE LEU LEU MET ILE ALA ALA SER ASP THR THR THR PHE ASN THR ARG VAL TRP TRP TRP SER ASN ASN PRO TYR TYR PRO PRO CYS LEU ARG GLY THR THR LEU LEU ILE ILE

SER	GLU	THR	LYS	LEU	GLY	ASP	VAL	TYR	SER	SER	MET	MET	ARG	ARG	SER	TRP	TRP	ASP	ASP	TRP	SER	SER	VAL	VAL	ARG	ARG	PRO	PRO	TYR	GLU	GLU	LYS	THR	THR	ANG	GLU	GLU	GLN	GLU	GLU	LYS	TYR	TYR	ILE	ILE	GLY	GLY	ARG	ARG	VAL	VAL	ASN	ASN	LEU	LEU	PHE	PHE	ASP	ASP	PHE	PHE	ALA	ALA	VAL	VAL	GLU	GLU	PRO	PRO	GLY	GLY	ILE	ILE	LYS	LYS	ILE	ILE	VAL	VAL	HIS	HIS	TRP	TRP	GLU	GLU	THR	THR	TYR	TYR	ARG	ARG	BCG	BCG
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LEU ASN HIS SER THR ARG GLU ILE THR TYR ALA GLN GLY ASN ASP PRO CYS ASP LEU TYR PRO GLU ASP ASP VAL ILE VAL VAL THR THR LYS PHE ASP ASP VAL VAL TYR TYR GLY GLN MET MET MET GLU MET MET ASN ASN GLN GLN GLN PHE PHE LYS MET HIS LYS ILE LEU LEU LYS

[illegible]

LEU SER SER PRO ILE THR ALA ASP PRO GLU LEU GLN ARG LEU THR LEU ALA ARG ARG PHE TYR ASP ILE ARG PRO ALA LEU ARG GLY GLN ALA LEU SER ARG GLN GLN ALA GLN SER THR TYR ASP GLU SER ILE LYS GLN ARG ASP THR

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	3400	Depositor
Resolution determination method	FSC 0.143 cut-off	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	80000	Depositor
Image detector	CCD	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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	307	0	0	1	0
1	B	307	0	0	1	0
1	C	307	0	0	1	0
1	D	307	0	0	1	0
1	E	307	0	0	1	0
1	F	307	0	0	1	0
2	G	141	0	0	3	0
2	I	141	0	0	3	0
2	K	141	0	0	3	0
3	G	22	0	20	0	0
3	I	22	0	20	0	0
3	K	22	0	20	0	0
All	All	2331	0	60	12	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 6.

The worst 5 of 12 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:E:415:GLY:CA	1:E:438:SER:CA	2.38	1.02
1:C:415:GLY:CA	1:C:438:SER:CA	2.38	1.02
1:D:415:GLY:CA	1:D:438:SER:CA	2.38	1.02
1:B:415:GLY:CA	1:B:438:SER:CA	2.38	1.01
1:A:415:GLY:CA	1:A:438:SER:CA	2.38	1.01

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands are 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
3	MNA	G	1000[A]	-	19,22,22	1.17	2 (10%)	17,32,32	0.80	1 (5%)
3	MNA	I	1000[B]	-	19,22,22	1.19	2 (10%)	17,32,32	0.80	1 (5%)
3	MNA	K	1000[C]	-	19,22,22	1.20	2 (10%)	17,32,32	0.81	1 (5%)

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
3	MNA	G	1000[A]	-	-	0/17/41/41	0/1/1/1
3	MNA	I	1000[B]	-	-	0/17/41/41	0/1/1/1
3	MNA	K	1000[C]	-	-	0/17/41/41	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1000[B]	MNA	C4-C5	2.13	1.55	1.53
3	G	1000[A]	MNA	C4-C5	2.13	1.55	1.53
3	K	1000[C]	MNA	C4-C5	2.18	1.55	1.53
3	G	1000[A]	MNA	C3-C2	3.67	1.55	1.52
3	K	1000[C]	MNA	C3-C2	3.72	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1000[B]	MNA	C12-O2-C2	2.06	117.33	115.29
3	G	1000[A]	MNA	C12-O2-C2	2.09	117.36	115.29
3	K	1000[C]	MNA	C12-O2-C2	2.11	117.39	115.29

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.